Digital Appendix
Computational Details

This chapter consists of research previously published under the following titles:

"Photocatalytic Hydrogen Evolution Driven by a Heteroleptic Ruthenium(II) Bis(terpyridine) Complex" in *Inorganic Chemistry*.

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"Electrochemical and photophysical study of homoleptic and heteroleptic methylated ruthenium(II) bis-terpyridine complexes" in *European Journal of Inorganic Chemistry*.

Reproduced with permission of Wiley-VCH, from *Electrochemical and photophysical study of homoleptic and heteroleptic methylated ruthenium(II) bis-terpyridine complexes*, Mira T. Rupp, Thomas Auvray, Garry S. Hanan, Dirk G. Kurth, *European Journal of Inorganic Chemistry* **2021**.

"Substituted 2,4-Di(pyridin-2-yl)pyrimidine-Based Ruthenium Photosensitizers for Hydrogen Photoevolution under Red Light" in *Inorganic Chemistry*.

Reproduced with permission of American Chemical Society from *Inorganic Chemistry*, **2021**, *60*, 292-302.

CCDC 2090569: Experimental Crystal Structure Determination, **2021**

and

submitted to *Dalton Transactions* as a full paper under the title

"Dinuclear 2,4-di(pyridin-2-yl)-pyrimidine based ruthenium photosensitizers for hydrogen photo-evolution under red light."

1. Comparison of experimental absorption spectra and predicted transitions

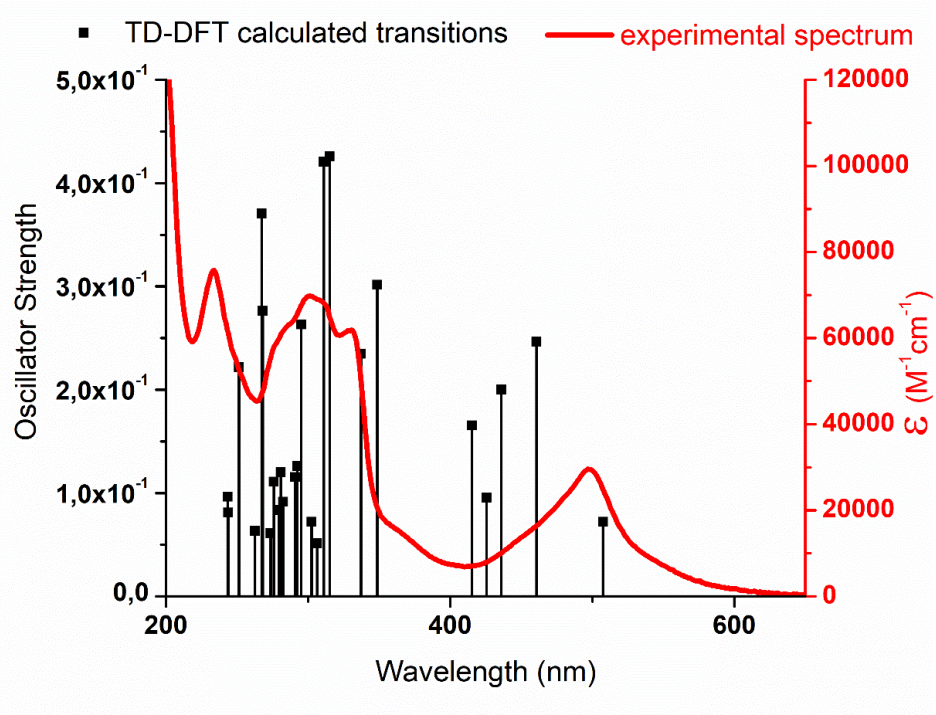

Figure 1. Comparison of the experimental absorption spectra with the predicted transitions (oscillator strength > 0.05) for complex **III-C1** in acetonitrile.

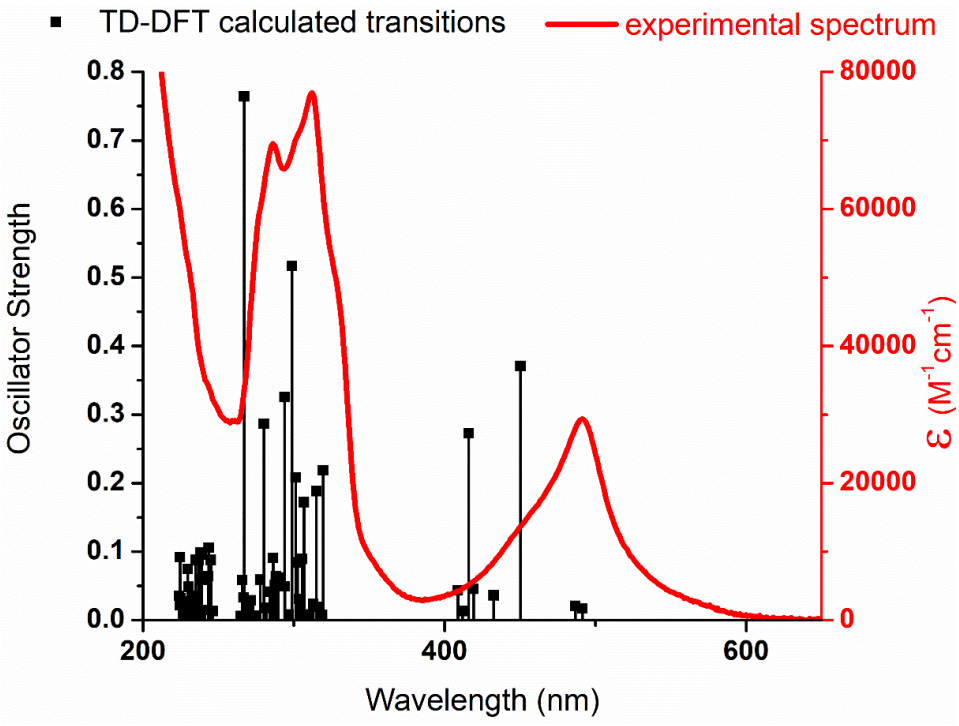

Figure 2. Comparison of the experimental absorption spectra with the predicted transitions (oscillator strength > 0.05) for complex **III-C2** in acetonitrile.

