Röntgenstrukturanalytische Daten für 48

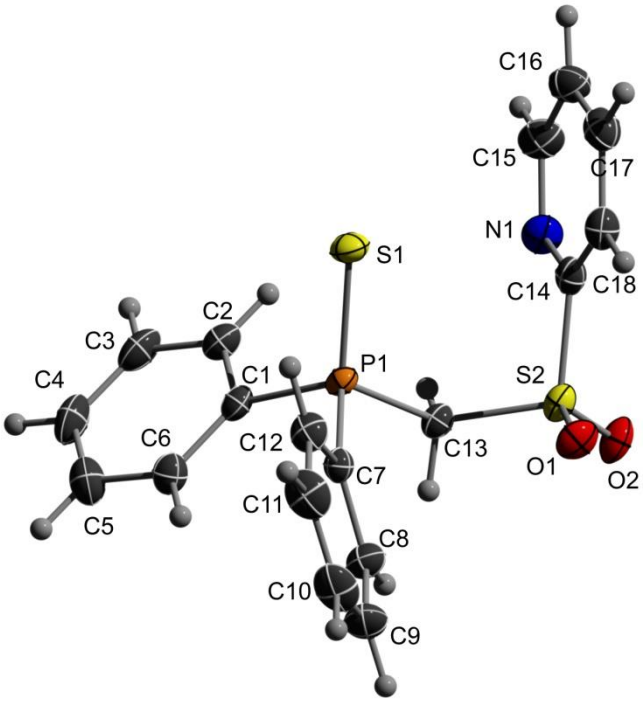

Table 48-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	C18 H16 N O2 P S2	
Formula weight	373.41	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 14.3098(4) Å	α = 90°.
	b = 13.3690(4) Å	β = 104.055(2)°.
	c = 9.3446(3) Å	γ = 90°.
Volume	1734.18(9) $Å^3$	
Z	4	
Density (calculated)	1.430 Mg/m^3	
Absorption coefficient	0.410 mm^{-1}	
F(000)	776	
Crystal size	0.40 x 0.35 x 0.15 mm^3	

Theta range for data collection	2.71 to 26.76°.
Index ranges	-18<=h<=18, -16<=k<=12, -11<=l<=11
Reflections collected	28287
Independent reflections	3670 [R(int) = 0.0330]
Completeness to theta = 26.76°	99.6 %
Max. and min. transmission	0.9411 and 0.8533
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3670 / 0 / 217
Goodness-of-fit on F^2	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0286, wR2 = 0.0705
R indices (all data)	R1 = 0.0394, wR2 = 0.0759
Largest diff. peak and hole	0.370 and -0.301 e.$Å^{-3}$

Table 48-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7902(1)	5323(1)	2832(2)	23(1)
C(2)	7394(1)	6222(1)	2747(2)	29(1)
C(3)	7513(1)	6829(1)	3974(2)	36(1)
C(4)	8138(1)	6548(1)	5286(2)	38(1)
C(5)	8632(1)	5654(2)	5380(2)	38(1)
C(6)	8516(1)	5035(1)	4156(2)	30(1)
C(7)	8577(1)	3548(1)	1545(2)	21(1)
C(8)	8342(1)	2698(1)	2241(2)	29(1)
C(9)	8958(1)	1885(1)	2478(2)	37(1)
C(10)	9816(1)	1923(2)	2055(2)	40(1)
C(11)	10060(1)	2764(2)	1393(2)	38(1)
C(12)	9446(1)	3579(1)	1126(2)	29(1)
C(13)	6546(1)	4147(1)	865(2)	22(1)
C(14)	5918(1)	4425(1)	-2179(2)	24(1)
C(15)	5454(1)	6009(1)	-2831(2)	35(1)
C(16)	5853(1)	5955(1)	-4040(2)	35(1)
C(17)	6277(1)	5075(1)	-4319(2)	33(1)

C(18)	6320(1)	4280(1)	-3360(2)	28(1)
N(1)	5473(1)	5250(1)	-1900(2)	29(1)
O(1)	6617(1)	2707(1)	-1052(1)	31(1)
O(2)	5042(1)	3238(1)	-676(1)	33(1)
P(1)	7786(1)	4618(1)	1136(1)	19(1)
S(1)	8015(1)	5449(1)	-454(1)	28(1)
S(2)	5996(1)	3499(1)	-788(1)	23(1)

Table 48-3. Bond lengths [Å] and angles [°] for sad.

C(1)-C(6)	1.386(2)
C(1)-C(2)	1.398(2)
C(1)-P(1)	1.8164(16)
C(2)-C(3)	1.381(2)
C(3)-C(4)	1.382(3)
C(4)-C(5)	1.380(3)
C(5)-C(6)	1.389(2)
C(7)-C(8)	1.391(2)
C(7)-C(12)	1.392(2)
C(7)-P(1)	1.8056(16)
C(8)-C(9)	1.383(2)
C(9)-C(10)	1.379(3)
C(10)-C(11)	1.369(3)
C(11)-C(12)	1.384(2)
C(13)-S(2)	1.7792(15)
C(13)-P(1)	1.8420(15)
C(14)-N(1)	1.330(2)
C(14)-C(18)	1.377(2)
C(14)-S(2)	1.7793(17)
C(15)-N(1)	1.332(2)
C(15)-C(16)	1.386(3)
C(16)-C(17)	1.378(3)
C(17)-C(18)	1.382(3)
O(1)-S(2)	1.4411(11)
O(2)-S(2)	1.4376(11)
P(1)-S(1)	1.9453(5)

C(6)-C(1)-C(2)	119.84(15)
C(6)-C(1)-P(1)	122.60(12)
C(2)-C(1)-P(1)	117.41(12)
C(3)-C(2)-C(1)	120.05(17)
C(2)-C(3)-C(4)	119.95(17)
C(5)-C(4)-C(3)	120.23(17)
C(4)-C(5)-C(6)	120.41(18)
C(1)-C(6)-C(5)	119.52(16)
C(8)-C(7)-C(12)	119.26(15)
C(8)-C(7)-P(1)	122.46(12)
C(12)-C(7)-P(1)	118.28(12)
C(9)-C(8)-C(7)	120.10(16)
C(10)-C(9)-C(8)	120.10(17)
C(11)-C(10)-C(9)	120.17(16)
C(10)-C(11)-C(12)	120.53(16)
C(11)-C(12)-C(7)	119.83(16)
S(2)-C(13)-P(1)	119.59(8)
N(1)-C(14)-C(18)	125.94(16)
N(1)-C(14)-S(2)	112.49(12)
C(18)-C(14)-S(2)	121.53(13)
N(1)-C(15)-C(16)	123.09(17)
C(17)-C(16)-C(15)	119.08(17)
C(16)-C(17)-C(18)	119.07(16)
C(14)-C(18)-C(17)	116.76(16)
C(14)-N(1)-C(15)	116.00(15)
C(7)-P(1)-C(1)	107.83(7)
C(7)-P(1)-C(13)	106.97(7)
C(1)-P(1)-C(13)	100.26(7)
C(7)-P(1)-S(1)	113.60(5)
C(1)-P(1)-S(1)	111.96(5)
C(13)-P(1)-S(1)	115.19(5)
O(2)-S(2)-O(1)	118.06(7)
O(2)-S(2)-C(13)	106.42(7)
O(1)-S(2)-C(13)	110.20(7)
O(2)-S(2)-C(14)	109.25(7)

O(1)-S(2)-C(14)	108.55(7)
C(13)-S(2)-C(14)	103.37(7)

Symmetry transformations used to generate equivalent atoms:

Table 48-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	21(1)	20(1)	28(1)	-2(1)	8(1)	-4(1)
C(2)	30(1)	22(1)	36(1)	0(1)	10(1)	-2(1)
C(3)	39(1)	21(1)	50(1)	-7(1)	19(1)	-5(1)
C(4)	41(1)	35(1)	42(1)	-18(1)	16(1)	-12(1)
C(5)	34(1)	46(1)	32(1)	-8(1)	2(1)	-4(1)
C(6)	26(1)	30(1)	32(1)	-4(1)	6(1)	0(1)
C(7)	18(1)	22(1)	22(1)	-2(1)	4(1)	0(1)
C(8)	27(1)	25(1)	34(1)	3(1)	9(1)	1(1)
C(9)	44(1)	25(1)	38(1)	6(1)	4(1)	5(1)
C(10)	37(1)	37(1)	41(1)	-4(1)	1(1)	18(1)
C(11)	24(1)	49(1)	42(1)	-1(1)	10(1)	11(1)
C(12)	23(1)	34(1)	31(1)	0(1)	9(1)	-1(1)
C(13)	19(1)	23(1)	26(1)	-2(1)	8(1)	-1(1)
C(14)	18(1)	24(1)	29(1)	-3(1)	2(1)	1(1)
C(15)	31(1)	29(1)	45(1)	4(1)	9(1)	9(1)
C(16)	29(1)	34(1)	39(1)	9(1)	4(1)	1(1)
C(17)	26(1)	43(1)	30(1)	-1(1)	7(1)	-3(1)
C(18)	23(1)	29(1)	31(1)	-6(1)	5(1)	1(1)
N(1)	26(1)	26(1)	35(1)	-1(1)	8(1)	7(1)
O(1)	32(1)	21(1)	40(1)	-3(1)	13(1)	5(1)
O(2)	23(1)	32(1)	44(1)	-8(1)	9(1)	-9(1)
P(1)	17(1)	17(1)	24(1)	1(1)	6(1)	-2(1)
S(1)	30(1)	25(1)	31(1)	7(1)	10(1)	-4(1)
S(2)	19(1)	19(1)	30(1)	-4(1)	7(1)	-1(1)

Table 48-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
H(2)	6966	6416	1845	35
H(3)	7166	7440	3916	43
H(4)	8227	6971	6125	46
H(5)	9054	5462	6289	46
H(6)	8856	4419	4225	35
H(8)	7758	2675	2553	34
H(9)	8790	1299	2934	44
H(10)	10238	1364	2223	48
H(11)	10656	2788	1116	46
H(12)	9617	4158	657	35
H(13A)	6534	3696	1701	27
H(13B)	6130	4726	945	27
H(15)	5153	6615	-2658	42
H(16)	5833	6517	-4668	42
H(17)	6537	5015	-5159	40
H(18)	6613	3663	-3509	33

Röntgenstrukturanalytische Daten für 49

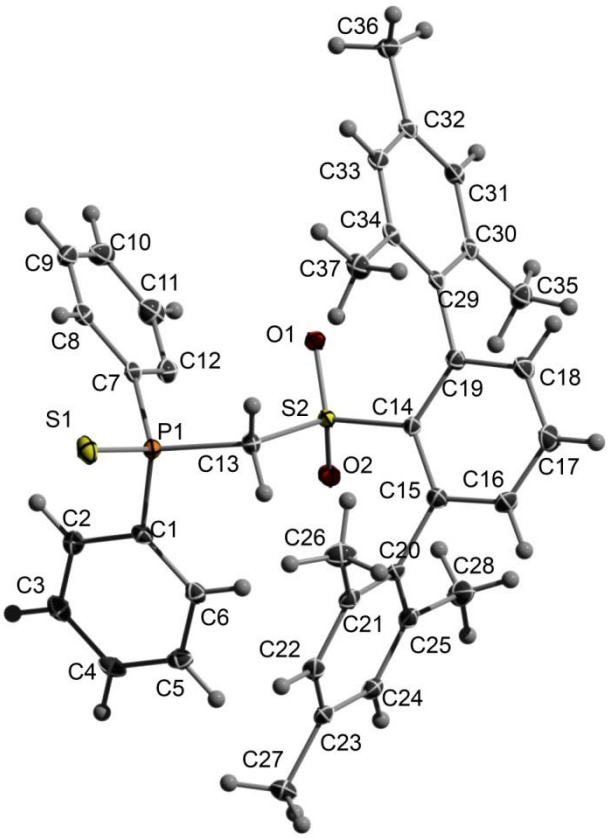

Table 49-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	C37 H37 O2 P S2	
Formula weight	608.76	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.6924(5) Å	α = 91.295(2)°.
	b = 10.6435(7) Å	β = 93.064(2)°.
	c = 16.8624(8) Å	γ = 96.496(2)°.
Volume	1547.19(15) $Å^3$	
Z	2	
Density (calculated)	1.307 Mg/m^3	
Absorption coefficient	0.257 mm^{-1}	

F(000)	644
Crystal size	0.32 x 0.32 x 0.17 mm^3
Theta range for data collection	1.93 to 26.44°.
Index ranges	-10<=h<=10, -13<=k<=13, -21<=l<=21
Reflections collected	21036
Independent reflections	6363 [R(int) = 0.0270]
Completeness to theta = 26.44°	99.9 %
Absorption correction	Empirical
Max. and min. transmission	0.9576 and 0.9223
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6363 / 0 / 385
Goodness-of-fit on F^2	1.018
Final R indices [I>2sigma(I)]	R1 = 0.0327, wR2 = 0.0803
R indices (all data)	R1 = 0.0398, wR2 = 0.0847
Largest diff. peak and hole	0.347 and -0.383 e.$Å^{-3}$

Table 49-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	8641(1)	3530(1)	2297(1)	19(1)
S(2)	8838(1)	7917(1)	2898(1)	11(1)
P(1)	7766(1)	4983(1)	2743(1)	12(1)
O(1)	9469(1)	7853(1)	3697(1)	16(1)
O(2)	7269(1)	8212(1)	2774(1)	16(1)
C(1)	5777(2)	5063(1)	2385(1)	13(1)
C(2)	4662(2)	4150(2)	2666(1)	17(1)
C(3)	3128(2)	4082(2)	2380(1)	19(1)
C(4)	2694(2)	4916(2)	1810(1)	16(1)
C(5)	3792(2)	5821(2)	1532(1)	16(1)
C(6)	5336(2)	5901(1)	1819(1)	14(1)
C(7)	7700(2)	5011(1)	3813(1)	14(1)
C(8)	8439(2)	4134(2)	4246(1)	18(1)
C(9)	8378(2)	4132(2)	5070(1)	23(1)

C(10)	7586(2)	5002(2)	5452(1)	24(1)
C(11)	6840(2)	5876(2)	5020(1)	22(1)
C(12)	6889(2)	5882(2)	4202(1)	17(1)
C(13)	8966(2)	6412(1)	2427(1)	13(1)
C(14)	10089(2)	9027(1)	2368(1)	12(1)
C(15)	9677(2)	9287(2)	1570(1)	16(1)
C(16)	10624(2)	10209(2)	1192(1)	22(1)
C(17)	11940(2)	10849(2)	1574(1)	25(1)
C(18)	12337(2)	10575(2)	2351(1)	20(1)
C(19)	11431(2)	9674(1)	2768(1)	13(1)
C(20)	8318(2)	8636(1)	1071(1)	15(1)
C(21)	8548(2)	7623(2)	558(1)	16(1)
C(22)	7304(2)	7060(2)	71(1)	16(1)
C(23)	5855(2)	7500(2)	54(1)	16(1)
C(24)	5676(2)	8543(2)	540(1)	17(1)
C(25)	6878(2)	9122(2)	1050(1)	16(1)
C(26)	10120(2)	7156(2)	498(1)	23(1)
C(27)	4530(2)	6867(2)	-478(1)	21(1)
C(28)	6622(2)	10261(2)	1552(1)	25(1)
C(29)	12013(2)	9503(1)	3607(1)	12(1)
C(30)	11670(2)	10345(1)	4207(1)	13(1)
C(31)	12285(2)	10209(1)	4977(1)	14(1)
C(32)	13225(2)	9272(1)	5162(1)	14(1)
C(33)	13593(2)	8482(1)	4547(1)	15(1)
C(34)	12998(2)	8581(1)	3773(1)	13(1)
C(35)	10662(2)	11378(2)	4033(1)	18(1)
C(36)	13831(2)	9094(2)	6003(1)	20(1)
C(37)	13426(2)	7709(2)	3124(1)	19(1)

Table 49-3. Bond lengths [Å] and angles [°] for sad.

S(1)-P(1)	1.9521(6)
S(2)-O(1)	1.4328(11)
S(2)-O(2)	1.4396(11)
S(2)-C(13)	1.7892(15)
S(2)-C(14)	1.7999(15)
P(1)-C(7)	1.8079(16)
P(1)-C(1)	1.8118(16)
P(1)-C(13)	1.8496(15)
C(1)-C(6)	1.390(2)
C(1)-C(2)	1.402(2)
C(2)-C(3)	1.387(2)
C(3)-C(4)	1.390(2)
C(4)-C(5)	1.385(2)
C(5)-C(6)	1.395(2)
C(7)-C(8)	1.391(2)
C(7)-C(12)	1.398(2)
C(8)-C(9)	1.392(2)
C(9)-C(10)	1.383(3)
C(10)-C(11)	1.389(3)
C(11)-C(12)	1.384(2)
C(14)-C(15)	1.415(2)
C(14)-C(19)	1.415(2)
C(15)-C(16)	1.397(2)
C(15)-C(20)	1.505(2)
C(16)-C(17)	1.383(2)
C(17)-C(18)	1.382(2)
C(18)-C(19)	1.399(2)
C(19)-C(29)	1.498(2)
C(20)-C(21)	1.406(2)
C(20)-C(25)	1.407(2)
C(21)-C(22)	1.392(2)
C(21)-C(26)	1.514(2)
C(22)-C(23)	1.392(2)
C(23)-C(24)	1.393(2)

C(23)-C(27)	1.508(2)
C(24)-C(25)	1.395(2)
C(25)-C(28)	1.507(2)
C(29)-C(34)	1.397(2)
C(29)-C(30)	1.403(2)
C(30)-C(31)	1.395(2)
C(30)-C(35)	1.506(2)
C(31)-C(32)	1.390(2)
C(32)-C(33)	1.393(2)
C(32)-C(36)	1.509(2)
C(33)-C(34)	1.390(2)
C(34)-C(37)	1.508(2)

O(1)-S(2)-O(2)	118.56(7)
O(1)-S(2)-C(13)	106.72(7)
O(2)-S(2)-C(13)	108.09(7)
O(1)-S(2)-C(14)	109.06(7)
O(2)-S(2)-C(14)	108.49(7)
C(13)-S(2)-C(14)	105.11(7)
C(7)-P(1)-C(1)	104.47(7)
C(7)-P(1)-C(13)	109.79(7)
C(1)-P(1)-C(13)	108.43(7)
C(7)-P(1)-S(1)	114.63(5)
C(1)-P(1)-S(1)	112.74(5)
C(13)-P(1)-S(1)	106.67(5)
C(6)-C(1)-C(2)	119.54(14)
C(6)-C(1)-P(1)	123.97(12)
C(2)-C(1)-P(1)	116.32(12)
C(3)-C(2)-C(1)	120.28(15)
C(2)-C(3)-C(4)	119.96(15)
C(5)-C(4)-C(3)	119.97(15)
C(4)-C(5)-C(6)	120.42(15)
C(1)-C(6)-C(5)	119.82(14)
C(8)-C(7)-C(12)	120.16(15)
C(8)-C(7)-P(1)	119.12(12)
C(12)-C(7)-P(1)	120.70(12)

C(7)-C(8)-C(9)	119.73(16)
C(10)-C(9)-C(8)	119.88(16)
C(9)-C(10)-C(11)	120.55(16)
C(12)-C(11)-C(10)	120.00(16)
C(11)-C(12)-C(7)	119.68(15)
S(2)-C(13)-P(1)	120.33(8)
C(15)-C(14)-C(19)	121.01(14)
C(15)-C(14)-S(2)	119.54(11)
C(19)-C(14)-S(2)	119.37(11)
C(16)-C(15)-C(14)	118.07(14)
C(16)-C(15)-C(20)	115.75(14)
C(14)-C(15)-C(20)	126.16(14)
C(17)-C(16)-C(15)	121.65(15)
C(18)-C(17)-C(16)	119.62(15)
C(17)-C(18)-C(19)	121.72(15)
C(18)-C(19)-C(14)	117.93(14)
C(18)-C(19)-C(29)	114.97(13)
C(14)-C(19)-C(29)	127.10(13)
C(21)-C(20)-C(25)	120.00(14)
C(21)-C(20)-C(15)	119.17(14)
C(25)-C(20)-C(15)	120.44(14)
C(22)-C(21)-C(20)	119.04(15)
C(22)-C(21)-C(26)	118.98(14)
C(20)-C(21)-C(26)	121.94(15)
C(21)-C(22)-C(23)	122.04(15)
C(22)-C(23)-C(24)	117.84(15)
C(22)-C(23)-C(27)	120.77(15)
C(24)-C(23)-C(27)	121.39(15)
C(23)-C(24)-C(25)	122.16(15)
C(24)-C(25)-C(20)	118.78(14)
C(24)-C(25)-C(28)	119.73(15)
C(20)-C(25)-C(28)	121.48(15)
C(34)-C(29)-C(30)	120.55(14)
C(34)-C(29)-C(19)	119.85(13)
C(30)-C(29)-C(19)	119.36(13)
C(31)-C(30)-C(29)	118.55(14)

C(31)-C(30)-C(35)	120.12(14)
C(29)-C(30)-C(35)	121.33(14)
C(32)-C(31)-C(30)	121.92(14)
C(31)-C(32)-C(33)	118.13(14)
C(31)-C(32)-C(36)	121.65(14)
C(33)-C(32)-C(36)	120.22(14)
C(34)-C(33)-C(32)	121.76(14)
C(33)-C(34)-C(29)	119.01(14)
C(33)-C(34)-C(37)	120.09(14)
C(29)-C(34)-C(37)	120.90(14)

Symmetry transformations used to generate equivalent atoms:

Table 49-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	18(1)	12(1)	26(1)	-3(1)	2(1)	3(1)
S(2)	12(1)	10(1)	10(1)	0(1)	0(1)	-1(1)
P(1)	12(1)	9(1)	13(1)	0(1)	0(1)	0(1)
O(1)	18(1)	17(1)	11(1)	2(1)	-1(1)	-4(1)
O(2)	14(1)	14(1)	19(1)	0(1)	1(1)	2(1)
C(1)	13(1)	12(1)	13(1)	-2(1)	0(1)	1(1)
C(2)	18(1)	15(1)	18(1)	2(1)	1(1)	0(1)
C(3)	17(1)	18(1)	20(1)	-2(1)	4(1)	-3(1)
C(4)	14(1)	21(1)	15(1)	-6(1)	0(1)	2(1)
C(5)	18(1)	18(1)	13(1)	-2(1)	-1(1)	4(1)
C(6)	16(1)	14(1)	13(1)	-2(1)	1(1)	0(1)
C(7)	13(1)	14(1)	14(1)	3(1)	-1(1)	-4(1)
C(8)	15(1)	14(1)	22(1)	2(1)	-3(1)	-3(1)
C(9)	22(1)	21(1)	23(1)	10(1)	-7(1)	-6(1)
C(10)	24(1)	30(1)	14(1)	5(1)	-1(1)	-7(1)
C(11)	21(1)	26(1)	18(1)	-1(1)	4(1)	-2(1)
C(12)	16(1)	18(1)	17(1)	3(1)	1(1)	-1(1)

C(13)	13(1)	11(1)	14(1)	0(1)	2(1)	1(1)
C(14)	14(1)	10(1)	11(1)	1(1)	1(1)	0(1)
C(15)	19(1)	14(1)	14(1)	0(1)	-1(1)	0(1)
C(16)	31(1)	23(1)	12(1)	6(1)	-3(1)	-5(1)
C(17)	30(1)	24(1)	18(1)	6(1)	1(1)	-11(1)
C(18)	19(1)	19(1)	18(1)	1(1)	-2(1)	-7(1)
C(19)	14(1)	12(1)	13(1)	0(1)	1(1)	2(1)
C(20)	20(1)	15(1)	9(1)	3(1)	-3(1)	-1(1)
C(21)	20(1)	16(1)	11(1)	4(1)	1(1)	2(1)
C(22)	24(1)	14(1)	11(1)	0(1)	1(1)	0(1)
C(23)	21(1)	16(1)	11(1)	5(1)	-2(1)	-3(1)
C(24)	20(1)	16(1)	16(1)	4(1)	-2(1)	4(1)
C(25)	24(1)	13(1)	13(1)	2(1)	-1(1)	3(1)
C(26)	22(1)	31(1)	18(1)	-1(1)	2(1)	6(1)
C(27)	23(1)	22(1)	18(1)	-2(1)	-5(1)	-1(1)
C(28)	35(1)	17(1)	24(1)	-4(1)	-7(1)	10(1)
C(29)	10(1)	11(1)	13(1)	0(1)	-1(1)	-3(1)
C(30)	11(1)	11(1)	16(1)	1(1)	1(1)	-2(1)
C(31)	15(1)	14(1)	13(1)	-2(1)	2(1)	-3(1)
C(32)	12(1)	16(1)	14(1)	2(1)	-1(1)	-4(1)
C(33)	12(1)	14(1)	19(1)	2(1)	-1(1)	1(1)
C(34)	10(1)	13(1)	16(1)	-1(1)	2(1)	-2(1)
C(35)	20(1)	16(1)	19(1)	0(1)	2(1)	4(1)
C(36)	20(1)	22(1)	16(1)	3(1)	-4(1)	-2(1)
C(37)	19(1)	18(1)	20(1)	-3(1)	1(1)	5(1)

Röntgenstrukturanalytische Daten für 50

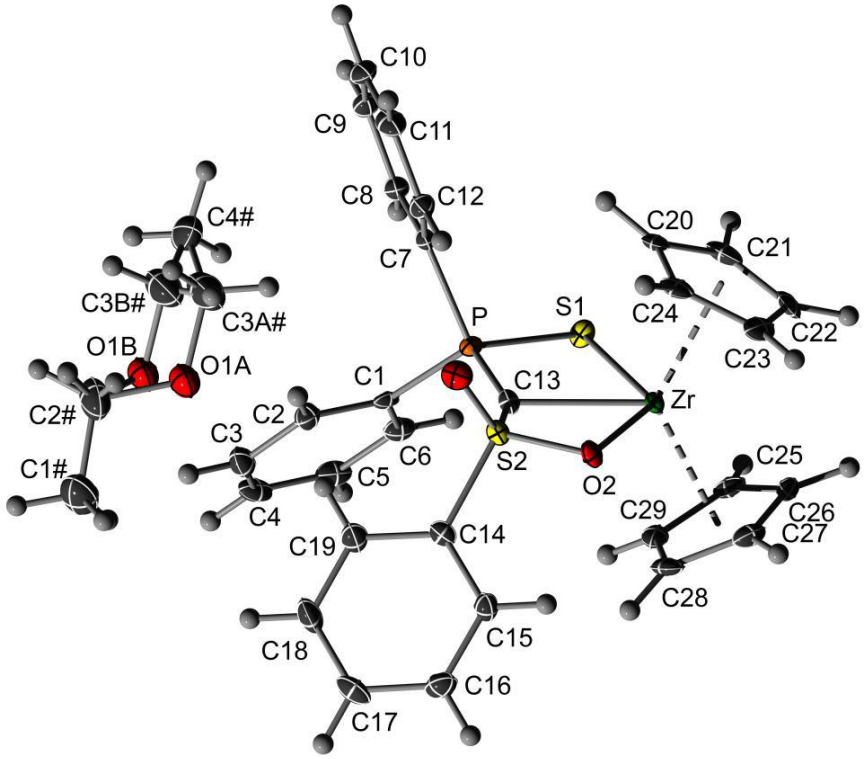

Table 50-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	$C_{33}H_{35}O_3PS_2Zr$	
Formula weight	665.92	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pna2(1)	
Unit cell dimensions	a = 25.4836(10) Å	α= 90°.
	b = 10.4001(3) Å	β= 90°.
	c = 11.3209(4) Å	γ = 90°.
Volume	3000.40(18) $Å^3$	
Z	4	
Density (calculated)	1.474 Mg/m^3	
Absorption coefficient	0.592 mm^{-1}	
F(000)	1376	

Crystal size	0.45 x 0.41 x 0.35 mm^3
Theta range for data collection	2.12 to 25.00°.
Index ranges	-30<=h<=30, -12<=k<=12, -12<=l<=13
Reflections collected	23102
Independent reflections	5087 [R(int) = 0.0215]
Completeness to theta = 25.00°	100.0 %
Absorption correction	Empirical
Max. and min. transmission	0.8195 and 0.7764
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5087 / 1 / 381
Goodness-of-fit on F^2	1.058
Final R indices [I>2sigma(I)]	R1 = 0.0177, wR2 = 0.0431
R indices (all data)	R1 = 0.0186, wR2 = 0.0435
Absolute structure parameter	-0.01(2)
Largest diff. peak and hole	0.214 and -0.199 e.$Å^{-3}$

Table 50-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zr(1)	7356(1)	121(1)	5714(1)	9(1)
S(1)	7179(1)	2451(1)	6813(1)	14(1)
S(2)	6419(1)	-84(1)	4225(1)	11(1)
P(1)	6503(1)	2363(1)	5882(1)	10(1)
O(1)	5921(1)	-694(1)	4488(1)	18(1)
O(2)	6884(1)	-983(1)	4309(1)	14(1)
C(1)	6377(1)	3851(2)	5089(2)	12(1)
C(2)	5934(1)	3902(2)	4371(2)	16(1)
C(3)	5836(1)	4988(2)	3692(2)	22(1)
C(4)	6175(1)	6033(2)	3744(2)	23(1)
C(5)	6613(1)	5986(2)	4466(2)	20(1)
C(6)	6717(1)	4893(2)	5129(2)	17(1)
C(7)	5948(1)	2231(2)	6882(2)	13(1)
C(8)	5840(1)	3247(2)	7647(2)	14(1)

C(9)	5438(1)	3143(2)	8464(2)	19(1)
C(10)	5139(1)	2023(2)	8515(2)	22(1)
C(11)	5243(1)	1020(2)	7754(2)	21(1)
C(12)	5648(1)	1110(2)	6938(2)	16(1)
C(13)	6628(1)	1078(2)	5037(2)	12(1)
C(14)	6384(1)	320(2)	2700(2)	13(1)
C(15)	6717(1)	-256(2)	1891(2)	17(1)
C(16)	6677(1)	68(2)	702(3)	21(1)
C(17)	6312(1)	966(2)	330(2)	22(1)
C(18)	5974(1)	1527(2)	1150(2)	26(1)
C(19)	6007(1)	1195(2)	2329(2)	21(1)
C(20)	6845(1)	-693(2)	7490(2)	15(1)
C(21)	7353(1)	-378(2)	7904(2)	22(1)
C(22)	7708(1)	-1261(2)	7424(2)	25(1)
C(23)	7428(1)	-2082(2)	6666(2)	23(1)
C(24)	6888(1)	-1746(2)	6737(2)	18(1)
C(25)	8226(1)	1266(2)	5497(2)	17(1)
C(26)	8350(1)	-50(2)	5460(2)	19(1)
C(27)	8119(1)	-577(2)	4451(2)	20(1)
C(28)	7874(1)	430(2)	3821(2)	19(1)
C(29)	7935(1)	1566(2)	4470(2)	17(1)
C11	4593(1)	3298(3)	1680(2)	42(1)
C21	4418(1)	3025(3)	2902(2)	37(1)
O1A1	4810(1)	2363(2)	3530(2)	28(1)
O1B1	4705(8)	3270(20)	3612(19)	28(1)
C3A1	4646(1)	1872(4)	4654(3)	42(1)
C3B1	4470(18)	2370(40)	4570(40)	42(1)
C4A1	4588(1)	2924(4)	5575(3)	51(1)

Table 50-3. Bond lengths [Å] and angles [°] for sad.

Zr(1)-C(13)	2.2419(18)
Zr(1)-O(2)	2.3019(14)
Zr(1)-C(27)	2.519(2)
Zr(1)-C(25)	2.5263(18)
Zr(1)-C(29)	2.5333(19)
Zr(1)-C(21)	2.534(2)
Zr(1)-C(28)	2.536(2)
Zr(1)-C(23)	2.539(2)
Zr(1)-C(20)	2.542(2)
Zr(1)-C(26)	2.5544(19)
Zr(1)-C(24)	2.557(2)
Zr(1)-C(22)	2.572(2)
S(1)-P(1)	2.0226(7)
S(2)-O(1)	1.4507(14)
S(2)-O(2)	1.5128(14)
S(2)-C(13)	1.609(2)
S(2)-C(14)	1.780(2)
P(1)-C(13)	1.673(2)
P(1)-C(7)	1.8169(19)
P(1)-C(1)	1.818(2)
C(1)-C(6)	1.388(3)
C(1)-C(2)	1.392(3)
C(2)-C(3)	1.389(3)
C(3)-C(4)	1.390(3)
C(4)-C(5)	1.385(3)
C(5)-C(6)	1.387(3)
C(7)-C(8)	1.393(3)
C(7)-C(12)	1.395(3)
C(8)-C(9)	1.384(3)
C(9)-C(10)	1.393(3)
C(10)-C(11)	1.378(3)
C(11)-C(12)	1.387(3)
C(14)-C(15)	1.386(3)
C(14)-C(19)	1.387(3)

C(15)-C(16)	1.391(4)
C(16)-C(17)	1.386(3)
C(17)-C(18)	1.393(3)
C(18)-C(19)	1.380(3)
C(20)-C(24)	1.392(3)
C(20)-C(21)	1.414(3)
C(21)-C(22)	1.399(3)
C(22)-C(23)	1.405(3)
C(23)-C(24)	1.422(3)
C(25)-C(26)	1.405(3)
C(25)-C(29)	1.414(3)
C(26)-C(27)	1.397(3)
C(27)-C(28)	1.413(3)
C(28)-C(29)	1.399(3)
C11-C21	1.481(4)
C21-O1B1	1.12(2)
C21-O1A1	1.406(3)
C21-C3B1	2.02(4)
O1A1-C3A1	1.433(4)
O1B1-C3B1	1.56(5)
C3A1-C4A1	1.518(5)
C3B1-C4A1	1.31(5)

C(13)-Zr(1)-O(2)	63.41(6)
C(13)-Zr(1)-C(27)	124.95(7)
O(2)-Zr(1)-C(27)	82.36(6)
C(13)-Zr(1)-C(25)	118.93(7)
O(2)-Zr(1)-C(25)	128.78(6)
C(27)-Zr(1)-C(25)	53.46(7)
C(13)-Zr(1)-C(29)	91.65(7)
O(2)-Zr(1)-C(29)	102.47(6)
C(27)-Zr(1)-C(29)	53.59(7)
C(25)-Zr(1)-C(29)	32.46(7)
C(13)-Zr(1)-C(21)	114.99(7)
O(2)-Zr(1)-C(21)	124.90(6)
C(27)-Zr(1)-C(21)	119.94(7)

C(25)-Zr(1)-C(21)	101.24(7)
C(29)-Zr(1)-C(21)	131.92(7)
C(13)-Zr(1)-C(28)	94.89(7)
O(2)-Zr(1)-C(28)	75.57(6)
C(27)-Zr(1)-C(28)	32.47(7)
C(25)-Zr(1)-C(28)	53.33(7)
C(29)-Zr(1)-C(28)	32.05(7)
C(21)-Zr(1)-C(28)	148.75(7)
C(13)-Zr(1)-C(23)	127.25(7)
O(2)-Zr(1)-C(23)	83.14(7)
C(27)-Zr(1)-C(23)	85.72(7)
C(25)-Zr(1)-C(23)	113.80(7)
C(29)-Zr(1)-C(23)	136.86(7)
C(21)-Zr(1)-C(23)	53.10(8)
C(28)-Zr(1)-C(23)	115.84(7)
C(13)-Zr(1)-C(20)	89.64(7)
O(2)-Zr(1)-C(20)	96.47(6)
C(27)-Zr(1)-C(20)	138.45(7)
C(25)-Zr(1)-C(20)	133.10(7)
C(29)-Zr(1)-C(20)	159.42(7)
C(21)-Zr(1)-C(20)	32.36(7)
C(28)-Zr(1)-C(20)	167.75(7)
C(23)-Zr(1)-C(20)	53.13(7)
C(13)-Zr(1)-C(26)	144.44(7)
O(2)-Zr(1)-C(26)	113.93(6)
C(27)-Zr(1)-C(26)	31.96(7)
C(25)-Zr(1)-C(26)	32.11(6)
C(29)-Zr(1)-C(26)	53.25(6)
C(21)-Zr(1)-C(26)	95.71(7)
C(28)-Zr(1)-C(26)	53.04(7)
C(23)-Zr(1)-C(26)	85.05(7)
C(20)-Zr(1)-C(26)	125.02(7)
C(13)-Zr(1)-C(24)	96.05(7)
O(2)-Zr(1)-C(24)	71.95(6)
C(27)-Zr(1)-C(24)	113.47(7)
C(25)-Zr(1)-C(24)	144.20(7)

C(29)-Zr(1)-C(24)	166.96(7)
C(21)-Zr(1)-C(24)	53.06(7)
C(28)-Zr(1)-C(24)	136.19(7)
C(23)-Zr(1)-C(24)	32.40(7)
C(20)-Zr(1)-C(24)	31.68(7)
C(26)-Zr(1)-C(24)	117.43(6)
C(13)-Zr(1)-C(22)	142.54(7)
O(2)-Zr(1)-C(22)	115.04(7)
C(27)-Zr(1)-C(22)	89.85(7)
C(25)-Zr(1)-C(22)	91.78(7)
C(29)-Zr(1)-C(22)	123.18(7)
C(21)-Zr(1)-C(22)	31.80(7)
C(28)-Zr(1)-C(22)	121.72(7)
C(23)-Zr(1)-C(22)	31.90(8)
C(20)-Zr(1)-C(22)	52.90(7)
C(26)-Zr(1)-C(22)	72.57(7)
C(24)-Zr(1)-C(22)	52.92(7)
P(1)-S(1)-Zr(1)	82.24(2)
O(1)-S(2)-O(2)	113.80(8)
O(1)-S(2)-C(13)	120.06(9)
O(2)-S(2)-C(13)	99.79(9)
O(1)-S(2)-C(14)	104.92(9)
O(2)-S(2)-C(14)	104.26(9)
C(13)-S(2)-C(14)	113.16(10)
O(1)-S(2)-Zr(1)	128.89(6)
O(2)-S(2)-Zr(1)	51.00(6)
C(13)-S(2)-Zr(1)	49.28(7)
C(14)-S(2)-Zr(1)	125.60(7)
C(13)-P(1)-C(7)	116.40(9)
C(13)-P(1)-C(1)	115.52(9)
C(7)-P(1)-C(1)	103.62(9)
C(13)-P(1)-S(1)	99.88(7)
C(7)-P(1)-S(1)	109.98(7)
C(1)-P(1)-S(1)	111.63(7)
S(2)-O(2)-Zr(1)	98.29(7)
C(6)-C(1)-C(2)	119.71(19)

C(6)-C(1)-P(1)	122.61(16)
C(2)-C(1)-P(1)	117.60(15)
C(3)-C(2)-C(1)	119.98(19)
C(2)-C(3)-C(4)	120.0(2)
C(5)-C(4)-C(3)	119.9(2)
C(4)-C(5)-C(6)	120.2(2)
C(5)-C(6)-C(1)	120.2(2)
C(8)-C(7)-C(12)	119.81(18)
C(8)-C(7)-P(1)	118.93(14)
C(12)-C(7)-P(1)	121.18(15)
C(9)-C(8)-C(7)	120.12(19)
C(8)-C(9)-C(10)	119.9(2)
C(11)-C(10)-C(9)	120.1(2)
C(10)-C(11)-C(12)	120.5(2)
C(11)-C(12)-C(7)	119.6(2)
S(2)-C(13)-P(1)	149.66(12)
S(2)-C(13)-Zr(1)	97.77(9)
P(1)-C(13)-Zr(1)	108.48(9)
C(15)-C(14)-C(19)	120.5(2)
C(15)-C(14)-S(2)	120.51(16)
C(19)-C(14)-S(2)	118.94(16)
C(14)-C(15)-C(16)	119.33(19)
C(17)-C(16)-C(15)	120.4(2)
C(16)-C(17)-C(18)	119.6(2)
C(19)-C(18)-C(17)	120.2(2)
C(18)-C(19)-C(14)	119.9(2)
C(24)-C(20)-C(21)	108.25(19)
C(24)-C(20)-Zr(1)	74.76(11)
C(21)-C(20)-Zr(1)	73.52(12)
C(22)-C(21)-C(20)	108.1(2)
C(22)-C(21)-Zr(1)	75.59(13)
C(20)-C(21)-Zr(1)	74.12(12)
C(21)-C(22)-C(23)	107.93(19)
C(21)-C(22)-Zr(1)	72.61(12)
C(23)-C(22)-Zr(1)	72.75(12)
C(22)-C(23)-C(24)	107.9(2)

C(22)-C(23)-Zr(1)	75.34(12)
C(24)-C(23)-Zr(1)	74.50(12)
C(20)-C(24)-C(23)	107.71(19)
C(20)-C(24)-Zr(1)	73.56(12)
C(23)-C(24)-Zr(1)	73.10(12)
C(26)-C(25)-C(29)	107.97(19)
C(26)-C(25)-Zr(1)	75.05(11)
C(29)-C(25)-Zr(1)	74.04(11)
C(27)-C(26)-C(25)	108.15(19)
C(27)-C(26)-Zr(1)	72.62(11)
C(25)-C(26)-Zr(1)	72.85(11)
C(26)-C(27)-C(28)	107.95(19)
C(26)-C(27)-Zr(1)	75.42(12)
C(28)-C(27)-Zr(1)	74.41(11)
C(29)-C(28)-C(27)	108.14(19)
C(29)-C(28)-Zr(1)	73.89(12)
C(27)-C(28)-Zr(1)	73.12(11)
C(28)-C(29)-C(25)	107.70(18)
C(28)-C(29)-Zr(1)	74.06(11)
C(25)-C(29)-Zr(1)	73.50(11)
O1B1-C21-O1A1	44.2(13)
O1B1-C21-C11	115.5(11)
O1A1-C21-C11	110.7(2)
O1B1-C21-C3B1	50.1(17)
O1A1-C21-C3B1	46.5(14)
C11-C21-C3B1	157.2(14)
C21-O1A1-C3A1	114.7(2)
C21-O1B1-C3B1	96(2)
O1A1-C3A1-C4A1	112.4(3)
C4A1-C3B1-O1B1	105(3)
C4A1-C3B1-C21	133(3)
O1B1-C3B1-C21	33.4(11)
C3B1-C4A1-C3A1	27(2)

Symmetry transformations used to generate equivalent atoms:

Table 50-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zr(1)	10(1)	9(1)	9(1)	1(1)	0(1)	0(1)
S(1)	12(1)	14(1)	16(1)	-5(1)	-1(1)	-1(1)
S(2)	13(1)	9(1)	12(1)	0(1)	-2(1)	-1(1)
P(1)	10(1)	9(1)	11(1)	0(1)	1(1)	-1(1)
O(1)	18(1)	17(1)	19(1)	-1(1)	-1(1)	-6(1)
O(2)	17(1)	9(1)	15(1)	1(1)	-2(1)	2(1)
C(1)	16(1)	9(1)	12(1)	0(1)	7(1)	4(1)
C(2)	17(1)	14(1)	19(1)	1(1)	2(1)	1(1)
C(3)	26(1)	21(1)	20(1)	2(1)	-2(1)	7(1)
C(4)	37(1)	14(1)	18(1)	4(1)	10(1)	6(1)
C(5)	29(1)	11(1)	20(1)	-1(1)	9(1)	-2(1)
C(6)	21(1)	13(1)	16(1)	-3(1)	5(1)	0(1)
C(7)	10(1)	16(1)	11(1)	4(1)	-1(1)	1(1)
C(8)	13(1)	16(1)	13(1)	1(1)	1(1)	1(1)
C(9)	18(1)	25(1)	15(1)	-3(1)	2(1)	6(1)
C(10)	12(1)	37(1)	18(1)	6(1)	3(1)	-1(1)
C(11)	16(1)	25(1)	22(1)	7(1)	-1(1)	-7(1)
C(12)	14(1)	17(1)	17(1)	2(1)	0(1)	-1(1)
C(13)	12(1)	11(1)	13(1)	1(1)	-2(1)	0(1)
C(14)	17(1)	11(1)	12(1)	-1(1)	-2(1)	-3(1)
C(15)	17(1)	18(1)	16(1)	-3(1)	-3(1)	3(1)
C(16)	20(1)	27(1)	17(1)	-6(1)	3(1)	1(1)
C(17)	31(1)	24(1)	13(1)	1(1)	-6(1)	-4(1)
C(18)	34(1)	24(1)	21(1)	2(1)	-9(1)	11(1)
C(19)	25(1)	22(1)	17(1)	-4(1)	-2(1)	8(1)
C(20)	19(1)	18(1)	9(1)	5(1)	4(1)	0(1)
C(21)	31(1)	25(1)	10(1)	5(1)	-3(1)	-9(1)
C(22)	19(1)	37(1)	20(1)	20(1)	-3(1)	1(1)
C(23)	33(1)	14(1)	22(1)	10(1)	11(1)	8(1)
C(24)	22(1)	17(1)	13(1)	7(1)	2(1)	-8(1)
C(25)	11(1)	24(1)	17(1)	-5(1)	5(1)	-5(1)

C(26)	11(1)	27(1)	20(2)	9(1)	4(1)	4(1)
C(27)	21(1)	18(1)	22(1)	-2(1)	10(1)	1(1)
C(28)	17(1)	30(1)	10(1)	1(1)	5(1)	-6(1)
C(29)	15(1)	16(1)	20(1)	8(1)	6(1)	1(1)
C11	50(2)	47(2)	28(2)	-5(1)	-8(1)	9(1)
C21	27(1)	43(2)	42(2)	9(1)	-10(1)	2(1)
O1A1	26(1)	31(1)	25(1)	2(1)	-5(1)	3(1)
O1B1	26(1)	31(1)	25(1)	2(1)	-5(1)	3(1)
C3A1	43(2)	50(2)	32(2)	11(2)	-7(2)	-2(2)
C3B1	43(2)	50(2)	32(2)	11(2)	-7(2)	-2(2)
C4A1	27(1)	94(2)	32(2)	4(2)	1(1)	22(2)

Table 50-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
H(2)	5699	3194	4345	20
H(3)	5537	5017	3192	27
H(4)	6106	6779	3286	27
H(5)	6843	6703	4508	24
H(6)	7021	4858	5612	20
H(8)	6042	4013	7607	17
H(9)	5366	3834	8988	23
H(10)	4863	1949	9076	27
H(11)	5036	261	7789	25
H(12)	5719	414	6420	19
H(15)	6970	-867	2145	20
H(16)	6902	-330	142	26
H(17)	6291	1199	-480	27
H(18)	5721	2139	898	31
H(19)	5772	1564	2884	26
H(20)	6509	-321	7792	18
H(21)	7433	249	8549	26

H(22)	8085	-1357	7653	30
H(23)	7572	-2871	6279	27
H(24)	6589	-2253	6405	21
H(25)	8374	1905	6067	21
H(26)	8596	-506	6007	23
H(27)	8179	-1468	4147	24
H(28)	7728	367	3003	23
H(29)	7844	2450	4191	21
H1A1	4654	2486	1263	62
H1B1	4919	3798	1702	62
H1C1	4321	3791	1267	62
H2A1	4337	3843	3310	45
H2B1	4094	2501	2881	45
H2C1	4090	3507	3050	45
H2D1	4335	2098	2962	45
H3AA1	4907	1236	4934	50
H3AB1	4306	1424	4561	50
H3BA1	4085	2292	4480	50
H3BB1	4629	1502	4527	50
H5A1	4372(11)	3530(30)	5370(20)	41(8)
H7A1	4473(12)	2440(30)	6350(30)	61(10)
H6A1	4923(11)	3350(30)	5690(30)	54(8)

Röntgenstrukturanalytische Daten für 52

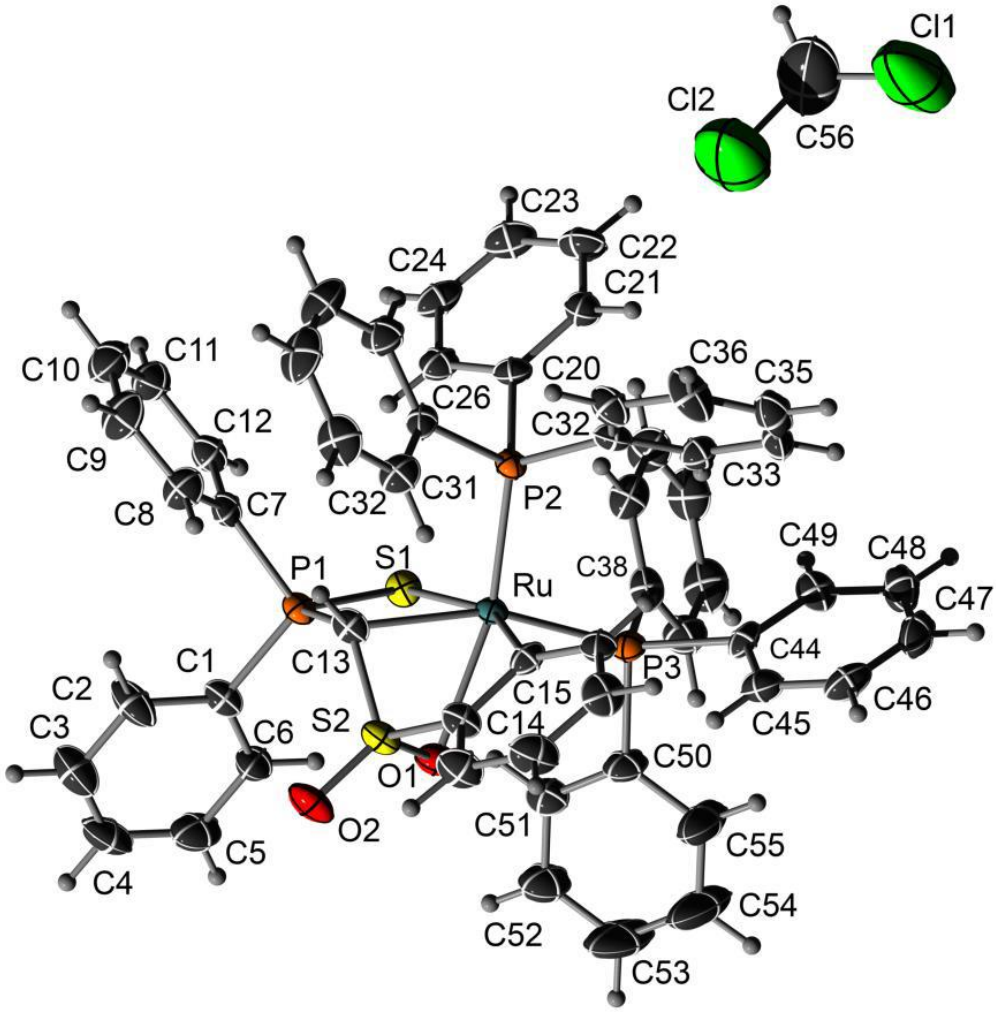

Table 52-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	C56 H47 Cl2 O2 P3 Ru S2	
Formula weight	1080.94	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 15.083(5) Å	α = 90°.
	b = 15.828(5) Å	β = 101.909(6)°.
	c = 21.542(8) Å	γ = 90°.
Volume	5032(3) Å^3	

Z	4
Density (calculated)	1.427 Mg/m^3
Absorption coefficient	0.638 mm^{-1}
F(000)	2216
Crystal size	0.24 x 0.05 x 0.05 mm^3
Theta range for data collection	1.38 to 25.00°.
Index ranges	-17<=h<=17, -18<=k<=18, -25<=l<=25
Reflections collected	43366
Independent reflections	8836 [R(int) = 0.0804]
Completeness to theta = 25.00°	100.0 %
Max. and min. transmission	0.9688 and 0.8619
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8836 / 0 / 599
Goodness-of-fit on F^2	1.077
Final R indices [I>2sigma(I)]	R1 = 0.0628, wR2 = 0.1729
R indices (all data)	R1 = 0.0859, wR2 = 0.1877
Largest diff. peak and hole	0.797 and -1.338 e.$Å^{-3}$

Table 52-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	1851(4)	-296(4)	4569(3)	25(1)
C(2)	1535(5)	-1118(5)	4478(3)	41(2)
C(3)	1025(5)	-1469(5)	4876(4)	49(2)
C(4)	821(5)	-998(5)	5366(4)	46(2)
C(5)	1124(5)	-176(5)	5460(3)	45(2)
C(6)	1638(5)	177(4)	5058(3)	34(2)
C(7)	3209(4)	-702(4)	3852(3)	26(1)
C(8)	2916(5)	-1214(4)	3326(3)	35(2)
C(9)	3440(5)	-1906(4)	3231(4)	46(2)
C(10)	4253(5)	-2061(5)	3637(4)	45(2)
C(11)	4541(5)	-1562(4)	4163(3)	36(2)
C(12)	4026(4)	-887(4)	4264(3)	29(1)

C(13)	1908(4)	549(4)	3307(3)	22(1)
C(14)	708(4)	1619(4)	2615(3)	24(1)
C(15)	1473(4)	2116(4)	2615(3)	24(1)
C(16)	1367(4)	2667(4)	2092(3)	27(1)
C(17)	555(5)	2713(4)	1640(3)	34(2)
C(18)	-104(5)	1617(5)	2165(3)	38(2)
C(19)	-174(5)	2189(5)	1669(3)	42(2)
C(20)	4720(4)	1577(4)	3181(3)	23(1)
C(21)	5386(4)	2092(4)	3031(3)	29(1)
C(22)	6514(5)	1426(5)	3838(3)	39(2)
C(23)	6280(4)	2029(5)	3371(3)	38(2)
C(24)	5865(4)	899(4)	3973(3)	33(2)
C(25)	4981(4)	963(4)	3651(3)	28(1)
C(26)	3359(4)	696(4)	2299(3)	24(1)
C(27)	4079(5)	178(4)	2238(3)	36(2)
C(28)	3950(6)	-495(5)	1812(4)	48(2)
C(29)	3108(6)	-654(5)	1441(4)	50(2)
C(30)	2505(4)	522(4)	1926(3)	32(1)
C(31)	2385(5)	-150(5)	1498(3)	42(2)
C(32)	3540(4)	2449(4)	2181(3)	22(1)
C(33)	3716(4)	3289(4)	2367(3)	26(1)
C(34)	3685(4)	3927(4)	1929(3)	29(1)
C(35)	3324(5)	2920(5)	1093(3)	41(2)
C(36)	3474(5)	3741(4)	1289(3)	39(2)
C(37)	3363(4)	2272(4)	1535(3)	32(1)
C(38)	3793(4)	3373(4)	4446(3)	27(1)
C(39)	3824(5)	3885(4)	4978(3)	37(2)
C(40)	4647(5)	4055(5)	5374(3)	45(2)
C(41)	5407(5)	3205(4)	4745(4)	41(2)
C(42)	5431(5)	3726(4)	5261(3)	42(2)
C(43)	4586(5)	3035(4)	4340(3)	35(2)
C(44)	2713(4)	4188(4)	3379(3)	24(1)
C(45)	1945(4)	4359(4)	2910(3)	33(2)
C(46)	1895(5)	5074(4)	2540(3)	39(2)
C(47)	2598(5)	5642(4)	2634(3)	41(2)
C(48)	3361(5)	5496(4)	3102(3)	39(2)

C(49)	3421(4)	4777(4)	3468(3)	28(1)
C(50)	1902(5)	3465(4)	4326(3)	33(2)
C(51)	1742(4)	2874(4)	4766(3)	32(2)
C(52)	1198(5)	3062(5)	5193(4)	47(2)
C(53)	811(7)	3840(7)	5195(5)	78(3)
C(54)	984(8)	4451(7)	4773(5)	88(4)
C(55)	1515(7)	4268(5)	4339(4)	63(3)
C(56)	9672(8)	3242(8)	3371(9)	127(6)
Cl(1)	9547(2)	4126(3)	2898(3)	166(2)
Cl(2)	8684(3)	2672(3)	3327(3)	159(2)
O(1)	1169(3)	1646(3)	3828(2)	29(1)
O(2)	109(3)	503(3)	3364(2)	37(1)
P(1)	2527(1)	165(1)	4046(1)	22(1)
P(2)	3504(1)	1659(1)	2796(1)	20(1)
P(3)	2738(1)	3210(1)	3842(1)	24(1)
Ru(1)	2460(1)	1834(1)	3407(1)	19(1)
S(1)	3257(1)	1149(1)	4448(1)	24(1)
S(2)	879(1)	1021(1)	3314(1)	26(1)

Table 52-3. Bond lengths [Å] and angles [°] for sad.

C(1)-C(6)	1.382(9)
C(1)-C(2)	1.386(9)
C(1)-P(1)	1.821(6)
C(2)-C(3)	1.381(10)
C(3)-C(4)	1.378(11)
C(4)-C(5)	1.380(11)
C(5)-C(6)	1.393(9)
C(7)-C(8)	1.389(9)
C(7)-C(12)	1.393(8)
C(7)-P(1)	1.815(6)
C(8)-C(9)	1.390(10)
C(9)-C(10)	1.373(11)
C(10)-C(11)	1.377(10)
C(11)-C(12)	1.365(9)
C(13)-S(2)	1.724(6)

C(13)-P(1)	1.779(6)
C(13)-Ru(1)	2.191(6)
C(14)-C(18)	1.396(9)
C(14)-C(15)	1.396(8)
C(14)-S(2)	1.753(6)
C(15)-C(16)	1.408(8)
C(15)-Ru(1)	2.070(6)
C(16)-C(17)	1.401(9)
C(17)-C(19)	1.389(10)
C(18)-C(19)	1.387(10)
C(20)-C(21)	1.383(8)
C(20)-C(25)	1.400(8)
C(20)-P(2)	1.855(6)
C(21)-C(23)	1.398(9)
C(22)-C(24)	1.363(10)
C(22)-C(23)	1.378(10)
C(24)-C(25)	1.373(9)
C(26)-C(27)	1.388(9)
C(26)-C(30)	1.398(9)
C(26)-P(2)	1.850(6)
C(27)-C(28)	1.393(10)
C(28)-C(29)	1.378(11)
C(29)-C(31)	1.376(11)
C(30)-C(31)	1.395(9)
C(32)-C(37)	1.390(8)
C(32)-C(33)	1.399(8)
C(32)-P(2)	1.832(6)
C(33)-C(34)	1.377(8)
C(34)-C(36)	1.381(9)
C(35)-C(36)	1.371(10)
C(35)-C(37)	1.391(9)
C(38)-C(43)	1.373(9)
C(38)-C(39)	1.395(9)
C(38)-P(3)	1.854(6)
C(39)-C(40)	1.381(10)
C(40)-C(42)	1.360(11)

C(41)-C(42)	1.377(10)
C(41)-C(43)	1.386(9)
C(44)-C(45)	1.398(9)
C(44)-C(49)	1.400(8)
C(44)-P(3)	1.837(6)
C(45)-C(46)	1.378(10)
C(46)-C(47)	1.373(10)
C(47)-C(48)	1.384(10)
C(48)-C(49)	1.377(9)
C(50)-C(51)	1.388(9)
C(50)-C(55)	1.401(10)
C(50)-P(3)	1.839(6)
C(51)-C(52)	1.386(9)
C(52)-C(53)	1.362(12)
C(53)-C(54)	1.389(13)
C(54)-C(55)	1.382(12)
C(56)-Cl(1)	1.719(14)
C(56)-Cl(2)	1.727(12)
O(1)-S(2)	1.483(4)
O(1)-Ru(1)	2.332(4)
O(2)-S(2)	1.443(4)
P(1)-S(1)	1.998(2)
P(2)-Ru(1)	2.2668(16)
P(3)-Ru(1)	2.3731(17)
Ru(1)-S(1)	2.5558(17)
Ru(1)-S(2)	2.6808(17)

C(6)-C(1)-C(2)	119.2(6)
C(6)-C(1)-P(1)	120.2(5)
C(2)-C(1)-P(1)	120.6(5)
C(3)-C(2)-C(1)	120.7(7)
C(4)-C(3)-C(2)	119.9(7)
C(3)-C(4)-C(5)	120.2(7)
C(4)-C(5)-C(6)	119.8(7)
C(1)-C(6)-C(5)	120.2(6)
C(8)-C(7)-C(12)	119.2(6)

C(8)-C(7)-P(1)	122.0(5)
C(12)-C(7)-P(1)	118.8(5)
C(7)-C(8)-C(9)	119.0(6)
C(10)-C(9)-C(8)	120.4(7)
C(9)-C(10)-C(11)	120.7(7)
C(12)-C(11)-C(10)	119.1(6)
C(11)-C(12)-C(7)	121.5(6)
S(2)-C(13)-P(1)	116.6(3)
S(2)-C(13)-Ru(1)	85.5(3)
P(1)-C(13)-Ru(1)	96.3(2)
C(18)-C(14)-C(15)	127.4(6)
C(18)-C(14)-S(2)	123.2(5)
C(15)-C(14)-S(2)	109.2(4)
C(14)-C(15)-C(16)	113.1(5)
C(14)-C(15)-Ru(1)	109.4(4)
C(16)-C(15)-Ru(1)	137.5(5)
C(17)-C(16)-C(15)	121.8(6)
C(19)-C(17)-C(16)	121.6(6)
C(19)-C(18)-C(14)	116.7(6)
C(18)-C(19)-C(17)	119.3(6)
C(21)-C(20)-C(25)	117.9(5)
C(21)-C(20)-P(2)	123.6(5)
C(25)-C(20)-P(2)	118.5(4)
C(20)-C(21)-C(23)	120.3(6)
C(24)-C(22)-C(23)	119.4(6)
C(22)-C(23)-C(21)	120.4(6)
C(22)-C(24)-C(25)	120.9(6)
C(24)-C(25)-C(20)	121.0(6)
C(27)-C(26)-C(30)	118.4(6)
C(27)-C(26)-P(2)	122.7(5)
C(30)-C(26)-P(2)	118.7(5)
C(26)-C(27)-C(28)	120.6(7)
C(29)-C(28)-C(27)	120.5(7)
C(31)-C(29)-C(28)	119.7(6)
C(31)-C(30)-C(26)	120.6(6)
C(29)-C(31)-C(30)	120.2(7)

C(37)-C(32)-C(33)	117.7(5)
C(37)-C(32)-P(2)	124.0(5)
C(33)-C(32)-P(2)	118.2(4)
C(34)-C(33)-C(32)	121.5(6)
C(33)-C(34)-C(36)	119.8(6)
C(36)-C(35)-C(37)	120.5(6)
C(35)-C(36)-C(34)	119.9(6)
C(32)-C(37)-C(35)	120.6(6)
C(43)-C(38)-C(39)	118.7(6)
C(43)-C(38)-P(3)	118.7(5)
C(39)-C(38)-P(3)	122.4(5)
C(40)-C(39)-C(38)	119.7(7)
C(42)-C(40)-C(39)	121.2(6)
C(42)-C(41)-C(43)	119.7(7)
C(40)-C(42)-C(41)	119.7(7)
C(38)-C(43)-C(41)	121.0(6)
C(45)-C(44)-C(49)	117.7(6)
C(45)-C(44)-P(3)	118.4(5)
C(49)-C(44)-P(3)	123.9(4)
C(46)-C(45)-C(44)	121.1(6)
C(47)-C(46)-C(45)	120.3(6)
C(46)-C(47)-C(48)	120.0(6)
C(49)-C(48)-C(47)	120.1(6)
C(48)-C(49)-C(44)	120.9(6)
C(51)-C(50)-C(55)	117.8(6)
C(51)-C(50)-P(3)	118.4(5)
C(55)-C(50)-P(3)	123.2(6)
C(52)-C(51)-C(50)	121.2(7)
C(53)-C(52)-C(51)	120.6(7)
C(52)-C(53)-C(54)	119.3(8)
C(55)-C(54)-C(53)	120.6(9)
C(54)-C(55)-C(50)	120.4(8)
Cl(1)-C(56)-Cl(2)	113.9(7)
S(2)-O(1)-Ru(1)	86.26(19)
C(13)-P(1)-C(7)	105.7(3)
C(13)-P(1)-C(1)	115.7(3)

C(7)-P(1)-C(1)	104.8(3)
C(13)-P(1)-S(1)	105.2(2)
C(7)-P(1)-S(1)	113.7(2)
C(1)-P(1)-S(1)	111.9(2)
C(32)-P(2)-C(26)	99.3(3)
C(32)-P(2)-C(20)	101.3(3)
C(26)-P(2)-C(20)	100.9(3)
C(32)-P(2)-Ru(1)	117.70(19)
C(26)-P(2)-Ru(1)	115.06(19)
C(20)-P(2)-Ru(1)	119.36(19)
C(44)-P(3)-C(50)	100.5(3)
C(44)-P(3)-C(38)	100.5(3)
C(50)-P(3)-C(38)	99.2(3)
C(44)-P(3)-Ru(1)	125.26(19)
C(50)-P(3)-Ru(1)	109.9(2)
C(38)-P(3)-Ru(1)	117.4(2)
C(15)-Ru(1)-C(13)	85.6(2)
C(15)-Ru(1)-P(2)	90.87(17)
C(13)-Ru(1)-P(2)	97.16(16)
C(15)-Ru(1)-O(1)	80.3(2)
C(13)-Ru(1)-O(1)	65.71(19)
P(2)-Ru(1)-O(1)	161.09(11)
C(15)-Ru(1)-P(3)	99.56(16)
C(13)-Ru(1)-P(3)	157.35(16)
P(2)-Ru(1)-P(3)	104.74(6)
O(1)-Ru(1)-P(3)	93.25(11)
C(15)-Ru(1)-S(1)	160.55(17)
C(13)-Ru(1)-S(1)	78.07(15)
P(2)-Ru(1)-S(1)	101.55(6)
O(1)-Ru(1)-S(1)	83.33(11)
P(3)-Ru(1)-S(1)	91.75(6)
C(15)-Ru(1)-S(2)	64.14(17)
C(13)-Ru(1)-S(2)	39.88(16)
P(2)-Ru(1)-S(2)	127.66(5)
O(1)-Ru(1)-S(2)	33.50(11)
P(3)-Ru(1)-S(2)	123.48(5)

S(1)-Ru(1)-S(2)	96.42(5)
P(1)-S(1)-Ru(1)	80.42(7)
O(2)-S(2)-O(1)	116.1(3)
O(2)-S(2)-C(13)	119.6(3)
O(1)-S(2)-C(13)	99.8(3)
O(2)-S(2)-C(14)	113.1(3)
O(1)-S(2)-C(14)	104.5(3)
C(13)-S(2)-C(14)	101.5(3)
O(2)-S(2)-Ru(1)	169.76(19)
O(1)-S(2)-Ru(1)	60.24(16)
C(13)-S(2)-Ru(1)	54.6(2)
C(14)-S(2)-Ru(1)	77.1(2)

Symmetry transformations used to generate equivalent atoms:

Table 52-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	22(3)	34(3)	17(3)	3(2)	1(2)	-5(3)
C(2)	50(4)	52(4)	25(3)	-4(3)	14(3)	-23(4)
C(3)	52(5)	53(5)	44(5)	4(4)	15(4)	-18(4)
C(4)	33(4)	67(5)	40(4)	19(4)	14(3)	-2(4)
C(5)	50(4)	55(5)	35(4)	10(3)	21(3)	13(4)
C(6)	41(4)	32(4)	32(4)	6(3)	19(3)	4(3)
C(7)	33(3)	22(3)	25(3)	5(2)	12(3)	0(3)
C(8)	36(4)	34(4)	32(4)	-5(3)	1(3)	2(3)
C(9)	57(5)	34(4)	45(4)	-17(3)	6(4)	-2(3)
C(10)	52(5)	36(4)	48(5)	-2(3)	16(4)	11(3)
C(11)	34(4)	37(4)	38(4)	9(3)	7(3)	6(3)
C(12)	30(3)	31(3)	25(3)	3(3)	6(3)	-1(3)
C(13)	22(3)	29(3)	15(3)	-3(2)	0(2)	-6(2)
C(14)	23(3)	33(3)	16(3)	2(2)	2(2)	-2(3)
C(15)	28(3)	23(3)	19(3)	-3(2)	5(2)	5(2)

C(16)	32(3)	27(3)	26(3)	-1(3)	13(3)	2(3)
C(17)	41(4)	42(4)	20(3)	7(3)	4(3)	5(3)
C(18)	30(4)	48(4)	34(4)	3(3)	2(3)	-3(3)
C(19)	31(4)	59(5)	33(4)	12(3)	2(3)	5(3)
C(20)	21(3)	27(3)	22(3)	-4(2)	7(2)	3(2)
C(21)	29(3)	29(3)	29(3)	1(3)	9(3)	1(3)
C(22)	26(3)	53(4)	34(4)	-5(3)	-3(3)	8(3)
C(23)	20(3)	48(4)	47(4)	-7(3)	7(3)	-2(3)
C(24)	34(4)	40(4)	22(3)	0(3)	1(3)	16(3)
C(25)	32(3)	31(3)	24(3)	2(3)	9(3)	6(3)
C(26)	35(3)	19(3)	20(3)	-1(2)	11(3)	0(2)
C(27)	40(4)	36(4)	34(4)	-5(3)	12(3)	3(3)
C(28)	60(5)	37(4)	48(5)	-8(3)	10(4)	16(4)
C(29)	77(6)	31(4)	40(4)	-17(3)	11(4)	-1(4)
C(30)	36(4)	33(3)	25(3)	-4(3)	4(3)	2(3)
C(31)	49(4)	43(4)	31(4)	-11(3)	-1(3)	-11(3)
C(32)	17(3)	31(3)	19(3)	2(2)	6(2)	1(2)
C(33)	27(3)	27(3)	24(3)	-1(2)	6(3)	3(3)
C(34)	32(3)	22(3)	33(4)	1(3)	8(3)	-6(3)
C(35)	49(4)	53(4)	18(3)	7(3)	0(3)	-17(4)
C(36)	36(4)	38(4)	41(4)	14(3)	4(3)	-2(3)
C(37)	34(3)	36(4)	26(3)	-1(3)	7(3)	-8(3)
C(38)	38(4)	25(3)	17(3)	-1(2)	3(3)	-6(3)
C(39)	40(4)	39(4)	32(4)	-3(3)	10(3)	0(3)
C(40)	65(5)	42(4)	26(4)	-13(3)	7(3)	-11(4)
C(41)	32(4)	39(4)	46(4)	-7(3)	-5(3)	-1(3)
C(42)	46(4)	41(4)	34(4)	-3(3)	-5(3)	-9(3)
C(43)	43(4)	31(4)	27(3)	-1(3)	2(3)	4(3)
C(44)	33(3)	19(3)	20(3)	-4(2)	6(2)	7(2)
C(45)	29(3)	35(4)	36(4)	-5(3)	10(3)	6(3)
C(46)	38(4)	40(4)	36(4)	0(3)	3(3)	17(3)
C(47)	57(5)	29(4)	39(4)	11(3)	16(4)	9(3)
C(48)	51(4)	29(4)	39(4)	-7(3)	11(3)	-9(3)
C(49)	35(3)	33(3)	18(3)	-1(3)	5(3)	-4(3)
C(50)	38(4)	38(4)	27(3)	-2(3)	16(3)	8(3)
C(51)	34(4)	37(4)	26(3)	-5(3)	7(3)	-2(3)

C(52)	49(4)	57(5)	38(4)	5(4)	20(4)	10(4)
C(53)	86(7)	100(8)	65(6)	18(6)	53(6)	43(6)
C(54)	109(9)	86(7)	89(8)	28(6)	68(7)	61(7)
C(55)	89(7)	52(5)	64(6)	17(4)	49(5)	33(5)
C(56)	73(8)	90(9)	199(17)	20(10)	-18(9)	-9(7)
Cl(1)	81(2)	188(4)	233(5)	113(4)	39(3)	20(3)
Cl(2)	92(3)	149(4)	237(6)	45(4)	37(3)	-4(3)
O(1)	25(2)	40(3)	23(2)	1(2)	6(2)	0(2)
O(2)	22(2)	54(3)	32(2)	7(2)	1(2)	-12(2)
P(1)	25(1)	25(1)	16(1)	0(1)	5(1)	-3(1)
P(2)	22(1)	21(1)	17(1)	-1(1)	5(1)	-1(1)
P(3)	26(1)	24(1)	21(1)	-2(1)	7(1)	1(1)
Ru(1)	19(1)	22(1)	16(1)	-1(1)	5(1)	-1(1)
S(1)	27(1)	27(1)	19(1)	-3(1)	2(1)	-2(1)
S(2)	21(1)	35(1)	21(1)	4(1)	4(1)	-4(1)

Table 52-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
H(2)	1671	-1443	4139	49
H(3)	815	-2035	4811	59
H(4)	470	-1240	5639	55
H(5)	982	148	5798	54
H(6)	1843	744	5120	40
H(8)	2366	-1093	3035	42
H(9)	3234	-2275	2883	55
H(10)	4621	-2517	3553	53
H(11)	5092	-1686	4453	44
H(12)	4228	-536	4623	35
H(16)	1861	3017	2044	33
H(17)	501	3112	1305	41
H(18)	-585	1244	2197	46

H(19)	-714	2221	1353	50
H(21)	5236	2491	2697	34
H(22)	7124	1378	4064	47
H(23)	6728	2404	3280	46
H(24)	6025	482	4293	39
H(25)	4540	585	3749	34
H(27)	4664	284	2488	44
H(28)	4448	-847	1777	58
H(29)	3026	-1110	1148	60
H(30)	2001	864	1965	38
H(31)	1802	-260	1244	51
H(33)	3861	3423	2807	31
H(34)	3809	4493	2066	35
H(35)	3193	2792	653	49
H(36)	3432	4182	985	47
H(37)	3266	1705	1394	38
H(39)	3282	4115	5066	44
H(40)	4667	4409	5733	53
H(41)	5951	2964	4668	49
H(42)	5993	3854	5536	51
H(43)	4573	2678	3983	41
H(45)	1451	3975	2844	40
H(46)	1371	5175	2219	46
H(47)	2561	6134	2378	49
H(48)	3845	5892	3170	47
H(49)	3950	4679	3786	34
H(51)	2011	2330	4774	39
H(52)	1094	2645	5487	56
H(53)	428	3962	5483	94
H(54)	734	5001	4783	106
H(55)	1619	4689	4048	76
H(56A)	9899	3417	3817	153
H(56B)	10134	2870	3248	153
H(13)	1920(40)	170(40)	2980(30)	22(16)

Röntgenstrukturanalytische Daten für 53

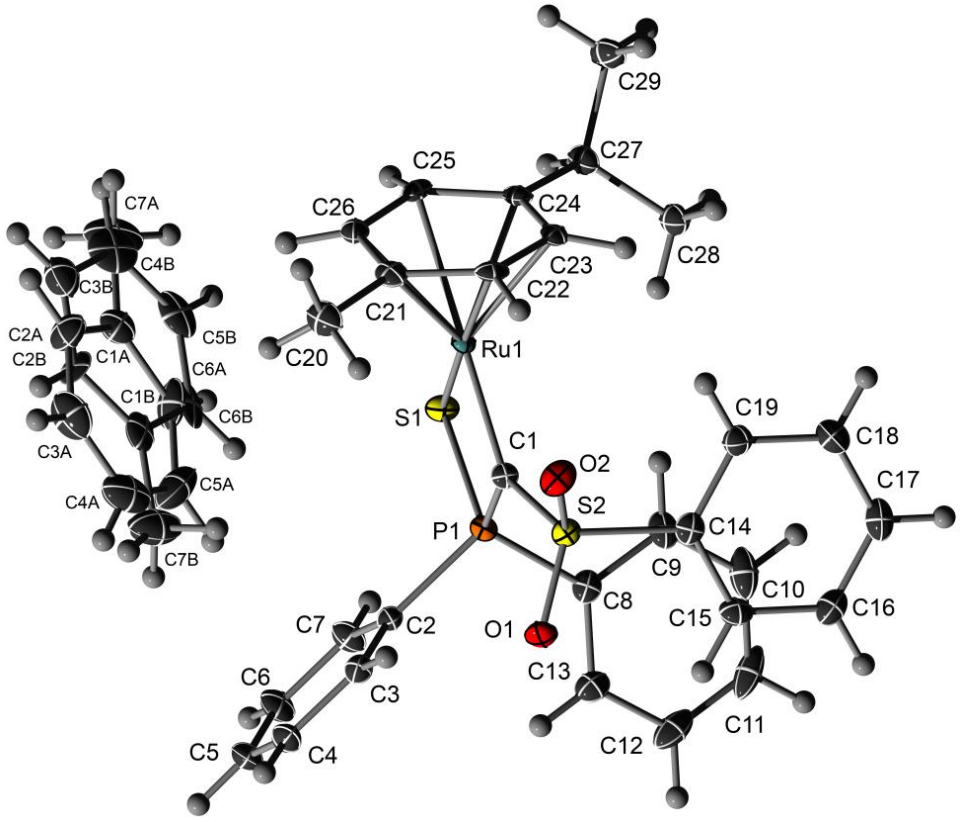

Table 53-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	$C_{36}H_{37}O_2PRuS_2$	
Formula weight	697.82	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 10.1990(11) Å	α = 90°.
	b = 13.0610(13) Å	β = 91.541(3)°.
	c = 23.982(3) Å	γ = 90°.
Volume	3193.5(6) $Å^3$	
Z	4	
Density (calculated)	1.451 Mg/m^3	
Absorption coefficient	0.703 mm^{-1}	

F(000)	1440
Crystal size	0.39 x 0.30 x 0.03 mm^3
Theta range for data collection	2.15 to 25.00°.
Index ranges	-12<=h<=12, -15<=k<=15, -28<=l<=28
Reflections collected	44418
Independent reflections	5626 [R(int) = 0.0328]
Completeness to theta = 25.00°	99.9 %
Max. and min. transmission	0.9792 and 0.7710
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5626 / 96 / 436
Goodness-of-fit on F^2	1.030
Final R indices [I>2sigma(I)]	R1 = 0.0222, wR2 = 0.0516
R indices (all data)	R1 = 0.0270, wR2 = 0.0538
Largest diff. peak and hole	0.732 and -0.527 e.$Å^{-3}$

Table 53-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	7135(1)	5358(1)	1101(1)	10(1)
S(1)	4959(1)	5768(1)	711(1)	14(1)
S(2)	6953(1)	6453(1)	2377(1)	12(1)
P(1)	4952(1)	6615(1)	1422(1)	11(1)
O(1)	6538(1)	7467(1)	2558(1)	18(1)
O(2)	8335(1)	6208(1)	2459(1)	18(1)
C(1)	6471(2)	6234(1)	1696(1)	12(1)
C(2)	4746(2)	7958(2)	1246(1)	14(1)
C(3)	5530(2)	8716(2)	1489(1)	16(1)
C(4)	5324(2)	9736(2)	1342(1)	20(1)
C(5)	4338(2)	9996(2)	958(1)	22(1)
C(6)	3552(2)	9239(2)	714(1)	22(1)
C(7)	3754(2)	8221(2)	856(1)	20(1)
C(8)	3552(2)	6334(2)	1848(1)	15(1)
C(9)	3195(2)	5314(2)	1926(1)	20(1)

C(10)	2159(2)	5081(2)	2268(1)	28(1)
C(11)	1489(2)	5858(2)	2533(1)	30(1)
C(12)	1850(2)	6870(2)	2460(1)	28(1)
C(13)	2881(2)	7112(2)	2119(1)	20(1)
C(14)	6067(2)	5559(2)	2784(1)	14(1)
C(15)	5065(2)	5902(2)	3117(1)	18(1)
C(16)	4354(2)	5193(2)	3423(1)	21(1)
C(17)	4654(2)	4160(2)	3388(1)	24(1)
C(18)	5661(2)	3823(2)	3057(1)	23(1)
C(19)	6375(2)	4522(2)	2753(1)	18(1)
C(20)	10110(2)	6396(2)	1024(1)	24(1)
C(21)	9240(2)	5467(2)	972(1)	16(1)
C(22)	9033(2)	4821(1)	1436(1)	14(1)
C(23)	8134(2)	3990(1)	1389(1)	13(1)
C(24)	7482(2)	3753(1)	868(1)	13(1)
C(25)	7792(2)	4351(2)	395(1)	13(1)
C(26)	8625(2)	5203(2)	446(1)	16(1)
C(27)	6479(2)	2897(2)	815(1)	16(1)
C(28)	5648(2)	2783(2)	1333(1)	20(1)
C(29)	7175(2)	1887(2)	682(1)	23(1)
C11	8121(3)	7401(2)	-531(1)	24(1)
C21	9308(2)	7918(2)	-472(1)	28(2)
C31	9464(2)	8674(2)	-68(1)	36(1)
C41	8433(3)	8913(2)	277(1)	39(1)
C51	7246(2)	8396(2)	217(1)	40(1)
C61	7090(2)	7640(2)	-187(1)	30(2)
C71	7931(7)	6568(6)	-952(3)	37(1)
C1B1	7990(9)	8218(7)	-6(4)	24(2)
C2B1	9110(12)	8169(11)	-336(6)	22(3)
C3B1	9213(10)	7420(8)	-757(4)	30(2)
C4B1	7095(8)	6791(7)	-534(4)	29(2)
C5B1	8288(18)	6810(17)	-901(11)	43(4)
C6B1	7057(12)	7509(13)	-119(7)	28(4)
C7B1	7922(13)	8987(11)	438(6)	42(4)

Table 53-3. Bond lengths [Å] and angles [°] for sad.

Ru(1)-C(1)	1.9647(19)
Ru(1)-C(23)	2.1612(18)
Ru(1)-C(21)	2.1814(19)
Ru(1)-C(22)	2.1911(19)
Ru(1)-C(24)	2.2000(19)
Ru(1)-C(26)	2.2240(19)
Ru(1)-C(25)	2.2595(19)
Ru(1)-S(1)	2.4441(5)
Ru(1)-P(1)	2.8875(6)
S(1)-P(1)	2.0312(7)
S(2)-O(2)	1.4538(14)
S(2)-O(1)	1.4595(14)
S(2)-C(1)	1.7168(19)
S(2)-C(14)	1.784(2)
P(1)-C(1)	1.7394(19)
P(1)-C(8)	1.815(2)
P(1)-C(2)	1.815(2)
C(2)-C(3)	1.390(3)
C(2)-C(7)	1.403(3)
C(3)-C(4)	1.393(3)
C(4)-C(5)	1.387(3)
C(5)-C(6)	1.392(3)
C(6)-C(7)	1.386(3)
C(8)-C(9)	1.395(3)
C(8)-C(13)	1.397(3)
C(9)-C(10)	1.388(3)
C(10)-C(11)	1.387(4)
C(11)-C(12)	1.385(4)
C(12)-C(13)	1.385(3)
C(14)-C(15)	1.388(3)
C(14)-C(19)	1.394(3)
C(15)-C(16)	1.395(3)
C(16)-C(17)	1.387(3)
C(17)-C(18)	1.387(3)

C(18)-C(19)	1.386(3)
C(20)-C(21)	1.507(3)
C(21)-C(22)	1.417(3)
C(21)-C(26)	1.435(3)
C(22)-C(23)	1.424(3)
C(23)-C(24)	1.435(3)
C(24)-C(25)	1.420(3)
C(24)-C(27)	1.518(3)
C(25)-C(26)	1.403(3)
C(27)-C(28)	1.530(3)
C(27)-C(29)	1.536(3)
C11-C21	1.3900
C11-C61	1.3900
C11-C71	1.493(6)
C21-C31	1.3900
C31-C41	1.3900
C41-C51	1.3900
C51-C61	1.3900
C1B1-C6B1	1.349(16)
C1B1-C2B1	1.409(17)
C1B1-C7B1	1.468(15)
C2B1-C3B1	1.412(15)
C3B1-C5B1	1.275(18)
C4B1-C6B1	1.370(17)
C4B1-C5B1	1.52(2)

C(1)-Ru(1)-C(23)	114.68(7)
C(1)-Ru(1)-C(21)	115.13(8)
C(23)-Ru(1)-C(21)	69.05(7)
C(1)-Ru(1)-C(22)	103.77(7)
C(23)-Ru(1)-C(22)	38.17(7)
C(21)-Ru(1)-C(22)	37.82(7)
C(1)-Ru(1)-C(24)	143.18(7)
C(23)-Ru(1)-C(24)	38.39(7)
C(21)-Ru(1)-C(24)	82.00(7)
C(22)-Ru(1)-C(24)	69.02(7)

C(1)-Ru(1)-C(26)	145.26(8)
C(23)-Ru(1)-C(26)	79.96(7)
C(21)-Ru(1)-C(26)	38.00(7)
C(22)-Ru(1)-C(26)	67.43(7)
C(24)-Ru(1)-C(26)	67.44(7)
C(1)-Ru(1)-C(25)	176.99(7)
C(23)-Ru(1)-C(25)	67.18(7)
C(21)-Ru(1)-C(25)	67.60(7)
C(22)-Ru(1)-C(25)	79.16(7)
C(24)-Ru(1)-C(25)	37.11(7)
C(26)-Ru(1)-C(25)	36.46(7)
C(1)-Ru(1)-S(1)	79.79(6)
C(23)-Ru(1)-S(1)	135.97(5)
C(21)-Ru(1)-S(1)	144.92(6)
C(22)-Ru(1)-S(1)	174.00(5)
C(24)-Ru(1)-S(1)	105.21(5)
C(26)-Ru(1)-S(1)	112.40(5)
C(25)-Ru(1)-S(1)	97.24(5)
C(1)-Ru(1)-P(1)	36.06(5)
C(23)-Ru(1)-P(1)	138.14(5)
C(21)-Ru(1)-P(1)	140.30(5)
C(22)-Ru(1)-P(1)	139.82(5)
C(24)-Ru(1)-P(1)	137.70(5)
C(26)-Ru(1)-P(1)	141.88(5)
C(25)-Ru(1)-P(1)	140.99(5)
S(1)-Ru(1)-P(1)	43.812(16)
P(1)-S(1)-Ru(1)	79.78(2)
O(2)-S(2)-O(1)	116.57(9)
O(2)-S(2)-C(1)	110.09(9)
O(1)-S(2)-C(1)	110.88(9)
O(2)-S(2)-C(14)	106.60(9)
O(1)-S(2)-C(14)	105.99(9)
C(1)-S(2)-C(14)	106.01(9)
C(1)-P(1)-C(8)	115.83(9)
C(1)-P(1)-C(2)	117.38(9)
C(8)-P(1)-C(2)	103.75(9)

C(1)-P(1)-S(1)	97.96(7)
C(8)-P(1)-S(1)	112.51(7)
C(2)-P(1)-S(1)	109.57(7)
C(1)-P(1)-Ru(1)	41.67(6)
C(8)-P(1)-Ru(1)	131.24(7)
C(2)-P(1)-Ru(1)	124.95(6)
S(1)-P(1)-Ru(1)	56.408(18)
S(2)-C(1)-P(1)	122.78(11)
S(2)-C(1)-Ru(1)	133.87(11)
P(1)-C(1)-Ru(1)	102.27(9)
C(3)-C(2)-C(7)	120.09(18)
C(3)-C(2)-P(1)	122.01(15)
C(7)-C(2)-P(1)	117.89(15)
C(2)-C(3)-C(4)	119.62(19)
C(5)-C(4)-C(3)	120.27(19)
C(4)-C(5)-C(6)	120.23(19)
C(7)-C(6)-C(5)	119.9(2)
C(6)-C(7)-C(2)	119.86(19)
C(9)-C(8)-C(13)	119.91(19)
C(9)-C(8)-P(1)	118.77(16)
C(13)-C(8)-P(1)	121.23(16)
C(10)-C(9)-C(8)	119.7(2)
C(11)-C(10)-C(9)	120.1(2)
C(12)-C(11)-C(10)	120.3(2)
C(11)-C(12)-C(13)	120.1(2)
C(12)-C(13)-C(8)	119.9(2)
C(15)-C(14)-C(19)	120.97(19)
C(15)-C(14)-S(2)	119.77(15)
C(19)-C(14)-S(2)	119.25(15)
C(14)-C(15)-C(16)	119.32(19)
C(17)-C(16)-C(15)	119.7(2)
C(16)-C(17)-C(18)	120.8(2)
C(19)-C(18)-C(17)	119.9(2)
C(18)-C(19)-C(14)	119.33(19)
C(22)-C(21)-C(26)	118.46(18)
C(22)-C(21)-C(20)	120.87(18)

C(26)-C(21)-C(20)	120.65(18)
C(22)-C(21)-Ru(1)	71.46(11)
C(26)-C(21)-Ru(1)	72.60(11)
C(20)-C(21)-Ru(1)	128.35(14)
C(21)-C(22)-C(23)	120.09(18)
C(21)-C(22)-Ru(1)	70.72(11)
C(23)-C(22)-Ru(1)	69.78(11)
C(22)-C(23)-C(24)	121.03(18)
C(22)-C(23)-Ru(1)	72.05(11)
C(24)-C(23)-Ru(1)	72.27(11)
C(25)-C(24)-C(23)	118.02(18)
C(25)-C(24)-C(27)	120.19(17)
C(23)-C(24)-C(27)	121.78(17)
C(25)-C(24)-Ru(1)	73.72(11)
C(23)-C(24)-Ru(1)	69.34(10)
C(27)-C(24)-Ru(1)	127.60(13)
C(26)-C(25)-C(24)	120.91(18)
C(26)-C(25)-Ru(1)	70.39(11)
C(24)-C(25)-Ru(1)	69.17(10)
C(25)-C(26)-C(21)	121.10(18)
C(25)-C(26)-Ru(1)	73.15(11)
C(21)-C(26)-Ru(1)	69.39(11)
C(24)-C(27)-C(28)	112.99(16)
C(24)-C(27)-C(29)	109.63(16)
C(28)-C(27)-C(29)	110.75(17)
C21-C11-C61	120.0
C21-C11-C71	121.4(3)
C61-C11-C71	118.6(3)
C11-C21-C31	120.0
C41-C31-C21	120.0
C31-C41-C51	120.0
C41-C51-C61	120.0
C51-C61-C11	120.0
C6B1-C1B1-C2B1	115.8(11)
C6B1-C1B1-C7B1	124.6(12)
C2B1-C1B1-C7B1	119.6(10)

C1B1-C2B1-C3B1	120.7(11)
C5B1-C3B1-C2B1	123.9(15)
C6B1-C4B1-C5B1	116.7(11)
C3B1-C5B1-C4B1	116.9(18)
C1B1-C6B1-C4B1	125.6(13)

Symmetry transformations used to generate equivalent atoms:

Table 53-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	11(1)	10(1)	10(1)	0(1)	-1(1)	2(1)
S(1)	14(1)	15(1)	13(1)	-4(1)	-5(1)	2(1)
S(2)	12(1)	14(1)	11(1)	-2(1)	-2(1)	-1(1)
P(1)	10(1)	10(1)	12(1)	-1(1)	-2(1)	0(1)
O(1)	25(1)	14(1)	15(1)	-5(1)	0(1)	-2(1)
O(2)	12(1)	27(1)	16(1)	-2(1)	-4(1)	-2(1)
C(1)	11(1)	12(1)	11(1)	0(1)	-2(1)	1(1)
C(2)	13(1)	13(1)	15(1)	1(1)	3(1)	2(1)
C(3)	15(1)	16(1)	16(1)	0(1)	2(1)	-1(1)
C(4)	24(1)	14(1)	22(1)	-3(1)	3(1)	-3(1)
C(5)	30(1)	11(1)	25(1)	2(1)	5(1)	4(1)
C(6)	23(1)	18(1)	25(1)	3(1)	-5(1)	6(1)
C(7)	20(1)	15(1)	23(1)	-1(1)	-5(1)	0(1)
C(8)	11(1)	21(1)	14(1)	2(1)	-2(1)	0(1)
C(9)	16(1)	21(1)	24(1)	5(1)	-4(1)	-1(1)
C(10)	20(1)	33(1)	30(1)	16(1)	-5(1)	-9(1)
C(11)	14(1)	57(2)	21(1)	15(1)	1(1)	-2(1)
C(12)	19(1)	46(2)	20(1)	0(1)	3(1)	8(1)
C(13)	17(1)	24(1)	18(1)	0(1)	0(1)	2(1)
C(14)	14(1)	17(1)	9(1)	0(1)	-4(1)	-2(1)
C(15)	18(1)	18(1)	17(1)	0(1)	-2(1)	4(1)
C(16)	17(1)	29(1)	18(1)	1(1)	3(1)	1(1)
C(17)	24(1)	26(1)	22(1)	7(1)	2(1)	-5(1)

C(18)	29(1)	16(1)	25(1)	2(1)	2(1)	2(1)
C(19)	19(1)	19(1)	16(1)	0(1)	1(1)	5(1)
C(20)	18(1)	20(1)	34(1)	-1(1)	2(1)	-3(1)
C(21)	9(1)	15(1)	23(1)	-1(1)	2(1)	3(1)
C(22)	12(1)	14(1)	16(1)	-3(1)	-2(1)	6(1)
C(23)	14(1)	12(1)	14(1)	1(1)	-1(1)	6(1)
C(24)	12(1)	10(1)	17(1)	-3(1)	1(1)	5(1)
C(25)	13(1)	16(1)	11(1)	-2(1)	0(1)	6(1)
C(26)	15(1)	15(1)	17(1)	3(1)	4(1)	5(1)
C(27)	16(1)	15(1)	18(1)	-1(1)	-2(1)	-1(1)
C(28)	18(1)	16(1)	26(1)	0(1)	5(1)	-3(1)
C(29)	23(1)	16(1)	32(1)	-7(1)	5(1)	-4(1)
C11	24(2)	21(2)	26(2)	3(1)	-4(1)	6(1)
C21	20(2)	33(3)	33(3)	4(2)	11(2)	1(2)
C31	30(2)	30(2)	48(2)	5(2)	-7(2)	-8(2)
C41	53(3)	31(2)	33(3)	-4(2)	-14(2)	15(2)
C51	32(2)	64(3)	24(2)	6(2)	11(2)	20(2)
C61	20(3)	40(4)	29(3)	14(2)	1(2)	-1(2)
C71	30(4)	31(4)	50(3)	0(2)	-6(3)	3(2)
C1B1	25(5)	23(5)	24(5)	11(4)	-3(4)	5(4)
C2B1	6(4)	37(6)	24(5)	1(5)	9(4)	5(5)
C3B1	27(5)	30(6)	33(6)	7(4)	8(4)	2(4)
C4B1	21(4)	25(5)	40(5)	11(4)	-13(4)	-2(4)
C5B1	11(8)	29(10)	89(10)	2(7)	-10(6)	4(5)
C6B1	16(8)	29(6)	37(7)	26(5)	0(6)	2(5)
C7B1	41(8)	44(7)	40(8)	-10(6)	-11(6)	19(6)

Table 53-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
H(3)	6203	8539	1753	19
H(4)	5862	10256	1505	24
H(5)	4198	10694	862	26
H(6)	2879	9419	451	27
H(7)	3221	7702	689	24
H(9)	3658	4782	1747	24
H(10)	1910	4388	2321	34
H(11)	777	5695	2765	36
H(12)	1392	7399	2645	34
H(13)	3130	7807	2070	24
H(15)	4865	6611	3137	21
H(16)	3667	5418	3653	26
H(17)	4164	3678	3593	29
H(18)	5862	3114	3038	28
H(19)	7068	4296	2527	22
H(20A)	11000	6217	915	36
H(20B)	10131	6635	1412	36
H(20C)	9765	6941	781	36
H(22)	9336	5053	1815	17
H(23)	7836	3647	1736	16
H(25)	7210	4296	54	16
H(26)	8630	5715	136	19
H(27)	5874	3063	493	20
H(28A)	5278	3450	1431	30
H(28B)	6199	2531	1645	30
H(28C)	4935	2296	1256	30
H(29A)	6520	1350	612	35
H(29B)	7748	1690	999	35
H(29C)	7702	1976	349	35
H21	10012	7754	-707	34

H31	10275	9027	-27	43
H41	8539	9430	553	47
H51	6542	8560	453	48
H61	6279	7287	-228	35
H7A1	7724	6869	-1318	55
H7B1	7208	6124	-842	55
H7C1	8737	6163	-972	55
H2B1	9804	8645	-275	27
H3B1	10019	7367	-945	36
H4B1	6410	6306	-591	34
H5B1	8341	6387	-1222	52
H6B1	6310	7508	110	33
H7B11	8007	8648	802	63
H7B21	7078	9344	410	63
H7B31	8636	9482	400	63

Röntgenstrukturanalytische Daten für 55

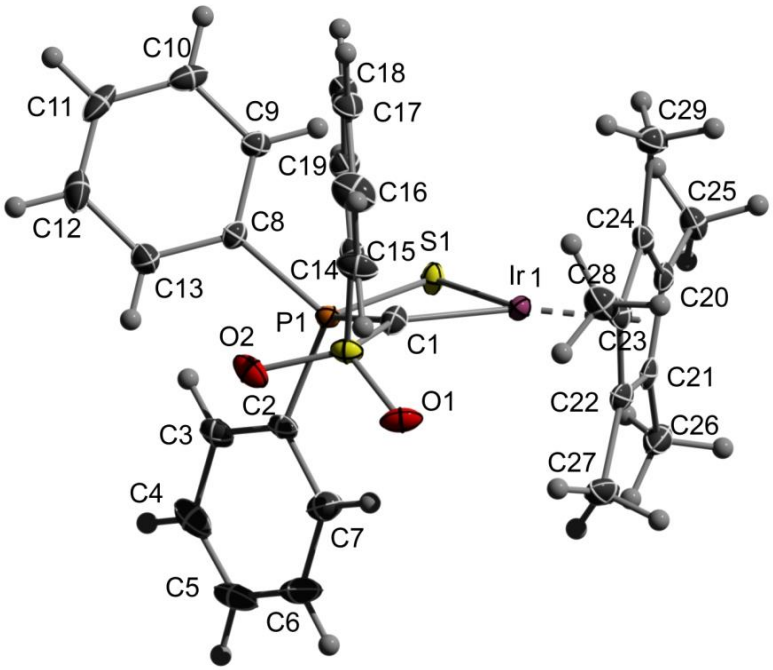

Table 55-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	$C_{29}H_{30}IrO_2PS_2$	
Formula weight	697.82	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	monoklin	
Space group	P 2(1)/n	
Unit cell dimensions	a = 11.6576(5) Å	α = 90°.
	b = 13.1445(6) Å	β = 103.5100(10)°.
	c = 17.7758(8) Å	γ = 90°.
Volume	2648.5(2) $Å^3$	
Z	4	
Density (calculated)	1.750 Mg/m^3	
Absorption coefficient	5.285 mm^{-1}	
F(000)	1376	
Crystal size	0.16 x 0.09 x 0.03 mm^3	
Theta range for data collection	1.95 to 25.00°.	
Index ranges	-13<=h<=13, -15<=k<=15, -18<=l<=21	
Reflections collected	19854	

Independent reflections	4652 [R(int) = 0.0216]
Completeness to theta = 25.00°	99.9 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4652 / 0 / 321
Goodness-of-fit on F^2	1.049
Final R indices [I>2sigma(I)]	R1 = 0.0207, wR2 = 0.0514
R indices (all data)	R1 = 0.0248, wR2 = 0.0539
Largest diff. peak and hole	1.396 and -0.768 e.Å^{-3}

Table 55-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	4860(1)	2822(1)	1220(1)	13(1)
S(1)	6241(1)	2069(1)	2279(1)	16(1)
S(2)	2469(1)	1356(1)	1212(1)	17(1)
P(5)	4775(1)	1269(1)	2364(1)	13(1)
O(1)	1692(2)	2221(2)	995(2)	24(1)
O(2)	2190(2)	664(2)	1778(2)	24(1)
C(1)	3904(3)	1726(3)	1510(2)	18(1)
C(2)	4334(3)	1659(3)	3231(2)	17(1)
C(3)	4824(3)	1220(3)	3946(2)	21(1)
C(4)	4579(3)	1624(3)	4616(2)	29(1)
C(5)	3854(4)	2470(3)	4564(3)	32(1)
C(6)	3358(4)	2895(3)	3857(3)	33(1)
C(7)	3593(4)	2498(3)	3191(2)	26(1)
C(8)	5072(3)	-79(3)	2440(2)	15(1)
C(9)	5955(3)	-455(3)	2106(2)	17(1)
C(10)	6196(3)	-1484(3)	2123(2)	23(1)
C(11)	5560(4)	-2136(3)	2477(2)	26(1)
C(12)	4666(4)	-1785(3)	2795(2)	29(1)
C(13)	4412(3)	-748(3)	2772(2)	23(1)
C(14)	2346(3)	641(3)	343(2)	16(1)
C(15)	1264(3)	641(3)	-187(2)	25(1)

C(16)	1096(4)	36(3)	-842(2)	31(1)
C(17)	2020(3)	-549(3)	-969(2)	24(1)
C(18)	3105(3)	-537(3)	-444(2)	23(1)
C(19)	3270(3)	53(3)	221(2)	20(1)
C(20)	5934(3)	3950(3)	741(2)	17(1)
C(21)	5221(3)	4444(3)	1178(2)	18(1)
C(22)	3986(3)	4216(3)	819(2)	19(1)
C(23)	3960(3)	3568(3)	167(2)	19(1)
C(24)	5175(3)	3385(3)	136(2)	16(1)
C(25)	7255(3)	3980(3)	892(2)	20(1)
C(26)	5659(4)	5075(3)	1888(2)	24(1)
C(27)	2949(4)	4616(3)	1089(2)	27(1)
C(28)	2897(3)	3192(3)	-410(2)	25(1)
C(29)	5566(3)	2769(3)	-467(2)	22(1)

Table 55-3. Bond lengths [Å] and angles [°] for sad.