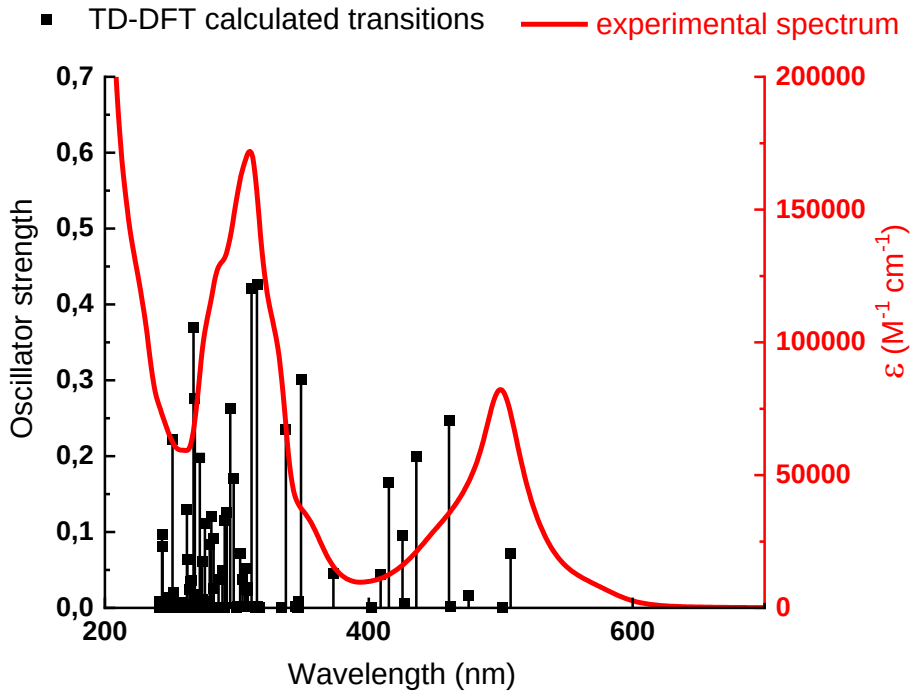

Figure 3. Comparison of the experimental absorption spectra with the predicted transitions (oscillator strength > 0.05) for complex **IV-C1** in acetonitrile.

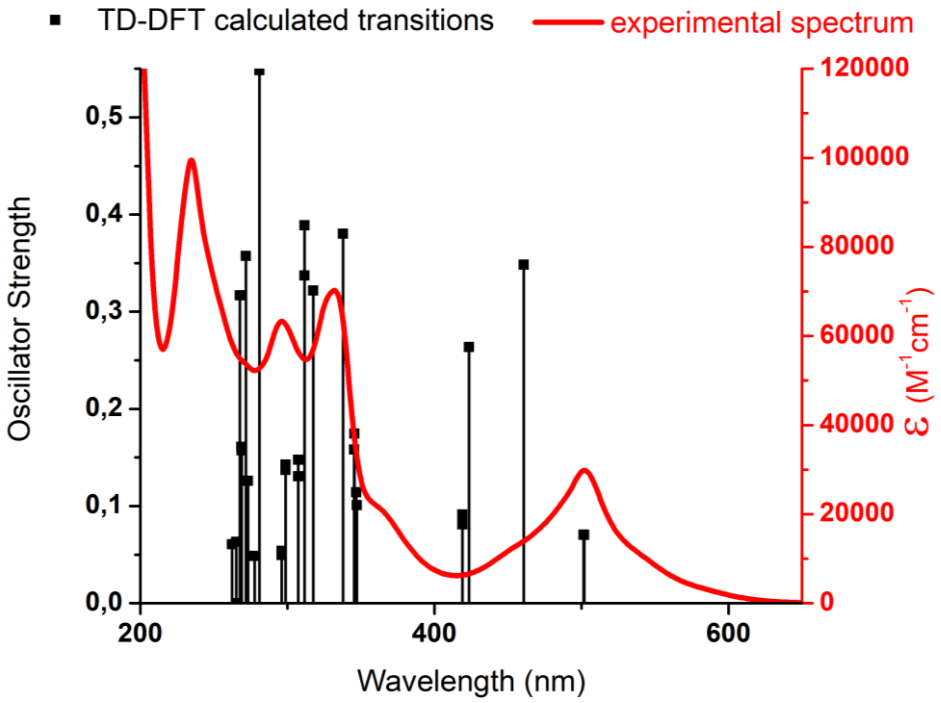

Figure 4. Comparison of the experimental absorption spectra with the predicted transitions (oscillator strength > 0.05) for complex **IV-C2** in acetonitrile.

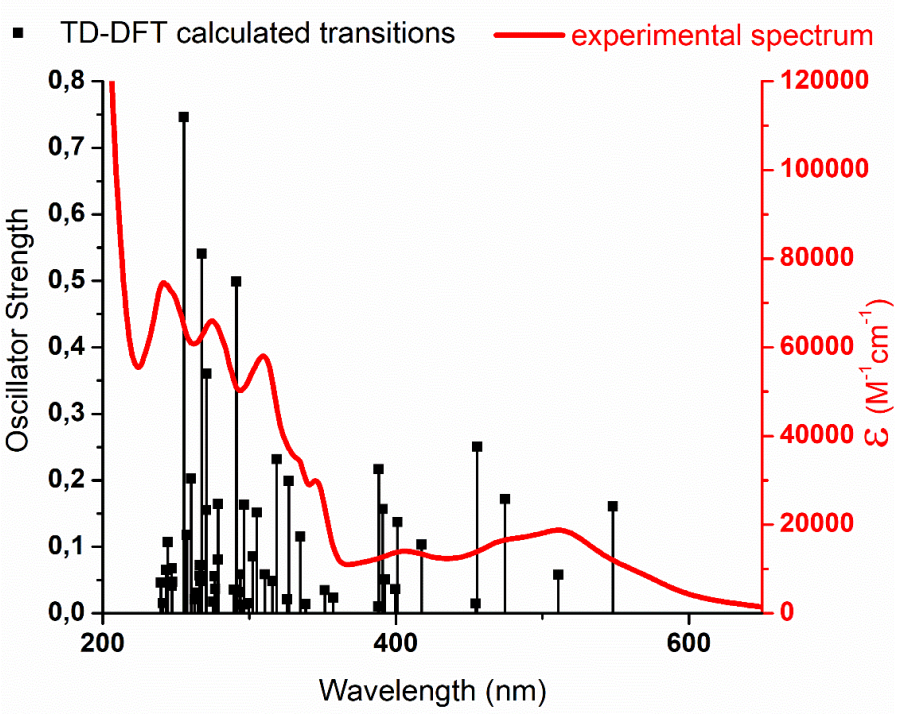

Figure 5. Comparison of the experimental absorption spectra with the predicted transitions (oscillator strength > 0.05) for complex **V-C1** in acetonitrile.

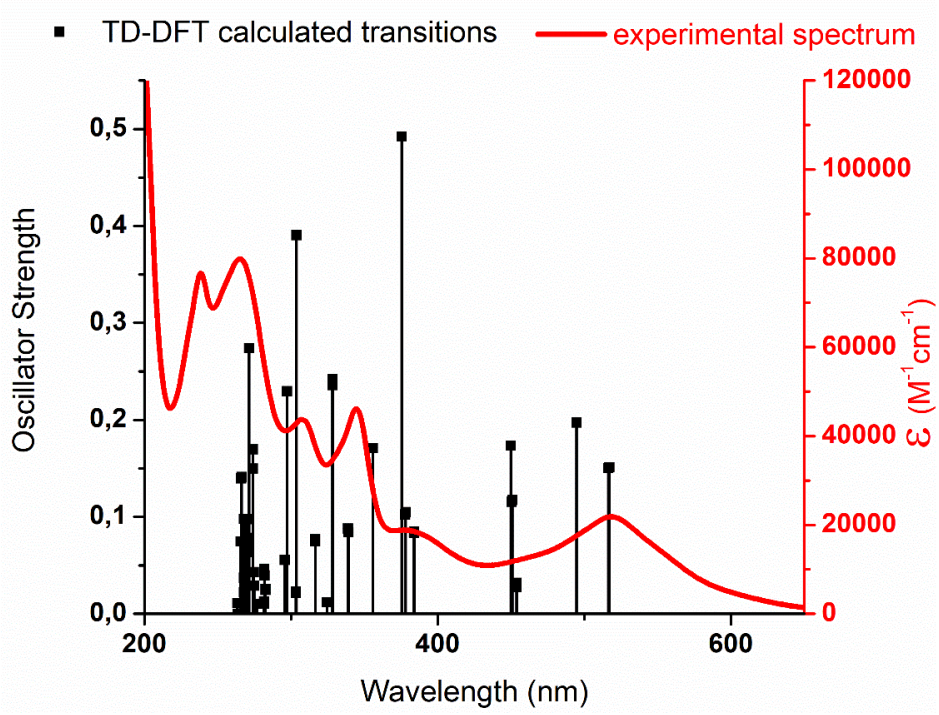

Figure 6. Comparison of the experimental absorption spectra with the predicted transitions (oscillator strength > 0.05) for complex **V-C2** in acetonitrile.