Ir(1)-C(1)	1.963(3)
Ir(1)-C(22)	2.136(3)
Ir(1)-C(23)	2.155(3)
Ir(1)-C(24)	2.173(3)
Ir(1)-C(21)	2.177(3)
Ir(1)-C(20)	2.233(3)
Ir(1)-S(1)	2.3876(9)
Ir(1)-P(5)	2.8992(9)
S(1)-P(5)	2.0412(12)
S(2)-O(1)	1.448(3)
S(2)-O(2)	1.449(3)
S(2)-C(1)	1.703(4)
S(2)-C(14)	1.785(3)
P(5)-C(1)	1.725(4)
P(5)-C(8)	1.805(3)
P(5)-C(2)	1.809(3)
C(2)-C(7)	1.392(5)
C(2)-C(3)	1.392(5)

C(3)-C(4)	1.393(5)
C(4)-C(5)	1.387(6)
C(5)-C(6)	1.374(7)
C(6)-C(7)	1.378(6)
C(8)-C(13)	1.387(5)
C(8)-C(9)	1.393(5)
C(9)-C(10)	1.380(5)
C(10)-C(11)	1.377(6)
C(11)-C(12)	1.377(6)
C(12)-C(13)	1.393(6)
C(14)-C(19)	1.384(5)
C(14)-C(15)	1.386(5)
C(15)-C(16)	1.386(5)
C(16)-C(17)	1.384(6)
C(17)-C(18)	1.385(5)
C(18)-C(19)	1.388(5)
C(20)-C(21)	1.421(5)
C(20)-C(24)	1.430(5)
C(20)-C(25)	1.501(5)
C(21)-C(22)	1.463(5)
C(21)-C(26)	1.497(5)
C(22)-C(23)	1.434(5)
C(22)-C(27)	1.496(5)
C(23)-C(24)	1.450(5)
C(23)-C(28)	1.495(5)
C(24)-C(29)	1.497(5)

C(1)-Ir(1)-C(22)	117.49(14)
C(1)-Ir(1)-C(23)	111.78(14)
C(22)-Ir(1)-C(23)	39.03(13)
C(1)-Ir(1)-C(24)	134.97(14)
C(22)-Ir(1)-C(24)	65.12(13)
C(23)-Ir(1)-C(24)	39.15(13)
C(1)-Ir(1)-C(21)	148.63(14)
C(22)-Ir(1)-C(21)	39.63(14)
C(23)-Ir(1)-C(21)	65.42(13)

C(24)-Ir(1)-C(21)	64.07(13)
C(1)-Ir(1)-C(20)	172.17(14)
C(22)-Ir(1)-C(20)	64.54(13)
C(23)-Ir(1)-C(20)	64.52(13)
C(24)-Ir(1)-C(20)	37.85(13)
C(21)-Ir(1)-C(20)	37.56(13)
C(1)-Ir(1)-S(1)	78.92(11)
C(22)-Ir(1)-S(1)	143.08(10)
C(23)-Ir(1)-S(1)	167.16(10)
C(24)-Ir(1)-S(1)	128.15(9)
C(21)-Ir(1)-S(1)	109.42(10)
C(20)-Ir(1)-S(1)	103.94(9)
C(1)-Ir(1)-P(5)	35.34(10)
C(22)-Ir(1)-P(5)	138.23(10)
C(23)-Ir(1)-P(5)	147.11(10)
C(24)-Ir(1)-P(5)	154.38(9)
C(21)-Ir(1)-P(5)	138.74(9)
C(20)-Ir(1)-P(5)	148.06(9)
S(1)-Ir(1)-P(5)	44.11(3)
P(5)-S(1)-Ir(1)	81.37(4)
O(1)-S(2)-O(2)	116.76(16)
O(1)-S(2)-C(1)	111.51(17)
O(2)-S(2)-C(1)	109.05(16)
O(1)-S(2)-C(14)	105.30(16)
O(2)-S(2)-C(14)	106.50(16)
C(1)-S(2)-C(14)	107.12(17)
C(1)-P(5)-C(8)	118.11(16)
C(1)-P(5)-C(2)	115.12(17)
C(8)-P(5)-C(2)	107.58(16)
C(1)-P(5)-S(1)	94.98(13)
C(8)-P(5)-S(1)	111.23(12)
C(2)-P(5)-S(1)	109.05(12)
C(1)-P(5)-Ir(1)	41.18(12)
C(8)-P(5)-Ir(1)	134.97(12)
C(2)-P(5)-Ir(1)	117.45(12)
S(1)-P(5)-Ir(1)	54.51(3)

S(2)-C(1)-P(5)	120.5(2)
S(2)-C(1)-Ir(1)	134.8(2)
P(5)-C(1)-Ir(1)	103.48(18)
C(7)-C(2)-C(3)	119.5(3)
C(7)-C(2)-P(5)	118.6(3)
C(3)-C(2)-P(5)	121.5(3)
C(2)-C(3)-C(4)	120.1(4)
C(5)-C(4)-C(3)	119.5(4)
C(6)-C(5)-C(4)	120.4(4)
C(5)-C(6)-C(7)	120.5(4)
C(6)-C(7)-C(2)	120.1(4)
C(13)-C(8)-C(9)	119.6(3)
C(13)-C(8)-P(5)	122.6(3)
C(9)-C(8)-P(5)	117.7(3)
C(10)-C(9)-C(8)	120.4(3)
C(11)-C(10)-C(9)	119.4(4)
C(10)-C(11)-C(12)	121.2(3)
C(11)-C(12)-C(13)	119.5(4)
C(8)-C(13)-C(12)	119.8(4)
C(19)-C(14)-C(15)	120.7(3)
C(19)-C(14)-S(2)	121.4(3)
C(15)-C(14)-S(2)	117.7(3)
C(16)-C(15)-C(14)	119.9(4)
C(17)-C(16)-C(15)	119.5(4)
C(16)-C(17)-C(18)	120.5(4)
C(17)-C(18)-C(19)	120.2(3)
C(14)-C(19)-C(18)	119.1(3)
C(21)-C(20)-C(24)	108.1(3)
C(21)-C(20)-C(25)	126.6(3)
C(24)-C(20)-C(25)	125.3(3)
C(21)-C(20)-Ir(1)	69.08(19)
C(24)-C(20)-Ir(1)	68.80(19)
C(25)-C(20)-Ir(1)	126.3(2)
C(20)-C(21)-C(22)	108.1(3)
C(20)-C(21)-C(26)	125.9(3)
C(22)-C(21)-C(26)	126.0(3)

C(20)-C(21)-Ir(1)	73.36(19)
C(22)-C(21)-Ir(1)	68.68(19)
C(26)-C(21)-Ir(1)	123.0(2)
C(23)-C(22)-C(21)	107.8(3)
C(23)-C(22)-C(27)	127.0(3)
C(21)-C(22)-C(27)	125.2(3)
C(23)-C(22)-Ir(1)	71.2(2)
C(21)-C(22)-Ir(1)	71.69(19)
C(27)-C(22)-Ir(1)	123.5(2)
C(22)-C(23)-C(24)	107.0(3)
C(22)-C(23)-C(28)	127.5(3)
C(24)-C(23)-C(28)	125.4(3)
C(22)-C(23)-Ir(1)	69.77(19)
C(24)-C(23)-Ir(1)	71.09(19)
C(28)-C(23)-Ir(1)	127.0(3)
C(20)-C(24)-C(23)	108.9(3)
C(20)-C(24)-C(29)	125.5(3)
C(23)-C(24)-C(29)	125.5(3)
C(20)-C(24)-Ir(1)	73.35(19)
C(23)-C(24)-Ir(1)	69.76(19)
C(29)-C(24)-Ir(1)	126.4(2)

Symmetry transformations used to generate equivalent atoms:

Table 55-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	13(1)	12(1)	14(1)	1(1)	3(1)	2(1)
S(1)	13(1)	15(1)	20(1)	3(1)	2(1)	-2(1)
S(2)	12(1)	20(1)	19(1)	-3(1)	4(1)	0(1)
P(5)	11(1)	12(1)	17(1)	0(1)	5(1)	0(1)
O(1)	16(1)	28(2)	28(2)	-6(1)	4(1)	8(1)
O(2)	19(1)	34(2)	22(1)	-2(1)	8(1)	-6(1)
C(1)	21(2)	14(2)	17(2)	1(1)	3(1)	0(1)
C(2)	14(2)	19(2)	19(2)	-6(1)	7(1)	-5(1)
C(3)	13(2)	26(2)	25(2)	-5(2)	8(2)	-5(2)
C(4)	23(2)	42(2)	22(2)	-8(2)	8(2)	-16(2)
C(5)	26(2)	39(2)	39(3)	-22(2)	21(2)	-15(2)
C(6)	28(2)	29(2)	46(3)	-14(2)	19(2)	1(2)
C(7)	25(2)	23(2)	32(2)	-5(2)	9(2)	3(2)
C(8)	14(2)	14(2)	14(2)	2(1)	1(1)	2(1)
C(9)	15(2)	19(2)	15(2)	1(1)	2(1)	4(1)
C(10)	24(2)	23(2)	19(2)	-4(2)	0(2)	10(2)
C(11)	37(2)	12(2)	22(2)	-2(2)	-5(2)	3(2)
C(12)	38(3)	19(2)	29(2)	3(2)	7(2)	-10(2)
C(13)	24(2)	22(2)	25(2)	-1(2)	11(2)	-3(2)
C(14)	14(2)	16(2)	19(2)	0(1)	6(1)	-2(1)
C(15)	14(2)	34(2)	26(2)	-6(2)	5(2)	2(2)
C(16)	22(2)	43(2)	25(2)	-8(2)	2(2)	-6(2)
C(17)	32(2)	23(2)	19(2)	-5(2)	11(2)	-6(2)
C(18)	28(2)	19(2)	26(2)	3(2)	14(2)	2(2)
C(19)	17(2)	22(2)	20(2)	2(2)	3(2)	1(2)
C(20)	21(2)	13(2)	18(2)	7(1)	5(1)	1(1)
C(21)	25(2)	10(2)	19(2)	8(1)	6(2)	3(1)
C(22)	23(2)	14(2)	18(2)	7(1)	6(2)	7(2)
C(23)	24(2)	19(2)	14(2)	5(1)	5(1)	2(2)
C(24)	18(2)	16(2)	15(2)	6(1)	5(1)	0(1)
C(25)	18(2)	24(2)	19(2)	4(2)	6(2)	-2(2)

C(26)	34(2)	16(2)	23(2)	-1(2)	8(2)	1(2)
C(27)	29(2)	25(2)	28(2)	5(2)	12(2)	13(2)
C(28)	19(2)	32(2)	23(2)	4(2)	4(2)	2(2)
C(29)	24(2)	24(2)	18(2)	0(2)	6(2)	4(2)

Röntgenstrukturanalytische Daten für 54

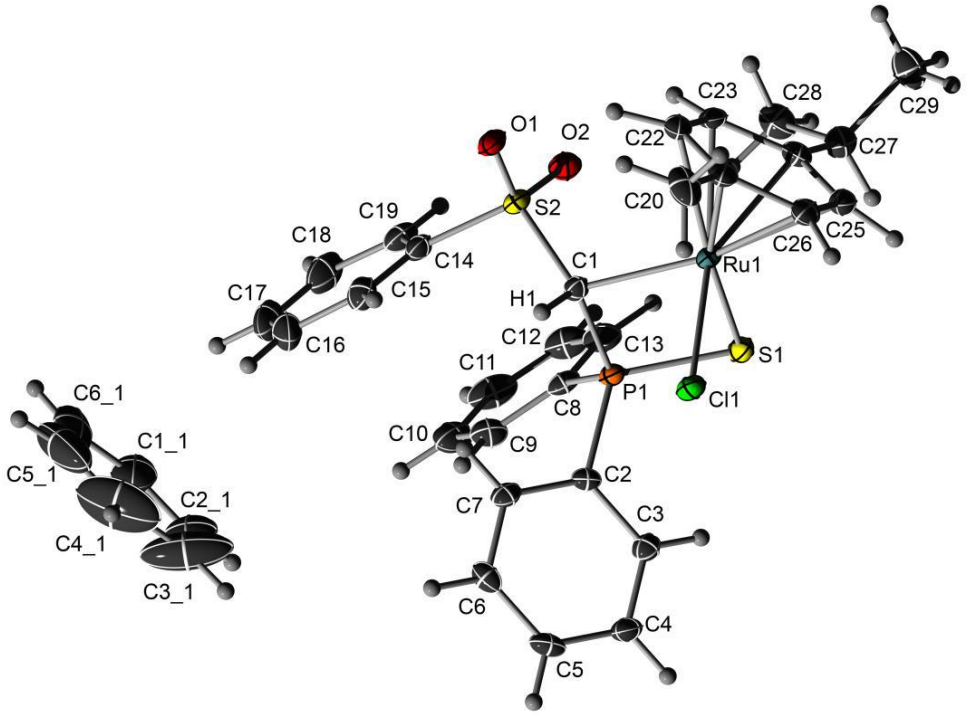

Table 54-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	C35 H36 Cl O2 P Ru S2	
Formula weight	720.25	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.1627(5) Å	α = 97.127(2)°.
	b = 12.0559(6) Å	β = 101.955(2)°.
	c = 12.7248(6) Å	γ = 104.9310(10)°.
Volume	1589.98(13) $Å^3$	
Z	2	
Density (calculated)	1.504 Mg/m^3	
Absorption coefficient	0.790 mm^{-1}	
F(000)	740	
Crystal size	0.31 x 0.11 x 0.09 mm^3	
Theta range for data collection	2.22 to 25.00°.	
Index ranges	-13<=h<=13, -14<=k<=14, -15<=l<=15	

Reflections collected	19240
Independent reflections	5590 [R(int) = 0.0302]
Completeness to theta = 25.00°	99.9 %
Absorption correction	Empirical
Max. and min. transmission	0.7454 and 0.7006
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5590 / 12 / 386
Goodness-of-fit on F^2	1.066
Final R indices [I>2sigma(I)]	R1 = 0.0406, wR2 = 0.0874
R indices (all data)	R1 = 0.0461, wR2 = 0.0901
Largest diff. peak and hole	2.499 and -1.297 e.$Å^{-3}$

Table 54-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	8069(1)	7913(1)	4683(1)	16(1)
Cl(3)	10108(1)	7718(1)	5654(1)	19(1)
S(1)	8997(1)	8447(1)	3159(1)	19(1)
S(2)	6245(1)	5368(1)	3011(1)	17(1)
P(1)	8877(1)	6745(1)	2869(1)	15(1)
O(1)	5594(3)	4975(2)	3827(2)	23(1)
O(2)	5681(3)	6014(2)	2274(2)	24(1)
C(1)	7821(3)	6188(3)	3692(3)	15(1)
C(2)	10386(3)	6439(3)	3344(3)	15(1)
C(3)	11509(4)	7282(3)	3362(3)	19(1)
C(4)	12670(4)	7056(4)	3653(3)	23(1)
C(5)	12728(4)	5994(4)	3925(3)	23(1)
C(6)	11610(4)	5150(3)	3904(3)	20(1)
C(7)	10439(4)	5370(3)	3614(3)	18(1)
C(8)	8419(3)	6142(3)	1414(3)	18(1)
C(9)	8769(4)	5188(4)	993(3)	25(1)
C(10)	8392(4)	4743(4)	-124(4)	31(1)
C(11)	7684(4)	5271(4)	-816(4)	34(1)

C(12)	7348(4)	6224(4)	-403(4)	31(1)
C(13)	7701(4)	6660(4)	706(3)	26(1)
C(14)	6348(4)	4106(3)	2191(3)	20(1)
C(15)	6961(4)	3358(3)	2676(4)	26(1)
C(16)	7065(5)	2401(4)	2007(4)	34(1)
C(17)	6528(5)	2185(4)	888(4)	37(1)
C(18)	5904(4)	2921(4)	427(4)	35(1)
C(19)	5826(4)	3896(4)	1075(3)	25(1)
C(20)	7763(5)	7466(4)	7210(4)	32(1)
C(21)	7407(4)	7997(3)	6229(3)	23(1)
C(22)	6372(4)	7398(3)	5338(3)	23(1)
C(23)	6080(4)	7893(3)	4407(3)	21(1)
C(24)	6810(4)	9032(3)	4346(3)	21(1)
C(25)	7874(4)	9650(3)	5254(3)	21(1)
C(26)	8164(4)	9132(3)	6154(3)	21(1)
C(27)	6498(4)	9646(4)	3409(3)	25(1)
C(28)	5718(4)	8831(4)	2341(3)	29(1)
C(29)	5786(5)	10512(4)	3768(4)	34(1)
C11	7588(5)	542(5)	-1386(5)	48(1)
C61	6931(7)	-321(5)	-949(7)	73(2)
C21	8740(5)	1310(5)	-812(4)	45(1)
C31	9277(6)	1238(9)	229(6)	95(3)
C41	8562(9)	288(9)	673(7)	99(3)
C51	7432(9)	-446(7)	36(8)	84(2)

Table 54-3. Bond lengths [Å] and angles [°] for sad.

Ru(1)-C(23)	2.168(4)
Ru(1)-C(26)	2.197(4)
Ru(1)-C(22)	2.201(4)
Ru(1)-C(24)	2.202(4)
Ru(1)-C(25)	2.210(4)
Ru(1)-C(1)	2.213(4)
Ru(1)-C(21)	2.240(4)
Ru(1)-Cl(3)	2.4385(9)

Ru(1)-S(1)	2.4587(10)
S(1)-P(1)	2.0038(13)
S(2)-O(2)	1.440(3)
S(2)-O(1)	1.444(3)
S(2)-C(1)	1.756(4)
S(2)-C(14)	1.778(4)
P(1)-C(1)	1.794(4)
P(1)-C(2)	1.814(4)
P(1)-C(8)	1.816(4)
C(2)-C(7)	1.386(5)
C(2)-C(3)	1.390(5)
C(3)-C(4)	1.378(5)
C(4)-C(5)	1.380(6)
C(5)-C(6)	1.386(6)
C(6)-C(7)	1.385(5)
C(8)-C(9)	1.389(6)
C(8)-C(13)	1.393(6)
C(9)-C(10)	1.390(6)
C(10)-C(11)	1.384(7)
C(11)-C(12)	1.375(7)
C(12)-C(13)	1.380(6)
C(14)-C(19)	1.384(6)
C(14)-C(15)	1.394(6)
C(15)-C(16)	1.391(6)
C(16)-C(17)	1.389(7)
C(17)-C(18)	1.377(7)
C(18)-C(19)	1.382(6)
C(20)-C(21)	1.500(6)
C(21)-C(22)	1.402(6)
C(21)-C(26)	1.438(6)
C(22)-C(23)	1.408(6)
C(23)-C(24)	1.425(5)
C(24)-C(25)	1.436(6)
C(24)-C(27)	1.507(6)
C(25)-C(26)	1.390(6)
C(27)-C(28)	1.519(6)

C(27)-C(29)	1.547(6)
C11-C61	1.360(8)
C11-C21	1.369(7)
C61-C51	1.306(11)
C21-C31	1.360(8)
C31-C41	1.465(12)
C41-C51	1.361(12)

C(23)-Ru(1)-C(26)	79.73(15)
C(23)-Ru(1)-C(22)	37.60(15)
C(26)-Ru(1)-C(22)	67.04(15)
C(23)-Ru(1)-C(24)	38.05(14)
C(26)-Ru(1)-C(24)	67.59(15)
C(22)-Ru(1)-C(24)	68.18(15)
C(23)-Ru(1)-C(25)	68.11(14)
C(26)-Ru(1)-C(25)	36.77(15)
C(22)-Ru(1)-C(25)	79.73(15)
C(24)-Ru(1)-C(25)	38.00(14)
C(23)-Ru(1)-C(1)	99.34(14)
C(26)-Ru(1)-C(1)	155.79(15)
C(22)-Ru(1)-C(1)	97.35(14)
C(24)-Ru(1)-C(1)	125.41(14)
C(25)-Ru(1)-C(1)	163.04(14)
C(23)-Ru(1)-C(21)	67.48(15)
C(26)-Ru(1)-C(21)	37.81(14)
C(22)-Ru(1)-C(21)	36.80(15)
C(24)-Ru(1)-C(21)	80.59(15)
C(25)-Ru(1)-C(21)	67.61(15)
C(1)-Ru(1)-C(21)	119.36(14)
C(23)-Ru(1)-Cl(3)	157.25(11)
C(26)-Ru(1)-Cl(3)	87.06(11)
C(22)-Ru(1)-Cl(3)	119.89(11)
C(24)-Ru(1)-Cl(3)	148.52(11)
C(25)-Ru(1)-Cl(3)	110.84(10)
C(1)-Ru(1)-Cl(3)	85.20(10)
C(21)-Ru(1)-Cl(3)	90.77(11)

C(23)-Ru(1)-S(1)	112.66(11)
C(26)-Ru(1)-S(1)	125.49(11)
C(22)-Ru(1)-S(1)	149.32(11)
C(24)-Ru(1)-S(1)	89.98(11)
C(25)-Ru(1)-S(1)	96.43(11)
C(1)-Ru(1)-S(1)	77.47(10)
C(21)-Ru(1)-S(1)	163.16(11)
Cl(3)-Ru(1)-S(1)	90.09(3)
P(1)-S(1)-Ru(1)	82.89(4)
O(2)-S(2)-O(1)	118.06(17)
O(2)-S(2)-C(1)	109.83(17)
O(1)-S(2)-C(1)	107.68(17)
O(2)-S(2)-C(14)	106.77(18)
O(1)-S(2)-C(14)	107.28(17)
C(1)-S(2)-C(14)	106.65(18)
C(1)-P(1)-C(2)	108.73(17)
C(1)-P(1)-C(8)	118.58(17)
C(2)-P(1)-C(8)	103.48(17)
C(1)-P(1)-S(1)	100.82(13)
C(2)-P(1)-S(1)	113.84(13)
C(8)-P(1)-S(1)	111.81(13)
S(2)-C(1)-P(1)	117.4(2)
S(2)-C(1)-Ru(1)	116.52(19)
P(1)-C(1)-Ru(1)	95.23(16)
C(7)-C(2)-C(3)	119.7(3)
C(7)-C(2)-P(1)	122.0(3)
C(3)-C(2)-P(1)	118.1(3)
C(4)-C(3)-C(2)	119.9(4)
C(3)-C(4)-C(5)	120.5(4)
C(4)-C(5)-C(6)	119.7(4)
C(7)-C(6)-C(5)	120.2(4)
C(6)-C(7)-C(2)	119.9(4)
C(9)-C(8)-C(13)	119.5(4)
C(9)-C(8)-P(1)	121.8(3)
C(13)-C(8)-P(1)	118.7(3)
C(8)-C(9)-C(10)	120.3(4)

C(11)-C(10)-C(9)	119.5(4)
C(12)-C(11)-C(10)	120.3(4)
C(11)-C(12)-C(13)	120.5(4)
C(12)-C(13)-C(8)	119.8(4)
C(19)-C(14)-C(15)	121.3(4)
C(19)-C(14)-S(2)	118.8(3)
C(15)-C(14)-S(2)	119.9(3)
C(16)-C(15)-C(14)	118.5(4)
C(17)-C(16)-C(15)	120.1(4)
C(18)-C(17)-C(16)	120.5(4)
C(17)-C(18)-C(19)	120.1(4)
C(18)-C(19)-C(14)	119.5(4)
C(22)-C(21)-C(26)	117.5(4)
C(22)-C(21)-C(20)	122.1(4)
C(26)-C(21)-C(20)	120.4(4)
C(22)-C(21)-Ru(1)	70.1(2)
C(26)-C(21)-Ru(1)	69.5(2)
C(20)-C(21)-Ru(1)	129.5(3)
C(21)-C(22)-C(23)	121.3(4)
C(21)-C(22)-Ru(1)	73.1(2)
C(23)-C(22)-Ru(1)	70.0(2)
C(22)-C(23)-C(24)	121.1(4)
C(22)-C(23)-Ru(1)	72.4(2)
C(24)-C(23)-Ru(1)	72.2(2)
C(23)-C(24)-C(25)	118.0(4)
C(23)-C(24)-C(27)	123.9(4)
C(25)-C(24)-C(27)	118.1(4)
C(23)-C(24)-Ru(1)	69.7(2)
C(25)-C(24)-Ru(1)	71.3(2)
C(27)-C(24)-Ru(1)	132.7(3)
C(26)-C(25)-C(24)	119.9(4)
C(26)-C(25)-Ru(1)	71.1(2)
C(24)-C(25)-Ru(1)	70.7(2)
C(25)-C(26)-C(21)	122.2(4)
C(25)-C(26)-Ru(1)	72.1(2)
C(21)-C(26)-Ru(1)	72.7(2)

C(24)-C(27)-C(28)	114.3(3)
C(24)-C(27)-C(29)	107.5(3)
C(28)-C(27)-C(29)	110.7(4)
C61-C11-C21	122.0(6)
C51-C61-C11	119.1(8)
C31-C21-C11	120.9(6)
C21-C31-C41	115.9(7)
C51-C41-C31	119.1(7)
C61-C51-C41	122.9(7)

Symmetry transformations used to generate equivalent atoms:

Table 54-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	11(1)	14(1)	21(1)	2(1)	4(1)	1(1)
Cl(3)	13(1)	21(1)	22(1)	2(1)	2(1)	3(1)
S(1)	15(1)	16(1)	26(1)	8(1)	6(1)	4(1)
S(2)	11(1)	16(1)	22(1)	2(1)	4(1)	1(1)
P(1)	11(1)	16(1)	18(1)	6(1)	4(1)	2(1)
O(1)	18(1)	19(1)	29(2)	1(1)	12(1)	-2(1)
O(2)	17(1)	24(2)	28(2)	3(1)	0(1)	5(1)
C(1)	13(2)	14(2)	17(2)	2(2)	1(2)	2(2)
C(2)	12(2)	21(2)	13(2)	2(2)	3(2)	6(2)
C(3)	19(2)	19(2)	18(2)	4(2)	7(2)	4(2)
C(4)	14(2)	25(2)	27(2)	2(2)	7(2)	3(2)
C(5)	15(2)	32(2)	21(2)	2(2)	4(2)	11(2)
C(6)	26(2)	22(2)	16(2)	7(2)	7(2)	13(2)
C(7)	16(2)	21(2)	16(2)	4(2)	8(2)	3(2)
C(8)	13(2)	23(2)	16(2)	5(2)	5(2)	0(2)
C(9)	20(2)	31(2)	24(2)	5(2)	5(2)	7(2)
C(10)	26(2)	36(3)	27(2)	-3(2)	11(2)	4(2)
C(11)	23(2)	55(3)	15(2)	5(2)	2(2)	0(2)

C(12)	23(2)	46(3)	26(2)	16(2)	6(2)	8(2)
C(13)	21(2)	33(2)	26(2)	12(2)	8(2)	7(2)
C(14)	15(2)	18(2)	22(2)	0(2)	4(2)	-1(2)
C(15)	27(2)	21(2)	27(2)	6(2)	9(2)	2(2)
C(16)	39(3)	20(2)	45(3)	6(2)	16(2)	8(2)
C(17)	42(3)	24(2)	41(3)	-9(2)	21(2)	0(2)
C(18)	35(3)	33(3)	27(2)	-8(2)	7(2)	-4(2)
C(19)	18(2)	26(2)	25(2)	1(2)	4(2)	-3(2)
C(20)	48(3)	27(2)	28(2)	7(2)	22(2)	15(2)
C(21)	23(2)	22(2)	26(2)	1(2)	14(2)	7(2)
C(22)	21(2)	18(2)	32(2)	4(2)	15(2)	6(2)
C(23)	12(2)	21(2)	28(2)	-2(2)	8(2)	2(2)
C(24)	19(2)	22(2)	26(2)	4(2)	9(2)	10(2)
C(25)	17(2)	19(2)	26(2)	0(2)	8(2)	4(2)
C(26)	21(2)	21(2)	22(2)	-2(2)	10(2)	5(2)
C(27)	24(2)	25(2)	27(2)	5(2)	8(2)	7(2)
C(28)	34(3)	34(2)	26(2)	10(2)	10(2)	16(2)
C(29)	42(3)	31(2)	30(2)	7(2)	6(2)	17(2)
C11	47(3)	49(3)	56(3)	8(3)	30(3)	14(3)
C61	92(5)	38(3)	109(6)	5(4)	73(5)	21(3)
C21	37(3)	66(4)	40(3)	24(3)	20(2)	13(3)
C31	40(4)	200(10)	58(4)	57(5)	15(3)	41(5)
C41	108(6)	170(7)	73(5)	76(5)	36(4)	100(5)
C51	108(6)	75(5)	131(6)	62(4)	82(5)	68(4)

Table 54-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
H(1)	8170(40)	5730(40)	4130(40)	27(12)
H(3)	11477	8014	3173	22
H(4)	13437	7635	3668	27
H(5)	13531	5843	4125	27

H(6)	11647	4418	4089	23
H(7)	9674	4790	3599	21
H(9)	9268	4837	1470	30
H(10)	8619	4082	-410	37
H(11)	7428	4973	-1581	40
H(12)	6868	6585	-885	38
H(13)	7455	7312	987	31
H(15)	7300	3498	3445	31
H(16)	7504	1894	2317	41
H(17)	6593	1525	437	45
H(18)	5526	2758	-337	42
H(19)	5417	4417	756	30
H(20A)	7235	6651	7076	47
H(20B)	7619	7906	7850	47
H(20C)	8669	7495	7345	47
H(22)	5956	6548	5296	27
H(23)	5449	7389	3733	25
H(25)	8508	10367	5171	25
H(26)	9011	9491	6694	25
H(27)	7322	10108	3285	30
H(28A)	5637	9284	1755	44
H(28B)	4865	8436	2418	44
H(28C)	6150	8248	2160	44
H(29A)	5582	10936	3178	50
H(29B)	6332	11069	4425	50
H(29C)	4992	10080	3927	50
H11	7237	614	-2113	58
H61	6119	-826	-1355	87
H21	9170	1902	-1145	55
H3A1	10068	1772	644	114
H41	8882	184	1395	118
H51	6988	-1076	321	101

Röntgenstrukturanalytische Daten für 56a

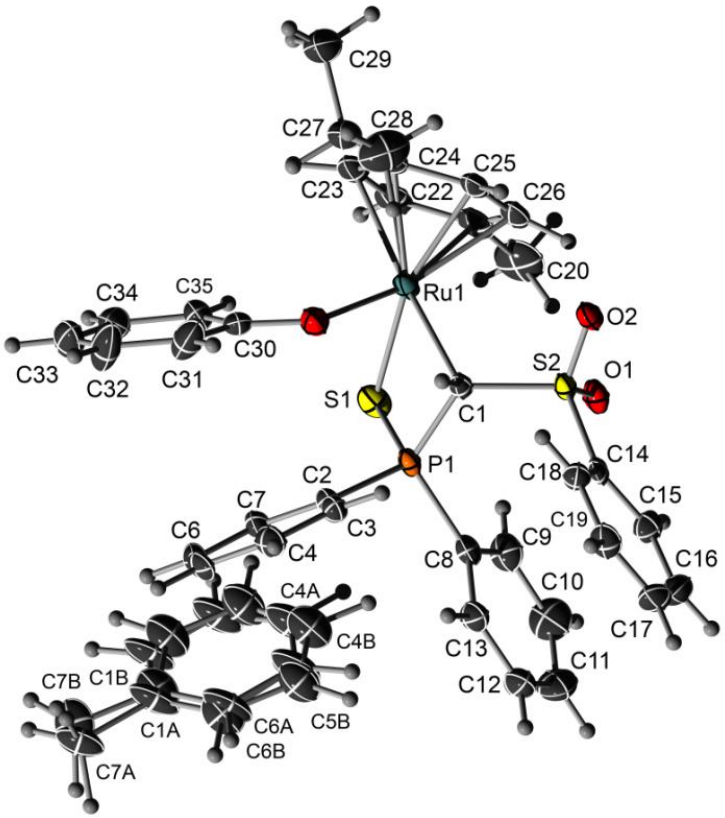

Table 56a-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	$C_{38.50}H_{39}O_3PRuS_2$	
Formula weight	745.86	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 10.8833(13) Å	α = 90°.
	b = 24.294(3) Å	β = 106.893(3)°.
	c = 13.4823(16) Å	γ = 90°.
Volume	3410.9(7) $Å^3$	
Z	4	
Density (calculated)	1.452 Mg/m^3	
Absorption coefficient	0.666 mm^{-1}	
F(000)	1540	

Crystal size	0.30 x 0.13 x 0.03 mm^3
Theta range for data collection	1.79 to 25.00°.
Index ranges	-12<=h<=12, -28<=k<=28, -16<=l<=16
Reflections collected	53809
Independent reflections	5997 [R(int) = 0.0419]
Completeness to theta = 25.00°	100.0 %
Absorption correction	Empirical
Max. and min. transmission	0.7643 and 0.6453
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5997 / 114 / 482
Goodness-of-fit on F^2	1.099
Final R indices [I>2sigma(I)]	R1 = 0.0428, wR2 = 0.1216
R indices (all data)	R1 = 0.0480, wR2 = 0.1265
Largest diff. peak and hole	1.170 and -0.769 e.$Å^{-3}$

Table 56a-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	5664(1)	2090(1)	6464(1)	23(1)
S(1)	4402(1)	1276(1)	5718(1)	27(1)
S(2)	7596(1)	1276(1)	8226(1)	18(1)
P(1)	4760(1)	1074(1)	7213(1)	18(1)
O(1)	7857(2)	939(1)	7428(2)	25(1)
O(2)	8429(2)	1740(1)	8614(2)	23(1)
O(3)	4243(3)	2306(1)	7161(2)	27(1)
C(1)	6042(3)	1535(2)	7810(3)	18(1)
C(2)	3430(3)	1201(2)	7732(3)	21(1)
C(3)	3629(4)	1344(2)	8766(3)	22(1)
C(4)	2582(4)	1422(2)	9144(3)	28(1)
C(5)	1344(4)	1352(2)	8495(3)	29(1)
C(6)	1143(4)	1206(2)	7472(3)	28(1)
C(7)	2185(4)	1135(2)	7082(3)	24(1)
C(8)	5092(3)	344(2)	7412(3)	22(1)

C(9)	5526(4)	51(2)	6695(3)	34(1)
C(10)	5768(5)	-508(2)	6830(4)	47(1)
C(11)	5600(5)	-775(2)	7694(4)	46(1)
C(12)	5186(4)	-487(2)	8423(4)	36(1)
C(13)	4919(4)	71(2)	8280(3)	28(1)
C(14)	7726(3)	843(2)	9320(3)	20(1)
C(15)	8094(4)	302(2)	9284(3)	26(1)
C(16)	8249(4)	-25(2)	10150(3)	33(1)
C(17)	8022(4)	183(2)	11034(3)	33(1)
C(18)	7665(4)	728(2)	11070(3)	31(1)
C(19)	7510(4)	1065(2)	10206(3)	23(1)
C(20)	7200(6)	1544(2)	4868(4)	55(2)
C(21)	6875(4)	2047(2)	5407(4)	36(1)
C(22)	5775(4)	2386(2)	4956(3)	37(1)
C(23)	5462(4)	2830(2)	5499(4)	35(1)
C(24)	6233(4)	2960(2)	6528(3)	30(1)
C(25)	7323(4)	2631(2)	6966(3)	29(1)
C(26)	7642(4)	2188(2)	6412(4)	33(1)
C(27)	5782(4)	3420(2)	7096(4)	38(1)
C(28)	6415(6)	3426(2)	8237(4)	59(2)
C(29)	5929(5)	3967(2)	6577(4)	50(1)
C(30)	3050(4)	2454(2)	6732(3)	29(1)
C(31)	2360(5)	2655(2)	7396(4)	47(1)
C(32)	1083(6)	2804(3)	7030(5)	62(2)
C(33)	444(5)	2752(2)	5990(5)	54(2)
C(34)	1089(4)	2563(2)	5314(4)	42(1)
C(35)	2384(4)	2418(2)	5675(4)	33(1)
C1A1	-621(14)	-56(7)	5249(10)	46(4)
C2A1	-572(16)	43(9)	4238(9)	48(4)
C3A1	606(18)	26(10)	4016(10)	51(4)
C4A1	1735(15)	-90(10)	4804(14)	50(4)
C5A1	1686(15)	-190(11)	5814(13)	49(4)
C6A1	508(17)	-173(10)	6037(9)	48(4)
C7A1	-1901(17)	-38(12)	5490(18)	42(5)
C1B1	-537(15)	-30(7)	5149(10)	45(4)
C2B1	-196(17)	104(8)	4254(9)	48(4)

C3B1	1084(18)	59(9)	4248(12)	48(4)
C4B1	2023(15)	-120(9)	5137(15)	47(4)
C5B1	1682(16)	-254(11)	6033(13)	46(4)
C6B1	402(18)	-209(10)	6038(10)	47(4)
C7B1	-1927(16)	20(12)	5155(17)	45(5)

Table 56a-3. Bond lengths [Å] and angles [°] for sad.

Ru(1)-O(3)	2.098(3)
Ru(1)-C(25)	2.177(4)
Ru(1)-C(26)	2.187(4)
Ru(1)-C(23)	2.192(4)
Ru(1)-C(22)	2.193(4)
Ru(1)-C(24)	2.198(4)
Ru(1)-C(1)	2.201(3)
Ru(1)-C(21)	2.207(4)
Ru(1)-S(1)	2.4501(11)
S(1)-P(1)	1.9997(13)
S(2)-O(1)	1.444(3)
S(2)-O(2)	1.445(3)
S(2)-C(1)	1.739(4)
S(2)-C(14)	1.784(4)
P(1)-C(1)	1.788(4)
P(1)-C(2)	1.807(4)
P(1)-C(8)	1.815(4)
O(3)-C(30)	1.308(5)
C(2)-C(7)	1.392(5)
C(2)-C(3)	1.392(5)
C(3)-C(4)	1.390(5)
C(4)-C(5)	1.387(6)
C(5)-C(6)	1.379(6)
C(6)-C(7)	1.393(6)
C(8)-C(9)	1.389(6)
C(8)-C(13)	1.404(6)
C(9)-C(10)	1.384(7)

C(10)-C(11)	1.392(8)
C(11)-C(12)	1.384(7)
C(12)-C(13)	1.390(6)
C(14)-C(15)	1.378(6)
C(14)-C(19)	1.391(5)
C(15)-C(16)	1.381(6)
C(16)-C(17)	1.381(6)
C(17)-C(18)	1.387(6)
C(18)-C(19)	1.392(6)
C(20)-C(21)	1.514(7)
C(21)-C(26)	1.412(7)
C(21)-C(22)	1.435(7)
C(22)-C(23)	1.400(7)
C(23)-C(24)	1.433(7)
C(24)-C(25)	1.409(6)
C(24)-C(27)	1.515(7)
C(25)-C(26)	1.410(7)
C(27)-C(28)	1.492(7)
C(27)-C(29)	1.531(6)
C(30)-C(35)	1.402(6)
C(30)-C(31)	1.412(6)
C(31)-C(32)	1.381(7)
C(32)-C(33)	1.377(9)
C(33)-C(34)	1.381(8)
C(34)-C(35)	1.396(6)
C1A1-C2A1	1.4001
C1A1-C6A1	1.4001
C1A1-C7A1	1.5200
C2A1-C3A1	1.3999
C3A1-C4A1	1.4000
C4A1-C5A1	1.4000
C5A1-C6A1	1.4000
C1B1-C2B1	1.4000
C1B1-C6B1	1.4001
C1B1-C7B1	1.5200
C2B1-C3B1	1.4000

C3B1-C4B1	1.4000
C4B1-C5B1	1.4000
C5B1-C6B1	1.4000

O(3)-Ru(1)-C(25)	111.24(15)
O(3)-Ru(1)-C(26)	147.99(16)
C(25)-Ru(1)-C(26)	37.70(17)
O(3)-Ru(1)-C(23)	95.75(15)
C(25)-Ru(1)-C(23)	67.67(16)
C(26)-Ru(1)-C(23)	79.72(16)
O(3)-Ru(1)-C(22)	125.43(15)
C(25)-Ru(1)-C(22)	79.96(17)
C(26)-Ru(1)-C(22)	67.33(16)
C(23)-Ru(1)-C(22)	37.25(19)
O(3)-Ru(1)-C(24)	88.68(14)
C(25)-Ru(1)-C(24)	37.58(16)
C(26)-Ru(1)-C(24)	68.13(17)
C(23)-Ru(1)-C(24)	38.11(17)
C(22)-Ru(1)-C(24)	68.30(18)
O(3)-Ru(1)-C(1)	76.65(12)
C(25)-Ru(1)-C(1)	100.04(14)
C(26)-Ru(1)-C(1)	98.26(14)
C(23)-Ru(1)-C(1)	162.48(17)
C(22)-Ru(1)-C(1)	156.64(17)
C(24)-Ru(1)-C(1)	124.97(15)
O(3)-Ru(1)-C(21)	163.32(15)
C(25)-Ru(1)-C(21)	68.42(17)
C(26)-Ru(1)-C(21)	37.49(18)
C(23)-Ru(1)-C(21)	68.37(18)
C(22)-Ru(1)-C(21)	38.06(18)
C(24)-Ru(1)-C(21)	81.76(17)
C(1)-Ru(1)-C(21)	120.02(16)
O(3)-Ru(1)-S(1)	89.29(8)
C(25)-Ru(1)-S(1)	158.55(12)
C(26)-Ru(1)-S(1)	120.99(13)
C(23)-Ru(1)-S(1)	118.05(13)

C(22)-Ru(1)-S(1)	93.41(13)
C(24)-Ru(1)-S(1)	155.54(12)
C(1)-Ru(1)-S(1)	78.05(10)
C(21)-Ru(1)-S(1)	93.77(13)
P(1)-S(1)-Ru(1)	82.09(4)
O(1)-S(2)-O(2)	118.26(16)
O(1)-S(2)-C(1)	110.43(17)
O(2)-S(2)-C(1)	106.45(17)
O(1)-S(2)-C(14)	107.22(18)
O(2)-S(2)-C(14)	105.64(16)
C(1)-S(2)-C(14)	108.42(17)
C(1)-P(1)-C(2)	109.12(18)
C(1)-P(1)-C(8)	116.73(17)
C(2)-P(1)-C(8)	104.85(17)
C(1)-P(1)-S(1)	101.43(12)
C(2)-P(1)-S(1)	113.89(13)
C(8)-P(1)-S(1)	111.16(13)
C(30)-O(3)-Ru(1)	129.6(3)
S(2)-C(1)-P(1)	118.5(2)
S(2)-C(1)-Ru(1)	114.75(18)
P(1)-C(1)-Ru(1)	94.45(15)
C(7)-C(2)-C(3)	120.0(3)
C(7)-C(2)-P(1)	118.6(3)
C(3)-C(2)-P(1)	121.4(3)
C(4)-C(3)-C(2)	119.7(4)
C(5)-C(4)-C(3)	120.1(4)
C(6)-C(5)-C(4)	120.4(4)
C(5)-C(6)-C(7)	120.0(4)
C(2)-C(7)-C(6)	119.8(4)
C(9)-C(8)-C(13)	119.5(4)
C(9)-C(8)-P(1)	119.4(3)
C(13)-C(8)-P(1)	121.0(3)
C(10)-C(9)-C(8)	120.1(4)
C(9)-C(10)-C(11)	120.1(4)
C(12)-C(11)-C(10)	120.5(4)
C(11)-C(12)-C(13)	119.5(4)

C(12)-C(13)-C(8)	120.2(4)
C(15)-C(14)-C(19)	121.5(4)
C(15)-C(14)-S(2)	119.1(3)
C(19)-C(14)-S(2)	119.3(3)
C(14)-C(15)-C(16)	119.0(4)
C(17)-C(16)-C(15)	120.7(4)
C(16)-C(17)-C(18)	120.1(4)
C(17)-C(18)-C(19)	119.9(4)
C(14)-C(19)-C(18)	118.8(4)
C(26)-C(21)-C(22)	117.1(4)
C(26)-C(21)-C(20)	120.1(5)
C(22)-C(21)-C(20)	122.8(5)
C(26)-C(21)-Ru(1)	70.5(2)
C(22)-C(21)-Ru(1)	70.4(2)
C(20)-C(21)-Ru(1)	127.9(3)
C(23)-C(22)-C(21)	121.4(4)
C(23)-C(22)-Ru(1)	71.3(2)
C(21)-C(22)-Ru(1)	71.5(2)
C(22)-C(23)-C(24)	120.9(4)
C(22)-C(23)-Ru(1)	71.4(2)
C(24)-C(23)-Ru(1)	71.2(2)
C(25)-C(24)-C(23)	117.7(4)
C(25)-C(24)-C(27)	124.3(4)
C(23)-C(24)-C(27)	117.9(4)
C(25)-C(24)-Ru(1)	70.4(2)
C(23)-C(24)-Ru(1)	70.7(2)
C(27)-C(24)-Ru(1)	126.9(3)
C(24)-C(25)-C(26)	121.2(4)
C(24)-C(25)-Ru(1)	72.0(2)
C(26)-C(25)-Ru(1)	71.5(2)
C(25)-C(26)-C(21)	121.7(4)
C(25)-C(26)-Ru(1)	70.8(2)
C(21)-C(26)-Ru(1)	72.0(2)
C(28)-C(27)-C(24)	114.0(4)
C(28)-C(27)-C(29)	112.6(4)
C(24)-C(27)-C(29)	108.5(4)

O(3)-C(30)-C(35)	125.9(4)
O(3)-C(30)-C(31)	117.1(4)
C(35)-C(30)-C(31)	116.9(4)
C(32)-C(31)-C(30)	121.9(5)
C(33)-C(32)-C(31)	119.9(5)
C(32)-C(33)-C(34)	119.9(5)
C(33)-C(34)-C(35)	120.6(5)
C(34)-C(35)-C(30)	120.7(4)
C2A1-C1A1-C6A1	120.0
C2A1-C1A1-C7A1	120.0
C6A1-C1A1-C7A1	120.0
C3A1-C2A1-C1A1	120.0
C2A1-C3A1-C4A1	120.0
C3A1-C4A1-C5A1	120.0
C6A1-C5A1-C4A1	120.0
C5A1-C6A1-C1A1	120.0
C2B1-C1B1-C6B1	120.0
C2B1-C1B1-C7B1	120.0
C6B1-C1B1-C7B1	120.0
C3B1-C2B1-C1B1	120.0
C2B1-C3B1-C4B1	120.0
C3B1-C4B1-C5B1	120.0
C6B1-C5B1-C4B1	120.0
C5B1-C6B1-C1B1	120.0

Symmetry transformations used to generate equivalent atoms:

Table 56a-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	16(1)	32(1)	19(1)	9(1)	5(1)	-2(1)
S(1)	25(1)	41(1)	16(1)	2(1)	5(1)	-6(1)
S(2)	13(1)	24(1)	17(1)	2(1)	6(1)	0(1)
P(1)	14(1)	26(1)	16(1)	2(1)	6(1)	-1(1)
O(1)	20(1)	35(2)	22(1)	0(1)	10(1)	2(1)
O(2)	16(1)	30(2)	21(1)	3(1)	3(1)	-3(1)
O(3)	21(1)	31(2)	29(2)	6(1)	8(1)	0(1)
C(1)	13(2)	24(2)	16(2)	4(2)	3(1)	0(1)
C(2)	15(2)	22(2)	26(2)	5(2)	8(2)	2(2)
C(3)	18(2)	24(2)	24(2)	4(2)	8(2)	2(2)
C(4)	28(2)	26(2)	33(2)	-2(2)	16(2)	0(2)
C(5)	21(2)	27(2)	46(3)	2(2)	22(2)	1(2)
C(6)	15(2)	27(2)	40(2)	4(2)	6(2)	2(2)
C(7)	16(2)	29(2)	25(2)	3(2)	4(2)	-1(2)
C(8)	15(2)	27(2)	23(2)	-2(2)	5(2)	-2(2)
C(9)	33(2)	38(3)	32(2)	-6(2)	14(2)	2(2)
C(10)	56(3)	38(3)	52(3)	-17(2)	24(3)	2(2)
C(11)	49(3)	23(2)	70(4)	-3(2)	23(3)	-2(2)
C(12)	31(2)	31(2)	51(3)	9(2)	21(2)	2(2)
C(13)	26(2)	27(2)	38(2)	2(2)	17(2)	2(2)
C(14)	9(2)	29(2)	21(2)	5(2)	1(1)	-1(1)
C(15)	26(2)	27(2)	24(2)	1(2)	4(2)	1(2)
C(16)	34(2)	24(2)	38(2)	5(2)	7(2)	5(2)
C(17)	33(2)	34(2)	30(2)	15(2)	6(2)	-1(2)
C(18)	27(2)	44(3)	24(2)	7(2)	11(2)	2(2)
C(19)	22(2)	25(2)	22(2)	4(2)	8(2)	2(2)
C(20)	64(4)	69(4)	47(3)	6(3)	41(3)	-4(3)
C(21)	30(2)	50(3)	34(2)	12(2)	20(2)	-7(2)
C(22)	32(2)	53(3)	25(2)	16(2)	9(2)	-10(2)
C(23)	23(2)	44(3)	35(2)	23(2)	4(2)	-5(2)
C(24)	21(2)	33(2)	37(2)	16(2)	8(2)	-5(2)

C(25)	18(2)	36(2)	34(2)	16(2)	6(2)	-6(2)
C(26)	20(2)	42(3)	40(3)	18(2)	14(2)	-3(2)
C(27)	31(2)	34(3)	48(3)	13(2)	11(2)	-3(2)
C(28)	78(4)	45(3)	51(3)	2(3)	14(3)	-4(3)
C(29)	43(3)	43(3)	61(3)	18(3)	9(3)	-3(2)
C(30)	25(2)	22(2)	42(2)	14(2)	13(2)	2(2)
C(31)	50(3)	49(3)	48(3)	21(2)	25(2)	24(2)
C(32)	48(3)	84(4)	65(4)	40(3)	35(3)	38(3)
C(33)	32(3)	62(4)	75(4)	34(3)	29(3)	14(2)
C(34)	28(2)	43(3)	50(3)	19(2)	4(2)	-2(2)
C(35)	21(2)	35(2)	42(3)	10(2)	9(2)	-1(2)
C1A1	49(6)	56(9)	39(6)	-2(6)	25(5)	-27(6)
C2A1	50(6)	62(9)	41(7)	3(6)	25(5)	-29(6)
C3A1	51(6)	66(9)	42(7)	0(6)	25(5)	-25(7)
C4A1	51(6)	64(9)	43(7)	-2(6)	25(5)	-23(7)
C5A1	49(6)	62(9)	43(7)	-1(6)	25(5)	-24(6)
C6A1	49(6)	61(9)	42(7)	0(6)	24(5)	-26(6)
C7A1	50(7)	47(10)	39(9)	0(8)	26(6)	-18(8)
C1B1	43(6)	55(9)	39(7)	-16(6)	15(4)	-8(6)
C2B1	45(6)	60(9)	40(7)	-7(6)	14(5)	-11(6)
C3B1	44(6)	62(9)	40(7)	-7(6)	13(5)	-13(6)
C4B1	44(6)	59(9)	38(7)	-7(6)	14(5)	-11(6)
C5B1	43(6)	58(9)	39(7)	-7(6)	17(5)	-9(6)
C6B1	44(6)	59(9)	41(7)	-10(6)	15(5)	-8(6)
C7B1	45(7)	52(11)	41(10)	-29(9)	17(6)	4(8)

Table 56a-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
H(1)	5890(40)	1750(18)	8380(30)	25(11)
H(3)	4477	1388	9212	26
H(4)	2714	1523	9848	33

H(5)	631	1405	8757	34
H(6)	293	1154	7034	33
H(7)	2047	1041	6374	29
H(9)	5657	234	6112	40
H(10)	6049	-709	6332	56
H(11)	5770	-1158	7784	55
H(12)	5086	-670	9018	43
H(13)	4619	269	8771	34
H(15)	8239	157	8673	32
H(16)	8516	-397	10137	39
H(17)	8110	-49	11618	39
H(18)	7526	873	11683	37
H(19)	7261	1439	10220	27
H(20A)	6443	1430	4311	82
H(20B)	7467	1244	5369	82
H(20C)	7901	1633	4574	82
H(22)	5121	2254	4315	44
H(23)	4596	3003	5231	42
H(25)	7772	2665	7724	35
H(26)	8301	1918	6799	40
H(27)	4842	3363	6991	45
H(28A)	7342	3476	8371	89
H(28B)	6252	3076	8538	89
H(28C)	6067	3729	8553	89
H(29A)	6837	4030	6638	76
H(29B)	5608	4268	6919	76
H(29C)	5435	3954	5843	76
H(31)	2787	2688	8116	56
H(32)	647	2942	7494	74
H(33)	-439	2846	5739	64
H(34)	647	2531	4596	50
H(35)	2818	2295	5199	39
H2A1	-1443	133	3630	58
H3A1	645	103	3236	61
H4A1	2645	-104	4632	60
H5A1	2557	-280	6422	59

H6A1	470	-249	6816	58
H7A1	-2664	58	4786	64
H7B1	-2088	-437	5787	64
H7C1	-1867	279	6071	64
H2B1	-921	243	3568	58
H3B1	1347	162	3558	58
H4B1	3011	-155	5133	56
H5B1	2407	-392	6719	55
H6B1	139	-312	6729	57
H7D1	-2513	164	4400	67
H7E1	-2273	-381	5318	67
H7F1	-1992	312	5751	67

Röntgenstrukturanalytische Daten für 56b

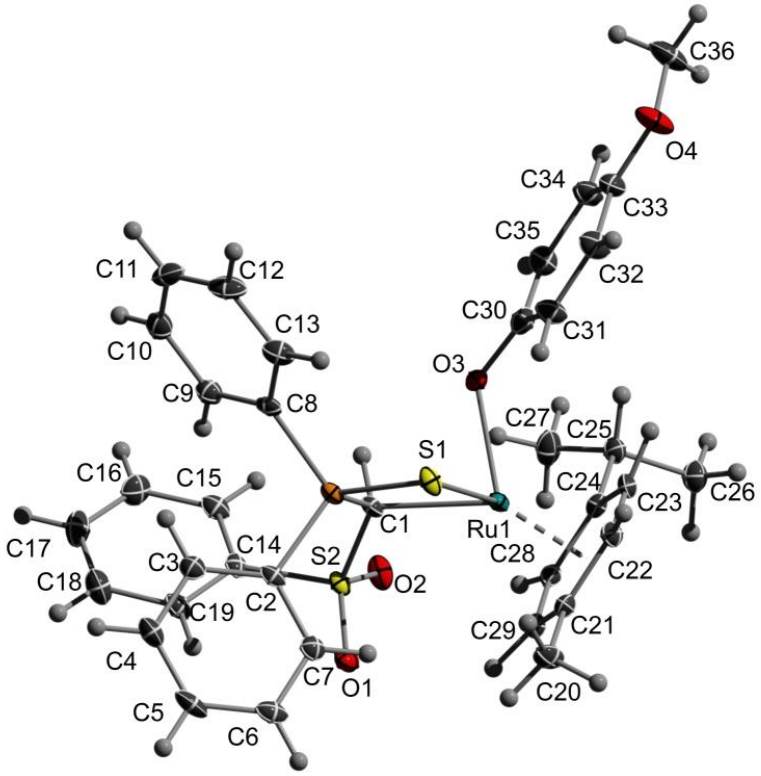

Table 56b-1. Crystal data and structure refinement for platon.

Identification code	platon	
Empirical formula	$C_{72}H_{74}O_8P_2Ru_2S_4$	
Formula weight	1459.63	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.1119(17) Å	α = 97.942(6)°.
	b = 12.265(2) Å	β = 96.127(5)°.
	c = 13.133(2) Å	γ = 92.149(5)°.
Volume	1601.7(4) $Å^3$	
Z	1	
Density (calculated)	1.513 Mg/m^3	
Absorption coefficient	0.709 mm^{-1}	
F(000)	752	

Crystal size	0.15 x 0.13 x 0.13 mm^3
Theta range for data collection	1.58 to 26.44°.
Index ranges	-12<=h<=12, -15<=k<=15, -16<=l<=16
Reflections collected	21517
Independent reflections	6574 [R(int) = 0.0366]
Completeness to theta = 26.44°	99.6 %
Absorption correction	Empirical
Max. and min. transmission	0.7454 and 0.6923
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6574 / 0 / 401
Goodness-of-fit on F^2	1.144
Final R indices [I>2sigma(I)]	R1 = 0.0303, wR2 = 0.0827
R indices (all data)	R1 = 0.0392, wR2 = 0.1047
Largest diff. peak and hole	1.004 and -0.576 e.$Å^{-3}$

Table 56b-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for platon. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(2)	4999(2)	898(2)	7278(2)	21(1)
S(2)	4123(1)	119(1)	7652(1)	14(1)
C(2)	1494(3)	-1278(2)	8588(2)	14(1)
C(1)	2557(3)	682(2)	7658(2)	13(1)
Ru(1)	2311(1)	2206(1)	8710(1)	12(1)
O(1)	4535(2)	-237(2)	8634(2)	19(1)
S(1)	395(1)	1060(1)	9003(1)	17(1)
P(1)	1130(1)	-60(1)	7991(1)	13(1)
C(5)	1954(3)	-3065(3)	9635(2)	22(1)
C(4)	1229(3)	-3227(3)	8659(2)	21(1)
O(4)	-2525(2)	5638(2)	6950(2)	30(1)
C(3)	994(3)	-2328(2)	8135(2)	18(1)
O(3)	1242(2)	2531(2)	7311(2)	16(1)
C(18)	3518(3)	-3015(3)	6193(3)	26(1)
C(17)	3491(3)	-2872(3)	5156(3)	28(1)

C(16)	3702(3)	-1835(3)	4889(2)	25(1)
C(15)	3918(3)	-926(3)	5654(2)	19(1)
C(14)	3937(3)	-1073(2)	6693(2)	15(1)
C(13)	-1405(3)	-332(3)	6930(2)	22(1)
C(12)	-2337(3)	-729(3)	6093(3)	26(1)
C(11)	-1938(3)	-1275(3)	5199(3)	26(1)
C(10)	-592(3)	-1418(3)	5115(3)	24(1)
C(9)	347(3)	-1046(2)	5956(2)	19(1)
C(8)	-53(3)	-505(2)	6870(2)	15(1)
C(7)	2217(3)	-1123(2)	9564(2)	17(1)
C(6)	2445(3)	-2018(3)	10093(2)	20(1)
C(19)	3756(3)	-2115(2)	6970(2)	20(1)
C(29)	4106(3)	2220(2)	9820(2)	16(1)
C(28)	4385(3)	2826(2)	9005(2)	16(1)
C(24)	3599(3)	3696(2)	8754(2)	16(1)
C(23)	2501(3)	3948(2)	9342(2)	17(1)
C(22)	2213(3)	3348(2)	10136(2)	18(1)
C(21)	3020(3)	2468(2)	10391(2)	17(1)
C(20)	2693(3)	1830(3)	11236(2)	22(1)
C(25)	3860(3)	4361(2)	7898(2)	18(1)
C(27)	4441(4)	3706(3)	6999(2)	27(1)
C(26)	4762(3)	5378(3)	8380(3)	23(1)
C(30)	389(3)	3310(3)	7267(2)	19(1)
C(32)	-1545(3)	4268(3)	7813(3)	23(1)
C(33)	-1516(3)	4915(3)	7014(2)	21(1)
C(34)	-534(3)	4785(3)	6368(2)	22(1)
C(35)	409(3)	3990(3)	6492(2)	22(1)
C(31)	-606(3)	3487(3)	7939(2)	23(1)
C(36)	-2594(4)	6248(3)	6108(3)	34(1)

Table 56b-3. Bond lengths [Å] and angles [°] for platon.

O(2)-S(2)	1.449(2)
S(2)-O(1)	1.443(2)
S(2)-C(1)	1.751(3)
S(2)-C(14)	1.783(3)
C(2)-C(7)	1.391(4)
C(2)-C(3)	1.394(4)
C(2)-P(1)	1.813(3)
C(1)-P(1)	1.801(3)
C(1)-Ru(1)	2.203(3)
C(1)-H(1)	1.0000
Ru(1)-O(3)	2.1237(19)
Ru(1)-C(23)	2.177(3)
Ru(1)-C(28)	2.180(3)
Ru(1)-C(22)	2.193(3)
Ru(1)-C(24)	2.195(3)
Ru(1)-C(29)	2.202(3)
Ru(1)-C(21)	2.223(3)
Ru(1)-S(1)	2.4459(8)
S(1)-P(1)	1.9975(10)
P(1)-C(8)	1.803(3)
C(5)-C(6)	1.390(5)
C(5)-C(4)	1.392(4)
C(5)-H(5)	0.9500
C(4)-C(3)	1.394(4)
C(4)-H(4)	0.9500
O(4)-C(33)	1.380(4)
O(4)-C(36)	1.415(4)
C(3)-H(3)	0.9500
O(3)-C(30)	1.314(4)
C(18)-C(19)	1.391(4)
C(18)-C(17)	1.395(5)
C(18)-H(18)	0.9500
C(17)-C(16)	1.380(5)
C(17)-H(17)	0.9500

C(16)-C(15)	1.387(4)
C(16)-H(16)	0.9500
C(15)-C(14)	1.400(4)
C(15)-H(15)	0.9500
C(14)-C(19)	1.386(4)
C(13)-C(12)	1.389(5)
C(13)-C(8)	1.401(4)
C(13)-H(13)	0.9500
C(12)-C(11)	1.376(5)
C(12)-H(12)	0.9500
C(11)-C(10)	1.393(5)
C(11)-H(11)	0.9500
C(10)-C(9)	1.390(4)
C(10)-H(10)	0.9500
C(9)-C(8)	1.395(4)
C(9)-H(9)	0.9500
C(7)-C(6)	1.392(4)
C(7)-H(7)	0.9500
C(6)-H(6)	0.9500
C(19)-H(19)	0.9500
C(29)-C(21)	1.414(4)
C(29)-C(28)	1.430(4)
C(29)-H(29)	1.0000
C(28)-C(24)	1.409(4)
C(28)-H(28)	1.0000
C(24)-C(23)	1.438(4)
C(24)-C(25)	1.516(4)
C(23)-C(22)	1.405(4)
C(23)-H(23)	1.0000
C(22)-C(21)	1.432(4)
C(22)-H(22)	1.0000
C(21)-C(20)	1.500(4)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(25)-C(27)	1.519(4)

C(25)-C(26)	1.537(4)
C(25)-H(25)	1.0000
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(30)-C(35)	1.404(4)
C(30)-C(31)	1.411(4)
C(32)-C(31)	1.388(4)
C(32)-C(33)	1.402(4)
C(32)-H(32)	0.9500
C(33)-C(34)	1.373(4)
C(34)-C(35)	1.402(4)
C(34)-H(34)	0.9500
C(35)-H(35)	0.9500
C(31)-H(31)	0.9500
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800

O(1)-S(2)-O(2)	118.06(13)
O(1)-S(2)-C(1)	110.68(13)
O(2)-S(2)-C(1)	107.23(13)
O(1)-S(2)-C(14)	107.57(13)
O(2)-S(2)-C(14)	106.00(13)
C(1)-S(2)-C(14)	106.67(13)
C(7)-C(2)-C(3)	120.3(3)
C(7)-C(2)-P(1)	117.4(2)
C(3)-C(2)-P(1)	122.1(2)
S(2)-C(1)-P(1)	122.11(16)
S(2)-C(1)-Ru(1)	119.68(14)
P(1)-C(1)-Ru(1)	95.24(12)
S(2)-C(1)-H(1)	106.1
P(1)-C(1)-H(1)	106.1

Ru(1)-C(1)-H(1)	106.1
O(3)-Ru(1)-C(23)	92.06(10)
O(3)-Ru(1)-C(28)	116.29(10)
C(23)-Ru(1)-C(28)	67.97(11)
O(3)-Ru(1)-C(22)	119.11(9)
C(23)-Ru(1)-C(22)	37.51(11)
C(28)-Ru(1)-C(22)	80.48(11)
O(3)-Ru(1)-C(24)	90.11(9)
C(23)-Ru(1)-C(24)	38.41(11)
C(28)-Ru(1)-C(24)	37.58(11)
C(22)-Ru(1)-C(24)	68.85(11)
O(3)-Ru(1)-C(29)	154.25(10)
C(23)-Ru(1)-C(29)	80.04(11)
C(28)-Ru(1)-C(29)	38.09(11)
C(22)-Ru(1)-C(29)	67.50(11)
C(24)-Ru(1)-C(29)	68.46(11)
O(3)-Ru(1)-C(1)	78.50(9)
C(23)-Ru(1)-C(1)	158.79(11)
C(28)-Ru(1)-C(1)	99.03(10)
C(22)-Ru(1)-C(1)	160.82(11)
C(24)-Ru(1)-C(1)	121.77(11)
C(29)-Ru(1)-C(1)	100.23(10)
O(3)-Ru(1)-C(21)	156.92(9)
C(23)-Ru(1)-C(21)	68.15(11)
C(28)-Ru(1)-C(21)	68.39(11)
C(22)-Ru(1)-C(21)	37.85(11)
C(24)-Ru(1)-C(21)	81.60(11)
C(29)-Ru(1)-C(21)	37.28(11)
C(1)-Ru(1)-C(21)	124.10(11)
O(3)-Ru(1)-S(1)	89.05(6)
C(23)-Ru(1)-S(1)	120.17(8)
C(28)-Ru(1)-S(1)	153.90(8)
C(22)-Ru(1)-S(1)	92.95(8)
C(24)-Ru(1)-S(1)	158.51(8)
C(29)-Ru(1)-S(1)	116.16(8)
C(1)-Ru(1)-S(1)	79.03(7)

C(21)-Ru(1)-S(1)	90.93(8)
P(1)-S(1)-Ru(1)	83.25(3)
C(1)-P(1)-C(8)	111.42(13)
C(1)-P(1)-C(2)	115.30(13)
C(8)-P(1)-C(2)	106.45(13)
C(1)-P(1)-S(1)	102.44(10)
C(8)-P(1)-S(1)	111.84(10)
C(2)-P(1)-S(1)	109.48(10)
C(6)-C(5)-C(4)	120.8(3)
C(6)-C(5)-H(5)	119.6
C(4)-C(5)-H(5)	119.6
C(5)-C(4)-C(3)	119.5(3)
C(5)-C(4)-H(4)	120.2
C(3)-C(4)-H(4)	120.2
C(33)-O(4)-C(36)	116.8(3)
C(2)-C(3)-C(4)	119.8(3)
C(2)-C(3)-H(3)	120.1
C(4)-C(3)-H(3)	120.1
C(30)-O(3)-Ru(1)	123.56(18)
C(19)-C(18)-C(17)	120.4(3)
C(19)-C(18)-H(18)	119.8
C(17)-C(18)-H(18)	119.8
C(16)-C(17)-C(18)	120.4(3)
C(16)-C(17)-H(17)	119.8
C(18)-C(17)-H(17)	119.8
C(17)-C(16)-C(15)	119.9(3)
C(17)-C(16)-H(16)	120.0
C(15)-C(16)-H(16)	120.0
C(16)-C(15)-C(14)	119.5(3)
C(16)-C(15)-H(15)	120.2
C(14)-C(15)-H(15)	120.2
C(19)-C(14)-C(15)	120.9(3)
C(19)-C(14)-S(2)	120.7(2)
C(15)-C(14)-S(2)	118.3(2)
C(12)-C(13)-C(8)	119.7(3)
C(12)-C(13)-H(13)	120.1

C(8)-C(13)-H(13)	120.1
C(11)-C(12)-C(13)	120.5(3)
C(11)-C(12)-H(12)	119.8
C(13)-C(12)-H(12)	119.8
C(12)-C(11)-C(10)	120.4(3)
C(12)-C(11)-H(11)	119.8
C(10)-C(11)-H(11)	119.8
C(9)-C(10)-C(11)	119.7(3)
C(9)-C(10)-H(10)	120.2
C(11)-C(10)-H(10)	120.2
C(10)-C(9)-C(8)	120.2(3)
C(10)-C(9)-H(9)	119.9
C(8)-C(9)-H(9)	119.9
C(9)-C(8)-C(13)	119.5(3)
C(9)-C(8)-P(1)	121.3(2)
C(13)-C(8)-P(1)	119.1(2)
C(2)-C(7)-C(6)	120.1(3)
C(2)-C(7)-H(7)	120.0
C(6)-C(7)-H(7)	120.0
C(5)-C(6)-C(7)	119.5(3)
C(5)-C(6)-H(6)	120.3
C(7)-C(6)-H(6)	120.3
C(14)-C(19)-C(18)	118.8(3)
C(14)-C(19)-H(19)	120.6
C(18)-C(19)-H(19)	120.6
C(21)-C(29)-C(28)	121.0(3)
C(21)-C(29)-Ru(1)	72.19(17)
C(28)-C(29)-Ru(1)	70.14(16)
C(21)-C(29)-H(29)	118.8
C(28)-C(29)-H(29)	118.8
Ru(1)-C(29)-H(29)	118.8
C(24)-C(28)-C(29)	121.2(3)
C(24)-C(28)-Ru(1)	71.78(16)
C(29)-C(28)-Ru(1)	71.78(16)
C(24)-C(28)-H(28)	118.8
C(29)-C(28)-H(28)	118.8

Ru(1)-C(28)-H(28)	118.8
C(28)-C(24)-C(23)	117.6(3)
C(28)-C(24)-C(25)	122.9(3)
C(23)-C(24)-C(25)	119.5(3)
C(28)-C(24)-Ru(1)	70.64(17)
C(23)-C(24)-Ru(1)	70.12(16)
C(25)-C(24)-Ru(1)	130.1(2)
C(22)-C(23)-C(24)	121.5(3)
C(22)-C(23)-Ru(1)	71.85(17)
C(24)-C(23)-Ru(1)	71.47(16)
C(22)-C(23)-H(23)	118.6
C(24)-C(23)-H(23)	118.6
Ru(1)-C(23)-H(23)	118.6
C(23)-C(22)-C(21)	120.7(3)
C(23)-C(22)-Ru(1)	70.64(16)
C(21)-C(22)-Ru(1)	72.24(16)
C(23)-C(22)-H(22)	119.1
C(21)-C(22)-H(22)	119.1
Ru(1)-C(22)-H(22)	119.1
C(29)-C(21)-C(22)	118.1(3)
C(29)-C(21)-C(20)	121.9(3)
C(22)-C(21)-C(20)	120.0(3)
C(29)-C(21)-Ru(1)	70.53(16)
C(22)-C(21)-Ru(1)	69.92(16)
C(20)-C(21)-Ru(1)	130.6(2)
C(21)-C(20)-H(20A)	109.5
C(21)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(21)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(24)-C(25)-C(27)	113.8(3)
C(24)-C(25)-C(26)	108.0(2)
C(27)-C(25)-C(26)	111.7(3)
C(24)-C(25)-H(25)	107.7
C(27)-C(25)-H(25)	107.7

C(26)-C(25)-H(25)	107.7
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
O(3)-C(30)-C(35)	119.7(3)
O(3)-C(30)-C(31)	123.6(3)
C(35)-C(30)-C(31)	116.7(3)
C(31)-C(32)-C(33)	120.5(3)
C(31)-C(32)-H(32)	119.8
C(33)-C(32)-H(32)	119.8
C(34)-C(33)-O(4)	125.6(3)
C(34)-C(33)-C(32)	119.4(3)
O(4)-C(33)-C(32)	114.9(3)
C(33)-C(34)-C(35)	120.1(3)
C(33)-C(34)-H(34)	120.0
C(35)-C(34)-H(34)	120.0
C(34)-C(35)-C(30)	121.9(3)
C(34)-C(35)-H(35)	119.0
C(30)-C(35)-H(35)	119.0
C(32)-C(31)-C(30)	121.4(3)
C(32)-C(31)-H(31)	119.3
C(30)-C(31)-H(31)	119.3
O(4)-C(36)-H(36A)	109.5
O(4)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
O(4)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5

H(36B)-C(36)-H(36C) 109.5

Symmetry transformations used to generate equivalent atoms:

Table 56b-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for platon. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(2)	19(1)	16(1)	31(1)	1(1)	11(1)	-1(1)
S(2)	13(1)	13(1)	18(1)	2(1)	5(1)	3(1)
C(2)	13(1)	14(1)	17(1)	6(1)	7(1)	5(1)
C(1)	12(1)	12(1)	17(1)	5(1)	2(1)	3(1)
Ru(1)	13(1)	11(1)	13(1)	2(1)	3(1)	3(1)
O(1)	18(1)	19(1)	19(1)	2(1)	1(1)	7(1)
S(1)	18(1)	14(1)	21(1)	2(1)	9(1)	4(1)
P(1)	12(1)	12(1)	16(1)	4(1)	4(1)	3(1)
C(5)	26(2)	20(2)	26(2)	14(1)	12(1)	13(1)
C(4)	25(2)	14(2)	27(2)	6(1)	7(1)	4(1)
O(4)	31(1)	31(1)	36(1)	17(1)	8(1)	17(1)
C(3)	16(1)	18(2)	18(2)	3(1)	2(1)	1(1)
O(3)	20(1)	16(1)	11(1)	1(1)	1(1)	3(1)
C(18)	32(2)	16(2)	32(2)	3(1)	11(2)	2(1)
C(17)	31(2)	24(2)	28(2)	-7(1)	8(2)	2(1)
C(16)	26(2)	31(2)	17(2)	0(1)	7(1)	5(1)
C(15)	16(1)	20(2)	23(2)	6(1)	7(1)	5(1)
C(14)	12(1)	15(2)	19(2)	0(1)	5(1)	5(1)
C(13)	20(2)	26(2)	22(2)	10(1)	6(1)	4(1)
C(12)	14(2)	35(2)	32(2)	16(2)	0(1)	1(1)
C(11)	25(2)	28(2)	24(2)	12(1)	-9(1)	-8(1)
C(10)	32(2)	18(2)	21(2)	5(1)	2(1)	0(1)
C(9)	17(1)	19(2)	23(2)	5(1)	3(1)	2(1)
C(8)	15(1)	13(1)	19(2)	8(1)	0(1)	0(1)
C(7)	15(1)	18(2)	18(2)	2(1)	4(1)	5(1)
C(6)	19(2)	26(2)	18(2)	8(1)	7(1)	11(1)
C(19)	22(2)	19(2)	21(2)	5(1)	8(1)	8(1)

C(29)	18(1)	13(2)	15(1)	-1(1)	0(1)	0(1)
C(28)	14(1)	17(2)	16(1)	-2(1)	-1(1)	0(1)
C(24)	17(1)	15(2)	15(1)	-1(1)	-1(1)	-1(1)
C(23)	20(2)	12(2)	18(2)	-2(1)	0(1)	4(1)
C(22)	19(1)	17(2)	16(2)	-1(1)	3(1)	6(1)
C(21)	22(2)	16(2)	13(1)	-1(1)	-1(1)	2(1)
C(20)	30(2)	26(2)	14(2)	6(1)	5(1)	9(1)
C(25)	20(2)	14(2)	20(2)	3(1)	1(1)	-2(1)
C(27)	42(2)	21(2)	19(2)	2(1)	7(2)	-3(1)
C(26)	24(2)	19(2)	26(2)	2(1)	5(1)	-3(1)
C(30)	16(1)	21(2)	19(2)	0(1)	1(1)	-1(1)
C(32)	21(2)	27(2)	24(2)	7(1)	9(1)	7(1)
C(33)	22(2)	20(2)	22(2)	4(1)	-1(1)	6(1)
C(34)	27(2)	23(2)	20(2)	8(1)	3(1)	5(1)
C(35)	23(2)	24(2)	20(2)	4(1)	7(1)	4(1)
C(31)	25(2)	25(2)	21(2)	10(1)	5(1)	6(1)
C(36)	42(2)	32(2)	34(2)	19(2)	12(2)	20(2)

Table 56b-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for platon.

	x	y	z	U(eq)
H(1)	2308	853	6942	16
H(5)	2115	-3678	9993	26
H(4)	897	-3946	8352	26
H(3)	493	-2429	7471	21
H(18)	3373	-3732	6370	31
H(17)	3327	-3491	4631	34
H(16)	3698	-1743	4182	30
H(15)	4051	-209	5474	22
H(13)	-1684	56	7540	26
H(12)	-3256	-623	6138	32
H(11)	-2584	-1556	4636	31

H(10)	-317	-1769	4487	28
H(9)	1264	-1159	5908	23
H(7)	2555	-406	9869	20
H(6)	2933	-1915	10761	24
H(19)	3793	-2212	7677	24
H(29)	4551	1514	9878	19
H(28)	5027	2533	8520	20
H(23)	1822	4447	9084	20
H(22)	1339	3433	10422	21
H(20A)	1749	1585	11122	34
H(20B)	2878	2302	11906	34
H(20C)	3240	1187	11232	34
H(25)	2989	4627	7622	22
H(27A)	3887	3028	6755	41
H(27B)	5348	3518	7227	41
H(27C)	4463	4150	6434	41
H(26A)	4945	5822	7840	35
H(26B)	5602	5140	8701	35
H(26C)	4315	5821	8907	35
H(32)	-2211	4366	8271	28
H(34)	-493	5235	5837	27
H(35)	1081	3910	6038	26
H(31)	-634	3062	8490	27
H(36A)	-2712	5739	5457	50
H(36B)	-1767	6702	6145	50
H(36C)	-3349	6724	6140	50

Röntgenstrukturanalytische Daten für 56c

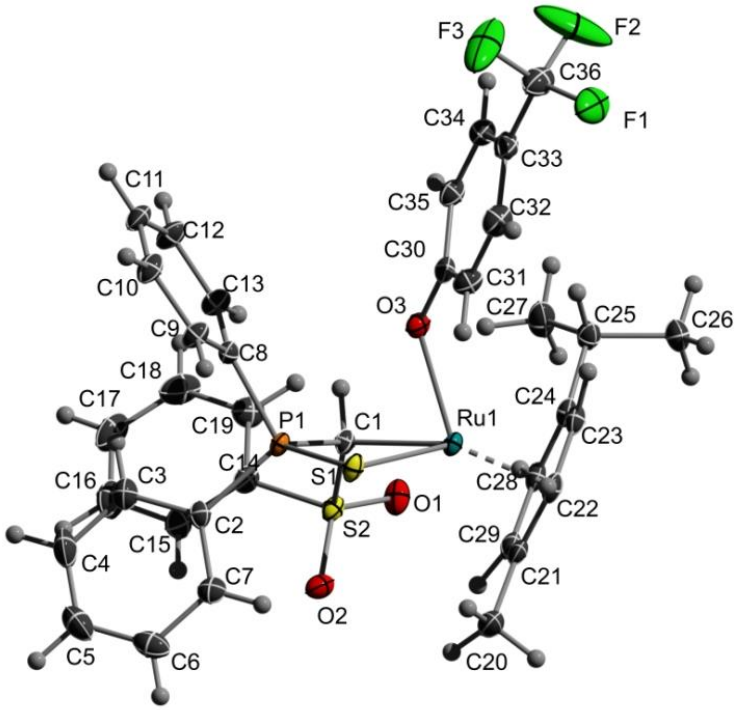

Table 56c-1. Crystal data and structure refinement for neu1.

Identification code	neu1	
Empirical formula	$C_{36}H_{34}F_3O_3PRuS_2$	
Formula weight	767.79	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.7150(4) Å	α = 117.6090(10)°.
	b = 13.5279(6) Å	β = 95.463(2)°.
	c = 14.5576(8) Å	γ = 95.3260(10)°.
Volume	1667.19(14) $Å^3$	
Z	2	
Density (calculated)	1.529 Mg/m^3	
Absorption coefficient	0.696 mm^{-1}	
F(000)	784	
Crystal size	0.15 x 0.14 x 0.13 mm^3	
Theta range for data collection	1.60 to 26.38°.	

Index ranges	-12<=h<=12, -16<=k<=16, -18<=l<=18
Reflections collected	20900
Independent reflections	6801 [R(int) = 0.0240]
Completeness to theta = 26.38°	99.9 %
Absorption correction	Empirical
Max. and min. transmission	0.7454 and 0.6362
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6801 / 0 / 418
Goodness-of-fit on F^2	1.046
Final R indices [I>2sigma(I)]	R1 = 0.0279, wR2 = 0.0717
R indices (all data)	R1 = 0.0326, wR2 = 0.0749
Largest diff. peak and hole	1.200 and -0.699 e.$Å^{-3}$

Table 56c-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for neu1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	3490(1)	2719(1)	2023(1)	13(1)
S(1)	3484(1)	4062(1)	3870(1)	17(1)
P(1)	2648(1)	2669(1)	3898(1)	14(1)
F(1)	-1422(2)	5867(1)	597(2)	44(1)
O(1)	3958(2)	-170(1)	1456(1)	25(1)
C(1)	2860(2)	1566(2)	2637(2)	14(1)
S(2)	3883(1)	537(1)	2549(1)	16(1)
F(2)	-2956(3)	4411(2)	-244(2)	93(1)
O(2)	5173(2)	1054(1)	3277(1)	23(1)
C(2)	3455(2)	2633(2)	5056(2)	18(1)
F(3)	-2988(2)	5531(2)	1357(2)	79(1)
O(3)	1284(2)	2510(1)	1801(1)	18(1)
C(3)	2705(3)	2110(2)	5526(2)	28(1)
C(4)	3345(3)	2098(2)	6412(2)	37(1)
C(5)	4711(3)	2598(2)	6833(2)	36(1)
C(6)	5460(3)	3129(2)	6376(2)	29(1)
C(7)	4830(2)	3151(2)	5492(2)	21(1)
C(8)	825(2)	2622(2)	4041(2)	16(1)

C(9)	420(2)	3596(2)	4804(2)	19(1)
C(10)	-941(2)	3584(2)	5018(2)	23(1)
C(11)	-1905(2)	2602(2)	4454(2)	23(1)
C(12)	-1509(2)	1632(2)	3694(2)	25(1)
C(13)	-144(2)	1640(2)	3493(2)	21(1)
C(14)	2913(2)	-334(2)	2953(2)	19(1)
C(15)	3337(3)	-267(2)	3917(2)	25(1)
C(16)	2556(3)	-940(2)	4228(2)	34(1)
C(17)	1371(3)	-1665(2)	3574(2)	37(1)
C(18)	966(3)	-1742(2)	2608(2)	36(1)
C(19)	1733(3)	-1077(2)	2281(2)	27(1)
C(20)	6819(2)	4045(2)	3014(2)	28(1)
C(21)	5692(2)	3368(2)	2086(2)	20(1)
C(22)	4791(2)	3931(2)	1710(2)	20(1)
C(23)	3712(2)	3314(2)	863(2)	19(1)
C(24)	3475(2)	2107(2)	346(2)	18(1)
C(25)	2230(2)	1486(2)	-526(2)	21(1)
C(26)	2659(3)	1387(2)	-1547(2)	24(1)
C(27)	1663(3)	339(2)	-638(2)	32(1)
C(28)	4383(2)	1549(2)	685(2)	19(1)
C(29)	5473(2)	2179(2)	1560(2)	21(1)
C(30)	506(2)	3125(2)	1569(2)	17(1)
C(31)	882(2)	4296(2)	1937(2)	22(1)
C(32)	27(2)	4898(2)	1647(2)	24(1)
C(33)	-1240(2)	4362(2)	975(2)	23(1)
C(34)	-1651(2)	3216(2)	620(2)	22(1)
C(35)	-803(2)	2611(2)	913(2)	21(1)
C(36)	-2140(3)	5021(2)	670(2)	32(1)

Table 56c-3. Bond lengths [Å] and angles [°] for neu1.