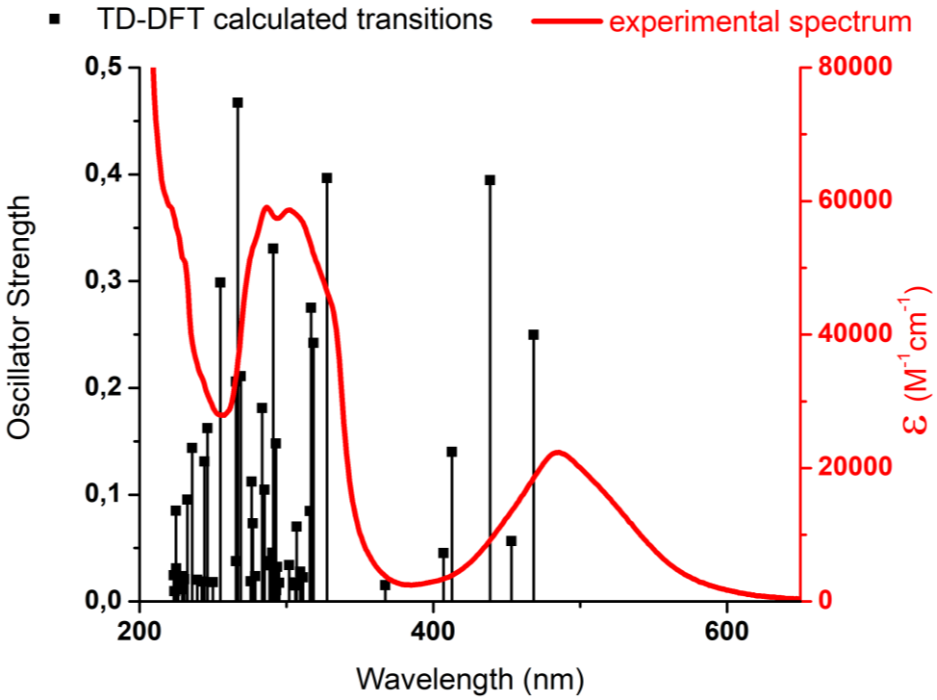

Figure 7. Comparison of the experimental absorption spectra with the predicted transitions (oscillator strength > 0.05) for complex **VI-C1** in acetonitrile.

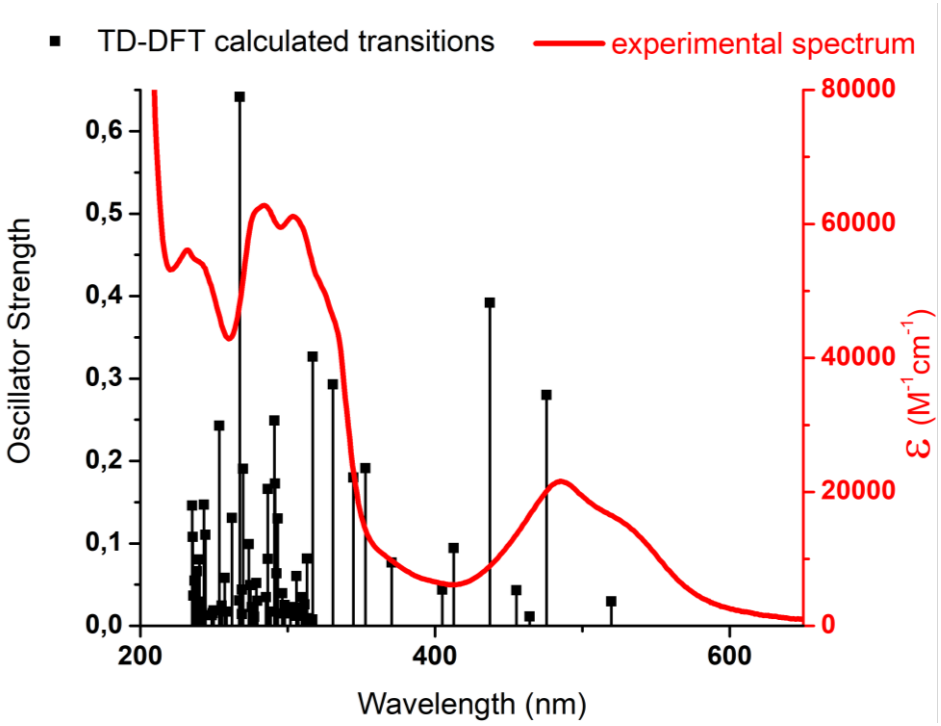

Figure 8. Comparison of the experimental absorption spectra with the predicted transitions (oscillator strength > 0.05) for complex **VI-C2** in acetonitrile.

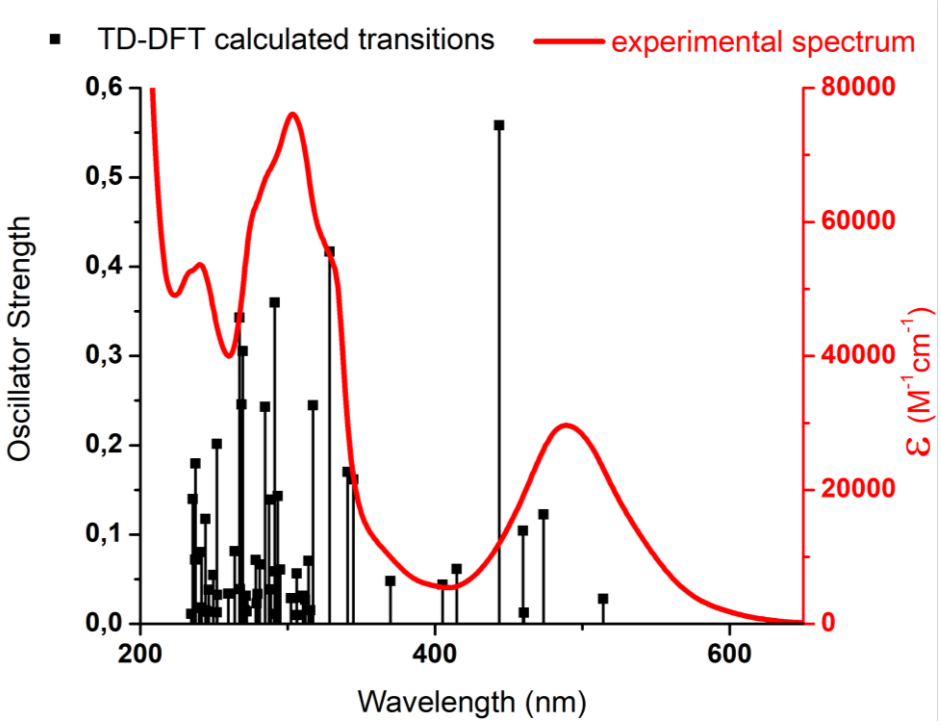

Figure 9. Comparison of the experimental absorption spectra with the predicted transitions (oscillator strength > 0.05) for complex **VI-C3** in acetonitrile.

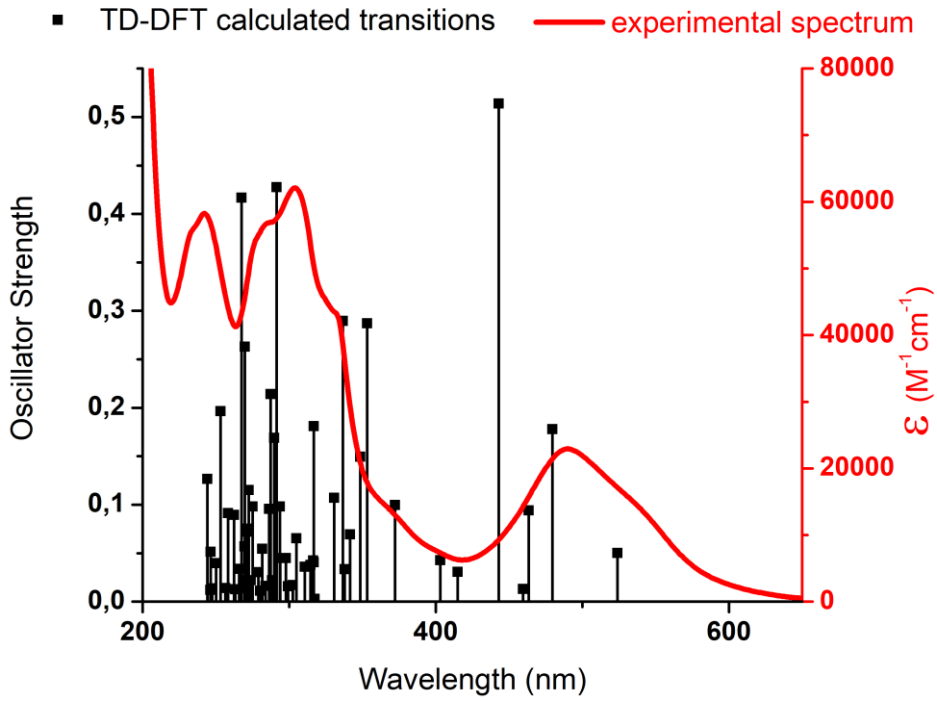

Figure 10. Comparison of the experimental absorption spectra with the predicted transitions (oscillator strength > 0.05) for complex **VI-C4** in acetonitrile.

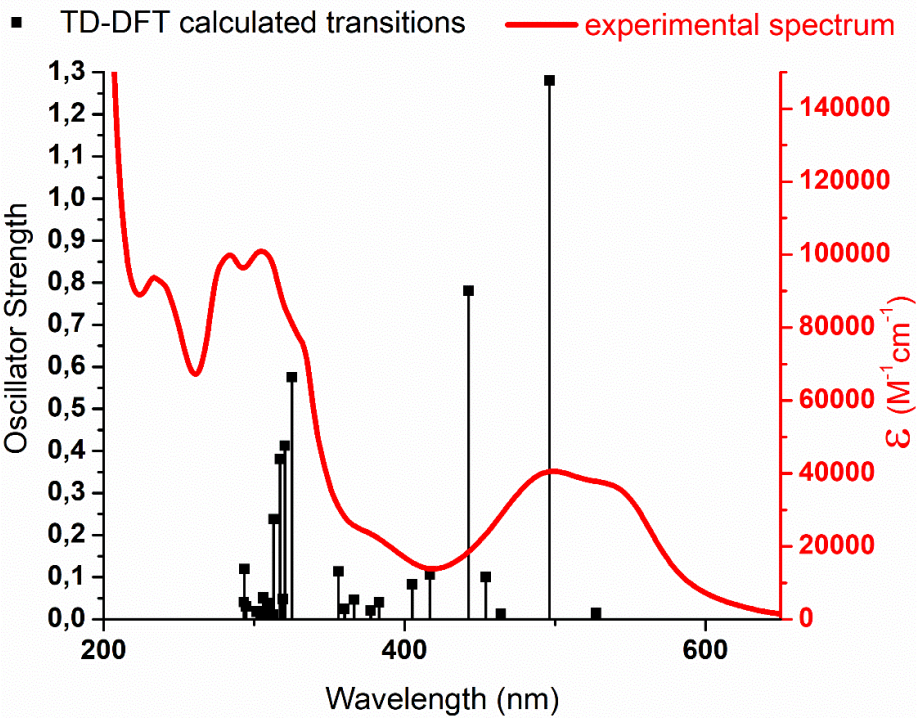

Figure 11. Comparison of the experimental absorption spectra with the predicted transitions (oscillator strength > 0.05) for complex **VII-C1** in acetonitrile.