Ru(1)-O(3)	2.1091(14)
Ru(1)-C(29)	2.179(2)
Ru(1)-C(24)	2.182(2)
Ru(1)-C(28)	2.185(2)
Ru(1)-C(1)	2.1965(19)
Ru(1)-C(23)	2.201(2)
Ru(1)-C(21)	2.213(2)
Ru(1)-C(22)	2.216(2)
Ru(1)-S(1)	2.4510(5)
S(1)-P(1)	2.0002(7)
P(1)-C(1)	1.797(2)
P(1)-C(8)	1.801(2)
P(1)-C(2)	1.815(2)
F(1)-C(36)	1.337(3)
O(1)-S(2)	1.4408(16)
C(1)-S(2)	1.749(2)
S(2)-O(2)	1.4427(16)
S(2)-C(14)	1.778(2)
F(2)-C(36)	1.320(3)
C(2)-C(7)	1.390(3)
C(2)-C(3)	1.396(3)
F(3)-C(36)	1.332(3)
O(3)-C(30)	1.307(3)
C(3)-C(4)	1.385(4)
C(4)-C(5)	1.374(4)
C(5)-C(6)	1.387(4)
C(6)-C(7)	1.385(3)
C(8)-C(13)	1.389(3)
C(8)-C(9)	1.396(3)
C(9)-C(10)	1.386(3)
C(10)-C(11)	1.388(3)
C(11)-C(12)	1.386(3)
C(12)-C(13)	1.385(3)
C(14)-C(15)	1.383(3)

C(14)-C(19)	1.394(3)
C(15)-C(16)	1.389(3)
C(16)-C(17)	1.382(4)
C(17)-C(18)	1.376(4)
C(18)-C(19)	1.390(3)
C(20)-C(21)	1.499(3)
C(21)-C(29)	1.408(3)
C(21)-C(22)	1.436(3)
C(22)-C(23)	1.398(3)
C(23)-C(24)	1.430(3)
C(24)-C(28)	1.405(3)
C(24)-C(25)	1.521(3)
C(25)-C(27)	1.525(3)
C(25)-C(26)	1.532(3)
C(28)-C(29)	1.429(3)
C(30)-C(31)	1.413(3)
C(30)-C(35)	1.415(3)
C(31)-C(32)	1.382(3)
C(32)-C(33)	1.395(3)
C(33)-C(34)	1.390(3)
C(33)-C(36)	1.481(3)
C(34)-C(35)	1.383(3)

O(3)-Ru(1)-C(29)	152.39(7)
O(3)-Ru(1)-C(24)	90.64(7)
C(29)-Ru(1)-C(24)	68.65(8)
O(3)-Ru(1)-C(28)	114.82(7)
C(29)-Ru(1)-C(28)	38.22(8)
C(24)-Ru(1)-C(28)	37.55(8)
O(3)-Ru(1)-C(1)	75.18(7)
C(29)-Ru(1)-C(1)	99.53(8)
C(24)-Ru(1)-C(1)	121.31(8)
C(28)-Ru(1)-C(1)	98.46(8)
O(3)-Ru(1)-C(23)	95.12(7)
C(29)-Ru(1)-C(23)	79.93(8)
C(24)-Ru(1)-C(23)	38.08(8)

C(28)-Ru(1)-C(23)	67.54(8)
C(1)-Ru(1)-C(23)	158.25(8)
O(3)-Ru(1)-C(21)	160.67(7)
C(29)-Ru(1)-C(21)	37.40(8)
C(24)-Ru(1)-C(21)	81.54(8)
C(28)-Ru(1)-C(21)	68.40(8)
C(1)-Ru(1)-C(21)	123.94(8)
C(23)-Ru(1)-C(21)	67.91(8)
O(3)-Ru(1)-C(22)	122.84(7)
C(29)-Ru(1)-C(22)	67.35(8)
C(24)-Ru(1)-C(22)	68.05(8)
C(28)-Ru(1)-C(22)	79.77(8)
C(1)-Ru(1)-C(22)	161.08(8)
C(23)-Ru(1)-C(22)	36.91(8)
C(21)-Ru(1)-C(22)	37.84(8)
O(3)-Ru(1)-S(1)	88.20(4)
C(29)-Ru(1)-S(1)	117.81(6)
C(24)-Ru(1)-S(1)	158.53(6)
C(28)-Ru(1)-S(1)	155.63(6)
C(1)-Ru(1)-S(1)	79.02(5)
C(23)-Ru(1)-S(1)	120.72(6)
C(21)-Ru(1)-S(1)	92.67(6)
C(22)-Ru(1)-S(1)	94.77(6)
P(1)-S(1)-Ru(1)	82.37(2)
C(1)-P(1)-C(8)	110.27(10)
C(1)-P(1)-C(2)	117.81(9)
C(8)-P(1)-C(2)	102.61(10)
C(1)-P(1)-S(1)	102.48(7)
C(8)-P(1)-S(1)	113.90(7)
C(2)-P(1)-S(1)	110.23(7)
S(2)-C(1)-P(1)	120.30(12)
S(2)-C(1)-Ru(1)	119.78(10)
P(1)-C(1)-Ru(1)	94.75(8)
O(1)-S(2)-O(2)	118.41(10)
O(1)-S(2)-C(1)	107.85(10)
O(2)-S(2)-C(1)	110.24(10)

O(1)-S(2)-C(14)	106.04(10)
O(2)-S(2)-C(14)	107.53(10)
C(1)-S(2)-C(14)	106.05(10)
C(7)-C(2)-C(3)	119.5(2)
C(7)-C(2)-P(1)	119.59(16)
C(3)-C(2)-P(1)	120.86(18)
C(30)-O(3)-Ru(1)	126.20(13)
C(4)-C(3)-C(2)	119.7(2)
C(5)-C(4)-C(3)	120.6(2)
C(4)-C(5)-C(6)	120.1(2)
C(7)-C(6)-C(5)	119.9(2)
C(6)-C(7)-C(2)	120.2(2)
C(13)-C(8)-C(9)	119.62(19)
C(13)-C(8)-P(1)	122.67(16)
C(9)-C(8)-P(1)	117.47(16)
C(10)-C(9)-C(8)	120.2(2)
C(9)-C(10)-C(11)	119.6(2)
C(12)-C(11)-C(10)	120.5(2)
C(13)-C(12)-C(11)	119.9(2)
C(12)-C(13)-C(8)	120.2(2)
C(15)-C(14)-C(19)	121.4(2)
C(15)-C(14)-S(2)	119.89(17)
C(19)-C(14)-S(2)	118.76(17)
C(14)-C(15)-C(16)	119.2(2)
C(17)-C(16)-C(15)	119.8(2)
C(18)-C(17)-C(16)	120.7(2)
C(17)-C(18)-C(19)	120.4(2)
C(18)-C(19)-C(14)	118.5(2)
C(29)-C(21)-C(22)	117.9(2)
C(29)-C(21)-C(20)	122.0(2)
C(22)-C(21)-C(20)	120.1(2)
C(29)-C(21)-Ru(1)	70.02(12)
C(22)-C(21)-Ru(1)	71.20(12)
C(20)-C(21)-Ru(1)	129.81(15)
C(23)-C(22)-C(21)	120.9(2)
C(23)-C(22)-Ru(1)	70.97(12)

C(21)-C(22)-Ru(1)	70.95(12)
C(22)-C(23)-C(24)	120.9(2)
C(22)-C(23)-Ru(1)	72.11(12)
C(24)-C(23)-Ru(1)	70.24(12)
C(28)-C(24)-C(23)	118.6(2)
C(28)-C(24)-C(25)	122.98(19)
C(23)-C(24)-C(25)	118.41(19)
C(28)-C(24)-Ru(1)	71.32(12)
C(23)-C(24)-Ru(1)	71.67(12)
C(25)-C(24)-Ru(1)	127.05(14)
C(24)-C(25)-C(27)	112.76(19)
C(24)-C(25)-C(26)	108.41(18)
C(27)-C(25)-C(26)	112.07(19)
C(24)-C(28)-C(29)	120.4(2)
C(24)-C(28)-Ru(1)	71.13(12)
C(29)-C(28)-Ru(1)	70.69(12)
C(21)-C(29)-C(28)	121.2(2)
C(21)-C(29)-Ru(1)	72.58(12)
C(28)-C(29)-Ru(1)	71.10(12)
O(3)-C(30)-C(31)	124.1(2)
O(3)-C(30)-C(35)	119.26(19)
C(31)-C(30)-C(35)	116.6(2)
C(32)-C(31)-C(30)	121.5(2)
C(31)-C(32)-C(33)	120.7(2)
C(34)-C(33)-C(32)	119.1(2)
C(34)-C(33)-C(36)	121.0(2)
C(32)-C(33)-C(36)	119.9(2)
C(35)-C(34)-C(33)	120.5(2)
C(34)-C(35)-C(30)	121.6(2)
F(2)-C(36)-F(3)	105.9(3)
F(2)-C(36)-F(1)	105.5(2)
F(3)-C(36)-F(1)	103.6(2)
F(2)-C(36)-C(33)	113.6(2)
F(3)-C(36)-C(33)	113.7(2)
F(1)-C(36)-C(33)	113.6(2)

Symmetry transformations used to generate equivalent atoms:

Table 56c-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for neu1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	15(1)	13(1)	15(1)	8(1)	5(1)	2(1)
S(1)	20(1)	13(1)	18(1)	7(1)	6(1)	-1(1)
P(1)	14(1)	13(1)	15(1)	7(1)	5(1)	1(1)
F(1)	39(1)	51(1)	71(1)	50(1)	12(1)	12(1)
O(1)	36(1)	20(1)	24(1)	12(1)	14(1)	12(1)
C(1)	17(1)	12(1)	16(1)	8(1)	5(1)	3(1)
S(2)	17(1)	14(1)	21(1)	10(1)	7(1)	4(1)
F(2)	100(2)	45(1)	115(2)	38(1)	-70(2)	2(1)
O(2)	16(1)	23(1)	33(1)	16(1)	5(1)	3(1)
C(2)	22(1)	18(1)	15(1)	7(1)	5(1)	5(1)
F(3)	77(1)	108(2)	135(2)	103(2)	78(2)	75(1)
O(3)	17(1)	17(1)	23(1)	12(1)	4(1)	3(1)
C(3)	28(1)	34(1)	27(1)	19(1)	6(1)	3(1)
C(4)	48(2)	46(2)	29(1)	27(1)	12(1)	8(1)
C(5)	47(2)	42(2)	22(1)	16(1)	3(1)	17(1)
C(6)	29(1)	26(1)	26(1)	7(1)	-1(1)	10(1)
C(7)	22(1)	19(1)	22(1)	8(1)	5(1)	7(1)
C(8)	15(1)	18(1)	18(1)	10(1)	4(1)	2(1)
C(9)	18(1)	15(1)	22(1)	7(1)	6(1)	1(1)
C(10)	24(1)	20(1)	26(1)	11(1)	12(1)	8(1)
C(11)	17(1)	27(1)	29(1)	16(1)	10(1)	5(1)
C(12)	18(1)	22(1)	29(1)	8(1)	5(1)	-4(1)
C(13)	19(1)	17(1)	22(1)	5(1)	5(1)	0(1)
C(14)	20(1)	14(1)	26(1)	11(1)	7(1)	4(1)
C(15)	27(1)	23(1)	29(1)	17(1)	5(1)	4(1)
C(16)	42(2)	32(1)	40(2)	26(1)	13(1)	9(1)
C(17)	35(1)	30(1)	61(2)	33(1)	19(1)	6(1)
C(18)	27(1)	23(1)	61(2)	25(1)	1(1)	-3(1)
C(19)	28(1)	19(1)	35(1)	15(1)	2(1)	2(1)

C(20)	21(1)	38(1)	25(1)	15(1)	4(1)	-1(1)
C(21)	16(1)	27(1)	21(1)	13(1)	8(1)	1(1)
C(22)	22(1)	19(1)	22(1)	11(1)	9(1)	-1(1)
C(23)	24(1)	19(1)	20(1)	13(1)	10(1)	4(1)
C(24)	20(1)	18(1)	16(1)	9(1)	8(1)	2(1)
C(25)	23(1)	21(1)	16(1)	8(1)	4(1)	1(1)
C(26)	31(1)	25(1)	17(1)	10(1)	5(1)	4(1)
C(27)	39(1)	30(1)	23(1)	12(1)	1(1)	-10(1)
C(28)	23(1)	19(1)	20(1)	10(1)	12(1)	5(1)
C(29)	20(1)	26(1)	23(1)	16(1)	12(1)	8(1)
C(30)	20(1)	18(1)	18(1)	10(1)	8(1)	5(1)
C(31)	20(1)	17(1)	25(1)	9(1)	4(1)	1(1)
C(32)	27(1)	17(1)	32(1)	12(1)	8(1)	5(1)
C(33)	23(1)	26(1)	29(1)	19(1)	10(1)	9(1)
C(34)	19(1)	26(1)	24(1)	14(1)	6(1)	4(1)
C(35)	21(1)	18(1)	25(1)	11(1)	7(1)	2(1)
C(36)	26(1)	36(1)	49(2)	29(1)	10(1)	9(1)

Table 56c-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for neu1.

	x	y	z	U(eq)
H(1)	1902	1161	2257	17
H(3)	1760	1763	5239	34
H(4)	2836	1741	6731	45
H(5)	5143	2581	7437	43
H(6)	6403	3478	6669	35
H(7)	5340	3520	5183	26
H(9)	1078	4270	5178	23
H(10)	-1211	4242	5547	27
H(11)	-2842	2595	4589	27
H(12)	-2174	963	3311	30
H(13)	130	972	2980	25

H(15)	4153	234	4361	30
H(16)	2836	-902	4889	40
H(17)	830	-2116	3794	44
H(18)	158	-2254	2162	43
H(19)	1458	-1127	1615	32
H(20A)	7643	4282	2783	42
H(20B)	7072	3581	3339	42
H(20C)	6477	4713	3525	42
H(22)	4792	4758	2159	24
H(23)	2973	3717	723	23
H(25)	1466	1959	-350	25
H(26A)	3398	915	-1745	36
H(26B)	3008	2141	-1444	36
H(26C)	1846	1043	-2106	36
H(27A)	773	34	-1121	48
H(27B)	1513	426	50	48
H(27C)	2339	-181	-916	48
H(28)	4131	718	420	23
H(29)	5960	1775	1889	25
H(31)	1742	4677	2394	26
H(32)	305	5685	1908	29
H(34)	-2520	2846	173	27
H(35)	-1107	1830	667	25

Röntgenstrukturanalytische Daten für 58a

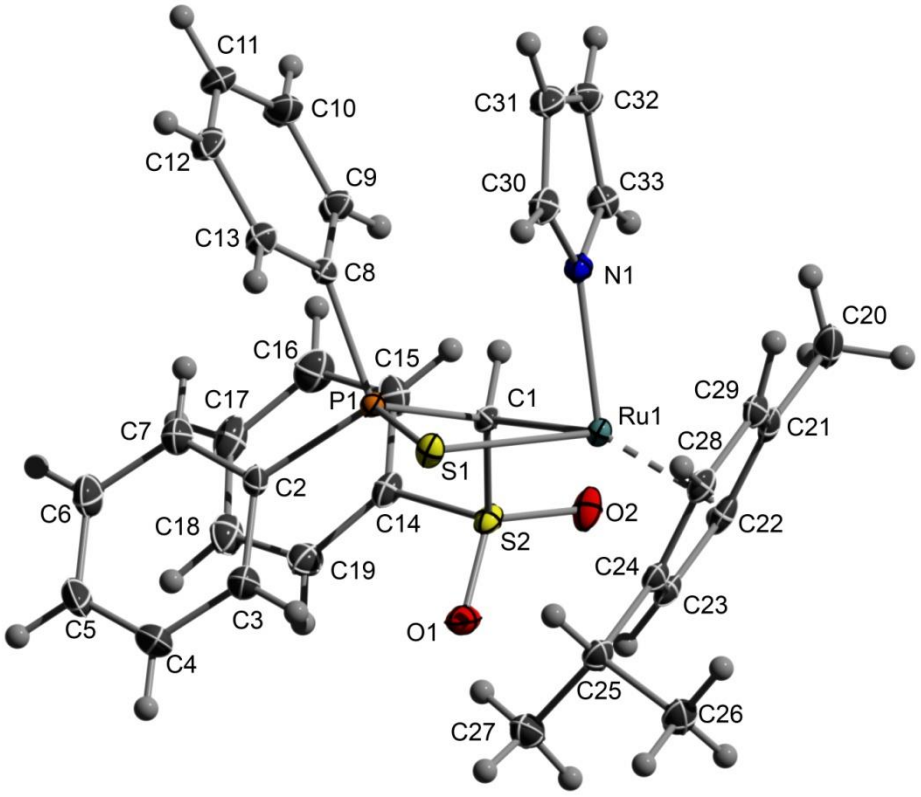

Table 58a-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	$C_{33}H_{34}NO_2PRuS_2$	
Formula weight	672.77	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 12.0085(9) Å	α = 90°.
	b = 19.2428(13) Å	β = 106.817(2)°.
	c = 13.4052(10) Å	γ = 90°.
Volume	2965.2(4) $Å^3$	
Z	4	
Density (calculated)	1.507 Mg/m^3	
Absorption coefficient	0.755 mm^{-1}	
F(000)	1384	

Crystal size	0.11 x 0.10 x 0.10 mm^3
Theta range for data collection	1.91 to 26.38°.
Index ranges	-14<=h<=15, -24<=k<=23, -16<=l<=10
Reflections collected	19368
Independent reflections	6048 [R(int) = 0.0186]
Completeness to theta = 26.38°	99.7 %
Absorption correction	Empirical
Max. and min. transmission	0.9276 and 0.9229
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6048 / 0 / 364
Goodness-of-fit on F^2	1.009
Final R indices [I>2sigma(I)]	R1 = 0.0205, wR2 = 0.0528
R indices (all data)	R1 = 0.0236, wR2 = 0.0548
Largest diff. peak and hole	0.415 and -0.329 e.$Å^{-3}$

Table 58a-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	9687(1)	1788(1)	3832(1)	11(1)
S(1)	8648(1)	2014(1)	2002(1)	15(1)
P(1)	10265(1)	2117(1)	1891(1)	11(1)
O(1)	11025(1)	445(1)	2556(1)	20(1)
N(1)	10166(1)	2842(1)	4005(1)	13(1)
C(1)	11117(1)	1763(1)	3117(1)	12(1)
S(2)	11824(1)	967(1)	3125(1)	14(1)
O(2)	12463(1)	829(1)	4202(1)	21(1)
C(2)	10399(2)	1708(1)	707(1)	15(1)
C(3)	9694(2)	1145(1)	284(1)	24(1)
C(4)	9788(2)	836(1)	-625(2)	31(1)
C(5)	10582(2)	1079(1)	-1103(2)	30(1)
C(6)	11296(2)	1637(1)	-682(2)	28(1)
C(7)	11199(2)	1955(1)	219(1)	21(1)
C(8)	10696(1)	3002(1)	1748(1)	13(1)
C(9)	11818(2)	3244(1)	2201(1)	19(1)

C(10)	12139(2)	3896(1)	1926(1)	25(1)
C(11)	11345(2)	4297(1)	1201(1)	24(1)
C(12)	10218(2)	4062(1)	761(1)	21(1)
C(13)	9889(2)	3417(1)	1035(1)	17(1)
C(14)	12893(1)	1101(1)	2465(1)	16(1)
C(15)	13771(2)	1587(1)	2862(1)	20(1)
C(16)	14592(2)	1702(1)	2337(2)	26(1)
C(17)	14548(2)	1332(1)	1435(2)	25(1)
C(18)	13693(2)	837(1)	1067(2)	24(1)
C(19)	12855(2)	720(1)	1579(1)	22(1)
C(20)	11093(2)	1899(1)	6410(1)	26(1)
C(21)	10156(2)	1583(1)	5532(1)	18(1)
C(22)	10378(2)	988(1)	5010(1)	18(1)
C(23)	9498(1)	675(1)	4179(1)	16(1)
C(24)	8377(1)	964(1)	3847(1)	16(1)
C(25)	7405(2)	655(1)	2973(1)	18(1)
C(26)	6533(2)	297(1)	3450(1)	23(1)
C(27)	7826(2)	150(1)	2285(2)	26(1)
C(28)	8141(1)	1574(1)	4367(1)	16(1)
C(29)	9014(2)	1879(1)	5185(1)	18(1)
C(30)	9477(2)	3407(1)	3635(1)	18(1)
C(31)	10096(2)	4013(1)	3965(1)	21(1)
C(32)	11217(2)	3812(1)	4563(1)	20(1)
C(33)	11230(2)	3092(1)	4574(1)	16(1)

Table 58a-3. Bond lengths [Å] and angles [°] for sad.

Ru(1)-N(1)	2.1023(13)
Ru(1)-C(22)	2.1890(16)
Ru(1)-C(29)	2.1949(16)
Ru(1)-C(1)	2.1962(16)
Ru(1)-C(28)	2.2129(16)
Ru(1)-C(23)	2.2179(16)
Ru(1)-C(21)	2.2190(16)
Ru(1)-C(24)	2.2380(16)
Ru(1)-S(1)	2.4482(4)

S(1)-P(1)	1.9989(6)
P(1)-C(1)	1.7998(16)
P(1)-C(8)	1.8056(16)
P(1)-C(2)	1.8201(17)
O(1)-S(2)	1.4445(13)
N(1)-C(30)	1.370(2)
N(1)-C(33)	1.371(2)
C(1)-S(2)	1.7503(15)
S(2)-O(2)	1.4495(13)
S(2)-C(14)	1.7762(16)
C(2)-C(3)	1.390(2)
C(2)-C(7)	1.393(2)
C(3)-C(4)	1.390(3)
C(4)-C(5)	1.375(3)
C(5)-C(6)	1.388(3)
C(6)-C(7)	1.389(3)
C(8)-C(9)	1.389(2)
C(8)-C(13)	1.398(2)
C(9)-C(10)	1.392(2)
C(10)-C(11)	1.383(3)
C(11)-C(12)	1.387(3)
C(12)-C(13)	1.384(2)
C(14)-C(19)	1.385(2)
C(14)-C(15)	1.394(2)
C(15)-C(16)	1.386(3)
C(16)-C(17)	1.391(3)
C(17)-C(18)	1.381(3)
C(18)-C(19)	1.391(2)
C(20)-C(21)	1.502(2)
C(21)-C(22)	1.408(3)
C(21)-C(29)	1.433(2)
C(22)-C(23)	1.428(2)
C(23)-C(24)	1.404(2)
C(24)-C(28)	1.436(2)
C(24)-C(25)	1.515(2)
C(25)-C(27)	1.523(2)

C(25)-C(26)	1.539(2)
C(28)-C(29)	1.406(2)
C(30)-C(31)	1.385(2)
C(31)-C(32)	1.407(3)
C(32)-C(33)	1.386(2)

N(1)-Ru(1)-C(22)	124.34(6)
N(1)-Ru(1)-C(29)	89.25(6)
C(22)-Ru(1)-C(29)	67.30(6)
N(1)-Ru(1)-C(1)	81.11(5)
C(22)-Ru(1)-C(1)	96.78(6)
C(29)-Ru(1)-C(1)	152.09(6)
N(1)-Ru(1)-C(28)	111.87(6)
C(22)-Ru(1)-C(28)	79.30(6)
C(29)-Ru(1)-C(28)	37.21(6)
C(1)-Ru(1)-C(28)	166.46(6)
N(1)-Ru(1)-C(23)	161.81(6)
C(22)-Ru(1)-C(23)	37.82(6)
C(29)-Ru(1)-C(23)	79.59(6)
C(1)-Ru(1)-C(23)	102.17(6)
C(28)-Ru(1)-C(23)	66.80(6)
N(1)-Ru(1)-C(21)	94.48(6)
C(22)-Ru(1)-C(21)	37.24(7)
C(29)-Ru(1)-C(21)	37.88(6)
C(1)-Ru(1)-C(21)	116.52(6)
C(28)-Ru(1)-C(21)	67.78(6)
C(23)-Ru(1)-C(21)	67.91(6)
N(1)-Ru(1)-C(24)	148.61(6)
C(22)-Ru(1)-C(24)	67.43(6)
C(29)-Ru(1)-C(24)	67.78(6)
C(1)-Ru(1)-C(24)	128.92(6)
C(28)-Ru(1)-C(24)	37.63(6)
C(23)-Ru(1)-C(24)	36.73(6)
C(21)-Ru(1)-C(24)	80.53(6)
N(1)-Ru(1)-S(1)	89.05(4)
C(22)-Ru(1)-S(1)	145.50(5)

C(29)-Ru(1)-S(1)	127.67(5)
C(1)-Ru(1)-S(1)	78.58(4)
C(28)-Ru(1)-S(1)	97.23(5)
C(23)-Ru(1)-S(1)	109.14(5)
C(21)-Ru(1)-S(1)	164.85(5)
C(24)-Ru(1)-S(1)	88.78(4)
P(1)-S(1)-Ru(1)	82.441(18)
C(1)-P(1)-C(8)	110.40(7)
C(1)-P(1)-C(2)	117.52(7)
C(8)-P(1)-C(2)	102.44(7)
C(1)-P(1)-S(1)	101.65(5)
C(8)-P(1)-S(1)	114.58(6)
C(2)-P(1)-S(1)	110.79(6)
C(30)-N(1)-C(33)	106.92(14)
C(30)-N(1)-Ru(1)	127.44(12)
C(33)-N(1)-Ru(1)	125.54(11)
S(2)-C(1)-P(1)	118.92(9)
S(2)-C(1)-Ru(1)	117.11(8)
P(1)-C(1)-Ru(1)	94.64(7)
O(1)-S(2)-O(2)	118.56(7)
O(1)-S(2)-C(1)	110.96(8)
O(2)-S(2)-C(1)	106.41(7)
O(1)-S(2)-C(14)	107.67(8)
O(2)-S(2)-C(14)	105.78(8)
C(1)-S(2)-C(14)	106.81(8)
C(3)-C(2)-C(7)	119.78(16)
C(3)-C(2)-P(1)	119.67(13)
C(7)-C(2)-P(1)	120.55(13)
C(4)-C(3)-C(2)	119.76(17)
C(5)-C(4)-C(3)	120.40(18)
C(4)-C(5)-C(6)	120.23(17)
C(5)-C(6)-C(7)	119.86(18)
C(6)-C(7)-C(2)	119.96(17)
C(9)-C(8)-C(13)	120.00(15)
C(9)-C(8)-P(1)	122.80(13)
C(13)-C(8)-P(1)	116.62(12)

C(8)-C(9)-C(10)	119.61(16)
C(11)-C(10)-C(9)	120.15(17)
C(10)-C(11)-C(12)	120.35(16)
C(13)-C(12)-C(11)	119.90(16)
C(12)-C(13)-C(8)	119.96(16)
C(19)-C(14)-C(15)	121.06(16)
C(19)-C(14)-S(2)	120.08(13)
C(15)-C(14)-S(2)	118.85(13)
C(16)-C(15)-C(14)	118.95(17)
C(15)-C(16)-C(17)	120.37(18)
C(18)-C(17)-C(16)	120.04(17)
C(17)-C(18)-C(19)	120.29(17)
C(14)-C(19)-C(18)	119.25(17)
C(22)-C(21)-C(29)	117.55(16)
C(22)-C(21)-C(20)	120.81(16)
C(29)-C(21)-C(20)	121.63(16)
C(22)-C(21)-Ru(1)	70.22(9)
C(29)-C(21)-Ru(1)	70.15(9)
C(20)-C(21)-Ru(1)	130.00(12)
C(21)-C(22)-C(23)	121.82(16)
C(21)-C(22)-Ru(1)	72.54(10)
C(23)-C(22)-Ru(1)	72.19(9)
C(24)-C(23)-C(22)	120.38(15)
C(24)-C(23)-Ru(1)	72.41(9)
C(22)-C(23)-Ru(1)	70.00(9)
C(23)-C(24)-C(28)	118.37(15)
C(23)-C(24)-C(25)	122.92(15)
C(28)-C(24)-C(25)	118.71(15)
C(23)-C(24)-Ru(1)	70.86(9)
C(28)-C(24)-Ru(1)	70.24(9)
C(25)-C(24)-Ru(1)	131.12(11)
C(24)-C(25)-C(27)	113.70(15)
C(24)-C(25)-C(26)	108.63(14)
C(27)-C(25)-C(26)	110.51(14)
C(29)-C(28)-C(24)	120.85(16)
C(29)-C(28)-Ru(1)	70.70(9)

C(24)-C(28)-Ru(1)	72.13(9)
C(28)-C(29)-C(21)	121.00(16)
C(28)-C(29)-Ru(1)	72.09(9)
C(21)-C(29)-Ru(1)	71.97(9)
N(1)-C(30)-C(31)	109.84(15)
C(30)-C(31)-C(32)	106.78(15)
C(33)-C(32)-C(31)	106.60(15)
N(1)-C(33)-C(32)	109.86(15)

Symmetry transformations used to generate equivalent atoms:

Table 58a-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	10(1)	12(1)	10(1)	2(1)	3(1)	0(1)
S(1)	10(1)	19(1)	13(1)	3(1)	2(1)	-1(1)
P(1)	11(1)	11(1)	10(1)	2(1)	3(1)	-1(1)
O(1)	26(1)	14(1)	26(1)	-2(1)	14(1)	-2(1)
N(1)	14(1)	13(1)	13(1)	1(1)	5(1)	1(1)
C(1)	12(1)	11(1)	12(1)	2(1)	3(1)	1(1)
S(2)	16(1)	12(1)	16(1)	3(1)	7(1)	3(1)
O(2)	21(1)	24(1)	18(1)	8(1)	7(1)	10(1)
C(2)	20(1)	15(1)	10(1)	2(1)	4(1)	1(1)
C(3)	32(1)	21(1)	18(1)	-1(1)	9(1)	-7(1)
C(4)	48(1)	22(1)	21(1)	-6(1)	8(1)	-9(1)
C(5)	50(1)	25(1)	16(1)	-3(1)	13(1)	4(1)
C(6)	37(1)	30(1)	21(1)	1(1)	17(1)	1(1)
C(7)	26(1)	21(1)	18(1)	-1(1)	9(1)	-3(1)
C(8)	17(1)	11(1)	13(1)	0(1)	6(1)	0(1)
C(9)	19(1)	18(1)	18(1)	4(1)	2(1)	-2(1)
C(10)	26(1)	22(1)	23(1)	0(1)	3(1)	-11(1)
C(11)	36(1)	14(1)	22(1)	2(1)	9(1)	-7(1)
C(12)	27(1)	15(1)	21(1)	5(1)	8(1)	4(1)
C(13)	16(1)	17(1)	18(1)	1(1)	4(1)	0(1)

C(14)	15(1)	16(1)	19(1)	6(1)	7(1)	6(1)
C(15)	18(1)	25(1)	19(1)	0(1)	6(1)	3(1)
C(16)	19(1)	31(1)	30(1)	2(1)	9(1)	-2(1)
C(17)	22(1)	31(1)	28(1)	9(1)	14(1)	8(1)
C(18)	30(1)	24(1)	23(1)	2(1)	14(1)	7(1)
C(19)	25(1)	18(1)	24(1)	0(1)	11(1)	2(1)
C(20)	26(1)	35(1)	14(1)	4(1)	2(1)	-9(1)
C(21)	20(1)	23(1)	12(1)	7(1)	5(1)	-6(1)
C(22)	16(1)	20(1)	18(1)	10(1)	7(1)	0(1)
C(23)	19(1)	15(1)	17(1)	6(1)	9(1)	0(1)
C(24)	17(1)	16(1)	15(1)	3(1)	8(1)	-3(1)
C(25)	18(1)	19(1)	17(1)	1(1)	6(1)	-6(1)
C(26)	21(1)	27(1)	22(1)	0(1)	7(1)	-10(1)
C(27)	31(1)	26(1)	23(1)	-6(1)	12(1)	-10(1)
C(28)	14(1)	19(1)	18(1)	2(1)	9(1)	-1(1)
C(29)	20(1)	21(1)	15(1)	0(1)	10(1)	-4(1)
C(30)	17(1)	18(1)	18(1)	3(1)	6(1)	4(1)
C(31)	28(1)	14(1)	23(1)	2(1)	10(1)	2(1)
C(32)	21(1)	18(1)	21(1)	-2(1)	8(1)	-5(1)
C(33)	14(1)	18(1)	16(1)	-1(1)	4(1)	0(1)

Table 58a-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
H(1)	11709	2117	3472	14
H(3)	9149	973	615	28
H(4)	9301	454	-918	37
H(5)	10643	863	-1722	36
H(6)	11849	1801	-1010	33
H(7)	11679	2342	503	25
H(9)	12364	2966	2695	23
H(10)	12904	4065	2238	30
H(11)	11574	4737	1004	29

H(12)	9673	4343	271	25
H(13)	9115	3257	740	20
H(15)	13806	1834	3484	25
H(16)	15189	2036	2593	31
H(17)	15105	1419	1071	30
H(18)	13678	576	462	29
H(19)	12263	383	1324	26
H(20A)	11855	1736	6378	39
H(20B)	10978	1761	7077	39
H(20C)	11058	2407	6349	39
H(22)	11203	835	5134	21
H(23)	9724	313	3739	20
H(25)	6992	1045	2524	22
H(26A)	5882	112	2891	35
H(26B)	6241	634	3861	35
H(26C)	6922	-85	3902	35
H(27A)	7177	28	1677	38
H(27B)	8126	-272	2683	38
H(27C)	8446	368	2054	38
H(28)	7409	1840	4049	19
H(29)	8878	2352	5436	21
H(30)	8691	3386	3214	21
H(31)	9818	4474	3817	25
H(32)	11843	4112	4895	24
H(33)	11878	2813	4923	19

Röntgenstrukturanalytische Daten für 59a

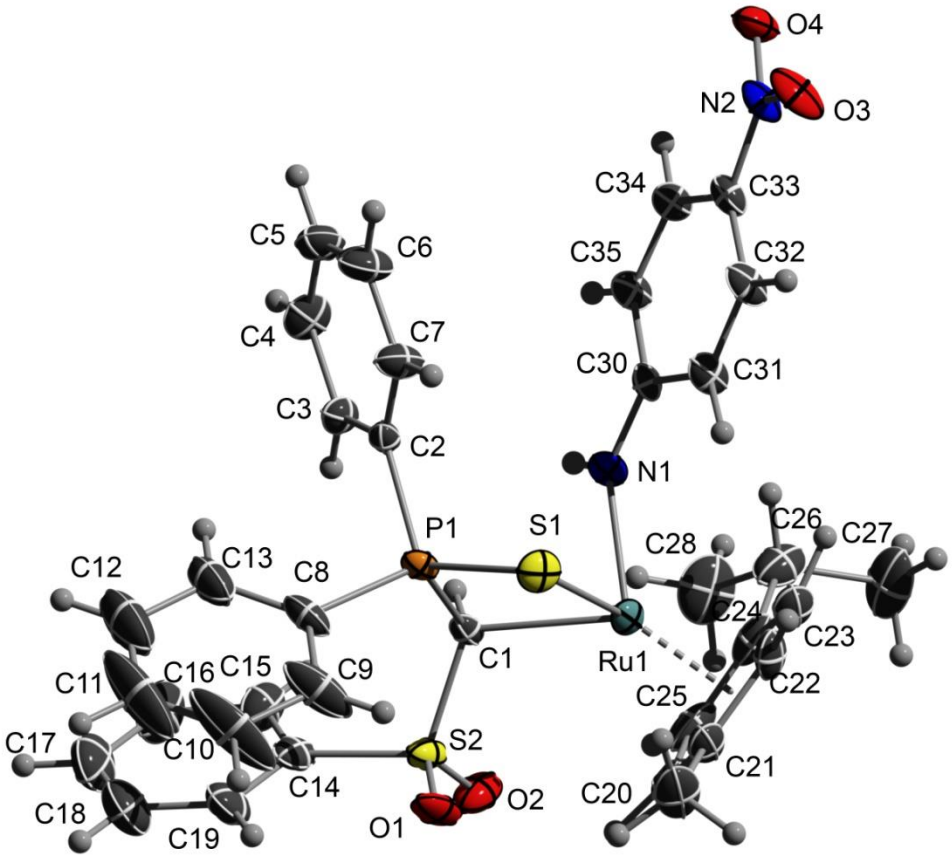

Table 59a-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	$C_{35}H_{35}N_2O_4PRuS_2$	
Formula weight	743.81	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 10.696(2) Å	α = 90°.
	b = 15.043(3) Å	β = 91.077(7)°.
	c = 20.901(4) Å	γ = 90°.
Volume	3362.6(12) $Å^3$	
Z	4	
Density (calculated)	1.469 Mg/m^3	

Absorption coefficient	0.679 mm^{-1}
F(000)	1528
Crystal size	0.160 x 0.113 x 0.023 mm^3
Theta range for data collection	1.67 to 25.00°.
Index ranges	-12<=h<=12, -17<=k<=17, -24<=l<=24
Reflections collected	38210
Independent reflections	5907 [R(int) = 0.0793]
Completeness to theta = 25.00°	100.0 %
Absorption correction	Empirical
Max. and min. transmission	0.7454 and 0.6161
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5907 / 0 / 441
Goodness-of-fit on F^2	1.063
Final R indices [I>2sigma(I)]	R1 = 0.0591, wR2 = 0.1293
R indices (all data)	R1 = 0.0820, wR2 = 0.1402
Largest diff. peak and hole	1.321 and -1.108 e.$Å^{-3}$

Table 59a-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	8059(1)	3702(1)	2086(1)	22(1)
S(1)	8456(1)	4568(1)	1116(1)	28(1)
S(2)	7098(1)	2031(1)	1157(1)	26(1)
P(1)	9050(1)	3390(1)	801(1)	19(1)
O(1)	6195(4)	2623(3)	864(2)	37(1)
O(2)	6717(4)	1521(3)	1704(2)	38(1)
O(3)	13442(4)	6883(3)	2739(2)	39(1)
O(4)	14709(4)	5826(3)	3041(2)	37(1)
N(1)	9981(4)	3605(3)	2238(2)	21(1)
N(2)	13649(5)	6074(3)	2841(2)	26(1)
C(1)	8429(5)	2637(4)	1381(3)	19(1)
C(2)	10734(5)	3301(4)	798(3)	20(1)
C(3)	11321(5)	2483(4)	885(3)	26(1)

C(4)	12624(6)	2430(4)	839(3)	36(2)
C(5)	13299(6)	3173(5)	711(3)	39(2)
C(6)	12723(6)	3986(5)	633(4)	43(2)
C(7)	11429(5)	4053(4)	683(3)	32(2)
C(8)	8594(6)	3216(4)	-27(3)	31(2)
C(9)	7519(8)	3621(5)	-262(4)	58(2)
C(10)	7154(12)	3484(6)	-891(5)	92(4)
C(11)	7863(14)	2950(7)	-1271(4)	97(5)
C(12)	8924(10)	2557(7)	-1049(4)	73(3)
C(13)	9308(8)	2685(5)	-427(3)	49(2)
C(14)	7505(5)	1248(4)	554(3)	30(1)
C(15)	8354(6)	579(4)	707(4)	39(2)
C(16)	8600(8)	-45(5)	238(4)	53(2)
C(17)	8025(8)	5(5)	-359(4)	55(2)
C(18)	7198(8)	674(5)	-501(4)	56(2)
C(19)	6930(6)	1301(5)	-40(3)	44(2)
C(20)	5439(7)	4791(5)	1657(3)	47(2)
C(21)	6182(6)	4318(4)	2170(3)	32(2)
C(22)	7067(6)	4803(4)	2562(3)	31(2)
C(23)	7802(6)	4354(4)	3019(3)	31(2)
C(24)	7726(6)	3409(5)	3104(3)	38(2)
C(25)	6841(6)	2955(5)	2722(4)	43(2)
C(26)	6059(6)	3401(4)	2264(4)	39(2)
C(27A)	8340(30)	2740(20)	3536(13)	37(7)
C(28A)	7504(19)	2271(15)	3982(11)	58(5)
C(29A)	9330(20)	3286(17)	3899(12)	58(5)
C(27B)	8750(18)	3040(11)	3592(11)	41(5)
C(28B)	8862(13)	2024(8)	3488(6)	55(4)
C(29B)	8347(13)	3236(10)	4280(5)	61(5)
C(30)	10841(5)	4202(3)	2395(3)	20(1)
C(31)	10576(6)	5136(4)	2427(3)	28(1)
C(32)	11471(6)	5729(4)	2582(3)	27(1)
C(33)	12695(6)	5456(4)	2728(3)	24(1)
C(34)	12979(5)	4542(4)	2727(3)	23(1)
C(35)	12095(5)	3942(3)	2558(3)	23(1)

Table 59a-3. Bond lengths [Å] and angles [°] for sad.

Ru(1)-N(1)	2.079(5)
Ru(1)-C(25)	2.190(7)
Ru(1)-C(23)	2.206(6)
Ru(1)-C(24)	2.209(6)
Ru(1)-C(22)	2.214(6)
Ru(1)-C(1)	2.218(5)
Ru(1)-C(21)	2.221(6)
Ru(1)-C(26)	2.225(6)
Ru(1)-S(1)	2.4538(17)
S(1)-P(1)	1.998(2)
S(2)-O(1)	1.441(4)
S(2)-O(2)	1.442(5)
S(2)-C(1)	1.747(5)
S(2)-C(14)	1.784(6)
P(1)-C(1)	1.795(6)
P(1)-C(2)	1.807(5)
P(1)-C(8)	1.808(6)
O(3)-N(2)	1.254(6)
O(4)-N(2)	1.257(6)
N(1)-C(30)	1.323(7)
N(2)-C(33)	1.398(7)
C(2)-C(7)	1.378(8)
C(2)-C(3)	1.391(8)
C(3)-C(4)	1.401(8)
C(4)-C(5)	1.361(9)
C(5)-C(6)	1.377(9)
C(6)-C(7)	1.393(9)
C(8)-C(9)	1.384(10)
C(8)-C(13)	1.393(10)
C(9)-C(10)	1.380(12)
C(10)-C(11)	1.369(16)
C(11)-C(12)	1.354(15)
C(12)-C(13)	1.371(10)
C(14)-C(19)	1.378(9)

C(14)-C(15)	1.389(9)
C(15)-C(16)	1.386(10)
C(16)-C(17)	1.384(11)
C(17)-C(18)	1.369(11)
C(18)-C(19)	1.383(10)
C(20)-C(21)	1.501(9)
C(21)-C(26)	1.400(9)
C(21)-C(22)	1.439(9)
C(22)-C(23)	1.400(8)
C(23)-C(24)	1.434(9)
C(24)-C(25)	1.405(10)
C(24)-C(27A)	1.49(2)
C(24)-C(27B)	1.58(2)
C(25)-C(26)	1.427(10)
C(27A)-C(28A)	1.48(3)
C(27A)-C(29A)	1.53(3)
C(27B)-C(29B)	1.54(2)
C(27B)-C(28B)	1.549(19)
C(30)-C(35)	1.432(8)
C(30)-C(31)	1.434(7)
C(31)-C(32)	1.344(8)
C(32)-C(33)	1.401(8)
C(33)-C(34)	1.408(8)
C(34)-C(35)	1.350(8)

N(1)-Ru(1)-C(25)	118.0(2)
N(1)-Ru(1)-C(23)	92.0(2)
C(25)-Ru(1)-C(23)	66.8(3)
N(1)-Ru(1)-C(24)	90.9(2)
C(25)-Ru(1)-C(24)	37.3(3)
C(23)-Ru(1)-C(24)	37.9(2)
N(1)-Ru(1)-C(22)	117.7(2)
C(25)-Ru(1)-C(22)	79.4(3)
C(23)-Ru(1)-C(22)	36.9(2)
C(24)-Ru(1)-C(22)	68.2(2)
N(1)-Ru(1)-C(1)	82.12(19)

C(25)-Ru(1)-C(1)	98.5(2)
C(23)-Ru(1)-C(1)	159.4(2)
C(24)-Ru(1)-C(1)	122.0(2)
C(22)-Ru(1)-C(1)	158.8(2)
N(1)-Ru(1)-C(21)	155.4(2)
C(25)-Ru(1)-C(21)	67.5(3)
C(23)-Ru(1)-C(21)	67.4(2)
C(24)-Ru(1)-C(21)	81.1(2)
C(22)-Ru(1)-C(21)	37.9(2)
C(1)-Ru(1)-C(21)	121.8(2)
N(1)-Ru(1)-C(26)	155.6(2)
C(25)-Ru(1)-C(26)	37.7(3)
C(23)-Ru(1)-C(26)	78.8(2)
C(24)-Ru(1)-C(26)	68.0(3)
C(22)-Ru(1)-C(26)	66.8(2)
C(1)-Ru(1)-C(26)	98.5(2)
C(21)-Ru(1)-C(26)	36.7(2)
N(1)-Ru(1)-S(1)	88.75(14)
C(25)-Ru(1)-S(1)	152.7(2)
C(23)-Ru(1)-S(1)	121.42(17)
C(24)-Ru(1)-S(1)	159.31(19)
C(22)-Ru(1)-S(1)	93.78(17)
C(1)-Ru(1)-S(1)	78.40(15)
C(21)-Ru(1)-S(1)	90.81(18)
C(26)-Ru(1)-S(1)	115.3(2)
P(1)-S(1)-Ru(1)	82.05(7)
O(1)-S(2)-O(2)	118.0(3)
O(1)-S(2)-C(1)	109.1(3)
O(2)-S(2)-C(1)	107.8(3)
O(1)-S(2)-C(14)	106.2(3)
O(2)-S(2)-C(14)	106.5(3)
C(1)-S(2)-C(14)	109.0(3)
C(1)-P(1)-C(2)	109.7(3)
C(1)-P(1)-C(8)	117.3(3)
C(2)-P(1)-C(8)	103.7(3)
C(1)-P(1)-S(1)	102.35(19)

C(2)-P(1)-S(1)	112.97(19)
C(8)-P(1)-S(1)	111.2(2)
C(30)-N(1)-Ru(1)	132.1(4)
O(3)-N(2)-O(4)	120.1(5)
O(3)-N(2)-C(33)	119.3(5)
O(4)-N(2)-C(33)	120.6(5)
S(2)-C(1)-P(1)	117.3(3)
S(2)-C(1)-Ru(1)	113.6(3)
P(1)-C(1)-Ru(1)	93.7(2)
C(7)-C(2)-C(3)	120.4(5)
C(7)-C(2)-P(1)	118.7(4)
C(3)-C(2)-P(1)	120.8(4)
C(2)-C(3)-C(4)	119.3(6)
C(5)-C(4)-C(3)	119.9(6)
C(4)-C(5)-C(6)	121.0(6)
C(5)-C(6)-C(7)	119.9(6)
C(2)-C(7)-C(6)	119.6(6)
C(9)-C(8)-C(13)	120.0(6)
C(9)-C(8)-P(1)	118.9(6)
C(13)-C(8)-P(1)	121.1(5)
C(10)-C(9)-C(8)	119.4(9)
C(11)-C(10)-C(9)	119.4(9)
C(12)-C(11)-C(10)	121.8(8)
C(11)-C(12)-C(13)	119.9(10)
C(12)-C(13)-C(8)	119.5(9)
C(19)-C(14)-C(15)	121.9(6)
C(19)-C(14)-S(2)	119.2(5)
C(15)-C(14)-S(2)	118.9(5)
C(16)-C(15)-C(14)	117.4(7)
C(17)-C(16)-C(15)	121.0(7)
C(18)-C(17)-C(16)	120.6(7)
C(17)-C(18)-C(19)	119.5(8)
C(14)-C(19)-C(18)	119.6(7)
C(26)-C(21)-C(22)	118.8(6)
C(26)-C(21)-C(20)	121.1(6)
C(22)-C(21)-C(20)	120.0(6)

C(26)-C(21)-Ru(1)	71.8(4)
C(22)-C(21)-Ru(1)	70.8(3)
C(20)-C(21)-Ru(1)	127.5(5)
C(23)-C(22)-C(21)	119.9(6)
C(23)-C(22)-Ru(1)	71.2(3)
C(21)-C(22)-Ru(1)	71.4(3)
C(22)-C(23)-C(24)	122.0(6)
C(22)-C(23)-Ru(1)	71.8(4)
C(24)-C(23)-Ru(1)	71.2(4)
C(25)-C(24)-C(23)	116.8(6)
C(25)-C(24)-C(27A)	107.5(13)
C(23)-C(24)-C(27A)	135.6(13)
C(25)-C(24)-C(27B)	130.2(8)
C(23)-C(24)-C(27B)	112.8(8)
C(27A)-C(24)-C(27B)	23.6(10)
C(25)-C(24)-Ru(1)	70.6(4)
C(23)-C(24)-Ru(1)	70.9(4)
C(27A)-C(24)-Ru(1)	129.8(12)
C(27B)-C(24)-Ru(1)	124.6(8)
C(24)-C(25)-C(26)	122.2(6)
C(24)-C(25)-Ru(1)	72.1(4)
C(26)-C(25)-Ru(1)	72.5(4)
C(21)-C(26)-C(25)	120.2(6)
C(21)-C(26)-Ru(1)	71.5(4)
C(25)-C(26)-Ru(1)	69.8(4)
C(28A)-C(27A)-C(24)	116(2)
C(28A)-C(27A)-C(29A)	111(2)
C(24)-C(27A)-C(29A)	104(2)
C(29B)-C(27B)-C(28B)	110.1(14)
C(29B)-C(27B)-C(24)	109.5(13)
C(28B)-C(27B)-C(24)	108.1(13)
N(1)-C(30)-C(35)	121.1(5)
N(1)-C(30)-C(31)	122.6(5)
C(35)-C(30)-C(31)	116.2(5)
C(32)-C(31)-C(30)	121.4(5)
C(31)-C(32)-C(33)	121.0(5)

N(2)-C(33)-C(32)	121.2(5)
N(2)-C(33)-C(34)	119.5(5)
C(32)-C(33)-C(34)	119.2(5)
C(35)-C(34)-C(33)	120.2(5)
C(34)-C(35)-C(30)	121.9(5)

Symmetry transformations used to generate equivalent atoms:

Table 59a-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	20(1)	18(1)	28(1)	-4(1)	-2(1)	6(1)
S(1)	28(1)	17(1)	39(1)	2(1)	-1(1)	7(1)
S(2)	18(1)	20(1)	42(1)	-7(1)	0(1)	0(1)
P(1)	18(1)	16(1)	23(1)	1(1)	-6(1)	2(1)
O(1)	18(2)	34(2)	59(3)	-13(2)	-14(2)	8(2)
O(2)	35(3)	25(2)	55(3)	-2(2)	17(2)	-6(2)
O(3)	57(3)	14(2)	45(3)	3(2)	-19(2)	-9(2)
O(4)	24(2)	35(2)	50(3)	-10(2)	-11(2)	-1(2)
N(1)	22(2)	18(3)	23(3)	2(2)	-6(2)	3(2)
N(2)	37(3)	14(2)	29(3)	-1(2)	-7(2)	-5(2)
C(1)	18(3)	17(3)	22(3)	-3(2)	-6(2)	4(2)
C(2)	18(3)	22(3)	19(3)	-4(2)	-3(2)	4(2)
C(3)	23(3)	21(3)	34(4)	-3(3)	0(3)	4(2)
C(4)	31(3)	29(3)	49(4)	-1(3)	-3(3)	16(3)
C(5)	21(3)	43(4)	53(4)	-9(3)	-6(3)	4(3)
C(6)	29(4)	35(4)	64(5)	-3(3)	-6(3)	-9(3)
C(7)	22(3)	24(3)	50(4)	0(3)	-3(3)	0(3)
C(8)	41(4)	28(3)	24(3)	4(3)	-14(3)	-12(3)
C(9)	74(6)	35(4)	62(5)	9(4)	-46(5)	-7(4)
C(10)	146(10)	46(5)	81(7)	18(5)	-91(8)	-13(6)
C(11)	184(13)	68(7)	36(5)	13(5)	-50(7)	-50(8)
C(12)	104(8)	85(7)	28(4)	-4(4)	-5(5)	-44(6)

C(13)	60(5)	61(5)	25(4)	-4(3)	-3(4)	-26(4)
C(14)	25(3)	20(3)	46(4)	-8(3)	3(3)	-7(3)
C(15)	41(4)	25(3)	51(4)	-1(3)	10(3)	3(3)
C(16)	61(5)	29(4)	68(6)	-6(4)	10(4)	17(4)
C(17)	68(6)	38(4)	58(5)	-20(4)	7(4)	-6(4)
C(18)	64(5)	50(5)	54(5)	-19(4)	-6(4)	-10(4)
C(19)	40(4)	37(4)	53(5)	-18(4)	-9(3)	-6(3)
C(20)	37(4)	57(5)	46(4)	-14(4)	-14(3)	29(4)
C(21)	24(3)	38(4)	36(4)	-11(3)	-2(3)	12(3)
C(22)	37(4)	29(3)	27(3)	-6(3)	2(3)	15(3)
C(23)	28(3)	34(4)	32(4)	-2(3)	-2(3)	9(3)
C(24)	38(4)	48(4)	28(4)	5(3)	14(3)	14(3)
C(25)	39(4)	33(4)	57(5)	2(3)	24(4)	9(3)
C(26)	26(3)	36(4)	56(5)	-18(3)	19(3)	4(3)
C(27A)	39(16)	50(20)	22(11)	26(13)	1(11)	16(13)
C(28A)	47(10)	61(11)	66(12)	18(9)	5(8)	2(8)
C(29A)	47(10)	61(11)	66(12)	18(9)	5(8)	2(8)
C(27B)	37(11)	25(9)	61(11)	2(7)	14(9)	-4(6)
C(28B)	73(9)	32(7)	61(9)	13(6)	3(7)	25(7)
C(29B)	69(10)	88(11)	25(7)	10(7)	-3(6)	34(8)
C(30)	25(3)	15(3)	18(3)	-1(2)	-2(2)	1(2)
C(31)	27(3)	17(3)	40(4)	-7(3)	-10(3)	10(2)
C(32)	34(3)	12(3)	36(4)	-3(2)	-11(3)	3(2)
C(33)	32(3)	19(3)	20(3)	0(2)	-5(3)	-5(2)
C(34)	25(3)	19(3)	24(3)	3(2)	-4(2)	0(2)
C(35)	27(3)	13(3)	29(3)	3(2)	-4(3)	0(2)

Table 59a-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
H(1)	9050(60)	2270(40)	1530(30)	26(16)
H(3)	10843	1967	974	31
H(4)	13036	1875	898	43
H(5)	14181	3132	675	47
H(6)	13206	4499	544	51
H(7)	11029	4614	638	38
H(9)	7037	3991	7	69
H(10)	6417	3758	-1059	111
H(11)	7603	2852	-1703	116
H(12)	9401	2193	-1324	87
H(13)	10054	2415	-269	59
H(15)	8750	549	1118	47
H(16)	9173	-513	328	63
H(17)	8206	-430	-674	66
H(18)	6812	707	-913	67
H(19)	6352	1765	-132	53
H(20A)	5982	5210	1434	70
H(20B)	4749	5116	1851	70
H(20C)	5102	4355	1350	70
H(100)	10260(60)	3100(40)	2230(30)	27(18)
H(22)	7275	5432	2450	37
H(23)	8530	4675	3218	38
H(25)	6875	2291	2710	51
H(26)	5573	3042	1943	47
H(27A)	8771	2292	3267	44
H(28A)	6878	1931	3736	87
H(28B)	7081	2705	4253	87
H(28C)	7999	1865	4251	87
H(29A)	8932	3786	4116	87
H(29B)	9946	3514	3597	87

H(29C)	9756	2907	4217	87
H(27B)	9572	3331	3510	49
H(28D)	8047	1744	3554	83
H(28E)	9476	1778	3793	83
H(28F)	9132	1907	3050	83
H(29D)	7488	3029	4337	91
H(29E)	8391	3877	4359	91
H(29F)	8907	2926	4582	91
H(31)	9750	5338	2337	34
H(32)	11270	6344	2592	33
H(34)	13796	4347	2845	27
H(35)	12310	3330	2547	28

Röntgenstrukturanalytische Daten für 61a

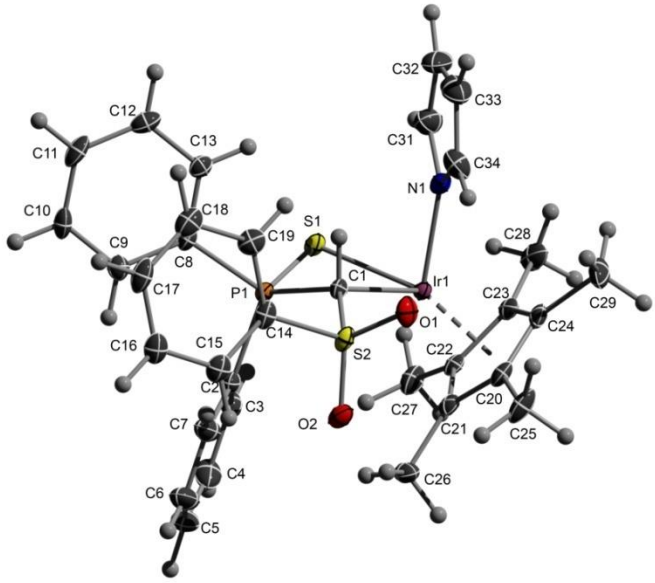

Table 61a-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	$C_{33}H_{35}IrNO_2PS_2$	
Formula weight	764.91	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 15.0129(7) Å	α = 90°.
	b = 12.6152(6) Å	β = 91.890(2)°.
	c = 16.0052(8) Å	γ = 90°.
Volume	3029.6(3) $Å^3$	
Z	4	
Density (calculated)	1.677 Mg/m^3	
Absorption coefficient	4.629 mm^{-1}	
F(000)	1520	
Crystal size	0.13 x 0.10 x 0.06 mm^3	
Theta range for data collection	1.83 to 26.48°.	
Index ranges	-18<=h<=18, -15<=k<=15, -20<=l<=20	

Reflections collected	49029
Independent reflections	6245 [R(int) = 0.0299]
Completeness to theta = 26.48°	99.8 %
Absorption correction	Empirical
Max. and min. transmission	0.7816 and 0.5844
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6245 / 0 / 366
Goodness-of-fit on F^2	1.140
Final R indices [I>2sigma(I)]	R1 = 0.0196, wR2 = 0.0579
R indices (all data)	R1 = 0.0235, wR2 = 0.0658
Largest diff. peak and hole	1.727 and -0.587 e.Å^{-3}

Table 61a-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	1396(1)	3276(1)	1812(1)	12(1)
S(1)	1727(1)	1630(1)	2563(1)	16(1)
P(1)	545(1)	1937(1)	3052(1)	12(1)
O(1)	-1038(2)	3918(2)	1435(1)	23(1)
N(1)	1081(2)	2330(2)	763(2)	17(1)
C(1)	107(2)	2730(2)	2214(2)	13(1)
S(2)	-820(1)	3562(1)	2274(1)	16(1)
O(2)	-693(1)	4354(2)	2920(1)	21(1)
C(2)	658(2)	2598(2)	4051(2)	17(1)
C(3)	1490(2)	2643(3)	4453(2)	22(1)
C(4)	1592(3)	3170(3)	5216(2)	32(1)
C(5)	864(3)	3640(3)	5572(2)	35(1)
C(6)	34(3)	3572(3)	5182(2)	33(1)
C(7)	-74(3)	3054(3)	4429(2)	25(1)
C(8)	-102(2)	744(2)	3193(2)	14(1)
C(9)	-487(2)	472(3)	3939(2)	19(1)
C(10)	-986(2)	-456(3)	3983(2)	24(1)
C(11)	-1101(2)	-1095(3)	3286(2)	25(1)

C(12)	-713(2)	-832(3)	2543(2)	23(1)
C(13)	-213(2)	87(2)	2500(2)	18(1)
C(14)	-1698(2)	2721(2)	2584(2)	17(1)
C(15)	-2177(2)	2964(3)	3285(2)	21(1)
C(16)	-2850(2)	2284(3)	3530(2)	23(1)
C(17)	-3029(2)	1379(3)	3070(2)	27(1)
C(18)	-2555(2)	1140(3)	2373(2)	25(1)
C(19)	-1891(2)	1816(2)	2119(2)	21(1)
C(20)	1343(2)	4993(2)	1681(2)	18(1)
C(21)	1723(2)	4732(2)	2502(2)	16(1)
C(22)	2522(2)	4147(2)	2378(2)	16(1)
C(23)	2645(2)	4033(2)	1494(2)	17(1)
C(24)	1916(2)	4573(2)	1074(2)	19(1)
C(25)	577(2)	5722(3)	1512(3)	29(1)
C(26)	1393(2)	5145(3)	3307(2)	24(1)
C(27)	3145(2)	3768(3)	3051(2)	24(1)
C(28)	3428(2)	3522(3)	1092(3)	29(1)
C(29)	1794(3)	4720(3)	151(2)	31(1)
C(30)	1488(3)	1428(3)	529(2)	31(1)
C(31)	1012(3)	962(3)	-126(2)	40(1)
C(32)	273(3)	1625(3)	-305(3)	36(1)
C(33)	340(2)	2452(3)	261(2)	28(1)

Table 61a-3. Bond lengths [Å] and angles [°] for sad.

Ir(1)-N(1)	2.100(2)
Ir(1)-C(1)	2.171(3)
Ir(1)-C(20)	2.177(3)
Ir(1)-C(24)	2.178(3)
Ir(1)-C(23)	2.179(3)
Ir(1)-C(22)	2.187(3)
Ir(1)-C(21)	2.191(3)
Ir(1)-S(1)	2.4420(8)
Ir(1)-P(1)	2.9310(8)
S(1)-P(1)	1.9994(11)
P(1)-C(1)	1.782(3)
P(1)-C(2)	1.806(3)
P(1)-C(8)	1.809(3)
O(1)-S(2)	1.445(2)
N(1)-C(30)	1.351(4)
N(1)-C(33)	1.360(4)
C(1)-S(2)	1.749(3)
S(2)-O(2)	1.445(2)
S(2)-C(14)	1.774(3)
C(2)-C(3)	1.387(4)
C(2)-C(7)	1.395(5)
C(3)-C(4)	1.394(5)
C(4)-C(5)	1.382(6)
C(5)-C(6)	1.379(6)
C(6)-C(7)	1.376(5)
C(8)-C(9)	1.387(4)
C(8)-C(13)	1.391(4)
C(9)-C(10)	1.392(4)
C(10)-C(11)	1.383(5)
C(11)-C(12)	1.382(5)
C(12)-C(13)	1.385(4)
C(14)-C(15)	1.388(5)
C(14)-C(19)	1.389(4)
C(15)-C(16)	1.391(5)

C(16)-C(17)	1.381(5)
C(17)-C(18)	1.376(5)
C(18)-C(19)	1.384(5)
C(20)-C(24)	1.421(4)
C(20)-C(21)	1.454(4)
C(20)-C(25)	1.490(4)
C(21)-C(22)	1.428(4)
C(21)-C(26)	1.489(4)
C(22)-C(23)	1.440(4)
C(22)-C(27)	1.483(4)
C(23)-C(24)	1.437(4)
C(23)-C(28)	1.504(5)
C(24)-C(29)	1.493(4)
C(30)-C(31)	1.381(5)
C(31)-C(32)	1.411(6)
C(32)-C(33)	1.383(5)

N(1)-Ir(1)-C(1)	82.94(11)
N(1)-Ir(1)-C(20)	118.76(11)
C(1)-Ir(1)-C(20)	108.30(11)
N(1)-Ir(1)-C(24)	93.92(11)
C(1)-Ir(1)-C(24)	137.53(11)
C(20)-Ir(1)-C(24)	38.07(12)
N(1)-Ir(1)-C(23)	103.59(11)
C(1)-Ir(1)-C(23)	171.96(11)
C(20)-Ir(1)-C(23)	64.56(11)
C(24)-Ir(1)-C(23)	38.52(12)
N(1)-Ir(1)-C(22)	140.07(10)
C(1)-Ir(1)-C(22)	136.13(11)
C(20)-Ir(1)-C(22)	64.25(11)
C(24)-Ir(1)-C(22)	63.99(11)
C(23)-Ir(1)-C(22)	38.51(11)
N(1)-Ir(1)-C(21)	156.91(11)
C(1)-Ir(1)-C(21)	107.67(11)
C(20)-Ir(1)-C(21)	38.87(11)
C(24)-Ir(1)-C(21)	64.24(12)

C(23)-Ir(1)-C(21)	64.55(11)
C(22)-Ir(1)-C(21)	38.08(11)
N(1)-Ir(1)-S(1)	86.99(7)
C(1)-Ir(1)-S(1)	75.71(8)
C(20)-Ir(1)-S(1)	154.09(9)
C(24)-Ir(1)-S(1)	146.65(9)
C(23)-Ir(1)-S(1)	108.98(9)
C(22)-Ir(1)-S(1)	94.67(8)
C(21)-Ir(1)-S(1)	115.22(9)
N(1)-Ir(1)-P(1)	97.03(7)
C(1)-Ir(1)-P(1)	37.28(8)
C(20)-Ir(1)-P(1)	128.56(8)
C(24)-Ir(1)-P(1)	166.48(9)
C(23)-Ir(1)-P(1)	143.92(9)
C(22)-Ir(1)-P(1)	110.92(8)
C(21)-Ir(1)-P(1)	103.71(8)
S(1)-Ir(1)-P(1)	42.49(2)
P(1)-S(1)-Ir(1)	81.94(3)
C(1)-P(1)-C(2)	115.36(14)
C(1)-P(1)-C(8)	111.99(14)
C(2)-P(1)-C(8)	107.97(14)
C(1)-P(1)-S(1)	97.14(10)
C(2)-P(1)-S(1)	112.19(11)
C(8)-P(1)-S(1)	112.02(10)
C(1)-P(1)-Ir(1)	47.54(9)
C(2)-P(1)-Ir(1)	107.63(10)
C(8)-P(1)-Ir(1)	144.26(10)
S(1)-P(1)-Ir(1)	55.58(3)
C(30)-N(1)-C(33)	107.5(3)
C(30)-N(1)-Ir(1)	127.5(2)
C(33)-N(1)-Ir(1)	124.5(2)
S(2)-C(1)-P(1)	124.74(17)
S(2)-C(1)-Ir(1)	123.02(15)
P(1)-C(1)-Ir(1)	95.18(13)
O(1)-S(2)-O(2)	118.06(14)
O(1)-S(2)-C(1)	106.92(14)

O(2)-S(2)-C(1)	111.61(14)
O(1)-S(2)-C(14)	107.33(14)
O(2)-S(2)-C(14)	107.22(15)
C(1)-S(2)-C(14)	104.86(14)
C(3)-C(2)-C(7)	119.4(3)
C(3)-C(2)-P(1)	119.1(2)
C(7)-C(2)-P(1)	121.5(3)
C(2)-C(3)-C(4)	119.8(3)
C(5)-C(4)-C(3)	120.0(4)
C(6)-C(5)-C(4)	120.1(3)
C(7)-C(6)-C(5)	120.3(4)
C(6)-C(7)-C(2)	120.2(3)
C(9)-C(8)-C(13)	119.8(3)
C(9)-C(8)-P(1)	123.7(2)
C(13)-C(8)-P(1)	116.5(2)
C(8)-C(9)-C(10)	119.5(3)
C(11)-C(10)-C(9)	120.2(3)
C(12)-C(11)-C(10)	120.7(3)
C(11)-C(12)-C(13)	119.2(3)
C(12)-C(13)-C(8)	120.7(3)
C(15)-C(14)-C(19)	120.7(3)
C(15)-C(14)-S(2)	120.2(3)
C(19)-C(14)-S(2)	119.1(2)
C(14)-C(15)-C(16)	119.5(3)
C(17)-C(16)-C(15)	119.3(3)
C(18)-C(17)-C(16)	121.1(3)
C(17)-C(18)-C(19)	120.1(3)
C(18)-C(19)-C(14)	119.3(3)
C(24)-C(20)-C(21)	107.8(3)
C(24)-C(20)-C(25)	125.9(3)
C(21)-C(20)-C(25)	125.5(3)
C(24)-C(20)-Ir(1)	71.01(18)
C(21)-C(20)-Ir(1)	71.07(17)
C(25)-C(20)-Ir(1)	131.1(2)
C(22)-C(21)-C(20)	107.3(3)
C(22)-C(21)-C(26)	127.3(3)

C(20)-C(21)-C(26)	124.9(3)
C(22)-C(21)-Ir(1)	70.80(17)
C(20)-C(21)-Ir(1)	70.06(17)
C(26)-C(21)-Ir(1)	130.9(2)
C(21)-C(22)-C(23)	108.9(3)
C(21)-C(22)-C(27)	125.3(3)
C(23)-C(22)-C(27)	125.7(3)
C(21)-C(22)-Ir(1)	71.12(16)
C(23)-C(22)-Ir(1)	70.46(16)
C(27)-C(22)-Ir(1)	126.8(2)
C(24)-C(23)-C(22)	107.0(3)
C(24)-C(23)-C(28)	126.7(3)
C(22)-C(23)-C(28)	126.2(3)
C(24)-C(23)-Ir(1)	70.71(17)
C(22)-C(23)-Ir(1)	71.02(16)
C(28)-C(23)-Ir(1)	127.1(2)
C(20)-C(24)-C(23)	109.0(3)
C(20)-C(24)-C(29)	125.0(3)
C(23)-C(24)-C(29)	126.0(3)
C(20)-C(24)-Ir(1)	70.92(18)
C(23)-C(24)-Ir(1)	70.77(17)
C(29)-C(24)-Ir(1)	126.5(2)
N(1)-C(30)-C(31)	110.0(3)
C(30)-C(31)-C(32)	106.6(4)
C(33)-C(32)-C(31)	105.9(4)
N(1)-C(33)-C(32)	110.0(3)

Symmetry transformations used to generate equivalent atoms:

Table 61a-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	12(1)	11(1)	14(1)	1(1)	1(1)	-1(1)
S(1)	13(1)	13(1)	21(1)	2(1)	3(1)	2(1)
P(1)	12(1)	10(1)	14(1)	1(1)	1(1)	0(1)
O(1)	21(1)	24(1)	22(1)	9(1)	-2(1)	4(1)
N(1)	18(1)	16(1)	18(1)	-1(1)	1(1)	-5(1)
C(1)	14(2)	12(2)	14(2)	2(1)	0(1)	0(1)
S(2)	12(1)	14(1)	22(1)	4(1)	1(1)	1(1)
O(2)	19(1)	15(1)	30(1)	-2(1)	4(1)	0(1)
C(2)	26(2)	12(2)	13(2)	3(1)	1(1)	-2(1)
C(3)	23(2)	26(2)	17(2)	4(1)	-1(1)	-6(1)
C(4)	39(2)	37(2)	21(2)	2(2)	-8(2)	-15(2)
C(5)	59(3)	26(2)	19(2)	-7(2)	-1(2)	-8(2)
C(6)	52(3)	25(2)	23(2)	-5(2)	5(2)	8(2)
C(7)	32(2)	23(2)	20(2)	-2(1)	0(2)	5(2)
C(8)	11(1)	10(1)	19(2)	3(1)	0(1)	-1(1)
C(9)	18(2)	21(2)	19(2)	2(1)	1(1)	-1(1)
C(10)	23(2)	24(2)	26(2)	10(2)	7(2)	-4(1)
C(11)	19(2)	17(2)	40(2)	7(2)	-3(2)	-7(1)
C(12)	20(2)	18(2)	32(2)	-5(1)	-4(2)	-1(1)
C(13)	18(2)	14(2)	21(2)	1(1)	-1(1)	3(1)
C(14)	9(1)	18(2)	24(2)	7(1)	-1(1)	1(1)
C(15)	16(2)	20(2)	26(2)	5(1)	-1(1)	5(1)
C(16)	18(2)	24(2)	28(2)	7(2)	2(1)	3(1)
C(17)	17(2)	24(2)	38(2)	12(2)	0(2)	-4(1)
C(18)	19(2)	22(2)	32(2)	4(2)	-7(2)	-2(1)
C(19)	14(2)	23(2)	26(2)	-1(1)	-3(1)	0(1)
C(20)	18(2)	11(2)	26(2)	4(1)	-2(1)	-3(1)
C(21)	14(2)	13(2)	20(2)	-1(1)	1(1)	-6(1)
C(22)	14(2)	12(2)	21(2)	0(1)	-2(1)	-6(1)
C(23)	14(2)	16(2)	21(2)	-2(1)	5(1)	-7(1)
C(24)	23(2)	16(2)	19(2)	5(1)	1(1)	-8(1)

C(25)	22(2)	16(2)	50(2)	11(2)	-4(2)	0(1)
C(26)	26(2)	21(2)	25(2)	-8(1)	6(2)	-7(1)
C(27)	21(2)	22(2)	29(2)	6(2)	-7(2)	-5(1)
C(28)	22(2)	24(2)	42(2)	-5(2)	16(2)	-8(2)
C(29)	42(2)	32(2)	18(2)	7(2)	-2(2)	-13(2)
C(30)	42(2)	24(2)	27(2)	-1(2)	0(2)	4(2)
C(31)	69(3)	25(2)	27(2)	-8(2)	-1(2)	-8(2)
C(32)	38(2)	43(2)	25(2)	-6(2)	-2(2)	-14(2)
C(33)	27(2)	38(2)	20(2)	0(2)	2(2)	0(2)

Table 61a-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
H(1)	-79	2199	1778	16
H(3)	1988	2316	4209	27
H(4)	2162	3206	5490	39
H(5)	937	4010	6087	41
H(6)	-467	3885	5434	40
H(7)	-649	3006	4165	30
H(9)	-412	914	4416	23
H(10)	-1249	-650	4493	29
H(11)	-1449	-1722	3318	30
H(12)	-790	-1277	2066	28
H(13)	58	271	1991	21
H(15)	-2047	3590	3596	25
H(16)	-3182	2441	4010	28
H(17)	-3488	913	3237	32
H(18)	-2684	510	2067	29
H(19)	-1570	1662	1631	25
H(25A)	226	5468	1026	44
H(25B)	802	6436	1398	44
H(25C)	201	5744	2000	44

H(26A)	1575	5887	3377	35
H(26B)	1646	4722	3771	35
H(26C)	741	5097	3303	35
H(27A)	3431	3111	2873	36
H(27B)	2815	3634	3559	36
H(27C)	3601	4308	3167	36
H(28A)	3237	3224	550	43
H(28B)	3665	2955	1454	43
H(28C)	3893	4055	1010	43
H(29A)	2185	4228	-138	46
H(29B)	1947	5451	4	46
H(29C)	1172	4578	-17	46
H(30)	2022	1154	779	37
H(31)	1154	320	-402	48
H(32)	-178	1524	-728	43
H(33)	-71	3022	293	34

Röntgenstrukturanalytische Daten für 61b

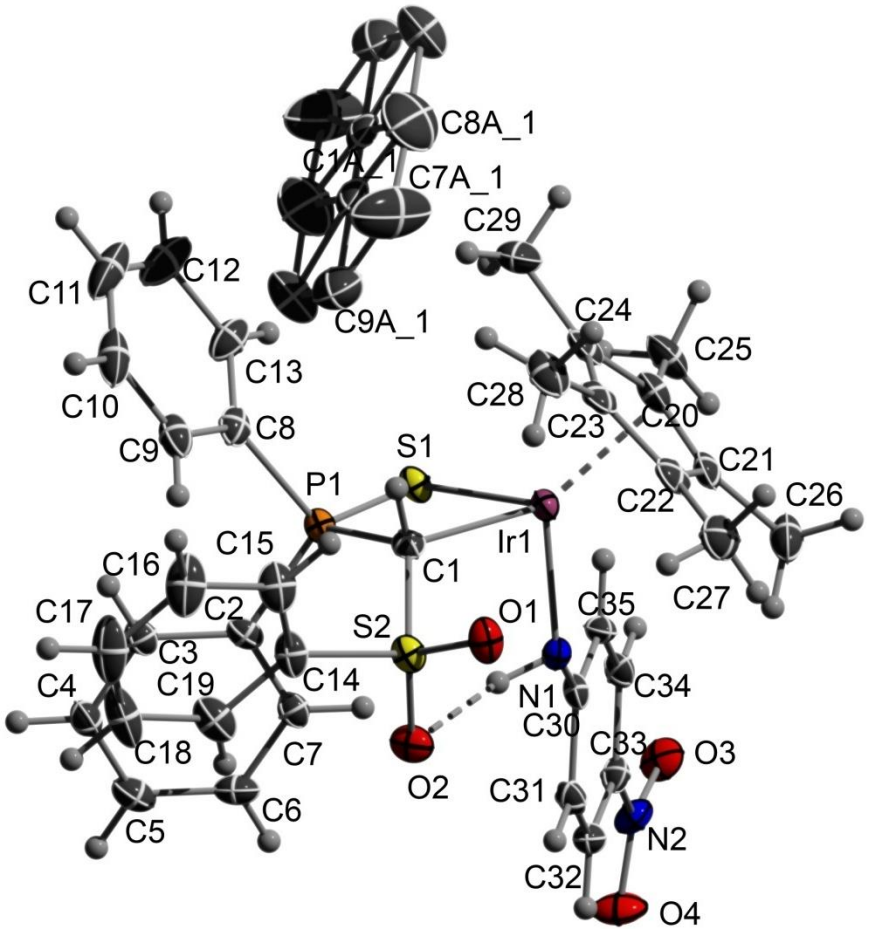

Table 61b-1. Crystal data and structure refinement for platon.

Identification code	platon	
Empirical formula	$C_{80}H_{72}Ir_2N_4O_8P_2S_4$	
Formula weight	1792.00	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.0547(7) Å	α = 110.166(2)°.
	b = 12.2581(7) Å	β = 104.434(2)°.
	c = 14.5894(9) Å	γ = 92.787(2)°.
Volume	1777.43(19) $Å^3$	
Z	1	
Density (calculated)	1.674 Mg/m^3	
Absorption coefficient	3.964 mm^{-1}	

F(000)	892
Crystal size	0.134 x 0.06 x 0.037 mm^3
Theta range for data collection	1.55 to 26.46°.
Index ranges	-13<=h<=13, -15<=k<=15, -18<=l<=18
Reflections collected	28148
Independent reflections	7298 [R(int) = 0.0282]
Completeness to theta = 26.46°	99.4 %
Absorption correction	Empirical
Max. and min. transmission	0.7454 and 0.6334
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7298 / 0 / 456
Goodness-of-fit on F^2	1.076
Final R indices [I>2sigma(I)]	R1 = 0.0254, wR2 = 0.0596
R indices (all data)	R1 = 0.0295, wR2 = 0.0612
Largest diff. peak and hole	1.387 and -0.791 e.$Å^{-3}$

Table 61b-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for platon. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	8035(1)	4852(1)	1812(1)	16(1)
S(1)	9304(1)	5241(1)	3556(1)	19(1)
P(1)	8276(1)	3763(1)	3392(1)	16(1)
O(1)	5160(2)	2736(2)	701(2)	25(1)
N(1)	6783(3)	5843(2)	2454(2)	18(1)
C(1)	7274(3)	3386(3)	2106(3)	17(1)
S(2)	5627(1)	3021(1)	1780(1)	19(1)
O(2)	5092(2)	3904(2)	2441(2)	25(1)
N(2)	7495(3)	10394(3)	5280(2)	24(1)
C(2)	7514(3)	4011(3)	4391(2)	17(1)
O(3)	8518(3)	11047(2)	5515(2)	30(1)
C(3)	7516(3)	3253(3)	4914(3)	21(1)
O(4)	6648(3)	10734(2)	5692(2)	35(1)
C(4)	6990(4)	3524(3)	5716(3)	24(1)
C(5)	6491(4)	4555(4)	6016(3)	27(1)

C(6)	6492(4)	5310(3)	5498(3)	26(1)
C(7)	6999(3)	5046(3)	4683(3)	21(1)
C(8)	9189(4)	2585(3)	3393(3)	22(1)
C(9)	8598(4)	1446(3)	3111(3)	28(1)
C(10)	9305(5)	545(4)	3077(3)	39(1)
C(11)	10606(5)	784(4)	3346(3)	45(1)
C(12)	11203(5)	1911(4)	3647(3)	43(1)
C(13)	10495(4)	2822(3)	3670(3)	29(1)
C(14)	5362(4)	1707(3)	1997(3)	22(1)
C(15)	5556(4)	666(3)	1317(3)	28(1)
C(16)	5371(5)	-366(3)	1480(3)	37(1)
C(17)	4998(5)	-342(4)	2324(3)	42(1)
C(18)	4809(5)	696(4)	3000(3)	41(1)
C(19)	4987(4)	1731(4)	2840(3)	29(1)
C(20)	9430(4)	5674(3)	1313(3)	26(1)
C(21)	8203(4)	5771(3)	788(3)	23(1)
C(22)	7499(4)	4601(3)	208(3)	25(1)
C(23)	8344(4)	3788(3)	378(3)	25(1)
C(24)	9517(4)	4438(3)	1071(3)	26(1)
C(25)	10498(4)	6645(4)	1972(3)	34(1)
C(26)	7684(5)	6891(4)	810(3)	36(1)
C(27)	6245(4)	4300(4)	-568(3)	34(1)
C(28)	8013(5)	2485(3)	-120(3)	34(1)
C(29)	10699(4)	3959(4)	1430(4)	40(1)
C(30)	6970(3)	6938(3)	3122(2)	17(1)
C(31)	5977(3)	7410(3)	3535(3)	19(1)
C(32)	6144(3)	8523(3)	4230(3)	20(1)
C(33)	7309(3)	9243(3)	4551(3)	19(1)
C(34)	8311(3)	8804(3)	4175(3)	21(1)
C(35)	8147(3)	7691(3)	3486(3)	20(1)
C1A1	9515(8)	-153(8)	-75(7)	35(2)
C4A1	8562(10)	-177(9)	534(7)	44(2)
C7A1	8510(12)	-964(14)	-1167(8)	82(5)
C8A1	9993(7)	-356(6)	-849(4)	74(2)
C9A1	8021(5)	-731(5)	-411(4)	50(1)

Table 61b-3. Bond lengths [Å] and angles [°] for platon.

Ir(1)-N(1)	2.072(3)
Ir(1)-C(1)	2.165(3)
Ir(1)-C(24)	2.167(4)
Ir(1)-C(23)	2.171(3)
Ir(1)-C(22)	2.172(3)
Ir(1)-C(21)	2.193(3)
Ir(1)-C(20)	2.200(4)
Ir(1)-S(1)	2.4465(9)
S(1)-P(1)	1.9992(12)
P(1)-C(8)	1.802(4)
P(1)-C(2)	1.805(3)
P(1)-C(1)	1.810(3)
O(1)-S(2)	1.437(3)
N(1)-C(30)	1.328(4)
N(1)-H(1A)	0.9000
N(1)-H(1B)	0.9000
C(1)-S(2)	1.756(4)
C(1)-H(1)	0.9800
S(2)-O(2)	1.441(3)
S(2)-C(14)	1.770(4)
N(2)-O(4)	1.247(4)
N(2)-O(3)	1.252(4)
N(2)-C(33)	1.412(4)
C(2)-C(7)	1.391(5)
C(2)-C(3)	1.391(5)
C(3)-C(4)	1.382(5)
C(3)-H(3)	0.9300
C(4)-C(5)	1.379(5)
C(4)-H(4)	0.9300
C(5)-C(6)	1.382(5)
C(5)-H(5)	0.9300
C(6)-C(7)	1.384(5)
C(6)-H(6)	0.9300
C(7)-H(7)	0.9300

C(8)-C(13)	1.385(6)
C(8)-C(9)	1.388(5)
C(9)-C(10)	1.378(6)
C(9)-H(9)	0.9300
C(10)-C(11)	1.381(7)
C(10)-H(10)	0.9300
C(11)-C(12)	1.374(7)
C(11)-H(11)	0.9300
C(12)-C(13)	1.390(6)
C(12)-H(12)	0.9300
C(13)-H(13)	0.9300
C(14)-C(15)	1.385(5)
C(14)-C(19)	1.385(5)
C(15)-C(16)	1.380(5)
C(15)-H(15)	0.9300
C(16)-C(17)	1.383(6)
C(16)-H(16)	0.9300
C(17)-C(18)	1.378(7)
C(17)-H(17)	0.9300
C(18)-C(19)	1.380(6)
C(18)-H(18)	0.9300
C(19)-H(19)	0.9300
C(20)-C(21)	1.414(5)
C(20)-C(24)	1.447(5)
C(20)-C(25)	1.497(5)
C(21)-C(22)	1.450(5)
C(21)-C(26)	1.507(5)
C(22)-C(23)	1.439(5)
C(22)-C(27)	1.490(5)
C(23)-C(24)	1.424(6)
C(23)-C(28)	1.491(5)
C(24)-C(29)	1.508(6)
C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600
C(25)-H(25C)	0.9600
C(26)-H(26A)	0.9600

C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600
C(27)-H(27A)	0.9600
C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600
C(29)-H(29A)	0.9600
C(29)-H(29B)	0.9600
C(29)-H(29C)	0.9600
C(30)-C(35)	1.424(5)
C(30)-C(31)	1.433(5)
C(31)-C(32)	1.362(5)
C(31)-H(31)	0.9300
C(32)-C(33)	1.400(5)
C(32)-H(32)	0.9300
C(33)-C(34)	1.406(5)
C(34)-C(35)	1.357(5)
C(34)-H(34)	0.9300
C(35)-H(35)	0.9300
C1A1-C1A1#1	1.062(18)
C1A1-C8A1#1	1.235(11)
C1A1-C8A1	1.317(10)
C1A1-C4A1	1.543(12)
C1A1-C7A1	1.637(15)
C1A1-C9A1	1.647(10)
C4A1-C9A1	1.275(10)
C4A1-C8A1#1	1.586(12)
C7A1-C9A1	1.297(13)
C7A1-C8A1	1.650(15)
C8A1-C1A1#1	1.235(11)
C8A1-C4A1#1	1.586(12)

N(1)-Ir(1)-C(1)	89.29(12)
N(1)-Ir(1)-C(24)	158.08(13)

C(1)-Ir(1)-C(24)	112.62(14)
N(1)-Ir(1)-C(23)	143.75(13)
C(1)-Ir(1)-C(23)	95.40(13)
C(24)-Ir(1)-C(23)	38.33(15)
N(1)-Ir(1)-C(22)	107.06(13)
C(1)-Ir(1)-C(22)	113.15(14)
C(24)-Ir(1)-C(22)	64.86(14)
C(23)-Ir(1)-C(22)	38.70(14)
N(1)-Ir(1)-C(21)	96.56(13)
C(1)-Ir(1)-C(21)	151.77(14)
C(24)-Ir(1)-C(21)	64.02(14)
C(23)-Ir(1)-C(21)	64.13(14)
C(22)-Ir(1)-C(21)	38.81(14)
N(1)-Ir(1)-C(20)	119.52(13)
C(1)-Ir(1)-C(20)	150.95(14)
C(24)-Ir(1)-C(20)	38.68(14)
C(23)-Ir(1)-C(20)	64.15(14)
C(22)-Ir(1)-C(20)	64.44(14)
C(21)-Ir(1)-C(20)	37.55(14)
N(1)-Ir(1)-S(1)	86.62(8)
C(1)-Ir(1)-S(1)	78.17(9)
C(24)-Ir(1)-S(1)	97.99(10)
C(23)-Ir(1)-S(1)	129.54(11)
C(22)-Ir(1)-S(1)	161.79(10)
C(21)-Ir(1)-S(1)	129.61(10)
C(20)-Ir(1)-S(1)	98.56(10)
P(1)-S(1)-Ir(1)	84.33(4)
C(8)-P(1)-C(2)	107.94(16)
C(8)-P(1)-C(1)	107.32(16)
C(2)-P(1)-C(1)	117.44(16)
C(8)-P(1)-S(1)	113.23(14)
C(2)-P(1)-S(1)	111.10(12)
C(1)-P(1)-S(1)	99.77(12)
C(30)-N(1)-Ir(1)	130.4(2)
C(30)-N(1)-H(1A)	104.7
Ir(1)-N(1)-H(1A)	104.7

C(30)-N(1)-H(1B)	104.7
Ir(1)-N(1)-H(1B)	104.7
H(1A)-N(1)-H(1B)	105.7
S(2)-C(1)-P(1)	122.42(19)
S(2)-C(1)-Ir(1)	118.59(17)
P(1)-C(1)-Ir(1)	97.73(15)
S(2)-C(1)-H(1)	105.5
P(1)-C(1)-H(1)	105.5
Ir(1)-C(1)-H(1)	105.5
O(1)-S(2)-O(2)	118.19(16)
O(1)-S(2)-C(1)	106.75(16)
O(2)-S(2)-C(1)	111.06(16)
O(1)-S(2)-C(14)	106.89(16)
O(2)-S(2)-C(14)	107.40(17)
C(1)-S(2)-C(14)	105.83(17)
O(4)-N(2)-O(3)	121.3(3)
O(4)-N(2)-C(33)	119.5(3)
O(3)-N(2)-C(33)	119.2(3)
C(7)-C(2)-C(3)	120.0(3)
C(7)-C(2)-P(1)	117.6(3)
C(3)-C(2)-P(1)	122.2(3)
C(4)-C(3)-C(2)	119.8(3)
C(4)-C(3)-H(3)	120.1
C(2)-C(3)-H(3)	120.1
C(5)-C(4)-C(3)	120.3(4)
C(5)-C(4)-H(4)	119.8
C(3)-C(4)-H(4)	119.8
C(4)-C(5)-C(6)	119.9(4)
C(4)-C(5)-H(5)	120.1
C(6)-C(5)-H(5)	120.1
C(5)-C(6)-C(7)	120.6(4)
C(5)-C(6)-H(6)	119.7
C(7)-C(6)-H(6)	119.7
C(6)-C(7)-C(2)	119.3(3)
C(6)-C(7)-H(7)	120.3
C(2)-C(7)-H(7)	120.3

C(13)-C(8)-C(9)	119.9(4)
C(13)-C(8)-P(1)	119.4(3)
C(9)-C(8)-P(1)	120.7(3)
C(10)-C(9)-C(8)	120.1(4)
C(10)-C(9)-H(9)	119.9
C(8)-C(9)-H(9)	119.9
C(9)-C(10)-C(11)	119.7(4)
C(9)-C(10)-H(10)	120.1
C(11)-C(10)-H(10)	120.1
C(12)-C(11)-C(10)	120.7(4)
C(12)-C(11)-H(11)	119.7
C(10)-C(11)-H(11)	119.7
C(11)-C(12)-C(13)	119.9(5)
C(11)-C(12)-H(12)	120.0
C(13)-C(12)-H(12)	120.0
C(8)-C(13)-C(12)	119.6(4)
C(8)-C(13)-H(13)	120.2
C(12)-C(13)-H(13)	120.2
C(15)-C(14)-C(19)	121.0(3)
C(15)-C(14)-S(2)	118.7(3)
C(19)-C(14)-S(2)	120.2(3)
C(16)-C(15)-C(14)	119.6(4)
C(16)-C(15)-H(15)	120.2
C(14)-C(15)-H(15)	120.2
C(15)-C(16)-C(17)	119.4(4)
C(15)-C(16)-H(16)	120.3
C(17)-C(16)-H(16)	120.3
C(18)-C(17)-C(16)	120.9(4)
C(18)-C(17)-H(17)	119.6
C(16)-C(17)-H(17)	119.6
C(17)-C(18)-C(19)	120.1(4)
C(17)-C(18)-H(18)	119.9
C(19)-C(18)-H(18)	119.9
C(18)-C(19)-C(14)	119.0(4)
C(18)-C(19)-H(19)	120.5
C(14)-C(19)-H(19)	120.5

C(21)-C(20)-C(24)	107.8(3)
C(21)-C(20)-C(25)	127.9(4)
C(24)-C(20)-C(25)	124.3(4)
C(21)-C(20)-Ir(1)	71.0(2)
C(24)-C(20)-Ir(1)	69.4(2)
C(25)-C(20)-Ir(1)	127.0(3)
C(20)-C(21)-C(22)	108.9(3)
C(20)-C(21)-C(26)	126.6(4)
C(22)-C(21)-C(26)	124.5(4)
C(20)-C(21)-Ir(1)	71.5(2)
C(22)-C(21)-Ir(1)	69.78(19)
C(26)-C(21)-Ir(1)	124.9(3)
C(23)-C(22)-C(21)	106.6(3)
C(23)-C(22)-C(27)	126.2(4)
C(21)-C(22)-C(27)	126.2(4)
C(23)-C(22)-Ir(1)	70.6(2)
C(21)-C(22)-Ir(1)	71.41(19)
C(27)-C(22)-Ir(1)	131.8(3)
C(24)-C(23)-C(22)	108.7(3)
C(24)-C(23)-C(28)	127.2(4)
C(22)-C(23)-C(28)	124.1(4)
C(24)-C(23)-Ir(1)	70.7(2)
C(22)-C(23)-Ir(1)	70.7(2)
C(28)-C(23)-Ir(1)	125.4(3)
C(23)-C(24)-C(20)	107.9(3)
C(23)-C(24)-C(29)	127.4(4)
C(20)-C(24)-C(29)	124.5(4)
C(23)-C(24)-Ir(1)	71.0(2)
C(20)-C(24)-Ir(1)	71.9(2)
C(29)-C(24)-Ir(1)	126.9(3)
C(20)-C(25)-H(25A)	109.5
C(20)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(20)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5

C(21)-C(26)-H(26A)	109.5
C(21)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(21)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(22)-C(27)-H(27A)	109.5
C(22)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(22)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(23)-C(28)-H(28A)	109.5
C(23)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(23)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(24)-C(29)-H(29A)	109.5
C(24)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(24)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
N(1)-C(30)-C(35)	123.1(3)
N(1)-C(30)-C(31)	120.5(3)
C(35)-C(30)-C(31)	116.4(3)
C(32)-C(31)-C(30)	121.9(3)
C(32)-C(31)-H(31)	119.1
C(30)-C(31)-H(31)	119.1
C(31)-C(32)-C(33)	119.8(3)
C(31)-C(32)-H(32)	120.1
C(33)-C(32)-H(32)	120.1
C(32)-C(33)-C(34)	120.0(3)
C(32)-C(33)-N(2)	120.2(3)
C(34)-C(33)-N(2)	119.8(3)

C(35)-C(34)-C(33)	120.2(3)
C(35)-C(34)-H(34)	119.9
C(33)-C(34)-H(34)	119.9
C(34)-C(35)-C(30)	121.7(3)
C(34)-C(35)-H(35)	119.1
C(30)-C(35)-H(35)	119.1
C1A1#1-C1A1-C8A1#1	69.5(10)
C1A1#1-C1A1-C8A1	61.4(9)
C8A1#1-C1A1-C8A1	131.0(8)
C1A1#1-C1A1-C4A1	138.1(13)
C8A1#1-C1A1-C4A1	68.6(6)
C8A1-C1A1-C4A1	160.4(9)
C1A1#1-C1A1-C7A1	128.1(13)
C8A1#1-C1A1-C7A1	161.7(9)
C8A1-C1A1-C7A1	66.9(7)
C4A1-C1A1-C7A1	93.5(8)
C1A1#1-C1A1-C9A1	174.3(13)
C8A1#1-C1A1-C9A1	115.6(7)
C8A1-C1A1-C9A1	113.4(7)
C4A1-C1A1-C9A1	47.0(5)
C7A1-C1A1-C9A1	46.5(6)
C9A1-C4A1-C1A1	70.8(6)
C9A1-C4A1-C8A1#1	117.2(7)
C1A1-C4A1-C8A1#1	46.4(5)
C9A1-C7A1-C1A1	67.1(6)
C9A1-C7A1-C8A1	114.4(8)
C1A1-C7A1-C8A1	47.2(5)
C1A1#1-C8A1-C1A1	49.0(8)
C1A1#1-C8A1-C4A1#1	64.9(6)
C1A1-C8A1-C4A1#1	114.0(7)
C1A1#1-C8A1-C7A1	114.8(7)
C1A1-C8A1-C7A1	65.9(6)
C4A1#1-C8A1-C7A1	177.4(8)
C4A1-C9A1-C7A1	128.4(8)
C4A1-C9A1-C1A1	62.2(6)
C7A1-C9A1-C1A1	66.3(7)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z

Table 61b-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for platon. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	19(1)	15(1)	15(1)	6(1)	7(1)	2(1)
S(1)	20(1)	19(1)	17(1)	6(1)	4(1)	-2(1)
P(1)	20(1)	14(1)	14(1)	4(1)	5(1)	0(1)
O(1)	28(2)	24(1)	19(1)	8(1)	1(1)	-4(1)
N(1)	20(2)	17(2)	19(1)	10(1)	7(1)	5(1)
C(1)	21(2)	14(2)	16(2)	3(1)	8(1)	3(1)
S(2)	20(1)	17(1)	18(1)	5(1)	4(1)	-2(1)
O(2)	24(1)	18(1)	29(1)	3(1)	9(1)	-1(1)
N(2)	24(2)	19(2)	28(2)	9(1)	6(1)	7(1)
C(2)	14(2)	18(2)	14(2)	3(1)	3(1)	-3(1)
O(3)	29(2)	16(1)	39(2)	7(1)	8(1)	1(1)
C(3)	21(2)	21(2)	22(2)	8(2)	6(2)	1(2)
O(4)	30(2)	26(2)	43(2)	1(1)	16(1)	9(1)
C(4)	23(2)	30(2)	24(2)	14(2)	7(2)	0(2)
C(5)	25(2)	34(2)	22(2)	7(2)	10(2)	1(2)
C(6)	20(2)	27(2)	32(2)	7(2)	12(2)	7(2)
C(7)	21(2)	20(2)	21(2)	7(1)	6(2)	-1(2)
C(8)	32(2)	22(2)	14(2)	6(1)	7(2)	7(2)
C(9)	43(3)	22(2)	23(2)	9(2)	16(2)	5(2)
C(10)	75(4)	22(2)	24(2)	12(2)	18(2)	15(2)
C(11)	70(4)	36(3)	25(2)	12(2)	3(2)	29(2)
C(12)	44(3)	44(3)	31(2)	9(2)	-4(2)	21(2)
C(13)	32(2)	26(2)	22(2)	6(2)	0(2)	10(2)
C(14)	28(2)	16(2)	18(2)	6(1)	1(2)	-6(2)
C(15)	37(2)	21(2)	18(2)	4(2)	2(2)	-5(2)
C(16)	56(3)	19(2)	22(2)	4(2)	-4(2)	-7(2)
C(17)	55(3)	26(2)	33(2)	14(2)	-6(2)	-16(2)

C(18)	53(3)	42(3)	26(2)	18(2)	6(2)	-14(2)
C(19)	31(2)	29(2)	23(2)	6(2)	7(2)	-6(2)
C(20)	30(2)	28(2)	23(2)	12(2)	13(2)	-1(2)
C(21)	32(2)	26(2)	19(2)	13(2)	13(2)	5(2)
C(22)	28(2)	35(2)	14(2)	10(2)	10(2)	3(2)
C(23)	33(2)	27(2)	22(2)	9(2)	20(2)	8(2)
C(24)	30(2)	36(2)	20(2)	14(2)	15(2)	3(2)
C(25)	31(2)	43(3)	31(2)	16(2)	14(2)	-7(2)
C(26)	56(3)	30(2)	30(2)	18(2)	18(2)	14(2)
C(27)	36(2)	44(3)	22(2)	14(2)	7(2)	6(2)
C(28)	53(3)	24(2)	28(2)	6(2)	22(2)	5(2)
C(29)	32(2)	58(3)	44(3)	26(2)	24(2)	20(2)
C(30)	22(2)	17(2)	15(2)	9(1)	6(1)	2(1)
C(31)	18(2)	20(2)	22(2)	10(1)	6(1)	-1(1)
C(32)	19(2)	25(2)	22(2)	11(2)	9(2)	8(2)
C(33)	23(2)	15(2)	20(2)	8(1)	6(2)	5(1)
C(34)	19(2)	19(2)	27(2)	12(2)	7(2)	-1(1)
C(35)	20(2)	19(2)	26(2)	10(2)	14(2)	7(2)
C1A1	44(5)	39(5)	36(5)	25(4)	18(5)	28(5)
C4A1	49(6)	47(6)	37(5)	15(4)	19(5)	-4(5)
C7A1	47(7)	144(13)	30(6)	10(7)	-2(5)	33(8)
C8A1	90(5)	105(5)	42(3)	32(3)	34(3)	32(4)
C9A1	50(3)	56(3)	54(3)	26(3)	22(3)	26(3)

Table 61b-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for platon.

	x	y	z	U(eq)
H(1A)	6158	5832	1919	21
H(1B)	6445	5407	2739	21
H(1)	7567	2696	1690	21
H(3)	7870	2566	4725	26
H(4)	6972	3008	6056	29
H(5)	6153	4743	6566	33
H(6)	6149	6003	5699	32
H(7)	6995	5555	4336	25
H(9)	7722	1291	2944	34
H(10)	8908	-220	2875	46
H(11)	11082	175	3322	54
H(12)	12080	2065	3836	52
H(13)	10896	3586	3869	35
H(15)	5810	663	755	33
H(16)	5495	-1070	1028	44
H(17)	4874	-1036	2436	50
H(18)	4561	699	3564	49
H(19)	4857	2433	3292	35
H(25A)	11133	6634	1626	51
H(25B)	10855	6537	2600	51
H(25C)	10189	7387	2113	51
H(26A)	7619	6983	173	53
H(26B)	8240	7547	1353	53
H(26C)	6864	6857	918	53
H(27A)	6362	4066	-1235	51
H(27B)	5813	4974	-448	51
H(27C)	5752	3666	-519	51
H(28A)	8115	2237	-793	51
H(28B)	7152	2258	-162	51
H(28C)	8559	2123	273	51

H(29A)	10483	3157	1349	59
H(29B)	11103	4418	2135	59
H(29C)	11264	3997	1034	59
H(31)	5197	6942	3323	23
H(32)	5486	8805	4491	24
H(34)	9090	9277	4399	25
H(35)	8820	7414	3246	24

Röntgenstrukturanalytische Daten für 63a

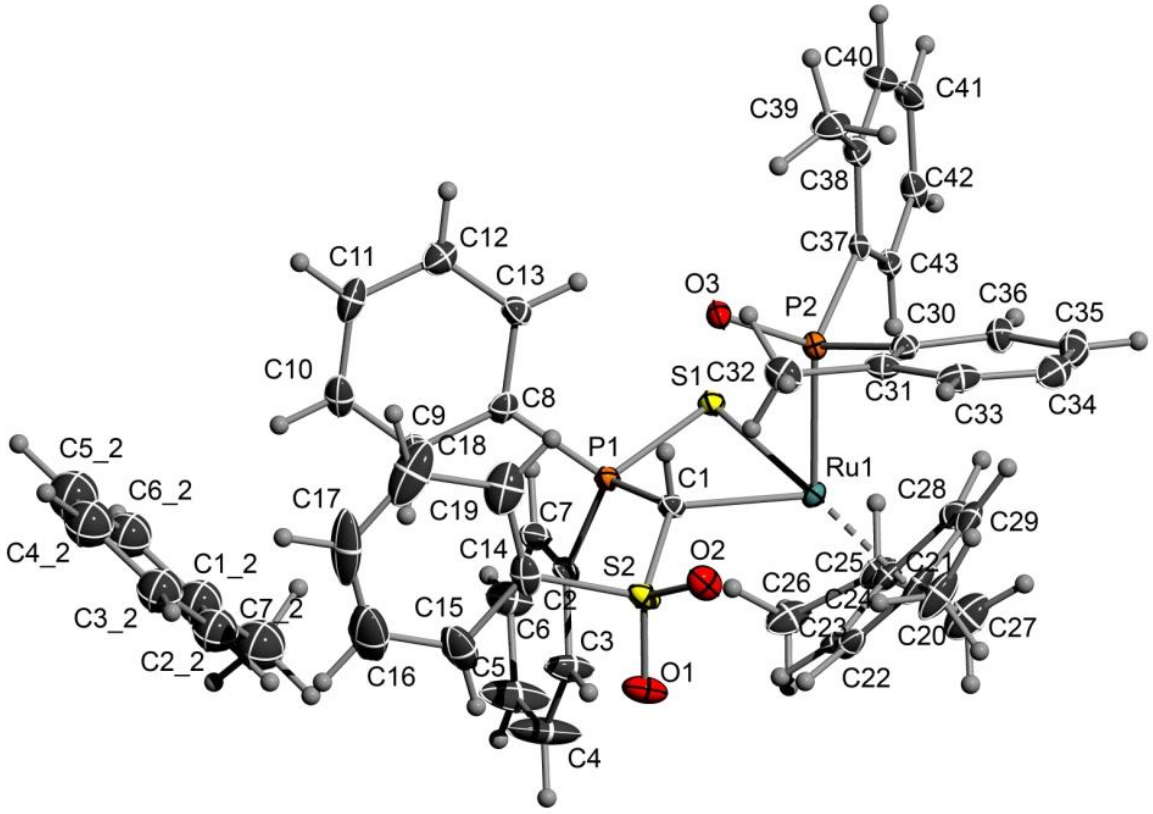

Table 63a-1. Crystal data and structure refinement for platon.