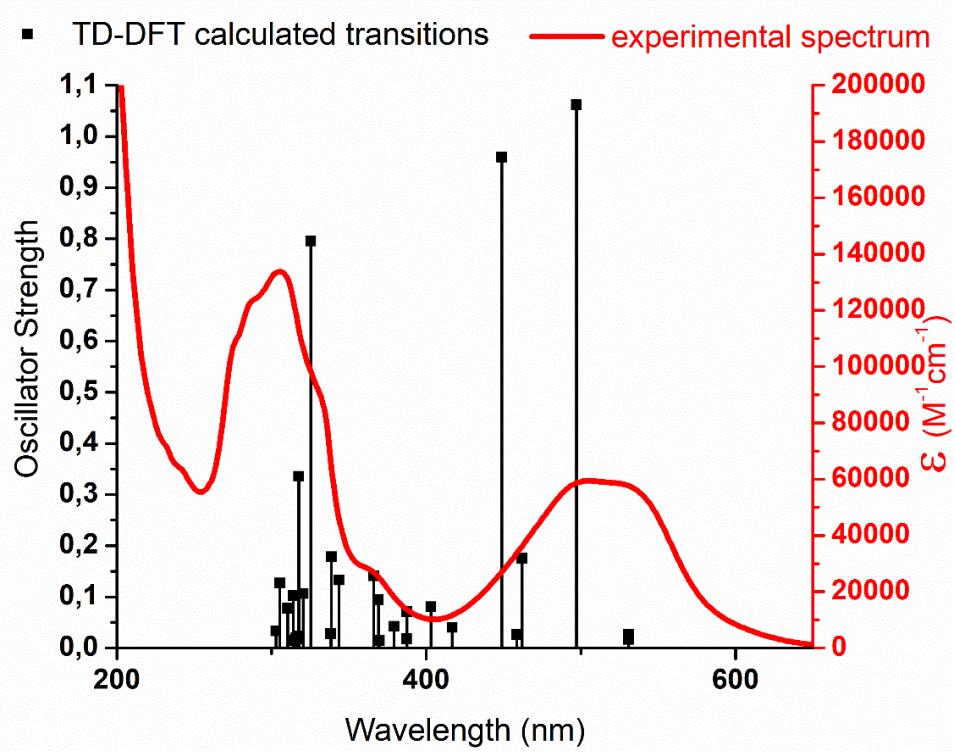

Figure 12. Comparison of the experimental absorption spectra with the predicted transitions (oscillator strength > 0.05) for complex **VII-C2** in acetonitrile.

2. Atomic coordinates of the optimized geometries

Table 1. Atomic coordinates oft he optimized geometry of **III-C1**.

Center	Atomic Number	Coordinates (Å)			Center	Atomic Number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	7	-2.923394	0.000793	0.000835	51	6	1.232591	-3.674667	0.044043
2	6	-5.704303	0.002070	0.001361	52	6	-1.064182	-4.385786	0.045091
3	6	-3.583832	0.015412	-1.188184	53	1	-2.488765	-2.764258	0.029282
4	6	-3.583408	0.013245	1.190080	54	1	2.294435	-3.888045	0.026778
5	6	-4.978981	0.008745	1.213591	55	1	-1.836649	-5.145203	0.072204
6	6	-4.979390	0.012222	-1.211141	56	6	-7.183720	0.002525	0.001178
7	1	-5.505657	0.009784	2.159695	57	6	-10.036216	0.005397	0.001458
8	1	-5.506573	0.005594	-2.156995	58	6	-7.909162	0.636709	-1.029144
9	6	-2.675422	0.024652	-2.347636	59	6	-7.910238	0.627860	1.033034
10	6	0.799770	0.044332	-4.388587	60	6	-9.309194	0.625585	1.030263
11	7	-1.330624	0.021419	-2.040677	61	6	-9.308116	0.639563	-1.024648
12	6	-3.106987	0.037761	-3.677772	62	1	-7.385903	1.160910	-1.823924
13	6	-2.163401	0.047393	-4.711439	63	1	-7.387965	-1.147788	1.831246
14	6	0.422513	0.031434	-3.043595	64	1	-9.843974	-1.125237	1.833769
15	1	-4.165529	0.040889	-3.907414	65	1	-9.842013	1.147887	-1.823274
16	1	-2.487020	0.057383	-5.746021	66	6	5.310324	0.000951	0.000605
17	1	0.621043	0.029156	-2.755113	67	6	8.117488	0.001475	0.001080
18	1	0.036805	0.051910	-5.157618	68	6	6.031178	-1.027116	0.643869
19	6	-2.674572	0.023135	2.349198	69	6	6.031343	1.024942	0.645328
20	6	0.798163	0.044171	4.389446	70	6	7.431073	1.030280	0.651266
21	6	-3.105641	0.036084	3.679497	71	6	7.430908	-1.032978	0.649333
22	7	-1.329884	0.020725	2.041738	72	1	5.509390	-1.818031	1.173722
23	6	0.421402	0.031396	3.044313	73	1	5.509673	1.816051	-1.175007
24	6	-2.161674	0.046396	4.712809	74	1	7.968239	1.822178	-1.161494
25	1	-4.164096	0.038585	3.909547	75	1	7.967950	-1.825076	1.159379
26	1	0.622047	0.029751	2.755440	76	6	-11.543780	0.016839	0.013216
27	1	-2.484913	0.056274	5.747510	77	1	-11.913923	0.896457	0.556560
28	1	0.034916	0.052296	5.158192	78	1	-11.952394	0.868802	0.510457
29	44	0.934165	0.000274	0.000460	79	1	-11.953939	0.063809	1.000734
30	7	1.052309	0.000120	0.000113	80	35	10.068307	0.001832	0.001401
31	6	3.829759	0.000667	0.000349	81	6	0.742346	-6.141731	0.076214
32	6	1.712035	-1.190167	0.011060	82	7	1.580971	-8.849833	0.117006
33	6	1.712509	1.189667	0.011075	83	6	0.024064	-7.154095	0.533274
34	6	3.108197	1.212136	0.014271	84	6	1.940952	-6.526833	0.708105
35	6	3.107714	-1.213188	0.014720	85	6	2.315742	-7.875616	0.704612
36	1	3.637166	2.156479	0.051854	86	6	0.428746	-8.477918	0.490022
37	1	3.636300	-2.157739	0.052471	87	1	0.946462	-6.926727	1.056161
38	7	0.541450	2.036498	0.022584	88	1	2.568810	-5.805344	-1.219563
39	6	0.303297	4.728394	0.055189	89	1	3.232723	-8.191617	-1.191551
40	6	0.802078	2.347756	0.028376	90	1	0.145558	-9.270074	0.959580
41	6	-1.442141	3.045883	0.030386	91	6	0.744802	6.141622	0.076493
42	6	-1.062419	4.386393	0.045997	92	7	1.584474	8.849402	0.116981
43	6	1.234071	3.674359	0.044195	93	6	1.943717	6.526284	0.708064
44	1	-2.487653	2.765447	0.030684	94	6	0.021379	7.154258	0.532830
45	1	-1.834575	5.146118	0.073353	95	6	0.431950	8.477909	0.489738
46	1	2.295996	3.887313	0.026564	96	6	2.319023	7.874923	0.704431
47	7	0.542269	-2.036100	0.021813	97	1	2.571425	5.804567	1.219386