Identification code	platon	
Empirical formula	$C_{372}H_{376}O_{24}P_{16}Ru_8S_{16}$	
Formula weight	7047.77	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 25.0763(13) Å	α = 90°.
	b = 12.6879(7) Å	β = 109.414(2)°.
	c = 26.8084(14) Å	γ = 90°.
Volume	8044.5(7) $Å^3$	
Z	1	
Density (calculated)	1.455 Mg/m^3	
Absorption coefficient	0.615 mm^{-1}	
F(000)	3648	

Crystal size	? x ? x ? mm^3
Theta range for data collection	1.61 to 25.00°.
Index ranges	-29<=h<=29, -15<=k<=15, -31<=l<=31
Reflections collected	59398
Independent reflections	7091 [R(int) = 0.0496]
Completeness to theta = 25.00°	100.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7091 / 0 / 517
Goodness-of-fit on F^2	1.098
Final R indices [I>2sigma(I)]	R1 = 0.0393, wR2 = 0.1030
R indices (all data)	R1 = 0.0466, wR2 = 0.1066
Largest diff. peak and hole	0.754 and -0.398 e.$Å^{-3}$

Table 63a-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for platon. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	8207(1)	10758(1)	8434(1)	12(1)
S(1)	8063(1)	9027(1)	7999(1)	13(1)
S(2)	8819(1)	9992(1)	9721(1)	16(1)
P(1)	8545(1)	8536(1)	8723(1)	12(1)
P(2)	7262(1)	10441(1)	8417(1)	12(1)
O(1)	9393(1)	10233(2)	9767(1)	24(1)
O(2)	8509(1)	10800(2)	9885(1)	21(1)
O(3)	7194(1)	9515(2)	8748(1)	15(1)
C(1)	8412(2)	9630(3)	9079(1)	13(1)
C(2)	9245(2)	8241(3)	8716(1)	16(1)
C(3)	9742(2)	8722(3)	9020(2)	30(1)
C(4)	10242(2)	8484(5)	8928(2)	56(2)
C(5)	10247(2)	7766(4)	8540(2)	52(2)
C(6)	9753(2)	7275(3)	8248(2)	30(1)
C(7)	9252(2)	7503(3)	8334(2)	20(1)
C(8)	8288(2)	7335(3)	8927(1)	16(1)
C(9)	8649(2)	6687(3)	9306(1)	19(1)
C(10)	8431(2)	5849(3)	9507(2)	24(1)

C(11)	7856(2)	5644(3)	9318(2)	24(1)
C(12)	7499(2)	6283(3)	8935(2)	22(1)
C(13)	7708(2)	7142(3)	8744(2)	18(1)
C(14)	8837(2)	8885(3)	10127(1)	22(1)
C(15)	8335(2)	8469(3)	10142(2)	34(1)
C(16)	8361(3)	7619(4)	10483(2)	48(1)
C(17)	8885(3)	7252(4)	10798(2)	55(2)
C(18)	9377(3)	7686(4)	10781(2)	53(2)
C(19)	9360(2)	8508(4)	10441(2)	36(1)
C(20)	8238(2)	12993(3)	9157(2)	34(1)
C(21)	8385(2)	12409(3)	8739(2)	22(1)
C(22)	8897(2)	11829(3)	8861(2)	20(1)
C(23)	9075(2)	11345(3)	8467(2)	17(1)
C(24)	8722(2)	11394(3)	7935(1)	16(1)
C(25)	8888(2)	10926(3)	7490(2)	22(1)
C(26)	9353(2)	10109(3)	7664(2)	27(1)
C(27)	9046(2)	11825(4)	7183(2)	36(1)
C(28)	8200(2)	11944(3)	7807(2)	19(1)
C(29)	8038(2)	12435(3)	8203(2)	23(1)
C(30)	6959(2)	11639(3)	8602(1)	15(1)
C(31)	6944(2)	11829(3)	9114(2)	18(1)
C(32)	7096(2)	11027(3)	9548(2)	23(1)
C(33)	6777(2)	12831(3)	9225(2)	23(1)
C(34)	6625(2)	13627(3)	8854(2)	26(1)
C(35)	6615(2)	13418(3)	8342(2)	26(1)
C(36)	6774(2)	12434(3)	8223(2)	19(1)
C(37)	6768(1)	10228(3)	7738(1)	14(1)
C(38)	6201(2)	9927(3)	7647(2)	19(1)
C(39)	5941(2)	9911(3)	8080(2)	25(1)
C(40)	5865(2)	9662(3)	7139(2)	24(1)
C(41)	6065(2)	9693(3)	6717(2)	23(1)
C(42)	6614(2)	10012(3)	6801(1)	20(1)
C(43)	6955(2)	10275(3)	7307(1)	14(1)
C12	9972(3)	4946(4)	9878(2)	51(5)
C22	9941(3)	5524(4)	10312(3)	47(3)
C32	9704(3)	5069(6)	10666(2)	46(3)

C42	9498(3)	4035(6)	10585(2)	49(3)
C52	9529(3)	3457(4)	10150(3)	53(3)
C62	9766(3)	3912(4)	9797(2)	43(3)
C72	10230(4)	5440(7)	9494(3)	55(3)

Table 63a-3. Bond lengths [Å] and angles [°] for platon.

Ru(1)-C(1)	2.171(4)
Ru(1)-C(22)	2.200(4)
Ru(1)-C(29)	2.218(4)
Ru(1)-C(21)	2.240(4)
Ru(1)-C(28)	2.251(4)
Ru(1)-C(23)	2.275(4)
Ru(1)-C(24)	2.293(4)
Ru(1)-P(2)	2.3897(9)
Ru(1)-S(1)	2.4548(9)
S(1)-P(1)	2.0141(12)
S(2)-O(1)	1.436(3)
S(2)-O(2)	1.440(3)
S(2)-C(1)	1.745(3)
S(2)-C(14)	1.768(4)
P(1)-C(1)	1.777(4)
P(1)-C(2)	1.802(4)
P(1)-C(8)	1.809(4)
P(2)-O(3)	1.516(3)
P(2)-C(30)	1.840(4)
P(2)-C(37)	1.850(4)
C(2)-C(3)	1.383(5)
C(2)-C(7)	1.394(5)
C(3)-C(4)	1.389(6)
C(4)-C(5)	1.386(6)
C(5)-C(6)	1.376(6)
C(6)-C(7)	1.380(5)
C(8)-C(9)	1.384(5)
C(8)-C(13)	1.393(5)

C(9)-C(10)	1.382(6)
C(10)-C(11)	1.386(6)
C(11)-C(12)	1.380(6)
C(12)-C(13)	1.379(5)
C(14)-C(15)	1.378(6)
C(14)-C(19)	1.387(6)
C(15)-C(16)	1.401(6)
C(16)-C(17)	1.385(8)
C(17)-C(18)	1.366(9)
C(18)-C(19)	1.376(7)
C(20)-C(21)	1.489(5)
C(21)-C(29)	1.412(6)
C(21)-C(22)	1.421(6)
C(22)-C(23)	1.417(5)
C(23)-C(24)	1.408(5)
C(24)-C(28)	1.422(5)
C(24)-C(25)	1.509(5)
C(25)-C(26)	1.512(6)
C(25)-C(27)	1.534(6)
C(28)-C(29)	1.402(5)
C(30)-C(36)	1.396(5)
C(30)-C(31)	1.407(5)
C(31)-C(33)	1.402(5)
C(31)-C(32)	1.496(5)
C(33)-C(34)	1.379(6)
C(34)-C(35)	1.390(6)
C(35)-C(36)	1.379(5)
C(37)-C(43)	1.386(5)
C(37)-C(38)	1.413(5)
C(38)-C(40)	1.384(5)
C(38)-C(39)	1.509(5)
C(40)-C(41)	1.384(6)
C(41)-C(42)	1.377(6)
C(42)-C(43)	1.381(5)
C12-C12#1	0.639(11)
C12-C22#1	0.857(12)

C12-C22	1.4000
C12-C62	1.4000
C12-C72	1.5200
C12-C62#1	1.706(11)
C12-C32#1	1.888(11)
C12-C72#1	1.975(11)
C22-C12#1	0.857(11)
C22-C62#1	1.130(13)
C22-C32	1.4001
C22-C72#1	1.449(12)
C32-C72#1	0.821(11)
C32-C42	1.4000
C32-C12#1	1.888(11)
C42-C72#1	1.024(12)
C42-C52	1.4000
C52-C62	1.4000
C52-C72#1	1.689(11)
C62-C22#1	1.130(13)
C62-C12#1	1.706(10)
C72-C32#1	0.82(2)
C72-C42#1	1.024(13)
C72-C22#1	1.449(14)
C72-C52#1	1.689(19)
C72-C12#1	1.975(11)

C(1)-Ru(1)-C(22)	93.15(14)
C(1)-Ru(1)-C(29)	145.83(14)
C(22)-Ru(1)-C(29)	66.21(15)
C(1)-Ru(1)-C(21)	111.08(14)
C(22)-Ru(1)-C(21)	37.32(15)
C(29)-Ru(1)-C(21)	36.92(15)
C(1)-Ru(1)-C(28)	167.53(14)
C(22)-Ru(1)-C(28)	77.62(14)
C(29)-Ru(1)-C(28)	36.55(14)
C(21)-Ru(1)-C(28)	66.32(14)
C(1)-Ru(1)-C(23)	102.40(14)

C(22)-Ru(1)-C(23)	36.87(14)
C(29)-Ru(1)-C(23)	77.76(14)
C(21)-Ru(1)-C(23)	66.87(14)
C(28)-Ru(1)-C(23)	65.20(14)
C(1)-Ru(1)-C(24)	131.83(14)
C(22)-Ru(1)-C(24)	65.66(13)
C(29)-Ru(1)-C(24)	65.89(13)
C(21)-Ru(1)-C(24)	78.51(13)
C(28)-Ru(1)-C(24)	36.46(13)
C(23)-Ru(1)-C(24)	35.91(13)
C(1)-Ru(1)-P(2)	82.80(10)
C(22)-Ru(1)-P(2)	135.85(10)
C(29)-Ru(1)-P(2)	93.44(11)
C(21)-Ru(1)-P(2)	103.91(10)
C(28)-Ru(1)-P(2)	109.66(10)
C(23)-Ru(1)-P(2)	170.49(10)
C(24)-Ru(1)-P(2)	142.73(10)
C(1)-Ru(1)-S(1)	75.38(9)
C(22)-Ru(1)-S(1)	139.97(11)
C(29)-Ru(1)-S(1)	137.86(11)
C(21)-Ru(1)-S(1)	171.84(10)
C(28)-Ru(1)-S(1)	106.27(10)
C(23)-Ru(1)-S(1)	107.40(10)
C(24)-Ru(1)-S(1)	93.47(9)
P(2)-Ru(1)-S(1)	81.52(3)
P(1)-S(1)-Ru(1)	82.71(4)
O(1)-S(2)-O(2)	116.64(16)
O(1)-S(2)-C(1)	112.45(17)
O(2)-S(2)-C(1)	106.82(16)
O(1)-S(2)-C(14)	107.29(18)
O(2)-S(2)-C(14)	106.49(17)
C(1)-S(2)-C(14)	106.57(18)
C(1)-P(1)-C(2)	121.64(18)
C(1)-P(1)-C(8)	110.30(17)
C(2)-P(1)-C(8)	105.95(17)
C(1)-P(1)-S(1)	96.69(12)

C(2)-P(1)-S(1)	109.15(13)
C(8)-P(1)-S(1)	113.12(13)
O(3)-P(2)-C(30)	110.29(15)
O(3)-P(2)-C(37)	107.11(15)
C(30)-P(2)-C(37)	100.64(16)
O(3)-P(2)-Ru(1)	114.97(10)
C(30)-P(2)-Ru(1)	110.61(12)
C(37)-P(2)-Ru(1)	112.25(12)
S(2)-C(1)-P(1)	125.6(2)
S(2)-C(1)-Ru(1)	121.24(18)
P(1)-C(1)-Ru(1)	97.10(16)
C(3)-C(2)-C(7)	120.1(3)
C(3)-C(2)-P(1)	126.4(3)
C(7)-C(2)-P(1)	113.4(3)
C(2)-C(3)-C(4)	119.2(4)
C(5)-C(4)-C(3)	120.8(4)
C(6)-C(5)-C(4)	119.5(4)
C(5)-C(6)-C(7)	120.6(4)
C(6)-C(7)-C(2)	119.9(4)
C(9)-C(8)-C(13)	120.4(3)
C(9)-C(8)-P(1)	120.7(3)
C(13)-C(8)-P(1)	118.4(3)
C(10)-C(9)-C(8)	119.7(4)
C(9)-C(10)-C(11)	120.0(4)
C(12)-C(11)-C(10)	120.0(4)
C(13)-C(12)-C(11)	120.5(4)
C(12)-C(13)-C(8)	119.3(4)
C(15)-C(14)-C(19)	122.6(4)
C(15)-C(14)-S(2)	119.1(3)
C(19)-C(14)-S(2)	118.2(3)
C(14)-C(15)-C(16)	117.9(5)
C(17)-C(16)-C(15)	119.1(5)
C(18)-C(17)-C(16)	121.8(5)
C(17)-C(18)-C(19)	119.9(5)
C(18)-C(19)-C(14)	118.5(5)
C(29)-C(21)-C(22)	116.8(3)

C(29)-C(21)-C(20)	122.1(4)
C(22)-C(21)-C(20)	121.0(4)
C(29)-C(21)-Ru(1)	70.7(2)
C(22)-C(21)-Ru(1)	69.8(2)
C(20)-C(21)-Ru(1)	132.2(3)
C(23)-C(22)-C(21)	122.5(3)
C(23)-C(22)-Ru(1)	74.4(2)
C(21)-C(22)-Ru(1)	72.9(2)
C(24)-C(23)-C(22)	119.2(3)
C(24)-C(23)-Ru(1)	72.7(2)
C(22)-C(23)-Ru(1)	68.7(2)
C(23)-C(24)-C(28)	119.0(3)
C(23)-C(24)-C(25)	122.5(3)
C(28)-C(24)-C(25)	118.5(3)
C(23)-C(24)-Ru(1)	71.4(2)
C(28)-C(24)-Ru(1)	70.2(2)
C(25)-C(24)-Ru(1)	132.8(2)
C(24)-C(25)-C(26)	114.4(3)
C(24)-C(25)-C(27)	108.6(3)
C(26)-C(25)-C(27)	111.4(3)
C(29)-C(28)-C(24)	120.7(4)
C(29)-C(28)-Ru(1)	70.4(2)
C(24)-C(28)-Ru(1)	73.4(2)
C(28)-C(29)-C(21)	121.7(4)
C(28)-C(29)-Ru(1)	73.0(2)
C(21)-C(29)-Ru(1)	72.4(2)
C(36)-C(30)-C(31)	118.5(3)
C(36)-C(30)-P(2)	117.9(3)
C(31)-C(30)-P(2)	123.4(3)
C(33)-C(31)-C(30)	118.0(4)
C(33)-C(31)-C(32)	117.9(3)
C(30)-C(31)-C(32)	124.1(3)
C(34)-C(33)-C(31)	122.7(4)
C(33)-C(34)-C(35)	118.9(4)
C(36)-C(35)-C(34)	119.3(4)
C(35)-C(36)-C(30)	122.5(4)

C(43)-C(37)-C(38)	118.0(3)
C(43)-C(37)-P(2)	120.8(3)
C(38)-C(37)-P(2)	121.0(3)
C(40)-C(38)-C(37)	118.8(3)
C(40)-C(38)-C(39)	118.5(3)
C(37)-C(38)-C(39)	122.6(3)
C(38)-C(40)-C(41)	122.1(4)
C(42)-C(41)-C(40)	119.1(4)
C(41)-C(42)-C(43)	119.4(4)
C(42)-C(43)-C(37)	122.4(3)
C12#1-C12-C22#1	138.4(18)
C12#1-C12-C22	24.0(11)
C22#1-C12-C22	162.4(9)
C12#1-C12-C62	107.7(9)
C22#1-C12-C62	53.8(9)
C22-C12-C62	120.0
C12#1-C12-C72	127.6(9)
C22#1-C12-C72	68.7(9)
C22-C12-C72	120.0
C62-C12-C72	120.0
C12#1-C12-C62#1	51.4(9)
C22#1-C12-C62#1	139.8(11)
C22-C12-C62#1	41.2(6)
C62-C12-C62#1	159.1(6)
C72-C12-C62#1	79.5(6)
C12#1-C12-C32#1	142.3(14)
C22#1-C12-C32#1	43.7(5)
C22-C12-C32#1	143.4(6)
C62-C12-C32#1	95.9(6)
C72-C12-C32#1	25.0(7)
C62#1-C12-C32#1	102.2(5)
C12#1-C12-C72#1	37.6(8)
C22#1-C12-C72#1	121.4(9)
C22-C12-C72#1	47.1(3)
C62-C12-C72#1	73.4(3)
C72-C12-C72#1	165.2(3)

C62#1-C12-C72#1	86.5(5)
C32#1-C12-C72#1	162.4(7)
C12#1-C22-C62#1	88.5(11)
C12#1-C22-C12	17.6(8)
C62#1-C22-C12	84.1(8)
C12#1-C22-C32	111.3(7)
C62#1-C22-C32	153.4(9)
C12-C22-C32	120.0
C12#1-C22-C72#1	77.8(7)
C62#1-C22-C72#1	157.2(14)
C12-C22-C72#1	87.8(4)
C32-C22-C72#1	33.4(4)
C72#1-C32-C42	46.4(8)
C72#1-C32-C22	76.6(8)
C42-C32-C22	120.0
C72#1-C32-C12#1	51.5(8)
C42-C32-C12#1	95.9(3)
C22-C32-C12#1	25.0(3)
C72#1-C42-C52	86.8(6)
C72#1-C42-C32	35.5(6)
C52-C42-C32	120.0
C42-C52-C62	120.0
C42-C52-C72#1	37.3(4)
C62-C52-C72#1	83.5(4)
C22#1-C62-C52	153.4(6)
C22#1-C62-C12	37.7(6)
C52-C62-C12	120.0
C22#1-C62-C12#1	54.7(4)
C52-C62-C12#1	100.5(4)
C12-C62-C12#1	20.9(4)
C32#1-C72-C42#1	98.1(13)
C32#1-C72-C22#1	70.0(11)
C42#1-C72-C22#1	156.9(19)
C32#1-C72-C12	103.4(10)
C42#1-C72-C12	150.4(13)
C22#1-C72-C12	33.4(4)

C32#1-C72-C52#1	148.1(17)
C42#1-C72-C52#1	55.9(9)
C22#1-C72-C52#1	126.2(10)
C12-C72-C52#1	96.5(6)
C32#1-C72-C12#1	113.7(12)
C42#1-C72-C12#1	135.5(16)
C22#1-C72-C12#1	45.1(3)
C12-C72-C12#1	14.9(3)
C52#1-C72-C12#1	82.5(7)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z+2

Table 63a-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for platon. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	13(1)	10(1)	13(1)	-1(1)	5(1)	0(1)
S(1)	14(1)	13(1)	12(1)	-1(1)	3(1)	0(1)
S(2)	14(1)	19(1)	13(1)	-4(1)	2(1)	1(1)
P(1)	11(1)	11(1)	13(1)	-1(1)	2(1)	0(1)
P(2)	13(1)	12(1)	12(1)	1(1)	4(1)	2(1)
O(1)	14(1)	33(2)	23(2)	-11(1)	4(1)	-2(1)
O(2)	22(1)	22(1)	19(1)	-5(1)	5(1)	4(1)
O(3)	14(1)	15(1)	16(1)	3(1)	5(1)	3(1)
C(1)	13(2)	12(2)	12(2)	-3(1)	2(2)	0(1)
C(2)	12(2)	15(2)	20(2)	0(2)	3(2)	5(1)
C(3)	16(2)	33(2)	37(2)	-21(2)	5(2)	-2(2)
C(4)	15(2)	71(4)	75(4)	-53(3)	8(2)	-7(2)
C(5)	16(2)	67(4)	72(4)	-44(3)	13(2)	2(2)
C(6)	21(2)	31(2)	37(3)	-18(2)	7(2)	4(2)
C(7)	15(2)	19(2)	23(2)	-4(2)	2(2)	0(2)
C(8)	22(2)	13(2)	14(2)	-5(2)	5(2)	-1(2)
C(9)	23(2)	16(2)	15(2)	-3(2)	1(2)	0(2)
C(10)	38(2)	17(2)	13(2)	-1(2)	4(2)	3(2)
C(11)	40(2)	13(2)	24(2)	2(2)	18(2)	1(2)
C(12)	23(2)	18(2)	28(2)	-4(2)	14(2)	-1(2)
C(13)	16(2)	17(2)	19(2)	-1(2)	4(2)	3(2)
C(14)	33(2)	21(2)	12(2)	1(2)	7(2)	5(2)
C(15)	52(3)	30(2)	30(2)	0(2)	27(2)	5(2)
C(16)	88(4)	31(3)	45(3)	-2(2)	50(3)	-5(3)
C(17)	113(5)	30(3)	20(3)	10(2)	21(3)	21(3)
C(18)	73(4)	40(3)	30(3)	5(2)	-3(3)	8(3)
C(19)	41(3)	33(3)	23(2)	-2(2)	-4(2)	9(2)
C(20)	56(3)	17(2)	42(3)	-8(2)	34(2)	-8(2)
C(21)	34(2)	9(2)	30(2)	-5(2)	21(2)	-8(2)
C(22)	26(2)	16(2)	14(2)	-1(2)	4(2)	-9(2)
C(23)	13(2)	14(2)	24(2)	0(2)	4(2)	-6(2)

C(24)	19(2)	11(2)	21(2)	-1(2)	8(2)	-4(2)
C(25)	26(2)	20(2)	23(2)	-3(2)	13(2)	-6(2)
C(26)	25(2)	28(2)	36(2)	-9(2)	21(2)	-6(2)
C(27)	50(3)	33(3)	34(3)	-6(2)	29(2)	-11(2)
C(28)	21(2)	17(2)	19(2)	1(2)	7(2)	-6(2)
C(29)	27(2)	14(2)	34(2)	5(2)	17(2)	-3(2)
C(30)	13(2)	16(2)	17(2)	-1(2)	6(2)	-1(1)
C(31)	14(2)	23(2)	18(2)	-2(2)	6(2)	-2(2)
C(32)	24(2)	32(2)	15(2)	0(2)	9(2)	1(2)
C(33)	17(2)	28(2)	27(2)	-11(2)	11(2)	-4(2)
C(34)	20(2)	19(2)	44(3)	-4(2)	15(2)	2(2)
C(35)	24(2)	20(2)	39(2)	7(2)	16(2)	6(2)
C(36)	21(2)	17(2)	21(2)	2(2)	8(2)	3(2)
C(37)	13(2)	10(2)	16(2)	2(1)	2(2)	3(1)
C(38)	17(2)	17(2)	23(2)	4(2)	7(2)	3(2)
C(39)	16(2)	31(2)	31(2)	1(2)	11(2)	-4(2)
C(40)	13(2)	25(2)	29(2)	2(2)	1(2)	-1(2)
C(41)	21(2)	20(2)	18(2)	-1(2)	-4(2)	2(2)
C(42)	25(2)	16(2)	15(2)	1(2)	4(2)	6(2)
C(43)	13(2)	13(2)	16(2)	3(1)	4(2)	2(1)
C12	18(5)	64(8)	54(14)	27(10)	-13(7)	9(5)
C22	26(6)	44(8)	57(8)	-3(6)	-7(5)	9(5)
C32	44(7)	37(7)	37(7)	1(5)	-13(5)	13(5)
C42	41(6)	40(6)	48(7)	17(5)	-10(5)	7(5)
C52	61(7)	44(6)	34(6)	17(5)	-9(5)	-5(5)
C62	25(5)	39(6)	45(6)	-1(5)	-13(5)	2(4)
C72	46(7)	63(9)	45(8)	20(7)	-1(6)	12(7)

Table 63a-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for platon.

	x	y	z	U(eq)
H(3)	9742	9210	9289	35
H(4)	10584	8817	9132	67
H(5)	10590	7614	8476	63
H(6)	9756	6774	7985	36
H(7)	8913	7157	8132	24
H(9)	9044	6818	9428	23
H(10)	8676	5414	9773	28
H(11)	7707	5063	9453	28
H(12)	7106	6131	8801	26
H(13)	7459	7596	8490	21
H(15)	7982	8750	9928	41
H(16)	8024	7298	10497	57
H(17)	8903	6682	11033	66
H(18)	9731	7422	11003	63
H(19)	9699	8811	10422	43
H(20A)	8457	13648	9240	50
H(20B)	8327	12556	9476	50
H(20C)	7833	13159	9030	50
H(22)	9113	11677	9241	24
H(23)	9405	10851	8572	21
H(25)	8546	10570	7244	26
H(26A)	9420	9813	7353	41
H(26B)	9239	9545	7858	41
H(26C)	9701	10440	7895	41
H(27A)	9121	11537	6874	53
H(27B)	9385	12184	7412	53
H(27C)	8733	12329	7067	53
H(28)	7916	11868	7444	23
H(29)	7643	12708	8112	28
H(32A)	6858	10401	9432	34

H(32B)	7034	11326	9862	34
H(32C)	7494	10830	9635	34
H(33)	6768	12968	9571	28
H(35)	6500	13947	8077	31
H(36)	6757	12292	7870	23
H(39A)	5836	10629	8145	38
H(39B)	6215	9628	8405	38
H(39C)	5602	9465	7972	38
H(40)	5485	9450	7079	28
H(41)	5828	9498	6372	27
H(42)	6756	10051	6515	23
H(43)	7332	10496	7361	17
H22	10100	6321	10374	57
H32	9680	5515	11001	55
H42	9315	3684	10857	59
H52	9370	2659	10088	63
H62	9790	3466	9462	51
H7A2	10365	6242	9620	66
H7B2	10593	4976	9487	66
H7C2	9915	5458	9099	66
H11	8068(18)	9460(30)	9105(15)	18(10)

Röntgenstrukturanalytische Daten für 63b

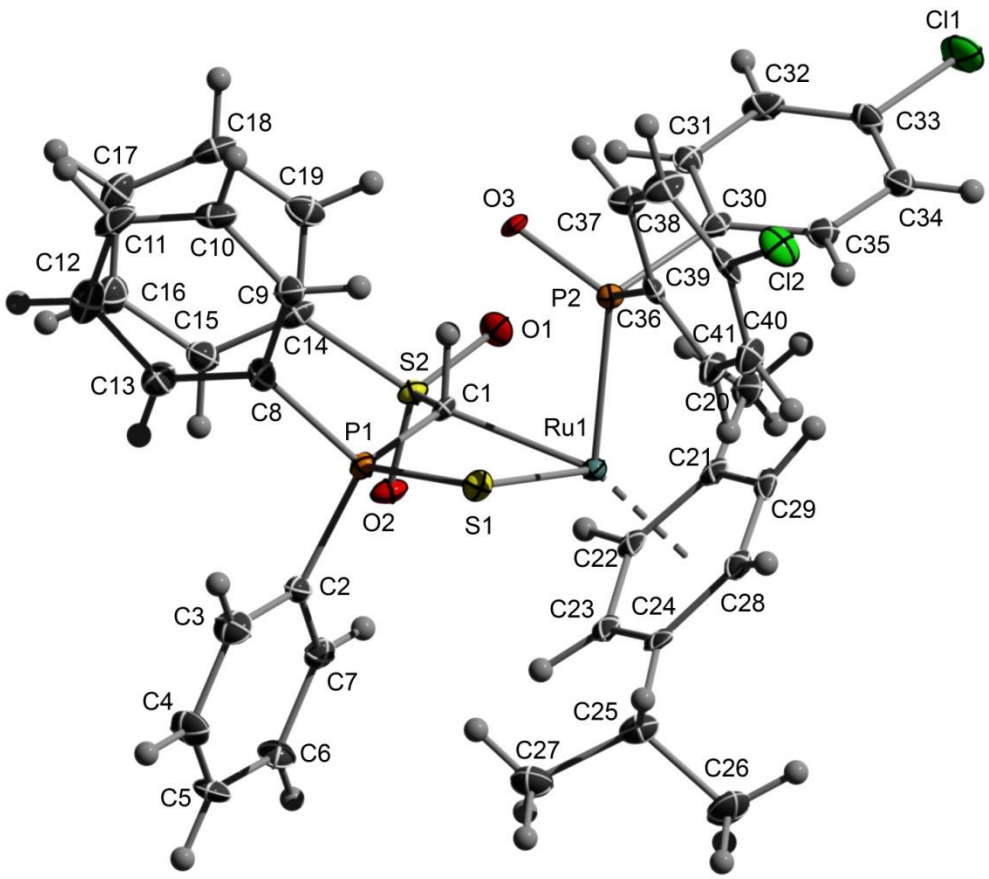

Table 63b-1. Crystal data and structure refinement for test.

Identification code	test	
Empirical formula	$C_{44}H_{41}Cl_2O_3P_2RuS_2$	
Formula weight	915.80	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 27.165(3) Å	α = 90°.
	b = 13.0735(13) Å	β = 118.508(3)°.
	c = 25.394(4) Å	γ = 90°.
Volume	7925.2(17) Å^3	
Z	8	
Density (calculated)	1.535 Mg/m^3	

Absorption coefficient	0.758 mm^{-1}
F(000)	3752
Crystal size	0.19 x 0.18 x 0.07 mm^3
Theta range for data collection	1.71 to 26.45°.
Index ranges	-33<=h<=33, -16<=k<=16, -31<=l<=31
Reflections collected	49447
Independent reflections	8141 [R(int) = 0.1049]
Completeness to theta = 26.45°	99.6 %
Absorption correction	Empirical
Max. and min. transmission	0.9467 and 0.8719
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8141 / 0 / 484
Goodness-of-fit on F^2	1.100
Final R indices [I>2sigma(I)]	R1 = 0.0432, wR2 = 0.1029
R indices (all data)	R1 = 0.0899, wR2 = 0.1581
Largest diff. peak and hole	0.764 and -1.336 e.$Å^{-3}$

Table 63b-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for test. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	1657(1)	43(1)	1484(1)	10(1)
Cl(1)	3495(1)	-3687(1)	1015(1)	30(1)
S(1)	1793(1)	1767(1)	1908(1)	13(1)
P(1)	1310(1)	2187(1)	1045(1)	11(1)
O(1)	1319(2)	-216(3)	-85(2)	18(1)
C(1)	1420(2)	1059(4)	728(2)	11(1)
Cl(2)	4475(1)	1353(1)	4222(1)	23(1)
S(2)	1025(1)	656(1)	-18(1)	12(1)
P(2)	2555(1)	357(1)	1594(1)	12(1)
O(2)	437(2)	521(3)	-195(2)	16(1)
C(2)	617(2)	2503(4)	916(2)	14(1)
O(3)	2607(2)	1164(3)	1194(2)	14(1)
C(3)	565(2)	3423(4)	1170(3)	22(1)
C(4)	65(2)	3676(4)	1162(3)	26(1)
C(5)	-383(2)	3017(4)	901(3)	21(1)
C(6)	-338(2)	2110(4)	654(2)	17(1)
C(7)	161(2)	1848(4)	655(2)	15(1)
C(8)	1576(2)	3301(4)	838(2)	14(1)
C(9)	2155(2)	3465(4)	1118(3)	17(1)
C(10)	2372(2)	4257(4)	929(3)	23(1)
C(11)	2017(3)	4885(4)	465(3)	23(1)
C(12)	1449(3)	4725(4)	177(3)	23(1)
C(13)	1224(2)	3944(4)	367(2)	18(1)
C(14)	1087(2)	1668(4)	-443(2)	14(1)
C(15)	628(2)	2262(4)	-805(2)	19(1)
C(16)	694(3)	3087(4)	-1115(3)	23(1)
C(17)	1219(2)	3304(4)	-1058(2)	21(1)
C(18)	1676(2)	2682(4)	-706(3)	22(1)
C(19)	1611(2)	1860(4)	-397(2)	20(1)
C(20)	1680(2)	-2224(4)	802(3)	20(1)
C(21)	1522(2)	-1608(4)	1203(2)	14(1)

C(22)	1003(2)	-1088(4)	969(2)	14(1)
C(23)	817(2)	-594(4)	1339(2)	15(1)
C(24)	1168(2)	-545(4)	1963(2)	14(1)
C(25)	998(2)	-70(4)	2388(2)	18(1)
C(26)	844(3)	-921(5)	2695(3)	30(2)
C(27)	530(2)	724(5)	2108(3)	25(1)
C(28)	1702(2)	-1018(4)	2202(2)	15(1)
C(29)	1870(2)	-1543(4)	1836(2)	15(1)
C(30)	2865(2)	-808(4)	1472(2)	13(1)
C(31)	2813(2)	-953(4)	905(2)	15(1)
C(32)	3011(2)	-1830(4)	764(3)	21(1)
C(33)	3258(2)	-2575(4)	1194(3)	18(1)
C(34)	3320(2)	-2465(4)	1766(3)	18(1)
C(35)	3132(2)	-1567(4)	1902(2)	16(1)
C(36)	3076(2)	694(4)	2363(2)	12(1)
C(37)	3541(2)	1270(4)	2441(3)	20(1)
C(38)	3966(2)	1488(4)	3008(3)	21(1)
C(39)	3924(2)	1135(4)	3500(2)	16(1)
C(40)	3459(2)	604(4)	3435(2)	19(1)
C(41)	3034(2)	388(4)	2865(2)	17(1)
C1A1	283(3)	6571(5)	-2329(3)	39(2)
C2A1	569(3)	5660(5)	-2155(3)	36(2)
C3A1	278(3)	4751(5)	-2337(3)	30(2)

Table 63b-3. Bond lengths [Å] and angles [°] for test.

Ru(1)-C(1)	2.164(5)
Ru(1)-C(22)	2.200(5)
Ru(1)-C(29)	2.222(5)
Ru(1)-C(28)	2.248(5)
Ru(1)-C(21)	2.248(5)
Ru(1)-C(23)	2.289(5)
Ru(1)-C(24)	2.320(5)
Ru(1)-P(2)	2.3535(14)
Ru(1)-S(1)	2.4491(14)
Cl(1)-C(33)	1.737(5)
S(1)-P(1)	2.0205(19)
P(1)-C(1)	1.773(5)
P(1)-C(2)	1.797(5)
P(1)-C(8)	1.812(5)
O(1)-S(2)	1.448(4)
C(1)-S(2)	1.753(5)
Cl(2)-C(39)	1.750(5)
S(2)-O(2)	1.447(4)
S(2)-C(14)	1.766(5)
P(2)-O(3)	1.519(4)
P(2)-C(30)	1.837(5)
P(2)-C(36)	1.837(5)
C(2)-C(7)	1.388(7)
C(2)-C(3)	1.402(8)
C(3)-C(4)	1.389(8)
C(4)-C(5)	1.377(8)
C(5)-C(6)	1.374(8)
C(6)-C(7)	1.397(7)
C(8)-C(9)	1.398(7)
C(8)-C(13)	1.401(7)
C(9)-C(10)	1.386(8)
C(10)-C(11)	1.381(8)
C(11)-C(12)	1.373(8)
C(12)-C(13)	1.389(8)

C(14)-C(15)	1.382(7)
C(14)-C(19)	1.393(7)
C(15)-C(16)	1.396(8)
C(16)-C(17)	1.392(8)
C(17)-C(18)	1.393(8)
C(18)-C(19)	1.392(8)
C(20)-C(21)	1.512(7)
C(21)-C(22)	1.416(7)
C(21)-C(29)	1.425(7)
C(22)-C(23)	1.417(7)
C(23)-C(24)	1.409(7)
C(24)-C(28)	1.419(7)
C(24)-C(25)	1.495(7)
C(25)-C(26)	1.527(8)
C(25)-C(27)	1.528(8)
C(28)-C(29)	1.397(8)
C(30)-C(31)	1.392(7)
C(30)-C(35)	1.396(7)
C(31)-C(32)	1.383(8)
C(32)-C(33)	1.376(8)
C(33)-C(34)	1.388(8)
C(34)-C(35)	1.387(8)
C(36)-C(41)	1.390(7)
C(36)-C(37)	1.400(7)
C(37)-C(38)	1.380(8)
C(38)-C(39)	1.388(8)
C(39)-C(40)	1.382(8)
C(40)-C(41)	1.384(7)
C1A1-C1A1#1	1.359(13)
C1A1-C2A1	1.375(9)
C2A1-C3A1	1.379(9)
C3A1-C3A1#1	1.333(13)

C(1)-Ru(1)-C(22)	94.10(19)
C(1)-Ru(1)-C(29)	147.07(19)
C(22)-Ru(1)-C(29)	65.98(19)

C(1)-Ru(1)-C(28)	167.47(19)
C(22)-Ru(1)-C(28)	77.4(2)
C(29)-Ru(1)-C(28)	36.41(19)
C(1)-Ru(1)-C(21)	111.94(19)
C(22)-Ru(1)-C(21)	37.11(19)
C(29)-Ru(1)-C(21)	37.18(19)
C(28)-Ru(1)-C(21)	66.55(19)
C(1)-Ru(1)-C(23)	103.24(19)
C(22)-Ru(1)-C(23)	36.75(19)
C(29)-Ru(1)-C(23)	76.90(19)
C(28)-Ru(1)-C(23)	64.47(19)
C(21)-Ru(1)-C(23)	66.44(19)
C(1)-Ru(1)-C(24)	131.77(19)
C(22)-Ru(1)-C(24)	65.57(19)
C(29)-Ru(1)-C(24)	65.45(19)
C(28)-Ru(1)-C(24)	36.15(19)
C(21)-Ru(1)-C(24)	78.51(19)
C(23)-Ru(1)-C(24)	35.58(18)
C(1)-Ru(1)-P(2)	81.45(14)
C(22)-Ru(1)-P(2)	133.28(14)
C(29)-Ru(1)-P(2)	93.38(14)
C(28)-Ru(1)-P(2)	111.08(14)
C(21)-Ru(1)-P(2)	102.03(14)
C(23)-Ru(1)-P(2)	168.44(14)
C(24)-Ru(1)-P(2)	144.64(14)
C(1)-Ru(1)-S(1)	75.15(13)
C(22)-Ru(1)-S(1)	142.17(14)
C(29)-Ru(1)-S(1)	136.58(14)
C(28)-Ru(1)-S(1)	105.84(14)
C(21)-Ru(1)-S(1)	172.26(14)
C(23)-Ru(1)-S(1)	109.59(14)
C(24)-Ru(1)-S(1)	94.48(13)
P(2)-Ru(1)-S(1)	81.75(5)
P(1)-S(1)-Ru(1)	83.65(6)
C(1)-P(1)-C(2)	119.9(2)
C(1)-P(1)-C(8)	111.1(2)

C(2)-P(1)-C(8)	106.9(2)
C(1)-P(1)-S(1)	95.92(17)
C(2)-P(1)-S(1)	109.99(18)
C(8)-P(1)-S(1)	112.95(18)
S(2)-C(1)-P(1)	126.2(3)
S(2)-C(1)-Ru(1)	122.9(3)
P(1)-C(1)-Ru(1)	98.7(2)
O(2)-S(2)-O(1)	117.1(2)
O(2)-S(2)-C(1)	112.9(2)
O(1)-S(2)-C(1)	106.0(2)
O(2)-S(2)-C(14)	108.3(2)
O(1)-S(2)-C(14)	107.3(2)
C(1)-S(2)-C(14)	104.3(2)
O(3)-P(2)-C(30)	105.4(2)
O(3)-P(2)-C(36)	105.9(2)
C(30)-P(2)-C(36)	101.2(2)
O(3)-P(2)-Ru(1)	117.67(15)
C(30)-P(2)-Ru(1)	111.60(17)
C(36)-P(2)-Ru(1)	113.43(17)
C(7)-C(2)-C(3)	119.1(5)
C(7)-C(2)-P(1)	124.3(4)
C(3)-C(2)-P(1)	116.1(4)
C(4)-C(3)-C(2)	120.7(5)
C(5)-C(4)-C(3)	119.4(5)
C(6)-C(5)-C(4)	120.6(5)
C(5)-C(6)-C(7)	120.6(5)
C(2)-C(7)-C(6)	119.6(5)
C(9)-C(8)-C(13)	119.1(5)
C(9)-C(8)-P(1)	118.9(4)
C(13)-C(8)-P(1)	121.7(4)
C(10)-C(9)-C(8)	120.0(5)
C(11)-C(10)-C(9)	120.0(5)
C(12)-C(11)-C(10)	120.9(5)
C(11)-C(12)-C(13)	119.7(6)
C(12)-C(13)-C(8)	120.2(5)
C(15)-C(14)-C(19)	121.0(5)

C(15)-C(14)-S(2)	120.5(4)
C(19)-C(14)-S(2)	118.4(4)
C(14)-C(15)-C(16)	119.4(5)
C(17)-C(16)-C(15)	119.9(5)
C(16)-C(17)-C(18)	120.3(5)
C(19)-C(18)-C(17)	119.8(5)
C(18)-C(19)-C(14)	119.4(5)
C(22)-C(21)-C(29)	115.9(5)
C(22)-C(21)-C(20)	121.3(5)
C(29)-C(21)-C(20)	122.8(5)
C(22)-C(21)-Ru(1)	69.6(3)
C(29)-C(21)-Ru(1)	70.4(3)
C(20)-C(21)-Ru(1)	132.0(4)
C(21)-C(22)-C(23)	122.7(5)
C(21)-C(22)-Ru(1)	73.3(3)
C(23)-C(22)-Ru(1)	75.1(3)
C(24)-C(23)-C(22)	120.2(5)
C(24)-C(23)-Ru(1)	73.4(3)
C(22)-C(23)-Ru(1)	68.2(3)
C(23)-C(24)-C(28)	117.7(5)
C(23)-C(24)-C(25)	123.6(5)
C(28)-C(24)-C(25)	118.6(5)
C(23)-C(24)-Ru(1)	71.0(3)
C(28)-C(24)-Ru(1)	69.1(3)
C(25)-C(24)-Ru(1)	133.8(4)
C(24)-C(25)-C(26)	108.7(5)
C(24)-C(25)-C(27)	115.0(5)
C(26)-C(25)-C(27)	111.2(5)
C(29)-C(28)-C(24)	121.5(5)
C(29)-C(28)-Ru(1)	70.8(3)
C(24)-C(28)-Ru(1)	74.7(3)
C(28)-C(29)-C(21)	121.8(5)
C(28)-C(29)-Ru(1)	72.8(3)
C(21)-C(29)-Ru(1)	72.4(3)
C(31)-C(30)-C(35)	118.0(5)
C(31)-C(30)-P(2)	117.4(4)

C(35)-C(30)-P(2)	124.5(4)
C(32)-C(31)-C(30)	121.4(5)
C(33)-C(32)-C(31)	118.9(5)
C(32)-C(33)-C(34)	121.8(5)
C(32)-C(33)-Cl(1)	119.0(4)
C(34)-C(33)-Cl(1)	119.2(4)
C(35)-C(34)-C(33)	118.2(5)
C(34)-C(35)-C(30)	121.5(5)
C(41)-C(36)-C(37)	119.3(5)
C(41)-C(36)-P(2)	123.1(4)
C(37)-C(36)-P(2)	117.6(4)
C(38)-C(37)-C(36)	120.5(5)
C(37)-C(38)-C(39)	118.9(5)
C(40)-C(39)-C(38)	121.6(5)
C(40)-C(39)-Cl(2)	118.9(4)
C(38)-C(39)-Cl(2)	119.4(4)
C(39)-C(40)-C(41)	119.0(5)
C(40)-C(41)-C(36)	120.6(5)
C1A1#1-C1A1-C2A1	120.0(4)
C1A1-C2A1-C3A1	119.5(6)
C3A1#1-C3A1-C2A1	120.5(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z-1/2

Table 63b-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for test. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	10(1)	10(1)	11(1)	1(1)	6(1)	-1(1)
Cl(1)	38(1)	20(1)	45(1)	-7(1)	31(1)	3(1)
S(1)	15(1)	14(1)	10(1)	-1(1)	5(1)	-1(1)
P(1)	12(1)	10(1)	12(1)	-1(1)	6(1)	-1(1)
O(1)	24(2)	13(2)	19(2)	-5(2)	13(2)	0(2)
C(1)	13(3)	11(3)	10(3)	3(2)	7(2)	0(2)
Cl(2)	15(1)	26(1)	22(1)	-5(1)	3(1)	-1(1)
S(2)	13(1)	13(1)	12(1)	-1(1)	6(1)	-2(1)
P(2)	11(1)	12(1)	14(1)	1(1)	7(1)	0(1)
O(2)	13(2)	20(2)	15(2)	-2(2)	7(2)	-5(2)
C(2)	12(3)	17(3)	14(3)	3(2)	7(2)	2(2)
O(3)	14(2)	14(2)	18(2)	7(2)	11(2)	-1(2)
C(3)	20(3)	18(3)	28(3)	-5(3)	12(3)	-5(2)
C(4)	29(4)	15(3)	42(4)	-6(3)	24(3)	0(2)
C(5)	13(3)	28(3)	28(3)	3(3)	14(3)	4(2)
C(6)	11(3)	22(3)	17(3)	-3(2)	5(2)	-2(2)
C(7)	18(3)	16(3)	12(3)	0(2)	8(2)	0(2)
C(8)	20(3)	8(3)	16(3)	-4(2)	10(2)	0(2)
C(9)	19(3)	13(3)	21(3)	-2(2)	12(3)	-1(2)
C(10)	22(3)	24(3)	30(3)	-5(3)	19(3)	-6(2)
C(11)	35(4)	16(3)	32(3)	-3(3)	25(3)	-10(3)
C(12)	38(4)	16(3)	16(3)	-1(2)	13(3)	0(3)
C(13)	19(3)	17(3)	17(3)	-3(2)	8(2)	-4(2)
C(14)	18(3)	16(3)	11(3)	-2(2)	9(2)	-6(2)
C(15)	17(3)	23(3)	18(3)	1(2)	9(3)	3(2)
C(16)	23(3)	24(3)	20(3)	6(3)	9(3)	2(3)
C(17)	27(3)	21(3)	16(3)	1(2)	10(3)	-4(3)
C(18)	23(3)	27(3)	21(3)	-1(3)	16(3)	-7(3)
C(19)	18(3)	25(3)	17(3)	-3(2)	9(3)	1(2)
C(20)	25(3)	10(3)	28(3)	-1(2)	16(3)	-2(2)
C(21)	14(2)	9(2)	20(2)	2(2)	9(2)	-5(2)

C(22)	14(2)	9(2)	20(2)	2(2)	9(2)	-5(2)
C(23)	13(3)	13(3)	19(3)	4(2)	8(2)	-3(2)
C(24)	18(3)	9(3)	20(3)	0(2)	14(3)	-5(2)
C(25)	19(3)	21(3)	17(3)	-3(2)	11(2)	-5(2)
C(26)	44(4)	33(4)	29(3)	6(3)	29(3)	3(3)
C(27)	26(3)	29(3)	27(3)	-1(3)	18(3)	3(3)
C(28)	16(3)	13(3)	17(3)	3(2)	8(2)	-3(2)
C(29)	14(3)	8(3)	20(3)	4(2)	6(2)	-2(2)
C(30)	11(3)	17(3)	12(3)	1(2)	5(2)	-3(2)
C(31)	12(3)	18(3)	14(3)	2(2)	5(2)	-1(2)
C(32)	28(3)	24(3)	17(3)	-5(3)	17(3)	-2(3)
C(33)	19(3)	13(3)	25(3)	-3(2)	13(3)	2(2)
C(34)	15(3)	17(3)	24(3)	0(2)	11(3)	1(2)
C(35)	17(3)	18(3)	17(3)	0(2)	10(2)	0(2)
C(36)	11(3)	11(3)	14(3)	2(2)	5(2)	5(2)
C(37)	16(3)	23(3)	20(3)	-1(2)	10(3)	-2(2)
C(38)	17(3)	21(3)	23(3)	-5(2)	8(3)	-11(2)
C(39)	9(3)	15(3)	16(3)	-3(2)	1(2)	5(2)
C(40)	22(3)	20(3)	15(3)	5(2)	7(3)	1(2)
C(41)	14(3)	15(3)	17(3)	3(2)	4(2)	-4(2)
C1A1	38(4)	35(4)	39(4)	3(3)	15(4)	-4(3)
C2A1	20(3)	41(4)	41(4)	14(3)	10(3)	-1(3)
C3A1	33(3)	29(4)	31(4)	5(3)	18(3)	3(3)

Table 63b-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for test.

	x	y	z	U(eq)
H(1)	1791	1204	751	13
H(3)	875	3877	1348	26
H(4)	33	4298	1337	31
H(5)	-727	3190	891	25
H(6)	-649	1656	481	21
H(7)	188	1225	477	18
H(9)	2399	3034	1438	20
H(10)	2765	4369	1119	27
H(11)	2169	5434	343	28
H(12)	1210	5148	-151	28
H(13)	830	3846	176	22
H(15)	270	2111	-842	22
H(16)	380	3499	-1365	27
H(17)	1265	3878	-1259	26
H(18)	2031	2820	-678	26
H(19)	1921	1433	-157	24
H(20A)	1422	-2802	633	29
H(20B)	2063	-2481	1037	29
H(20C)	1657	-1789	477	29
H(22)	779	-1000	525	17
H(23)	476	-149	1150	18
H(25)	1334	287	2705	21
H(26A)	501	-1261	2401	46
H(26B)	783	-627	3014	46
H(26C)	1150	-1420	2868	46
H(27A)	648	1280	1935	38
H(27B)	450	1002	2418	38
H(27C)	192	401	1794	38
H(28)	1984	-880	2628	18
H(29)	2268	-1774	2012	18

H(31)	2638	-440	608	18
H(32)	2978	-1915	377	25
H(34)	3486	-2990	2057	22
H(35)	3187	-1467	2297	20
H(37)	3563	1512	2100	23
H(38)	4283	1873	3061	25
H(40)	3431	390	3778	23
H(41)	2711	27	2815	20
H1A1	481	7201	-2209	47
H2A1	965	5657	-1911	43
H3A1	476	4121	-2228	35

Röntgenstrukturanalytische Daten für 65a

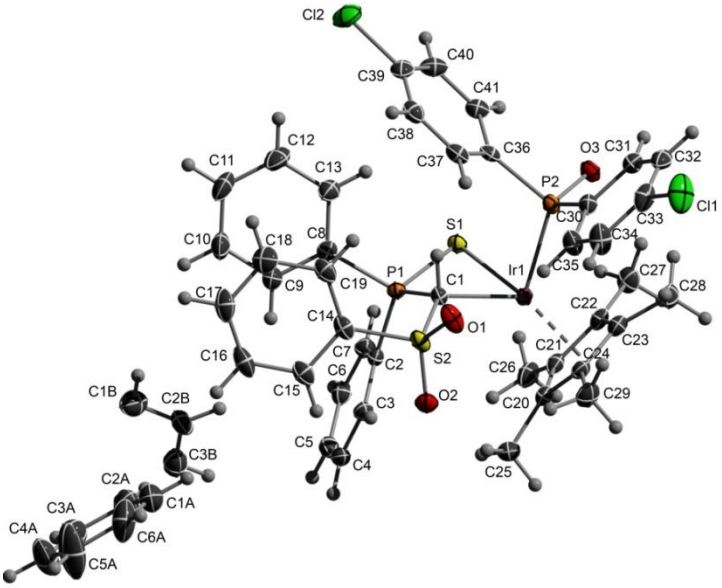

Table 65a-1. Crystal data and structure refinement for platon.

Identification code	platon	
Empirical formula	$C_{50}H_{48}Cl_2IrO_3P_2S_2$	
Formula weight	4344.18	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 13.0188(6) Å	α = 90°.
	b = 23.4359(10) Å	β = 128.022(2)°.
	c = 18.8971(7) Å	γ = 90°.
Volume	4542.0(3) $Å^3$	
Z	4	
Density (calculated)	1.588 Mg/m^3	
Absorption coefficient	3.262 mm^{-1}	
F(000)	2180	
Crystal size	0.14 x 0.14 x 0.06 mm^3	

Theta range for data collection	1.62 to 26.52°.
Index ranges	-16<=h<=16, -29<=k<=29, -23<=l<=23
Reflections collected	74061
Independent reflections	9352 [R(int) = 0.0368]
Completeness to theta = 26.52°	99.1 %
Absorption correction	Empirical
Max. and min. transmission	0.8410 and 0.6580
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9352 / 0 / 546
Goodness-of-fit on F^2	1.030
Final R indices [I>2sigma(I)]	R1 = 0.0218, wR2 = 0.0489
R indices (all data)	R1 = 0.0280, wR2 = 0.0514
Largest diff. peak and hole	0.984 and -0.429 e.$Å^{-3}$

Table 65a-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for platon. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	8154(1)	590(1)	1621(1)	16(1)
Cl(1)	12016(1)	3126(1)	1856(1)	46(1)
Cl(2)	3177(1)	3050(1)	-218(1)	39(1)
S(1)	5819(1)	468(1)	789(1)	19(1)
S(2)	8832(1)	1301(1)	3497(1)	20(1)
P(1)	6290(1)	630(1)	1997(1)	16(1)
P(2)	7588(1)	1325(1)	640(1)	18(1)
O(1)	9592(2)	836(1)	4098(1)	26(1)
O(2)	9519(2)	1775(1)	3477(1)	29(1)
O(3)	7074(2)	1126(1)	-282(1)	23(1)
C(1)	7690(2)	1063(1)	2384(2)	16(1)
C(2)	6478(2)	-21(1)	2574(2)	18(1)
C(3)	7401(2)	-115(1)	3490(2)	20(1)
C(4)	7334(3)	-607(1)	3868(2)	24(1)
C(5)	6335(3)	-994(1)	3340(2)	26(1)
C(6)	5419(3)	-906(1)	2427(2)	25(1)

C(7)	5492(2)	-421(1)	2043(2)	22(1)
C(8)	5000(2)	1005(1)	1911(2)	20(1)
C(9)	4645(3)	868(1)	2448(2)	26(1)
C(10)	3662(3)	1169(1)	2365(2)	35(1)
C(11)	3029(3)	1602(1)	1746(2)	39(1)
C(12)	3378(3)	1744(1)	1213(2)	36(1)
C(13)	4359(3)	1446(1)	1292(2)	26(1)
C(14)	7883(2)	1574(1)	3801(2)	21(1)
C(15)	7958(3)	1320(1)	4492(2)	26(1)
C(16)	7196(3)	1531(1)	4710(2)	32(1)
C(17)	6360(3)	1978(1)	4240(2)	34(1)
C(18)	6292(3)	2234(1)	3554(2)	34(1)
C(19)	7065(3)	2035(1)	3336(2)	27(1)
C(20)	9574(2)	-115(1)	2584(2)	23(1)
C(21)	8620(3)	-356(1)	1733(2)	23(1)
C(22)	8665(2)	-75(1)	1074(2)	22(1)
C(23)	9709(2)	329(1)	1545(2)	22(1)
C(24)	10212(2)	338(1)	2465(2)	22(1)
C(25)	9994(3)	-335(1)	3467(2)	32(1)
C(26)	7721(3)	-842(1)	1519(2)	30(1)
C(27)	7920(3)	-243(1)	111(2)	30(1)
C(28)	10256(3)	633(1)	1156(2)	28(1)
C(29)	11387(3)	656(1)	3212(2)	32(1)
C(30)	8912(2)	1831(1)	1036(2)	21(1)
C(31)	8994(2)	2079(1)	404(2)	24(1)
C(32)	9941(3)	2475(1)	649(2)	28(1)
C(33)	10808(3)	2631(1)	1541(2)	29(1)
C(34)	10758(3)	2393(1)	2182(2)	33(1)
C(35)	9814(3)	1987(1)	1929(2)	27(1)
C(36)	6378(2)	1833(1)	472(2)	19(1)
C(37)	6636(3)	2281(1)	1051(2)	22(1)
C(38)	5669(3)	2659(1)	849(2)	25(1)
C(39)	4428(3)	2587(1)	58(2)	25(1)
C(40)	4136(3)	2153(1)	-532(2)	27(1)
C(122)	5108(2)	1781(1)	-327(2)	22(1)
C(1A)	8835(3)	1426(2)	7345(2)	45(1)

C(2A)	7951(3)	1001(2)	7104(2)	45(1)
C(3A)	7639(3)	852(2)	7654(2)	44(1)
C(4A)	8228(4)	1132(2)	8449(2)	63(1)
C(5A)	9138(5)	1553(2)	8693(3)	86(2)
C(6A)	9415(4)	1706(2)	8133(3)	55(1)
C(1B)	5061(3)	562(1)	4836(2)	41(1)
C(2B)	5533(3)	151(2)	4589(2)	43(1)
C(3B)	4536(3)	411(2)	5251(2)	39(1)

Table 65a-3. Bond lengths [Å] and angles [°] for platon.

Ir(1)-C(1)	2.178(2)
Ir(1)-C(22)	2.188(2)
Ir(1)-C(24)	2.192(2)
Ir(1)-C(23)	2.204(2)
Ir(1)-C(21)	2.274(3)
Ir(1)-P(2)	2.2947(6)
Ir(1)-C(20)	2.306(2)
Ir(1)-S(1)	2.4310(6)
Ir(1)-P(1)	2.9199(7)
Cl(1)-C(33)	1.737(3)
Cl(2)-C(39)	1.749(3)
S(1)-P(1)	2.0015(9)
S(2)-O(1)	1.4394(19)
S(2)-O(2)	1.4413(18)
S(2)-C(1)	1.759(2)
S(2)-C(14)	1.770(3)
P(1)-C(1)	1.802(2)
P(1)-C(2)	1.802(2)
P(1)-C(8)	1.811(3)
P(2)-O(3)	1.5050(17)
P(2)-C(30)	1.829(3)
P(2)-C(36)	1.840(3)
C(2)-C(3)	1.387(3)
C(2)-C(7)	1.397(3)

C(3)-C(4)	1.388(3)
C(4)-C(5)	1.384(4)
C(5)-C(6)	1.381(4)
C(6)-C(7)	1.382(4)
C(8)-C(9)	1.387(4)
C(8)-C(13)	1.389(4)
C(9)-C(10)	1.384(4)
C(10)-C(11)	1.374(4)
C(11)-C(12)	1.377(4)
C(12)-C(13)	1.381(4)
C(14)-C(15)	1.382(3)
C(14)-C(19)	1.388(4)
C(15)-C(16)	1.380(4)
C(16)-C(17)	1.373(4)
C(17)-C(18)	1.380(4)
C(18)-C(19)	1.380(4)
C(20)-C(21)	1.410(4)
C(20)-C(24)	1.449(4)
C(20)-C(25)	1.491(4)
C(21)-C(22)	1.440(4)
C(21)-C(26)	1.498(4)
C(22)-C(23)	1.430(4)
C(22)-C(27)	1.495(4)
C(23)-C(24)	1.433(4)
C(23)-C(28)	1.482(4)
C(24)-C(29)	1.493(4)
C(30)-C(35)	1.385(4)
C(30)-C(31)	1.391(3)
C(31)-C(32)	1.375(4)
C(32)-C(33)	1.380(4)
C(33)-C(34)	1.373(4)
C(34)-C(35)	1.385(4)
C(36)-C(122)	1.397(3)
C(36)-C(37)	1.399(3)
C(37)-C(38)	1.387(4)
C(38)-C(39)	1.378(4)

C(39)-C(40)	1.378(4)
C(40)-C(122)	1.382(4)
C(1A)-C(6A)	1.354(5)
C(1A)-C(2A)	1.370(5)
C(2A)-C(3A)	1.374(4)
C(3A)-C(4A)	1.362(5)
C(4A)-C(5A)	1.384(5)
C(5A)-C(6A)	1.360(5)
C(1B)-C(3B)	1.367(4)
C(1B)-C(2B)	1.369(5)
C(2B)-C(3B)#1	1.366(4)
C(3B)-C(2B)#1	1.366(4)

C(1)-Ir(1)-C(22)	164.64(9)
C(1)-Ir(1)-C(24)	111.62(9)
C(22)-Ir(1)-C(24)	63.95(9)
C(1)-Ir(1)-C(23)	145.63(9)
C(22)-Ir(1)-C(23)	38.00(9)
C(24)-Ir(1)-C(23)	38.04(9)
C(1)-Ir(1)-C(21)	127.04(9)
C(22)-Ir(1)-C(21)	37.60(9)
C(24)-Ir(1)-C(21)	62.17(10)
C(23)-Ir(1)-C(21)	62.06(9)
C(1)-Ir(1)-P(2)	94.03(7)
C(22)-Ir(1)-P(2)	101.11(7)
C(24)-Ir(1)-P(2)	115.49(7)
C(23)-Ir(1)-P(2)	90.36(7)
C(21)-Ir(1)-P(2)	137.84(7)
C(1)-Ir(1)-C(20)	104.91(9)
C(22)-Ir(1)-C(20)	62.16(9)
C(24)-Ir(1)-C(20)	37.48(9)
C(23)-Ir(1)-C(20)	61.99(9)
C(21)-Ir(1)-C(20)	35.85(9)
P(2)-Ir(1)-C(20)	151.43(6)
C(1)-Ir(1)-S(1)	75.05(6)
C(22)-Ir(1)-S(1)	103.50(7)

C(24)-Ir(1)-S(1)	156.91(7)
C(23)-Ir(1)-S(1)	139.32(7)
C(21)-Ir(1)-S(1)	95.80(7)
P(2)-Ir(1)-S(1)	85.11(2)
C(20)-Ir(1)-S(1)	120.07(7)
C(1)-Ir(1)-P(1)	38.00(6)
C(22)-Ir(1)-P(1)	132.70(7)
C(24)-Ir(1)-P(1)	131.16(7)
C(23)-Ir(1)-P(1)	163.71(7)
C(21)-Ir(1)-P(1)	102.92(7)
P(2)-Ir(1)-P(1)	105.72(2)
C(20)-Ir(1)-P(1)	102.34(6)
S(1)-Ir(1)-P(1)	42.722(19)
P(1)-S(1)-Ir(1)	81.79(3)
O(1)-S(2)-O(2)	117.87(11)
O(1)-S(2)-C(1)	111.55(11)
O(2)-S(2)-C(1)	107.07(11)
O(1)-S(2)-C(14)	107.21(12)
O(2)-S(2)-C(14)	107.36(12)
C(1)-S(2)-C(14)	104.96(11)
C(1)-P(1)-C(2)	120.33(11)
C(1)-P(1)-C(8)	114.44(11)
C(2)-P(1)-C(8)	103.75(11)
C(1)-P(1)-S(1)	95.33(8)
C(2)-P(1)-S(1)	111.15(8)
C(8)-P(1)-S(1)	111.95(8)
C(1)-P(1)-Ir(1)	48.09(7)
C(2)-P(1)-Ir(1)	107.24(8)
C(8)-P(1)-Ir(1)	149.01(9)
S(1)-P(1)-Ir(1)	55.49(2)
O(3)-P(2)-C(30)	108.08(11)
O(3)-P(2)-C(36)	106.12(10)
C(30)-P(2)-C(36)	98.15(11)
O(3)-P(2)-Ir(1)	113.26(8)
C(30)-P(2)-Ir(1)	113.77(8)
C(36)-P(2)-Ir(1)	116.12(8)

S(2)-C(1)-P(1)	124.19(13)
S(2)-C(1)-Ir(1)	125.35(12)
P(1)-C(1)-Ir(1)	93.91(10)
C(3)-C(2)-C(7)	119.7(2)
C(3)-C(2)-P(1)	125.45(19)
C(7)-C(2)-P(1)	114.35(18)
C(2)-C(3)-C(4)	119.6(2)
C(5)-C(4)-C(3)	120.2(2)
C(6)-C(5)-C(4)	120.6(2)
C(5)-C(6)-C(7)	119.5(2)
C(6)-C(7)-C(2)	120.4(2)
C(9)-C(8)-C(13)	119.3(2)
C(9)-C(8)-P(1)	122.0(2)
C(13)-C(8)-P(1)	118.7(2)
C(10)-C(9)-C(8)	120.1(3)
C(11)-C(10)-C(9)	120.0(3)
C(10)-C(11)-C(12)	120.4(3)
C(11)-C(12)-C(13)	119.9(3)
C(12)-C(13)-C(8)	120.2(3)
C(15)-C(14)-C(19)	120.8(2)
C(15)-C(14)-S(2)	119.6(2)
C(19)-C(14)-S(2)	119.6(2)
C(16)-C(15)-C(14)	118.9(3)
C(17)-C(16)-C(15)	120.6(3)
C(16)-C(17)-C(18)	120.5(3)
C(17)-C(18)-C(19)	119.7(3)
C(18)-C(19)-C(14)	119.5(3)
C(21)-C(20)-C(24)	107.6(2)
C(21)-C(20)-C(25)	126.7(2)
C(24)-C(20)-C(25)	125.2(2)
C(21)-C(20)-Ir(1)	70.86(14)
C(24)-C(20)-Ir(1)	67.01(13)
C(25)-C(20)-Ir(1)	133.93(18)
C(20)-C(21)-C(22)	109.1(2)
C(20)-C(21)-C(26)	127.1(2)
C(22)-C(21)-C(26)	123.7(2)

C(20)-C(21)-Ir(1)	73.29(15)
C(22)-C(21)-Ir(1)	67.95(14)
C(26)-C(21)-Ir(1)	126.55(19)
C(23)-C(22)-C(21)	107.1(2)
C(23)-C(22)-C(27)	125.9(2)
C(21)-C(22)-C(27)	126.2(2)
C(23)-C(22)-Ir(1)	71.61(14)
C(21)-C(22)-Ir(1)	74.45(15)
C(27)-C(22)-Ir(1)	127.22(18)
C(22)-C(23)-C(24)	108.2(2)
C(22)-C(23)-C(28)	125.0(2)
C(24)-C(23)-C(28)	126.4(2)
C(22)-C(23)-Ir(1)	70.39(14)
C(24)-C(23)-Ir(1)	70.54(14)
C(28)-C(23)-Ir(1)	129.72(19)
C(23)-C(24)-C(20)	107.5(2)
C(23)-C(24)-C(29)	126.3(2)
C(20)-C(24)-C(29)	124.8(2)
C(23)-C(24)-Ir(1)	71.42(14)
C(20)-C(24)-Ir(1)	75.51(14)
C(29)-C(24)-Ir(1)	129.36(19)
C(35)-C(30)-C(31)	118.7(2)
C(35)-C(30)-P(2)	123.2(2)
C(31)-C(30)-P(2)	118.09(19)
C(32)-C(31)-C(30)	121.3(3)
C(31)-C(32)-C(33)	118.7(3)
C(34)-C(33)-C(32)	121.4(3)
C(34)-C(33)-Cl(1)	119.6(2)
C(32)-C(33)-Cl(1)	118.9(2)
C(33)-C(34)-C(35)	119.3(3)
C(30)-C(35)-C(34)	120.5(3)
C(122)-C(36)-C(37)	117.8(2)
C(122)-C(36)-P(2)	116.53(19)
C(37)-C(36)-P(2)	125.60(19)
C(38)-C(37)-C(36)	121.5(2)
C(39)-C(38)-C(37)	118.7(2)

C(38)-C(39)-C(40)	121.5(2)
C(38)-C(39)-Cl(2)	120.1(2)
C(40)-C(39)-Cl(2)	118.4(2)
C(39)-C(40)-C(122)	119.4(2)
C(40)-C(122)-C(36)	121.1(2)
C(6A)-C(1A)-C(2A)	120.2(3)
C(1A)-C(2A)-C(3A)	120.8(3)
C(4A)-C(3A)-C(2A)	118.9(3)
C(3A)-C(4A)-C(5A)	119.8(3)
C(6A)-C(5A)-C(4A)	120.8(4)
C(1A)-C(6A)-C(5A)	119.4(4)
C(3B)-C(1B)-C(2B)	120.0(3)
C(3B)#1-C(2B)-C(1B)	119.9(3)
C(2B)#1-C(3B)-C(1B)	120.1(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z+1

Table 65a-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for platon. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	14(1)	19(1)	14(1)	-1(1)	8(1)	-1(1)
Cl(1)	51(1)	34(1)	73(1)	-18(1)	48(1)	-21(1)
Cl(2)	38(1)	30(1)	41(1)	3(1)	21(1)	14(1)
S(1)	16(1)	23(1)	14(1)	-2(1)	8(1)	-2(1)
S(2)	20(1)	26(1)	14(1)	-4(1)	10(1)	-7(1)
P(1)	15(1)	18(1)	15(1)	-1(1)	8(1)	-1(1)
P(2)	18(1)	21(1)	15(1)	-1(1)	10(1)	-2(1)
O(1)	19(1)	35(1)	16(1)	-1(1)	7(1)	0(1)
O(2)	32(1)	34(1)	25(1)	-9(1)	19(1)	-17(1)
O(3)	25(1)	28(1)	16(1)	-2(1)	13(1)	-1(1)
C(1)	17(1)	18(1)	15(1)	-1(1)	11(1)	-2(1)
C(2)	17(1)	19(1)	21(1)	2(1)	13(1)	3(1)

C(3)	17(1)	23(1)	19(1)	0(1)	10(1)	0(1)
C(4)	24(1)	28(2)	20(1)	5(1)	13(1)	8(1)
C(5)	35(2)	23(2)	33(2)	5(1)	27(1)	4(1)
C(6)	26(1)	23(2)	29(2)	-2(1)	19(1)	-2(1)
C(7)	19(1)	24(1)	19(1)	-2(1)	11(1)	-1(1)
C(8)	18(1)	21(1)	20(1)	-4(1)	11(1)	-2(1)
C(9)	24(1)	29(2)	28(2)	1(1)	18(1)	2(1)
C(10)	37(2)	39(2)	46(2)	2(1)	34(2)	3(1)
C(11)	30(2)	36(2)	60(2)	1(2)	32(2)	6(1)
C(12)	33(2)	25(2)	50(2)	9(1)	26(2)	9(1)
C(13)	26(1)	22(2)	33(2)	3(1)	19(1)	1(1)
C(14)	25(1)	22(1)	18(1)	-8(1)	14(1)	-9(1)
C(15)	33(2)	25(2)	22(1)	-6(1)	18(1)	-7(1)
C(16)	45(2)	34(2)	30(2)	-12(1)	30(2)	-15(1)
C(17)	44(2)	31(2)	43(2)	-15(1)	35(2)	-10(1)
C(18)	41(2)	25(2)	34(2)	-7(1)	23(2)	0(1)
C(19)	35(2)	26(2)	22(1)	-5(1)	19(1)	-5(1)
C(20)	19(1)	27(2)	26(1)	5(1)	15(1)	6(1)
C(21)	21(1)	19(1)	34(2)	2(1)	20(1)	4(1)
C(22)	21(1)	21(1)	27(1)	-2(1)	16(1)	3(1)
C(23)	18(1)	23(1)	26(1)	0(1)	14(1)	2(1)
C(24)	15(1)	26(1)	21(1)	2(1)	10(1)	5(1)
C(25)	30(2)	38(2)	30(2)	13(1)	20(1)	13(1)
C(26)	28(1)	22(2)	44(2)	0(1)	25(1)	0(1)
C(27)	31(2)	31(2)	27(2)	-8(1)	17(1)	0(1)
C(28)	26(1)	30(2)	36(2)	2(1)	24(1)	2(1)
C(29)	16(1)	44(2)	27(2)	-4(1)	10(1)	-1(1)
C(30)	22(1)	21(1)	24(1)	-1(1)	16(1)	0(1)
C(31)	21(1)	27(2)	26(1)	4(1)	14(1)	5(1)
C(32)	28(1)	23(2)	38(2)	11(1)	23(1)	7(1)
C(33)	28(2)	20(2)	47(2)	-7(1)	27(2)	-6(1)
C(34)	31(2)	39(2)	34(2)	-16(1)	23(1)	-15(1)
C(35)	28(1)	34(2)	24(2)	-5(1)	18(1)	-7(1)
C(36)	21(1)	19(1)	16(1)	3(1)	12(1)	-2(1)
C(37)	25(1)	23(1)	17(1)	0(1)	12(1)	-5(1)
C(38)	35(2)	21(1)	25(2)	0(1)	21(1)	-2(1)

C(39)	29(1)	18(1)	30(2)	7(1)	19(1)	5(1)
C(40)	24(1)	23(2)	22(1)	2(1)	9(1)	-2(1)
C(122)	25(1)	19(1)	20(1)	0(1)	12(1)	-2(1)
C(1A)	43(2)	58(2)	43(2)	8(2)	32(2)	9(2)
C(2A)	39(2)	63(2)	33(2)	-7(2)	22(2)	5(2)
C(3A)	40(2)	49(2)	44(2)	0(2)	25(2)	-1(2)
C(4A)	62(3)	98(3)	45(2)	-7(2)	41(2)	-15(2)
C(5A)	83(3)	132(4)	72(3)	-62(3)	63(3)	-52(3)
C(6A)	61(2)	52(2)	80(3)	-23(2)	58(2)	-14(2)
C(1B)	32(2)	40(2)	50(2)	11(2)	24(2)	-1(1)
C(2B)	37(2)	65(2)	35(2)	14(2)	27(2)	4(2)
C(3B)	37(2)	51(2)	34(2)	-4(1)	24(2)	2(2)

Table 65a-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for platon.

	x	y	z	U(eq)
H(1)	7306	1418	2042	20
H(3)	8060	150	3848	25
H(4)	7963	-676	4479	28
H(5)	6279	-1317	3601	32
H(6)	4758	-1172	2072	29
H(7)	4880	-362	1428	26
H(9)	5068	573	2864	31
H(10)	3429	1079	2729	42
H(11)	2361	1800	1687	46
H(12)	2953	2040	800	43
H(13)	4592	1541	930	31
H(15)	8513	1012	4804	31
H(16)	7249	1368	5181	39
H(17)	5836	2111	4384	41
H(18)	5728	2539	3239	40
H(19)	7036	2210	2883	32

H(25A)	10163	-19	3850	48
H(25B)	10774	-557	3743	48
H(25C)	9317	-569	3376	48
H(26A)	7665	-888	1999	45
H(26B)	8052	-1186	1451	45
H(26C)	6870	-762	971	45
H(27A)	7090	-397	-106	45
H(27B)	8403	-526	58	45
H(27C)	7790	86	-239	45
H(28A)	10868	391	1177	42
H(28B)	10690	974	1496	42
H(28C)	9563	733	544	42
H(29A)	12153	430	3455	47
H(29B)	11306	735	3675	47
H(29C)	11457	1009	2987	47
H(31)	8396	1976	-197	29
H(32)	9995	2634	222	33
H(34)	11350	2503	2780	40
H(35)	9786	1818	2362	33
H(37)	7477	2326	1584	26
H(38)	5854	2954	1240	30
H(40)	3293	2111	-1063	32
H(122)	4914	1490	-728	27
H(1A)	9037	1522	6967	54
H(2A)	7558	811	6562	55
H(3A)	7035	564	7486	53
H(4A)	8019	1041	8826	76
H(5A)	9564	1733	9247	103
H(6A)	9998	2002	8290	66
H(1B)	5098	945	4721	50
H(2B)	5899	254	4314	51
H(3B)	4226	690	5425	47

Röntgenstrukturanalytische Daten für 65b

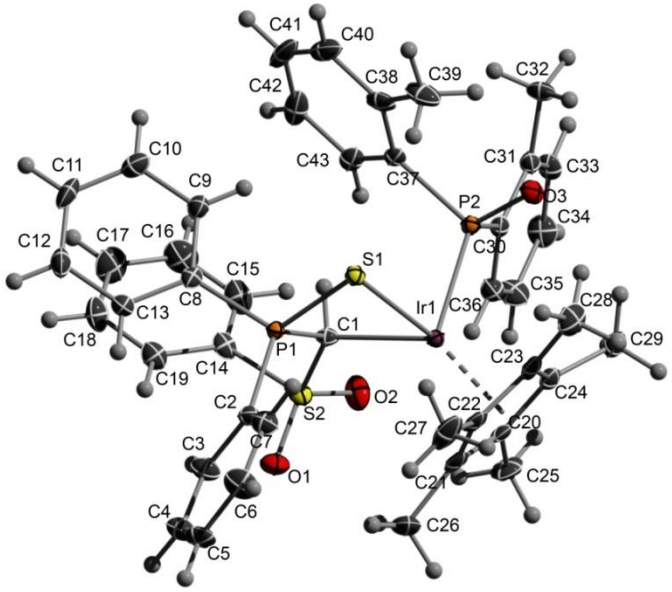

Table 65b-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	$C_{43}H_{45}IrO_3P_2S_2$	
Formula weight	928.05	
Temperature	102(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P(2)1/c	
Unit cell dimensions	a = 11.5779(12) Å	α = 90°.
	b = 19.1195(19) Å	β = 96.535(3)°.
	c = 17.1015(17) Å	γ = 90°.
Volume	3761.1(7) $Å^3$	
Z	4	
Density (calculated)	1.639 Mg/m^3	
Absorption coefficient	3.787 mm^{-1}	
F(000)	1864	
Crystal size	0.31 x 0.28 x 0.21 mm^3	
Theta range for data collection	1.60 to 26.44°.	
Index ranges	-14<=h<=14, -23<=k<=23, -21<=l<=21	

Reflections collected	50945
Independent reflections	7715 [R(int) = 0.0449]
Completeness to theta = 26.44°	99.6 %
Absorption correction	Empirical
Max. and min. transmission	0.5021 and 0.3894
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7715 / 0 / 461
Goodness-of-fit on F^2	1.145
Final R indices [I>2sigma(I)]	R1 = 0.0213, wR2 = 0.0498
R indices (all data)	R1 = 0.0290, wR2 = 0.0643
Largest diff. peak and hole	0.562 and -0.491 e.$Å^{-3}$

Table 65b-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	1859(1)	1312(1)	8491(1)	12(1)
S(1)	2992(1)	360(1)	9142(1)	14(1)
P(1)	4333(1)	870(1)	8749(1)	12(1)
O(1)	4632(2)	2448(1)	7835(2)	25(1)
C(1)	3453(3)	1264(2)	7922(2)	14(1)
S(2)	3972(1)	1940(1)	7353(1)	17(1)
P(2)	879(1)	506(1)	7643(1)	13(1)
O(2)	3021(2)	2189(1)	6818(2)	27(1)
C(2)	5090(3)	1443(2)	9485(2)	16(1)
O(3)	-127(2)	187(1)	8002(1)	20(1)
C(3)	5894(3)	1946(2)	9304(2)	22(1)
C(4)	6517(3)	2321(2)	9896(2)	26(1)
C(5)	6344(3)	2209(2)	10669(2)	25(1)
C(6)	5578(3)	1706(2)	10854(2)	28(1)
C(7)	4954(3)	1320(2)	10267(2)	21(1)
C(8)	5433(3)	286(2)	8457(2)	14(1)
C(9)	5064(3)	-247(2)	7932(2)	20(1)
C(10)	5863(3)	-689(2)	7650(2)	26(1)

C(11)	7021(3)	-601(2)	7883(2)	27(1)
C(12)	7403(3)	-84(2)	8412(2)	26(1)
C(13)	6609(3)	359(2)	8709(2)	19(1)
C(14)	4923(3)	1501(2)	6770(2)	18(1)
C(15)	4472(3)	1257(2)	6040(2)	28(1)
C(16)	5183(4)	885(2)	5590(2)	34(1)
C(17)	6323(4)	764(2)	5873(2)	36(1)
C(18)	6772(3)	1011(2)	6599(2)	28(1)
C(19)	6074(3)	1388(2)	7057(2)	22(1)
C(20)	1125(3)	2378(2)	8433(2)	19(1)
C(21)	1980(3)	2372(2)	9127(2)	22(1)
C(22)	1635(3)	1865(2)	9651(2)	22(1)
C(23)	567(3)	1539(2)	9300(2)	19(1)
C(24)	229(3)	1889(2)	8569(2)	18(1)
C(25)	1058(4)	2919(2)	7805(2)	30(1)
C(26)	2972(3)	2873(2)	9271(3)	35(1)
C(27)	2199(4)	1690(2)	10454(2)	34(1)
C(28)	-148(3)	1023(2)	9692(2)	29(1)
C(29)	-935(3)	1805(2)	8097(2)	24(1)
C(30)	313(3)	853(2)	6662(2)	15(1)
C(31)	-409(3)	439(2)	6118(2)	16(1)
C(32)	-774(3)	-295(2)	6294(2)	21(1)
C(33)	-789(3)	726(2)	5382(2)	22(1)
C(34)	-513(3)	1401(2)	5184(2)	26(1)
C(35)	174(3)	1805(2)	5721(2)	27(1)
C(36)	592(3)	1525(2)	6448(2)	20(1)
C(37)	1801(3)	-206(2)	7306(2)	15(1)
C(38)	1893(3)	-874(2)	7650(2)	23(1)
C(39)	1303(4)	-1074(2)	8357(2)	31(1)
C(40)	2549(4)	-1381(2)	7309(2)	30(1)
C(41)	3127(4)	-1239(2)	6672(2)	35(1)
C(42)	3056(3)	-583(2)	6334(2)	29(1)
C(43)	2392(3)	-72(2)	6651(2)	20(1)

Table 65b-3. Bond lengths [Å] and angles [°] for sad.

Ir(1)-C(1)	2.185(3)
Ir(1)-C(23)	2.193(3)
Ir(1)-C(24)	2.203(3)
Ir(1)-C(20)	2.205(3)
Ir(1)-C(22)	2.288(3)
Ir(1)-C(21)	2.297(3)
Ir(1)-P(2)	2.3217(8)
Ir(1)-S(1)	2.4365(8)
S(1)-P(1)	2.0129(12)
P(1)-C(8)	1.807(3)
P(1)-C(1)	1.810(3)
P(1)-C(2)	1.817(3)
O(1)-S(2)	1.436(3)
C(1)-S(2)	1.764(3)
S(2)-O(2)	1.431(2)
S(2)-C(14)	1.779(4)
P(2)-O(3)	1.506(2)
P(2)-C(30)	1.854(3)
P(2)-C(37)	1.861(3)
C(2)-C(7)	1.385(5)
C(2)-C(3)	1.396(5)
C(3)-C(4)	1.376(5)
C(4)-C(5)	1.376(5)
C(5)-C(6)	1.370(5)
C(6)-C(7)	1.381(5)
C(8)-C(13)	1.387(5)
C(8)-C(9)	1.393(5)
C(9)-C(10)	1.381(5)
C(10)-C(11)	1.365(5)
C(11)-C(12)	1.380(5)
C(12)-C(13)	1.387(5)
C(14)-C(15)	1.380(5)
C(14)-C(19)	1.383(5)
C(15)-C(16)	1.386(6)

C(16)-C(17)	1.373(6)
C(17)-C(18)	1.374(5)
C(18)-C(19)	1.389(5)
C(20)-C(24)	1.435(5)
C(20)-C(21)	1.457(5)
C(20)-C(25)	1.486(5)
C(21)-C(22)	1.408(5)
C(21)-C(26)	1.493(5)
C(22)-C(23)	1.452(5)
C(22)-C(27)	1.490(5)
C(23)-C(24)	1.432(5)
C(23)-C(28)	1.495(5)
C(24)-C(29)	1.498(5)
C(30)-C(36)	1.383(5)
C(30)-C(31)	1.420(4)
C(31)-C(33)	1.398(5)
C(31)-C(32)	1.506(5)
C(33)-C(34)	1.381(5)
C(34)-C(35)	1.380(5)
C(35)-C(36)	1.389(5)
C(37)-C(43)	1.402(5)
C(37)-C(38)	1.407(5)
C(38)-C(40)	1.399(5)
C(38)-C(39)	1.503(5)
C(40)-C(41)	1.368(6)
C(41)-C(42)	1.380(6)
C(42)-C(43)	1.390(5)

C(1)-Ir(1)-C(23)	163.95(13)
C(1)-Ir(1)-C(24)	145.19(12)
C(23)-Ir(1)-C(24)	38.03(13)
C(1)-Ir(1)-C(20)	111.06(12)
C(23)-Ir(1)-C(20)	63.82(13)
C(24)-Ir(1)-C(20)	38.01(13)
C(1)-Ir(1)-C(22)	126.21(13)
C(23)-Ir(1)-C(22)	37.75(13)

C(24)-Ir(1)-C(22)	62.22(12)
C(20)-Ir(1)-C(22)	62.03(13)
C(1)-Ir(1)-C(21)	103.82(12)
C(23)-Ir(1)-C(21)	62.38(13)
C(24)-Ir(1)-C(21)	62.39(13)
C(20)-Ir(1)-C(21)	37.69(13)
C(22)-Ir(1)-C(21)	35.77(13)
C(1)-Ir(1)-P(2)	94.08(9)
C(23)-Ir(1)-P(2)	101.84(10)
C(24)-Ir(1)-P(2)	90.49(9)
C(20)-Ir(1)-P(2)	115.24(9)
C(22)-Ir(1)-P(2)	138.81(10)
C(21)-Ir(1)-P(2)	151.71(9)
C(1)-Ir(1)-S(1)	74.57(8)
C(23)-Ir(1)-S(1)	103.32(10)
C(24)-Ir(1)-S(1)	140.06(9)
C(20)-Ir(1)-S(1)	153.55(9)
C(22)-Ir(1)-S(1)	93.33(9)
C(21)-Ir(1)-S(1)	116.25(9)
P(2)-Ir(1)-S(1)	89.36(3)
P(1)-S(1)-Ir(1)	83.19(4)
C(8)-P(1)-C(1)	113.17(15)
C(8)-P(1)-C(2)	105.35(15)
C(1)-P(1)-C(2)	118.34(15)
C(8)-P(1)-S(1)	112.78(11)
C(1)-P(1)-S(1)	94.32(11)
C(2)-P(1)-S(1)	112.97(12)
S(2)-C(1)-P(1)	122.63(19)
S(2)-C(1)-Ir(1)	124.94(17)
P(1)-C(1)-Ir(1)	95.63(14)
O(2)-S(2)-O(1)	117.64(16)
O(2)-S(2)-C(1)	108.12(15)
O(1)-S(2)-C(1)	111.79(15)
O(2)-S(2)-C(14)	106.24(16)
O(1)-S(2)-C(14)	108.49(16)
C(1)-S(2)-C(14)	103.51(16)

O(3)-P(2)-C(30)	107.67(14)
O(3)-P(2)-C(37)	109.12(15)
C(30)-P(2)-C(37)	97.90(15)
O(3)-P(2)-Ir(1)	111.11(10)
C(30)-P(2)-Ir(1)	115.16(11)
C(37)-P(2)-Ir(1)	114.96(10)
C(7)-C(2)-C(3)	118.9(3)
C(7)-C(2)-P(1)	117.9(3)
C(3)-C(2)-P(1)	122.8(3)
C(4)-C(3)-C(2)	120.2(3)
C(3)-C(4)-C(5)	120.2(3)
C(6)-C(5)-C(4)	120.0(3)
C(5)-C(6)-C(7)	120.4(3)
C(6)-C(7)-C(2)	120.2(3)
C(13)-C(8)-C(9)	119.5(3)
C(13)-C(8)-P(1)	123.4(3)
C(9)-C(8)-P(1)	117.1(3)
C(10)-C(9)-C(8)	120.3(3)
C(11)-C(10)-C(9)	119.8(4)
C(10)-C(11)-C(12)	120.7(3)
C(11)-C(12)-C(13)	120.1(3)
C(8)-C(13)-C(12)	119.5(3)
C(15)-C(14)-C(19)	121.2(3)
C(15)-C(14)-S(2)	118.1(3)
C(19)-C(14)-S(2)	120.6(3)
C(14)-C(15)-C(16)	119.2(4)
C(17)-C(16)-C(15)	120.0(4)
C(16)-C(17)-C(18)	120.7(4)
C(17)-C(18)-C(19)	120.2(4)
C(14)-C(19)-C(18)	118.7(4)
C(24)-C(20)-C(21)	107.5(3)
C(24)-C(20)-C(25)	126.3(3)
C(21)-C(20)-C(25)	124.6(3)
C(24)-C(20)-Ir(1)	70.89(19)
C(21)-C(20)-Ir(1)	74.58(19)
C(25)-C(20)-Ir(1)	131.6(2)

C(22)-C(21)-C(20)	107.9(3)
C(22)-C(21)-C(26)	127.3(3)
C(20)-C(21)-C(26)	124.6(4)
C(22)-C(21)-Ir(1)	71.74(19)
C(20)-C(21)-Ir(1)	67.73(18)
C(26)-C(21)-Ir(1)	130.4(2)
C(21)-C(22)-C(23)	108.9(3)
C(21)-C(22)-C(27)	127.8(4)
C(23)-C(22)-C(27)	123.2(4)
C(21)-C(22)-Ir(1)	72.5(2)
C(23)-C(22)-Ir(1)	67.57(18)
C(27)-C(22)-Ir(1)	127.8(2)
C(24)-C(23)-C(22)	107.2(3)
C(24)-C(23)-C(28)	126.1(3)
C(22)-C(23)-C(28)	125.9(3)
C(24)-C(23)-Ir(1)	71.37(19)
C(22)-C(23)-Ir(1)	74.69(19)
C(28)-C(23)-Ir(1)	127.2(2)
C(23)-C(24)-C(20)	108.3(3)
C(23)-C(24)-C(29)	124.1(3)
C(20)-C(24)-C(29)	127.2(3)
C(23)-C(24)-Ir(1)	70.60(19)
C(20)-C(24)-Ir(1)	71.10(18)
C(29)-C(24)-Ir(1)	129.7(2)
C(36)-C(30)-C(31)	118.9(3)
C(36)-C(30)-P(2)	120.2(3)
C(31)-C(30)-P(2)	121.0(2)
C(33)-C(31)-C(30)	118.2(3)
C(33)-C(31)-C(32)	118.6(3)
C(30)-C(31)-C(32)	123.2(3)
C(34)-C(33)-C(31)	122.0(3)
C(35)-C(34)-C(33)	119.4(3)
C(34)-C(35)-C(36)	119.7(3)
C(30)-C(36)-C(35)	121.7(3)
C(43)-C(37)-C(38)	118.7(3)
C(43)-C(37)-P(2)	117.6(3)

C(38)-C(37)-P(2)	123.6(3)
C(40)-C(38)-C(37)	118.3(4)
C(40)-C(38)-C(39)	118.6(3)
C(37)-C(38)-C(39)	123.2(3)
C(41)-C(40)-C(38)	122.2(4)
C(40)-C(41)-C(42)	120.1(4)
C(41)-C(42)-C(43)	119.0(4)
C(42)-C(43)-C(37)	121.7(3)

Symmetry transformations used to generate equivalent atoms:

Table 65b-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	12(1)	11(1)	12(1)	-2(1)	0(1)	1(1)
S(1)	13(1)	13(1)	14(1)	1(1)	2(1)	0(1)
P(1)	12(1)	11(1)	13(1)	0(1)	1(1)	0(1)
O(1)	26(2)	16(1)	32(2)	0(1)	3(1)	-5(1)
C(1)	16(2)	11(2)	13(2)	1(1)	0(1)	0(1)
S(2)	16(1)	16(1)	19(1)	6(1)	1(1)	-1(1)
P(2)	13(1)	13(1)	13(1)	-2(1)	2(1)	-1(1)
O(2)	21(1)	31(2)	29(2)	17(1)	-1(1)	3(1)
C(2)	16(2)	14(2)	17(2)	-2(1)	-1(1)	1(1)
O(3)	20(1)	21(1)	19(1)	-3(1)	7(1)	-5(1)
C(3)	26(2)	22(2)	17(2)	1(1)	-1(2)	-5(2)
C(4)	28(2)	19(2)	28(2)	1(2)	-4(2)	-7(2)
C(5)	27(2)	22(2)	24(2)	-7(2)	-10(2)	-3(2)
C(6)	34(2)	36(2)	13(2)	0(2)	-4(2)	-5(2)
C(7)	23(2)	19(2)	20(2)	3(1)	-1(2)	-1(1)
C(8)	16(2)	13(2)	14(2)	4(1)	4(1)	0(1)
C(9)	17(2)	20(2)	23(2)	-1(1)	1(1)	4(1)
C(10)	32(2)	21(2)	25(2)	-6(2)	3(2)	5(2)
C(11)	26(2)	25(2)	32(2)	4(2)	14(2)	13(2)

C(12)	14(2)	27(2)	37(2)	5(2)	5(2)	3(2)
C(13)	16(2)	17(2)	24(2)	-1(1)	2(1)	-2(1)
C(14)	18(2)	22(2)	15(2)	7(1)	4(1)	-4(1)
C(15)	24(2)	38(2)	22(2)	9(2)	2(2)	-3(2)
C(16)	37(3)	46(3)	20(2)	-3(2)	4(2)	-5(2)
C(17)	38(3)	48(3)	25(2)	-3(2)	13(2)	-1(2)
C(18)	19(2)	40(2)	26(2)	4(2)	7(2)	0(2)
C(19)	22(2)	27(2)	18(2)	3(2)	3(2)	-4(2)
C(20)	22(2)	10(2)	24(2)	-3(1)	3(1)	7(1)
C(21)	23(1)	19(1)	24(1)	-13(1)	0(1)	8(1)
C(22)	23(1)	19(1)	24(1)	-13(1)	0(1)	8(1)
C(23)	19(2)	20(2)	18(2)	-7(1)	5(1)	7(1)
C(24)	18(2)	19(2)	19(2)	-5(1)	2(1)	5(1)
C(25)	38(2)	12(2)	40(2)	4(2)	6(2)	6(2)
C(26)	29(2)	22(2)	53(3)	-19(2)	-1(2)	-2(2)
C(27)	37(2)	42(3)	22(2)	-15(2)	-5(2)	20(2)
C(28)	32(2)	33(2)	25(2)	1(2)	14(2)	2(2)
C(29)	21(2)	25(2)	26(2)	-4(2)	0(2)	8(2)
C(30)	12(2)	18(2)	14(2)	-1(1)	1(1)	2(1)
C(31)	13(2)	18(2)	17(2)	-1(1)	1(1)	0(1)
C(32)	25(2)	19(2)	19(2)	-6(1)	-2(2)	-5(2)
C(33)	19(2)	29(2)	17(2)	-5(2)	-1(1)	0(2)
C(34)	28(2)	34(2)	16(2)	6(2)	-1(2)	2(2)
C(35)	31(2)	22(2)	26(2)	9(2)	1(2)	-4(2)
C(36)	18(2)	21(2)	21(2)	-1(1)	2(1)	-2(1)
C(37)	15(2)	16(2)	12(2)	-5(1)	-4(1)	1(1)
C(38)	24(2)	17(2)	23(2)	-2(1)	-11(2)	-3(1)
C(39)	36(2)	19(2)	35(2)	7(2)	-6(2)	-10(2)
C(40)	34(2)	18(2)	34(2)	-7(2)	-15(2)	5(2)
C(41)	32(2)	35(3)	34(2)	-23(2)	-12(2)	19(2)
C(42)	21(2)	48(3)	16(2)	-12(2)	-4(2)	10(2)
C(43)	20(2)	24(2)	14(2)	-6(1)	-2(1)	3(1)

Table 65b-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
H(1)	3311	877	7547	16
H(3)	6008	2027	8782	26
H(4)	7057	2652	9773	31
H(5)	6748	2474	11066	30
H(6)	5476	1624	11377	34
H(7)	4442	975	10398	25
H(9)	4276	-304	7770	24
H(10)	5613	-1047	7302	31
H(11)	7559	-894	7682	32
H(12)	8194	-31	8569	31
H(13)	6863	702	9074	23
H(15)	3699	1341	5851	33
H(16)	4889	718	5097	41
H(17)	6797	512	5570	43
H(18)	7546	925	6785	34
H(19)	6375	1561	7546	27
H(25A)	1804	2965	7616	45
H(25B)	838	3358	8015	45
H(25C)	491	2782	7380	45
H(26A)	3322	2937	8794	53
H(26B)	3538	2689	9672	53
H(26C)	2692	3314	9440	53
H(27A)	2386	1201	10479	51
H(27B)	1677	1797	10835	51
H(27C)	2898	1960	10565	51
H(28A)	-479	689	9311	44
H(28B)	-759	1264	9916	44
H(28C)	337	784	10100	44
H(29A)	-888	1957	7566	36
H(29B)	-1499	2084	8326	36

H(29C)	-1163	1323	8096	36
H(32A)	-1326	-459	5873	32
H(32B)	-1124	-298	6777	32
H(32C)	-105	-595	6345	32
H(33)	-1240	454	5014	26
H(34)	-789	1583	4693	32
H(35)	356	2262	5596	32
H(36)	1072	1796	6800	24
H(39A)	488	-972	8257	46
H(39B)	1636	-812	8806	46
H(39C)	1409	-1564	8459	46
H(40)	2593	-1830	7521	36
H(41)	3569	-1586	6467	42
H(42)	3447	-484	5902	35
H(43)	2337	369	6421	23

Röntgenstrukturanalytische Daten für 66a

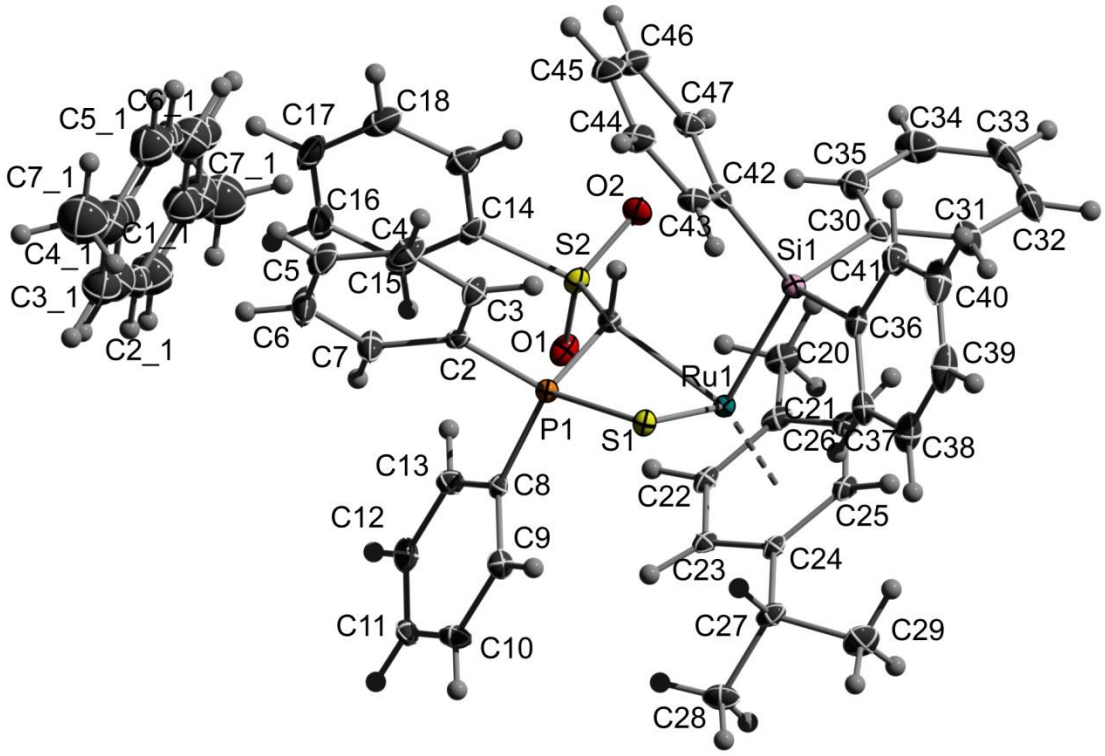

Table 66a-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	$C_{50.50}H_{49}O_2PRuS_2Si$	
Formula weight	912.15	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P-1(2)	
Unit cell dimensions	a = 9.3712(7) Å	α = 97.379(2)°.
	b = 13.5265(9) Å	β = 97.740(2)°.
	c = 17.6717(12) Å	γ = 101.302(2)°.
Volume	2148.8(3) $Å^3$	
Z	2	
Density (calculated)	1.410 Mg/m^3	
Absorption coefficient	0.568 mm^{-1}	
F(000)	946	
Crystal size	0.30 x 0.20 x 0.20 mm^3	

Theta range for data collection	3.11 to 25.00°.
Index ranges	-11<=h<=11, -16<=k<=16, -20<=l<=20
Reflections collected	25734
Independent reflections	7520 [R(int) = 0.0359]
Completeness to theta = 25.00°	99.8 %
Max. and min. transmission	0.8949 and 0.8481
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7520 / 42 / 558
Goodness-of-fit on F^2	1.051
Final R indices [I>2sigma(I)]	R1 = 0.0287, wR2 = 0.0756
R indices (all data)	R1 = 0.0369, wR2 = 0.0804
Largest diff. peak and hole	0.569 and -0.524 e.$Å^{-3}$

Table 66a-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	2828(1)	3288(1)	1440(1)	9(1)
S(1)	618(1)	3996(1)	1430(1)	12(1)
S(2)	5104(1)	4896(1)	2997(1)	14(1)
P(1)	2165(1)	5176(1)	2038(1)	10(1)
Si(1)	1565(1)	2118(1)	2183(1)	12(1)
O(1)	6102(2)	5290(1)	2499(1)	18(1)
O(2)	5457(2)	4101(1)	3416(1)	19(1)
C(1)	3306(2)	4433(2)	2492(1)	11(1)
C(2)	1381(3)	5990(2)	2690(1)	12(1)
C(3)	148(3)	5562(2)	2983(1)	19(1)
C(4)	-481(3)	6164(2)	3475(1)	22(1)
C(5)	110(3)	7192(2)	3677(2)	26(1)
C(6)	1342(3)	7631(2)	3389(2)	33(1)
C(7)	1981(3)	7036(2)	2899(2)	22(1)
C(8)	2986(3)	6017(2)	1420(1)	12(1)
C(9)	2129(3)	6076(2)	729(1)	16(1)
C(10)	2627(3)	6795(2)	276(1)	19(1)

C(11)	3988(3)	7460(2)	508(1)	17(1)
C(12)	4853(3)	7395(2)	1191(2)	19(1)
C(13)	4368(3)	6683(2)	1649(1)	17(1)
C(14)	5052(3)	5952(2)	3700(1)	17(1)
C(15)	5925(3)	6904(2)	3685(2)	22(1)
C(16)	5914(3)	7719(2)	4243(2)	31(1)
C(17)	5037(3)	7584(2)	4805(2)	34(1)
C(18)	4178(3)	6633(2)	4825(2)	32(1)
C(19)	4186(3)	5811(2)	4272(1)	24(1)
C(20)	6374(3)	2883(2)	1822(2)	21(1)
C(21)	5033(3)	2945(2)	1282(1)	15(1)
C(22)	4917(2)	3861(2)	974(1)	14(1)
C(23)	3754(2)	3897(2)	405(1)	13(1)
C(24)	2593(2)	3018(2)	122(1)	13(1)
C(25)	2698(3)	2100(2)	414(1)	14(1)
C(26)	3895(3)	2074(2)	990(1)	15(1)
C(27)	1307(3)	3072(2)	-490(1)	16(1)
C(28)	1739(3)	3856(2)	-1015(2)	23(1)
C(29)	592(3)	2044(2)	-992(2)	29(1)
C(30)	2699(3)	1157(2)	2463(1)	16(1)
C(31)	2294(3)	127(2)	2122(2)	23(1)
C(32)	3173(3)	-558(2)	2279(2)	29(1)
C(33)	4464(3)	-243(2)	2794(2)	31(1)
C(34)	4916(3)	772(2)	3140(2)	30(1)
C(35)	4048(3)	1461(2)	2967(2)	22(1)
C(36)	-276(3)	1304(2)	1631(1)	16(1)
C(37)	-831(3)	1362(2)	871(2)	17(1)
C(38)	-2200(3)	778(2)	486(2)	25(1)
C(39)	-3059(3)	139(2)	877(2)	28(1)
C(40)	-2542(3)	72(2)	1638(2)	30(1)
C(41)	-1173(3)	638(2)	2004(2)	23(1)
C(42)	973(3)	2675(2)	3113(1)	13(1)
C(43)	-460(3)	2841(2)	3092(1)	19(1)
C(44)	-939(3)	3279(2)	3742(2)	23(1)
C(45)	4(3)	3558(2)	4439(2)	25(1)
C(46)	1422(3)	3402(2)	4484(2)	23(1)

C(47)	1904(3)	2967(2)	3835(1)	17(1)
C11	8896(9)	10244(6)	5003(4)	37(2)
C21	9334(9)	9599(5)	5527(4)	23(1)
C31	10692(9)	9335(5)	5523(4)	36(2)
C41	11644(10)	9634(6)	5051(5)	45(2)
C51	11229(10)	10265(6)	4521(5)	47(2)
C61	9879(11)	10570(6)	4514(5)	41(2)
C71	7408(9)	10532(6)	5001(5)	63(2)

Table 66a-3. Bond lengths [Å] and angles [°] for sad.

Ru(1)-C(1)	2.194(2)
Ru(1)-C(26)	2.202(2)
Ru(1)-C(25)	2.237(2)
Ru(1)-C(21)	2.249(2)
Ru(1)-C(22)	2.262(2)
Ru(1)-C(24)	2.285(2)
Ru(1)-C(23)	2.305(2)
Ru(1)-Si(1)	2.4168(7)
Ru(1)-S(1)	2.4454(6)
Ru(1)-P(1)	2.8510(6)
S(1)-P(1)	2.0091(8)
S(2)-O(1)	1.4417(17)
S(2)-O(2)	1.4478(17)
S(2)-C(1)	1.750(2)
S(2)-C(14)	1.781(2)
P(1)-C(1)	1.788(2)
P(1)-C(8)	1.811(2)
P(1)-C(2)	1.817(2)
Si(1)-C(30)	1.906(2)
Si(1)-C(36)	1.915(2)
Si(1)-C(42)	1.916(2)
C(2)-C(3)	1.383(3)
C(2)-C(7)	1.397(3)
C(3)-C(4)	1.382(3)
C(4)-C(5)	1.373(4)

C(5)-C(6)	1.383(4)
C(6)-C(7)	1.380(3)
C(8)-C(9)	1.387(3)
C(8)-C(13)	1.400(3)
C(9)-C(10)	1.389(3)
C(10)-C(11)	1.385(3)
C(11)-C(12)	1.383(4)
C(12)-C(13)	1.383(3)
C(14)-C(19)	1.389(4)
C(14)-C(15)	1.390(4)
C(15)-C(16)	1.384(4)
C(16)-C(17)	1.380(4)
C(17)-C(18)	1.386(4)
C(18)-C(19)	1.384(4)
C(20)-C(21)	1.496(3)
C(21)-C(26)	1.412(3)
C(21)-C(22)	1.432(3)
C(22)-C(23)	1.393(3)
C(23)-C(24)	1.428(3)
C(24)-C(25)	1.421(3)
C(24)-C(27)	1.526(3)
C(25)-C(26)	1.419(3)
C(27)-C(29)	1.526(4)
C(27)-C(28)	1.528(3)
C(30)-C(35)	1.400(4)
C(30)-C(31)	1.402(3)
C(31)-C(32)	1.385(4)
C(32)-C(33)	1.369(4)
C(33)-C(34)	1.387(4)
C(34)-C(35)	1.389(4)
C(36)-C(37)	1.390(3)
C(36)-C(41)	1.400(3)
C(37)-C(38)	1.401(3)
C(38)-C(39)	1.381(4)
C(39)-C(40)	1.387(4)
C(40)-C(41)	1.384(4)

C(42)-C(43)	1.401(3)
C(42)-C(47)	1.407(3)
C(43)-C(44)	1.393(3)
C(44)-C(45)	1.378(4)
C(45)-C(46)	1.379(4)
C(46)-C(47)	1.393(3)
C11-C61	1.394(11)
C11-C21	1.426(10)
C11-C71	1.520(11)
C21-C31	1.389(10)
C31-C41	1.341(11)
C41-C51	1.412(12)
C51-C61	1.404(12)

C(1)-Ru(1)-C(26)	134.42(9)
C(1)-Ru(1)-C(25)	171.24(8)
C(26)-Ru(1)-C(25)	37.28(8)
C(1)-Ru(1)-C(21)	104.46(8)
C(26)-Ru(1)-C(21)	36.96(9)
C(25)-Ru(1)-C(21)	66.88(8)
C(1)-Ru(1)-C(22)	96.68(9)
C(26)-Ru(1)-C(22)	65.75(9)
C(25)-Ru(1)-C(22)	77.19(8)
C(21)-Ru(1)-C(22)	37.01(8)
C(1)-Ru(1)-C(24)	145.79(8)
C(26)-Ru(1)-C(24)	66.67(8)
C(25)-Ru(1)-C(24)	36.61(8)
C(21)-Ru(1)-C(24)	78.97(8)
C(22)-Ru(1)-C(24)	65.25(8)
C(1)-Ru(1)-C(23)	113.41(8)
C(26)-Ru(1)-C(23)	77.19(8)
C(25)-Ru(1)-C(23)	65.01(8)
C(21)-Ru(1)-C(23)	65.73(8)
C(22)-Ru(1)-C(23)	35.50(8)
C(24)-Ru(1)-C(23)	36.25(8)
C(1)-Ru(1)-Si(1)	86.89(6)

C(26)-Ru(1)-Si(1)	88.81(6)
C(25)-Ru(1)-Si(1)	94.97(6)
C(21)-Ru(1)-Si(1)	110.86(6)
C(22)-Ru(1)-Si(1)	147.54(6)
C(24)-Ru(1)-Si(1)	124.35(6)
C(23)-Ru(1)-Si(1)	159.71(6)
C(1)-Ru(1)-S(1)	75.33(6)
C(26)-Ru(1)-S(1)	148.86(6)
C(25)-Ru(1)-S(1)	113.38(6)
C(21)-Ru(1)-S(1)	165.84(6)
C(22)-Ru(1)-S(1)	128.87(6)
C(24)-Ru(1)-S(1)	93.29(6)
C(23)-Ru(1)-S(1)	101.07(6)
Si(1)-Ru(1)-S(1)	83.30(2)
C(1)-Ru(1)-P(1)	38.83(6)
C(26)-Ru(1)-P(1)	165.50(6)
C(25)-Ru(1)-P(1)	147.86(6)
C(21)-Ru(1)-P(1)	128.76(6)
C(22)-Ru(1)-P(1)	100.49(6)
C(24)-Ru(1)-P(1)	112.92(6)
C(23)-Ru(1)-P(1)	94.25(6)
Si(1)-Ru(1)-P(1)	102.22(2)
S(1)-Ru(1)-P(1)	43.754(18)
P(1)-S(1)-Ru(1)	78.92(3)
O(1)-S(2)-O(2)	117.97(10)
O(1)-S(2)-C(1)	111.68(11)
O(2)-S(2)-C(1)	106.40(11)
O(1)-S(2)-C(14)	106.25(11)
O(2)-S(2)-C(14)	106.89(11)
C(1)-S(2)-C(14)	107.10(11)
C(1)-P(1)-C(8)	116.98(11)
C(1)-P(1)-C(2)	115.43(11)
C(8)-P(1)-C(2)	104.33(10)
C(1)-P(1)-S(1)	96.75(8)
C(8)-P(1)-S(1)	112.00(8)
C(2)-P(1)-S(1)	111.53(8)

C(1)-P(1)-Ru(1)	50.32(7)
C(8)-P(1)-Ru(1)	101.54(7)
C(2)-P(1)-Ru(1)	154.13(8)
S(1)-P(1)-Ru(1)	57.32(2)
C(30)-Si(1)-C(36)	104.84(11)
C(30)-Si(1)-C(42)	106.27(10)
C(36)-Si(1)-C(42)	101.08(10)
C(30)-Si(1)-Ru(1)	111.50(8)
C(36)-Si(1)-Ru(1)	113.57(8)
C(42)-Si(1)-Ru(1)	118.27(7)
S(2)-C(1)-P(1)	125.73(13)
S(2)-C(1)-Ru(1)	121.64(12)
P(1)-C(1)-Ru(1)	90.85(10)
C(3)-C(2)-C(7)	119.2(2)
C(3)-C(2)-P(1)	118.95(18)
C(7)-C(2)-P(1)	121.85(18)
C(4)-C(3)-C(2)	120.3(2)
C(5)-C(4)-C(3)	120.4(2)
C(4)-C(5)-C(6)	120.0(2)
C(7)-C(6)-C(5)	120.1(3)
C(6)-C(7)-C(2)	120.1(2)
C(9)-C(8)-C(13)	119.1(2)
C(9)-C(8)-P(1)	117.74(18)
C(13)-C(8)-P(1)	122.72(18)
C(8)-C(9)-C(10)	120.5(2)
C(11)-C(10)-C(9)	120.2(2)
C(12)-C(11)-C(10)	119.5(2)
C(13)-C(12)-C(11)	120.8(2)
C(12)-C(13)-C(8)	119.9(2)
C(19)-C(14)-C(15)	120.6(2)
C(19)-C(14)-S(2)	120.0(2)
C(15)-C(14)-S(2)	119.4(2)
C(16)-C(15)-C(14)	119.4(3)
C(17)-C(16)-C(15)	120.1(3)
C(16)-C(17)-C(18)	120.6(3)
C(19)-C(18)-C(17)	119.9(3)

C(18)-C(19)-C(14)	119.5(3)
C(26)-C(21)-C(22)	116.9(2)
C(26)-C(21)-C(20)	121.3(2)
C(22)-C(21)-C(20)	121.5(2)
C(26)-C(21)-Ru(1)	69.70(13)
C(22)-C(21)-Ru(1)	71.98(13)
C(20)-C(21)-Ru(1)	134.33(17)
C(23)-C(22)-C(21)	122.1(2)
C(23)-C(22)-Ru(1)	73.94(13)
C(21)-C(22)-Ru(1)	71.01(13)
C(22)-C(23)-C(24)	120.7(2)
C(22)-C(23)-Ru(1)	70.56(13)
C(24)-C(23)-Ru(1)	71.11(13)
C(25)-C(24)-C(23)	117.9(2)
C(25)-C(24)-C(27)	121.7(2)
C(23)-C(24)-C(27)	120.3(2)
C(25)-C(24)-Ru(1)	69.83(13)
C(23)-C(24)-Ru(1)	72.64(13)
C(27)-C(24)-Ru(1)	129.85(15)
C(26)-C(25)-C(24)	120.6(2)
C(26)-C(25)-Ru(1)	70.04(13)
C(24)-C(25)-Ru(1)	73.56(13)
C(21)-C(26)-C(25)	121.7(2)
C(21)-C(26)-Ru(1)	73.34(13)
C(25)-C(26)-Ru(1)	72.68(13)
C(29)-C(27)-C(24)	113.3(2)
C(29)-C(27)-C(28)	108.9(2)
C(24)-C(27)-C(28)	112.7(2)
C(35)-C(30)-C(31)	116.5(2)
C(35)-C(30)-Si(1)	121.59(19)
C(31)-C(30)-Si(1)	121.7(2)
C(32)-C(31)-C(30)	121.9(3)
C(33)-C(32)-C(31)	120.1(3)
C(32)-C(33)-C(34)	119.9(3)
C(33)-C(34)-C(35)	119.7(3)
C(34)-C(35)-C(30)	121.8(3)

C(37)-C(36)-C(41)	116.4(2)
C(37)-C(36)-Si(1)	123.64(18)
C(41)-C(36)-Si(1)	119.90(19)
C(36)-C(37)-C(38)	122.6(2)
C(39)-C(38)-C(37)	119.2(3)
C(38)-C(39)-C(40)	119.6(3)
C(41)-C(40)-C(39)	120.4(3)
C(40)-C(41)-C(36)	121.8(3)
C(43)-C(42)-C(47)	116.0(2)
C(43)-C(42)-Si(1)	119.63(18)
C(47)-C(42)-Si(1)	124.33(18)
C(44)-C(43)-C(42)	122.4(2)
C(45)-C(44)-C(43)	120.0(2)
C(44)-C(45)-C(46)	119.4(2)
C(45)-C(46)-C(47)	120.7(2)
C(46)-C(47)-C(42)	121.5(2)
C61-C11-C21	117.0(7)
C61-C11-C71	123.8(8)
C21-C11-C71	119.3(7)
C31-C21-C11	118.9(7)
C41-C31-C21	124.8(8)
C31-C41-C51	117.4(9)
C61-C51-C41	119.9(8)
C11-C61-C51	122.0(8)

Symmetry transformations used to generate equivalent atoms:

Table 66a-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	7(1)	11(1)	10(1)	1(1)	1(1)	3(1)
S(1)	9(1)	12(1)	14(1)	0(1)	1(1)	3(1)
S(2)	11(1)	15(1)	14(1)	0(1)	-2(1)	3(1)
P(1)	9(1)	11(1)	11(1)	2(1)	1(1)	2(1)
Si(1)	11(1)	12(1)	14(1)	3(1)	3(1)	2(1)
O(1)	12(1)	20(1)	19(1)	-2(1)	3(1)	1(1)
O(2)	18(1)	21(1)	19(1)	3(1)	-3(1)	9(1)
C(1)	9(1)	12(1)	13(1)	2(1)	1(1)	2(1)
C(2)	14(1)	16(1)	9(1)	3(1)	1(1)	6(1)
C(3)	16(1)	18(1)	19(1)	-2(1)	2(1)	0(1)
C(4)	14(1)	31(2)	18(1)	-1(1)	6(1)	5(1)
C(5)	29(2)	29(2)	22(2)	-2(1)	10(1)	15(1)
C(6)	48(2)	16(1)	38(2)	-2(1)	22(2)	5(1)
C(7)	27(2)	16(1)	26(2)	2(1)	15(1)	2(1)
C(8)	14(1)	11(1)	13(1)	1(1)	5(1)	6(1)
C(9)	12(1)	15(1)	19(1)	2(1)	3(1)	2(1)
C(10)	20(1)	24(1)	17(1)	8(1)	2(1)	10(1)
C(11)	23(1)	13(1)	20(1)	5(1)	11(1)	5(1)
C(12)	13(1)	16(1)	25(2)	0(1)	4(1)	-1(1)
C(13)	16(1)	18(1)	16(1)	3(1)	0(1)	3(1)
C(14)	16(1)	20(1)	12(1)	-3(1)	-5(1)	6(1)
C(15)	23(1)	22(1)	19(1)	2(1)	-5(1)	5(1)
C(16)	41(2)	19(2)	27(2)	-4(1)	-10(1)	7(1)
C(17)	47(2)	29(2)	21(2)	-10(1)	-9(1)	17(2)
C(18)	35(2)	46(2)	16(2)	1(1)	2(1)	19(2)
C(19)	24(2)	31(2)	17(1)	1(1)	-1(1)	8(1)
C(20)	13(1)	31(2)	21(1)	4(1)	3(1)	9(1)
C(21)	10(1)	25(1)	13(1)	2(1)	4(1)	8(1)
C(22)	10(1)	17(1)	14(1)	-2(1)	5(1)	1(1)
C(23)	14(1)	16(1)	11(1)	2(1)	7(1)	5(1)
C(24)	12(1)	14(1)	12(1)	-1(1)	5(1)	4(1)

C(25)	12(1)	16(1)	14(1)	1(1)	7(1)	3(1)
C(26)	14(1)	19(1)	15(1)	5(1)	8(1)	9(1)
C(27)	14(1)	22(1)	12(1)	0(1)	1(1)	8(1)
C(28)	22(1)	31(2)	18(1)	8(1)	-1(1)	8(1)
C(29)	27(2)	30(2)	21(2)	1(1)	-10(1)	0(1)
C(30)	19(1)	16(1)	17(1)	7(1)	10(1)	7(1)
C(31)	22(1)	17(1)	32(2)	7(1)	9(1)	5(1)
C(32)	35(2)	17(1)	43(2)	11(1)	17(2)	11(1)
C(33)	37(2)	27(2)	45(2)	23(2)	24(2)	23(1)
C(34)	23(2)	44(2)	27(2)	10(1)	4(1)	17(1)
C(35)	24(2)	23(1)	22(1)	4(1)	7(1)	10(1)
C(36)	14(1)	12(1)	20(1)	-2(1)	5(1)	2(1)
C(37)	14(1)	12(1)	25(1)	1(1)	4(1)	3(1)
C(38)	19(1)	20(1)	32(2)	-3(1)	-5(1)	6(1)
C(39)	12(1)	19(1)	47(2)	-7(1)	3(1)	0(1)
C(40)	23(2)	18(1)	47(2)	-3(1)	19(1)	-4(1)
C(41)	26(2)	18(1)	24(2)	1(1)	10(1)	1(1)
C(42)	13(1)	12(1)	18(1)	7(1)	6(1)	4(1)
C(43)	19(1)	23(1)	16(1)	6(1)	2(1)	5(1)
C(44)	21(1)	31(2)	22(1)	8(1)	9(1)	14(1)
C(45)	32(2)	30(2)	17(1)	5(1)	11(1)	13(1)
C(46)	26(2)	28(2)	13(1)	2(1)	1(1)	6(1)
C(47)	16(1)	20(1)	17(1)	6(1)	2(1)	5(1)
C11	38(2)	36(2)	37(2)	4(1)	3(1)	8(1)
C21	23(2)	23(2)	24(2)	3(1)	3(1)	6(1)
C31	36(2)	35(2)	36(2)	4(1)	5(1)	9(1)
C41	44(2)	44(2)	45(2)	4(1)	8(1)	9(1)
C51	47(2)	46(2)	47(2)	6(1)	8(1)	9(1)
C61	41(2)	41(2)	41(2)	5(1)	7(1)	9(1)
C71	63(2)	62(2)	63(2)	10(1)	8(1)	14(1)

Table 66a-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
H(1)	2730(30)	4187(18)	2869(14)	16(7)
H(3)	-269	4852	2844	22
H(4)	-1326	5864	3674	26
H(5)	-328	7602	4015	31
H(6)	1750	8342	3529	40
H(7)	2830	7338	2703	27
H(9)	1196	5621	566	19
H(10)	2032	6831	-195	23
H(11)	4324	7957	201	21
H(12)	5792	7844	1348	22
H(13)	4971	6646	2117	20
H(15)	6525	6995	3296	26
H(16)	6511	8372	4238	37
H(17)	5023	8148	5182	41
H(18)	3584	6545	5217	38
H(19)	3603	5155	4285	29
H(20A)	7087	2649	1524	31
H(20B)	6093	2401	2173	31
H(20C)	6820	3560	2124	31
H(22)	5584	4518	1242	17
H(23)	3607	4578	288	16
H(25)	1834	1506	285	16
H(26)	3855	1458	1251	18
H(27)	537	3295	-210	19
H(28A)	2561	3697	-1261	35
H(28B)	2041	4540	-706	35
H(28C)	893	3834	-1413	35
H(29A)	-226	2126	-1369	43
H(29B)	218	1554	-664	43
H(29C)	1325	1791	-1265	43

H(31)	1391	-108	1773	27
H(32)	2880	-1248	2029	35
H(33)	5049	-719	2914	37
H(34)	5815	994	3494	36
H(35)	4379	2158	3196	26
H(37)	-259	1815	603	21
H(38)	-2532	821	-39	30
H(39)	-3998	-252	628	34
H(40)	-3132	-366	1910	36
H(41)	-832	572	2522	28
H(43)	-1130	2647	2618	23
H(44)	-1917	3386	3705	27
H(45)	-318	3856	4884	30
H(46)	2076	3593	4964	27
H(47)	2885	2866	3879	21
H21	8707	9355	5874	28
H31	10967	8910	5880	43
H41	12561	9431	5074	54
H51	11862	10482	4169	56
H61	9628	11012	4165	50
H71	6964	10290	5433	95
H7B1	6758	10216	4512	95
H7C1	7542	11276	5055	95

Röntgenstrukturanalytische Daten für 66b

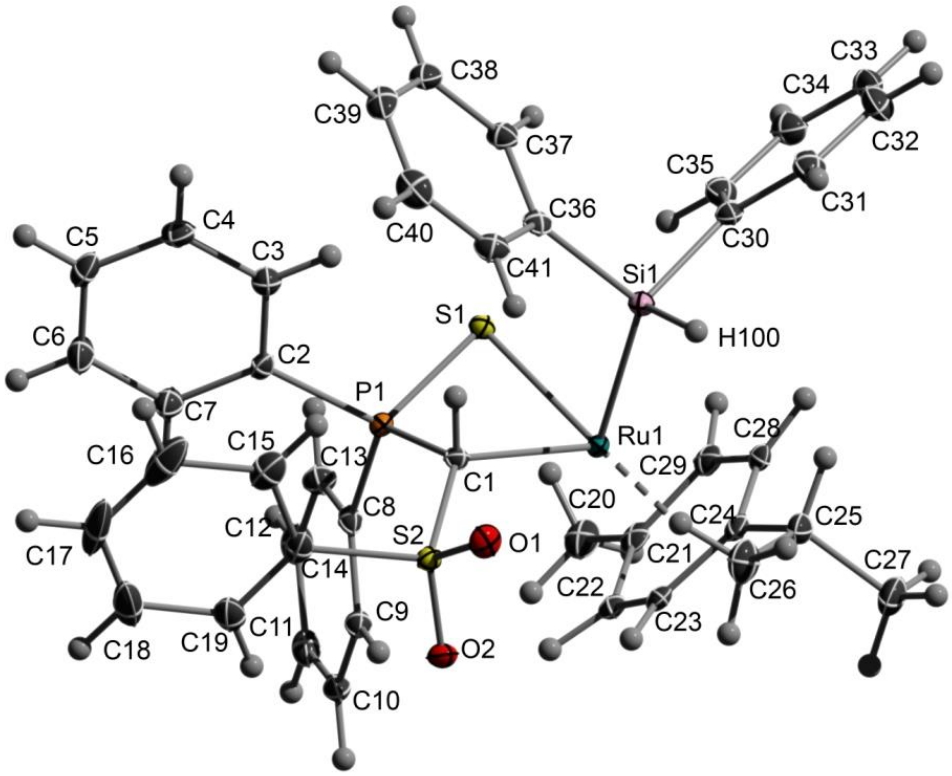

Table 66b-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	C41 H41 O2 P Ru S2 Si	
Formula weight	789.99	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.7262(4) Å	α = 87.9340(10)°.
	b = 12.1957(4) Å	β = 75.0580(10)°.
	c = 13.2281(4) Å	γ = 82.3080(10)°.
Volume	1811.33(10) $Å^3$	
Z	2	
Density (calculated)	1.448 Mg/m^3	
Absorption coefficient	0.661 mm^{-1}	
F(000)	816	
Crystal size	0.27 x 0.23 x 0.07 mm^3	

Theta range for data collection	1.59 to 26.42°.
Index ranges	-14<=h<=14, -14<=k<=15, -16<=l<=16
Reflections collected	23640
Independent reflections	7439 [R(int) = 0.0143]
Completeness to theta = 26.42°	99.9 %
Max. and min. transmission	0.9552 and 0.8438
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7439 / 0 / 440
Goodness-of-fit on F^2	1.172
Final R indices [I>2sigma(I)]	R1 = 0.0208, wR2 = 0.0576
R indices (all data)	R1 = 0.0231, wR2 = 0.0661
Largest diff. peak and hole	0.555 and -0.415 e.$Å^{-3}$

Table 66b-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	7092(1)	6489(1)	2156(1)	10(1)
S(1)	5866(1)	7099(1)	943(1)	12(1)
P(1)	4590(1)	7146(1)	2299(1)	10(1)
Si(1)	7929(1)	8166(1)	1652(1)	12(1)
O(1)	5862(1)	8071(1)	4830(1)	17(1)
C(1)	5507(1)	7469(1)	3109(1)	11(1)
S(2)	5093(1)	7425(1)	4476(1)	11(1)
O(2)	5040(1)	6305(1)	4861(1)	16(1)
C(2)	3340(1)	8205(1)	2328(1)	12(1)
C(3)	3586(2)	9285(1)	2085(1)	15(1)
C(4)	2669(2)	10131(2)	2102(1)	18(1)
C(5)	1499(2)	9912(2)	2360(2)	20(1)
C(6)	1250(2)	8848(2)	2620(2)	22(1)
C(7)	2160(2)	7989(2)	2604(1)	17(1)
C(8)	3981(1)	5842(1)	2476(1)	13(1)
C(9)	3912(1)	5140(1)	3336(1)	14(1)
C(10)	3482(2)	4127(1)	3327(2)	17(1)

C(11)	3107(2)	3827(2)	2479(2)	19(1)
C(12)	3166(2)	4531(2)	1623(2)	20(1)
C(13)	3605(2)	5530(2)	1615(1)	17(1)
C(14)	3629(2)	8137(2)	4861(1)	16(1)
C(15)	3463(2)	9283(2)	4765(2)	24(1)
C(16)	2313(2)	9834(2)	5055(2)	36(1)
C(17)	1360(2)	9252(2)	5433(2)	42(1)
C(18)	1533(2)	8112(2)	5522(2)	36(1)
C(19)	2675(2)	7541(2)	5233(1)	24(1)
C(20)	6527(2)	4011(2)	1274(2)	23(1)
C(21)	7233(2)	4612(1)	1817(1)	16(1)
C(22)	6923(2)	4744(1)	2901(1)	15(1)
C(23)	7570(2)	5392(1)	3382(1)	14(1)
C(24)	8610(2)	5815(1)	2804(1)	15(1)
C(25)	9433(2)	6327(2)	3307(2)	18(1)
C(26)	8811(2)	6964(2)	4301(2)	25(1)
C(27)	10370(2)	5403(2)	3506(2)	28(1)
C(28)	8922(2)	5662(1)	1694(1)	16(1)
C(29)	8230(2)	5111(1)	1214(1)	17(1)
C(30)	9036(2)	8042(1)	318(1)	15(1)
C(31)	10091(2)	8524(2)	139(2)	21(1)
C(32)	10945(2)	8413(2)	-813(2)	26(1)
C(33)	10770(2)	7816(2)	-1617(2)	23(1)
C(34)	9731(2)	7336(2)	-1467(2)	22(1)
C(35)	8881(2)	7450(2)	-513(1)	19(1)
C(36)	6908(2)	9498(1)	1618(1)	13(1)
C(37)	6605(2)	9877(1)	699(1)	15(1)
C(38)	5854(2)	10857(2)	674(2)	19(1)
C(39)	5385(2)	11479(1)	1577(2)	20(1)
C(40)	5665(2)	11128(2)	2503(2)	22(1)
C(41)	6425(2)	10147(2)	2518(1)	18(1)

Table 66b-3. Bond lengths [Å] and angles [°] for sad.

Ru(1)-C(1)	2.1858(16)
Ru(1)-C(28)	2.1873(16)
Ru(1)-C(23)	2.2018(16)
Ru(1)-C(29)	2.2024(17)
Ru(1)-C(24)	2.2192(16)
Ru(1)-C(22)	2.3243(16)
Ru(1)-C(21)	2.3247(16)
Ru(1)-Si(1)	2.3856(5)
Ru(1)-S(1)	2.4520(4)
Ru(1)-P(1)	2.8954(4)
S(1)-P(1)	2.0146(6)
P(1)-C(1)	1.7898(16)
P(1)-C(2)	1.8121(16)
P(1)-C(8)	1.8131(17)
Si(1)-C(36)	1.8900(17)
Si(1)-C(30)	1.8998(18)
O(1)-S(2)	1.4445(12)
C(1)-S(2)	1.7471(16)
S(2)-O(2)	1.4450(12)
S(2)-C(14)	1.7732(17)
C(2)-C(3)	1.394(2)
C(2)-C(7)	1.396(2)
C(3)-C(4)	1.383(2)
C(4)-C(5)	1.386(3)
C(5)-C(6)	1.381(3)
C(6)-C(7)	1.388(2)
C(8)-C(9)	1.391(2)
C(8)-C(13)	1.403(2)
C(9)-C(10)	1.396(2)
C(10)-C(11)	1.383(3)
C(11)-C(12)	1.390(3)
C(12)-C(13)	1.384(3)
C(14)-C(19)	1.388(3)
C(14)-C(15)	1.391(3)

C(15)-C(16)	1.387(3)
C(16)-C(17)	1.380(4)
C(17)-C(18)	1.383(4)
C(18)-C(19)	1.389(3)
C(20)-C(21)	1.498(3)
C(21)-C(22)	1.395(3)
C(21)-C(29)	1.432(3)
C(22)-C(23)	1.432(2)
C(23)-C(24)	1.413(2)
C(24)-C(28)	1.431(3)
C(24)-C(25)	1.512(2)
C(25)-C(26)	1.514(3)
C(25)-C(27)	1.531(2)
C(28)-C(29)	1.399(3)
C(30)-C(35)	1.399(3)
C(30)-C(31)	1.402(2)
C(31)-C(32)	1.390(3)
C(32)-C(33)	1.383(3)
C(33)-C(34)	1.387(3)
C(34)-C(35)	1.390(3)
C(36)-C(37)	1.400(2)
C(36)-C(41)	1.401(2)
C(37)-C(38)	1.391(2)
C(38)-C(39)	1.387(3)
C(39)-C(40)	1.387(3)
C(40)-C(41)	1.395(3)

C(1)-Ru(1)-C(28)	158.57(7)
C(1)-Ru(1)-C(23)	99.08(6)
C(28)-Ru(1)-C(23)	66.98(6)
C(1)-Ru(1)-C(29)	160.13(7)
C(28)-Ru(1)-C(29)	37.17(7)
C(23)-Ru(1)-C(29)	78.67(7)
C(1)-Ru(1)-C(24)	121.73(6)
C(28)-Ru(1)-C(24)	37.90(7)
C(23)-Ru(1)-C(24)	37.27(6)

C(29)-Ru(1)-C(24)	67.77(7)
C(1)-Ru(1)-C(22)	101.63(6)
C(28)-Ru(1)-C(22)	77.25(6)
C(23)-Ru(1)-C(22)	36.75(6)
C(29)-Ru(1)-C(22)	64.71(6)
C(24)-Ru(1)-C(22)	66.33(6)
C(1)-Ru(1)-C(21)	124.35(6)
C(28)-Ru(1)-C(21)	66.23(6)
C(23)-Ru(1)-C(21)	65.51(6)
C(29)-Ru(1)-C(21)	36.75(6)
C(24)-Ru(1)-C(21)	78.80(6)
C(22)-Ru(1)-C(21)	34.93(6)
C(1)-Ru(1)-Si(1)	88.55(4)
C(28)-Ru(1)-Si(1)	86.04(5)
C(23)-Ru(1)-Si(1)	122.52(5)
C(29)-Ru(1)-Si(1)	109.45(5)
C(24)-Ru(1)-Si(1)	91.43(5)
C(22)-Ru(1)-Si(1)	157.72(4)
C(21)-Ru(1)-Si(1)	146.00(5)
C(1)-Ru(1)-S(1)	75.00(4)
C(28)-Ru(1)-S(1)	124.90(5)
C(23)-Ru(1)-S(1)	152.82(5)
C(29)-Ru(1)-S(1)	97.87(5)
C(24)-Ru(1)-S(1)	162.71(5)
C(22)-Ru(1)-S(1)	117.41(4)
C(21)-Ru(1)-S(1)	95.50(4)
Si(1)-Ru(1)-S(1)	84.241(15)
C(1)-Ru(1)-P(1)	38.12(4)
C(28)-Ru(1)-P(1)	162.86(5)
C(23)-Ru(1)-P(1)	117.95(4)
C(29)-Ru(1)-P(1)	125.83(5)
C(24)-Ru(1)-P(1)	153.47(5)
C(22)-Ru(1)-P(1)	97.37(4)
C(21)-Ru(1)-P(1)	99.98(4)
Si(1)-Ru(1)-P(1)	102.701(14)
S(1)-Ru(1)-P(1)	43.279(13)

P(1)-S(1)-Ru(1)	80.167(18)
C(1)-P(1)-C(2)	112.87(7)
C(1)-P(1)-C(8)	119.58(8)
C(2)-P(1)-C(8)	105.86(8)
C(1)-P(1)-S(1)	95.99(5)
C(2)-P(1)-S(1)	113.54(6)
C(8)-P(1)-S(1)	108.97(6)
C(1)-P(1)-Ru(1)	48.93(5)
C(2)-P(1)-Ru(1)	150.92(6)
C(8)-P(1)-Ru(1)	103.19(5)
S(1)-P(1)-Ru(1)	56.554(15)
C(36)-Si(1)-C(30)	105.98(7)
C(36)-Si(1)-Ru(1)	119.39(5)
C(30)-Si(1)-Ru(1)	111.75(5)
S(2)-C(1)-P(1)	124.08(9)
S(2)-C(1)-Ru(1)	123.45(8)
P(1)-C(1)-Ru(1)	92.95(7)
O(1)-S(2)-O(2)	117.46(7)
O(1)-S(2)-C(1)	106.63(8)
O(2)-S(2)-C(1)	111.63(7)
O(1)-S(2)-C(14)	107.30(8)
O(2)-S(2)-C(14)	107.14(8)
C(1)-S(2)-C(14)	106.05(8)
C(3)-C(2)-C(7)	119.42(15)
C(3)-C(2)-P(1)	117.53(12)
C(7)-C(2)-P(1)	123.04(13)
C(4)-C(3)-C(2)	120.22(16)
C(3)-C(4)-C(5)	120.27(17)
C(6)-C(5)-C(4)	119.70(16)
C(5)-C(6)-C(7)	120.73(17)
C(6)-C(7)-C(2)	119.64(17)
C(9)-C(8)-C(13)	119.68(16)
C(9)-C(8)-P(1)	126.42(13)
C(13)-C(8)-P(1)	113.82(13)
C(8)-C(9)-C(10)	119.47(16)
C(11)-C(10)-C(9)	120.61(17)

C(10)-C(11)-C(12)	119.97(16)
C(13)-C(12)-C(11)	120.05(17)
C(12)-C(13)-C(8)	120.21(17)
C(19)-C(14)-C(15)	121.56(17)
C(19)-C(14)-S(2)	119.56(14)
C(15)-C(14)-S(2)	118.87(15)
C(16)-C(15)-C(14)	118.6(2)
C(17)-C(16)-C(15)	120.3(2)
C(16)-C(17)-C(18)	120.59(19)
C(17)-C(18)-C(19)	120.1(2)
C(14)-C(19)-C(18)	118.7(2)
C(22)-C(21)-C(29)	118.13(16)
C(22)-C(21)-C(20)	122.12(16)
C(29)-C(21)-C(20)	119.70(16)
C(22)-C(21)-Ru(1)	72.52(10)
C(29)-C(21)-Ru(1)	66.98(9)
C(20)-C(21)-Ru(1)	129.94(12)
C(21)-C(22)-C(23)	120.25(16)
C(21)-C(22)-Ru(1)	72.55(10)
C(23)-C(22)-Ru(1)	66.97(9)
C(24)-C(23)-C(22)	121.94(16)
C(24)-C(23)-Ru(1)	72.03(9)
C(22)-C(23)-Ru(1)	76.28(10)
C(23)-C(24)-C(28)	116.76(16)
C(23)-C(24)-C(25)	123.33(16)
C(28)-C(24)-C(25)	119.73(15)
C(23)-C(24)-Ru(1)	70.70(9)
C(28)-C(24)-Ru(1)	69.84(9)
C(25)-C(24)-Ru(1)	134.12(12)
C(24)-C(25)-C(26)	114.37(15)
C(24)-C(25)-C(27)	107.89(15)
C(26)-C(25)-C(27)	110.95(16)
C(29)-C(28)-C(24)	121.15(16)
C(29)-C(28)-Ru(1)	72.01(10)
C(24)-C(28)-Ru(1)	72.26(9)
C(28)-C(29)-C(21)	121.33(16)

C(28)-C(29)-Ru(1)	70.83(10)
C(21)-C(29)-Ru(1)	76.27(10)
C(35)-C(30)-C(31)	116.62(16)
C(35)-C(30)-Si(1)	123.28(13)
C(31)-C(30)-Si(1)	120.06(14)
C(32)-C(31)-C(30)	121.76(18)
C(33)-C(32)-C(31)	120.24(18)
C(32)-C(33)-C(34)	119.37(18)
C(33)-C(34)-C(35)	120.06(18)
C(34)-C(35)-C(30)	121.94(17)
C(37)-C(36)-C(41)	117.29(16)
C(37)-C(36)-Si(1)	121.60(13)
C(41)-C(36)-Si(1)	121.11(13)
C(38)-C(37)-C(36)	121.60(16)
C(39)-C(38)-C(37)	119.82(17)
C(38)-C(39)-C(40)	120.11(17)
C(39)-C(40)-C(41)	119.61(17)
C(40)-C(41)-C(36)	121.57(17)

Symmetry transformations used to generate equivalent atoms:

Table 66b-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	9(1)	9(1)	11(1)	1(1)	-2(1)	0(1)
S(1)	12(1)	13(1)	10(1)	0(1)	-2(1)	0(1)
P(1)	10(1)	9(1)	10(1)	1(1)	-3(1)	0(1)
Si(1)	11(1)	11(1)	13(1)	2(1)	-3(1)	-2(1)
O(1)	18(1)	21(1)	15(1)	-2(1)	-7(1)	-4(1)
C(1)	11(1)	11(1)	10(1)	1(1)	-3(1)	-2(1)
S(2)	11(1)	12(1)	10(1)	0(1)	-3(1)	0(1)
O(2)	19(1)	15(1)	14(1)	4(1)	-4(1)	-1(1)
C(2)	12(1)	13(1)	11(1)	-1(1)	-4(1)	2(1)

C(3)	14(1)	15(1)	16(1)	1(1)	-4(1)	-2(1)
C(4)	22(1)	13(1)	17(1)	2(1)	-4(1)	0(1)
C(5)	18(1)	19(1)	22(1)	-1(1)	-7(1)	6(1)
C(6)	13(1)	23(1)	30(1)	-1(1)	-6(1)	-1(1)
C(7)	15(1)	16(1)	22(1)	1(1)	-6(1)	-2(1)
C(8)	10(1)	11(1)	16(1)	-2(1)	-2(1)	-1(1)
C(9)	12(1)	14(1)	16(1)	0(1)	-3(1)	-1(1)
C(10)	13(1)	13(1)	23(1)	4(1)	-2(1)	-1(1)
C(11)	14(1)	12(1)	30(1)	-4(1)	-3(1)	-2(1)
C(12)	18(1)	20(1)	23(1)	-7(1)	-7(1)	-2(1)
C(13)	19(1)	17(1)	15(1)	0(1)	-5(1)	-2(1)
C(14)	14(1)	23(1)	9(1)	-2(1)	-3(1)	4(1)
C(15)	28(1)	23(1)	17(1)	-5(1)	-7(1)	7(1)
C(16)	44(1)	37(1)	24(1)	-11(1)	-13(1)	24(1)
C(17)	23(1)	73(2)	21(1)	-9(1)	-6(1)	26(1)
C(18)	15(1)	71(2)	19(1)	4(1)	-2(1)	1(1)
C(19)	17(1)	38(1)	15(1)	4(1)	-4(1)	-2(1)
C(20)	24(1)	15(1)	29(1)	-5(1)	-7(1)	-1(1)
C(21)	17(1)	7(1)	24(1)	-1(1)	-6(1)	4(1)
C(22)	14(1)	9(1)	22(1)	4(1)	-4(1)	1(1)
C(23)	14(1)	12(1)	17(1)	4(1)	-4(1)	3(1)
C(24)	12(1)	11(1)	22(1)	3(1)	-5(1)	2(1)
C(25)	12(1)	20(1)	24(1)	5(1)	-7(1)	-2(1)
C(26)	20(1)	29(1)	29(1)	-5(1)	-11(1)	-2(1)
C(27)	18(1)	29(1)	37(1)	4(1)	-12(1)	3(1)
C(28)	11(1)	13(1)	22(1)	4(1)	0(1)	3(1)
C(29)	18(1)	13(1)	17(1)	-1(1)	-2(1)	5(1)
C(30)	14(1)	11(1)	17(1)	4(1)	-1(1)	0(1)
C(31)	18(1)	19(1)	25(1)	1(1)	-3(1)	-5(1)
C(32)	16(1)	27(1)	31(1)	5(1)	0(1)	-6(1)
C(33)	19(1)	22(1)	21(1)	5(1)	4(1)	4(1)
C(34)	26(1)	19(1)	18(1)	0(1)	-3(1)	0(1)
C(35)	18(1)	17(1)	20(1)	2(1)	-2(1)	-4(1)
C(36)	14(1)	10(1)	16(1)	1(1)	-3(1)	-4(1)
C(37)	18(1)	13(1)	14(1)	0(1)	-2(1)	-2(1)
C(38)	20(1)	16(1)	21(1)	6(1)	-6(1)	-3(1)

C(39)	18(1)	10(1)	32(1)	0(1)	-4(1)	-1(1)
C(40)	24(1)	16(1)	23(1)	-7(1)	-1(1)	-3(1)
C(41)	21(1)	17(1)	16(1)	0(1)	-4(1)	-5(1)

Table 66b-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for sad.

	x	y	z	U(eq)
H(1)	5637	8255	2935	13
H(3)	4387	9440	1907	18
H(4)	2842	10865	1936	22
H(5)	872	10491	2357	24
H(6)	446	8702	2813	27
H(7)	1980	7258	2780	21
H(9)	4156	5348	3926	17
H(10)	3447	3640	3908	20
H(11)	2809	3139	2482	23
H(12)	2905	4326	1042	24
H(13)	3653	6006	1025	21
H(15)	4123	9680	4507	28
H(16)	2182	10617	4992	44
H(17)	577	9638	5635	50
H(18)	870	7719	5781	44
H(19)	2802	6758	5288	28
H(20A)	6248	4505	762	34
H(20B)	5841	3775	1790	34
H(20C)	7030	3361	914	34
H(22)	6122	4576	3312	18
H(23)	7234	5612	4131	17
H(25)	9853	6854	2791	22
H(26A)	8144	7481	4178	38
H(26B)	9374	7377	4509	38
H(26C)	8510	6446	4859	38
H(27A)	10791	5030	2845	41

H(27B)	9979	4867	4001	41
H(27C)	10939	5720	3801	41
H(28)	9554	6071	1247	20
H(29)	8378	5141	435	20
H(31)	10226	8937	683	25
H(32)	11652	8748	-911	31
H(33)	11355	7735	-2266	28
H(34)	9600	6929	-2017	26
H(35)	8174	7117	-423	22
H(37)	6920	9455	76	18
H(38)	5663	11098	39	23
H(39)	4871	12148	1562	24
H(40)	5342	11552	3123	26
H(41)	6619	9914	3153	21
H(100)	8611(14)	8540(13)	2403(12)	-5(4)

Röntgenstrukturanalytische Daten für 66c

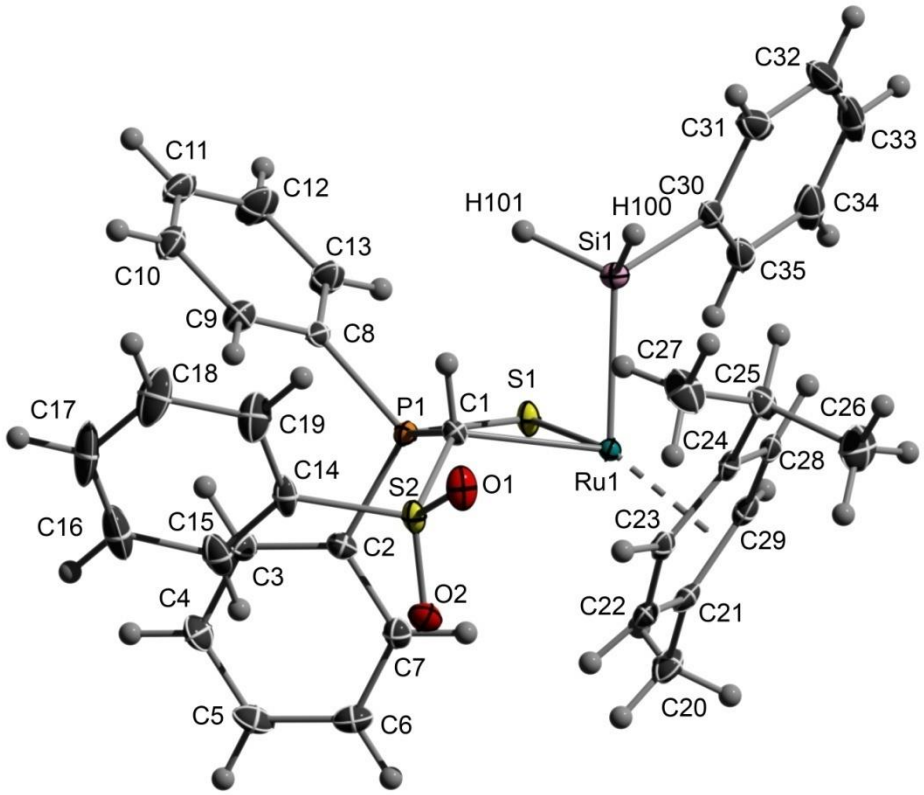

Table 66c-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	$C_{35}H_{37}O_2PRu\ S_2Si$	
Formula weight	713.90	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 19.0170(9) Å	α = 90°.
	b = 8.5520(4) Å	β = 105.150(2)°.
	c = 20.5995(10) Å	γ = 90°.
Volume	3233.7(3) $Å^3$	
Z	4	

Density (calculated)	1.466 Mg/m^3
Absorption coefficient	0.732 mm^{-1}
F(000)	1472
Crystal size	0.14 x 0.14 x 0.04 mm^3
Theta range for data collection	1.30 to 26.42°.
Index ranges	-23<=h<=23, -10<=k<=10, -25<=l<=25
Reflections collected	50602
Independent reflections	6636 [R(int) = 0.0264]
Completeness to theta = 26.42°	99.9 %
Absorption correction	Empirical
Max. and min. transmission	0.9734 and 0.9045
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6636 / 0 / 390
Goodness-of-fit on F^2	1.019
Final R indices [I>2sigma(I)]	R1 = 0.0201, wR2 = 0.0504
R indices (all data)	R1 = 0.0247, wR2 = 0.0528
Largest diff. peak and hole	0.447 and -0.294 $e.Å^{-3}$

Table 66c-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
ru(1)	146(1)	5837(1)	2068(1)	10(1)
s(1)	-778(1)	7853(1)	1921(1)	15(1)
p(1)	-1415(1)	6175(1)	1392(1)	11(1)
si(1)	-184(1)	5389(1)	3077(1)	15(1)
o(1)	-321(1)	1849(1)	1332(1)	21(1)
c(1)	-844(1)	4472(2)	1599(1)	11(1)
s(2)	-759(1)	3115(1)	980(1)	14(1)
o(2)	-534(1)	3877(1)	445(1)	20(1)
c(2)	-1670(1)	6709(2)	515(1)	13(1)
c(3)	-2391(1)	6736(2)	140(1)	18(1)
c(4)	-2566(1)	7246(2)	-523(1)	25(1)
c(5)	-2022(1)	7734(2)	-808(1)	24(1)
c(6)	-1301(1)	7725(2)	-434(1)	20(1)
c(7)	-1124(1)	7219(2)	224(1)	16(1)
c(8)	-2261(1)	5970(2)	1629(1)	14(1)
c(9)	-2704(1)	4659(2)	1451(1)	19(1)
c(10)	-3369(1)	4577(2)	1608(1)	22(1)
c(11)	-3595(1)	5804(2)	1938(1)	25(1)
c(12)	-3158(1)	7101(2)	2118(1)	30(1)
c(13)	-2489(1)	7187(2)	1970(1)	23(1)
c(14)	-1642(1)	2338(2)	625(1)	18(1)
c(15)	-2069(1)	2965(2)	31(1)	23(1)
c(16)	-2778(1)	2435(3)	-212(1)	34(1)
c(17)	-3048(1)	1298(3)	129(1)	42(1)
c(18)	-2611(1)	645(2)	710(1)	38(1)
c(19)	-1903(1)	1168(2)	965(1)	26(1)
c(20)	730(1)	8597(2)	1038(1)	21(1)
c(21)	880(1)	7218(2)	1504(1)	16(1)
c(22)	825(1)	5690(2)	1271(1)	15(1)
c(23)	944(1)	4415(2)	1737(1)	14(1)
c(24)	1201(1)	4644(2)	2438(1)	15(1)

c(25)	1457(1)	3320(2)	2928(1)	18(1)
c(26)	2279(1)	3130(3)	3028(1)	33(1)
c(27)	1066(1)	1783(2)	2715(1)	29(1)
c(28)	1255(1)	6219(2)	2673(1)	15(1)
c(29)	1062(1)	7470(2)	2217(1)	16(1)
c(30)	172(1)	6881(2)	3769(1)	20(1)
c(31)	329(1)	6429(3)	4445(1)	29(1)
c(32)	582(1)	7496(3)	4963(1)	39(1)
c(33)	679(1)	9038(3)	4818(1)	37(1)
c(34)	530(1)	9526(3)	4156(1)	31(1)
c(35)	285(1)	8445(2)	3639(1)	22(1)

Table 66c-3. Bond lengths [Å] and angles [°] for sad.

ru(1)-c(28)	2.1764(16)
ru(1)-c(23)	2.1881(15)
ru(1)-c(29)	2.1919(16)
ru(1)-c(24)	2.2027(16)
ru(1)-c(1)	2.2101(15)
ru(1)-c(22)	2.3434(16)
ru(1)-c(21)	2.3544(16)
ru(1)-si(1)	2.3547(5)
ru(1)-s(1)	2.4237(4)
s(1)-p(1)	2.0062(6)
p(1)-c(1)	1.8006(16)
p(1)-c(2)	1.8041(16)
p(1)-c(8)	1.8077(16)
si(1)-c(30)	1.9016(18)
o(1)-s(2)	1.4403(12)
c(1)-s(2)	1.7616(16)
s(2)-o(2)	1.4390(13)
s(2)-c(14)	1.7749(17)
c(2)-c(3)	1.388(2)
c(2)-c(7)	1.397(2)
c(3)-c(4)	1.387(2)
c(4)-c(5)	1.382(3)
c(5)-c(6)	1.385(3)
c(6)-c(7)	1.377(2)
c(8)-c(13)	1.387(2)
c(8)-c(9)	1.392(2)
c(9)-c(10)	1.388(2)
c(10)-c(11)	1.379(3)
c(11)-c(12)	1.378(3)
c(12)-c(13)	1.386(3)
c(14)-c(19)	1.387(3)
c(14)-c(15)	1.387(2)
c(15)-c(16)	1.386(3)
c(16)-c(17)	1.376(3)

c(17)-c(18)	1.383(3)
c(18)-c(19)	1.385(3)
c(20)-c(21)	1.499(2)
c(21)-c(22)	1.388(2)
c(21)-c(29)	1.434(2)
c(22)-c(23)	1.431(2)
c(23)-c(24)	1.412(2)
c(24)-c(28)	1.426(2)
c(24)-c(25)	1.511(2)
c(25)-c(27)	1.517(3)
c(25)-c(26)	1.531(2)
c(28)-c(29)	1.407(2)
c(30)-c(35)	1.391(3)
c(30)-c(31)	1.400(3)
c(31)-c(32)	1.390(3)
c(32)-c(33)	1.375(4)
c(33)-c(34)	1.383(3)
c(34)-c(35)	1.395(3)

c(28)-ru(1)-c(23)	67.34(6)
c(28)-ru(1)-c(29)	37.59(6)
c(23)-ru(1)-c(29)	78.86(6)
c(28)-ru(1)-c(24)	38.01(6)
c(23)-ru(1)-c(24)	37.53(6)
c(29)-ru(1)-c(24)	68.10(6)
c(28)-ru(1)-c(1)	156.43(6)
c(23)-ru(1)-c(1)	98.67(6)
c(29)-ru(1)-c(1)	162.33(6)
c(24)-ru(1)-c(1)	120.08(6)
c(28)-ru(1)-c(22)	77.29(6)
c(23)-ru(1)-c(22)	36.61(6)
c(29)-ru(1)-c(22)	64.43(6)
c(24)-ru(1)-c(22)	66.29(6)
c(1)-ru(1)-c(22)	103.16(6)
c(28)-ru(1)-c(21)	66.17(6)
c(23)-ru(1)-c(21)	64.91(6)

c(29)-ru(1)-c(21)	36.56(6)
c(24)-ru(1)-c(21)	78.38(6)
c(1)-ru(1)-c(21)	126.62(6)
c(22)-ru(1)-c(21)	34.36(6)
c(28)-ru(1)-si(1)	87.72(5)
c(23)-ru(1)-si(1)	123.45(4)
c(29)-ru(1)-si(1)	111.41(5)
c(24)-ru(1)-si(1)	92.74(4)
c(1)-ru(1)-si(1)	84.70(4)
c(22)-ru(1)-si(1)	158.88(4)
c(21)-ru(1)-si(1)	147.80(4)
c(28)-ru(1)-s(1)	121.78(5)
c(23)-ru(1)-s(1)	153.63(4)
c(29)-ru(1)-s(1)	95.05(5)
c(24)-ru(1)-s(1)	159.71(5)
c(1)-ru(1)-s(1)	79.34(4)
c(22)-ru(1)-s(1)	117.76(4)
c(21)-ru(1)-s(1)	94.92(4)
si(1)-ru(1)-s(1)	82.755(16)
p(1)-s(1)-ru(1)	82.731(18)
c(1)-p(1)-c(2)	115.40(7)
c(1)-p(1)-c(8)	112.50(7)
c(2)-p(1)-c(8)	105.67(7)
c(1)-p(1)-s(1)	102.07(5)
c(2)-p(1)-s(1)	109.22(6)
c(8)-p(1)-s(1)	112.11(6)
c(30)-si(1)-ru(1)	115.34(6)
s(2)-c(1)-p(1)	121.71(9)
s(2)-c(1)-ru(1)	115.87(8)
p(1)-c(1)-ru(1)	93.90(7)
o(2)-s(2)-o(1)	118.48(8)
o(2)-s(2)-c(1)	110.94(7)
o(1)-s(2)-c(1)	106.31(7)
o(2)-s(2)-c(14)	106.98(8)
o(1)-s(2)-c(14)	106.66(8)
c(1)-s(2)-c(14)	106.86(8)

c(3)-c(2)-c(7)	119.59(15)
c(3)-c(2)-p(1)	121.97(12)
c(7)-c(2)-p(1)	118.27(12)
c(4)-c(3)-c(2)	120.09(16)
c(5)-c(4)-c(3)	119.90(17)
c(4)-c(5)-c(6)	120.27(16)
c(7)-c(6)-c(5)	120.09(16)
c(6)-c(7)-c(2)	120.06(16)
c(13)-c(8)-c(9)	119.44(15)
c(13)-c(8)-p(1)	118.74(13)
c(9)-c(8)-p(1)	121.75(13)
c(10)-c(9)-c(8)	120.26(16)
c(11)-c(10)-c(9)	119.85(17)
c(12)-c(11)-c(10)	120.03(17)
c(11)-c(12)-c(13)	120.59(18)
c(12)-c(13)-c(8)	119.81(17)
c(19)-c(14)-c(15)	121.35(17)
c(19)-c(14)-s(2)	119.10(14)
c(15)-c(14)-s(2)	119.47(14)
c(16)-c(15)-c(14)	118.85(19)
c(17)-c(16)-c(15)	120.3(2)
c(16)-c(17)-c(18)	120.43(19)
c(17)-c(18)-c(19)	120.2(2)
c(18)-c(19)-c(14)	118.80(19)
c(22)-c(21)-c(29)	118.18(15)
c(22)-c(21)-c(20)	122.32(16)
c(29)-c(21)-c(20)	119.46(15)
c(22)-c(21)-ru(1)	72.39(9)
c(29)-c(21)-ru(1)	65.54(9)
c(20)-c(21)-ru(1)	132.18(11)
c(21)-c(22)-c(23)	120.07(15)
c(21)-c(22)-ru(1)	73.25(9)
c(23)-c(22)-ru(1)	65.78(9)
c(24)-c(23)-c(22)	122.15(15)
c(24)-c(23)-ru(1)	71.80(9)
c(22)-c(23)-ru(1)	77.61(9)

c(23)-c(24)-c(28)	116.96(15)
c(23)-c(24)-c(25)	123.00(15)
c(28)-c(24)-c(25)	119.94(15)
c(23)-c(24)-ru(1)	70.68(9)
c(28)-c(24)-ru(1)	70.00(9)
c(25)-c(24)-ru(1)	133.14(11)
c(24)-c(25)-c(27)	114.09(14)
c(24)-c(25)-c(26)	108.00(15)
c(27)-c(25)-c(26)	110.70(16)
c(29)-c(28)-c(24)	120.53(15)
c(29)-c(28)-ru(1)	71.80(9)
c(24)-c(28)-ru(1)	71.99(9)
c(28)-c(29)-c(21)	121.38(15)
c(28)-c(29)-ru(1)	70.61(9)
c(21)-c(29)-ru(1)	77.90(9)
c(35)-c(30)-c(31)	116.97(17)
c(35)-c(30)-si(1)	122.91(13)
c(31)-c(30)-si(1)	120.11(15)
c(32)-c(31)-c(30)	121.5(2)
c(33)-c(32)-c(31)	120.1(2)
c(32)-c(33)-c(34)	119.92(19)
c(33)-c(34)-c(35)	119.6(2)
c(30)-c(35)-c(34)	121.82(19)

Symmetry transformations used to generate equivalent atoms:

Table 66c-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
ru(1)	9(1)	10(1)	10(1)	0(1)	2(1)	0(1)
s(1)	12(1)	12(1)	18(1)	-3(1)	1(1)	1(1)
p(1)	10(1)	12(1)	11(1)	0(1)	2(1)	0(1)
si(1)	15(1)	19(1)	13(1)	1(1)	5(1)	0(1)
o(1)	18(1)	13(1)	28(1)	-3(1)	-1(1)	4(1)
c(1)	12(1)	11(1)	10(1)	-1(1)	2(1)	0(1)
s(2)	12(1)	12(1)	16(1)	-3(1)	1(1)	1(1)
o(2)	21(1)	22(1)	17(1)	-5(1)	7(1)	-1(1)
c(2)	16(1)	11(1)	12(1)	1(1)	4(1)	2(1)
c(3)	15(1)	23(1)	17(1)	4(1)	5(1)	1(1)
c(4)	19(1)	34(1)	18(1)	7(1)	-1(1)	3(1)
c(5)	31(1)	25(1)	15(1)	7(1)	5(1)	4(1)
c(6)	25(1)	18(1)	20(1)	2(1)	12(1)	1(1)
c(7)	15(1)	16(1)	17(1)	-1(1)	4(1)	0(1)
c(8)	11(1)	18(1)	11(1)	3(1)	3(1)	2(1)
c(9)	17(1)	19(1)	22(1)	1(1)	7(1)	0(1)
c(10)	17(1)	24(1)	26(1)	4(1)	6(1)	-4(1)
c(11)	15(1)	36(1)	26(1)	6(1)	10(1)	3(1)
c(12)	26(1)	32(1)	37(1)	-8(1)	18(1)	3(1)
c(13)	21(1)	24(1)	26(1)	-6(1)	10(1)	-2(1)
c(14)	15(1)	14(1)	23(1)	-8(1)	-1(1)	1(1)
c(15)	23(1)	24(1)	20(1)	-9(1)	0(1)	3(1)
c(16)	25(1)	36(1)	32(1)	-14(1)	-10(1)	4(1)
c(17)	19(1)	33(1)	62(2)	-17(1)	-7(1)	-8(1)
c(18)	27(1)	20(1)	65(2)	-4(1)	6(1)	-9(1)
c(19)	22(1)	14(1)	39(1)	-1(1)	1(1)	-1(1)
c(20)	18(1)	19(1)	27(1)	5(1)	7(1)	-4(1)
c(21)	10(1)	18(1)	22(1)	3(1)	8(1)	-2(1)
c(22)	10(1)	20(1)	16(1)	-1(1)	5(1)	-1(1)
c(23)	9(1)	16(1)	17(1)	-2(1)	5(1)	1(1)
c(24)	8(1)	20(1)	17(1)	1(1)	3(1)	1(1)

c(25)	15(1)	21(1)	17(1)	1(1)	0(1)	5(1)
c(26)	19(1)	40(1)	38(1)	7(1)	2(1)	12(1)
c(27)	37(1)	19(1)	27(1)	7(1)	-2(1)	2(1)
c(28)	9(1)	20(1)	17(1)	-4(1)	3(1)	-3(1)
c(29)	11(1)	16(1)	23(1)	-5(1)	7(1)	-4(1)
c(30)	10(1)	34(1)	15(1)	-5(1)	3(1)	4(1)
c(31)	21(1)	48(1)	17(1)	0(1)	6(1)	8(1)
c(32)	24(1)	77(2)	14(1)	-9(1)	2(1)	12(1)
c(33)	16(1)	65(2)	28(1)	-28(1)	0(1)	6(1)
c(34)	17(1)	39(1)	35(1)	-19(1)	5(1)	0(1)
c(35)	14(1)	33(1)	19(1)	-7(1)	2(1)	1(1)

Table 66c-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
h(1)	-992	3888	1962	13
h(3)	-2765	6406	337	22
h(4)	-3060	7259	-780	30
h(5)	-2142	8077	-1262	29
h(6)	-929	8069	-631	24
h(7)	-629	7216	480	20
h(9)	-2549	3816	1220	23
h(10)	-3669	3678	1488	27
h(11)	-4053	5756	2042	30
h(12)	-3316	7942	2346	36
h(13)	-2187	8079	2101	27
h(15)	-1879	3743	-205	28
h(16)	-3079	2860	-616	41
h(17)	-3538	958	-35	50
h(18)	-2797	-164	934	46
h(19)	-1602	733	1367	32
h(20a)	566	8230	572	32

h(20b)	1175	9216	1095	32
h(20c)	349	9246	1143	32
h(22)	564	5485	790	18
h(23)	804	3336	1563	17
h(25)	1371	3629	3369	22
h(26a)	2377	2825	2602	50
h(26b)	2463	2320	3367	50
h(26c)	2524	4123	3181	50
h(27a)	539	1944	2623	44
h(27b)	1222	1014	3077	44
h(27c)	1184	1399	2308	44
h(28)	1343	6425	3166	18
h(29)	1012	8543	2393	20
h(31)	260	5370	4552	34
h(32)	687	7159	5417	46
h(33)	848	9767	5172	45
h(34)	595	10591	4054	37
h(35)	192	8786	3186	27
h(100)	41(11)	3930(20)	3393(11)	32(6)
h(101)	-951(10)	5380(20)	2985(9)	21(5)

Röntgenstrukturanalytische Daten für 71b

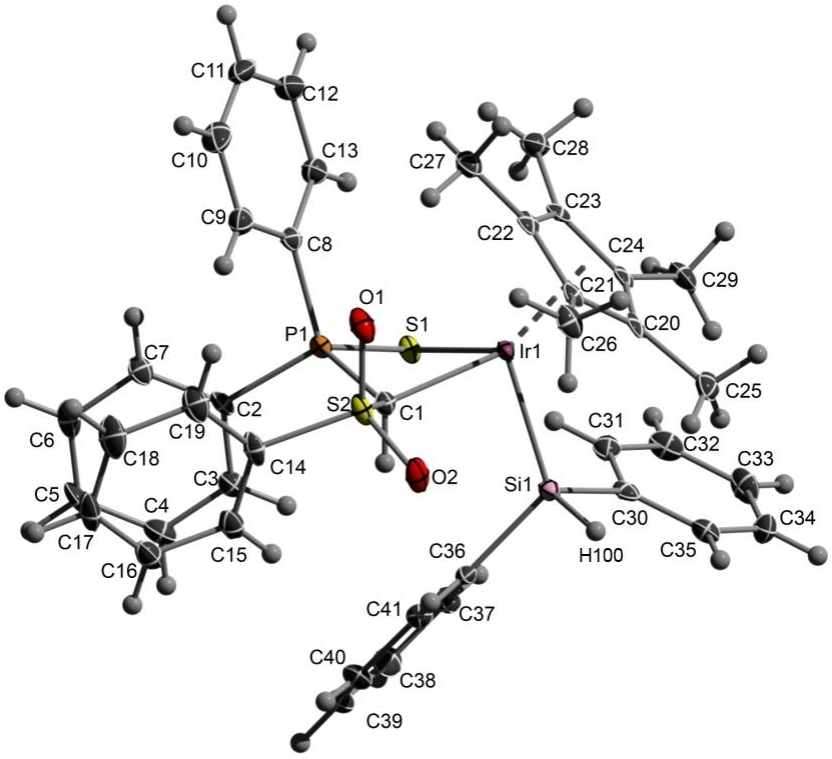

Table 71b-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	C41 H42 Ir O2 P S2 Si	
Formula weight	882.13	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P212121	
Unit cell dimensions	a = 11.5635(11) Å	α = 90°.
	b = 14.6143(14) Å	β = 90°.
	c = 21.630(2) Å	γ = 90°.
Volume	3655.3(6) $Å^3$	
Z	4	
Density (calculated)	1.603 Mg/m^3	
Absorption coefficient	3.879 mm^{-1}	
F(000)	1768	
Crystal size	0.17 x 0.12 x 0.08 mm^3	

Theta range for data collection	1.68 to 26.44°.
Index ranges	-14<=h<=14, -16<=k<=18, -27<=l<=27
Reflections collected	39569
Independent reflections	7467 [R(int) = 0.0396]
Completeness to theta = 26.44°	99.7 %
Absorption correction	Empirical
Max. and min. transmission	0.7466 and 0.5585
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7467 / 0 / 442
Goodness-of-fit on F^2	1.016
Final R indices [I>2sigma(I)]	R1 = 0.0174, wR2 = 0.0416
R indices (all data)	R1 = 0.0186, wR2 = 0.0421
Absolute structure parameter	0.013(3)
Largest diff. peak and hole	1.261 and -0.959 e.$Å^{-3}$

Table 71b-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	3446(1)	-5(1)	-4441(1)	10(1)
S(1)	4539(1)	-1287(1)	-4864(1)	13(1)
P(1)	4759(1)	-1549(1)	-3957(1)	11(1)
Si(1)	4827(1)	1010(1)	-4838(1)	12(1)
O(1)	3407(2)	-342(1)	-2692(1)	22(1)
C(1)	4666(2)	-375(2)	-3718(1)	12(1)
S(2)	4485(1)	-12(1)	-2950(1)	16(1)
O(2)	4710(2)	955(1)	-2946(1)	21(1)
C(2)	6149(2)	-2068(2)	-3787(1)	13(1)
C(3)	7120(2)	-1678(2)	-4068(1)	17(1)
C(4)	8208(2)	-2025(2)	-3948(1)	22(1)
C(5)	8339(2)	-2761(2)	-3552(1)	25(1)
C(6)	7378(2)	-3148(2)	-3270(1)	24(1)
C(7)	6284(2)	-2809(2)	-3386(1)	18(1)
C(8)	3660(2)	-2293(2)	-3657(1)	14(1)

C(9)	3535(2)	-2454(2)	-3023(1)	19(1)
C(10)	2706(2)	-3061(2)	-2810(1)	28(1)
C(11)	1996(3)	-3516(2)	-3225(1)	29(1)
C(12)	2123(2)	-3378(2)	-3849(1)	29(1)
C(13)	2953(2)	-2774(2)	-4071(1)	20(1)
C(14)	5616(2)	-550(2)	-2518(1)	18(1)
C(15)	6755(2)	-446(2)	-2703(1)	20(1)
C(16)	7621(2)	-842(2)	-2355(1)	24(1)
C(17)	7351(3)	-1317(2)	-1820(1)	26(1)
C(18)	6223(3)	-1414(2)	-1634(1)	31(1)
C(19)	5333(3)	-1029(2)	-1987(1)	24(1)
C(20)	2111(2)	1039(2)	-4606(1)	15(1)
C(21)	1974(2)	661(2)	-3995(1)	13(1)
C(22)	1612(2)	-282(2)	-4050(1)	14(1)
C(23)	1610(2)	-502(2)	-4690(1)	14(1)
C(24)	1943(2)	304(2)	-5035(1)	14(1)
C(25)	2230(2)	2025(2)	-4758(1)	20(1)
C(26)	1946(2)	1213(2)	-3404(1)	20(1)
C(27)	1191(2)	-871(2)	-3534(1)	20(1)
C(28)	1253(2)	-1376(2)	-4988(1)	20(1)
C(29)	1816(2)	404(2)	-5724(1)	22(1)
C(30)	4667(2)	1167(2)	-5705(1)	14(1)
C(31)	4605(2)	414(2)	-6110(1)	19(1)
C(32)	4425(2)	545(2)	-6740(1)	21(1)
C(33)	4313(2)	1410(2)	-6983(1)	24(1)
C(34)	4373(2)	2155(2)	-6597(1)	22(1)
C(35)	4549(2)	2035(2)	-5961(1)	17(1)
C(36)	6422(2)	779(2)	-4717(1)	15(1)
C(37)	7132(2)	422(2)	-5181(1)	20(1)
C(38)	8302(3)	256(2)	-5089(1)	28(1)
C(39)	8793(3)	447(2)	-4513(1)	31(1)
C(40)	8114(2)	791(2)	-4052(1)	26(1)
C(41)	6951(2)	974(2)	-4148(1)	20(1)

Table 71b-3. Bond lengths [Å] and angles [°] for sad.

Ir(1)-C(1)	2.175(2)
Ir(1)-C(21)	2.185(2)
Ir(1)-C(20)	2.199(3)
Ir(1)-C(24)	2.208(2)
Ir(1)-C(23)	2.307(3)
Ir(1)-C(22)	2.319(3)
Ir(1)-Si(1)	2.3428(8)
Ir(1)-S(1)	2.4388(7)
Ir(1)-P(1)	2.9141(7)
S(1)-P(1)	2.0155(8)
P(1)-C(8)	1.794(3)
P(1)-C(1)	1.795(2)
P(1)-C(2)	1.815(3)
Si(1)-C(36)	1.893(3)
Si(1)-C(30)	1.899(2)
O(1)-S(2)	1.4488(19)
C(1)-S(2)	1.756(2)
S(2)-O(2)	1.437(2)
S(2)-C(14)	1.789(2)
C(2)-C(7)	1.396(4)
C(2)-C(3)	1.398(3)
C(3)-C(4)	1.382(4)
C(4)-C(5)	1.383(4)
C(5)-C(6)	1.388(4)
C(6)-C(7)	1.381(4)
C(8)-C(9)	1.398(3)
C(8)-C(13)	1.402(4)
C(9)-C(10)	1.385(4)
C(10)-C(11)	1.386(4)
C(11)-C(12)	1.372(4)
C(12)-C(13)	1.389(4)
C(14)-C(19)	1.384(4)
C(14)-C(15)	1.385(4)
C(15)-C(16)	1.380(4)

C(16)-C(17)	1.384(4)
C(17)-C(18)	1.372(4)
C(18)-C(19)	1.400(4)
C(20)-C(24)	1.433(4)
C(20)-C(21)	1.440(3)
C(20)-C(25)	1.485(4)
C(21)-C(22)	1.445(4)
C(21)-C(26)	1.512(3)
C(22)-C(23)	1.421(3)
C(22)-C(27)	1.491(3)
C(23)-C(24)	1.446(4)
C(23)-C(28)	1.490(4)
C(24)-C(29)	1.505(3)
C(30)-C(35)	1.391(4)
C(30)-C(31)	1.408(3)
C(31)-C(32)	1.392(3)
C(32)-C(33)	1.375(4)
C(33)-C(34)	1.375(4)
C(34)-C(35)	1.400(3)
C(36)-C(37)	1.398(3)
C(36)-C(41)	1.404(4)
C(37)-C(38)	1.389(4)
C(38)-C(39)	1.398(4)
C(39)-C(40)	1.364(4)
C(40)-C(41)	1.387(4)

C(1)-Ir(1)-C(21)	107.38(9)
C(1)-Ir(1)-C(20)	138.10(9)
C(21)-Ir(1)-C(20)	38.35(9)
C(1)-Ir(1)-C(24)	168.53(9)
C(21)-Ir(1)-C(24)	63.43(9)
C(20)-Ir(1)-C(24)	37.96(9)
C(1)-Ir(1)-C(23)	133.34(9)
C(21)-Ir(1)-C(23)	61.75(9)
C(20)-Ir(1)-C(23)	62.29(10)
C(24)-Ir(1)-C(23)	37.29(9)

C(1)-Ir(1)-C(22)	106.72(9)
C(21)-Ir(1)-C(22)	37.29(10)
C(20)-Ir(1)-C(22)	62.50(9)
C(24)-Ir(1)-C(22)	61.83(8)
C(23)-Ir(1)-C(22)	35.77(9)
C(1)-Ir(1)-Si(1)	88.79(7)
C(21)-Ir(1)-Si(1)	114.23(8)
C(20)-Ir(1)-Si(1)	88.83(7)
C(24)-Ir(1)-Si(1)	101.18(7)
C(23)-Ir(1)-Si(1)	137.82(7)
C(22)-Ir(1)-Si(1)	150.18(7)
C(1)-Ir(1)-S(1)	75.09(6)
C(21)-Ir(1)-S(1)	155.75(8)
C(20)-Ir(1)-S(1)	146.71(7)
C(24)-Ir(1)-S(1)	110.28(7)
C(23)-Ir(1)-S(1)	98.48(7)
C(22)-Ir(1)-S(1)	118.49(7)
Si(1)-Ir(1)-S(1)	89.76(3)
C(1)-Ir(1)-P(1)	37.91(6)
C(21)-Ir(1)-P(1)	126.32(7)
C(20)-Ir(1)-P(1)	163.95(7)
C(24)-Ir(1)-P(1)	141.03(7)
C(23)-Ir(1)-P(1)	108.63(7)
C(22)-Ir(1)-P(1)	102.15(7)
Si(1)-Ir(1)-P(1)	105.47(2)
S(1)-Ir(1)-P(1)	43.105(19)
P(1)-S(1)-Ir(1)	81.12(3)
C(8)-P(1)-C(1)	115.65(12)
C(8)-P(1)-C(2)	107.46(12)
C(1)-P(1)-C(2)	113.22(12)
C(8)-P(1)-S(1)	112.20(9)
C(1)-P(1)-S(1)	95.28(8)
C(2)-P(1)-S(1)	112.85(8)
C(8)-P(1)-Ir(1)	103.33(8)
C(1)-P(1)-Ir(1)	48.13(8)
C(2)-P(1)-Ir(1)	149.09(9)

S(1)-P(1)-Ir(1)	55.78(2)
C(36)-Si(1)-C(30)	104.64(11)
C(36)-Si(1)-Ir(1)	120.01(8)
C(30)-Si(1)-Ir(1)	111.86(8)
S(2)-C(1)-P(1)	124.64(14)
S(2)-C(1)-Ir(1)	121.87(13)
P(1)-C(1)-Ir(1)	93.96(10)
O(2)-S(2)-O(1)	118.73(12)
O(2)-S(2)-C(1)	106.34(11)
O(1)-S(2)-C(1)	111.50(12)
O(2)-S(2)-C(14)	107.23(12)
O(1)-S(2)-C(14)	106.37(12)
C(1)-S(2)-C(14)	105.92(12)
C(7)-C(2)-C(3)	119.8(2)
C(7)-C(2)-P(1)	123.3(2)
C(3)-C(2)-P(1)	116.9(2)
C(4)-C(3)-C(2)	120.0(2)
C(3)-C(4)-C(5)	120.1(3)
C(4)-C(5)-C(6)	120.0(3)
C(7)-C(6)-C(5)	120.5(3)
C(6)-C(7)-C(2)	119.5(3)
C(9)-C(8)-C(13)	118.8(2)
C(9)-C(8)-P(1)	122.0(2)
C(13)-C(8)-P(1)	119.08(19)
C(10)-C(9)-C(8)	120.4(3)
C(9)-C(10)-C(11)	120.1(3)
C(12)-C(11)-C(10)	120.2(3)
C(11)-C(12)-C(13)	120.4(3)
C(12)-C(13)-C(8)	120.1(3)
C(19)-C(14)-C(15)	121.4(2)
C(19)-C(14)-S(2)	118.9(2)
C(15)-C(14)-S(2)	119.7(2)
C(16)-C(15)-C(14)	119.0(3)
C(15)-C(16)-C(17)	120.2(3)
C(18)-C(17)-C(16)	120.7(3)
C(17)-C(18)-C(19)	119.8(3)

C(14)-C(19)-C(18)	118.8(3)
C(24)-C(20)-C(21)	107.0(2)
C(24)-C(20)-C(25)	126.6(2)
C(21)-C(20)-C(25)	125.9(2)
C(24)-C(20)-Ir(1)	71.37(14)
C(21)-C(20)-Ir(1)	70.31(14)
C(25)-C(20)-Ir(1)	130.14(19)
C(20)-C(21)-C(22)	108.8(2)
C(20)-C(21)-C(26)	125.0(2)
C(22)-C(21)-C(26)	124.9(2)
C(20)-C(21)-Ir(1)	71.34(14)
C(22)-C(21)-Ir(1)	76.36(16)
C(26)-C(21)-Ir(1)	128.86(18)
C(23)-C(22)-C(21)	107.2(2)
C(23)-C(22)-C(27)	126.7(2)
C(21)-C(22)-C(27)	125.7(2)
C(23)-C(22)-Ir(1)	71.66(15)
C(21)-C(22)-Ir(1)	66.35(14)
C(27)-C(22)-Ir(1)	132.21(18)
C(22)-C(23)-C(24)	108.6(2)
C(22)-C(23)-C(28)	128.1(2)
C(24)-C(23)-C(28)	123.2(2)
C(22)-C(23)-Ir(1)	72.57(15)
C(24)-C(23)-Ir(1)	67.66(14)
C(28)-C(23)-Ir(1)	128.79(19)
C(20)-C(24)-C(23)	108.2(2)
C(20)-C(24)-C(29)	125.6(2)
C(23)-C(24)-C(29)	124.4(2)
C(20)-C(24)-Ir(1)	70.67(14)
C(23)-C(24)-Ir(1)	75.06(14)
C(29)-C(24)-Ir(1)	132.29(18)
C(35)-C(30)-C(31)	117.4(2)
C(35)-C(30)-Si(1)	120.86(18)
C(31)-C(30)-Si(1)	121.70(19)
C(32)-C(31)-C(30)	120.7(3)
C(33)-C(32)-C(31)	120.9(2)

C(34)-C(33)-C(32)	119.5(2)
C(33)-C(34)-C(35)	120.2(3)
C(30)-C(35)-C(34)	121.3(2)
C(37)-C(36)-C(41)	116.6(2)
C(37)-C(36)-Si(1)	122.7(2)
C(41)-C(36)-Si(1)	120.7(2)
C(38)-C(37)-C(36)	122.4(3)
C(37)-C(38)-C(39)	119.2(3)
C(40)-C(39)-C(38)	119.4(3)
C(39)-C(40)-C(41)	121.4(3)
C(40)-C(41)-C(36)	121.0(3)

Symmetry transformations used to generate equivalent atoms:

Table 71b-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	7(1)	12(1)	10(1)	1(1)	-1(1)	1(1)
S(1)	13(1)	16(1)	11(1)	-1(1)	-1(1)	4(1)
P(1)	10(1)	13(1)	12(1)	0(1)	-1(1)	1(1)
Si(1)	10(1)	15(1)	12(1)	1(1)	0(1)	-1(1)
O(1)	18(1)	31(1)	16(1)	1(1)	1(1)	8(1)
C(1)	12(1)	12(1)	12(1)	-1(1)	1(1)	2(1)
S(2)	15(1)	19(1)	13(1)	-4(1)	-3(1)	6(1)
O(2)	25(1)	15(1)	23(1)	-6(1)	-8(1)	7(1)
C(2)	9(1)	16(2)	15(1)	-4(1)	-3(1)	3(1)
C(3)	15(1)	18(2)	17(1)	-2(1)	-1(1)	1(1)
C(4)	14(2)	27(2)	26(1)	-3(1)	-1(1)	-1(1)
C(5)	12(2)	33(2)	28(1)	-4(1)	-7(1)	8(1)
C(6)	26(2)	25(2)	20(1)	1(1)	-7(1)	9(1)
C(7)	15(1)	21(2)	17(1)	-1(1)	1(1)	4(1)
C(8)	10(1)	12(2)	21(1)	0(1)	0(1)	2(1)
C(9)	19(2)	17(2)	22(1)	3(1)	1(1)	3(1)

C(10)	22(2)	32(2)	29(2)	13(1)	7(1)	1(1)
C(11)	19(2)	19(2)	49(2)	13(1)	3(1)	-3(1)
C(12)	21(2)	19(2)	46(2)	2(1)	-6(1)	-5(1)
C(13)	18(2)	18(2)	24(1)	0(1)	-2(1)	0(1)
C(14)	21(2)	19(2)	13(1)	-5(1)	-7(1)	7(1)
C(15)	21(2)	19(2)	21(1)	-3(1)	-8(1)	2(1)
C(16)	18(2)	22(2)	31(2)	-5(1)	-9(1)	2(1)
C(17)	32(2)	23(2)	23(1)	-2(1)	-17(1)	8(1)
C(18)	37(2)	39(2)	17(1)	4(1)	-7(1)	9(2)
C(19)	25(2)	30(2)	16(1)	-1(1)	-2(1)	6(1)
C(20)	6(1)	21(2)	19(1)	3(1)	-1(1)	6(1)
C(21)	8(1)	15(2)	17(1)	-1(1)	0(1)	5(1)
C(22)	6(1)	19(2)	18(1)	1(1)	2(1)	5(1)
C(23)	5(1)	19(2)	19(1)	2(1)	-1(1)	0(1)
C(24)	5(1)	20(2)	18(1)	3(1)	-1(1)	4(1)
C(25)	14(1)	21(2)	24(1)	5(1)	2(1)	6(1)
C(26)	18(2)	24(2)	19(1)	-6(1)	0(1)	9(1)
C(27)	13(1)	26(2)	20(1)	4(1)	1(1)	1(1)
C(28)	16(1)	20(2)	24(1)	-2(1)	-2(1)	-2(1)
C(29)	12(1)	37(2)	17(1)	4(1)	-3(1)	2(1)
C(30)	8(1)	22(2)	14(1)	1(1)	2(1)	-2(1)
C(31)	14(1)	21(2)	21(1)	3(1)	3(1)	1(1)
C(32)	21(2)	26(2)	16(1)	-8(1)	0(1)	-1(1)
C(33)	24(2)	37(2)	12(1)	3(1)	-3(1)	3(1)
C(34)	22(2)	21(2)	21(1)	9(1)	-2(1)	1(1)
C(35)	12(1)	21(2)	17(1)	-2(1)	-2(1)	-1(1)
C(36)	11(1)	12(2)	22(1)	7(1)	1(1)	-1(1)
C(37)	15(1)	20(2)	23(1)	5(1)	2(1)	3(1)
C(38)	18(2)	25(2)	40(2)	8(1)	9(1)	5(1)
C(39)	13(2)	25(2)	54(2)	16(1)	-4(1)	-2(1)
C(40)	18(2)	26(2)	35(2)	6(1)	-11(1)	-5(1)
C(41)	16(2)	17(2)	27(1)	5(1)	-4(1)	-2(1)

Table 71b-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
H(1)	5400	-102	-3848	15
H(3)	7033	-1186	-4336	20
H(4)	8854	-1764	-4134	26
H(5)	9072	-2996	-3474	29
H(6)	7471	-3639	-3002	28
H(7)	5642	-3073	-3198	21
H(9)	4011	-2152	-2743	23
H(10)	2625	-3164	-2388	33
H(11)	1432	-3915	-3080	35
H(12)	1650	-3691	-4125	34
H(13)	3039	-2689	-4494	24
H(15)	6934	-115	-3058	24
H(16)	8388	-788	-2479	28
H(17)	7941	-1574	-1585	32
H(18)	6051	-1735	-1274	37
H(19)	4565	-1094	-1867	28
H(25A)	2693	2092	-5124	30
H(25B)	2595	2338	-4420	30
H(25C)	1478	2283	-4829	30
H(100)	4710(20)	1921(17)	-4581(10)	12(6)
H(26A)	2623	1591	-3381	31
H(26B)	1928	806	-3056	31
H(26C)	1268	1593	-3400	31
H(27A)	419	-693	-3424	30
H(27B)	1691	-800	-3183	30
H(27C)	1193	-1499	-3664	30
H(28A)	553	-1280	-5218	30
H(28B)	1123	-1831	-4676	30
H(28C)	1852	-1579	-5263	30
H(29A)	2236	933	-5861	33

H(29B)	1013	473	-5827	33
H(29C)	2118	-132	-5925	33
H(31)	4686	-176	-5955	23
H(32)	4381	40	-7001	25
H(33)	4196	1490	-7405	29
H(34)	4297	2742	-6758	26
H(35)	4587	2545	-5705	20
H(37)	6810	291	-5564	24
H(38)	8754	21	-5408	33
H(39)	9576	340	-4444	37
H(40)	8438	904	-3666	31
H(41)	6516	1231	-3831	24

Röntgenstrukturanalytische Daten für 72

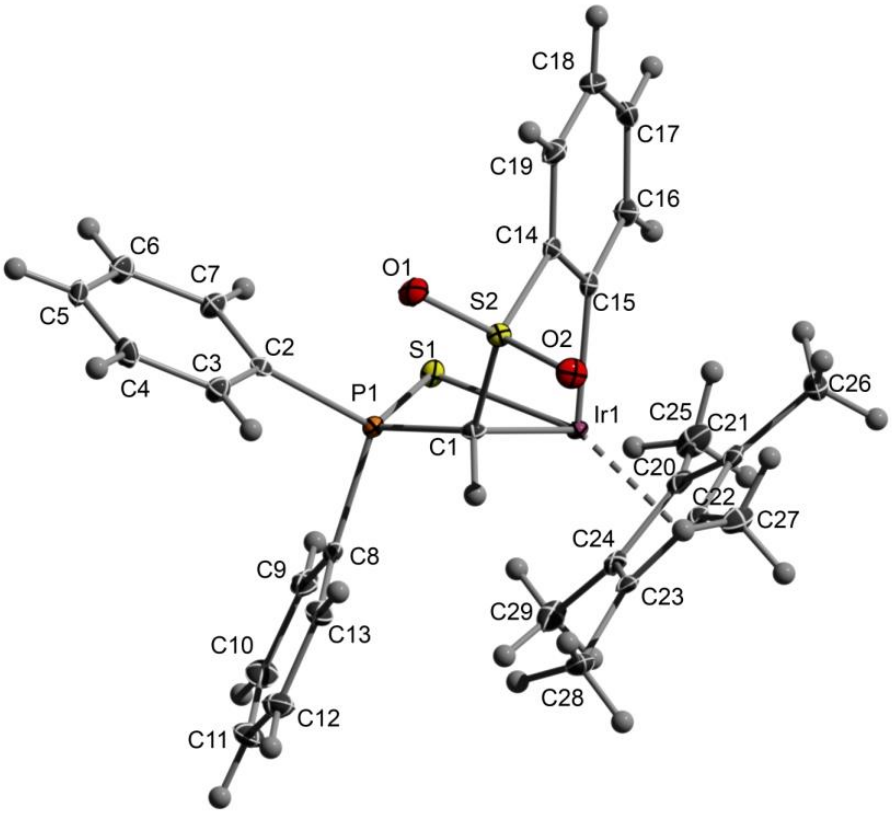

Table 72-1. Crystal data and structure refinement for platon.