48	6	0.301395	-4.728332	0.054742	98	1	0.943999	6.927226	-1.055471
49	6	-1.443367	-3.045125	0.029334	99	1	0.142171	9.270271	0.959173
50	6	0.801135	-2.347893	0.028061	100	1	3.236249	8.190590	1.191124

Table 2. Atomic coordinates oft he optimized geometry of **III-C2**.

Center number	Atomic number	Coordinates (Å)			Center number	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	7	-2.847162	-0.011133	0.000378	54	1	2.385259	-3.875109	-0.057718
2	6	-5.628802	-0.017624	0.000947	55	1	-1.733578	-5.157224	-0.093110
3	6	-3.508292	0.008236	-1.188700	56	6	-7.108462	-0.021006	0.000847
4	6	-3.507729	-0.033817	1.189689	57	6	-9.961303	-0.025194	0.001538
5	6	-4.903418	-0.033302	1.213006	58	6	-7.835802	0.618255	-1.024960
6	6	-4.903952	0.001238	-1.211420	59	6	-7.833442	-0.660100	1.028390
7	1	-5.430195	-0.021664	2.159237	60	6	-9.232484	-0.661144	1.025966
8	1	-5.431214	-0.012724	-2.157369	61	6	-9.234848	0.617493	-1.020385
9	6	-2.599723	0.026878	-2.347583	62	1	-7.313831	1.148973	-1.816278
10	6	-0.723113	0.065078	-4.387439	63	1	-7.309634	-1.183960	1.823041
11	7	-1.254932	0.025873	-2.039500	64	1	-9.765876	-1.167381	1.826304
12	6	-3.030665	0.046917	-3.678120	65	1	-9.770100	1.129747	-1.815624
13	6	-2.086771	0.065911	-4.711228	66	6	5.385203	0.014281	0.000003
14	6	-0.346596	0.044944	-3.042395	67	6	8.192760	0.023154	-0.000809
15	1	-4.089188	0.048373	-3.908135	68	6	6.109879	-1.011459	0.640898
16	1	-2.409812	0.081404	-5.745955	69	6	6.103036	1.044590	-0.641257
17	1	0.696707	0.044128	-2.752796	70	6	7.502824	1.054829	-0.647304
18	1	0.040186	0.079814	-5.156109	71	6	7.509712	-1.012821	0.646124
19	6	-2.598696	-0.048330	2.348253	72	1	5.590588	-1.805994	1.167789
20	6	-0.721279	-0.077545	4.387511	73	1	5.578370	1.835794	-1.167827
21	6	-3.029106	-0.070810	3.678921	74	1	8.037264	1.850357	-1.154784
22	7	-1.254032	-0.040506	2.039740	75	1	8.049465	-1.804949	1.153298
23	6	-0.345298	-0.055287	3.042354	76	6	-11.468890	-0.051043	-0.013062
24	6	-2.084812	-0.085273	4.711733	77	1	-11.837139	-0.928013	-0.561950
25	1	-4.087531	-0.077560	3.909278	78	1	-11.879733	0.836832	-0.504486
26	1	0.697901	-0.049179	2.752453	79	1	-11.878745	-0.105436	1.000658
27	1	-2.407448	-0.102562	5.746558	80	35	10.143935	0.029227	-0.001474
28	1	0.042331	-0.088629	5.155933	81	6	0.795947	6.208929	0.105920
29	44	-0.860647	-0.005792	0.000066	82	6	2.324734	6.380142	0.107121
30	7	1.127404	0.000333	0.000171	83	1	2.787131	5.921114	0.989547
31	6	3.904374	0.009588	0.000212	84	1	2.566546	7.448560	0.126116
32	6	1.790780	-1.187882	-0.015242	85	1	2.784954	5.953300	-0.792421
33	6	1.783042	1.193169	0.015827	86	6	0.220189	6.916643	-1.144559
34	6	3.178989	1.219870	0.018929	87	1	0.614639	6.469996	-2.064981
35	6	3.186741	-1.205407	-0.018377	88	1	0.503571	7.975570	-1.128219
36	1	3.704078	2.166220	0.059618	89	1	-0.873623	6.862767	-1.178249
37	1	3.718087	-2.148282	-0.059127	90	6	0.223484	6.871115	1.382586
38	7	-0.469605	2.033668	0.034384	91	1	0.619481	6.390928	2.285291
39	6	0.376996	4.738172	0.080137	92	1	-0.870309	6.817063	1.416695
40	6	0.869598	2.349445	0.037321	93	1	0.507870	7.929671	1.404147
41	6	-1.370061	3.044374	0.053841	94	6	0.901895	-6.189452	-0.104269
42	6	-0.988369	4.382975	0.076741	95	6	1.762485	-6.447773	1.156345
43	6	1.300103	3.679858	0.059289	96	1	2.129592	-7.480736	1.142748
44	1	-2.415702	2.762794	0.051110	97	1	1.173390	-6.304943	2.070008
45	1	-1.766067	5.137979	0.091711	98	1	2.633457	-5.784303	1.202019
46	1	2.362291	3.886121	0.060163	99	6	1.766110	-6.402496	-1.370936
47	7	-0.459870	-2.043664	-0.034543	100	1	2.134801	-7.434757	-1.392422
48	6	0.402179	-4.743883	-0.079555	101	1	2.636111	-5.736461	-1.391372
49	6	-1.350345	-3.058327	-0.054658	102	1	1.179037	-6.228803	-2.280547
50	6	0.885226	-2.350836	-0.036775	103	6	-0.257026	-7.200919	-0.124075
51	6	1.320348	-3.675017	-0.058038	104	1	0.152359	-8.217034	-0.141855
52	6	-0.961020	-4.399439	-0.077529	105	1	-0.887318	-7.081951	-1.013661
53	1	-2.398441	-2.785185	-0.052548	106	1	-0.889823	-7.114097	0.767482