Identification code	platon	
Empirical formula	C29 H30 Ir O2 P S2	
Formula weight	1395.64	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.1798(11) Å	α = 99.467(3)°.
	b = 11.1962(11) Å	β = 105.272(3)°.
	c = 11.4825(11) Å	γ = 105.876(3)°.
Volume	1289.6(2) $Å^3$	
Z	2	
Density (calculated)	1.797 Mg/m^3	
Absorption coefficient	5.427 mm^{-1}	

F(000)	688
Crystal size	0.286 x 0.176 x 0.052 mm^3
Theta range for data collection	1.90 to 26.44°.
Index ranges	-14<=h<=13, -14<=k<=14, -14<=l<=14
Reflections collected	17332
Independent reflections	5298 [R(int) = 0.0235]
Completeness to theta = 26.44°	99.8 %
Absorption correction	Empirical
Max. and min. transmission	0.7454 and 0.5306
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5298 / 0 / 321
Goodness-of-fit on F^2	1.319
Final R indices [I>2sigma(I)]	R1 = 0.0149, wR2 = 0.0410
R indices (all data)	R1 = 0.0169, wR2 = 0.0644
Largest diff. peak and hole	0.702 and -0.675 e.$Å^{-3}$

Table 72-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for platon. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ir(1)	986(1)	3084(1)	7560(1)	7(1)
S(1)	1035(1)	904(1)	6905(1)	11(1)
P(1)	2951(1)	1936(1)	7503(1)	8(1)
O(1)	4400(2)	3209(2)	10720(2)	15(1)
C(1)	3034(3)	3408(3)	8463(3)	9(1)
S(2)	3389(1)	3691(1)	10100(1)	9(1)
O(2)	3635(2)	5053(2)	10563(2)	15(1)
C(2)	3991(3)	1050(3)	8102(3)	10(1)
C(3)	5348(3)	1705(3)	8679(3)	12(1)
C(4)	6170(3)	1007(3)	9005(3)	14(1)
C(5)	5674(3)	-322(3)	8777(3)	14(1)
C(6)	4336(4)	-962(3)	8225(3)	15(1)
C(7)	3491(3)	-279(3)	7893(3)	12(1)
C(8)	3518(3)	2359(3)	6231(3)	10(1)

C(9)	2877(3)	1541(3)	5037(3)	14(1)
C(10)	3388(4)	1743(4)	4085(3)	19(1)
C(11)	4521(4)	2771(4)	4305(3)	20(1)
C(12)	5145(4)	3598(4)	5486(3)	18(1)
C(13)	4660(3)	3388(3)	6460(3)	14(1)
C(14)	1877(3)	2794(3)	10191(3)	10(1)
C(15)	782(3)	2502(3)	9129(3)	10(1)
C(16)	-402(3)	1722(3)	9208(3)	14(1)
C(17)	-452(3)	1307(3)	10279(3)	15(1)
C(18)	658(4)	1668(3)	11327(3)	15(1)
C(19)	1848(3)	2417(3)	11281(3)	14(1)
C(20)	-837(3)	3136(3)	6250(3)	13(1)
C(21)	-453(3)	4105(3)	7376(3)	12(1)
C(22)	847(3)	4971(3)	7574(3)	11(1)
C(23)	1210(3)	4569(3)	6485(3)	11(1)
C(24)	194(3)	3448(3)	5689(3)	11(1)
C(25)	-2137(4)	2063(4)	5666(4)	21(1)
C(26)	-1294(4)	4251(4)	8176(4)	20(1)
C(27)	1613(4)	6176(3)	8590(3)	17(1)
C(28)	2438(4)	5275(3)	6253(4)	17(1)
C(29)	140(4)	2728(4)	4447(3)	18(1)

Table 72-3. Bond lengths [Å] and angles [°] for platon.

Ir(1)-C(15)	2.060(3)
Ir(1)-C(1)	2.149(3)
Ir(1)-C(22)	2.158(3)
Ir(1)-C(21)	2.201(3)
Ir(1)-C(20)	2.212(3)
Ir(1)-C(23)	2.227(3)
Ir(1)-C(24)	2.247(3)
Ir(1)-S(1)	2.4536(9)
Ir(1)-P(1)	2.8413(9)
S(1)-P(1)	2.0011(12)
P(1)-C(1)	1.790(3)

P(1)-C(2)	1.802(3)
P(1)-C(8)	1.819(3)
O(1)-S(2)	1.453(2)
C(1)-S(2)	1.771(3)
C(1)-H(1)	1.0000
S(2)-O(2)	1.452(2)
S(2)-C(14)	1.753(3)
C(2)-C(7)	1.393(5)
C(2)-C(3)	1.407(5)
C(3)-C(4)	1.378(5)
C(3)-H(3)	0.9500
C(4)-C(5)	1.391(5)
C(4)-H(4)	0.9500
C(5)-C(6)	1.385(5)
C(5)-H(5)	0.9500
C(6)-C(7)	1.386(5)
C(6)-H(6)	0.9500
C(7)-H(7)	0.9500
C(8)-C(9)	1.394(5)
C(8)-C(13)	1.396(5)
C(9)-C(10)	1.383(5)
C(9)-H(9)	0.9500
C(10)-C(11)	1.390(5)
C(10)-H(10)	0.9500
C(11)-C(12)	1.385(5)
C(11)-H(11)	0.9500
C(12)-C(13)	1.391(5)
C(12)-H(12)	0.9500
C(13)-H(13)	0.9500
C(14)-C(19)	1.390(5)
C(14)-C(15)	1.399(5)
C(15)-C(16)	1.407(5)
C(16)-C(17)	1.394(5)
C(16)-H(16)	0.9500
C(17)-C(18)	1.389(5)
C(17)-H(17)	0.9500

C(18)-C(19)	1.385(5)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500
C(20)-C(21)	1.422(5)
C(20)-C(24)	1.452(5)
C(20)-C(25)	1.507(5)
C(21)-C(22)	1.445(5)
C(21)-C(26)	1.498(5)
C(22)-C(23)	1.453(5)
C(22)-C(27)	1.496(5)
C(23)-C(24)	1.413(5)
C(23)-C(28)	1.500(5)
C(24)-C(29)	1.496(5)
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800

C(15)-Ir(1)-C(1)	83.25(12)
C(15)-Ir(1)-C(22)	113.33(13)
C(1)-Ir(1)-C(22)	105.10(13)
C(15)-Ir(1)-C(21)	97.43(12)
C(1)-Ir(1)-C(21)	140.68(12)
C(22)-Ir(1)-C(21)	38.71(12)
C(15)-Ir(1)-C(20)	115.25(13)

C(1)-Ir(1)-C(20)	160.91(13)
C(22)-Ir(1)-C(20)	64.39(13)
C(21)-Ir(1)-C(20)	37.60(13)
C(15)-Ir(1)-C(23)	151.57(13)
C(1)-Ir(1)-C(23)	98.44(12)
C(22)-Ir(1)-C(23)	38.66(12)
C(21)-Ir(1)-C(23)	63.44(12)
C(20)-Ir(1)-C(23)	63.17(12)
C(15)-Ir(1)-C(24)	153.06(13)
C(1)-Ir(1)-C(24)	123.68(12)
C(22)-Ir(1)-C(24)	63.61(12)
C(21)-Ir(1)-C(24)	62.82(12)
C(20)-Ir(1)-C(24)	38.01(12)
C(23)-Ir(1)-C(24)	36.82(12)
C(15)-Ir(1)-S(1)	82.56(9)
C(1)-Ir(1)-S(1)	80.36(9)
C(22)-Ir(1)-S(1)	163.49(9)
C(21)-Ir(1)-S(1)	138.89(9)
C(20)-Ir(1)-S(1)	105.62(9)
C(23)-Ir(1)-S(1)	125.81(9)
C(24)-Ir(1)-S(1)	100.26(9)
C(15)-Ir(1)-P(1)	91.36(9)
C(1)-Ir(1)-P(1)	39.02(9)
C(22)-Ir(1)-P(1)	135.41(9)
C(21)-Ir(1)-P(1)	171.10(9)
C(20)-Ir(1)-P(1)	138.18(9)
C(23)-Ir(1)-P(1)	107.88(9)
C(24)-Ir(1)-P(1)	109.28(9)
S(1)-Ir(1)-P(1)	43.65(3)
P(1)-S(1)-Ir(1)	78.54(4)
C(1)-P(1)-C(2)	120.37(15)
C(1)-P(1)-C(8)	106.16(15)
C(2)-P(1)-C(8)	101.87(15)
C(1)-P(1)-S(1)	103.44(11)
C(2)-P(1)-S(1)	113.07(11)
C(8)-P(1)-S(1)	111.88(12)

C(1)-P(1)-Ir(1)	49.11(10)
C(2)-P(1)-Ir(1)	152.69(11)
C(8)-P(1)-Ir(1)	105.37(11)
S(1)-P(1)-Ir(1)	57.81(3)
S(2)-C(1)-P(1)	122.74(18)
S(2)-C(1)-Ir(1)	110.41(16)
P(1)-C(1)-Ir(1)	91.86(13)
S(2)-C(1)-H(1)	110.1
P(1)-C(1)-H(1)	110.1
Ir(1)-C(1)-H(1)	110.1
O(2)-S(2)-O(1)	115.44(15)
O(2)-S(2)-C(14)	109.93(15)
O(1)-S(2)-C(14)	108.76(15)
O(2)-S(2)-C(1)	106.04(15)
O(1)-S(2)-C(1)	114.65(15)
C(14)-S(2)-C(1)	101.03(15)
C(7)-C(2)-C(3)	120.1(3)
C(7)-C(2)-P(1)	120.8(3)
C(3)-C(2)-P(1)	118.7(2)
C(4)-C(3)-C(2)	118.9(3)
C(4)-C(3)-H(3)	120.5
C(2)-C(3)-H(3)	120.5
C(3)-C(4)-C(5)	121.0(3)
C(3)-C(4)-H(4)	119.5
C(5)-C(4)-H(4)	119.5
C(6)-C(5)-C(4)	120.0(3)
C(6)-C(5)-H(5)	120.0
C(4)-C(5)-H(5)	120.0
C(5)-C(6)-C(7)	120.1(3)
C(5)-C(6)-H(6)	120.0
C(7)-C(6)-H(6)	120.0
C(6)-C(7)-C(2)	119.9(3)
C(6)-C(7)-H(7)	120.0
C(2)-C(7)-H(7)	120.0
C(9)-C(8)-C(13)	120.1(3)
C(9)-C(8)-P(1)	118.4(3)

C(13)-C(8)-P(1)	121.1(3)
C(10)-C(9)-C(8)	119.8(3)
C(10)-C(9)-H(9)	120.1
C(8)-C(9)-H(9)	120.1
C(9)-C(10)-C(11)	120.4(3)
C(9)-C(10)-H(10)	119.8
C(11)-C(10)-H(10)	119.8
C(12)-C(11)-C(10)	119.8(3)
C(12)-C(11)-H(11)	120.1
C(10)-C(11)-H(11)	120.1
C(11)-C(12)-C(13)	120.4(3)
C(11)-C(12)-H(12)	119.8
C(13)-C(12)-H(12)	119.8
C(12)-C(13)-C(8)	119.5(3)
C(12)-C(13)-H(13)	120.2
C(8)-C(13)-H(13)	120.2
C(19)-C(14)-C(15)	125.0(3)
C(19)-C(14)-S(2)	118.9(3)
C(15)-C(14)-S(2)	116.1(2)
C(14)-C(15)-C(16)	114.6(3)
C(14)-C(15)-Ir(1)	120.7(2)
C(16)-C(15)-Ir(1)	124.6(2)
C(17)-C(16)-C(15)	121.4(3)
C(17)-C(16)-H(16)	119.3
C(15)-C(16)-H(16)	119.3
C(18)-C(17)-C(16)	121.5(3)
C(18)-C(17)-H(17)	119.2
C(16)-C(17)-H(17)	119.2
C(19)-C(18)-C(17)	118.8(3)
C(19)-C(18)-H(18)	120.6
C(17)-C(18)-H(18)	120.6
C(18)-C(19)-C(14)	118.5(3)
C(18)-C(19)-H(19)	120.8
C(14)-C(19)-H(19)	120.8
C(21)-C(20)-C(24)	107.5(3)
C(21)-C(20)-C(25)	126.5(3)

C(24)-C(20)-C(25)	125.7(3)
C(21)-C(20)-Ir(1)	70.78(19)
C(24)-C(20)-Ir(1)	72.27(18)
C(25)-C(20)-Ir(1)	127.5(2)
C(20)-C(21)-C(22)	108.6(3)
C(20)-C(21)-C(26)	125.6(3)
C(22)-C(21)-C(26)	125.7(3)
C(20)-C(21)-Ir(1)	71.62(19)
C(22)-C(21)-Ir(1)	69.02(18)
C(26)-C(21)-Ir(1)	128.2(2)
C(21)-C(22)-C(23)	106.9(3)
C(21)-C(22)-C(27)	127.6(3)
C(23)-C(22)-C(27)	124.9(3)
C(21)-C(22)-Ir(1)	72.27(19)
C(23)-C(22)-Ir(1)	73.23(18)
C(27)-C(22)-Ir(1)	126.8(2)
C(24)-C(23)-C(22)	108.3(3)
C(24)-C(23)-C(28)	127.0(3)
C(22)-C(23)-C(28)	124.6(3)
C(24)-C(23)-Ir(1)	72.35(18)
C(22)-C(23)-Ir(1)	68.11(18)
C(28)-C(23)-Ir(1)	126.9(2)
C(23)-C(24)-C(20)	108.5(3)
C(23)-C(24)-C(29)	126.4(3)
C(20)-C(24)-C(29)	125.0(3)
C(23)-C(24)-Ir(1)	70.83(18)
C(20)-C(24)-Ir(1)	69.72(18)
C(29)-C(24)-Ir(1)	127.5(2)
C(20)-C(25)-H(25A)	109.5
C(20)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(20)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(21)-C(26)-H(26A)	109.5
C(21)-C(26)-H(26B)	109.5

H(26A)-C(26)-H(26B)	109.5
C(21)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(22)-C(27)-H(27A)	109.5
C(22)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(22)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(23)-C(28)-H(28A)	109.5
C(23)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(23)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(24)-C(29)-H(29A)	109.5
C(24)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(24)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 72-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for platon. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	7(1)	7(1)	7(1)	2(1)	2(1)	3(1)
S(1)	9(1)	8(1)	13(1)	1(1)	2(1)	2(1)
P(1)	8(1)	8(1)	8(1)	2(1)	2(1)	3(1)
O(1)	12(1)	19(1)	13(1)	6(1)	0(1)	5(1)
C(1)	9(2)	8(2)	8(2)	2(1)	2(1)	2(1)
S(2)	9(1)	9(1)	8(1)	2(1)	2(1)	2(1)
O(2)	16(1)	10(1)	13(1)	-1(1)	3(1)	1(1)
C(2)	12(2)	12(2)	7(2)	3(1)	5(1)	6(1)
C(3)	12(2)	11(2)	13(2)	3(1)	3(1)	4(1)
C(4)	9(2)	16(2)	18(2)	4(1)	5(1)	5(1)
C(5)	18(2)	18(2)	13(2)	7(1)	7(1)	13(1)
C(6)	20(2)	10(2)	18(2)	4(1)	8(2)	6(1)
C(7)	13(2)	10(2)	13(2)	3(1)	3(1)	4(1)
C(8)	12(2)	13(2)	9(2)	5(1)	4(1)	8(1)
C(9)	17(2)	16(2)	10(2)	4(1)	2(1)	7(1)
C(10)	26(2)	25(2)	10(2)	5(1)	6(2)	12(2)
C(11)	22(2)	31(2)	16(2)	12(2)	12(2)	12(2)
C(12)	15(2)	22(2)	19(2)	10(2)	7(2)	5(1)
C(13)	16(2)	16(2)	13(2)	4(1)	6(1)	6(1)
C(14)	13(2)	7(2)	13(2)	3(1)	6(1)	5(1)
C(15)	11(2)	9(2)	12(2)	3(1)	5(1)	6(1)
C(16)	10(2)	16(2)	14(2)	5(1)	3(1)	5(1)
C(17)	15(2)	16(2)	21(2)	8(1)	11(2)	8(1)
C(18)	21(2)	17(2)	14(2)	9(1)	9(1)	10(1)
C(19)	17(2)	14(2)	12(2)	5(1)	3(1)	7(1)
C(20)	11(2)	14(2)	13(2)	7(1)	1(1)	7(1)
C(21)	13(2)	12(2)	14(2)	7(1)	3(1)	7(1)
C(22)	15(2)	11(2)	11(2)	6(1)	4(1)	7(1)
C(23)	12(2)	11(2)	12(2)	7(1)	4(1)	6(1)
C(24)	14(2)	14(2)	7(2)	4(1)	0(1)	9(1)
C(25)	13(2)	17(2)	27(2)	9(2)	-1(2)	2(1)

C(26)	23(2)	26(2)	20(2)	11(2)	13(2)	16(2)
C(27)	24(2)	12(2)	13(2)	3(1)	3(2)	5(1)
C(28)	19(2)	16(2)	22(2)	13(2)	11(2)	8(1)
C(29)	27(2)	19(2)	9(2)	2(1)	2(2)	13(2)

Table 72-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for platon.

	x	y	z	U(eq)
H(1)	3589	4156	8257	10
H(3)	5693	2613	8842	15
H(4)	7088	1441	9391	17
H(5)	6253	-790	8999	17
H(6)	3996	-1869	8073	19
H(7)	2572	-717	7523	15
H(9)	2091	848	4877	17
H(10)	2963	1174	3275	23
H(11)	4865	2908	3646	24
H(12)	5909	4311	5632	21
H(13)	5103	3943	7275	17
H(16)	-1185	1474	8516	16
H(17)	-1264	764	10293	18
H(18)	601	1406	12062	18
H(19)	2627	2667	11978	17
H(25A)	-2779	2375	5158	31
H(25B)	-2451	1770	6324	31
H(25C)	-2026	1348	5136	31
H(26A)	-1862	4729	7845	30
H(26B)	-731	4719	9032	30
H(26C)	-1839	3400	8176	30
H(27A)	2550	6276	8829	26
H(27B)	1314	6127	9316	26
H(27C)	1475	6915	8291	26

H(28A)	2663	4678	5692	25
H(28B)	3161	5645	7047	25
H(28C)	2292	5964	5867	25
H(29A)	-472	2924	3782	27
H(29B)	-163	1804	4382	27
H(29C)	1018	2986	4363	27

Röntgenstrukturanalytische Daten für 73

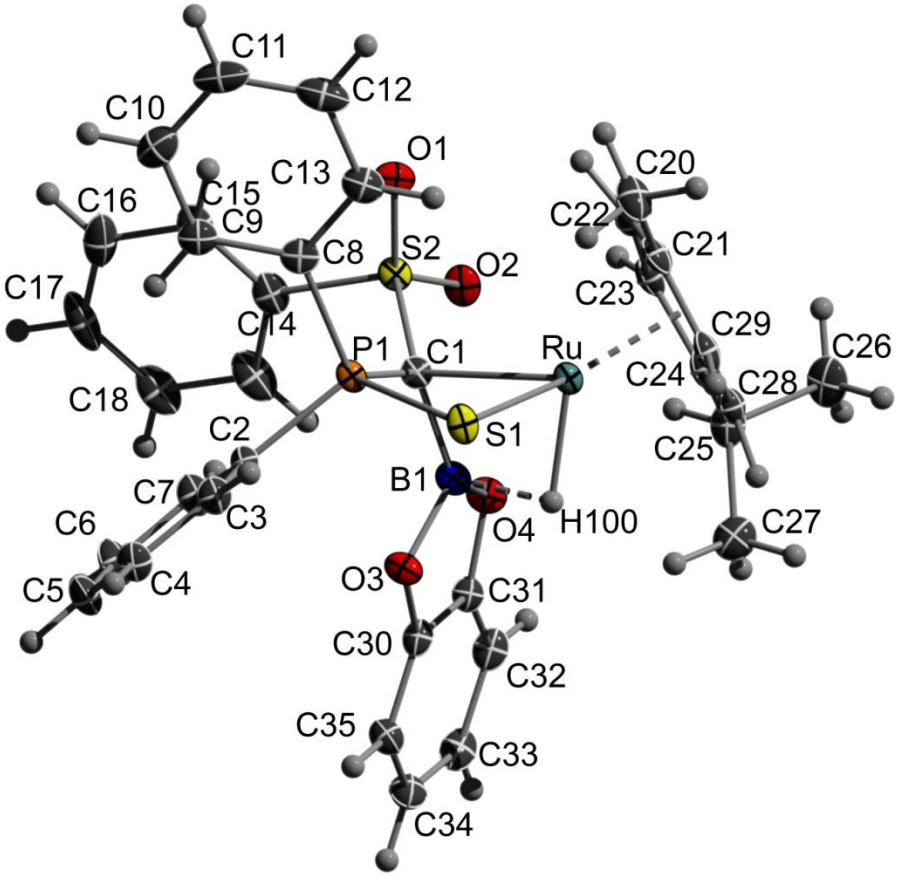

Table 73-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	C35 H34 B O4 P Ru S2	
Formula weight	725.59	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 10.3903(7) Å	α = 90°.
	b = 15.3003(11) Å	β = 101.767(3)°.
	c = 20.3638(14) Å	γ = 90°.
Volume	3169.3(4) $Å^3$	
Z	4	
Density (calculated)	1.521 Mg/m^3	
Absorption coefficient	0.716 mm^{-1}	
F(000)	1488	

Crystal size	0.19 x 0.07 x 0.03 mm^3
Theta range for data collection	1.68 to 26.52°.
Index ranges	-13<=h<=10, -19<=k<=19, -25<=l<=25
Reflections collected	46107
Independent reflections	6534 [R(int) = 0.0727]
Completeness to theta = 26.52°	99.3 %
Absorption correction	Empirical
Max. and min. transmission	0.9816 and 0.8771
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6534 / 0 / 392
Goodness-of-fit on F^2	1.060
Final R indices [I>2sigma(I)]	R1 = 0.0475, wR2 = 0.1297
R indices (all data)	R1 = 0.0562, wR2 = 0.1417
Largest diff. peak and hole	2.171 and -1.601 e.$Å^{-3}$

Table 73-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	5810(1)	2683(1)	54(1)	12(1)
S(1)	8151(1)	2668(1)	41(1)	16(1)
P(1)	7543(1)	1968(1)	-803(1)	12(1)
O(1)	5038(2)	556(2)	-874(1)	20(1)
C(1)	5824(3)	2184(2)	-956(2)	13(1)
B(1)	5446(4)	3171(2)	-1117(2)	17(1)
S(2)	4691(1)	1353(1)	-1244(1)	14(1)
O(2)	3377(2)	1689(2)	-1279(1)	20(1)
C(2)	8397(3)	2327(2)	-1453(2)	15(1)
O(3)	6354(2)	3733(2)	-1374(1)	17(1)
C(3)	9746(3)	2469(2)	-1272(2)	18(1)
O(4)	4132(2)	3452(2)	-1400(1)	18(1)
C(4)	10440(4)	2747(2)	-1744(2)	22(1)
C(5)	9782(4)	2901(3)	-2398(2)	26(1)
C(6)	8433(4)	2757(3)	-2584(2)	27(1)

C(7)	7740(4)	2467(2)	-2111(2)	21(1)
C(8)	7966(3)	821(2)	-687(2)	16(1)
C(9)	8346(3)	351(2)	-1199(2)	20(1)
C(10)	8739(4)	-515(2)	-1094(2)	29(1)
C(11)	8744(4)	-901(2)	-475(2)	29(1)
C(12)	8354(4)	-442(2)	30(2)	27(1)
C(13)	7964(3)	425(2)	-72(2)	21(1)
C(14)	4837(3)	1136(2)	-2086(2)	20(1)
C(15)	5316(3)	343(2)	-2251(2)	20(1)
C(16)	5363(4)	181(3)	-2918(2)	34(1)
C(17)	4946(4)	806(3)	-3401(2)	35(1)
C(18)	4482(4)	1603(3)	-3230(2)	29(1)
C(19)	4398(4)	1777(3)	-2571(2)	29(1)
C(20)	7077(4)	1370(3)	1421(2)	28(1)
C(21)	5989(4)	1938(2)	1043(2)	20(1)
C(22)	4935(3)	1591(2)	586(2)	21(1)
C(23)	3951(3)	2162(2)	221(2)	18(1)
C(24)	3954(3)	3069(2)	337(2)	17(1)
C(25)	2836(3)	3629(2)	-28(2)	22(1)
C(26)	1732(4)	3610(3)	371(2)	31(1)
C(27)	3211(4)	4568(2)	-146(2)	28(1)
C(28)	5026(3)	3416(2)	818(2)	17(1)
C(29)	6036(3)	2863(2)	1149(2)	19(1)
C(30)	5584(3)	4366(2)	-1730(2)	16(1)
C(31)	4263(3)	4200(2)	-1739(2)	16(1)
C(32)	3286(3)	4749(2)	-2073(2)	20(1)
C(33)	3683(4)	5460(2)	-2416(2)	24(1)
C(34)	4989(4)	5615(2)	-2410(2)	25(1)
C(35)	5980(3)	5070(2)	-2059(2)	21(1)

Table 73-3. Bond lengths [Å] and angles [°] for sad.

Ru(1)-C(23)	2.179(3)
Ru(1)-C(1)	2.198(3)
Ru(1)-C(24)	2.202(3)
Ru(1)-C(28)	2.203(3)
Ru(1)-C(29)	2.211(3)
Ru(1)-C(22)	2.279(3)
Ru(1)-C(21)	2.288(3)
Ru(1)-S(1)	2.4377(9)
Ru(1)-B(1)	2.454(4)
S(1)-P(1)	2.0147(11)
P(1)-C(1)	1.780(3)
P(1)-C(8)	1.812(3)
P(1)-C(2)	1.822(3)
O(1)-S(2)	1.439(2)
C(1)-B(1)	1.578(5)
C(1)-S(2)	1.751(3)
B(1)-O(4)	1.435(4)
B(1)-O(3)	1.450(4)
S(2)-O(2)	1.447(2)
S(2)-C(14)	1.784(3)
C(2)-C(3)	1.392(5)
C(2)-C(7)	1.392(5)
O(3)-C(30)	1.368(4)
C(3)-C(4)	1.381(5)
O(4)-C(31)	1.358(4)
C(4)-C(5)	1.388(5)
C(5)-C(6)	1.392(6)
C(6)-C(7)	1.388(5)
C(8)-C(9)	1.389(5)
C(8)-C(13)	1.391(5)
C(9)-C(10)	1.390(5)
C(10)-C(11)	1.391(6)
C(11)-C(12)	1.373(6)
C(12)-C(13)	1.390(5)

C(14)-C(15)	1.379(5)
C(14)-C(19)	1.399(5)
C(15)-C(16)	1.392(5)
C(16)-C(17)	1.375(6)
C(17)-C(18)	1.382(6)
C(18)-C(19)	1.389(5)
C(20)-C(21)	1.507(5)
C(21)-C(22)	1.390(5)
C(21)-C(29)	1.430(5)
C(22)-C(23)	1.432(5)
C(23)-C(24)	1.407(5)
C(24)-C(28)	1.427(5)
C(24)-C(25)	1.512(5)
C(25)-C(27)	1.521(5)
C(25)-C(26)	1.535(5)
C(28)-C(29)	1.409(5)
C(30)-C(35)	1.375(5)
C(30)-C(31)	1.392(5)
C(31)-C(32)	1.385(4)
C(32)-C(33)	1.399(5)
C(33)-C(34)	1.374(5)
C(34)-C(35)	1.402(5)

C(23)-Ru(1)-C(1)	101.19(12)
C(23)-Ru(1)-C(24)	37.46(13)
C(1)-Ru(1)-C(24)	120.73(12)
C(23)-Ru(1)-C(28)	67.00(12)
C(1)-Ru(1)-C(28)	155.70(12)
C(24)-Ru(1)-C(28)	37.80(12)
C(23)-Ru(1)-C(29)	78.68(13)
C(1)-Ru(1)-C(29)	165.42(12)
C(24)-Ru(1)-C(29)	67.79(12)
C(28)-Ru(1)-C(29)	37.24(12)
C(23)-Ru(1)-C(22)	37.38(13)
C(1)-Ru(1)-C(22)	105.62(12)
C(24)-Ru(1)-C(22)	67.48(13)

C(28)-Ru(1)-C(22)	78.33(12)
C(29)-Ru(1)-C(22)	65.36(12)
C(23)-Ru(1)-C(21)	66.17(13)
C(1)-Ru(1)-C(21)	129.50(12)
C(24)-Ru(1)-C(21)	79.73(12)
C(28)-Ru(1)-C(21)	66.92(12)
C(29)-Ru(1)-C(21)	37.03(13)
C(22)-Ru(1)-C(21)	35.45(12)
C(23)-Ru(1)-S(1)	156.36(10)
C(1)-Ru(1)-S(1)	77.84(8)
C(24)-Ru(1)-S(1)	159.08(9)
C(28)-Ru(1)-S(1)	121.72(9)
C(29)-Ru(1)-S(1)	96.37(9)
C(22)-Ru(1)-S(1)	119.59(9)
C(21)-Ru(1)-S(1)	95.90(9)
C(23)-Ru(1)-B(1)	107.28(12)
C(1)-Ru(1)-B(1)	39.17(12)
C(24)-Ru(1)-B(1)	101.70(12)
C(28)-Ru(1)-B(1)	121.66(12)
C(29)-Ru(1)-B(1)	154.95(13)
C(22)-Ru(1)-B(1)	133.43(12)
C(21)-Ru(1)-B(1)	167.34(13)
S(1)-Ru(1)-B(1)	87.06(9)
P(1)-S(1)-Ru(1)	82.79(4)
C(1)-P(1)-C(8)	114.29(15)
C(1)-P(1)-C(2)	115.83(15)
C(8)-P(1)-C(2)	104.18(15)
C(1)-P(1)-S(1)	100.35(11)
C(8)-P(1)-S(1)	112.25(11)
C(2)-P(1)-S(1)	110.17(11)
B(1)-C(1)-S(2)	120.3(2)
B(1)-C(1)-P(1)	114.4(2)
S(2)-C(1)-P(1)	120.39(18)
B(1)-C(1)-Ru(1)	79.20(18)
S(2)-C(1)-Ru(1)	115.64(16)
P(1)-C(1)-Ru(1)	95.61(13)

O(4)-B(1)-O(3)	108.3(3)
O(4)-B(1)-C(1)	123.1(3)
O(3)-B(1)-C(1)	119.3(3)
O(4)-B(1)-Ru(1)	115.2(2)
O(3)-B(1)-Ru(1)	123.2(2)
C(1)-B(1)-Ru(1)	61.63(16)
O(1)-S(2)-O(2)	117.42(14)
O(1)-S(2)-C(1)	111.12(14)
O(2)-S(2)-C(1)	108.77(14)
O(1)-S(2)-C(14)	106.52(16)
O(2)-S(2)-C(14)	106.46(15)
C(1)-S(2)-C(14)	105.82(15)
C(3)-C(2)-C(7)	120.0(3)
C(3)-C(2)-P(1)	117.9(3)
C(7)-C(2)-P(1)	122.0(3)
C(30)-O(3)-B(1)	104.9(2)
C(4)-C(3)-C(2)	120.3(3)
C(31)-O(4)-B(1)	105.7(2)
C(3)-C(4)-C(5)	119.7(3)
C(4)-C(5)-C(6)	120.3(3)
C(7)-C(6)-C(5)	119.9(3)
C(6)-C(7)-C(2)	119.7(4)
C(9)-C(8)-C(13)	120.2(3)
C(9)-C(8)-P(1)	120.2(2)
C(13)-C(8)-P(1)	119.6(3)
C(8)-C(9)-C(10)	119.9(3)
C(9)-C(10)-C(11)	119.4(4)
C(12)-C(11)-C(10)	121.0(3)
C(11)-C(12)-C(13)	119.8(3)
C(12)-C(13)-C(8)	119.8(3)
C(15)-C(14)-C(19)	121.8(3)
C(15)-C(14)-S(2)	120.2(3)
C(19)-C(14)-S(2)	117.9(3)
C(14)-C(15)-C(16)	118.7(3)
C(17)-C(16)-C(15)	120.3(4)
C(16)-C(17)-C(18)	120.6(3)

C(17)-C(18)-C(19)	120.4(4)
C(18)-C(19)-C(14)	118.1(4)
C(22)-C(21)-C(29)	118.5(3)
C(22)-C(21)-C(20)	121.8(3)
C(29)-C(21)-C(20)	119.6(3)
C(22)-C(21)-Ru(1)	71.90(19)
C(29)-C(21)-Ru(1)	68.57(17)
C(20)-C(21)-Ru(1)	130.9(2)
C(21)-C(22)-C(23)	119.7(3)
C(21)-C(22)-Ru(1)	72.64(19)
C(23)-C(22)-Ru(1)	67.53(18)
C(24)-C(23)-C(22)	122.6(3)
C(24)-C(23)-Ru(1)	72.16(18)
C(22)-C(23)-Ru(1)	75.08(19)
C(23)-C(24)-C(28)	117.2(3)
C(23)-C(24)-C(25)	120.2(3)
C(28)-C(24)-C(25)	122.6(3)
C(23)-C(24)-Ru(1)	70.38(18)
C(28)-C(24)-Ru(1)	71.12(18)
C(25)-C(24)-Ru(1)	130.5(2)
C(24)-C(25)-C(27)	114.7(3)
C(24)-C(25)-C(26)	108.2(3)
C(27)-C(25)-C(26)	110.2(3)
C(29)-C(28)-C(24)	120.4(3)
C(29)-C(28)-Ru(1)	71.70(19)
C(24)-C(28)-Ru(1)	71.08(18)
C(28)-C(29)-C(21)	121.5(3)
C(28)-C(29)-Ru(1)	71.06(18)
C(21)-C(29)-Ru(1)	74.41(18)
O(3)-C(30)-C(35)	127.8(3)
O(3)-C(30)-C(31)	110.2(3)
C(35)-C(30)-C(31)	122.0(3)
O(4)-C(31)-C(32)	128.4(3)
O(4)-C(31)-C(30)	110.4(3)
C(32)-C(31)-C(30)	121.1(3)
C(31)-C(32)-C(33)	117.1(3)

C(34)-C(33)-C(32)	121.4(3)
C(33)-C(34)-C(35)	121.5(3)
C(30)-C(35)-C(34)	116.9(3)

Symmetry transformations used to generate equivalent atoms:

Table 73-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	8(1)	18(1)	9(1)	0(1)	-2(1)	-1(1)
S(1)	8(1)	28(1)	10(1)	-3(1)	-3(1)	-2(1)
P(1)	7(1)	19(1)	9(1)	1(1)	-3(1)	0(1)
O(1)	18(1)	21(1)	16(1)	2(1)	-6(1)	-5(1)
C(1)	7(2)	18(2)	11(2)	1(1)	-3(1)	0(1)
B(1)	11(2)	22(2)	16(2)	2(1)	-1(1)	0(1)
S(2)	9(1)	20(1)	10(1)	0(1)	-4(1)	-2(1)
O(2)	7(1)	29(1)	20(1)	-4(1)	-3(1)	-3(1)
C(2)	13(2)	18(2)	13(2)	1(1)	2(1)	1(1)
O(3)	9(1)	22(1)	18(1)	7(1)	-2(1)	1(1)
C(3)	14(2)	24(2)	14(2)	0(1)	-2(1)	0(1)
O(4)	8(1)	24(1)	20(1)	3(1)	-5(1)	0(1)
C(4)	15(2)	29(2)	21(2)	-4(1)	2(1)	-4(1)
C(5)	26(2)	33(2)	21(2)	2(2)	11(2)	-2(2)
C(6)	24(2)	43(2)	15(2)	6(1)	2(2)	4(2)
C(7)	15(2)	32(2)	14(2)	3(1)	-2(1)	3(1)
C(8)	5(2)	21(2)	19(2)	2(1)	-6(1)	-1(1)
C(9)	14(2)	23(2)	21(2)	0(1)	-2(1)	-2(1)
C(10)	20(2)	25(2)	38(2)	-4(2)	2(2)	2(2)
C(11)	14(2)	19(2)	48(2)	7(2)	-5(2)	-1(1)
C(12)	15(2)	30(2)	30(2)	13(2)	-7(1)	-5(1)
C(13)	15(2)	25(2)	20(2)	3(1)	-4(1)	-2(1)
C(14)	10(1)	33(1)	16(1)	-4(1)	-4(1)	-7(1)
C(15)	10(1)	33(1)	16(1)	-4(1)	-4(1)	-7(1)

C(16)	22(2)	48(2)	32(2)	-20(2)	8(2)	-11(2)
C(17)	19(2)	72(3)	13(2)	-8(2)	3(1)	-19(2)
C(18)	14(1)	54(2)	15(1)	5(1)	-7(1)	-6(1)
C(19)	14(1)	54(2)	15(1)	5(1)	-7(1)	-6(1)
C(20)	28(2)	38(2)	18(2)	9(2)	5(2)	11(2)
C(21)	21(2)	29(2)	12(2)	7(1)	5(1)	2(1)
C(22)	20(2)	25(2)	20(2)	0(1)	7(1)	-4(1)
C(23)	11(2)	29(2)	14(2)	-1(1)	3(1)	-6(1)
C(24)	10(2)	31(2)	12(1)	0(1)	3(1)	1(1)
C(25)	10(2)	35(2)	20(2)	-5(1)	-2(1)	1(1)
C(26)	11(2)	44(2)	38(2)	-6(2)	3(2)	0(2)
C(27)	20(2)	32(2)	29(2)	0(2)	-3(2)	5(2)
C(28)	15(2)	24(2)	14(2)	-2(1)	3(1)	-2(1)
C(29)	15(2)	31(2)	10(2)	0(1)	3(1)	-1(1)
C(30)	12(2)	21(2)	13(1)	-1(1)	-2(1)	6(1)
C(31)	13(2)	21(2)	14(2)	-1(1)	-1(1)	1(1)
C(32)	11(2)	28(2)	17(2)	-3(1)	-6(1)	5(1)
C(33)	28(2)	27(2)	13(2)	2(1)	-5(1)	12(1)
C(34)	29(2)	25(2)	20(2)	6(1)	4(1)	6(2)
C(35)	17(2)	25(2)	19(2)	4(1)	2(1)	2(1)

Table 73-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
H(3)	10192	2374	-822	22
H(4)	11363	2833	-1621	26
H(5)	10254	3106	-2721	31
H(6)	7989	2858	-3034	33
H(7)	6820	2365	-2236	25
H(9)	8338	620	-1620	24
H(10)	9001	-840	-1442	34
H(11)	9022	-1490	-400	35

H(12)	8350	-716	448	32
H(13)	7697	746	276	25
H(15)	5608	-85	-1915	24
H(16)	5684	-363	-3041	40
H(17)	4979	688	-3855	42
H(18)	4218	2034	-3566	35
H(19)	4052	2315	-2452	35
H(20A)	6868	755	1316	42
H(20B)	7166	1466	1904	42
H(20C)	7905	1520	1288	42
H(22)	4986	974	429	26
H(23)	3312	1920	-171	22
H(25)	2491	3356	-475	27
H(26A)	963	3923	121	47
H(26B)	2036	3893	807	47
H(26C)	1492	3003	440	47
H(27A)	3979	4572	-357	42
H(27B)	3423	4878	284	42
H(27C)	2474	4860	-441	42
H(28)	5152	4064	850	21
H(29)	6865	3130	1407	22
H(32)	2385	4647	-2071	24
H(33)	3038	5844	-2657	28
H(34)	5224	6102	-2650	30
H(35)	6883	5182	-2050	25
H(100)	5870(30)	2110(20)	13(13)	-11(6)

Röntgenstrukturanalytische Daten für 76

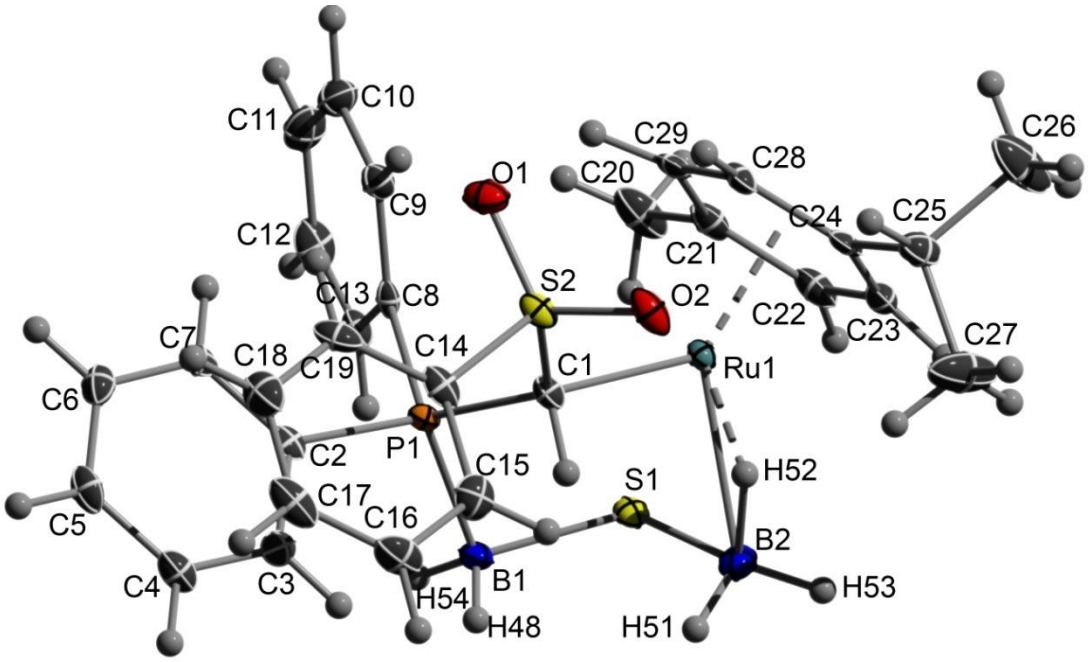

Table 76-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	C29 H35 B2 O2 P Ru S2	
Formula weight	633.35	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 11.586(2) Å	α = 90°.
	b = 14.210(3) Å	β = 90°.
	c = 17.491(4) Å	γ = 90°.
Volume	2879.5(10) $Å^3$	
Z	4	
Density (calculated)	1.461 Mg/m^3	
Absorption coefficient	0.771 mm^{-1}	
F(000)	1304	
Crystal size	0.09 x 0.08 x 0.01 mm^3	

Theta range for data collection	1.85 to 26.42°.
Index ranges	-14<=h<=14, -17<=k<=17, -21<=l<=21
Reflections collected	46800
Independent reflections	5916 [R(int) = 0.0648]
Completeness to theta = 26.42°	99.9 %
Absorption correction	Empirical
Max. and min. transmission	0.9923 and 0.9346
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5916 / 0 / 357
Goodness-of-fit on F^2	1.069
Final R indices [I>2sigma(I)]	R1 = 0.0288, wR2 = 0.0650
R indices (all data)	R1 = 0.0329, wR2 = 0.0682
Absolute structure parameter	-0.04(3)
Largest diff. peak and hole	1.093 and -0.339 e.$Å^{-3}$

Table 76-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	7346(1)	7606(1)	1731(1)	12(1)
S(1)	7288(1)	5976(1)	1401(1)	15(1)
P(1)	5796(1)	6225(1)	2806(1)	11(1)
O(1)	5737(2)	8474(2)	3569(1)	22(1)
C(1)	6897(3)	7123(2)	2882(2)	14(1)
B(1)	6645(3)	5276(3)	2254(2)	16(1)
S(2)	6850(1)	7998(1)	3589(1)	16(1)
O(2)	7871(2)	8571(2)	3523(1)	22(1)
C(2)	5299(3)	5806(2)	3731(2)	13(1)
B(2)	8777(3)	6389(3)	1713(2)	20(1)
C(3)	6049(3)	5247(2)	4158(2)	16(1)
C(4)	5710(3)	4916(2)	4870(2)	19(1)
C(5)	4625(3)	5127(2)	5158(2)	20(1)
C(6)	3879(3)	5674(2)	4734(2)	20(1)
C(7)	4203(3)	6017(2)	4025(2)	15(1)

C(8)	4486(3)	6575(2)	2316(2)	12(1)
C(9)	3881(2)	7409(2)	2485(2)	16(1)
C(10)	2817(3)	7573(2)	2143(2)	22(1)
C(11)	2331(3)	6923(2)	1651(2)	26(1)
C(12)	2923(3)	6100(2)	1483(2)	23(1)
C(13)	4002(3)	5933(2)	1806(2)	16(1)
C(14)	6963(3)	7424(2)	4491(2)	17(1)
C(15)	7992(3)	6952(2)	4678(2)	22(1)
C(16)	8074(3)	6516(2)	5388(2)	24(1)
C(17)	7154(3)	6566(2)	5896(2)	24(1)
C(18)	6167(3)	7041(3)	5710(2)	25(1)
C(19)	6065(3)	7465(2)	4994(2)	21(1)
C(20)	5130(3)	7567(3)	458(2)	30(1)
C(21)	6091(3)	8094(2)	840(2)	19(1)
C(22)	7236(3)	8059(2)	530(2)	21(1)
C(23)	8148(3)	8534(2)	879(2)	19(1)
C(24)	7989(3)	9071(2)	1560(2)	15(1)
C(25)	8965(3)	9622(2)	1912(2)	21(1)
C(26)	9149(4)	10518(3)	1446(3)	43(1)
C(27)	10081(3)	9066(3)	1995(3)	47(1)
C(28)	6864(3)	9097(2)	1867(2)	15(1)
C(29)	5922(3)	8623(2)	1514(2)	16(1)

Table 76-3. Bond lengths [Å] and angles [°] for sad.

Ru(1)-C(1)	2.190(3)
Ru(1)-C(23)	2.197(3)
Ru(1)-C(22)	2.201(3)
Ru(1)-C(28)	2.204(3)
Ru(1)-C(29)	2.226(3)
Ru(1)-C(24)	2.232(3)
Ru(1)-C(21)	2.241(3)
Ru(1)-S(1)	2.3875(9)
Ru(1)-B(2)	2.395(4)
S(1)-B(2)	1.902(4)

S(1)-B(1)	1.941(4)
P(1)-C(1)	1.809(3)
P(1)-C(8)	1.813(3)
P(1)-C(2)	1.818(3)
P(1)-B(1)	1.928(4)
O(1)-S(2)	1.456(2)
C(1)-S(2)	1.753(3)
S(2)-O(2)	1.440(2)
S(2)-C(14)	1.782(3)
C(2)-C(3)	1.394(4)
C(2)-C(7)	1.402(4)
C(3)-C(4)	1.387(4)
C(4)-C(5)	1.388(5)
C(5)-C(6)	1.378(5)
C(6)-C(7)	1.385(4)
C(8)-C(13)	1.393(4)
C(8)-C(9)	1.409(4)
C(9)-C(10)	1.390(4)
C(10)-C(11)	1.381(5)
C(11)-C(12)	1.387(5)
C(12)-C(13)	1.393(4)
C(14)-C(19)	1.364(4)
C(14)-C(15)	1.407(5)
C(15)-C(16)	1.391(5)
C(16)-C(17)	1.391(5)
C(17)-C(18)	1.366(5)
C(18)-C(19)	1.395(5)
C(20)-C(21)	1.499(4)
C(21)-C(29)	1.411(5)
C(21)-C(22)	1.435(5)
C(22)-C(23)	1.395(5)
C(23)-C(24)	1.427(4)
C(24)-C(28)	1.410(4)
C(24)-C(25)	1.507(4)
C(25)-C(27)	1.523(5)
C(25)-C(26)	1.526(5)

C(28)-C(29)	1.423(4)

C(1)-Ru(1)-C(23)	155.82(12)
C(1)-Ru(1)-C(22)	162.84(13)
C(23)-Ru(1)-C(22)	36.99(12)
C(1)-Ru(1)-C(28)	98.10(11)
C(23)-Ru(1)-C(28)	66.62(12)
C(22)-Ru(1)-C(28)	78.89(11)
C(1)-Ru(1)-C(29)	100.56(12)
C(23)-Ru(1)-C(29)	78.94(12)
C(22)-Ru(1)-C(29)	66.72(12)
C(28)-Ru(1)-C(29)	37.47(11)
C(1)-Ru(1)-C(24)	119.63(11)
C(23)-Ru(1)-C(24)	37.57(11)
C(22)-Ru(1)-C(24)	67.56(11)
C(28)-Ru(1)-C(24)	37.06(11)
C(29)-Ru(1)-C(24)	67.58(12)
C(1)-Ru(1)-C(21)	125.57(12)
C(23)-Ru(1)-C(21)	67.48(13)
C(22)-Ru(1)-C(21)	37.68(12)
C(28)-Ru(1)-C(21)	67.22(12)
C(29)-Ru(1)-C(21)	36.83(12)
C(24)-Ru(1)-C(21)	80.45(11)
C(1)-Ru(1)-S(1)	84.94(8)
C(23)-Ru(1)-S(1)	115.53(9)
C(22)-Ru(1)-S(1)	92.97(8)
C(28)-Ru(1)-S(1)	162.07(8)
C(29)-Ru(1)-S(1)	124.60(9)
C(24)-Ru(1)-S(1)	151.92(8)
C(21)-Ru(1)-S(1)	96.58(9)
C(1)-Ru(1)-B(2)	87.17(13)
C(23)-Ru(1)-B(2)	97.59(13)
C(22)-Ru(1)-B(2)	103.82(14)
C(28)-Ru(1)-B(2)	150.52(12)
C(29)-Ru(1)-B(2)	168.36(13)
C(24)-Ru(1)-B(2)	116.16(12)

C(21)-Ru(1)-B(2)	131.59(13)
S(1)-Ru(1)-B(2)	46.87(9)
B(2)-S(1)-B(1)	106.59(18)
B(2)-S(1)-Ru(1)	66.78(11)
B(1)-S(1)-Ru(1)	108.80(11)
C(1)-P(1)-C(8)	115.56(14)
C(1)-P(1)-C(2)	112.91(14)
C(8)-P(1)-C(2)	104.23(14)
C(1)-P(1)-B(1)	99.82(16)
C(8)-P(1)-B(1)	112.45(16)
C(2)-P(1)-B(1)	112.21(15)
S(2)-C(1)-P(1)	122.02(18)
S(2)-C(1)-Ru(1)	115.70(15)
P(1)-C(1)-Ru(1)	108.70(14)
P(1)-B(1)-S(1)	102.84(17)
O(2)-S(2)-O(1)	117.59(14)
O(2)-S(2)-C(1)	108.61(14)
O(1)-S(2)-C(1)	109.85(14)
O(2)-S(2)-C(14)	105.59(14)
O(1)-S(2)-C(14)	107.38(14)
C(1)-S(2)-C(14)	107.31(15)
C(3)-C(2)-C(7)	119.4(3)
C(3)-C(2)-P(1)	117.8(2)
C(7)-C(2)-P(1)	122.8(2)
S(1)-B(2)-Ru(1)	66.35(12)
C(4)-C(3)-C(2)	119.8(3)
C(3)-C(4)-C(5)	120.7(3)
C(6)-C(5)-C(4)	119.6(3)
C(5)-C(6)-C(7)	120.7(3)
C(6)-C(7)-C(2)	119.8(3)
C(13)-C(8)-C(9)	119.0(3)
C(13)-C(8)-P(1)	117.4(2)
C(9)-C(8)-P(1)	123.2(2)
C(10)-C(9)-C(8)	119.5(3)
C(11)-C(10)-C(9)	121.1(3)
C(10)-C(11)-C(12)	119.7(3)

C(11)-C(12)-C(13)	120.1(3)
C(8)-C(13)-C(12)	120.6(3)
C(19)-C(14)-C(15)	121.2(3)
C(19)-C(14)-S(2)	119.8(2)
C(15)-C(14)-S(2)	119.1(2)
C(16)-C(15)-C(14)	118.5(3)
C(15)-C(16)-C(17)	119.7(3)
C(18)-C(17)-C(16)	121.0(3)
C(17)-C(18)-C(19)	119.8(3)
C(14)-C(19)-C(18)	119.8(3)
C(29)-C(21)-C(22)	117.6(3)
C(29)-C(21)-C(20)	122.4(3)
C(22)-C(21)-C(20)	120.0(3)
C(29)-C(21)-Ru(1)	71.01(18)
C(22)-C(21)-Ru(1)	69.63(18)
C(20)-C(21)-Ru(1)	129.6(2)
C(23)-C(22)-C(21)	121.2(3)
C(23)-C(22)-Ru(1)	71.37(18)
C(21)-C(22)-Ru(1)	72.69(18)
C(22)-C(23)-C(24)	121.7(3)
C(22)-C(23)-Ru(1)	71.64(18)
C(24)-C(23)-Ru(1)	72.53(17)
C(28)-C(24)-C(23)	116.9(3)
C(28)-C(24)-C(25)	121.6(3)
C(23)-C(24)-C(25)	121.5(3)
C(28)-C(24)-Ru(1)	70.41(17)
C(23)-C(24)-Ru(1)	69.90(17)
C(25)-C(24)-Ru(1)	132.8(2)
C(24)-C(25)-C(27)	114.0(3)
C(24)-C(25)-C(26)	108.6(3)
C(27)-C(25)-C(26)	111.4(3)
C(24)-C(28)-C(29)	122.1(3)
C(24)-C(28)-Ru(1)	72.53(18)
C(29)-C(28)-Ru(1)	72.10(17)
C(21)-C(29)-C(28)	120.5(3)
C(21)-C(29)-Ru(1)	72.16(19)

C(28)-C(29)-Ru(1) 70.43(18)

Symmetry transformations used to generate equivalent atoms:

Table 76-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	14(1)	10(1)	12(1)	0(1)	0(1)	-1(1)
S(1)	20(1)	11(1)	14(1)	-2(1)	2(1)	1(1)
P(1)	13(1)	9(1)	13(1)	0(1)	-1(1)	0(1)
O(1)	28(1)	19(1)	20(1)	-2(1)	1(1)	7(1)
C(1)	17(2)	11(2)	15(2)	1(1)	0(1)	-2(1)
B(1)	19(2)	11(2)	17(2)	1(2)	1(2)	3(2)
S(2)	22(1)	13(1)	14(1)	0(1)	-2(1)	-2(1)
O(2)	31(1)	18(1)	17(1)	3(1)	-6(1)	-9(1)
C(2)	18(2)	7(2)	14(2)	-3(1)	-2(1)	-5(1)
B(2)	20(2)	16(2)	23(2)	-5(2)	5(2)	0(2)
C(3)	14(2)	14(2)	20(2)	-3(1)	-2(1)	-2(1)
C(4)	24(2)	16(2)	17(2)	3(1)	-5(2)	-5(2)
C(5)	29(2)	19(2)	11(2)	1(1)	2(2)	-6(2)
C(6)	21(2)	17(2)	21(2)	-4(1)	7(2)	-4(2)
C(7)	18(2)	10(2)	19(2)	-1(1)	-3(1)	-2(1)
C(8)	13(2)	16(2)	8(2)	3(1)	-1(1)	-4(1)
C(9)	17(1)	16(2)	15(2)	1(1)	-1(1)	0(2)
C(10)	20(2)	26(2)	21(2)	2(1)	1(1)	6(2)
C(11)	17(2)	36(2)	26(2)	5(2)	-4(2)	1(2)
C(12)	25(2)	24(2)	21(2)	0(1)	-8(2)	-11(2)
C(13)	22(2)	12(2)	15(2)	1(1)	2(2)	-4(1)
C(14)	25(2)	13(2)	14(2)	-1(1)	-4(1)	-7(1)
C(15)	20(2)	23(2)	22(2)	-4(2)	-3(2)	-5(2)
C(16)	23(2)	21(2)	30(2)	4(2)	-13(2)	-3(2)
C(17)	39(2)	17(2)	15(2)	1(1)	-11(2)	-9(2)
C(18)	36(2)	23(2)	18(2)	-2(2)	5(2)	0(2)

C(19)	31(2)	12(2)	20(2)	-2(1)	-4(1)	4(2)
C(20)	39(2)	24(2)	27(2)	8(2)	-18(2)	-10(2)
C(21)	22(2)	16(2)	19(2)	6(1)	-7(2)	-2(2)
C(22)	36(2)	13(2)	14(2)	2(1)	0(2)	-1(2)
C(23)	23(2)	13(2)	20(2)	5(1)	5(2)	2(2)
C(24)	20(2)	6(1)	20(2)	4(1)	-1(1)	0(1)
C(25)	21(2)	14(2)	27(2)	1(1)	-4(2)	-1(1)
C(26)	46(3)	27(2)	56(3)	13(2)	-24(2)	-18(2)
C(27)	27(2)	26(2)	87(4)	-4(2)	-24(2)	2(2)
C(28)	23(2)	8(2)	15(2)	2(1)	2(1)	0(1)
C(29)	19(2)	9(2)	21(2)	7(1)	-2(1)	2(1)

Table 76-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
H(1)	7593	6751	3032	17
H(3)	6790	5092	3962	19
H(4)	6226	4542	5163	23
H(5)	4397	4896	5645	24
H(6)	3135	5816	4930	23
H(7)	3684	6396	3738	19
H(9)	4197	7855	2831	19
H(10)	2416	8141	2250	27
H(11)	1597	7040	1429	32
H(12)	2591	5650	1146	28
H(13)	4412	5375	1678	20
H(15)	8617	6931	4327	26
H(16)	8757	6186	5525	29
H(17)	7212	6266	6380	28
H(18)	5551	7081	6068	30
H(19)	5372	7781	4858	25
H(20A)	4928	7880	-23	45

H(20B)	4455	7554	794	45
H(20C)	5380	6921	351	45
H(22)	7410	7593	117	25
H(23)	8953	8394	707	22
H(25)	8715	9816	2436	25
H(26A)	9336	10351	917	65
H(26B)	9786	10880	1667	65
H(26C)	8443	10897	1455	65
H(27A)	10341	8855	1490	70
H(27B)	9947	8518	2324	70
H(27C)	10675	9468	2226	70
H(28)	6757	9349	2396	18
H(29)	5181	8554	1802	20
H(48)	7240(30)	5040(20)	2623(16)	12(8)
H(51)	9110(20)	5990(19)	2257(15)	-1(7)
H(52)	8630(30)	7220(30)	2080(20)	45(12)
H(53)	9420(30)	6430(20)	1268(19)	23(10)
H(54)	6050(30)	4700(30)	2049(19)	32(11)

Röntgenstrukturanalytische Daten für 77

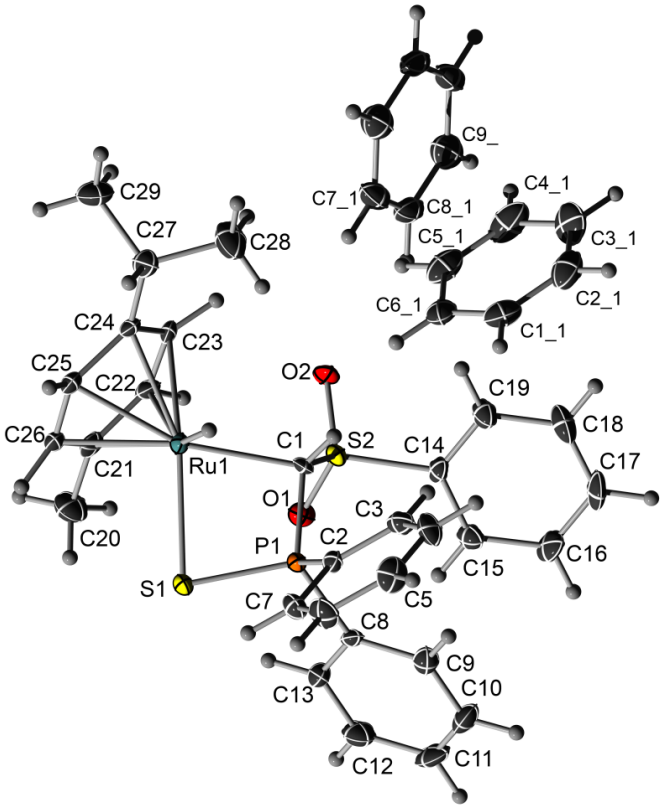

Table 77-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	$C_{38}H_{40}O_2PRuS_2$	
Formula weight	724.86	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 9.9058(13) Å	α = 90°.
	b = 18.783(2) Å	β = 93.682(6)°.
	c = 18.593(2) Å	γ = 90°.
Volume	3452.3(7) $Å^3$	
Z	4	
Density (calculated)	1.395 Mg/m^3	
Absorption coefficient	0.654 mm^{-1}	
F(000)	1500	
Crystal size	0.25 x 0.21 x 0.12 mm^3	

Theta range for data collection	2.17 to 25.00°.
Index ranges	-11<=h<=7, -21<=k<=20, -22<=l<=21
Reflections collected	16617
Independent reflections	5955 [R(int) = 0.0536]
Completeness to theta = 25.00°	97.9 %
Absorption correction	Empirical
Max. and min. transmission	0.9257 and 0.8537
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5955 / 1 / 407
Goodness-of-fit on F^2	1.040
Final R indices [I>2sigma(I)]	R1 = 0.0503, wR2 = 0.0827
R indices (all data)	R1 = 0.0856, wR2 = 0.0942
Largest diff. peak and hole	1.526 and -0.986 e.$Å^{-3}$

Table 77-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	9121(1)	624(1)	6176(1)	15(1)
O(1)	7488(3)	2031(2)	7205(2)	18(1)
C(1)	9828(5)	1513(2)	6859(2)	13(1)
S(1)	8743(1)	1625(1)	5347(1)	19(1)
P(1)	9913(1)	2109(1)	6114(1)	13(1)
S(2)	8736(1)	1749(1)	7536(1)	15(1)
O(2)	8662(3)	1155(2)	8029(2)	19(1)
C(3)	12705(5)	2277(2)	6436(3)	21(1)
C(4)	14015(5)	2393(2)	6247(3)	26(1)
C(5)	14300(5)	2427(3)	5529(3)	28(1)
C(6)	13277(5)	2332(2)	4995(3)	26(1)
C(7)	11975(5)	2213(2)	5180(2)	20(1)
C(8)	9357(5)	3021(2)	6223(2)	15(1)
C(9)	10254(5)	3570(2)	6426(2)	21(1)
C(10)	9768(5)	4256(2)	6506(3)	28(1)
C(11)	8429(6)	4407(3)	6368(3)	33(1)

C(12)	7519(5)	3865(3)	6166(3)	29(1)
C(13)	7992(5)	3174(2)	6092(2)	22(1)
C(14)	9567(5)	2438(2)	8049(2)	16(1)
C(15)	9100(5)	3132(2)	8001(2)	21(1)
C(16)	9785(6)	3652(3)	8405(3)	29(1)
C(17)	10922(6)	3480(3)	8844(3)	31(1)
C(18)	11365(5)	2785(3)	8888(3)	30(1)
C(19)	10694(5)	2264(3)	8492(2)	24(1)
C(20)	5633(5)	654(3)	5855(3)	33(1)
C(21)	6917(5)	255(2)	6082(3)	21(1)
C(22)	7384(5)	210(2)	6800(2)	19(1)
C(23)	8632(5)	-147(2)	6999(2)	17(1)
C(24)	9383(5)	-493(2)	6481(2)	17(1)
C(25)	8884(5)	-459(2)	5746(2)	20(1)
C(26)	7707(5)	-73(2)	5551(2)	19(1)
C(27)	10634(5)	-929(2)	6684(3)	24(1)
C(28)	11533(5)	-611(3)	7296(3)	42(2)
C(29)	10216(6)	-1689(3)	6864(3)	38(2)
C(2)	11658(4)	2186(2)	5902(2)	15(1)
C11	9208(5)	540(3)	9701(3)	32(1)
C121	9186(5)	395(3)	10434(3)	37(2)
C91	14765(7)	1193(3)	9325(3)	46(2)
C101	15520(6)	1412(3)	8753(3)	38(2)
C111	14982(5)	1336(3)	8062(3)	30(1)
C61	13507(6)	894(3)	9184(3)	43(2)
C71	12995(6)	818(3)	8493(3)	35(1)
C81	13737(5)	1037(2)	7929(3)	28(1)
C21	10010(5)	153(3)	9272(3)	32(1)

Table 77-3. Bond lengths [Å] and angles [°] for sad.

Ru(1)-C(23)	2.183(4)
Ru(1)-C(1)	2.185(4)
Ru(1)-C(24)	2.185(4)
Ru(1)-C(25)	2.192(4)
Ru(1)-C(26)	2.195(4)
Ru(1)-C(22)	2.273(5)
Ru(1)-C(21)	2.286(5)
Ru(1)-S(1)	2.4458(12)
Ru(1)-P(1)	2.9016(12)
O(1)-S(2)	1.445(3)
C(1)-S(2)	1.768(5)
C(1)-P(1)	1.787(4)
S(1)-P(1)	1.9971(16)
P(1)-C(2)	1.804(5)
P(1)-C(8)	1.815(4)
S(2)-O(2)	1.449(3)
S(2)-C(14)	1.779(4)
C(3)-C(4)	1.384(6)
C(3)-C(2)	1.399(6)
C(4)-C(5)	1.383(7)
C(5)-C(6)	1.383(6)
C(6)-C(7)	1.375(6)
C(7)-C(2)	1.399(6)
C(8)-C(13)	1.389(6)
C(8)-C(9)	1.396(6)
C(9)-C(10)	1.387(6)
C(10)-C(11)	1.365(7)
C(11)-C(12)	1.395(7)
C(12)-C(13)	1.391(6)
C(14)-C(19)	1.382(6)
C(14)-C(15)	1.384(6)
C(15)-C(16)	1.383(6)
C(16)-C(17)	1.386(7)
C(17)-C(18)	1.379(7)

C(18)-C(19)	1.370(6)
C(20)-C(21)	1.512(6)
C(21)-C(22)	1.387(6)
C(21)-C(26)	1.438(6)
C(22)-C(23)	1.434(6)
C(23)-C(24)	1.413(6)
C(24)-C(25)	1.424(6)
C(24)-C(27)	1.513(6)
C(25)-C(26)	1.401(6)
C(27)-C(28)	1.521(6)
C(27)-C(29)	1.531(6)
C11-C21	1.371(7)
C11-C121	1.392(7)
C121-C21#1	1.390(7)
C91-C61	1.376(8)
C91-C101	1.400(8)
C101-C111	1.366(7)
C111-C81	1.363(7)
C61-C71	1.358(7)
C71-C81	1.382(7)
C21-C121#1	1.390(7)

C(23)-Ru(1)-C(1)	100.22(16)
C(23)-Ru(1)-C(24)	37.74(16)
C(1)-Ru(1)-C(24)	123.72(17)
C(23)-Ru(1)-C(25)	67.45(17)
C(1)-Ru(1)-C(25)	160.63(17)
C(24)-Ru(1)-C(25)	37.96(15)
C(23)-Ru(1)-C(26)	79.24(17)
C(1)-Ru(1)-C(26)	158.95(18)
C(24)-Ru(1)-C(26)	68.04(16)
C(25)-Ru(1)-C(26)	37.25(16)
C(23)-Ru(1)-C(22)	37.49(15)
C(1)-Ru(1)-C(22)	100.95(17)
C(24)-Ru(1)-C(22)	67.70(16)
C(25)-Ru(1)-C(22)	78.58(17)

C(26)-Ru(1)-C(22)	65.71(17)
C(23)-Ru(1)-C(21)	66.36(17)
C(1)-Ru(1)-C(21)	123.03(18)
C(24)-Ru(1)-C(21)	79.97(17)
C(25)-Ru(1)-C(21)	67.14(17)
C(26)-Ru(1)-C(21)	37.36(16)
C(22)-Ru(1)-C(21)	35.42(16)
C(23)-Ru(1)-S(1)	156.94(13)
C(1)-Ru(1)-S(1)	78.97(12)
C(24)-Ru(1)-S(1)	155.93(12)
C(25)-Ru(1)-S(1)	118.38(12)
C(26)-Ru(1)-S(1)	93.31(12)
C(22)-Ru(1)-S(1)	119.64(12)
C(21)-Ru(1)-S(1)	94.48(12)
C(23)-Ru(1)-P(1)	137.59(12)
C(1)-Ru(1)-P(1)	37.93(12)
C(24)-Ru(1)-P(1)	154.91(12)
C(25)-Ru(1)-P(1)	154.17(13)
C(26)-Ru(1)-P(1)	135.79(12)
C(22)-Ru(1)-P(1)	124.36(12)
C(21)-Ru(1)-P(1)	123.20(12)
S(1)-Ru(1)-P(1)	42.81(4)
S(2)-C(1)-P(1)	117.1(3)
S(2)-C(1)-Ru(1)	114.6(2)
P(1)-C(1)-Ru(1)	93.33(19)
P(1)-S(1)-Ru(1)	80.86(5)
C(1)-P(1)-C(2)	108.2(2)
C(1)-P(1)-C(8)	118.4(2)
C(2)-P(1)-C(8)	104.5(2)
C(1)-P(1)-S(1)	102.39(16)
C(2)-P(1)-S(1)	113.64(15)
C(8)-P(1)-S(1)	110.05(15)
C(1)-P(1)-Ru(1)	48.74(14)
C(2)-P(1)-Ru(1)	110.56(14)
C(8)-P(1)-Ru(1)	144.91(16)
S(1)-P(1)-Ru(1)	56.33(4)

O(1)-S(2)-O(2)	118.34(19)
O(1)-S(2)-C(1)	109.6(2)
O(2)-S(2)-C(1)	108.36(19)
O(1)-S(2)-C(14)	108.38(19)
O(2)-S(2)-C(14)	105.13(19)
C(1)-S(2)-C(14)	106.3(2)
C(4)-C(3)-C(2)	120.2(4)
C(5)-C(4)-C(3)	120.3(5)
C(4)-C(5)-C(6)	120.1(5)
C(7)-C(6)-C(5)	119.8(5)
C(6)-C(7)-C(2)	121.2(4)
C(13)-C(8)-C(9)	119.4(4)
C(13)-C(8)-P(1)	118.3(3)
C(9)-C(8)-P(1)	122.3(3)
C(10)-C(9)-C(8)	119.7(5)
C(11)-C(10)-C(9)	120.8(5)
C(10)-C(11)-C(12)	120.2(5)
C(13)-C(12)-C(11)	119.5(5)
C(8)-C(13)-C(12)	120.4(4)
C(19)-C(14)-C(15)	121.0(4)
C(19)-C(14)-S(2)	118.4(3)
C(15)-C(14)-S(2)	120.6(3)
C(16)-C(15)-C(14)	118.7(4)
C(15)-C(16)-C(17)	120.4(5)
C(18)-C(17)-C(16)	120.0(5)
C(19)-C(18)-C(17)	120.1(5)
C(18)-C(19)-C(14)	119.8(5)
C(22)-C(21)-C(26)	118.2(4)
C(22)-C(21)-C(20)	121.4(4)
C(26)-C(21)-C(20)	120.4(4)
C(22)-C(21)-Ru(1)	71.7(3)
C(26)-C(21)-Ru(1)	67.8(3)
C(20)-C(21)-Ru(1)	130.8(3)
C(21)-C(22)-C(23)	120.3(4)
C(21)-C(22)-Ru(1)	72.8(3)
C(23)-C(22)-Ru(1)	67.9(3)

C(24)-C(23)-C(22)	121.5(4)
C(24)-C(23)-Ru(1)	71.2(3)
C(22)-C(23)-Ru(1)	74.7(3)
C(23)-C(24)-C(25)	117.8(4)
C(23)-C(24)-C(27)	122.5(4)
C(25)-C(24)-C(27)	119.5(4)
C(23)-C(24)-Ru(1)	71.0(2)
C(25)-C(24)-Ru(1)	71.3(2)
C(27)-C(24)-Ru(1)	131.8(3)
C(26)-C(25)-C(24)	120.3(4)
C(26)-C(25)-Ru(1)	71.5(2)
C(24)-C(25)-Ru(1)	70.7(3)
C(25)-C(26)-C(21)	121.6(4)
C(25)-C(26)-Ru(1)	71.3(2)
C(21)-C(26)-Ru(1)	74.8(3)
C(24)-C(27)-C(28)	113.9(4)
C(24)-C(27)-C(29)	109.3(4)
C(28)-C(27)-C(29)	110.8(4)
C(7)-C(2)-C(3)	118.4(4)
C(7)-C(2)-P(1)	119.3(3)
C(3)-C(2)-P(1)	122.1(4)
C21-C11-C121	120.8(5)
C21#1-C121-C11	119.0(5)
C61-C91-C101	119.8(6)
C111-C101-C91	119.2(6)
C81-C111-C101	120.5(5)
C71-C61-C91	120.1(6)
C61-C71-C81	120.2(5)
C111-C81-C71	120.2(5)
C11-C21-C121#1	120.2(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z+2

Table 77-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	21(1)	11(1)	12(1)	-1(1)	0(1)	-2(1)
O(1)	15(2)	22(2)	19(2)	4(2)	2(1)	-1(1)
C(1)	17(3)	13(3)	10(2)	2(2)	-5(2)	2(2)
S(1)	27(1)	16(1)	12(1)	1(1)	-5(1)	-5(1)
P(1)	18(1)	12(1)	10(1)	0(1)	-1(1)	-2(1)
S(2)	21(1)	15(1)	11(1)	-1(1)	0(1)	-1(1)
O(2)	31(2)	18(2)	10(2)	4(1)	2(1)	-2(2)
C(3)	26(3)	20(3)	17(3)	4(2)	3(2)	1(2)
C(4)	19(3)	33(3)	26(3)	-3(3)	-6(2)	-1(2)
C(5)	18(3)	33(3)	35(3)	-3(3)	6(3)	-3(2)
C(6)	31(3)	34(3)	14(3)	1(2)	5(2)	-4(3)
C(7)	22(3)	23(3)	14(3)	-2(2)	-1(2)	0(2)
C(8)	23(3)	10(2)	12(2)	3(2)	1(2)	1(2)
C(9)	23(3)	22(3)	19(3)	-1(2)	3(2)	-4(2)
C(10)	37(4)	15(3)	33(3)	-3(2)	5(3)	-7(2)
C(11)	56(4)	12(3)	30(3)	2(3)	6(3)	8(3)
C(12)	31(3)	26(3)	29(3)	3(3)	-3(3)	9(3)
C(13)	29(3)	14(3)	21(3)	-2(2)	-4(2)	0(2)
C(14)	21(3)	14(3)	14(3)	-5(2)	3(2)	-1(2)
C(15)	25(3)	23(3)	15(3)	-1(2)	1(2)	4(2)
C(16)	48(4)	17(3)	24(3)	-9(2)	6(3)	3(3)
C(17)	39(3)	34(3)	21(3)	-16(3)	2(3)	-12(3)
C(18)	25(3)	42(3)	22(3)	-13(3)	-3(2)	1(3)
C(19)	26(3)	24(3)	21(3)	-7(2)	-3(2)	5(2)
C(20)	25(3)	36(3)	37(3)	4(3)	-6(2)	3(3)
C(21)	18(3)	14(3)	29(3)	4(2)	-1(2)	-9(2)
C(22)	26(3)	10(3)	21(3)	3(2)	2(2)	0(2)
C(23)	25(3)	10(3)	16(3)	-2(2)	-3(2)	-6(2)
C(24)	26(3)	7(3)	17(2)	1(2)	0(2)	-1(2)
C(25)	30(3)	10(3)	20(3)	0(2)	-2(2)	-5(2)
C(26)	29(3)	11(3)	16(3)	2(2)	-4(2)	-6(2)

C(27)	31(3)	20(3)	21(3)	-3(2)	0(2)	3(2)
C(28)	37(4)	42(4)	45(4)	-12(3)	-15(3)	12(3)
C(29)	51(4)	25(3)	38(3)	8(3)	-6(3)	9(3)
C(2)	19(3)	11(2)	15(3)	-2(2)	1(2)	-1(2)
C11	29(3)	23(3)	44(4)	12(3)	-11(3)	-9(3)
C121	33(4)	40(4)	38(4)	4(3)	-1(3)	-8(3)
C91	70(5)	42(4)	27(3)	-16(3)	7(3)	-1(3)
C101	32(4)	27(3)	55(4)	-10(3)	1(3)	2(3)
C111	30(3)	22(3)	39(4)	7(3)	8(3)	4(2)
C61	54(4)	31(3)	47(4)	-6(3)	28(3)	-9(3)
C71	32(4)	23(3)	51(4)	-2(3)	12(3)	3(2)
C81	31(3)	17(3)	34(3)	0(2)	-4(3)	6(2)
C21	27(3)	38(3)	28(3)	12(3)	-7(3)	-11(3)

Table 77-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
H(1RU)	10706(9)	590(20)	6050(20)	22
H(1)	10620(40)	1445(19)	7090(20)	2(11)
H(3)	12515	2259	6930	25
H(4)	14723	2449	6612	31
H(5)	15199	2515	5402	34
H(6)	13474	2350	4502	31
H(7)	11277	2148	4811	24
H(9)	11192	3473	6508	26
H(10)	10376	4626	6658	34
H(11)	8115	4882	6411	39
H(12)	6583	3968	6079	35
H(13)	7377	2803	5950	26
H(15)	8325	3249	7697	25
H(16)	9473	4131	8381	35
H(17)	11395	3842	9114	38

H(18)	12138	2666	9194	36
H(19)	11002	1786	8521	29
H(20A)	5800	969	5451	49
H(20B)	5347	937	6261	49
H(20C)	4920	313	5707	49
H(22)	6981	530	7159	23
H(23)	9047	-88	7500	21
H(25)	9476	-620	5362	24
H(26)	7487	36	5030	23
H(27)	11180	-954	6251	29
H(28A)	12369	-889	7362	63
H(28B)	11056	-623	7742	63
H(28C)	11753	-118	7180	63
H(29A)	9647	-1885	6461	58
H(29B)	9707	-1685	7299	58
H(29C)	11026	-1985	6948	58
H11	8661	913	9496	39
H121	8630	665	10730	45
H91	15120	1250	9808	56
H101	16396	1610	8844	46
H111	15479	1493	7672	36
H61	12995	742	9571	51
H71	12126	612	8397	42
H81	13377	980	7446	33
H21	10017	259	8773	38

Röntgenstrukturanalytische Daten für 78

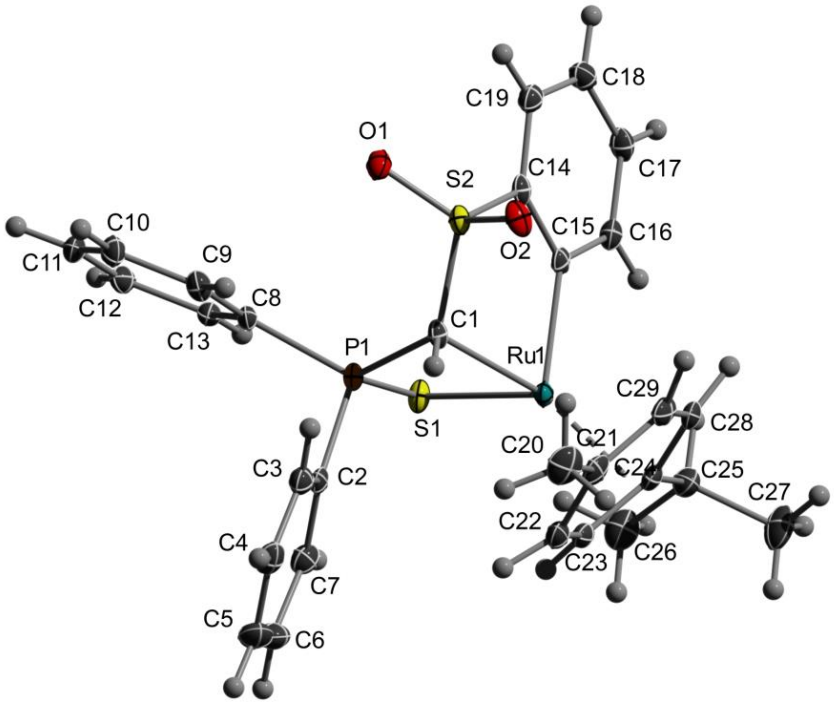

Table 78-1. Crystal data and structure refinement for test.

Identification code	test	
Empirical formula	$C_{29}H_{29}O_2PRuS_2$	
Formula weight	605.68	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 11.3790(5) Å	α = 90°.
	b = 20.9671(9) Å	β = 91.898(2)°.
	c = 10.7092(5) Å	γ = 90°.
Volume	2553.6(2) $Å^3$	
Z	4	
Density (calculated)	1.575 Mg/m^3	
Absorption coefficient	0.866 mm^{-1}	
F(000)	1240	
Crystal size	0.11 x 0.08 x 0.05 mm^3	
Theta range for data collection	1.94 to 26.49°.	

Index ranges	-9<=h<=14, -26<=k<=26, -13<=l<=13
Reflections collected	27904
Independent reflections	5269 [R(int) = 0.0293]
Completeness to theta = 26.49°	99.6 %
Absorption correction	Empirical
Max. and min. transmission	0.9547 and 0.9122
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5269 / 0 / 319
Goodness-of-fit on F^2	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0251, wR2 = 0.0596
R indices (all data)	R1 = 0.0315, wR2 = 0.0630
Largest diff. peak and hole	0.545 and -0.366 e.$Å^{-3}$

Table 78-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for test. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	8539(1)	1046(1)	1615(1)	12(1)
S(1)	7590(1)	1262(1)	3600(1)	15(1)
P(1)	6218(1)	1031(1)	2477(1)	12(1)
O(1)	5974(1)	-568(1)	1593(1)	19(1)
C(1)	6856(2)	600(1)	1243(2)	13(1)
S(2)	6988(1)	-227(1)	1158(1)	14(1)
O(2)	7305(1)	-363(1)	-112(1)	19(1)
C(2)	5560(2)	1708(1)	1673(2)	14(1)
C(3)	4885(2)	1612(1)	585(2)	17(1)
C(4)	4321(2)	2120(1)	3(2)	21(1)
C(5)	4408(2)	2721(1)	512(2)	24(1)
C(6)	5073(2)	2820(1)	1598(2)	25(1)
C(7)	5652(2)	2317(1)	2183(2)	20(1)
C(8)	5013(2)	706(1)	3325(2)	13(1)
C(9)	4059(2)	427(1)	2688(2)	17(1)
C(10)	3079(2)	252(1)	3334(2)	19(1)
C(11)	3040(2)	358(1)	4609(2)	19(1)
C(12)	3989(2)	627(1)	5244(2)	18(1)
C(13)	4985(2)	799(1)	4607(2)	14(1)
C(14)	8202(2)	-362(1)	2168(2)	14(1)
C(15)	8921(2)	162(1)	2406(2)	14(1)
C(16)	9896(2)	36(1)	3200(2)	16(1)
C(17)	10127(2)	-567(1)	3679(2)	19(1)
C(18)	9389(2)	-1075(1)	3388(2)	20(1)
C(19)	8400(2)	-974(1)	2632(2)	17(1)
C(20)	7738(2)	1276(1)	-1399(2)	28(1)
C(21)	8588(2)	1404(1)	-328(2)	20(1)
C(22)	8443(2)	1943(1)	449(2)	19(1)
C(23)	9203(2)	2036(1)	1492(2)	17(1)
C(24)	10190(2)	1633(1)	1752(2)	16(1)
C(25)	11081(2)	1759(1)	2808(2)	21(1)

C(26)	10640(2)	2199(1)	3812(2)	29(1)
C(27)	12208(2)	2018(1)	2267(2)	33(1)
C(28)	10341(2)	1110(1)	945(2)	18(1)
C(29)	9556(2)	992(1)	-86(2)	19(1)

Table 78-3. Bond lengths [Å] and angles [°] for test.

Ru(1)-C(15)	2.079(2)
Ru(1)-C(1)	2.157(2)
Ru(1)-C(29)	2.192(2)
Ru(1)-C(28)	2.198(2)
Ru(1)-C(23)	2.213(2)
Ru(1)-C(21)	2.214(2)
Ru(1)-C(24)	2.246(2)
Ru(1)-C(22)	2.258(2)
Ru(1)-S(1)	2.4581(5)
Ru(1)-P(1)	2.8268(6)
S(1)-P(1)	1.9971(7)
P(1)-C(1)	1.776(2)
P(1)-C(8)	1.803(2)
P(1)-C(2)	1.810(2)
O(1)-S(2)	1.4482(15)
C(1)-S(2)	1.742(2)
S(2)-O(2)	1.4464(15)
S(2)-C(14)	1.749(2)
C(2)-C(3)	1.388(3)
C(2)-C(7)	1.391(3)
C(3)-C(4)	1.382(3)
C(4)-C(5)	1.374(3)
C(5)-C(6)	1.383(3)
C(6)-C(7)	1.382(3)
C(8)-C(13)	1.389(3)
C(8)-C(9)	1.392(3)
C(9)-C(10)	1.381(3)
C(10)-C(11)	1.385(3)
C(11)-C(12)	1.377(3)
C(12)-C(13)	1.389(3)
C(14)-C(15)	1.389(3)
C(14)-C(19)	1.391(3)
C(15)-C(16)	1.400(3)
C(16)-C(17)	1.386(3)

C(17)-C(18)	1.385(3)
C(18)-C(19)	1.381(3)
C(20)-C(21)	1.500(3)
C(21)-C(22)	1.416(3)
C(21)-C(29)	1.417(3)
C(22)-C(23)	1.404(3)
C(23)-C(24)	1.425(3)
C(24)-C(28)	1.412(3)
C(24)-C(25)	1.516(3)
C(25)-C(26)	1.515(3)
C(25)-C(27)	1.524(3)
C(28)-C(29)	1.419(3)

C(15)-Ru(1)-C(1)	81.97(8)
C(15)-Ru(1)-C(29)	100.57(8)
C(1)-Ru(1)-C(29)	108.28(8)
C(15)-Ru(1)-C(28)	90.12(8)
C(1)-Ru(1)-C(28)	142.93(8)
C(29)-Ru(1)-C(28)	37.70(8)
C(15)-Ru(1)-C(23)	142.50(8)
C(1)-Ru(1)-C(23)	134.31(8)
C(29)-Ru(1)-C(23)	78.97(8)
C(28)-Ru(1)-C(23)	66.44(8)
C(15)-Ru(1)-C(21)	132.37(8)
C(1)-Ru(1)-C(21)	91.33(8)
C(29)-Ru(1)-C(21)	37.50(8)
C(28)-Ru(1)-C(21)	67.69(8)
C(23)-Ru(1)-C(21)	66.88(8)
C(15)-Ru(1)-C(24)	107.41(8)
C(1)-Ru(1)-C(24)	170.15(8)
C(29)-Ru(1)-C(24)	67.66(8)
C(28)-Ru(1)-C(24)	37.02(8)
C(23)-Ru(1)-C(24)	37.25(8)
C(21)-Ru(1)-C(24)	80.15(8)
C(15)-Ru(1)-C(22)	166.91(8)
C(1)-Ru(1)-C(22)	103.44(8)

C(29)-Ru(1)-C(22)	66.48(8)
C(28)-Ru(1)-C(22)	78.36(8)
C(23)-Ru(1)-C(22)	36.59(8)
C(21)-Ru(1)-C(22)	36.90(8)
C(24)-Ru(1)-C(22)	66.75(8)
C(15)-Ru(1)-S(1)	84.46(6)
C(1)-Ru(1)-S(1)	79.99(5)
C(29)-Ru(1)-S(1)	170.74(6)
C(28)-Ru(1)-S(1)	135.45(6)
C(23)-Ru(1)-S(1)	92.29(6)
C(21)-Ru(1)-S(1)	140.86(6)
C(24)-Ru(1)-S(1)	103.50(6)
C(22)-Ru(1)-S(1)	108.10(6)
C(15)-Ru(1)-P(1)	92.40(6)
C(1)-Ru(1)-P(1)	38.91(5)
C(29)-Ru(1)-P(1)	142.65(6)
C(28)-Ru(1)-P(1)	177.19(6)
C(23)-Ru(1)-P(1)	110.75(6)
C(21)-Ru(1)-P(1)	111.31(6)
C(24)-Ru(1)-P(1)	140.62(6)
C(22)-Ru(1)-P(1)	99.27(6)
S(1)-Ru(1)-P(1)	43.716(16)
P(1)-S(1)-Ru(1)	78.01(2)
C(1)-P(1)-C(8)	121.22(10)
C(1)-P(1)-C(2)	102.59(10)
C(8)-P(1)-C(2)	103.07(9)
C(1)-P(1)-S(1)	103.93(7)
C(8)-P(1)-S(1)	112.37(7)
C(2)-P(1)-S(1)	113.57(7)
C(1)-P(1)-Ru(1)	49.72(7)
C(8)-P(1)-Ru(1)	154.57(7)
C(2)-P(1)-Ru(1)	102.26(7)
S(1)-P(1)-Ru(1)	58.27(2)
S(2)-C(1)-P(1)	125.72(12)
S(2)-C(1)-Ru(1)	111.31(10)
P(1)-C(1)-Ru(1)	91.37(9)

O(2)-S(2)-O(1)	115.53(9)
O(2)-S(2)-C(1)	105.72(9)
O(1)-S(2)-C(1)	113.78(9)
O(2)-S(2)-C(14)	109.46(9)
O(1)-S(2)-C(14)	109.96(10)
C(1)-S(2)-C(14)	101.37(10)
C(3)-C(2)-C(7)	119.7(2)
C(3)-C(2)-P(1)	119.60(16)
C(7)-C(2)-P(1)	120.53(16)
C(4)-C(3)-C(2)	120.1(2)
C(5)-C(4)-C(3)	120.1(2)
C(4)-C(5)-C(6)	120.1(2)
C(7)-C(6)-C(5)	120.4(2)
C(6)-C(7)-C(2)	119.6(2)
C(13)-C(8)-C(9)	119.99(19)
C(13)-C(8)-P(1)	119.21(16)
C(9)-C(8)-P(1)	120.43(15)
C(10)-C(9)-C(8)	119.7(2)
C(9)-C(10)-C(11)	120.2(2)
C(12)-C(11)-C(10)	120.2(2)
C(11)-C(12)-C(13)	120.1(2)
C(8)-C(13)-C(12)	119.7(2)
C(15)-C(14)-C(19)	125.18(19)
C(15)-C(14)-S(2)	115.66(16)
C(19)-C(14)-S(2)	119.12(16)
C(14)-C(15)-C(16)	114.35(19)
C(14)-C(15)-Ru(1)	121.16(15)
C(16)-C(15)-Ru(1)	124.50(16)
C(17)-C(16)-C(15)	122.3(2)
C(18)-C(17)-C(16)	120.8(2)
C(19)-C(18)-C(17)	119.4(2)
C(18)-C(19)-C(14)	118.1(2)
C(22)-C(21)-C(29)	119.0(2)
C(22)-C(21)-C(20)	120.5(2)
C(29)-C(21)-C(20)	120.5(2)
C(22)-C(21)-Ru(1)	73.23(12)

C(29)-C(21)-Ru(1)	70.40(12)
C(20)-C(21)-Ru(1)	128.49(16)
C(23)-C(22)-C(21)	119.8(2)
C(23)-C(22)-Ru(1)	69.97(12)
C(21)-C(22)-Ru(1)	69.88(12)
C(22)-C(23)-C(24)	122.3(2)
C(22)-C(23)-Ru(1)	73.44(13)
C(24)-C(23)-Ru(1)	72.64(12)
C(28)-C(24)-C(23)	116.9(2)
C(28)-C(24)-C(25)	119.99(19)
C(23)-C(24)-C(25)	123.07(19)
C(28)-C(24)-Ru(1)	69.65(12)
C(23)-C(24)-Ru(1)	70.11(12)
C(25)-C(24)-Ru(1)	132.90(15)
C(26)-C(25)-C(24)	113.98(19)
C(26)-C(25)-C(27)	110.8(2)
C(24)-C(25)-C(27)	109.16(19)
C(24)-C(28)-C(29)	121.6(2)
C(24)-C(28)-Ru(1)	73.34(12)
C(29)-C(28)-Ru(1)	70.91(12)
C(21)-C(29)-C(28)	120.2(2)
C(21)-C(29)-Ru(1)	72.09(12)
C(28)-C(29)-Ru(1)	71.39(12)

Symmetry transformations used to generate equivalent atoms:

Table 78-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for test. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	10(1)	15(1)	12(1)	0(1)	4(1)	1(1)
S(1)	11(1)	23(1)	13(1)	-3(1)	2(1)	-2(1)
P(1)	9(1)	16(1)	11(1)	-1(1)	2(1)	0(1)
O(1)	14(1)	20(1)	22(1)	-4(1)	3(1)	-3(1)
C(1)	11(1)	18(1)	11(1)	-1(1)	2(1)	2(1)
S(2)	12(1)	17(1)	13(1)	-3(1)	1(1)	1(1)
O(2)	19(1)	26(1)	13(1)	-7(1)	0(1)	4(1)
C(2)	11(1)	17(1)	14(1)	3(1)	7(1)	1(1)
C(3)	15(1)	19(1)	18(1)	-1(1)	5(1)	-1(1)
C(4)	18(1)	27(1)	17(1)	7(1)	1(1)	-1(1)
C(5)	26(1)	19(1)	28(1)	9(1)	1(1)	1(1)
C(6)	30(1)	15(1)	28(1)	2(1)	3(1)	-1(1)
C(7)	20(1)	22(1)	17(1)	1(1)	3(1)	-2(1)
C(8)	11(1)	14(1)	15(1)	1(1)	4(1)	2(1)
C(9)	15(1)	21(1)	15(1)	0(1)	1(1)	3(1)
C(10)	12(1)	21(1)	23(1)	-2(1)	1(1)	0(1)
C(11)	15(1)	18(1)	24(1)	4(1)	8(1)	1(1)
C(12)	20(1)	16(1)	17(1)	0(1)	6(1)	2(1)
C(13)	14(1)	13(1)	16(1)	0(1)	3(1)	0(1)
C(14)	12(1)	19(1)	10(1)	-2(1)	3(1)	2(1)
C(15)	12(1)	18(1)	11(1)	0(1)	6(1)	1(1)
C(16)	12(1)	21(1)	17(1)	-1(1)	3(1)	-1(1)
C(17)	14(1)	26(1)	16(1)	2(1)	0(1)	4(1)
C(18)	21(1)	20(1)	20(1)	4(1)	4(1)	5(1)
C(19)	17(1)	18(1)	18(1)	-2(1)	5(1)	-2(1)
C(20)	32(1)	37(2)	16(1)	5(1)	2(1)	-2(1)
C(21)	21(1)	23(1)	15(1)	4(1)	7(1)	-4(1)
C(22)	16(1)	20(1)	21(1)	6(1)	7(1)	1(1)
C(23)	18(1)	14(1)	20(1)	1(1)	10(1)	-1(1)
C(24)	13(1)	16(1)	20(1)	2(1)	6(1)	-3(1)
C(25)	17(1)	19(1)	27(1)	2(1)	1(1)	-2(1)

C(26)	27(1)	37(2)	23(1)	-3(1)	2(1)	-6(1)
C(27)	19(1)	43(2)	37(1)	-7(1)	3(1)	-11(1)
C(28)	13(1)	18(1)	23(1)	3(1)	9(1)	-1(1)
C(29)	22(1)	18(1)	18(1)	-1(1)	12(1)	-2(1)

Table 78-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for test.

	x	y	z	U(eq)
H(1)	6528	759	444	16
H(3)	4812	1205	248	21
H(4)	3882	2055	-734	25
H(5)	4019	3061	124	29
H(6)	5131	3228	1938	30
H(7)	6100	2385	2913	23
H(9)	4081	358	1831	21
H(10)	2442	63	2911	23
H(11)	2372	248	5036	22
H(12)	3963	692	6102	21
H(13)	5628	976	5038	17
H(16)	10406	368	3413	20
H(17)	10785	-632	4202	22
H(18)	9558	-1480	3699	24
H(19)	7882	-1305	2439	21
H(20A)	8041	1451	-2151	42
H(20B)	6995	1471	-1235	42
H(20C)	7635	824	-1496	42
H(22)	7702	2182	390	23
H(23)	8977	2343	2130	21
H(25)	11270	1349	3203	25
H(26A)	10503	2616	3465	43
H(26B)	11218	2227	4483	43
H(26C)	9920	2034	4124	43

H(27A)	12482	1727	1648	49
H(27B)	12797	2063	2923	49
H(27C)	12054	2426	1889	49
H(28)	10907	777	1194	22
H(29)	9600	587	-537	23

Röntgenstrukturanalytische Daten für 80a

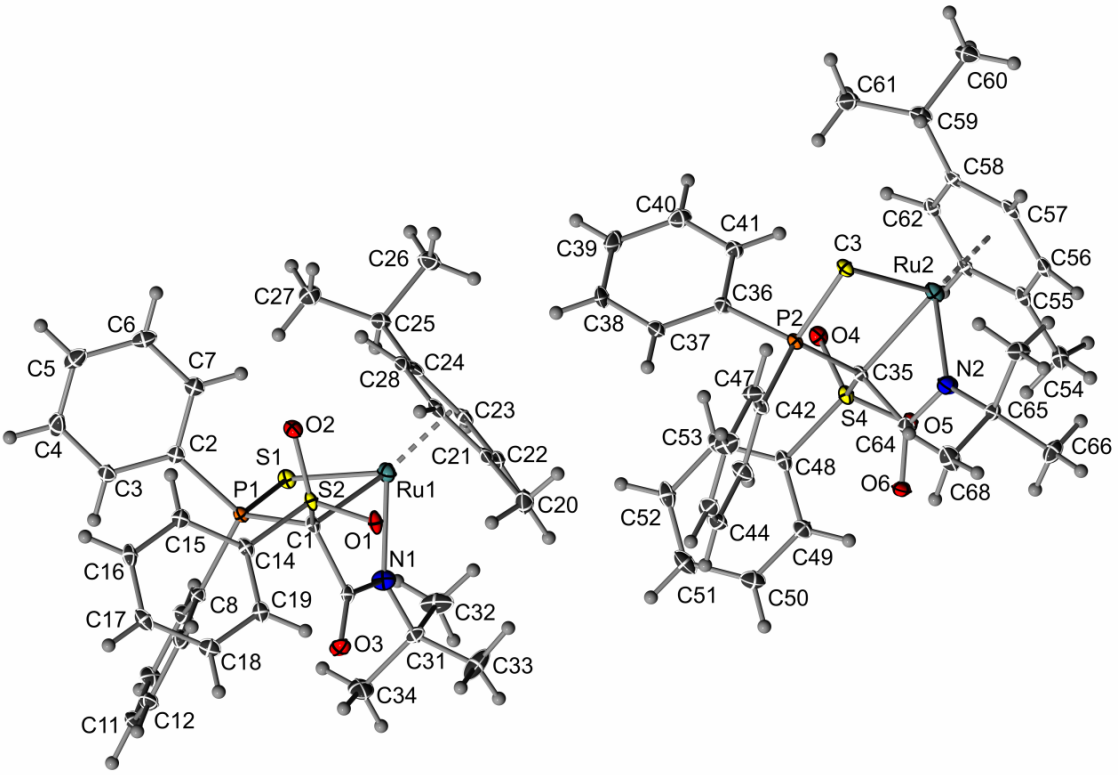

Table 80a-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	C34 H38 N O3 P Ru S2	
Formula weight	704.81	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.9184(7) Å	α = 89.739(2)°.
	b = 14.2275(9) Å	β = 85.986(2)°.
	c = 21.9330(14) Å	γ = 71.341(2)°.
Volume	3219.5(4) $Å^3$	
Z	4	
Density (calculated)	1.454 Mg/m^3	
Absorption coefficient	0.701 mm^{-1}	

F(000)	1456
Crystal size	0.13 x 0.08 x 0.05 mm^3
Theta range for data collection	0.93 to 26.45°.
Index ranges	-13<=h<=13, -17<=k<=17, -27<=l<=27
Reflections collected	43538
Independent reflections	13245 [R(int) = 0.0340]
Completeness to theta = 26.45°	99.8 %
Absorption correction	Empirical
Max. and min. transmission	0.9644 and 0.9125
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13245 / 0 / 769
Goodness-of-fit on F^2	1.004
Final R indices [I>2sigma(I)]	R1 = 0.0305, wR2 = 0.0686
R indices (all data)	R1 = 0.0419, wR2 = 0.0747
Largest diff. peak and hole	0.568 and -0.508 e.$Å^{-3}$

Table 80a-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	5648(1)	8022(1)	2116(1)	13(1)
S(1)	4979(1)	9295(1)	1341(1)	17(1)
P(1)	5708(1)	8120(1)	768(1)	14(1)
O(1)	7174(2)	5374(1)	1689(1)	20(1)
N(1)	7526(2)	7961(1)	1796(1)	15(1)
C(1)	6462(2)	7151(2)	1279(1)	14(1)
Ru(2)	5263(1)	6811(1)	7185(1)	13(1)
S(2)	6362(1)	5945(1)	1238(1)	15(1)
P(2)	5573(1)	6546(1)	5843(1)	14(1)
O(2)	5019(2)	5993(1)	1282(1)	19(1)
N(2)	7180(2)	5917(1)	6979(1)	15(1)
C(2)	4427(2)	7929(2)	355(1)	16(1)
S(3)	4715(1)	5802(1)	6414(1)	17(1)
O(3)	8845(2)	6678(1)	1148(1)	23(1)

C(3)	4423(3)	8039(2)	-276(1)	21(1)
S(4)	6237(1)	8403(1)	6275(1)	16(1)
O(4)	4917(2)	9047(1)	6243(1)	20(1)
C(4)	3363(3)	7991(2)	-574(1)	30(1)
O(5)	6963(2)	8602(1)	6752(1)	21(1)
C(5)	2335(3)	7816(2)	-253(1)	30(1)
O(6)	8642(2)	6445(1)	6347(1)	21(1)
C(6)	2329(3)	7702(2)	377(1)	25(1)
C(7)	3370(2)	7766(2)	682(1)	19(1)
C(8)	6870(2)	8315(2)	197(1)	16(1)
C(9)	6885(3)	9272(2)	86(1)	22(1)
C(10)	7780(3)	9439(2)	-344(1)	25(1)
C(11)	8673(3)	8646(2)	-662(1)	25(1)
C(12)	8669(2)	7692(2)	-555(1)	23(1)
C(13)	7775(2)	7519(2)	-126(1)	20(1)
C(14)	7033(2)	5406(2)	514(1)	16(1)
C(15)	6219(3)	5484(2)	40(1)	18(1)
C(16)	6749(3)	5050(2)	-524(1)	20(1)
C(17)	8065(3)	4555(2)	-614(1)	21(1)
C(18)	8862(3)	4470(2)	-136(1)	22(1)
C(19)	8350(2)	4893(2)	430(1)	18(1)
C(20)	7245(3)	6227(2)	3079(1)	30(1)
C(21)	6066(3)	7074(2)	2938(1)	20(1)
C(22)	5908(3)	8070(2)	3096(1)	21(1)
C(23)	4798(3)	8857(2)	2980(1)	20(1)
C(24)	3782(2)	8670(2)	2674(1)	19(1)
C(25)	2581(2)	9544(2)	2579(1)	22(1)
C(26)	1698(3)	9721(2)	3173(1)	30(1)
C(27)	1848(3)	9432(2)	2037(1)	29(1)
C(28)	3912(2)	7687(2)	2510(1)	19(1)
C(29)	5053(2)	6908(2)	2628(1)	19(1)
C(30)	7814(2)	7207(2)	1396(1)	16(1)
C(31)	8488(2)	8437(2)	1951(1)	18(1)
C(32)	7790(3)	9400(2)	2292(2)	40(1)
C(33)	9466(3)	7750(2)	2341(2)	43(1)
C(34)	9131(3)	8684(3)	1362(1)	40(1)

C(35)	6265(2)	7175(2)	6359(1)	14(1)
C(36)	4401(2)	7387(2)	5385(1)	17(1)
C(37)	4531(3)	7338(2)	4747(1)	22(1)
C(38)	3563(3)	7961(2)	4418(1)	30(1)
C(39)	2481(3)	8629(2)	4716(1)	31(1)
C(40)	2348(3)	8681(2)	5349(1)	25(1)
C(41)	3301(2)	8063(2)	5680(1)	20(1)
C(42)	6783(2)	5726(2)	5315(1)	17(1)
C(43)	7734(3)	6043(2)	5010(1)	25(1)
C(44)	8660(3)	5406(2)	4609(1)	28(1)
C(45)	8637(3)	4455(2)	4505(1)	27(1)
C(46)	7693(3)	4139(2)	4807(1)	29(1)
C(47)	6770(3)	4768(2)	5214(1)	24(1)
C(48)	7074(3)	8519(2)	5570(1)	18(1)
C(49)	8425(3)	8224(2)	5528(1)	22(1)
C(50)	9067(3)	8302(2)	4969(1)	29(1)
C(51)	8366(3)	8677(2)	4469(1)	32(1)
C(52)	7033(3)	8983(2)	4519(1)	26(1)
C(53)	6373(3)	8897(2)	5071(1)	20(1)
C(54)	6667(3)	7923(2)	8163(1)	26(1)
C(55)	5514(2)	7650(2)	7989(1)	19(1)
C(56)	5331(3)	6746(2)	8179(1)	20(1)
C(57)	4251(2)	6486(2)	8030(1)	20(1)
C(58)	3296(2)	7127(2)	7671(1)	17(1)
C(59)	2118(2)	6831(2)	7545(1)	22(1)
C(60)	1199(3)	7055(2)	8126(1)	32(1)
C(61)	1412(3)	7310(2)	6993(1)	30(1)
C(62)	3459(2)	8027(2)	7480(1)	18(1)
C(63)	4576(2)	8265(2)	7623(1)	18(1)
C(64)	7562(2)	6458(2)	6559(1)	17(1)
C(65)	8085(2)	5007(2)	7223(1)	18(1)
C(66)	8982(3)	5275(2)	7650(1)	29(1)
C(67)	7298(3)	4440(2)	7562(1)	26(1)
C(68)	8880(3)	4367(2)	6685(1)	32(1)

Table 80a-3. Bond lengths [Å] and angles [°] for sad.

Ru(1)-N(1)	2.095(2)
Ru(1)-C(29)	2.177(2)
Ru(1)-C(1)	2.187(2)
Ru(1)-C(22)	2.192(2)
Ru(1)-C(28)	2.216(2)
Ru(1)-C(23)	2.221(2)
Ru(1)-C(24)	2.227(2)
Ru(1)-C(21)	2.233(2)
Ru(1)-S(1)	2.4485(7)
S(1)-P(1)	2.0087(9)
P(1)-C(1)	1.794(2)
P(1)-C(8)	1.805(3)
P(1)-C(2)	1.809(2)
O(1)-S(2)	1.4404(18)
N(1)-C(30)	1.331(3)
N(1)-C(31)	1.478(3)
C(1)-C(30)	1.543(3)
C(1)-S(2)	1.757(2)
Ru(2)-N(2)	2.091(2)
Ru(2)-C(63)	2.165(2)
Ru(2)-C(56)	2.186(2)
Ru(2)-C(35)	2.196(2)
Ru(2)-C(57)	2.214(2)
Ru(2)-C(55)	2.215(2)
Ru(2)-C(62)	2.223(2)
Ru(2)-C(58)	2.240(2)
Ru(2)-S(3)	2.4495(6)
S(2)-O(2)	1.4433(18)
S(2)-C(14)	1.771(2)
P(2)-C(35)	1.793(2)
P(2)-C(42)	1.805(2)
P(2)-C(36)	1.808(3)
P(2)-S(3)	2.0057(9)
N(2)-C(64)	1.328(3)

N(2)-C(65)	1.479(3)
C(2)-C(3)	1.393(3)
C(2)-C(7)	1.397(3)
O(3)-C(30)	1.227(3)
C(3)-C(4)	1.389(4)
S(4)-O(5)	1.4386(18)
S(4)-O(4)	1.4452(18)
S(4)-C(35)	1.747(2)
S(4)-C(48)	1.773(3)
C(4)-C(5)	1.374(4)
C(5)-C(6)	1.390(4)
O(6)-C(64)	1.231(3)
C(6)-C(7)	1.386(4)
C(8)-C(9)	1.388(3)
C(8)-C(13)	1.397(3)
C(9)-C(10)	1.386(4)
C(10)-C(11)	1.385(4)
C(11)-C(12)	1.378(4)
C(12)-C(13)	1.385(4)
C(14)-C(19)	1.389(3)
C(14)-C(15)	1.396(3)
C(15)-C(16)	1.387(3)
C(16)-C(17)	1.383(4)
C(17)-C(18)	1.388(4)
C(18)-C(19)	1.383(3)
C(20)-C(21)	1.505(4)
C(21)-C(22)	1.414(4)
C(21)-C(29)	1.419(4)
C(22)-C(23)	1.400(4)
C(23)-C(24)	1.431(4)
C(24)-C(28)	1.405(3)
C(24)-C(25)	1.517(3)
C(25)-C(27)	1.515(4)
C(25)-C(26)	1.537(4)
C(28)-C(29)	1.417(4)
C(31)-C(33)	1.510(4)

C(31)-C(32)	1.510(4)
C(31)-C(34)	1.521(4)
C(35)-C(64)	1.547(3)
C(36)-C(41)	1.395(3)
C(36)-C(37)	1.397(3)
C(37)-C(38)	1.387(4)
C(38)-C(39)	1.380(4)
C(39)-C(40)	1.386(4)
C(40)-C(41)	1.378(4)
C(42)-C(47)	1.387(4)
C(42)-C(43)	1.389(4)
C(43)-C(44)	1.383(4)
C(44)-C(45)	1.381(4)
C(45)-C(46)	1.379(4)
C(46)-C(47)	1.385(4)
C(48)-C(53)	1.387(4)
C(48)-C(49)	1.395(4)
C(49)-C(50)	1.391(4)
C(50)-C(51)	1.388(4)
C(51)-C(52)	1.375(4)
C(52)-C(53)	1.390(4)
C(54)-C(55)	1.504(4)
C(55)-C(63)	1.412(4)
C(55)-C(56)	1.419(3)
C(56)-C(57)	1.404(4)
C(57)-C(58)	1.428(4)
C(58)-C(62)	1.406(3)
C(58)-C(59)	1.518(4)
C(59)-C(61)	1.519(4)
C(59)-C(60)	1.534(4)
C(62)-C(63)	1.421(4)
C(65)-C(67)	1.513(3)
C(65)-C(68)	1.528(4)
C(65)-C(66)	1.533(4)

N(1)-Ru(1)-C(29)	127.97(9)

N(1)-Ru(1)-C(1)	63.03(8)
C(29)-Ru(1)-C(1)	98.54(9)
N(1)-Ru(1)-C(22)	97.53(9)
C(29)-Ru(1)-C(22)	66.86(10)
C(1)-Ru(1)-C(22)	142.16(9)
N(1)-Ru(1)-C(28)	165.37(9)
C(29)-Ru(1)-C(28)	37.61(9)
C(1)-Ru(1)-C(28)	111.38(9)
C(22)-Ru(1)-C(28)	78.95(9)
N(1)-Ru(1)-C(23)	118.49(9)
C(29)-Ru(1)-C(23)	79.18(9)
C(1)-Ru(1)-C(23)	177.72(9)
C(22)-Ru(1)-C(23)	36.99(10)
C(28)-Ru(1)-C(23)	66.71(9)
N(1)-Ru(1)-C(24)	153.75(9)
C(29)-Ru(1)-C(24)	67.43(9)
C(1)-Ru(1)-C(24)	141.40(9)
C(22)-Ru(1)-C(24)	67.33(10)
C(28)-Ru(1)-C(24)	36.87(9)
C(23)-Ru(1)-C(24)	37.53(9)
N(1)-Ru(1)-C(21)	100.73(9)
C(29)-Ru(1)-C(21)	37.52(9)
C(1)-Ru(1)-C(21)	110.91(9)
C(22)-Ru(1)-C(21)	37.25(10)
C(28)-Ru(1)-C(21)	67.82(9)
C(23)-Ru(1)-C(21)	67.36(9)
C(24)-Ru(1)-C(21)	80.36(9)
N(1)-Ru(1)-S(1)	84.07(6)
C(29)-Ru(1)-S(1)	143.20(7)
C(1)-Ru(1)-S(1)	79.11(6)
C(22)-Ru(1)-S(1)	133.80(7)
C(28)-Ru(1)-S(1)	108.71(7)
C(23)-Ru(1)-S(1)	102.62(7)
C(24)-Ru(1)-S(1)	91.43(7)
C(21)-Ru(1)-S(1)	169.97(7)
P(1)-S(1)-Ru(1)	82.42(3)

C(1)-P(1)-C(8)	111.58(11)
C(1)-P(1)-C(2)	115.62(11)
C(8)-P(1)-C(2)	106.13(11)
C(1)-P(1)-S(1)	102.02(8)
C(8)-P(1)-S(1)	111.70(9)
C(2)-P(1)-S(1)	109.90(8)
C(30)-N(1)-C(31)	122.2(2)
C(30)-N(1)-Ru(1)	100.39(15)
C(31)-N(1)-Ru(1)	137.03(16)
C(30)-C(1)-S(2)	115.00(16)
C(30)-C(1)-P(1)	108.82(16)
S(2)-C(1)-P(1)	123.74(14)
C(30)-C(1)-Ru(1)	90.03(14)
S(2)-C(1)-Ru(1)	117.47(12)
P(1)-C(1)-Ru(1)	95.33(10)
N(2)-Ru(2)-C(63)	128.07(9)
N(2)-Ru(2)-C(56)	96.29(9)
C(63)-Ru(2)-C(56)	67.29(9)
N(2)-Ru(2)-C(35)	63.32(8)
C(63)-Ru(2)-C(35)	98.91(9)
C(56)-Ru(2)-C(35)	141.77(9)
N(2)-Ru(2)-C(57)	117.34(9)
C(63)-Ru(2)-C(57)	79.50(9)
C(56)-Ru(2)-C(57)	37.20(10)
C(35)-Ru(2)-C(57)	178.37(9)
N(2)-Ru(2)-C(55)	100.18(9)
C(63)-Ru(2)-C(55)	37.61(9)
C(56)-Ru(2)-C(55)	37.62(9)
C(35)-Ru(2)-C(55)	110.71(9)
C(57)-Ru(2)-C(55)	67.78(9)
N(2)-Ru(2)-C(62)	165.78(9)
C(63)-Ru(2)-C(62)	37.76(9)
C(56)-Ru(2)-C(62)	79.06(9)
C(35)-Ru(2)-C(62)	112.47(9)
C(57)-Ru(2)-C(62)	66.50(9)
C(55)-Ru(2)-C(62)	67.91(9)

N(2)-Ru(2)-C(58)	152.57(8)
C(63)-Ru(2)-C(58)	67.63(9)
C(56)-Ru(2)-C(58)	67.48(9)
C(35)-Ru(2)-C(58)	142.31(9)
C(57)-Ru(2)-C(58)	37.40(9)
C(55)-Ru(2)-C(58)	80.61(9)
C(62)-Ru(2)-C(58)	36.72(9)
N(2)-Ru(2)-S(3)	85.45(6)
C(63)-Ru(2)-S(3)	141.86(7)
C(56)-Ru(2)-S(3)	134.16(7)
C(35)-Ru(2)-S(3)	79.05(6)
C(57)-Ru(2)-S(3)	102.44(7)
C(55)-Ru(2)-S(3)	170.11(7)
C(62)-Ru(2)-S(3)	107.49(7)
C(58)-Ru(2)-S(3)	90.64(7)
O(1)-S(2)-O(2)	117.39(11)
O(1)-S(2)-C(1)	106.79(11)
O(2)-S(2)-C(1)	109.43(11)
O(1)-S(2)-C(14)	107.14(11)
O(2)-S(2)-C(14)	106.72(11)
C(1)-S(2)-C(14)	109.17(11)
C(35)-P(2)-C(42)	112.27(11)
C(35)-P(2)-C(36)	112.95(11)
C(42)-P(2)-C(36)	106.54(12)
C(35)-P(2)-S(3)	102.38(8)
C(42)-P(2)-S(3)	112.05(9)
C(36)-P(2)-S(3)	110.77(9)
C(64)-N(2)-C(65)	122.2(2)
C(64)-N(2)-Ru(2)	100.64(15)
C(65)-N(2)-Ru(2)	136.71(16)
C(3)-C(2)-C(7)	119.8(2)
C(3)-C(2)-P(1)	120.6(2)
C(7)-C(2)-P(1)	119.27(19)
P(2)-S(3)-Ru(2)	82.35(3)
C(4)-C(3)-C(2)	119.6(3)
O(5)-S(4)-O(4)	117.42(11)

O(5)-S(4)-C(35)	106.45(11)
O(4)-S(4)-C(35)	109.95(11)
O(5)-S(4)-C(48)	106.93(11)
O(4)-S(4)-C(48)	106.39(11)
C(35)-S(4)-C(48)	109.53(11)
C(5)-C(4)-C(3)	120.4(3)
C(4)-C(5)-C(6)	120.5(3)
C(7)-C(6)-C(5)	119.6(3)
C(6)-C(7)-C(2)	120.1(2)
C(9)-C(8)-C(13)	119.4(2)
C(9)-C(8)-P(1)	119.30(19)
C(13)-C(8)-P(1)	121.32(19)
C(10)-C(9)-C(8)	120.3(2)
C(11)-C(10)-C(9)	119.9(2)
C(12)-C(11)-C(10)	120.2(3)
C(11)-C(12)-C(13)	120.3(2)
C(12)-C(13)-C(8)	119.9(2)
C(19)-C(14)-C(15)	121.1(2)
C(19)-C(14)-S(2)	119.64(19)
C(15)-C(14)-S(2)	119.29(19)
C(16)-C(15)-C(14)	118.9(2)
C(17)-C(16)-C(15)	120.3(2)
C(16)-C(17)-C(18)	120.3(2)
C(19)-C(18)-C(17)	120.3(2)
C(18)-C(19)-C(14)	119.2(2)
C(22)-C(21)-C(29)	116.4(2)
C(22)-C(21)-C(20)	122.5(2)
C(29)-C(21)-C(20)	121.1(2)
C(22)-C(21)-Ru(1)	69.83(15)
C(29)-C(21)-Ru(1)	69.12(14)
C(20)-C(21)-Ru(1)	130.91(18)
C(23)-C(22)-C(21)	122.7(2)
C(23)-C(22)-Ru(1)	72.63(14)
C(21)-C(22)-Ru(1)	72.92(14)
C(22)-C(23)-C(24)	119.8(2)
C(22)-C(23)-Ru(1)	70.38(14)

C(24)-C(23)-Ru(1)	71.43(14)
C(28)-C(24)-C(23)	118.7(2)
C(28)-C(24)-C(25)	123.5(2)
C(23)-C(24)-C(25)	117.7(2)
C(28)-C(24)-Ru(1)	71.16(14)
C(23)-C(24)-Ru(1)	71.04(14)
C(25)-C(24)-Ru(1)	132.65(18)
C(27)-C(25)-C(24)	114.8(2)
C(27)-C(25)-C(26)	110.8(2)
C(24)-C(25)-C(26)	107.9(2)
C(24)-C(28)-C(29)	120.1(2)
C(24)-C(28)-Ru(1)	71.98(14)
C(29)-C(28)-Ru(1)	69.70(14)
C(28)-C(29)-C(21)	122.2(2)
C(28)-C(29)-Ru(1)	72.69(14)
C(21)-C(29)-Ru(1)	73.37(14)
O(3)-C(30)-N(1)	132.3(2)
O(3)-C(30)-C(1)	125.5(2)
N(1)-C(30)-C(1)	102.2(2)
N(1)-C(31)-C(33)	109.5(2)
N(1)-C(31)-C(32)	108.7(2)
C(33)-C(31)-C(32)	110.4(3)
N(1)-C(31)-C(34)	108.8(2)
C(33)-C(31)-C(34)	111.7(3)
C(32)-C(31)-C(34)	107.6(2)
C(64)-C(35)-S(4)	114.46(17)
C(64)-C(35)-P(2)	109.89(16)
S(4)-C(35)-P(2)	123.73(14)
C(64)-C(35)-Ru(2)	89.50(14)
S(4)-C(35)-Ru(2)	117.77(12)
P(2)-C(35)-Ru(2)	94.92(10)
C(41)-C(36)-C(37)	119.4(2)
C(41)-C(36)-P(2)	118.62(19)
C(37)-C(36)-P(2)	121.9(2)
C(38)-C(37)-C(36)	119.5(3)
C(39)-C(38)-C(37)	120.6(3)

C(38)-C(39)-C(40)	120.2(3)
C(41)-C(40)-C(39)	119.7(3)
C(40)-C(41)-C(36)	120.6(2)
C(47)-C(42)-C(43)	119.5(2)
C(47)-C(42)-P(2)	119.8(2)
C(43)-C(42)-P(2)	120.69(19)
C(44)-C(43)-C(42)	120.2(3)
C(45)-C(44)-C(43)	120.3(3)
C(46)-C(45)-C(44)	119.7(2)
C(45)-C(46)-C(47)	120.5(3)
C(46)-C(47)-C(42)	119.9(3)
C(53)-C(48)-C(49)	121.2(2)
C(53)-C(48)-S(4)	119.4(2)
C(49)-C(48)-S(4)	119.4(2)
C(50)-C(49)-C(48)	118.7(3)
C(51)-C(50)-C(49)	120.1(3)
C(52)-C(51)-C(50)	120.7(3)
C(51)-C(52)-C(53)	120.1(3)
C(48)-C(53)-C(52)	119.2(3)
C(63)-C(55)-C(56)	116.7(2)
C(63)-C(55)-C(54)	122.1(2)
C(56)-C(55)-C(54)	121.2(2)
C(63)-C(55)-Ru(2)	69.28(14)
C(56)-C(55)-Ru(2)	70.11(14)
C(54)-C(55)-Ru(2)	130.44(18)
C(57)-C(56)-C(55)	122.0(2)
C(57)-C(56)-Ru(2)	72.46(14)
C(55)-C(56)-Ru(2)	72.27(14)
C(56)-C(57)-C(58)	120.5(2)
C(56)-C(57)-Ru(2)	70.33(14)
C(58)-C(57)-Ru(2)	72.28(14)
C(62)-C(58)-C(57)	118.3(2)
C(62)-C(58)-C(59)	123.2(2)
C(57)-C(58)-C(59)	118.4(2)
C(62)-C(58)-Ru(2)	70.99(14)
C(57)-C(58)-Ru(2)	70.31(14)

C(59)-C(58)-Ru(2)	133.15(17)
C(58)-C(59)-C(61)	115.4(2)
C(58)-C(59)-C(60)	107.7(2)
C(61)-C(59)-C(60)	110.9(2)
C(58)-C(62)-C(63)	120.3(2)
C(58)-C(62)-Ru(2)	72.29(14)
C(63)-C(62)-Ru(2)	68.90(13)
C(55)-C(63)-C(62)	122.1(2)
C(55)-C(63)-Ru(2)	73.11(14)
C(62)-C(63)-Ru(2)	73.34(14)
O(6)-C(64)-N(2)	132.4(2)
O(6)-C(64)-C(35)	124.8(2)
N(2)-C(64)-C(35)	102.9(2)
N(2)-C(65)-C(67)	108.4(2)
N(2)-C(65)-C(68)	108.4(2)
C(67)-C(65)-C(68)	108.8(2)
N(2)-C(65)-C(66)	110.3(2)
C(67)-C(65)-C(66)	110.6(2)
C(68)-C(65)-C(66)	110.2(2)

Symmetry transformations used to generate equivalent atoms:

Table 80a-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	14(1)	13(1)	12(1)	-2(1)	0(1)	-5(1)
S(1)	20(1)	12(1)	17(1)	-1(1)	0(1)	-2(1)
P(1)	15(1)	13(1)	13(1)	1(1)	0(1)	-4(1)
O(1)	29(1)	14(1)	14(1)	3(1)	-4(1)	-4(1)
N(1)	14(1)	13(1)	19(1)	-2(1)	0(1)	-5(1)
C(1)	18(1)	12(1)	12(1)	-1(1)	0(1)	-5(1)
Ru(2)	15(1)	11(1)	11(1)	1(1)	1(1)	-3(1)
S(2)	21(1)	12(1)	12(1)	0(1)	0(1)	-5(1)

P(2)	15(1)	14(1)	13(1)	-1(1)	1(1)	-5(1)
O(2)	23(1)	18(1)	18(1)	-2(1)	1(1)	-10(1)
N(2)	14(1)	15(1)	16(1)	3(1)	1(1)	-3(1)
C(2)	17(1)	11(1)	17(1)	-2(1)	-1(1)	-2(1)
S(3)	20(1)	17(1)	16(1)	0(1)	2(1)	-8(1)
O(3)	16(1)	23(1)	25(1)	-8(1)	-1(1)	1(1)
C(3)	19(1)	23(1)	18(1)	-2(1)	1(1)	-2(1)
S(4)	21(1)	13(1)	14(1)	1(1)	-1(1)	-6(1)
O(4)	23(1)	15(1)	20(1)	2(1)	0(1)	-4(1)
C(4)	28(2)	36(2)	19(1)	-8(1)	-4(1)	0(1)
O(5)	28(1)	19(1)	18(1)	-1(1)	-4(1)	-11(1)
C(5)	21(2)	31(2)	36(2)	-11(1)	-7(1)	-4(1)
O(6)	15(1)	25(1)	24(1)	7(1)	2(1)	-6(1)
C(6)	18(1)	20(1)	38(2)	-3(1)	0(1)	-6(1)
C(7)	20(1)	16(1)	21(1)	-1(1)	0(1)	-6(1)
C(8)	15(1)	18(1)	16(1)	3(1)	-1(1)	-4(1)
C(9)	21(1)	17(1)	24(1)	4(1)	2(1)	-3(1)
C(10)	25(2)	21(1)	30(2)	12(1)	-1(1)	-8(1)
C(11)	19(1)	32(2)	23(1)	11(1)	0(1)	-8(1)
C(12)	18(1)	26(1)	20(1)	2(1)	4(1)	-2(1)
C(13)	21(1)	19(1)	19(1)	3(1)	-1(1)	-5(1)
C(14)	24(1)	11(1)	13(1)	0(1)	1(1)	-7(1)
C(15)	21(1)	15(1)	19(1)	1(1)	-3(1)	-7(1)
C(16)	32(2)	19(1)	15(1)	3(1)	-6(1)	-14(1)
C(17)	32(2)	17(1)	16(1)	-3(1)	4(1)	-11(1)
C(18)	21(1)	17(1)	26(1)	-4(1)	4(1)	-5(1)
C(19)	23(1)	15(1)	17(1)	0(1)	-2(1)	-5(1)
C(20)	31(2)	34(2)	21(2)	4(1)	-5(1)	-3(1)
C(21)	22(1)	27(1)	10(1)	3(1)	2(1)	-5(1)
C(22)	22(1)	33(2)	12(1)	-3(1)	0(1)	-14(1)
C(23)	26(1)	20(1)	15(1)	-5(1)	7(1)	-12(1)
C(24)	18(1)	21(1)	17(1)	-1(1)	7(1)	-8(1)
C(25)	16(1)	23(1)	26(2)	1(1)	2(1)	-6(1)
C(26)	22(2)	33(2)	30(2)	3(1)	6(1)	-4(1)
C(27)	24(2)	31(2)	31(2)	1(1)	-3(1)	-7(1)
C(28)	20(1)	25(1)	15(1)	2(1)	1(1)	-13(1)

C(29)	26(1)	17(1)	12(1)	0(1)	4(1)	-9(1)
C(30)	18(1)	14(1)	14(1)	3(1)	-3(1)	-4(1)
C(31)	15(1)	16(1)	23(1)	-3(1)	-3(1)	-5(1)
C(32)	30(2)	31(2)	61(2)	-24(2)	8(2)	-17(1)
C(33)	43(2)	28(2)	67(2)	12(2)	-36(2)	-16(1)
C(34)	42(2)	61(2)	35(2)	0(2)	0(2)	-40(2)
C(35)	16(1)	14(1)	13(1)	0(1)	1(1)	-5(1)
C(36)	19(1)	18(1)	18(1)	3(1)	-2(1)	-9(1)
C(37)	21(1)	31(2)	16(1)	1(1)	2(1)	-11(1)
C(38)	30(2)	46(2)	16(1)	12(1)	-5(1)	-15(1)
C(39)	26(2)	36(2)	30(2)	17(1)	-11(1)	-9(1)
C(40)	21(1)	21(1)	33(2)	3(1)	-2(1)	-5(1)
C(41)	20(1)	20(1)	20(1)	1(1)	-1(1)	-7(1)
C(42)	17(1)	19(1)	15(1)	-3(1)	-1(1)	-3(1)
C(43)	28(2)	23(1)	24(1)	-5(1)	5(1)	-11(1)
C(44)	23(2)	38(2)	23(2)	-5(1)	6(1)	-12(1)
C(45)	21(1)	32(2)	24(2)	-13(1)	2(1)	-2(1)
C(46)	27(2)	21(1)	37(2)	-13(1)	0(1)	-5(1)
C(47)	19(1)	26(1)	27(2)	-7(1)	3(1)	-10(1)
C(48)	26(1)	15(1)	15(1)	2(1)	-1(1)	-10(1)
C(49)	24(1)	22(1)	24(1)	7(1)	-3(1)	-10(1)
C(50)	24(2)	29(2)	35(2)	3(1)	5(1)	-10(1)
C(51)	43(2)	29(2)	23(2)	2(1)	8(1)	-14(1)
C(52)	42(2)	20(1)	18(1)	3(1)	-3(1)	-12(1)
C(53)	25(1)	16(1)	18(1)	3(1)	-1(1)	-8(1)
C(54)	33(2)	28(2)	17(1)	1(1)	-4(1)	-12(1)
C(55)	23(1)	18(1)	13(1)	-3(1)	2(1)	-5(1)
C(56)	25(1)	19(1)	10(1)	2(1)	2(1)	-2(1)
C(57)	23(1)	18(1)	14(1)	-1(1)	7(1)	-3(1)
C(58)	20(1)	15(1)	14(1)	-4(1)	6(1)	-3(1)
C(59)	20(1)	21(1)	25(1)	-1(1)	5(1)	-7(1)
C(60)	27(2)	38(2)	32(2)	-5(1)	9(1)	-14(1)
C(61)	21(2)	35(2)	35(2)	2(1)	-1(1)	-9(1)
C(62)	19(1)	15(1)	14(1)	-2(1)	3(1)	0(1)
C(63)	24(1)	13(1)	13(1)	-1(1)	5(1)	-2(1)
C(64)	17(1)	15(1)	16(1)	-1(1)	-1(1)	-3(1)

C(65)	15(1)	15(1)	20(1)	4(1)	-1(1)	-1(1)
C(66)	31(2)	25(2)	32(2)	8(1)	-13(1)	-10(1)
C(67)	18(1)	20(1)	37(2)	13(1)	-1(1)	-4(1)
C(68)	35(2)	22(1)	26(2)	2(1)	3(1)	7(1)

Table 80a-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
H(3)	5126	8144	-496	25
H(4)	3349	8079	-995	36
H(5)	1637	7773	-458	36
H(6)	1630	7584	593	30
H(7)	3365	7700	1104	23
H(9)	6290	9805	302	26
H(10)	7781	10083	-420	30
H(11)	9277	8757	-949	30
H(12)	9268	7162	-770	27
H(13)	7777	6874	-53	24
H(15)	5335	5821	101	22
H(16)	6218	5093	-844	25
H(17)	8417	4277	-995	26
H(18)	9744	4127	-198	26
H(19)	8882	4835	751	22
H(20A)	7573	5817	2720	46
H(20B)	7015	5839	3400	46
H(20C)	7899	6484	3209	46
H(22)	6665	8228	3222	26
H(23)	4799	9541	3029	23
H(25)	2855	10131	2513	26
H(26A)	964	10305	3136	45
H(26B)	2173	9809	3508	45
H(26C)	1404	9159	3246	45

H(27A)	2408	9343	1670	44
H(27B)	1112	10017	2006	44
H(27C)	1558	8865	2092	44
H(28)	3309	7562	2235	22
H(29)	5207	6257	2434	22
H(32A)	8395	9744	2364	60
H(32B)	7407	9264	2675	60
H(32C)	7123	9806	2052	60
H(33A)	9947	7162	2109	65
H(33B)	9023	7572	2694	65
H(33C)	10049	8080	2469	65
H(34A)	9548	8087	1125	60
H(34B)	9765	8988	1458	60
H(34C)	8487	9135	1130	60
H(37)	5261	6892	4544	26
H(38)	3644	7928	3993	36
H(39)	1840	9046	4491	37
H(40)	1618	9131	5549	30
H(41)	3210	8097	6105	24
H(43)	7749	6684	5076	29
H(44)	9300	5619	4409	33
H(45)	9255	4031	4232	33
H(46)	7677	3499	4737	35
H(47)	6141	4548	5420	28
H(49)	8887	7980	5866	27
H(50)	9968	8103	4930	35
H(51)	8801	8722	4095	38
H(52)	6573	9249	4183	31
H(53)	5473	9090	5104	24
H(54A)	7049	8152	7809	38
H(54B)	7294	7351	8319	38
H(54C)	6395	8440	8470	38
H(56)	6054	6239	8351	23
H(57)	4246	5806	8099	23
H(59)	2413	6111	7473	26
H(60A)	905	7756	8212	48

H(60B)	1648	6710	8463	48
H(60C)	467	6838	8066	48
H(61A)	2001	7152	6634	46
H(61B)	1089	8017	7055	46
H(61C)	702	7065	6942	46
H(62)	2917	8408	7168	21
H(63)	4763	8819	7413	21
H(66A)	9585	4678	7792	43
H(66B)	8474	5658	7992	43
H(66C)	9448	5656	7432	43
H(67A)	6690	4330	7299	39
H(67B)	6839	4818	7916	39
H(67C)	7868	3814	7686	39
H(68A)	8307	4253	6403	47
H(68B)	9410	3744	6833	47
H(68C)	9424	4703	6482	47

Röntgenstrukturanalytische Daten für 81a

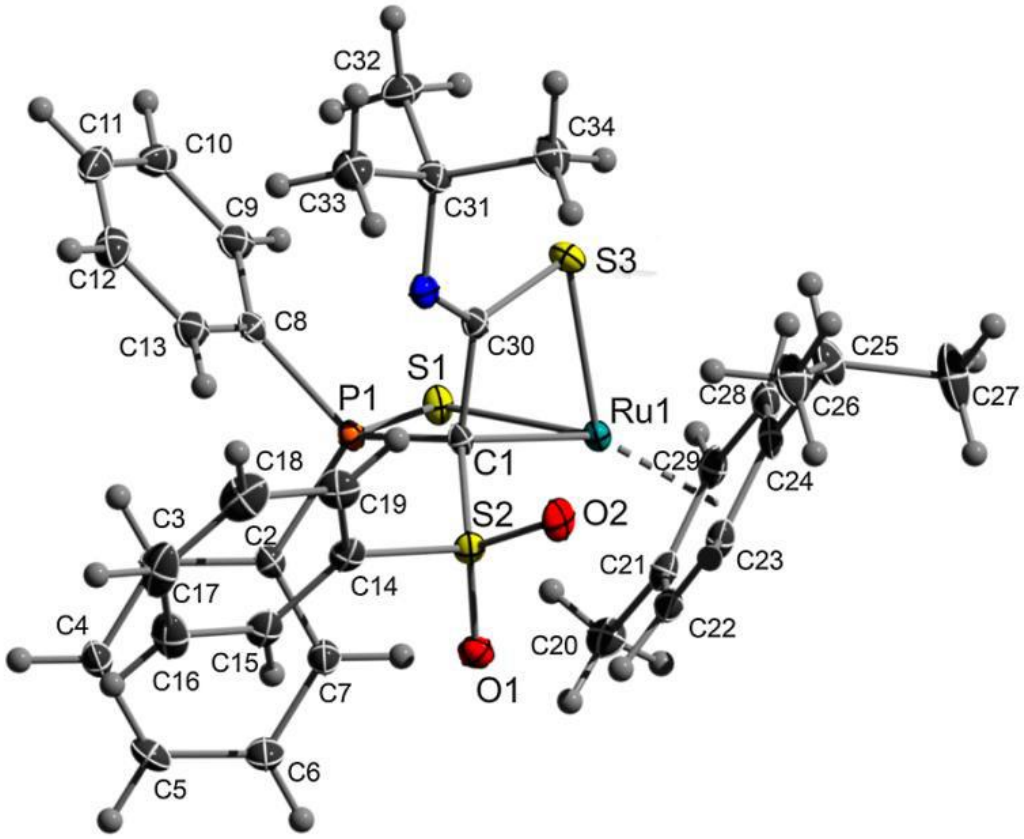

Table 81a-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	$C_{34}H_{38}NO_2PRuS_3$	
Formula weight	720.87	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 10.8646(11) Å	α = 90°.
	b = 17.7665(17) Å	β = 95.704(4)°.
	c = 16.7228(16) Å	γ = 90°.
Volume	3212.0(5) $Å^3$	
Z	4	

Density (calculated)	1.491 Mg/m^3
Absorption coefficient	0.765 mm^{-1}
F(000)	1488
Crystal size	0.21 x 0.18 x 0.11 mm^3
Theta range for data collection	1.68 to 26.46°.
Index ranges	-13<=h<=13, -22<=k<=22, -20<=l<=20
Reflections collected	48301
Independent reflections	6609 [R(int) = 0.0560]
Completeness to theta = 26.46°	99.5 %
Absorption correction	Empirical
Max. and min. transmission	0.9233 and 0.8534
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6609 / 0 / 385
Goodness-of-fit on F^2	1.142
Final R indices [I>2sigma(I)]	R1 = 0.0271, wR2 = 0.0728
R indices (all data)	R1 = 0.0354, wR2 = 0.0859
Largest diff. peak and hole	0.868 and -0.537 $e.Å^{-3}$

Table 81a-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	6766(1)	102(1)	2173(1)	12(1)
S(1)	6672(1)	21(1)	713(1)	16(1)
P(1)	7017(1)	1126(1)	787(1)	12(1)
O(1)	5328(2)	1907(1)	2247(1)	19(1)
N(1)	9478(2)	1708(1)	2122(1)	16(1)
C(1)	7350(2)	1246(1)	1866(1)	13(1)
S(2)	6655(1)	1977(1)	2391(1)	14(1)
O(2)	7205(2)	1950(1)	3211(1)	20(1)
C(2)	5719(2)	1662(1)	317(1)	14(1)
S(3)	8947(1)	174(1)	2213(1)	17(1)
C(3)	5855(2)	2179(1)	-300(1)	17(1)
C(4)	4824(2)	2544(1)	-670(1)	19(1)

C(5)	3665(2)	2399(1)	-433(1)	21(1)
C(6)	3517(2)	1882(1)	174(1)	22(1)
C(7)	4541(2)	1507(1)	542(1)	18(1)
C(8)	8331(2)	1399(1)	266(1)	14(1)
C(9)	8889(2)	871(1)	-194(1)	19(1)
C(10)	9873(2)	1078(2)	-623(1)	24(1)
C(11)	10290(2)	1812(2)	-588(1)	26(1)
C(12)	9750(2)	2340(2)	-122(1)	24(1)
C(13)	8778(2)	2136(1)	314(1)	19(1)
C(14)	7026(2)	2869(1)	2005(1)	17(1)
C(15)	6197(2)	3214(1)	1433(1)	19(1)
C(16)	6479(3)	3920(1)	1149(2)	26(1)
C(17)	7562(3)	4276(1)	1445(2)	29(1)
C(18)	8378(3)	3934(1)	2023(2)	29(1)
C(19)	8112(2)	3225(1)	2309(2)	22(1)
C(20)	3827(2)	-460(1)	1520(2)	23(1)
C(21)	4851(2)	-390(1)	2185(1)	18(1)
C(22)	4974(2)	241(1)	2695(1)	18(1)
C(23)	5978(2)	304(1)	3307(1)	18(1)
C(24)	6869(2)	-274(1)	3433(1)	19(1)
C(25)	7950(3)	-256(2)	4076(1)	25(1)
C(26)	8321(3)	529(2)	4372(2)	28(1)
C(27)	7649(3)	-774(2)	4764(2)	39(1)
C(28)	6735(2)	-918(1)	2916(1)	20(1)
C(29)	5760(2)	-971(1)	2301(1)	19(1)
C(30)	8745(2)	1154(1)	2084(1)	14(1)
C(31)	10835(2)	1622(1)	2302(1)	18(1)
C(32)	11376(2)	1097(1)	1703(2)	23(1)
C(33)	11381(2)	2407(1)	2219(2)	25(1)
C(34)	11148(2)	1343(1)	3165(1)	23(1)

Table 81a-3. Bond lengths [Å] and angles [°] for sad.

Ru(1)-C(23)	2.186(2)
Ru(1)-C(28)	2.198(2)
Ru(1)-C(24)	2.202(2)
Ru(1)-C(1)	2.205(2)
Ru(1)-C(29)	2.217(2)
Ru(1)-C(22)	2.225(2)
Ru(1)-C(21)	2.258(2)
Ru(1)-S(3)	2.3675(6)
Ru(1)-S(1)	2.4378(6)
S(1)-P(1)	2.0013(8)
P(1)-C(8)	1.811(2)
P(1)-C(2)	1.815(2)
P(1)-C(1)	1.817(2)
O(1)-S(2)	1.4433(17)
N(1)-C(30)	1.263(3)
N(1)-C(31)	1.483(3)
C(1)-C(30)	1.531(3)
C(1)-S(2)	1.778(2)
S(2)-O(2)	1.4407(16)
S(2)-C(14)	1.773(2)
C(2)-C(7)	1.397(3)
C(2)-C(3)	1.400(3)
S(3)-C(30)	1.765(2)
C(3)-C(4)	1.385(3)
C(4)-C(5)	1.381(3)
C(5)-C(6)	1.391(3)
C(6)-C(7)	1.387(3)
C(8)-C(9)	1.390(3)
C(8)-C(13)	1.396(3)
C(9)-C(10)	1.394(3)
C(10)-C(11)	1.381(4)
C(11)-C(12)	1.386(4)
C(12)-C(13)	1.389(3)
C(14)-C(19)	1.389(3)

C(14)-C(15)	1.389(3)
C(15)-C(16)	1.386(3)
C(16)-C(17)	1.384(4)
C(17)-C(18)	1.385(4)
C(18)-C(19)	1.388(4)
C(20)-C(21)	1.498(3)
C(21)-C(22)	1.406(3)
C(21)-C(29)	1.428(3)
C(22)-C(23)	1.424(3)
C(23)-C(24)	1.411(3)
C(24)-C(28)	1.434(3)
C(24)-C(25)	1.512(3)
C(25)-C(26)	1.520(4)
C(25)-C(27)	1.534(4)
C(28)-C(29)	1.404(3)
C(31)-C(33)	1.528(3)
C(31)-C(32)	1.529(3)
C(31)-C(34)	1.532(3)

C(23)-Ru(1)-C(28)	67.44(9)
C(23)-Ru(1)-C(24)	37.53(9)
C(28)-Ru(1)-C(24)	38.04(9)
C(23)-Ru(1)-C(1)	101.38(8)
C(28)-Ru(1)-C(1)	155.82(8)
C(24)-Ru(1)-C(1)	120.91(8)
C(23)-Ru(1)-C(29)	79.53(9)
C(28)-Ru(1)-C(29)	37.06(9)
C(24)-Ru(1)-C(29)	68.06(9)
C(1)-Ru(1)-C(29)	166.02(8)
C(23)-Ru(1)-C(22)	37.66(9)
C(28)-Ru(1)-C(22)	78.89(9)
C(24)-Ru(1)-C(22)	67.79(9)
C(1)-Ru(1)-C(22)	105.77(8)
C(29)-Ru(1)-C(22)	66.36(9)
C(23)-Ru(1)-C(21)	67.37(9)
C(28)-Ru(1)-C(21)	67.07(9)

C(24)-Ru(1)-C(21)	80.42(9)
C(1)-Ru(1)-C(21)	130.16(8)
C(29)-Ru(1)-C(21)	37.21(9)
C(22)-Ru(1)-C(21)	36.55(8)
C(23)-Ru(1)-S(3)	116.34(7)
C(28)-Ru(1)-S(3)	95.78(7)
C(24)-Ru(1)-S(3)	91.95(7)
C(1)-Ru(1)-S(3)	69.26(6)
C(29)-Ru(1)-S(3)	123.09(7)
C(22)-Ru(1)-S(3)	153.54(6)
C(21)-Ru(1)-S(3)	160.29(6)
C(23)-Ru(1)-S(1)	153.78(7)
C(28)-Ru(1)-S(1)	121.02(6)
C(24)-Ru(1)-S(1)	158.98(7)
C(1)-Ru(1)-S(1)	78.77(6)
C(29)-Ru(1)-S(1)	94.22(6)
C(22)-Ru(1)-S(1)	116.59(6)
C(21)-Ru(1)-S(1)	92.23(6)
S(3)-Ru(1)-S(1)	88.51(2)
P(1)-S(1)-Ru(1)	83.77(2)
C(8)-P(1)-C(2)	105.47(10)
C(8)-P(1)-C(1)	110.99(10)
C(2)-P(1)-C(1)	116.03(10)
C(8)-P(1)-S(1)	112.64(8)
C(2)-P(1)-S(1)	110.78(8)
C(1)-P(1)-S(1)	101.14(7)
C(30)-N(1)-C(31)	122.62(19)
C(30)-C(1)-S(2)	114.76(15)
C(30)-C(1)-P(1)	108.57(14)
S(2)-C(1)-P(1)	121.53(12)
C(30)-C(1)-Ru(1)	98.48(13)
S(2)-C(1)-Ru(1)	114.38(11)
P(1)-C(1)-Ru(1)	95.19(9)
O(2)-S(2)-O(1)	117.93(10)
O(2)-S(2)-C(14)	106.81(10)
O(1)-S(2)-C(14)	106.02(10)

O(2)-S(2)-C(1)	106.77(10)
O(1)-S(2)-C(1)	108.72(10)
C(14)-S(2)-C(1)	110.53(10)
C(7)-C(2)-C(3)	119.6(2)
C(7)-C(2)-P(1)	118.26(17)
C(3)-C(2)-P(1)	121.96(17)
C(30)-S(3)-Ru(1)	86.45(8)
C(4)-C(3)-C(2)	119.7(2)
C(5)-C(4)-C(3)	120.3(2)
C(4)-C(5)-C(6)	120.5(2)
C(7)-C(6)-C(5)	119.6(2)
C(6)-C(7)-C(2)	120.2(2)
C(9)-C(8)-C(13)	119.8(2)
C(9)-C(8)-P(1)	119.60(18)
C(13)-C(8)-P(1)	120.64(17)
C(8)-C(9)-C(10)	120.4(2)
C(11)-C(10)-C(9)	119.4(2)
C(10)-C(11)-C(12)	120.5(2)
C(11)-C(12)-C(13)	120.3(2)
C(12)-C(13)-C(8)	119.5(2)
C(19)-C(14)-C(15)	121.4(2)
C(19)-C(14)-S(2)	119.25(18)
C(15)-C(14)-S(2)	119.30(18)
C(16)-C(15)-C(14)	119.0(2)
C(17)-C(16)-C(15)	120.0(2)
C(16)-C(17)-C(18)	120.7(2)
C(17)-C(18)-C(19)	119.9(2)
C(18)-C(19)-C(14)	119.0(2)
C(22)-C(21)-C(29)	118.1(2)
C(22)-C(21)-C(20)	122.3(2)
C(29)-C(21)-C(20)	119.5(2)
C(22)-C(21)-Ru(1)	70.45(13)
C(29)-C(21)-Ru(1)	69.83(13)
C(20)-C(21)-Ru(1)	129.95(16)
C(21)-C(22)-C(23)	121.1(2)
C(21)-C(22)-Ru(1)	73.00(13)

C(23)-C(22)-Ru(1)	69.65(13)
C(24)-C(23)-C(22)	121.1(2)
C(24)-C(23)-Ru(1)	71.85(13)
C(22)-C(23)-Ru(1)	72.69(13)
C(23)-C(24)-C(28)	117.6(2)
C(23)-C(24)-C(25)	124.3(2)
C(28)-C(24)-C(25)	118.1(2)
C(23)-C(24)-Ru(1)	70.62(13)
C(28)-C(24)-Ru(1)	70.86(13)
C(25)-C(24)-Ru(1)	129.52(17)
C(24)-C(25)-C(26)	114.4(2)
C(24)-C(25)-C(27)	108.2(2)
C(26)-C(25)-C(27)	112.1(2)
C(29)-C(28)-C(24)	121.3(2)
C(29)-C(28)-Ru(1)	72.20(13)
C(24)-C(28)-Ru(1)	71.10(13)
C(28)-C(29)-C(21)	120.8(2)
C(28)-C(29)-Ru(1)	70.74(13)
C(21)-C(29)-Ru(1)	72.96(13)
N(1)-C(30)-C(1)	122.2(2)
N(1)-C(30)-S(3)	133.73(18)
C(1)-C(30)-S(3)	104.02(15)
N(1)-C(31)-C(33)	105.92(19)
N(1)-C(31)-C(32)	111.67(18)
C(33)-C(31)-C(32)	108.6(2)
N(1)-C(31)-C(34)	110.32(19)
C(33)-C(31)-C(34)	109.27(19)
C(32)-C(31)-C(34)	110.9(2)

Symmetry transformations used to generate equivalent atoms:

Table 81a-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	15(1)	11(1)	11(1)	0(1)	0(1)	1(1)
S(1)	22(1)	13(1)	12(1)	-1(1)	0(1)	-1(1)
P(1)	14(1)	12(1)	11(1)	0(1)	0(1)	1(1)
O(1)	19(1)	15(1)	22(1)	0(1)	4(1)	2(1)
N(1)	17(1)	17(1)	12(1)	0(1)	1(1)	0(1)
C(1)	16(1)	10(1)	11(1)	1(1)	0(1)	1(1)
S(2)	18(1)	12(1)	13(1)	-2(1)	3(1)	1(1)
O(2)	30(1)	20(1)	11(1)	-3(1)	2(1)	1(1)
C(2)	16(1)	12(1)	12(1)	-2(1)	-1(1)	1(1)
S(3)	16(1)	14(1)	20(1)	1(1)	0(1)	3(1)
C(3)	18(1)	17(1)	15(1)	-1(1)	1(1)	-1(1)
C(4)	23(1)	18(1)	17(1)	3(1)	1(1)	2(1)
C(5)	17(1)	23(1)	23(1)	2(1)	-4(1)	4(1)
C(6)	14(1)	26(1)	24(1)	2(1)	1(1)	-1(1)
C(7)	18(1)	19(1)	17(1)	2(1)	1(1)	-1(1)
C(8)	14(1)	18(1)	12(1)	2(1)	-2(1)	1(1)
C(9)	19(1)	23(1)	15(1)	-2(1)	-1(1)	4(1)
C(10)	19(1)	36(2)	16(1)	-3(1)	3(1)	7(1)
C(11)	17(1)	43(2)	18(1)	7(1)	2(1)	-2(1)
C(12)	21(1)	27(1)	23(1)	5(1)	-1(1)	-6(1)
C(13)	20(1)	21(1)	16(1)	0(1)	0(1)	1(1)
C(14)	22(1)	12(1)	17(1)	-4(1)	6(1)	1(1)
C(15)	25(1)	15(1)	18(1)	-3(1)	6(1)	1(1)
C(16)	41(2)	15(1)	23(1)	-1(1)	7(1)	4(1)
C(17)	47(2)	14(1)	28(1)	-2(1)	14(1)	-6(1)
C(18)	31(2)	20(1)	36(2)	-9(1)	8(1)	-10(1)
C(19)	24(1)	18(1)	24(1)	-5(1)	2(1)	-1(1)
C(20)	21(1)	22(1)	25(1)	-1(1)	1(1)	-5(1)
C(21)	20(1)	18(1)	17(1)	2(1)	5(1)	-5(1)
C(22)	20(1)	17(1)	16(1)	3(1)	6(1)	0(1)
C(23)	25(1)	17(1)	14(1)	2(1)	6(1)	-2(1)

C(24)	25(1)	19(1)	13(1)	7(1)	0(1)	-3(1)
C(25)	33(2)	26(1)	16(1)	4(1)	-2(1)	3(1)
C(26)	34(2)	31(2)	18(1)	2(1)	-6(1)	-4(1)
C(27)	64(2)	32(2)	20(1)	10(1)	-9(1)	-6(2)
C(28)	26(1)	16(1)	19(1)	6(1)	4(1)	2(1)
C(29)	26(1)	14(1)	18(1)	1(1)	5(1)	-5(1)
C(30)	17(1)	16(1)	9(1)	0(1)	1(1)	3(1)
C(31)	15(1)	21(1)	18(1)	2(1)	-2(1)	0(1)
C(32)	16(1)	29(1)	24(1)	-2(1)	3(1)	0(1)
C(33)	21(1)	25(1)	29(1)	3(1)	-3(1)	-6(1)
C(34)	24(1)	25(1)	18(1)	0(1)	-5(1)	-3(1)

Table 81a-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
H(3)	6651	2279	-465	20
H(4)	4915	2895	-1088	23
H(5)	2964	2655	-687	25
H(6)	2718	1785	336	26
H(7)	4441	1144	947	22
H(9)	8597	367	-217	23
H(10)	10253	716	-937	29
H(11)	10953	1957	-885	31
H(12)	10046	2843	-100	29
H(13)	8421	2496	642	23
H(15)	5449	2969	1239	23
H(16)	5928	4159	751	31
H(17)	7748	4761	1250	35
H(18)	9118	4184	2223	35
H(19)	8664	2986	2707	27
H(20A)	4179	-552	1012	34
H(20B)	3345	7	1479	34

H(20C)	3287	-880	1634	34
H(22)	4462	698	2548	21
H(23)	6135	797	3586	22
H(25)	8676	-478	3838	30
H(26A)	8486	844	3913	43
H(26B)	9069	497	4750	43
H(26C)	7649	751	4642	43
H(27A)	6925	-579	5004	59
H(27B)	8359	-792	5174	59
H(27C)	7471	-1282	4555	59
H(28)	7437	-1282	2919	24
H(29)	5792	-1368	1880	23
H(32A)	11054	1237	1155	34
H(32B)	11142	577	1808	34
H(32C)	12280	1141	1760	34
H(33A)	11161	2593	1671	38
H(33B)	12283	2383	2327	38
H(33C)	11048	2748	2604	38
H(34A)	10804	837	3219	34
H(34B)	10791	1686	3538	34
H(34C)	12048	1326	3289	34

Röntgenstrukturanalytische Daten für 81b

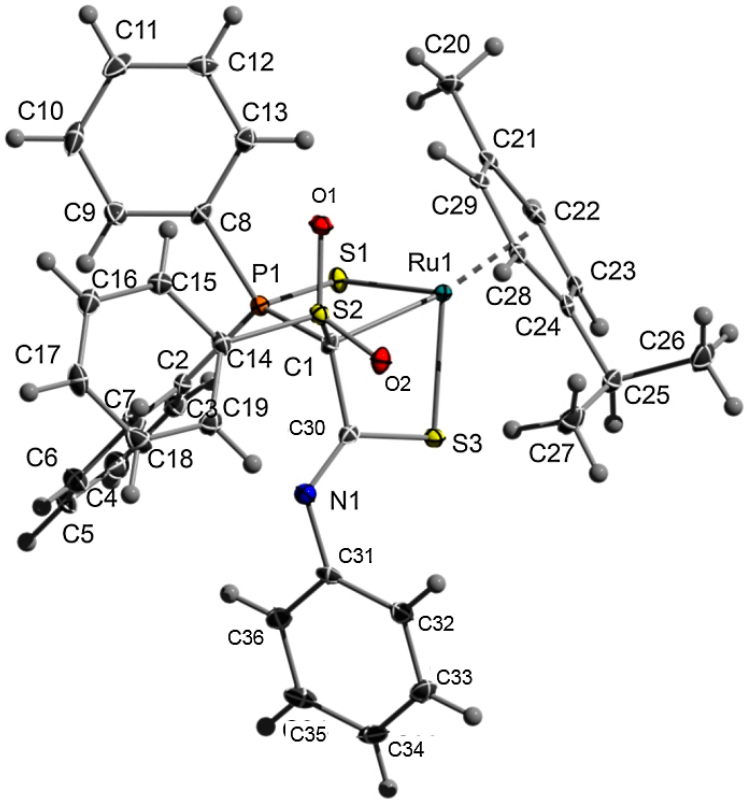

Table 81b-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	$C_{36}H_{34}NO_2PRuS_3$	
Formula weight	740.86	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.1992(4) Å	α = 98.611(2)°.
	b = 12.5648(5) Å	β = 110.524(2)°.
	c = 13.5614(6) Å	γ = 95.420(2)°.
Volume	1588.85(11) $Å^3$	
Z	2	
Density (calculated)	1.549 Mg/m^3	
Absorption coefficient	0.776 mm^{-1}	
F(000)	760	
Crystal size	0.14 x 0.12 x 0.09 mm^3	

Theta range for data collection	1.64 to 26.49°.
Index ranges	-12<=h<=12, -15<=k<=15, -16<=l<=16
Reflections collected	18401
Independent reflections	6544 [R(int) = 0.0237]
Completeness to theta = 26.49°	99.6 %
Absorption correction	Empirical
Max. and min. transmission	0.9363 and 0.8984
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6544 / 0 / 400
Goodness-of-fit on F^2	1.108
Final R indices [I>2sigma(I)]	R1 = 0.0279, wR2 = 0.0692
R indices (all data)	R1 = 0.0364, wR2 = 0.0826
Largest diff. peak and hole	0.600 and -0.565 e.$Å^{-3}$

Table 81b-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	9691(1)	5170(1)	3017(1)	8(1)
S(1)	11575(1)	4118(1)	3770(1)	12(1)
P(1)	10432(1)	2996(1)	2450(1)	10(1)
O(1)	8788(2)	4085(1)	233(1)	13(1)
N(1)	7005(2)	2270(2)	2318(2)	12(1)
C(1)	8777(3)	3515(2)	2003(2)	10(1)
S(2)	7848(1)	3506(1)	629(1)	10(1)
O(2)	6533(2)	3893(1)	549(1)	14(1)
C(2)	10199(3)	1640(2)	2747(2)	12(1)
S(3)	8336(1)	4165(1)	3766(1)	12(1)
C(3)	9221(3)	791(2)	1993(2)	17(1)
C(4)	9075(3)	-229(2)	2248(2)	21(1)
C(5)	9888(3)	-408(2)	3245(2)	19(1)
C(6)	10841(3)	431(2)	3998(2)	19(1)
C(7)	10997(3)	1463(2)	3754(2)	14(1)
C(8)	11334(3)	2890(2)	1510(2)	12(1)

C(9)	11631(3)	1900(2)	1104(2)	16(1)
C(10)	12492(3)	1884(2)	504(2)	22(1)
C(11)	13057(3)	2839(2)	320(2)	19(1)
C(12)	12748(3)	3824(2)	712(2)	15(1)
C(13)	11885(3)	3854(2)	1305(2)	14(1)
C(14)	7369(3)	2171(2)	-173(2)	12(1)
C(15)	8167(3)	1842(2)	-771(2)	14(1)
C(16)	7701(3)	866(2)	-1509(2)	17(1)
C(17)	6437(3)	230(2)	-1647(2)	18(1)
C(18)	5657(3)	554(2)	-1030(2)	18(1)
C(19)	6116(3)	1524(2)	-288(2)	14(1)
C(20)	12617(3)	6602(2)	2807(2)	14(1)
C(21)	11157(3)	6543(2)	2835(2)	12(1)
C(22)	11010(3)	6769(2)	3857(2)	11(1)
C(23)	9666(3)	6759(2)	3929(2)	11(1)
C(24)	8409(3)	6487(2)	2982(2)	11(1)
C(25)	6983(3)	6507(2)	3090(2)	14(1)
C(26)	6667(3)	7685(2)	3163(2)	22(1)
C(27)	5766(3)	5740(2)	2193(2)	21(1)
C(28)	8557(3)	6215(2)	1981(2)	11(1)
C(29)	9929(3)	6258(2)	1909(2)	11(1)
C(30)	7872(3)	3163(2)	2615(2)	10(1)
C(31)	6324(3)	2053(2)	3040(2)	13(1)
C(32)	5272(3)	2632(2)	3161(2)	16(1)
C(33)	4631(3)	2397(2)	3867(2)	20(1)
C(34)	5013(3)	1586(2)	4449(2)	20(1)
C(35)	6057(3)	1006(2)	4322(2)	21(1)
C(36)	6706(3)	1237(2)	3625(2)	17(1)

Table 81b-3. Bond lengths [Å] and angles [°] for sad.

Ru(1)-C(28)	2.176(2)
Ru(1)-C(23)	2.192(2)
Ru(1)-C(24)	2.200(2)
Ru(1)-C(22)	2.208(2)

Ru(1)-C(1)	2.228(2)
Ru(1)-C(29)	2.235(2)
Ru(1)-C(21)	2.274(2)
Ru(1)-S(3)	2.3609(6)
Ru(1)-S(1)	2.4472(6)
S(1)-P(1)	2.0055(9)
P(1)-C(1)	1.803(3)
P(1)-C(8)	1.813(3)
P(1)-C(2)	1.821(3)
O(1)-S(2)	1.4430(18)
N(1)-C(30)	1.277(3)
N(1)-C(31)	1.427(3)
C(1)-C(30)	1.518(3)
C(1)-S(2)	1.768(3)
S(2)-O(2)	1.4432(18)
S(2)-C(14)	1.778(3)
C(2)-C(7)	1.387(4)
C(2)-C(3)	1.391(4)
S(3)-C(30)	1.740(3)
C(3)-C(4)	1.384(4)
C(4)-C(5)	1.382(4)
C(5)-C(6)	1.374(4)
C(6)-C(7)	1.393(4)
C(8)-C(9)	1.388(3)
C(8)-C(13)	1.393(4)
C(9)-C(10)	1.389(4)
C(10)-C(11)	1.378(4)
C(11)-C(12)	1.381(4)
C(12)-C(13)	1.385(3)
C(14)-C(15)	1.386(3)
C(14)-C(19)	1.394(3)
C(15)-C(16)	1.385(4)
C(16)-C(17)	1.387(4)
C(17)-C(18)	1.388(4)
C(18)-C(19)	1.382(4)
C(20)-C(21)	1.499(3)

C(21)-C(29)	1.397(4)
C(21)-C(22)	1.435(3)
C(22)-C(23)	1.406(3)
C(23)-C(24)	1.428(4)
C(24)-C(28)	1.413(3)
C(24)-C(25)	1.514(3)
C(25)-C(27)	1.521(4)
C(25)-C(26)	1.540(4)
C(28)-C(29)	1.433(3)
C(31)-C(36)	1.392(4)
C(31)-C(32)	1.393(4)
C(32)-C(33)	1.385(4)
C(33)-C(34)	1.383(4)
C(34)-C(35)	1.390(4)
C(35)-C(36)	1.378(4)
C(28)-Ru(1)-C(23)	67.82(9)
C(28)-Ru(1)-C(24)	37.67(9)
C(23)-Ru(1)-C(24)	37.95(9)
C(28)-Ru(1)-C(22)	79.71(10)
C(23)-Ru(1)-C(22)	37.28(9)
C(24)-Ru(1)-C(22)	67.91(9)
C(28)-Ru(1)-C(1)	102.07(9)
C(23)-Ru(1)-C(1)	156.20(9)
C(24)-Ru(1)-C(1)	121.86(9)
C(22)-Ru(1)-C(1)	165.83(9)
C(28)-Ru(1)-C(29)	37.89(9)
C(23)-Ru(1)-C(29)	79.40(9)
C(24)-Ru(1)-C(29)	67.96(9)
C(22)-Ru(1)-C(29)	66.44(9)
C(1)-Ru(1)-C(29)	106.25(9)
C(28)-Ru(1)-C(21)	66.99(9)
C(23)-Ru(1)-C(21)	67.23(9)
C(24)-Ru(1)-C(21)	79.90(9)
C(22)-Ru(1)-C(21)	37.30(9)
C(1)-Ru(1)-C(21)	130.33(9)
C(29)-Ru(1)-C(21)	36.09(9)

C(28)-Ru(1)-S(3)	115.18(7)
C(23)-Ru(1)-S(3)	94.82(7)
C(24)-Ru(1)-S(3)	90.97(7)
C(22)-Ru(1)-S(3)	122.93(7)
C(1)-Ru(1)-S(3)	69.34(6)
C(29)-Ru(1)-S(3)	152.65(7)
C(21)-Ru(1)-S(3)	160.22(7)
C(28)-Ru(1)-S(1)	156.73(7)
C(23)-Ru(1)-S(1)	119.93(7)
C(24)-Ru(1)-S(1)	157.52(7)
C(22)-Ru(1)-S(1)	94.63(7)
C(1)-Ru(1)-S(1)	78.15(6)
C(29)-Ru(1)-S(1)	119.25(7)
C(21)-Ru(1)-S(1)	94.83(7)
S(3)-Ru(1)-S(1)	86.93(2)
P(1)-S(1)-Ru(1)	82.88(3)
C(1)-P(1)-C(8)	115.19(12)
C(1)-P(1)-C(2)	111.77(12)
C(8)-P(1)-C(2)	106.11(12)
C(1)-P(1)-S(1)	101.48(9)
C(8)-P(1)-S(1)	110.19(9)
C(2)-P(1)-S(1)	112.25(9)
C(30)-N(1)-C(31)	115.5(2)
C(30)-C(1)-S(2)	115.53(17)
C(30)-C(1)-P(1)	109.79(17)
S(2)-C(1)-P(1)	121.30(14)
C(30)-C(1)-Ru(1)	96.98(15)
S(2)-C(1)-Ru(1)	114.51(12)
P(1)-C(1)-Ru(1)	94.13(11)
O(1)-S(2)-O(2)	118.46(11)
O(1)-S(2)-C(1)	108.27(11)
O(2)-S(2)-C(1)	106.66(11)
O(1)-S(2)-C(14)	104.97(11)
O(2)-S(2)-C(14)	106.06(11)
C(1)-S(2)-C(14)	112.55(12)
C(7)-C(2)-C(3)	119.7(2)

C(7)-C(2)-P(1)	119.0(2)
C(3)-C(2)-P(1)	121.3(2)
C(30)-S(3)-Ru(1)	86.43(8)
C(4)-C(3)-C(2)	119.7(3)
C(5)-C(4)-C(3)	120.5(3)
C(6)-C(5)-C(4)	120.0(2)
C(5)-C(6)-C(7)	120.1(3)
C(2)-C(7)-C(6)	120.0(3)
C(9)-C(8)-C(13)	120.1(2)
C(9)-C(8)-P(1)	121.66(19)
C(13)-C(8)-P(1)	117.79(19)
C(8)-C(9)-C(10)	119.3(2)
C(11)-C(10)-C(9)	120.6(3)
C(10)-C(11)-C(12)	120.1(2)
C(11)-C(12)-C(13)	120.0(2)
C(12)-C(13)-C(8)	119.9(2)
C(15)-C(14)-C(19)	120.9(2)
C(15)-C(14)-S(2)	118.82(19)
C(19)-C(14)-S(2)	119.9(2)
C(16)-C(15)-C(14)	119.5(2)
C(15)-C(16)-C(17)	119.9(2)
C(16)-C(17)-C(18)	120.2(3)
C(19)-C(18)-C(17)	120.3(3)
C(18)-C(19)-C(14)	119.1(2)
C(29)-C(21)-C(22)	118.5(2)
C(29)-C(21)-C(20)	122.7(2)
C(22)-C(21)-C(20)	118.8(2)
C(29)-C(21)-Ru(1)	70.44(14)
C(22)-C(21)-Ru(1)	68.83(14)
C(20)-C(21)-Ru(1)	131.82(17)
C(23)-C(22)-C(21)	121.1(2)
C(23)-C(22)-Ru(1)	70.77(14)
C(21)-C(22)-Ru(1)	73.86(14)
C(22)-C(23)-C(24)	120.6(2)
C(22)-C(23)-Ru(1)	71.95(14)
C(24)-C(23)-Ru(1)	71.32(14)

C(28)-C(24)-C(23)	118.1(2)
C(28)-C(24)-C(25)	122.9(2)
C(23)-C(24)-C(25)	119.0(2)
C(28)-C(24)-Ru(1)	70.25(14)
C(23)-C(24)-Ru(1)	70.73(14)
C(25)-C(24)-Ru(1)	130.72(17)
C(24)-C(25)-C(27)	114.1(2)
C(24)-C(25)-C(26)	108.9(2)
C(27)-C(25)-C(26)	110.3(2)
C(24)-C(28)-C(29)	121.1(2)
C(24)-C(28)-Ru(1)	72.07(14)
C(29)-C(28)-Ru(1)	73.28(14)
C(21)-C(29)-C(28)	120.5(2)
C(21)-C(29)-Ru(1)	73.47(14)
C(28)-C(29)-Ru(1)	68.83(13)
N(1)-C(30)-C(1)	124.0(2)
N(1)-C(30)-S(3)	129.5(2)
C(1)-C(30)-S(3)	106.43(17)
C(36)-C(31)-C(32)	119.3(2)
C(36)-C(31)-N(1)	119.3(2)
C(32)-C(31)-N(1)	121.4(2)
C(33)-C(32)-C(31)	119.9(3)
C(34)-C(33)-C(32)	120.8(3)
C(33)-C(34)-C(35)	119.2(3)
C(36)-C(35)-C(34)	120.4(3)
C(35)-C(36)-C(31)	120.4(3)

Symmetry transformations used to generate equivalent atoms:

Table 81b-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	9(1)	8(1)	8(1)	2(1)	4(1)	1(1)
S(1)	12(1)	11(1)	11(1)	2(1)	2(1)	3(1)
P(1)	11(1)	9(1)	11(1)	3(1)	5(1)	2(1)
O(1)	16(1)	11(1)	11(1)	2(1)	7(1)	-1(1)
N(1)	13(1)	10(1)	12(1)	2(1)	5(1)	1(1)
C(1)	9(1)	11(1)	10(1)	1(1)	4(1)	3(1)
S(2)	11(1)	9(1)	9(1)	1(1)	3(1)	1(1)
O(2)	13(1)	14(1)	14(1)	2(1)	4(1)	5(1)
C(2)	14(1)	10(1)	17(1)	4(1)	9(1)	4(1)
S(3)	15(1)	11(1)	11(1)	1(1)	7(1)	-1(1)
C(3)	18(2)	16(1)	19(2)	5(1)	7(1)	4(1)
C(4)	20(2)	13(1)	28(2)	2(1)	10(1)	0(1)
C(5)	24(2)	12(1)	31(2)	10(1)	17(1)	6(1)
C(6)	20(2)	20(1)	22(2)	11(1)	10(1)	9(1)
C(7)	13(1)	14(1)	18(1)	5(1)	7(1)	2(1)
C(8)	9(1)	15(1)	12(1)	3(1)	5(1)	4(1)
C(9)	22(2)	13(1)	17(1)	5(1)	10(1)	5(1)
C(10)	34(2)	21(2)	18(2)	6(1)	15(1)	16(1)
C(11)	19(2)	29(2)	17(1)	11(1)	12(1)	12(1)
C(12)	13(1)	19(1)	13(1)	7(1)	4(1)	1(1)
C(13)	16(1)	14(1)	13(1)	1(1)	6(1)	2(1)
C(14)	14(1)	9(1)	10(1)	2(1)	3(1)	2(1)
C(15)	13(1)	14(1)	14(1)	4(1)	5(1)	1(1)
C(16)	21(2)	16(1)	16(1)	3(1)	8(1)	7(1)
C(17)	22(2)	12(1)	17(2)	-1(1)	4(1)	2(1)
C(18)	14(1)	14(1)	21(2)	3(1)	4(1)	-1(1)
C(19)	11(1)	16(1)	15(1)	3(1)	4(1)	3(1)
C(20)	11(1)	16(1)	16(1)	3(1)	6(1)	0(1)
C(21)	15(1)	7(1)	14(1)	3(1)	7(1)	0(1)
C(22)	13(1)	7(1)	12(1)	2(1)	4(1)	-1(1)
C(23)	15(1)	6(1)	12(1)	0(1)	6(1)	1(1)

C(24)	15(1)	5(1)	14(1)	2(1)	7(1)	3(1)
C(25)	13(1)	16(1)	18(1)	4(1)	9(1)	6(1)
C(26)	16(2)	23(2)	29(2)	2(1)	10(1)	7(1)
C(27)	12(1)	24(2)	24(2)	-2(1)	8(1)	2(1)
C(28)	14(1)	7(1)	11(1)	2(1)	4(1)	2(1)
C(29)	15(1)	8(1)	12(1)	5(1)	8(1)	2(1)
C(30)	10(1)	12(1)	9(1)	4(1)	4(1)	4(1)
C(31)	11(1)	12(1)	13(1)	1(1)	3(1)	-4(1)
C(32)	16(1)	13(1)	17(1)	3(1)	5(1)	1(1)
C(33)	13(1)	20(1)	27(2)	0(1)	12(1)	0(1)
C(34)	19(2)	24(2)	20(2)	4(1)	12(1)	-2(1)
C(35)	21(2)	21(2)	24(2)	10(1)	9(1)	0(1)
C(36)	12(1)	17(1)	22(2)	3(1)	7(1)	2(1)

Table 81b-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
H(3)	8668	908	1322	21
H(4)	8425	-798	1743	25
H(5)	9791	-1098	3407	23
H(6)	11382	311	4672	22
H(7)	11636	2032	4266	17
H(9)	11258	1253	1232	19
H(10)	12688	1222	226	26
H(11)	13648	2822	-70	23
H(12)	13119	4467	577	18
H(13)	11673	4517	1567	17
H(15)	9011	2274	-679	17
H(16)	8234	638	-1910	20
H(17)	6112	-415	-2156	22
H(18)	4821	117	-1116	21
H(19)	5597	1741	128	17
H(20A)	12551	6359	2083	22

H(20B)	13137	6144	3256	22
H(20C)	13098	7341	3062	22
H(22)	11841	6809	4512	13
H(23)	9586	6800	4632	13
H(25)	7054	6286	3768	17
H(26A)	6573	7916	2501	33
H(26B)	7431	8157	3743	33
H(26C)	5801	7715	3289	33
H(27A)	5580	6003	1535	31
H(27B)	4933	5709	2370	31
H(27C)	6017	5024	2106	31
H(28)	7716	5886	1343	13
H(29)	10003	5936	1230	13
H(32)	5002	3174	2769	19
H(33)	3936	2790	3951	23
H(34)	4576	1431	4921	24
H(35)	6319	458	4710	25
H(36)	7404	844	3546	20

Röntgenstrukturanalytische Daten für 82

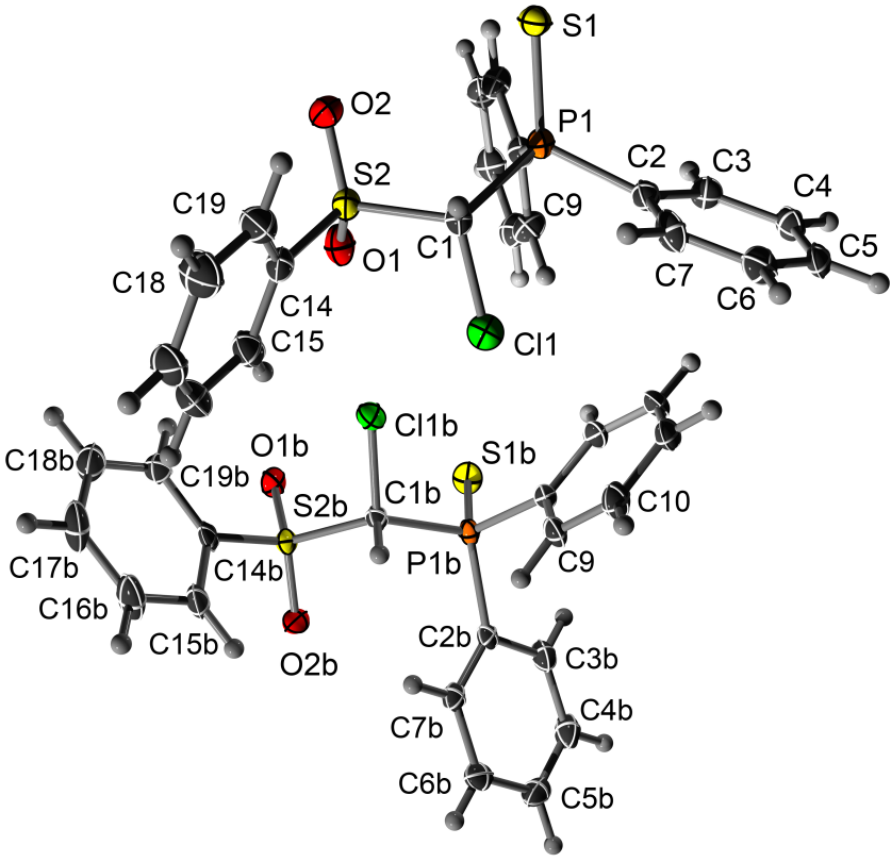

Table 82-1. Crystal data and structure refinement for test.

Identification code	test	
Empirical formula	C38 H32 Cl2 O4 P2 S4	
Formula weight	813.72	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 14.6305(10) Å	α = 90°.
	b = 24.0872(16) Å	β = 98.829(2)°.
	c = 10.8747(8) Å	γ = 90°.
Volume	3786.9(5) $Å^3$	
Z	4	
Density (calculated)	1.427 Mg/m^3	
Absorption coefficient	0.517 mm^{-1}	

F(000)	1680
Crystal size	0.31 x 0.30 x 0.27 mm^3
Theta range for data collection	1.41 to 25.00°.
Index ranges	-17<=h<=17, -28<=k<=28, -12<=l<=12
Reflections collected	45022
Independent reflections	6660 [R(int) = 0.0406]
Completeness to theta = 25.00°	100.0 %
Max. and min. transmission	0.8735 and 0.8563
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6660 / 0 / 451
Goodness-of-fit on F^2	1.057
Final R indices [I>2sigma(I)]	R1 = 0.0461, wR2 = 0.1227
R indices (all data)	R1 = 0.0571, wR2 = 0.1277
Largest diff. peak and hole	1.328 and -1.013 e.$Å^{-3}$

Table 82-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for test. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1A)	3863(1)	4848(1)	2886(1)	20(1)
S(1A)	5097(1)	4517(1)	3137(1)	24(1)
Cl(1)	2799(1)	5799(1)	3838(1)	34(1)
S(2)	4342(1)	6096(1)	2600(1)	25(1)
O(1)	3644(2)	6254(1)	1590(2)	32(1)
O(2)	5212(2)	5893(1)	2342(3)	36(1)
C(1)	3886(2)	5569(1)	3538(3)	22(1)
C(2)	3062(2)	4484(1)	3706(3)	22(1)
C(3)	2470(2)	4091(1)	3094(3)	23(1)
C(4)	1927(2)	3765(1)	3760(3)	25(1)
C(5)	1973(2)	3836(1)	5019(3)	25(1)
C(6)	2560(3)	4227(2)	5638(3)	27(1)
C(7)	3112(2)	4549(1)	4996(3)	26(1)
C(8)	3317(2)	4902(1)	1287(3)	23(1)
C(9)	2411(2)	5093(2)	1007(3)	27(1)

C(10)	2002(3)	5138(2)	-212(3)	29(1)
C(11)	2484(3)	4995(2)	-1162(3)	29(1)
C(12)	3390(3)	4809(2)	-903(3)	28(1)
C(13)	3809(3)	4756(2)	328(3)	27(1)
C(14)	4547(2)	6656(1)	3649(3)	25(1)
C(15)	3942(3)	7102(2)	3574(4)	30(1)
C(16)	4129(3)	7530(2)	4424(4)	38(1)
C(17)	4895(3)	7509(2)	5345(4)	39(1)
C(18)	5499(3)	7065(2)	5398(4)	43(1)
C(19)	5328(3)	6636(2)	4561(4)	35(1)
Cl12	1692(1)	6690(1)	1429(1)	25(1)
S12	-542(1)	6344(1)	-639(1)	25(1)
S22	605(1)	7668(1)	626(1)	18(1)
P12	-339(1)	6552(1)	1103(1)	15(1)
O12	810(2)	7544(1)	-595(2)	21(1)
O22	-261(2)	7927(1)	752(2)	26(1)
C12	647(2)	7038(1)	1537(3)	15(1)
C22	-1335(2)	6842(1)	1667(3)	16(1)
C32	-2177(2)	6583(1)	1252(3)	25(1)
C42	-2964(2)	6735(2)	1737(4)	30(1)
C52	-2922(2)	7147(2)	2616(4)	29(1)
C62	-2091(2)	7414(1)	3026(3)	25(1)
C72	-1294(2)	7260(1)	2564(3)	19(1)
C82	210(2)	6080(1)	3438(3)	21(1)
C92	21(2)	5987(1)	2159(3)	16(1)
C102	121(2)	5454(1)	1704(3)	23(1)
C112	416(2)	5027(1)	2519(4)	28(1)
C122	633(2)	5125(1)	3772(4)	27(1)
C132	526(3)	5654(2)	4239(3)	26(1)
C142	1524(2)	8063(1)	1419(3)	19(1)
C152	1418(3)	8316(1)	2536(4)	32(1)
C162	2151(3)	8616(2)	3161(4)	41(1)
C172	2966(3)	8665(2)	2672(4)	40(1)
C182	3063(3)	8413(2)	1565(4)	33(1)
C192	2342(2)	8101(1)	934(3)	26(1)

Table 82-3. Bond lengths [Å] and angles [°] for test.

P(1A)-C(8)	1.804(4)
P(1A)-C(2)	1.804(3)
P(1A)-C(1)	1.874(3)
P(1A)-S(1A)	1.9541(12)
Cl(1)-C(1)	1.762(3)
S(2)-O(2)	1.430(3)
S(2)-O(1)	1.432(3)
S(2)-C(14)	1.764(4)
S(2)-C(1)	1.818(3)
C(2)-C(3)	1.384(5)
C(2)-C(7)	1.402(5)
C(3)-C(4)	1.397(5)
C(4)-C(5)	1.371(5)
C(5)-C(6)	1.380(5)
C(6)-C(7)	1.384(5)
C(8)-C(9)	1.392(5)
C(8)-C(13)	1.400(5)
C(9)-C(10)	1.372(5)
C(10)-C(11)	1.380(5)
C(11)-C(12)	1.387(5)
C(12)-C(13)	1.390(5)
C(14)-C(15)	1.385(5)
C(14)-C(19)	1.395(5)
C(15)-C(16)	1.385(6)
C(16)-C(17)	1.383(6)
C(17)-C(18)	1.384(6)
C(18)-C(19)	1.375(6)
Cl12-C12	1.763(3)
S12-P12	1.9375(11)
S22-O22	1.437(2)
S22-O12	1.437(2)
S22-C142	1.760(3)
S22-C12	1.810(3)
P12-C22	1.806(3)

P12-C92	1.808(3)
P12-C12	1.861(3)
C22-C32	1.393(5)
C22-C72	1.396(5)
C32-C42	1.387(5)
C42-C52	1.372(5)
C52-C62	1.387(5)
C62-C72	1.390(5)
C82-C132	1.379(5)
C82-C92	1.394(5)
C92-C102	1.390(4)
C102-C112	1.384(5)
C112-C122	1.372(5)
C122-C132	1.389(5)
C142-C192	1.384(5)
C142-C152	1.388(5)
C152-C162	1.382(6)
C162-C172	1.383(6)
C172-C182	1.375(6)
C182-C192	1.386(5)

C(8)-P(1A)-C(2)	106.65(16)
C(8)-P(1A)-C(1)	106.14(16)
C(2)-P(1A)-C(1)	103.83(15)
C(8)-P(1A)-S(1A)	115.24(12)
C(2)-P(1A)-S(1A)	112.87(12)
C(1)-P(1A)-S(1A)	111.26(12)
O(2)-S(2)-O(1)	119.47(17)
O(2)-S(2)-C(14)	108.65(17)
O(1)-S(2)-C(14)	108.78(17)
O(2)-S(2)-C(1)	106.61(16)
O(1)-S(2)-C(1)	109.72(16)
C(14)-S(2)-C(1)	102.23(16)
Cl(1)-C(1)-S(2)	107.70(17)
Cl(1)-C(1)-P(1A)	113.35(18)
S(2)-C(1)-P(1A)	114.93(18)

C(3)-C(2)-C(7)	119.4(3)
C(3)-C(2)-P(1A)	120.1(3)
C(7)-C(2)-P(1A)	120.1(3)
C(2)-C(3)-C(4)	120.0(3)
C(5)-C(4)-C(3)	120.2(3)
C(4)-C(5)-C(6)	120.2(3)
C(5)-C(6)-C(7)	120.4(3)
C(6)-C(7)-C(2)	119.8(3)
C(9)-C(8)-C(13)	120.1(3)
C(9)-C(8)-P(1A)	120.0(3)
C(13)-C(8)-P(1A)	119.9(3)
C(10)-C(9)-C(8)	119.8(3)
C(9)-C(10)-C(11)	120.4(4)
C(10)-C(11)-C(12)	120.7(3)
C(11)-C(12)-C(13)	119.5(3)
C(12)-C(13)-C(8)	119.5(3)
C(15)-C(14)-C(19)	121.1(3)
C(15)-C(14)-S(2)	120.8(3)
C(19)-C(14)-S(2)	118.2(3)
C(14)-C(15)-C(16)	118.6(4)
C(17)-C(16)-C(15)	120.8(4)
C(16)-C(17)-C(18)	119.9(4)
C(19)-C(18)-C(17)	120.3(4)
C(18)-C(19)-C(14)	119.3(4)
O22-S22-O12	119.34(14)
O22-S22-C142	109.75(15)
O12-S22-C142	108.25(15)
O22-S22-C12	105.56(14)
O12-S22-C12	109.67(14)
C142-S22-C12	103.06(15)
C22-P12-C92	104.30(14)
C22-P12-C12	107.78(14)
C92-P12-C12	99.95(14)
C22-P12-S12	114.97(11)
C92-P12-S12	114.31(11)
C12-P12-S12	114.06(11)

Cl12-C12-S22	108.60(16)
Cl12-C12-P12	109.38(16)
S22-C12-P12	115.37(16)
C32-C22-C72	119.4(3)
C32-C22-P12	115.8(2)
C72-C22-P12	124.5(2)
C42-C32-C22	120.2(3)
C52-C42-C32	120.3(3)
C42-C52-C62	120.2(3)
C52-C62-C72	120.2(3)
C62-C72-C22	119.7(3)
C132-C82-C92	120.4(3)
C102-C92-C82	119.3(3)
C102-C92-P12	120.3(3)
C82-C92-P12	120.4(2)
C112-C102-C92	119.8(3)
C122-C112-C102	120.7(3)
C112-C122-C132	120.0(3)
C82-C132-C122	119.8(3)
C192-C142-C152	121.6(3)
C192-C142-S22	119.3(3)
C152-C142-S22	119.1(3)
C162-C152-C142	118.5(4)
C152-C162-C172	120.4(4)
C182-C172-C162	120.6(4)
C172-C182-C192	120.0(4)
C142-C192-C182	118.9(3)

Symmetry transformations used to generate equivalent atoms:

Table 82-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for test. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1A)	20(1)	18(1)	24(1)	0(1)	4(1)	-1(1)
S(1A)	20(1)	22(1)	29(1)	-2(1)	3(1)	3(1)
Cl(1)	33(1)	29(1)	40(1)	0(1)	11(1)	1(1)
S(2)	27(1)	20(1)	30(1)	1(1)	10(1)	-4(1)
O(1)	40(2)	28(1)	28(1)	5(1)	6(1)	-5(1)
O(2)	33(2)	29(1)	50(2)	-4(1)	22(1)	-4(1)
C(1)	22(2)	17(2)	26(2)	1(1)	6(1)	-2(1)
C(2)	21(2)	18(2)	25(2)	4(1)	2(1)	0(1)
C(3)	26(2)	24(2)	20(2)	-3(1)	3(1)	-1(1)
C(4)	25(2)	18(2)	32(2)	-2(2)	1(2)	-4(1)
C(5)	25(2)	18(2)	32(2)	11(2)	5(2)	1(1)
C(6)	36(2)	28(2)	19(2)	4(2)	4(2)	5(2)
C(7)	30(2)	19(2)	27(2)	-1(2)	-7(2)	-5(2)
C(8)	24(2)	19(2)	26(2)	1(1)	5(1)	-3(1)
C(9)	25(2)	33(2)	24(2)	0(2)	6(2)	-2(2)
C(10)	25(2)	30(2)	30(2)	0(2)	2(2)	-5(2)
C(11)	37(2)	26(2)	23(2)	-2(2)	1(2)	-5(2)
C(12)	39(2)	24(2)	26(2)	-3(2)	12(2)	-2(2)
C(13)	26(2)	26(2)	30(2)	2(2)	9(2)	-3(2)
C(14)	27(2)	21(2)	30(2)	2(2)	10(2)	-5(1)
C(15)	30(2)	23(2)	37(2)	6(2)	3(2)	1(2)
C(16)	39(2)	21(2)	54(3)	-1(2)	11(2)	2(2)
C(17)	35(2)	27(2)	55(3)	-14(2)	7(2)	-6(2)
C(18)	37(2)	36(2)	52(3)	-11(2)	-3(2)	-5(2)
C(19)	30(2)	27(2)	50(3)	-3(2)	5(2)	1(2)
Cl12	23(1)	20(1)	32(1)	4(1)	4(1)	3(1)
S12	33(1)	28(1)	14(1)	-5(1)	2(1)	-6(1)
S22	21(1)	15(1)	19(1)	5(1)	6(1)	2(1)
P12	19(1)	14(1)	14(1)	-1(1)	2(1)	-2(1)
O12	28(1)	21(1)	16(1)	5(1)	5(1)	0(1)
O22	23(1)	22(1)	34(1)	12(1)	11(1)	8(1)

C12	18(2)	13(2)	15(2)	2(1)	3(1)	0(1)
C22	18(2)	13(2)	18(2)	5(1)	2(1)	2(1)
C32	23(2)	19(2)	32(2)	1(2)	0(2)	-3(1)
C42	20(2)	26(2)	44(2)	6(2)	2(2)	-4(2)
C52	22(2)	29(2)	37(2)	14(2)	11(2)	8(2)
C62	30(2)	22(2)	24(2)	6(2)	9(2)	7(2)
C72	19(2)	17(2)	20(2)	5(1)	3(1)	0(1)
C82	30(2)	12(2)	21(2)	-1(1)	4(1)	-2(1)
C92	17(2)	12(2)	20(2)	1(1)	5(1)	0(1)
C102	24(2)	17(2)	30(2)	-5(1)	8(2)	-3(1)
C112	28(2)	13(2)	44(2)	-3(2)	12(2)	2(1)
C122	26(2)	20(2)	37(2)	10(2)	8(2)	2(1)
C132	33(2)	24(2)	22(2)	8(2)	5(2)	0(2)
C142	29(2)	9(1)	21(2)	4(1)	7(1)	-2(1)
C152	52(2)	15(2)	35(2)	-3(2)	24(2)	-9(2)
C162	69(3)	26(2)	32(2)	-12(2)	18(2)	-21(2)
C172	54(3)	28(2)	38(2)	-2(2)	4(2)	-22(2)
C182	35(2)	29(2)	36(2)	2(2)	10(2)	-10(2)
C192	31(2)	20(2)	27(2)	0(2)	11(2)	-1(2)

Table 82-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for test.

	x	y	z	U(eq)
H(1)	4305	5559	4357	26
H(3)	2433	4042	2221	28
H(4)	1524	3493	3340	30
H(5)	1599	3614	5467	30
H(6)	2586	4276	6510	33
H(7)	3523	4814	5428	32
H(9)	2077	5192	1657	33
H(10)	1384	5267	-404	34
H(11)	2192	5025	-2002	35

H(12)	3722	4718	-1561	34
H(13)	4425	4621	518	32
H(15)	3410	7113	2952	36
H(16)	3728	7842	4375	45
H(17)	5006	7800	5939	47
H(18)	6033	7056	6015	51
H(19)	5738	6328	4603	43
H12	657	7146	2427	18
H32	-2213	6302	634	30
H42	-3535	6553	1459	36
H52	-3463	7249	2945	35
H62	-2067	7702	3626	30
H72	-723	7439	2856	23
H82	119	6439	3760	25
H102	-14	5384	835	28
H112	469	4662	2207	33
H122	856	4831	4321	33
H132	670	5722	5108	32
H152	855	8284	2863	38
H162	2095	8789	3930	50
H172	3463	8875	3105	48
H182	3623	8452	1233	39
H192	2410	7917	180	31

Röntgenstrukturanalytische Daten für 83

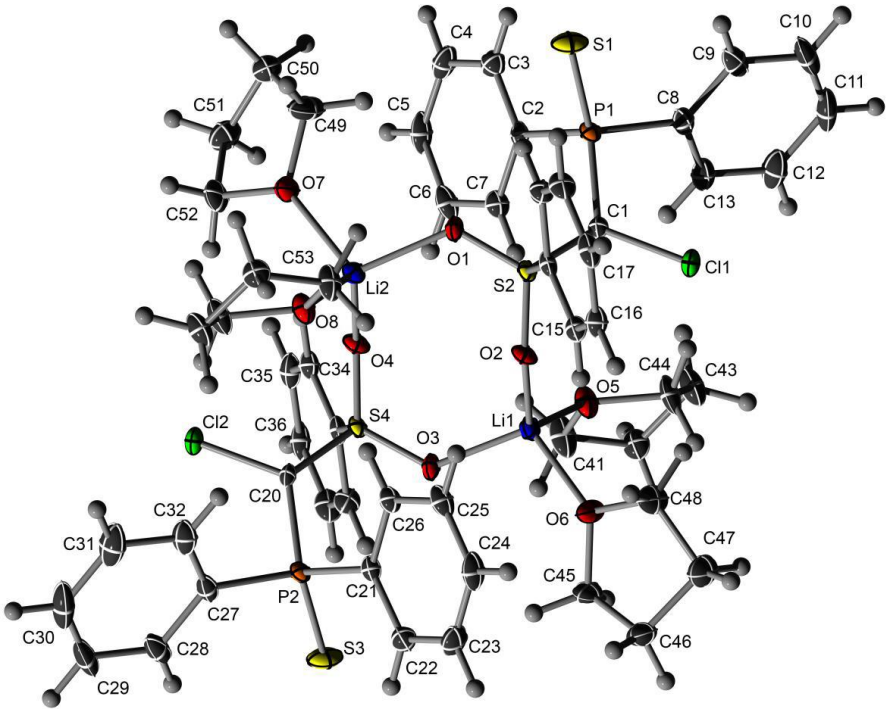

Table 83-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	C54 H62 Cl2 Li2 O8 P2 S4	
Formula weight	1114.00	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.7495(7) Å	α = 84.130(2)°.
	b = 14.3410(10) Å	β = 75.385(2)°.
	c = 18.4656(13) Å	γ = 84.843(2)°.
Volume	2734.0(3) $Å^3$	
Z	2	
Density (calculated)	1.353 Mg/m^3	
Absorption coefficient	0.382 mm^{-1}	
F(000)	1168	
Crystal size	0.18 x 0.18 x 0.06 mm^3	
Theta range for data collection	1.14 to 25.00°.	
Index ranges	-12<=h<=12, -17<=k<=16, -21<=l<=21	

Reflections collected	28561
Independent reflections	9559 [R(int) = 0.0337]
Completeness to theta = 25.00°	99.2 %
Max. and min. transmission	0.9774 and 0.9343
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9559 / 0 / 649
Goodness-of-fit on F^2	1.033
Final R indices [I>2sigma(I)]	R1 = 0.0477, wR2 = 0.1270
R indices (all data)	R1 = 0.0625, wR2 = 0.1412
Largest diff. peak and hole	1.246 and -0.391 e.$Å^{-3}$

Table 83-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1A)	-3809(1)	1449(1)	2217(1)	17(1)
Cl(2A)	3681(1)	3639(1)	2733(1)	17(1)
S(1A)	-2513(1)	-874(1)	3599(1)	24(1)
S(2A)	-2003(1)	1847(1)	3001(1)	11(1)
S(3A)	2404(1)	6042(1)	1449(1)	23(1)
S(4A)	1866(1)	3314(1)	1930(1)	11(1)
P(1A)	-1975(1)	-145(1)	2624(1)	13(1)
P(2A)	1844(1)	5263(1)	2398(1)	12(1)
O(1)	-962(2)	1410(1)	3318(1)	14(1)
O(2)	-1750(2)	2742(1)	2566(1)	16(1)
O(3)	829(2)	3778(1)	1619(1)	14(1)
O(4)	1608(2)	2397(1)	2326(1)	15(1)
O(5)	-409(2)	2500(1)	755(1)	18(1)
O(6)	-1905(2)	4281(1)	1321(1)	24(1)
O(7)	1849(2)	788(1)	3466(1)	26(1)
O(8)	408(2)	2497(1)	4184(1)	19(1)
C(2)	-233(2)	-305(2)	2253(1)	12(1)
C(1A)	-2397(2)	1061(2)	2506(1)	12(1)
C(3)	389(2)	-1158(2)	2416(2)	19(1)

C(4)	1700(3)	-1332(2)	2110(2)	25(1)
C(5)	2392(3)	-633(2)	1650(2)	25(1)
C(6)	1790(2)	223(2)	1492(2)	20(1)
C(7)	471(2)	392(2)	1784(1)	16(1)
C(8)	-2622(2)	-577(2)	1910(2)	19(1)
C(9)	-3530(3)	-1254(2)	2099(2)	27(1)
C(10)	-4042(3)	-1538(2)	1538(2)	40(1)
C(11)	-3659(3)	-1159(2)	807(2)	43(1)
C(12)	-2751(3)	-484(2)	619(2)	36(1)
C(13)	-2231(3)	-208(2)	1168(2)	23(1)
C(14)	-3345(2)	2124(2)	3758(1)	13(1)
C(15)	-4061(2)	2964(2)	3731(1)	16(1)
C(16)	-5141(2)	3141(2)	4313(2)	21(1)
C(17)	-5487(2)	2469(2)	4905(2)	21(1)
C(18)	-4777(2)	1626(2)	4923(2)	22(1)
C(19)	-3691(2)	1440(2)	4346(1)	18(1)
C(21)	106(2)	5423(2)	2770(1)	13(1)
C(20A)	2255(2)	4048(2)	2468(1)	12(1)
C(22)	-494(2)	6307(2)	2663(2)	19(1)
C(23)	-1793(3)	6485(2)	2989(2)	24(1)
C(24)	-2506(3)	5767(2)	3414(2)	25(1)
C(25)	-1927(2)	4887(2)	3515(2)	21(1)
C(26)	-609(2)	4710(2)	3201(1)	15(1)
C(27)	2473(2)	5640(2)	3142(2)	17(1)
C(28)	3375(2)	6320(2)	2985(2)	24(1)
C(29)	3860(3)	6576(2)	3568(2)	34(1)
C(30)	3455(3)	6159(2)	4290(2)	37(1)
C(31)	2554(3)	5487(2)	4441(2)	31(1)
C(32)	2060(3)	5236(2)	3870(2)	22(1)
C(33)	3222(2)	3080(2)	1173(1)	13(1)
C(34)	3939(2)	2235(2)	1185(1)	14(1)
C(35)	5043(2)	2081(2)	611(1)	18(1)
C(36)	5402(2)	2775(2)	37(1)	18(1)
C(37)	4689(2)	3622(2)	34(1)	19(1)
C(38)	3589(2)	3789(2)	604(1)	16(1)
C(41)	751(3)	2573(2)	155(2)	23(1)

C(42)	373(3)	2444(2)	-566(2)	21(1)
C(43)	-808(3)	1875(2)	-283(2)	24(1)
C(44)	-1458(3)	2323(2)	439(2)	24(1)
C(45)	-1563(3)	5221(2)	1099(2)	34(1)
C(46)	-2765(3)	5860(2)	1351(2)	24(1)
C(47)	-3790(3)	5186(2)	1755(2)	31(1)
C(48)	-3279(3)	4284(2)	1425(2)	27(1)
C(49)	1510(3)	-72(2)	3908(2)	25(1)
C(50)	2748(3)	-685(2)	3813(2)	28(1)
C(52)	3236(3)	804(2)	3223(2)	31(1)
C(51A)	3740(3)	50(2)	3706(2)	33(1)
C(53)	-695(3)	2317(2)	4796(2)	29(1)
C(54)	-316(3)	2452(2)	5516(2)	22(1)
C(55)	831(3)	3049(2)	5238(2)	27(1)
C(56)	1467(3)	2655(2)	4491(2)	27(1)
Li(1)	-794(4)	3276(3)	1613(2)	16(1)
Li(2)	713(4)	1823(3)	3277(2)	15(1)

Table 83-3. Bond lengths [Å] and angles [°] for sad.

Cl(1A)-C(1A)	1.759(2)
Cl(2A)-C(20A)	1.758(2)
S(1A)-P(1A)	1.9684(9)
S(2A)-O(2)	1.4517(18)
S(2A)-O(1)	1.4560(18)
S(2A)-C(1A)	1.665(2)
S(2A)-C(14)	1.785(2)
S(3A)-P(2A)	1.9669(9)
S(4A)-O(4)	1.4529(18)
S(4A)-O(3)	1.4582(17)
S(4A)-C(20A)	1.665(2)
S(4A)-C(33)	1.781(2)
P(1A)-C(1A)	1.754(3)
P(1A)-C(8)	1.820(3)
P(1A)-C(2)	1.826(2)

P(2A)-C(20A)	1.759(3)
P(2A)-C(27)	1.822(3)
P(2A)-C(21)	1.823(2)
O(1)-Li(2)	1.926(4)
O(2)-Li(1)	1.922(5)
O(3)-Li(1)	1.949(4)
O(4)-Li(2)	1.917(4)
O(5)-C(44)	1.445(3)
O(5)-C(41)	1.447(3)
O(5)-Li(1)	1.967(5)
O(6)-C(45)	1.422(3)
O(6)-C(48)	1.440(3)
O(6)-Li(1)	1.911(5)
O(7)-C(49)	1.430(3)
O(7)-C(52)	1.446(3)
O(7)-Li(2)	1.897(5)
O(8)-C(56)	1.438(3)
O(8)-C(53)	1.438(3)
O(8)-Li(2)	1.962(5)
C(2)-C(3)	1.384(4)
C(2)-C(7)	1.396(3)
C(3)-C(4)	1.389(4)
C(4)-C(5)	1.386(4)
C(5)-C(6)	1.374(4)
C(6)-C(7)	1.393(4)
C(8)-C(13)	1.391(4)
C(8)-C(9)	1.395(4)
C(9)-C(10)	1.398(4)
C(10)-C(11)	1.376(5)
C(11)-C(12)	1.393(5)
C(12)-C(13)	1.382(4)
C(14)-C(15)	1.373(4)
C(14)-C(19)	1.388(4)
C(15)-C(16)	1.393(4)
C(16)-C(17)	1.381(4)
C(17)-C(18)	1.373(4)

C(18)-C(19)	1.394(4)
C(21)-C(22)	1.388(4)
C(21)-C(26)	1.392(4)
C(22)-C(23)	1.386(4)
C(23)-C(24)	1.392(4)
C(24)-C(25)	1.372(4)
C(25)-C(26)	1.399(4)
C(27)-C(32)	1.389(4)
C(27)-C(28)	1.395(4)
C(28)-C(29)	1.402(4)
C(29)-C(30)	1.383(5)
C(30)-C(31)	1.387(5)
C(31)-C(32)	1.384(4)
C(33)-C(34)	1.378(4)
C(33)-C(38)	1.392(4)
C(34)-C(35)	1.395(4)
C(35)-C(36)	1.381(4)
C(36)-C(37)	1.377(4)
C(37)-C(38)	1.391(4)
C(41)-C(42)	1.520(4)
C(42)-C(43)	1.522(4)
C(43)-C(44)	1.518(4)
C(45)-C(46)	1.516(4)
C(46)-C(47)	1.527(4)
C(47)-C(48)	1.488(4)
C(49)-C(50)	1.509(4)
C(50)-C(51A)	1.529(4)
C(52)-C(51A)	1.484(4)
C(53)-C(54)	1.521(4)
C(54)-C(55)	1.516(4)
C(55)-C(56)	1.517(4)

O(2)-S(2A)-O(1)	115.69(10)
O(2)-S(2A)-C(1A)	112.08(11)
O(1)-S(2A)-C(1A)	107.33(11)
O(2)-S(2A)-C(14)	103.86(11)

O(1)-S(2A)-C(14)	108.10(11)
C(1A)-S(2A)-C(14)	109.59(11)
O(4)-S(4A)-O(3)	115.41(10)
O(4)-S(4A)-C(20A)	111.71(11)
O(3)-S(4A)-C(20A)	108.01(11)
O(4)-S(4A)-C(33)	103.87(11)
O(3)-S(4A)-C(33)	108.42(11)
C(20A)-S(4A)-C(33)	109.20(11)
C(1A)-P(1A)-C(8)	100.57(12)
C(1A)-P(1A)-C(2)	107.03(11)
C(8)-P(1A)-C(2)	103.51(11)
C(1A)-P(1A)-S(1A)	121.78(9)
C(8)-P(1A)-S(1A)	111.64(9)
C(2)-P(1A)-S(1A)	110.50(9)
C(20A)-P(2A)-C(27)	101.08(12)
C(20A)-P(2A)-C(21)	107.05(11)
C(27)-P(2A)-C(21)	102.72(11)
C(20A)-P(2A)-S(3A)	121.46(9)
C(27)-P(2A)-S(3A)	111.73(9)
C(21)-P(2A)-S(3A)	110.88(9)
S(2A)-O(1)-Li(2)	131.03(17)
S(2A)-O(2)-Li(1)	141.68(17)
S(4A)-O(3)-Li(1)	127.70(17)
S(4A)-O(4)-Li(2)	141.22(17)
C(44)-O(5)-C(41)	108.80(19)
C(44)-O(5)-Li(1)	118.11(19)
C(41)-O(5)-Li(1)	122.42(19)
C(45)-O(6)-C(48)	107.0(2)
C(45)-O(6)-Li(1)	125.2(2)
C(48)-O(6)-Li(1)	126.7(2)
C(49)-O(7)-C(52)	109.7(2)
C(49)-O(7)-Li(2)	127.1(2)
C(52)-O(7)-Li(2)	123.0(2)
C(56)-O(8)-C(53)	108.4(2)
C(56)-O(8)-Li(2)	120.2(2)
C(53)-O(8)-Li(2)	119.97(19)

C(3)-C(2)-C(7)	119.5(2)
C(3)-C(2)-P(1A)	118.68(19)
C(7)-C(2)-P(1A)	121.79(19)
S(2A)-C(1A)-P(1A)	122.91(14)
S(2A)-C(1A)-Cl(1A)	111.07(14)
P(1A)-C(1A)-Cl(1A)	120.04(13)
C(2)-C(3)-C(4)	120.7(2)
C(5)-C(4)-C(3)	119.3(3)
C(6)-C(5)-C(4)	120.5(2)
C(5)-C(6)-C(7)	120.3(3)
C(6)-C(7)-C(2)	119.6(2)
C(13)-C(8)-C(9)	119.5(3)
C(13)-C(8)-P(1A)	119.4(2)
C(9)-C(8)-P(1A)	121.1(2)
C(8)-C(9)-C(10)	119.1(3)
C(11)-C(10)-C(9)	120.8(3)
C(10)-C(11)-C(12)	120.1(3)
C(13)-C(12)-C(11)	119.4(3)
C(12)-C(13)-C(8)	121.0(3)
C(15)-C(14)-C(19)	121.3(2)
C(15)-C(14)-S(2A)	120.77(19)
C(19)-C(14)-S(2A)	117.80(19)
C(14)-C(15)-C(16)	119.5(2)
C(17)-C(16)-C(15)	119.8(3)
C(18)-C(17)-C(16)	120.5(2)
C(17)-C(18)-C(19)	120.4(3)
C(14)-C(19)-C(18)	118.6(2)
C(22)-C(21)-C(26)	119.5(2)
C(22)-C(21)-P(2A)	118.34(19)
C(26)-C(21)-P(2A)	121.94(19)
S(4A)-C(20A)-Cl(2A)	111.34(13)
S(4A)-C(20A)-P(2A)	122.73(15)
Cl(2A)-C(20A)-P(2A)	119.15(13)
C(23)-C(22)-C(21)	120.5(2)
C(22)-C(23)-C(24)	119.7(3)
C(25)-C(24)-C(23)	120.3(2)

C(24)-C(25)-C(26)	120.2(3)
C(21)-C(26)-C(25)	119.8(2)
C(32)-C(27)-C(28)	119.8(3)
C(32)-C(27)-P(2A)	119.5(2)
C(28)-C(27)-P(2A)	120.7(2)
C(27)-C(28)-C(29)	119.1(3)
C(30)-C(29)-C(28)	120.7(3)
C(29)-C(30)-C(31)	119.8(3)
C(32)-C(31)-C(30)	120.0(3)
C(31)-C(32)-C(27)	120.7(3)
C(34)-C(33)-C(38)	121.2(2)
C(34)-C(33)-S(4A)	119.98(19)
C(38)-C(33)-S(4A)	118.64(19)
C(33)-C(34)-C(35)	119.4(2)
C(36)-C(35)-C(34)	119.7(2)
C(37)-C(36)-C(35)	120.5(2)
C(36)-C(37)-C(38)	120.6(2)
C(37)-C(38)-C(33)	118.6(2)
O(5)-C(41)-C(42)	106.5(2)
C(41)-C(42)-C(43)	102.4(2)
C(44)-C(43)-C(42)	101.0(2)
O(5)-C(44)-C(43)	104.5(2)
O(6)-C(45)-C(46)	107.4(2)
C(45)-C(46)-C(47)	104.0(2)
C(48)-C(47)-C(46)	102.9(2)
O(6)-C(48)-C(47)	104.4(2)
O(7)-C(49)-C(50)	105.4(2)
C(49)-C(50)-C(51A)	101.4(2)
O(7)-C(52)-C(51A)	105.2(2)
C(52)-C(51A)-C(50)	101.7(2)
O(8)-C(53)-C(54)	107.2(2)
C(55)-C(54)-C(53)	102.6(2)
C(54)-C(55)-C(56)	101.3(2)
O(8)-C(56)-C(55)	104.3(2)
O(6)-Li(1)-O(2)	105.2(2)
O(6)-Li(1)-O(3)	108.5(2)

O(2)-Li(1)-O(3)	115.5(2)
O(6)-Li(1)-O(5)	102.6(2)
O(2)-Li(1)-O(5)	117.9(2)
O(3)-Li(1)-O(5)	106.1(2)
O(7)-Li(2)-O(4)	103.7(2)
O(7)-Li(2)-O(1)	110.6(2)
O(4)-Li(2)-O(1)	115.9(2)
O(7)-Li(2)-O(8)	102.9(2)
O(4)-Li(2)-O(8)	120.0(2)
O(1)-Li(2)-O(8)	103.1(2)

Symmetry transformations used to generate equivalent atoms:

Table 83-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1A)	12(1)	22(1)	18(1)	-3(1)	-6(1)	0(1)
Cl(2A)	13(1)	22(1)	17(1)	-3(1)	-6(1)	0(1)
S(1A)	23(1)	20(1)	21(1)	8(1)	4(1)	-2(1)
S(2A)	9(1)	14(1)	9(1)	-1(1)	0(1)	-3(1)
S(3A)	26(1)	18(1)	18(1)	6(1)	5(1)	-3(1)
S(4A)	8(1)	14(1)	10(1)	-1(1)	-1(1)	-3(1)
P(1A)	10(1)	13(1)	14(1)	0(1)	-1(1)	-3(1)
P(2A)	10(1)	13(1)	12(1)	0(1)	-1(1)	-2(1)
O(1)	9(1)	22(1)	12(1)	-2(1)	-3(1)	-3(1)
O(2)	15(1)	16(1)	17(1)	0(1)	1(1)	-5(1)
O(3)	10(1)	19(1)	15(1)	-1(1)	-4(1)	-2(1)
O(4)	13(1)	15(1)	14(1)	0(1)	2(1)	-5(1)
O(5)	14(1)	25(1)	13(1)	-3(1)	0(1)	-4(1)
O(6)	13(1)	17(1)	43(1)	3(1)	-8(1)	-1(1)
O(7)	11(1)	20(1)	42(1)	11(1)	-3(1)	-2(1)
O(8)	14(1)	31(1)	11(1)	-1(1)	0(1)	-9(1)
C(2)	10(1)	16(1)	11(1)	-3(1)	-3(1)	-1(1)

C(1A)	7(1)	19(1)	12(1)	-2(1)	-5(1)	-1(1)
C(3)	18(1)	21(2)	19(1)	-3(1)	-6(1)	-1(1)
C(4)	22(2)	24(2)	31(2)	-6(1)	-11(1)	7(1)
C(5)	9(1)	38(2)	27(2)	-12(1)	-2(1)	2(1)
C(6)	13(1)	28(2)	18(1)	-5(1)	0(1)	-6(1)
C(7)	14(1)	19(1)	14(1)	-1(1)	-3(1)	-3(1)
C(8)	13(1)	16(1)	30(2)	-8(1)	-7(1)	1(1)
C(9)	14(1)	18(2)	50(2)	-8(1)	-8(1)	-1(1)
C(10)	19(2)	27(2)	81(3)	-24(2)	-20(2)	1(1)
C(11)	32(2)	49(2)	61(3)	-36(2)	-30(2)	14(2)
C(12)	33(2)	46(2)	34(2)	-23(2)	-16(2)	10(2)
C(13)	21(1)	26(2)	25(2)	-9(1)	-8(1)	1(1)
C(14)	10(1)	20(1)	11(1)	-4(1)	-5(1)	-4(1)
C(15)	14(1)	22(1)	14(1)	-4(1)	-4(1)	-3(1)
C(16)	15(1)	29(2)	22(2)	-11(1)	-8(1)	5(1)
C(17)	11(1)	39(2)	16(1)	-11(1)	-2(1)	-2(1)
C(18)	17(1)	34(2)	14(1)	1(1)	-1(1)	-9(1)
C(19)	14(1)	23(2)	16(1)	1(1)	-2(1)	-3(1)
C(21)	11(1)	17(1)	9(1)	-3(1)	-2(1)	-2(1)
C(20A)	10(1)	15(1)	12(1)	-2(1)	-3(1)	0(1)
C(22)	18(1)	20(1)	19(1)	-5(1)	-6(1)	0(1)
C(23)	24(2)	24(2)	28(2)	-8(1)	-12(1)	9(1)
C(24)	11(1)	42(2)	23(2)	-15(1)	-4(1)	4(1)
C(25)	13(1)	35(2)	16(1)	-9(1)	1(1)	-9(1)
C(26)	13(1)	19(1)	14(1)	-4(1)	-3(1)	-2(1)
C(27)	12(1)	16(1)	25(2)	-9(1)	-5(1)	2(1)
C(28)	13(1)	19(2)	40(2)	-12(1)	-2(1)	-1(1)
C(29)	16(1)	30(2)	64(2)	-26(2)	-14(2)	2(1)
C(30)	28(2)	48(2)	46(2)	-28(2)	-22(2)	7(2)
C(31)	31(2)	39(2)	27(2)	-14(1)	-14(1)	7(1)
C(32)	19(1)	26(2)	21(2)	-7(1)	-6(1)	-1(1)
C(33)	9(1)	21(1)	10(1)	-3(1)	-3(1)	-5(1)
C(34)	14(1)	20(1)	10(1)	-2(1)	-2(1)	-5(1)
C(35)	15(1)	22(2)	16(1)	-4(1)	-5(1)	-1(1)
C(36)	13(1)	33(2)	9(1)	-7(1)	0(1)	-8(1)
C(37)	18(1)	27(2)	12(1)	2(1)	-2(1)	-9(1)

C(38)	15(1)	19(1)	14(1)	-1(1)	-2(1)	-3(1)
C(41)	16(1)	38(2)	13(1)	-4(1)	0(1)	-6(1)
C(42)	21(1)	24(2)	16(1)	-1(1)	-3(1)	-4(1)
C(43)	23(2)	27(2)	24(2)	-9(1)	-5(1)	-7(1)
C(44)	18(1)	33(2)	24(2)	-10(1)	-4(1)	-10(1)
C(45)	24(2)	21(2)	52(2)	11(2)	-5(2)	-3(1)
C(46)	28(2)	19(2)	28(2)	2(1)	-12(1)	-1(1)
C(47)	24(2)	31(2)	36(2)	-3(1)	-6(1)	5(1)
C(48)	13(1)	27(2)	43(2)	-4(1)	-8(1)	-3(1)
C(49)	21(1)	21(2)	31(2)	10(1)	-7(1)	-7(1)
C(50)	27(2)	22(2)	35(2)	9(1)	-9(1)	-3(1)
C(52)	10(1)	29(2)	49(2)	6(2)	-2(1)	-3(1)
C(51A)	21(2)	34(2)	41(2)	7(2)	-6(1)	-3(1)
C(53)	16(1)	52(2)	19(2)	-10(1)	2(1)	-12(1)
C(54)	22(1)	31(2)	13(1)	-2(1)	-3(1)	-6(1)
C(55)	21(2)	40(2)	23(2)	-11(1)	-3(1)	-8(1)
C(56)	16(1)	44(2)	23(2)	-11(1)	-2(1)	-14(1)
Li(1)	15(2)	18(2)	15(2)	-2(2)	-3(2)	-2(2)
Li(2)	11(2)	19(2)	13(2)	2(2)	-1(2)	-1(2)

Table 83-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
H(3)	-85	-1630	2741	23
H(4)	2117	-1924	2215	30
H(5)	3289	-747	1441	30
H(6)	2276	700	1183	24
H(7)	53	979	1665	19
H(9)	-3798	-1519	2602	32
H(10)	-4661	-1999	1662	48
H(11)	-4015	-1357	432	51
H(12)	-2491	-216	116	43

H(13)	-1596	242	1038	28
H(15)	-3822	3420	3319	19
H(16)	-5638	3723	4302	25
H(17)	-6223	2591	5302	25
H(18)	-5026	1167	5332	27
H(19)	-3198	856	4356	22
H(22)	-10	6793	2364	22
H(23)	-2195	7094	2923	29
H(24)	-3398	5886	3636	30
H(25)	-2421	4397	3799	25
H(26)	-204	4105	3282	18
H(28)	3658	6606	2489	29
H(29)	4473	7039	3467	41
H(30)	3793	6334	4681	45
H(31)	2276	5198	4935	37
H(32)	1431	4783	3978	26
H(34)	3684	1761	1581	17
H(35)	5545	1502	614	21
H(36)	6146	2667	-358	22
H(37)	4951	4096	-360	23
H(38)	3099	4374	605	20
H(41A)	1417	2081	243	27
H(41B)	1099	3196	126	27
H(42A)	1070	2096	-915	25
H(42B)	159	3056	-822	25
H(43A)	-1364	1947	-642	29
H(43B)	-565	1200	-186	29
H(44A)	-1952	2917	334	29
H(44B)	-2050	1893	786	29
H(45A)	-1233	5308	547	41
H(45B)	-882	5368	1336	41
H(46A)	-3011	6219	916	29
H(46B)	-2634	6306	1696	29
H(47A)	-3878	5130	2304	37
H(47B)	-4638	5395	1653	37
H(48A)	-3629	3743	1770	32

H(48B)	-3501	4257	939	32
H(49A)	864	-373	3727	30
H(49B)	1149	43	4442	30
H(50A)	2902	-1049	3368	34
H(50B)	2750	-1121	4264	34
H(52A)	3518	1422	3289	37
H(52B)	3544	679	2687	37
H(51A)	3762	275	4192	39
H(51B)	4613	-200	3454	39
H(53A)	-946	1668	4804	35
H(53B)	-1434	2759	4740	35
H(54A)	-1026	2781	5872	26
H(54B)	-73	1842	5765	26
H(55A)	1410	2965	5584	33
H(55B)	556	3723	5171	33
H(56A)	2038	3110	4157	32
H(56B)	1981	2060	4565	32

Röntgenstrukturanalytische Daten für 85

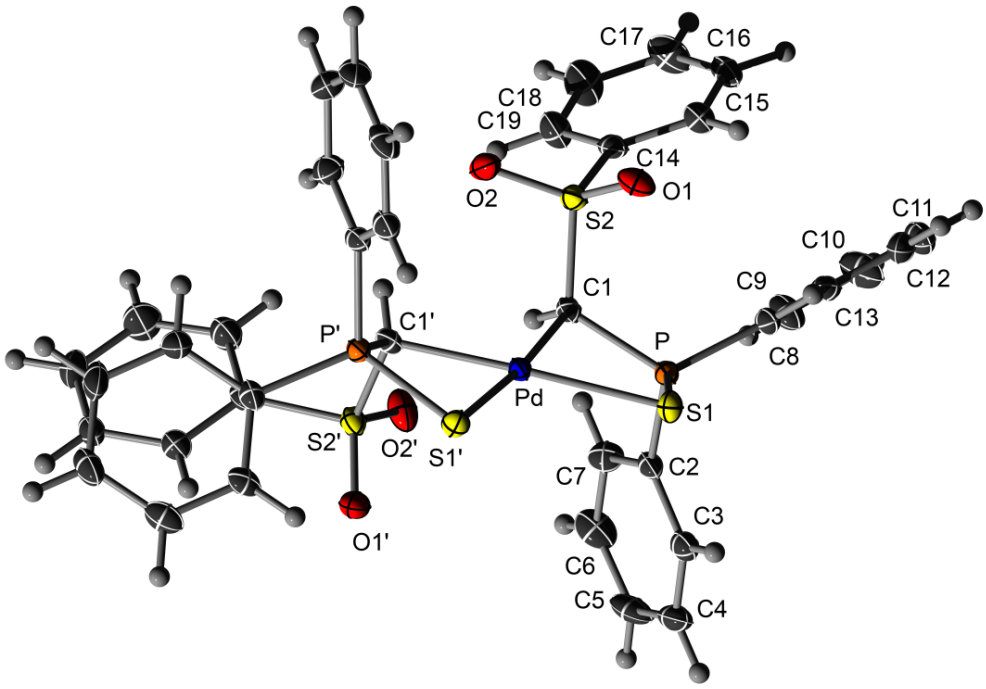

Table 85-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	C98 H80 P4 Pd2 S2 Si2	
Formula weight	1714.60	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 25.8179(13) Å	α = 90°.
	b = 11.4035(6) Å	β = 93.8160(10)°.
	c = 27.4898(14) Å	γ = 90°.
Volume	8075.4(7) $Å^3$	
Z	4	
Density (calculated)	1.410 Mg/m^3	
Absorption coefficient	0.655 mm^{-1}	
F(000)	3520	
Crystal size	0.32 x 0.22 x 0.12 mm^3	

Theta range for data collection	1.05 to 25.00°.
Index ranges	-30<=h<=30, -13<=k<=13, -32<=l<=32
Reflections collected	96001
Independent reflections	14233 [R(int) = 0.0393]
Completeness to theta = 25.00°	99.9 %
Absorption correction	Empirical
Max. and min. transmission	0.5624 and 0.5126
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14233 / 13 / 998
Goodness-of-fit on F^2	1.092
Final R indices [I>2sigma(I)]	R1 = 0.0280, wR2 = 0.0676
R indices (all data)	R1 = 0.0359, wR2 = 0.0715
Largest diff. peak and hole	1.147 and -0.515 e.$Å^{-3}$

Table 85-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd11	6502(1)	484(1)	9056(1)	13(1)
S11	6788(1)	-489(1)	9823(1)	18(1)
P11	6400(1)	894(1)	10073(1)	12(1)
P21	6861(1)	-855(1)	8549(1)	16(1)
Si11	6473(1)	3033(1)	9288(1)	12(1)
C11	6198(1)	1700(2)	9555(1)	12(1)
C21	5844(1)	460(2)	10402(1)	14(1)
C31	5387(1)	1104(2)	10371(1)	23(1)
C41	4974(1)	775(3)	10642(1)	28(1)
C51	5018(1)	-185(2)	10945(1)	25(1)
C61	5468(1)	-831(2)	10976(1)	25(1)
C71	5881(1)	-519(2)	10706(1)	21(1)
C81	6809(1)	1716(2)	10512(1)	16(1)
C91	6638(1)	2798(2)	10681(1)	22(1)
C101	6966(1)	3462(3)	10990(1)	30(1)
C111	7464(1)	3068(3)	11124(1)	32(1)

C121	7630(1)	1997(3)	10965(1)	30(1)
C131	7304(1)	1314(2)	10659(1)	23(1)
C141	6227(1)	4457(2)	9537(1)	15(1)
C151	5696(1)	4655(2)	9547(1)	21(1)
C161	5501(1)	5717(2)	9705(1)	27(1)
C171	5836(1)	6599(2)	9865(1)	28(1)
C181	6363(1)	6421(2)	9867(1)	29(1)
C191	6555(1)	5367(2)	9701(1)	24(1)
C201	7202(1)	3100(2)	9308(1)	14(1)
C211	7441(1)	3038(2)	8871(1)	23(1)
C221	7975(1)	3139(3)	8853(1)	30(1)
C231	8284(1)	3282(2)	9278(1)	24(1)
C241	8059(1)	3333(2)	9718(1)	21(1)
C251	7524(1)	3267(2)	9732(1)	18(1)
C261	6212(1)	2777(2)	8646(1)	15(1)
C271	6190(1)	1566(2)	8529(1)	17(1)
C281	5953(1)	1248(3)	8077(1)	28(1)
C291	5767(1)	2089(3)	7744(1)	30(1)
C301	5811(1)	3267(2)	7853(1)	23(1)
C311	6029(1)	3614(2)	8306(1)	18(1)
C321	6368(1)	-1877(2)	8297(1)	16(1)
C331	6306(1)	-2194(2)	7811(1)	26(1)
C341	5909(1)	-2942(2)	7652(1)	29(1)
C351	5567(1)	-3364(2)	7966(1)	26(1)
C361	5622(1)	-3050(3)	8453(1)	29(1)
C371	6020(1)	-2311(2)	8619(1)	26(1)
C381	7351(1)	-1781(2)	8873(1)	18(1)
C391	7802(1)	-1239(3)	9059(1)	34(1)
C401	8210(1)	-1891(3)	9268(1)	38(1)
C411	8167(1)	-3087(3)	9313(1)	30(1)
C421	7720(1)	-3633(3)	9137(1)	38(1)
C431	7311(1)	-2983(2)	8917(1)	31(1)
C441	7223(1)	-429(2)	8026(1)	23(1)
C45B1	7644(5)	-954(11)	7867(6)	27(3)
C451	7520(5)	-1321(9)	7816(5)	37(3)
C461	7850(1)	-894(3)	7443(1)	43(1)

C471	7875(3)	145(6)	7314(2)	38(1)
C481	7602(3)	980(6)	7546(3)	58(2)
C491	7287(2)	689(5)	7919(2)	39(1)
C47B1	7647(4)	60(9)	7111(3)	38(1)
C48B1	7198(3)	612(6)	7209(3)	38(2)
C49B1	6974(3)	396(6)	7642(3)	39(1)
Pd12	4481(1)	2196(1)	6667(1)	10(1)
S22	3760(1)	3401(1)	6908(1)	14(1)
P12	3803(1)	2232(1)	7460(1)	11(1)
P22	4680(1)	3326(1)	6014(1)	12(1)
Si12	4248(1)	-240(1)	7032(1)	12(1)
C12	4283(1)	1239(2)	7306(1)	12(1)
C22	3178(1)	1617(2)	7569(1)	15(1)
C32	2728(1)	2111(2)	7359(1)	23(1)
C42	2247(1)	1681(3)	7469(1)	32(1)
C52	2219(1)	762(3)	7791(1)	36(1)
C62	2664(1)	259(3)	8006(1)	32(1)
C72	3148(1)	683(2)	7895(1)	25(1)
C82	4007(1)	2955(2)	8031(1)	14(1)
C92	3672(1)	3091(2)	8403(1)	22(1)
C102	3845(1)	3644(2)	8836(1)	26(1)
C112	4346(1)	4043(2)	8901(1)	23(1)
C122	4681(1)	3922(2)	8528(1)	23(1)
C132	4509(1)	3383(2)	8096(1)	17(1)
C142	4219(1)	-1475(2)	7483(1)	13(1)
C152	4151(1)	-2632(2)	7322(1)	18(1)
C162	4125(1)	-3554(2)	7647(1)	25(1)
C172	4153(1)	-3323(3)	8143(1)	30(1)
C182	4225(1)	-2199(3)	8310(1)	28(1)
C192	4267(1)	-1287(2)	7984(1)	20(1)
C202	3693(1)	-502(2)	6561(1)	15(1)
C212	3769(1)	-438(2)	6063(1)	20(1)
C222	3373(1)	-701(2)	5714(1)	27(1)
C232	2893(1)	-1031(2)	5852(1)	30(1)
C242	2811(1)	-1116(3)	6343(1)	32(1)
C252	3206(1)	-854(2)	6693(1)	23(1)

C262	4885(1)	-206(2)	6748(1)	13(1)
C272	5236(1)	-1135(2)	6741(1)	18(1)
C282	5724(1)	-969(2)	6568(1)	21(1)
C292	5853(1)	117(2)	6386(1)	17(1)
C302	5504(1)	1034(2)	6377(1)	14(1)
C312	5016(1)	912(2)	6569(1)	12(1)
C322	4824(1)	2555(2)	5457(1)	13(1)
C332	4487(1)	1657(2)	5298(1)	17(1)
C342	4554(1)	1065(2)	4869(1)	21(1)
C352	4966(1)	1341(2)	4594(1)	22(1)
C362	5313(1)	2207(2)	4751(1)	23(1)
C372	5244(1)	2817(2)	5180(1)	18(1)
C382	5233(1)	4295(2)	6148(1)	14(1)
C392	5571(1)	4072(2)	6550(1)	18(1)
C402	6010(1)	4767(2)	6642(1)	25(1)
C412	6106(1)	5688(2)	6338(1)	27(1)
C422	5765(1)	5938(2)	5943(1)	26(1)
C432	5331(1)	5249(2)	5846(1)	23(1)
C442	4166(1)	4355(2)	5809(1)	14(1)
C452	4062(1)	5313(2)	6102(1)	17(1)
C462	3660(1)	6082(2)	5973(1)	22(1)
C472	3354(1)	5902(2)	5547(1)	26(1)
C482	3450(1)	4952(3)	5256(1)	30(1)
C492	3853(1)	4180(2)	5382(1)	23(1)

Table 85-3. Bond lengths [Å] and angles [°] for sad.

Pd11-C271	2.027(2)
Pd11-C11	2.137(2)
Pd11-P21	2.3031(6)
Pd11-S11	2.4544(6)
Pd11-P11	2.8646(6)
Pd11-Si11	2.9786(7)
S11-P11	2.0142(9)
P11-C11	1.746(2)
P11-C81	1.811(2)

P11-C21	1.818(2)
P21-C321	1.827(2)
P21-C441	1.831(3)
P21-C381	1.834(3)
Si11-C11	1.850(2)
Si11-C261	1.869(2)
Si11-C201	1.881(2)
Si11-C141	1.888(2)
C21-C31	1.387(4)
C21-C71	1.392(3)
C31-C41	1.391(4)
C41-C51	1.376(4)
C51-C61	1.374(4)
C61-C71	1.386(4)
C81-C131	1.393(4)
C81-C91	1.400(4)
C91-C101	1.384(4)
C101-C111	1.388(4)
C111-C121	1.375(4)
C121-C131	1.388(4)
C141-C151	1.392(4)
C141-C191	1.393(4)
C151-C161	1.393(4)
C161-C171	1.379(4)
C171-C181	1.376(4)
C181-C191	1.388(4)
C201-C211	1.388(3)
C201-C251	1.401(3)
C211-C221	1.386(4)
C221-C231	1.381(4)
C231-C241	1.378(4)
C241-C251	1.385(3)
C261-C311	1.396(3)
C261-C271	1.418(4)
C271-C281	1.397(3)
C281-C291	1.389(4)

C291-C301	1.380(4)
C301-C311	1.388(3)
C321-C331	1.384(4)
C321-C371	1.393(4)
C331-C341	1.382(4)
C341-C351	1.364(4)
C351-C361	1.382(4)
C361-C371	1.383(4)
C381-C431	1.381(4)
C381-C391	1.385(4)
C391-C401	1.383(4)
C401-C411	1.375(4)
C411-C421	1.371(4)
C421-C431	1.393(4)
C441-C491	1.322(6)
C441-C45B1	1.341(17)
C441-C451	1.419(13)
C441-C49B1	1.524(9)
C45B1-C461	1.316(17)
C451-C461	1.462(12)
C461-C471	1.239(8)
C461-C47B1	1.492(10)
C471-C481	1.367(9)
C481-C491	1.390(8)
C47B1-C48B1	1.361(12)
C48B1-C49B1	1.380(10)
Pd12-C312	2.043(2)
Pd12-C12	2.157(2)
Pd12-P22	2.2950(6)
Pd12-S22	2.4385(6)
Pd12-P12	2.8838(6)
Pd12-Si12	3.0268(7)
S22-P12	2.0170(8)
P12-C12	1.750(2)
P12-C22	1.804(2)
P12-C82	1.820(2)

P22-C382	1.823(2)
P22-C322	1.827(2)
P22-C442	1.832(2)
Si12-C12	1.848(2)
Si12-C262	1.867(2)
Si12-C142	1.881(2)
Si12-C202	1.891(2)
C22-C32	1.382(4)
C22-C72	1.397(3)
C32-C42	1.386(4)
C42-C52	1.377(4)
C52-C62	1.382(4)
C62-C72	1.392(4)
C82-C132	1.386(3)
C82-C92	1.392(3)
C92-C102	1.394(4)
C102-C112	1.371(4)
C112-C122	1.391(4)
C122-C132	1.384(3)
C142-C192	1.391(3)
C142-C152	1.398(3)
C152-C162	1.385(4)
C162-C172	1.385(4)
C172-C182	1.371(4)
C182-C192	1.383(4)
C202-C252	1.391(3)
C202-C212	1.397(3)
C212-C222	1.388(4)
C222-C232	1.374(4)
C232-C242	1.383(4)
C242-C252	1.385(4)
C262-C272	1.396(3)
C262-C312	1.415(3)
C272-C282	1.388(3)
C282-C292	1.384(4)
C292-C302	1.381(3)

C302-C312	1.404(3)
C322-C332	1.395(3)
C322-C372	1.396(3)
C332-C342	1.380(3)
C342-C352	1.382(4)
C352-C362	1.382(4)
C362-C372	1.391(4)
C382-C392	1.385(3)
C382-C432	1.401(3)
C392-C402	1.392(4)
C402-C412	1.376(4)
C412-C422	1.382(4)
C422-C432	1.379(4)
C442-C492	1.394(3)
C442-C452	1.394(3)
C452-C462	1.387(3)
C462-C472	1.384(4)
C472-C482	1.379(4)
C482-C492	1.389(4)

C271-Pd11-C11	85.28(9)
C271-Pd11-P21	97.37(7)
C11-Pd11-P21	177.07(7)
C271-Pd11-S11	166.31(7)
C11-Pd11-S11	81.03(6)
P21-Pd11-S11	96.32(2)
C271-Pd11-P11	122.65(7)
C11-Pd11-P11	37.41(6)
P21-Pd11-P11	139.97(2)
S11-Pd11-P11	43.660(19)
C271-Pd11-Si11	62.88(7)
C11-Pd11-Si11	38.12(6)
P21-Pd11-Si11	142.54(2)
S11-Pd11-Si11	105.53(2)
P11-Pd11-Si11	68.045(17)
P11-S11-Pd11	79.07(3)

C11-P11-C81	113.63(11)
C11-P11-C21	110.25(11)
C81-P11-C21	104.71(11)
C11-P11-S11	105.26(8)
C81-P11-S11	110.58(9)
C21-P11-S11	112.59(8)
C11-P11-Pd11	48.04(8)
C81-P11-Pd11	130.39(8)
C21-P11-Pd11	124.66(8)
S11-P11-Pd11	57.27(2)
C321-P21-C441	104.51(12)
C321-P21-C381	104.92(11)
C441-P21-C381	99.36(12)
C321-P21-Pd11	110.74(8)
C441-P21-Pd11	123.09(9)
C381-P21-Pd11	112.34(8)
C11-Si11-C261	97.04(11)
C11-Si11-C201	115.53(11)
C261-Si11-C201	109.28(11)
C11-Si11-C141	114.60(11)
C261-Si11-C141	111.64(11)
C201-Si11-C141	108.30(11)
C11-Si11-Pd11	45.48(7)
C261-Si11-Pd11	69.99(8)
C201-Si11-Pd11	90.31(7)
C141-Si11-Pd11	158.63(8)
P11-C11-Si11	130.87(13)
P11-C11-Pd11	94.55(10)
Si11-C11-Pd11	96.40(10)
C31-C21-C71	119.2(2)
C31-C21-P11	121.41(19)
C71-C21-P11	119.40(19)
C21-C31-C41	120.1(2)
C51-C41-C31	120.2(3)
C61-C51-C41	120.0(2)
C51-C61-C71	120.4(2)

C61-C71-C21	120.1(2)
C131-C81-C91	119.8(2)
C131-C81-P11	120.4(2)
C91-C81-P11	119.7(2)
C101-C91-C81	119.5(3)
C91-C101-C111	120.2(3)
C121-C111-C101	120.4(3)
C111-C121-C131	120.2(3)
C121-C131-C81	119.9(3)
C151-C141-C191	116.8(2)
C151-C141-Si11	120.03(19)
C191-C141-Si11	123.15(19)
C141-C151-C161	121.5(3)
C171-C161-C151	120.2(3)
C181-C171-C161	119.5(3)
C171-C181-C191	120.0(3)
C181-C191-C141	122.0(3)
C211-C201-C251	116.9(2)
C211-C201-Si11	118.41(18)
C251-C201-Si11	124.57(18)
C221-C211-C201	121.8(2)
C231-C221-C211	120.1(3)
C241-C231-C221	119.5(2)
C231-C241-C251	120.2(2)
C241-C251-C201	121.5(2)
C311-C261-C271	120.5(2)
C311-C261-Si11	127.62(19)
C271-C261-Si11	111.86(17)
C281-C271-C261	117.6(2)
C281-C271-Pd11	127.3(2)
C261-C271-Pd11	115.05(17)
C291-C281-C271	121.2(3)
C301-C291-C281	120.7(2)
C291-C301-C311	119.6(2)
C301-C311-C261	120.3(2)
C331-C321-C371	118.8(2)

C331-C321-P21	124.5(2)
C371-C321-P21	116.66(19)
C341-C331-C321	120.2(3)
C351-C341-C331	121.0(3)
C341-C351-C361	119.5(3)
C351-C361-C371	120.2(3)
C361-C371-C321	120.3(2)
C431-C381-C391	118.4(3)
C431-C381-P21	124.1(2)
C391-C381-P21	117.3(2)
C401-C391-C381	120.8(3)
C411-C401-C391	120.4(3)
C421-C411-C401	119.3(3)
C411-C421-C431	120.5(3)
C381-C431-C421	120.5(3)
C491-C441-C45B1	103.9(6)
C491-C441-C451	121.4(5)
C45B1-C441-C451	22.3(6)
C491-C441-C49B1	45.9(4)
C45B1-C441-C49B1	111.3(7)
C451-C441-C49B1	112.0(6)
C491-C441-P21	120.6(3)
C45B1-C441-P21	127.2(6)
C451-C441-P21	116.5(5)
C49B1-C441-P21	119.6(3)
C461-C45B1-C441	130.6(10)
C441-C451-C461	113.8(7)
C471-C461-C45B1	109.5(7)
C471-C461-C451	124.2(6)
C45B1-C461-C451	21.6(6)
C471-C461-C47B1	32.0(4)
C45B1-C461-C47B1	115.6(7)
C451-C461-C47B1	118.3(7)
C461-C471-C481	119.7(6)
C471-C481-C491	121.5(7)
C441-C491-C481	118.9(5)

C48B1-C47B1-C461	119.1(7)
C47B1-C48B1-C49B1	120.0(7)
C48B1-C49B1-C441	121.7(6)
C312-Pd12-C12	86.79(9)
C312-Pd12-P22	96.37(7)
C12-Pd12-P22	176.20(6)
C312-Pd12-S22	166.92(7)
C12-Pd12-S22	80.66(6)
P22-Pd12-S22	96.32(2)
C312-Pd12-P12	124.01(6)
C12-Pd12-P12	37.22(6)
P22-Pd12-P12	139.57(2)
S22-Pd12-P12	43.545(18)
C312-Pd12-Si12	62.40(7)
C12-Pd12-Si12	37.21(6)
P22-Pd12-Si12	146.50(2)
S22-Pd12-Si12	104.820(19)
P12-Pd12-Si12	67.641(17)
P12-S22-Pd12	80.06(3)
C12-P12-C22	116.32(11)
C12-P12-C82	109.43(11)
C22-P12-C82	104.08(11)
C12-P12-S22	104.46(8)
C22-P12-S22	112.22(9)
C82-P12-S22	110.39(8)
C12-P12-Pd12	48.23(7)
C22-P12-Pd12	135.65(8)
C82-P12-Pd12	120.20(8)
S22-P12-Pd12	56.40(2)
C382-P22-C322	105.07(11)
C382-P22-C442	102.39(11)
C322-P22-C442	103.47(11)
C382-P22-Pd12	113.34(8)
C322-P22-Pd12	117.04(8)
C442-P22-Pd12	113.95(8)
C12-Si12-C262	97.55(11)

C12-Si12-C142	114.67(10)
C262-Si12-C142	111.47(10)
C12-Si12-C202	115.91(10)
C262-Si12-C202	111.52(10)
C142-Si12-C202	105.77(10)
C12-Si12-Pd12	44.92(7)
C262-Si12-Pd12	69.06(7)
C142-Si12-Pd12	157.32(8)
C202-Si12-Pd12	94.38(7)
P12-C12-Si12	132.37(14)
P12-C12-Pd12	94.55(10)
Si12-C12-Pd12	97.87(10)
C32-C22-C72	119.8(2)
C32-C22-P12	120.53(19)
C72-C22-P12	119.53(19)
C22-C32-C42	120.3(3)
C52-C42-C32	119.8(3)
C42-C52-C62	120.8(3)
C52-C62-C72	119.7(3)
C62-C72-C22	119.7(3)
C132-C82-C92	119.3(2)
C132-C82-P12	119.03(18)
C92-C82-P12	121.71(19)
C82-C92-C102	119.8(2)
C112-C102-C92	120.5(2)
C102-C112-C122	119.9(2)
C132-C122-C112	119.8(3)
C122-C132-C82	120.7(2)
C192-C142-C152	117.3(2)
C192-C142-Si12	122.16(18)
C152-C142-Si12	120.51(18)
C162-C152-C142	121.6(2)
C152-C162-C172	119.3(2)
C182-C172-C162	120.3(2)
C172-C182-C192	120.1(3)
C182-C192-C142	121.4(2)

C252-C202-C212	117.4(2)
C252-C202-Si12	121.68(19)
C212-C202-Si12	120.77(19)
C222-C212-C202	121.4(2)
C232-C222-C212	120.3(3)
C222-C232-C242	119.3(3)
C232-C242-C252	120.6(3)
C242-C252-C202	121.2(3)
C272-C262-C312	120.6(2)
C272-C262-Si12	125.48(18)
C312-C262-Si12	113.66(17)
C282-C272-C262	120.4(2)
C292-C282-C272	119.5(2)
C302-C292-C282	120.7(2)
C292-C302-C312	121.3(2)
C302-C312-C262	117.4(2)
C302-C312-Pd12	127.57(18)
C262-C312-Pd12	114.88(16)
C332-C322-C372	118.5(2)
C332-C322-P22	117.24(18)
C372-C322-P22	124.27(19)
C342-C332-C322	121.0(2)
C332-C342-C352	120.1(2)
C342-C352-C362	119.8(2)
C352-C362-C372	120.4(2)
C362-C372-C322	120.2(2)
C392-C382-C432	119.0(2)
C392-C382-P22	119.51(18)
C432-C382-P22	121.45(19)
C382-C392-C402	120.2(2)
C412-C402-C392	120.1(2)
C402-C412-C422	120.2(3)
C432-C422-C412	120.1(2)
C422-C432-C382	120.3(2)
C492-C442-C452	118.4(2)
C492-C442-P22	122.40(19)

C452-C442-P22	119.12(18)
C462-C452-C442	121.2(2)
C472-C462-C452	119.8(2)
C482-C472-C462	119.6(2)
C472-C482-C492	120.9(2)
C482-C492-C442	120.2(2)

Symmetry transformations used to generate equivalent atoms:

Table 85-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd11	14(1)	13(1)	11(1)	-3(1)	3(1)	-2(1)
S11	23(1)	17(1)	16(1)	-1(1)	2(1)	6(1)
P11	14(1)	11(1)	11(1)	0(1)	2(1)	-2(1)
P21	15(1)	16(1)	16(1)	-5(1)	4(1)	-1(1)
Si11	13(1)	11(1)	11(1)	0(1)	1(1)	0(1)
C11	12(1)	12(1)	12(1)	-2(1)	1(1)	-2(1)
C21	15(1)	15(1)	12(1)	-2(1)	2(1)	-4(1)
C31	25(2)	28(2)	17(1)	7(1)	4(1)	4(1)
C41	18(1)	44(2)	24(2)	5(1)	4(1)	5(1)
C51	22(2)	39(2)	14(1)	-2(1)	4(1)	-14(1)
C61	35(2)	19(1)	21(1)	6(1)	4(1)	-9(1)
C71	24(2)	19(1)	19(1)	2(1)	3(1)	-2(1)
C81	21(1)	20(1)	8(1)	1(1)	3(1)	-8(1)
C91	24(2)	25(2)	19(1)	-4(1)	7(1)	-4(1)
C101	39(2)	28(2)	24(2)	-9(1)	8(1)	-13(1)
C111	42(2)	35(2)	18(2)	1(1)	-8(1)	-21(1)
C121	29(2)	35(2)	24(2)	10(1)	-12(1)	-10(1)
C131	23(2)	24(2)	22(1)	5(1)	-5(1)	-3(1)
C141	22(1)	14(1)	9(1)	1(1)	2(1)	2(1)
C151	23(1)	20(1)	18(1)	-2(1)	1(1)	4(1)
C161	28(2)	31(2)	21(2)	-2(1)	5(1)	13(1)
C171	50(2)	19(2)	17(1)	-1(1)	6(1)	13(1)

C181	45(2)	16(1)	26(2)	-5(1)	2(1)	-1(1)
C191	28(2)	19(1)	25(2)	-1(1)	2(1)	1(1)
C201	15(1)	9(1)	19(1)	3(1)	1(1)	-2(1)
C211	18(1)	31(2)	20(1)	-3(1)	2(1)	-1(1)
C221	21(2)	43(2)	28(2)	-5(1)	10(1)	0(1)
C231	13(1)	21(1)	40(2)	0(1)	4(1)	1(1)
C241	17(1)	18(1)	26(1)	5(1)	-5(1)	-2(1)
C251	18(1)	19(1)	18(1)	3(1)	2(1)	-3(1)
C261	11(1)	20(1)	13(1)	0(1)	3(1)	0(1)
C271	18(1)	21(1)	12(1)	1(1)	4(1)	-2(1)
C281	43(2)	25(2)	16(1)	-2(1)	-2(1)	-11(1)
C291	38(2)	41(2)	11(1)	-1(1)	-5(1)	-8(1)
C301	24(2)	33(2)	12(1)	7(1)	0(1)	2(1)
C311	17(1)	20(1)	17(1)	2(1)	4(1)	3(1)
C321	18(1)	14(1)	17(1)	-1(1)	2(1)	0(1)
C331	30(2)	28(2)	20(1)	-4(1)	5(1)	-4(1)
C341	34(2)	32(2)	20(2)	-5(1)	-5(1)	-1(1)
C351	21(2)	25(2)	32(2)	0(1)	-10(1)	-5(1)
C361	25(2)	32(2)	30(2)	-1(1)	5(1)	-9(1)
C371	26(2)	34(2)	19(1)	-6(1)	6(1)	-7(1)
C381	18(1)	22(1)	15(1)	-5(1)	5(1)	0(1)
C391	30(2)	28(2)	42(2)	2(1)	-7(1)	-5(1)
C401	26(2)	47(2)	39(2)	-2(2)	-12(1)	-3(1)
C411	26(2)	38(2)	26(2)	-2(1)	3(1)	14(1)
C421	32(2)	25(2)	58(2)	2(1)	11(2)	8(1)
C431	21(2)	25(2)	45(2)	-5(1)	4(1)	1(1)
C441	24(2)	21(1)	25(2)	-5(1)	10(1)	-4(1)
C45B1	23(6)	31(8)	26(5)	13(6)	5(4)	9(5)
C451	48(7)	23(5)	43(5)	0(4)	28(4)	-3(4)
C461	33(2)	72(3)	25(2)	-5(2)	11(1)	13(2)
C471	36(4)	47(3)	33(4)	9(3)	21(2)	1(3)
C481	59(2)	56(2)	59(2)	2(1)	9(1)	0(1)
C491	44(3)	24(2)	52(3)	3(2)	31(2)	1(2)
C47B1	36(4)	47(3)	33(4)	9(3)	21(2)	1(3)
C48B1	50(5)	32(4)	36(4)	20(3)	20(4)	4(3)
C49B1	44(3)	24(2)	52(3)	3(2)	31(2)	1(2)

Pd12	11(1)	9(1)	9(1)	2(1)	3(1)	1(1)
S22	15(1)	13(1)	13(1)	3(1)	4(1)	4(1)
P12	13(1)	11(1)	10(1)	1(1)	3(1)	1(1)
P22	13(1)	11(1)	10(1)	2(1)	2(1)	0(1)
Si12	13(1)	10(1)	12(1)	1(1)	3(1)	1(1)
C12	13(1)	12(1)	12(1)	2(1)	2(1)	2(1)
C22	17(1)	15(1)	15(1)	-3(1)	7(1)	-3(1)
C32	20(1)	25(2)	24(2)	0(1)	3(1)	-3(1)
C42	17(2)	41(2)	36(2)	1(1)	2(1)	-4(1)
C52	25(2)	38(2)	47(2)	0(2)	14(1)	-12(1)
C62	38(2)	24(2)	35(2)	6(1)	16(1)	-9(1)
C72	25(2)	21(2)	30(2)	6(1)	10(1)	1(1)
C82	21(1)	12(1)	10(1)	2(1)	1(1)	4(1)
C92	20(1)	29(2)	17(1)	-3(1)	2(1)	5(1)
C102	31(2)	31(2)	17(1)	-2(1)	7(1)	8(1)
C112	37(2)	21(1)	12(1)	-1(1)	-4(1)	5(1)
C122	28(2)	19(1)	21(1)	1(1)	0(1)	-1(1)
C132	23(1)	14(1)	14(1)	-1(1)	6(1)	-2(1)
C142	11(1)	12(1)	16(1)	2(1)	3(1)	1(1)
C152	17(1)	16(1)	21(1)	0(1)	0(1)	3(1)
C162	20(1)	11(1)	44(2)	5(1)	0(1)	-1(1)
C172	22(2)	28(2)	40(2)	23(1)	4(1)	4(1)
C182	31(2)	35(2)	19(1)	10(1)	3(1)	7(1)
C192	24(1)	18(1)	19(1)	2(1)	1(1)	3(1)
C202	17(1)	10(1)	18(1)	1(1)	1(1)	2(1)
C212	24(1)	17(1)	20(1)	1(1)	2(1)	0(1)
C222	39(2)	22(2)	18(1)	0(1)	-6(1)	4(1)
C232	29(2)	23(2)	36(2)	-3(1)	-15(1)	4(1)
C242	17(2)	34(2)	45(2)	1(1)	-2(1)	-3(1)
C252	20(1)	24(2)	25(2)	2(1)	2(1)	1(1)
C262	15(1)	14(1)	11(1)	-2(1)	2(1)	2(1)
C272	21(1)	15(1)	18(1)	1(1)	5(1)	2(1)
C282	18(1)	20(1)	23(1)	0(1)	7(1)	7(1)
C292	13(1)	22(1)	19(1)	0(1)	7(1)	1(1)
C302	19(1)	14(1)	10(1)	0(1)	2(1)	-1(1)
C312	15(1)	14(1)	7(1)	-1(1)	-1(1)	0(1)

C322	17(1)	14(1)	9(1)	3(1)	1(1)	5(1)
C332	17(1)	15(1)	20(1)	4(1)	1(1)	1(1)
C342	25(2)	17(1)	20(1)	-1(1)	-3(1)	6(1)
C352	32(2)	24(2)	11(1)	-1(1)	2(1)	12(1)
C362	23(2)	32(2)	15(1)	7(1)	9(1)	8(1)
C372	19(1)	20(1)	15(1)	6(1)	0(1)	2(1)
C382	16(1)	12(1)	16(1)	-1(1)	4(1)	0(1)
C392	22(1)	15(1)	15(1)	0(1)	1(1)	0(1)
C402	25(2)	26(2)	22(1)	-5(1)	-5(1)	-1(1)
C412	26(2)	22(2)	34(2)	-5(1)	4(1)	-9(1)
C422	31(2)	20(2)	29(2)	7(1)	4(1)	-8(1)
C432	26(2)	20(1)	21(1)	5(1)	1(1)	-2(1)
C442	15(1)	16(1)	13(1)	7(1)	2(1)	-1(1)
C452	21(1)	16(1)	14(1)	5(1)	1(1)	0(1)
C462	25(2)	15(1)	26(2)	3(1)	4(1)	3(1)
C472	21(2)	23(2)	34(2)	7(1)	-3(1)	7(1)
C482	28(2)	31(2)	29(2)	1(1)	-13(1)	7(1)
C492	23(2)	22(1)	22(1)	-2(1)	-4(1)	5(1)

Table 85-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
H11	5810	1717	9513	14
H31	5356	1772	10164	28
H41	4661	1215	10617	34
H51	4737	-400	11133	30
H61	5496	-1497	11184	30
H71	6190	-973	10727	25
H91	6300	3074	10585	27
H101	6850	4190	11111	36
H111	7691	3541	11327	38
H121	7968	1724	11065	36

H131	7419	574	10550	28
H151	5461	4051	9442	25
H161	5137	5835	9704	32
H171	5704	7325	9974	34
H181	6597	7019	9982	35
H191	6920	5263	9698	29
H211	7234	2923	8576	28
H221	8127	3110	8548	36
H231	8650	3344	9268	29
H241	8270	3415	10012	25
H251	7373	3336	10036	22
H281	5917	440	7996	34
H291	5609	1850	7438	36
H301	5692	3838	7620	28
H311	6054	4424	8384	22
H331	6536	-1896	7585	31
H341	5874	-3166	7318	35
H351	5293	-3869	7852	31
H361	5385	-3342	8674	35
H371	6057	-2099	8953	31
H391	7832	-410	9042	40
H401	8522	-1510	9382	45
H411	8444	-3532	9465	36
H421	7689	-4460	9164	46
H431	7003	-3370	8797	37
H45B1	7823	-1451	8099	32
H451	7505	-2121	7910	45
H46A1	8060	-1449	7288	51
H46B1	8112	-1424	7353	51
H471	8082	360	7056	46
H481	7628	1777	7450	69
H491	7122	1285	8094	46
H47B1	7828	279	6835	46
H48B1	7039	1145	6979	46
H49B1	6656	772	7702	46
H12	4580	1273	7558	15

H32	2748	2747	7138	27
H42	1939	2020	7323	38
H52	1889	470	7866	43
H62	2640	-372	8229	38
H72	3456	338	8039	30
H92	3326	2807	8362	26
H102	3615	3746	9088	31
H112	4464	4401	9200	28
H122	5027	4207	8570	27
H132	4738	3306	7841	21
H152	4122	-2789	6982	22
H162	4089	-4337	7532	30
H172	4122	-3947	8368	36
H182	4245	-2046	8650	34
H192	4330	-515	8104	24
H212	4099	-210	5962	24
H222	3435	-652	5377	32
H232	2620	-1200	5614	36
H242	2482	-1355	6442	38
H252	3142	-917	7028	28
H272	5142	-1885	6857	21
H282	5966	-1596	6573	25
H292	6187	233	6268	21
H302	5595	1762	6238	17
H332	4207	1449	5489	21
H342	4317	466	4763	25
H352	5010	938	4297	27
H362	5600	2385	4565	28
H372	5482	3414	5285	22
H392	5503	3442	6763	21
H402	6243	4605	6916	29
H412	6408	6155	6400	33
H422	5829	6584	5737	32
H432	5098	5422	5574	27
H452	4271	5440	6395	21
H462	3595	6731	6177	26

H472	3080	6430	5456	32
H482	3237	4822	4966	36
H492	3916	3533	5177	27

Röntgenstrukturanalytische Daten für 90

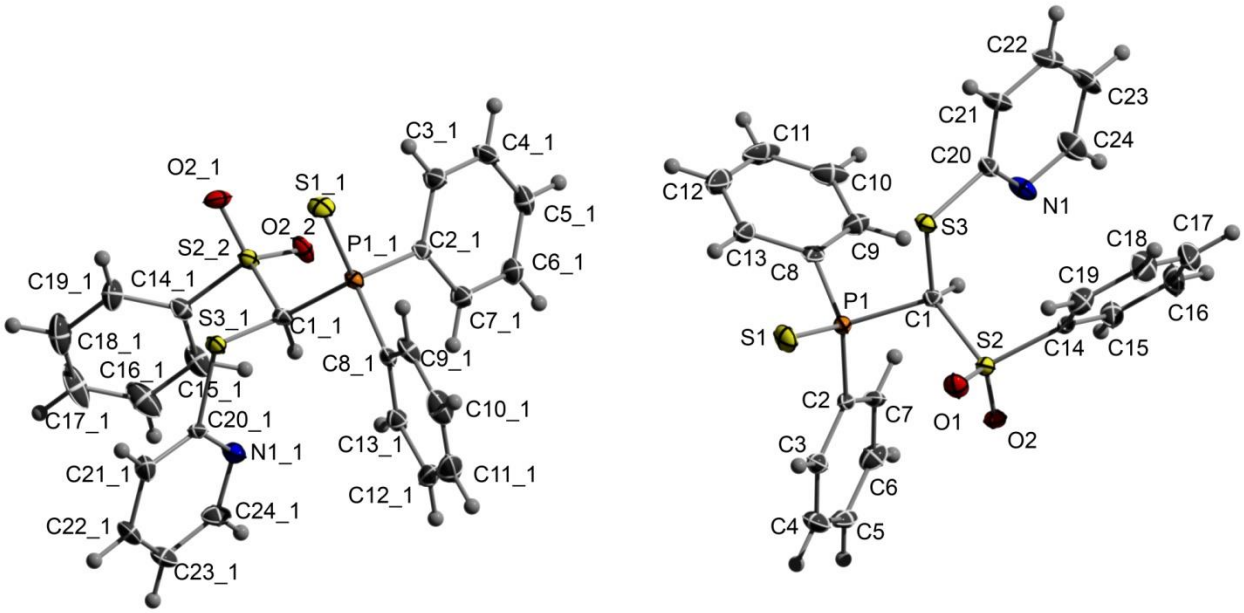

Table 90-1. Crystal data and structure refinement for sad.

Identification code	sad	
Empirical formula	$C_{24}H_{20}NO_2PS_3$	
Formula weight	481.56	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbc2(1)	
Unit cell dimensions	a = 10.0319(14) Å	α = 90°.
	b = 11.8863(16) Å	β = 90°.
	c = 38.635(5) Å	γ = 90°.
Volume	4606.9(11) $Å^3$	
Z	8	
Density (calculated)	1.389 Mg/m^3	
Absorption coefficient	0.413 mm^{-1}	
F(000)	2000	
Crystal size	0.16 x 0.12 x 0.08 mm^3	
Theta range for data collection	2.03 to 25.00°.	
Index ranges	-11<=h<=11, -14<=k<=14, -45<=l<=45	
Reflections collected	50624	
Independent reflections	8100 [R(int) = 0.0601]	

Completeness to theta = 25.00°	99.9 %
Absorption correction	Empirical
Max. and min. transmission	0.9681 and 0.9376
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8100 / 1 / 568
Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0328, wR2 = 0.0681
R indices (all data)	R1 = 0.0400, wR2 = 0.0721
Absolute structure parameter	0.47(5)
Largest diff. peak and hole	0.289 and -0.284 e.$Å^{-3}$

Table 90-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for sad. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	7182(1)	4124(1)	8038(1)	24(1)
S(2)	6346(1)	6176(1)	8792(1)	15(1)
S(3)	4234(1)	4729(1)	8477(1)	15(1)
P(1)	6314(1)	5580(1)	8014(1)	13(1)
O(1)	7092(2)	5191(2)	8882(1)	22(1)
O(2)	7048(2)	7214(2)	8725(1)	22(1)
N(1)	2696(3)	6561(2)	8557(1)	22(1)
C(1)	5338(3)	5905(2)	8409(1)	13(1)
C(2)	7458(3)	6735(2)	7935(1)	14(1)
C(3)	8822(3)	6514(2)	7946(1)	19(1)
C(4)	9725(4)	7364(3)	7871(1)	27(1)
C(5)	9283(4)	8426(3)	7788(1)	24(1)
C(6)	7923(4)	8649(3)	7779(1)	25(1)
C(7)	7022(3)	7807(2)	7854(1)	18(1)
C(8)	5052(3)	5686(2)	7676(1)	17(1)
C(9)	4093(4)	6528(3)	7674(1)	23(1)
C(10)	3227(4)	6628(3)	7397(1)	32(1)
C(11)	3303(4)	5889(3)	7124(1)	39(1)
C(12)	4232(4)	5038(4)	7126(1)	41(1)

C(13)	5116(4)	4926(3)	7402(1)	26(1)
C(14)	5144(3)	6418(3)	9120(1)	18(1)
C(15)	4504(4)	7441(3)	9134(1)	25(1)
C(16)	3540(4)	7603(3)	9387(1)	35(1)
C(17)	3236(4)	6750(3)	9616(1)	38(1)
C(18)	3883(4)	5738(3)	9598(1)	36(1)
C(19)	4850(4)	5559(3)	9346(1)	26(1)
C(20)	2706(3)	5448(2)	8563(1)	17(1)
C(21)	1593(3)	4788(3)	8628(1)	22(1)
C(22)	413(3)	5334(3)	8710(1)	27(1)
C(23)	391(4)	6491(3)	8720(1)	29(1)
C(24)	1545(4)	7071(3)	8642(1)	29(1)
S11	7834(1)	-572(1)	6134(1)	21(1)
S21	8620(1)	1456(1)	5369(1)	16(1)
S31	10759(1)	25(1)	5675(1)	16(1)
P11	8708(1)	883(1)	6149(1)	13(1)
O11	7935(2)	2497(2)	5432(1)	21(1)
O21	7858(2)	468(2)	5286(1)	25(1)
N11	12272(3)	1867(2)	5590(1)	22(1)
C11	9640(3)	1186(3)	5745(1)	13(1)
C21	7559(3)	2033(2)	6221(1)	14(1)
C31	6195(3)	1828(2)	6196(1)	22(1)
C41	5298(3)	2689(3)	6249(1)	25(1)
C51	5733(4)	3755(3)	6326(1)	24(1)
C61	7100(3)	3966(3)	6356(1)	24(1)
C71	8007(3)	3112(2)	6304(1)	20(1)
C81	10003(3)	998(2)	6477(1)	14(1)
C91	9983(3)	247(3)	6753(1)	22(1)
C101	10899(4)	362(3)	7021(1)	31(1)
C111	11820(4)	1214(3)	7016(1)	32(1)
C121	11858(3)	1960(3)	6742(1)	24(1)
C131	10954(3)	1846(2)	6469(1)	19(1)
C141	9793(3)	1668(2)	5034(1)	17(1)
C151	10457(3)	2687(3)	5009(1)	27(1)
C161	11397(4)	2824(3)	4748(1)	39(1)
C171	11642(4)	1964(3)	4520(1)	43(1)

C181	10973(5)	956(3)	4545(1)	40(1)
C191	10035(4)	797(3)	4804(1)	27(1)
C201	12283(3)	757(2)	5583(1)	16(1)
C211	13392(3)	107(3)	5503(1)	24(1)
C221	14548(4)	666(3)	5418(1)	31(1)
C231	14562(4)	1821(3)	5411(1)	31(1)
C241	13414(3)	2382(3)	5502(1)	30(1)

Table 90-3. Bond lengths [Å] and angles [°] for sad.

S(1)-P(1)	1.9384(11)
S(2)-O(1)	1.433(2)
S(2)-O(2)	1.444(2)
S(2)-C(14)	1.772(3)
S(2)-C(1)	1.819(3)
S(3)-C(20)	1.786(3)
S(3)-C(1)	1.803(3)
P(1)-C(2)	1.816(3)
P(1)-C(8)	1.823(3)
P(1)-C(1)	1.854(3)
N(1)-C(20)	1.323(4)
N(1)-C(24)	1.345(4)
C(2)-C(7)	1.382(4)
C(2)-C(3)	1.394(4)
C(3)-C(4)	1.387(5)
C(4)-C(5)	1.376(5)
C(5)-C(6)	1.390(5)
C(6)-C(7)	1.379(4)
C(8)-C(9)	1.389(5)
C(8)-C(13)	1.395(5)
C(9)-C(10)	1.382(5)
C(10)-C(11)	1.375(6)
C(11)-C(12)	1.375(6)
C(12)-C(13)	1.391(5)
C(14)-C(15)	1.376(4)

C(14)-C(19)	1.378(5)
C(15)-C(16)	1.386(5)
C(16)-C(17)	1.382(5)
C(17)-C(18)	1.369(5)
C(18)-C(19)	1.391(5)
C(20)-C(21)	1.389(4)
C(21)-C(22)	1.386(5)
C(22)-C(23)	1.376(4)
C(23)-C(24)	1.380(5)
S11-P11	1.9397(10)
S21-O21	1.436(2)
S21-O11	1.436(2)
S21-C141	1.766(3)
S21-C11	1.807(3)
S31-C201	1.795(3)
S31-C11	1.799(3)
P11-C21	1.810(3)
P11-C81	1.823(3)
P11-C11	1.854(3)
N11-C201	1.319(4)
N11-C241	1.344(4)
C21-C31	1.393(4)
C21-C71	1.396(4)
C31-C41	1.378(4)
C41-C51	1.372(5)
C51-C61	1.400(5)
C61-C71	1.378(4)
C81-C131	1.388(4)
C81-C91	1.390(4)
C91-C101	1.391(5)
C101-C111	1.371(5)
C111-C121	1.384(5)
C121-C131	1.396(5)
C141-C151	1.386(4)
C141-C191	1.387(4)
C151-C161	1.391(5)

C161-C171	1.371(6)
C171-C181	1.376(6)
C181-C191	1.385(5)
C201-C211	1.389(5)
C211-C221	1.376(5)
C221-C231	1.373(5)
C231-C241	1.376(5)

O(1)-S(2)-O(2)	119.11(15)
O(1)-S(2)-C(14)	108.27(15)
O(2)-S(2)-C(14)	108.66(14)
O(1)-S(2)-C(1)	110.14(14)
O(2)-S(2)-C(1)	106.14(14)
C(14)-S(2)-C(1)	103.39(15)
C(20)-S(3)-C(1)	100.56(14)
C(2)-P(1)-C(8)	105.37(14)
C(2)-P(1)-C(1)	108.36(13)
C(8)-P(1)-C(1)	102.00(14)
C(2)-P(1)-S(1)	113.55(11)
C(8)-P(1)-S(1)	114.10(10)
C(1)-P(1)-S(1)	112.56(10)
C(20)-N(1)-C(24)	116.9(3)
S(3)-C(1)-S(2)	111.14(16)
S(3)-C(1)-P(1)	106.42(15)
S(2)-C(1)-P(1)	114.35(16)
C(7)-C(2)-C(3)	119.4(3)
C(7)-C(2)-P(1)	122.4(2)
C(3)-C(2)-P(1)	118.2(2)
C(4)-C(3)-C(2)	119.8(3)
C(5)-C(4)-C(3)	120.5(3)
C(4)-C(5)-C(6)	119.8(3)
C(7)-C(6)-C(5)	120.0(3)
C(6)-C(7)-C(2)	120.6(3)
C(9)-C(8)-C(13)	119.5(3)
C(9)-C(8)-P(1)	122.5(2)
C(13)-C(8)-P(1)	117.9(3)

C(10)-C(9)-C(8)	120.2(3)
C(11)-C(10)-C(9)	120.2(4)
C(10)-C(11)-C(12)	120.2(4)
C(11)-C(12)-C(13)	120.4(4)
C(12)-C(13)-C(8)	119.4(3)
C(15)-C(14)-C(19)	122.0(3)
C(15)-C(14)-S(2)	119.4(3)
C(19)-C(14)-S(2)	118.6(3)
C(14)-C(15)-C(16)	118.5(3)
C(17)-C(16)-C(15)	120.3(3)
C(18)-C(17)-C(16)	120.4(4)
C(17)-C(18)-C(19)	120.1(3)
C(14)-C(19)-C(18)	118.7(3)
N(1)-C(20)-C(21)	124.2(3)
N(1)-C(20)-S(3)	118.8(2)
C(21)-C(20)-S(3)	117.0(2)
C(22)-C(21)-C(20)	117.6(3)
C(23)-C(22)-C(21)	119.2(3)
C(22)-C(23)-C(24)	118.7(3)
N(1)-C(24)-C(23)	123.2(3)
O21-S21-O11	119.19(15)
O21-S21-C141	108.06(14)
O11-S21-C141	108.68(14)
O21-S21-C11	109.51(14)
O11-S21-C11	106.65(14)
C141-S21-C11	103.66(15)
C201-S31-C11	100.93(14)
C21-P11-C81	106.82(14)
C21-P11-C11	107.76(14)
C81-P11-C11	102.24(15)
C21-P11-S11	112.96(11)
C81-P11-S11	114.14(10)
C11-P11-S11	112.17(11)
C201-N11-C241	116.3(3)
S31-C11-S21	111.62(17)
S31-C11-P11	107.01(16)

S21-C11-P11	115.19(17)
C31-C21-C71	119.5(3)
C31-C21-P11	118.9(2)
C71-C21-P11	121.6(2)
C41-C31-C21	120.1(3)
C51-C41-C31	120.6(3)
C41-C51-C61	119.7(3)
C71-C61-C51	120.1(3)
C61-C71-C21	119.8(3)
C131-C81-C91	119.6(3)
C131-C81-P11	121.9(2)
C91-C81-P11	118.4(2)
C81-C91-C101	119.8(3)
C111-C101-C91	120.5(3)
C101-C111-C121	120.1(4)
C111-C121-C131	119.9(3)
C81-C131-C121	119.9(3)
C151-C141-C191	121.6(3)
C151-C141-S21	119.8(3)
C191-C141-S21	118.7(3)
C141-C151-C161	118.6(3)
C171-C161-C151	120.0(3)
C161-C171-C181	121.0(4)
C171-C181-C191	120.1(3)
C181-C191-C141	118.7(3)
N11-C201-C211	124.6(3)
N11-C201-S31	118.2(2)
C211-C201-S31	117.2(2)
C221-C211-C201	117.3(3)
C231-C221-C211	119.7(3)
C221-C231-C241	118.1(3)
N11-C241-C231	123.9(3)

Symmetry transformations used to generate equivalent atoms:

Table 90-4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for sad. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	22(1)	16(1)	34(1)	-2(1)	5(1)	5(1)
S(2)	12(1)	20(1)	14(1)	-2(1)	0(1)	-1(1)
S(3)	12(1)	14(1)	20(1)	1(1)	2(1)	-1(1)
P(1)	12(1)	13(1)	14(1)	-2(1)	2(1)	0(1)
O(1)	20(1)	28(1)	19(1)	1(1)	-2(1)	6(1)
O(2)	19(1)	27(1)	19(1)	-5(1)	3(1)	-11(1)
N(1)	14(2)	23(1)	28(2)	5(1)	4(1)	3(1)
C(1)	12(2)	15(1)	13(2)	1(1)	-1(1)	1(1)
C(2)	13(2)	18(2)	12(2)	-3(1)	1(1)	-4(1)
C(3)	15(2)	22(2)	18(2)	0(1)	1(1)	0(1)
C(4)	16(2)	35(2)	31(2)	0(2)	4(2)	-5(2)
C(5)	20(2)	34(2)	18(2)	2(1)	1(2)	-14(2)
C(6)	33(2)	17(2)	26(2)	2(1)	-3(2)	-4(1)
C(7)	10(2)	21(2)	24(2)	-3(1)	-2(2)	-2(1)
C(8)	14(2)	19(2)	19(2)	1(1)	3(1)	-8(1)
C(9)	23(2)	25(2)	21(2)	2(1)	-5(2)	-5(1)
C(10)	22(2)	40(2)	33(2)	16(2)	-7(2)	-7(2)
C(11)	30(2)	70(3)	18(2)	10(2)	-11(2)	-20(2)
C(12)	36(2)	68(3)	19(2)	-11(2)	6(2)	-23(2)
C(13)	21(2)	39(2)	18(2)	-7(2)	2(2)	-9(2)
C(14)	17(2)	23(2)	13(2)	-6(1)	0(2)	-6(1)
C(15)	29(2)	20(2)	26(2)	-4(1)	9(2)	-5(2)
C(16)	37(2)	26(2)	41(2)	-14(2)	16(2)	-2(2)
C(17)	34(3)	46(2)	35(3)	-15(2)	18(2)	-11(2)
C(18)	45(3)	41(2)	22(2)	3(2)	13(2)	-15(2)
C(19)	32(2)	24(2)	23(2)	1(1)	-2(2)	-3(2)
C(20)	14(2)	23(2)	14(2)	1(1)	2(1)	2(1)
C(21)	11(2)	27(2)	28(2)	5(1)	-1(1)	-1(1)
C(22)	14(2)	38(2)	29(2)	7(2)	0(2)	-5(2)
C(23)	12(2)	44(2)	29(2)	7(2)	3(2)	8(2)
C(24)	25(2)	28(2)	35(2)	7(2)	3(2)	8(2)

S11	20(1)	14(1)	30(1)	2(1)	3(1)	-4(1)
S21	12(1)	21(1)	14(1)	1(1)	0(1)	1(1)
S31	12(1)	15(1)	20(1)	-1(1)	2(1)	2(1)
P11	12(1)	13(1)	15(1)	1(1)	2(1)	0(1)
O11	16(1)	29(1)	19(1)	4(1)	3(1)	9(1)
O21	18(1)	30(1)	26(1)	-1(1)	-6(1)	-8(1)
N11	15(2)	19(1)	31(2)	-2(1)	3(1)	-2(1)
C11	12(2)	11(1)	16(2)	1(1)	2(1)	-1(1)
C21	13(2)	19(2)	11(2)	2(1)	2(1)	-1(1)
C31	17(2)	21(2)	27(2)	-2(1)	0(2)	0(1)
C41	11(2)	35(2)	29(2)	0(2)	1(2)	2(2)
C51	25(2)	28(2)	19(2)	1(1)	4(2)	11(2)
C61	23(2)	23(2)	27(2)	-5(1)	0(2)	3(1)
C71	16(2)	19(2)	25(2)	-2(1)	0(2)	2(1)
C81	12(2)	19(2)	12(2)	0(1)	2(1)	4(1)
C91	19(2)	24(2)	22(2)	5(1)	8(2)	3(1)
C101	34(2)	43(2)	15(2)	12(2)	2(2)	12(2)
C111	27(2)	47(2)	23(2)	-8(2)	-7(2)	10(2)
C121	20(2)	27(2)	24(2)	-9(1)	-6(2)	3(1)
C131	17(2)	21(2)	19(2)	0(1)	0(2)	2(1)
C141	15(2)	22(2)	14(2)	5(1)	2(1)	2(1)
C151	29(2)	22(2)	31(2)	7(2)	11(2)	6(2)
C161	36(2)	31(2)	50(3)	19(2)	19(2)	7(2)
C171	52(3)	52(2)	25(2)	18(2)	24(2)	20(2)
C181	54(3)	44(2)	21(2)	-2(2)	8(2)	14(2)
C191	35(2)	28(2)	19(2)	-2(1)	4(2)	2(2)
C201	9(2)	25(2)	13(2)	-3(1)	-1(1)	-2(1)
C211	23(2)	27(2)	23(2)	-6(1)	3(2)	4(2)
C221	14(2)	43(2)	37(2)	-13(2)	8(2)	1(2)
C231	17(2)	44(2)	33(2)	-7(2)	7(2)	-10(2)
C241	22(2)	27(2)	40(2)	-5(2)	6(2)	-12(2)

Table 90-5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for sad.

	x	y	z	U(eq)
H(1)	4820(30)	6560(20)	8378(8)	10(8)
H(3)	9133	5783	8005	22
H(4)	10654	7211	7876	33
H(5)	9905	9005	7737	28
H(6)	7614	9381	7722	30
H(7)	6094	7964	7849	22
H(9)	4031	7037	7863	27
H(10)	2577	7209	7396	38
H(11)	2712	5966	6934	47
H(12)	4271	4524	6939	49
H(13)	5756	4337	7403	31
H(15)	4719	8024	8975	30
H(16)	3087	8304	9401	41
H(17)	2573	6867	9788	46
H(18)	3670	5157	9757	43
H(19)	5300	4857	9331	32
H(21)	1639	3990	8618	26
H(22)	-372	4914	8758	32
H(23)	-402	6883	8779	34
H(24)	1525	7870	8650	35
H11	10100(30)	1790(20)	5752(8)	10(8)
H31	5883	1094	6143	26
H41	4369	2543	6231	30
H51	5108	4346	6358	29
H61	7404	4701	6413	29
H71	8935	3257	6324	24
H91	9345	-344	6759	26
H101	10886	-154	7209	37
H111	12433	1293	7202	39
H121	12498	2548	6738	29

H131	10989	2349	6278	23
H151	10273	3280	5167	33
H161	11870	3513	4727	47
H171	12283	2065	4342	51
H181	11156	369	4385	48
H191	9566	105	4823	33
H211	13354	-692	5508	29
H221	15332	254	5364	37
H231	15342	2221	5346	38
H241	13430	3181	5501	35