Table 3. Atomic coordinates oft he optimized geometry of **IV-C1**.

Center	Atomic number	Coordinates (Å)			Center	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	7	1.987853	0.000451	0.001340	44	1	1.557928	1.948709	1.941918
2	6	4.768921	0.002308	0.000561	45	1	0.903070	3.648817	3.642179
3	6	2.648356	0.838043	0.842741	46	1	-3.226524	2.762642	2.769063
4	6	2.648406	0.839718	0.844592	47	1	-1.546616	4.063158	4.063167
5	6	4.044142	0.859332	0.857016	48	7	0.394265	-1.443071	-1.444422
6	6	4.044050	0.855786	0.857025	49	6	-1.223803	-3.331822	-3.334470
7	1	4.572691	1.546466	-1.506036	50	6	0.514916	-2.152233	-2.152640
8	1	4.572757	-1.541966	1.506949	51	6	-1.739068	-1.660392	-1.663237
9	6	1.739047	-1.659548	1.660563	52	6	-2.168692	-2.601056	-2.605213
10	6	0.139511	-3.104284	3.099906	53	6	0.139511	-3.103534	-3.104159
11	7	0.394258	-1.443057	1.440935	54	1	1.557920	-1.947312	-1.946792
12	6	2.168682	-2.600176	2.602572	55	1	-3.226534	-2.764134	-2.771109
13	6	1.223803	-3.331743	3.331036	56	1	0.903076	-3.647432	-3.647062
14	6	0.514920	-2.152992	2.148383	57	1	-1.546609	-4.063248	-4.066591
15	1	3.226524	-2.762642	2.769063	58	6	6.248373	0.003036	0.002139
16	1	1.546616	-4.063158	4.063167	59	6	9.100943	0.006248	0.006476
17	1	-1.557928	-1.948709	1.941918	60	6	6.972952	0.293806	1.175456
18	1	0.903070	-3.648817	3.642179	61	6	6.975822	0.304240	-1.168262
19	6	1.739068	1.660392	-1.663237	62	6	8.374785	0.304391	-1.163570
20	6	0.139511	3.103534	-3.104159	63	6	8.371907	0.288146	1.175686
21	6	2.168692	2.601056	-2.605213	64	1	6.448548	0.499175	2.104487
22	7	0.394265	1.443071	-1.444422	65	1	6.453828	0.514789	-2.097478
23	6	0.514916	2.152233	-2.152640	66	1	8.910315	0.532916	-2.081341
24	6	1.223803	3.331822	-3.334470	67	1	8.904986	0.506579	2.097298
25	1	3.226534	2.764134	-2.771109	68	6	-6.248373	0.003036	0.002139
26	1	-1.557920	1.947312	-1.946792	69	6	-9.100943	0.006248	0.006476
27	1	1.546609	4.063248	-4.066591	70	6	-6.975822	0.304240	-1.168262
28	1	0.903076	3.647432	-3.647062	71	6	-6.972952	0.293806	1.175456
29	44	0.000000	0.000000	0.001735	72	6	-8.371907	0.288146	1.175686
30	7	-1.987853	0.000451	0.001340	73	6	-8.374785	0.304391	-1.163570
31	6	-4.768921	0.002308	0.000561	74	1	-6.453828	0.514789	-2.097478
32	6	-2.648406	0.839718	0.844592	75	1	-6.448548	0.499175	2.104487
33	6	-2.648356	0.838043	0.842741	76	1	-8.904986	0.506579	2.097298
34	6	-4.044050	0.855786	0.857025	77	1	-8.910315	0.532916	-2.081341
35	6	-4.044142	0.859332	0.857016	78	6	-10.608544	0.019270	0.001893
36	1	-4.572757	1.541966	1.506949	79	1	-11.018902	0.676444	0.737108
37	1	-4.572691	-1.546466	-1.506036	80	1	-10.979319	1.021416	0.251471
38	7	0.394258	1.443057	1.440935	81	1	-11.016379	0.240086	0.984231
39	6	-1.223803	3.331743	3.331036	82	6	10.608544	0.019270	0.001893
40	6	-1.739047	1.659548	1.660563	83	1	10.979319	-1.021416	0.251471
41	6	0.514920	2.152992	2.148383	84	1	11.016379	0.240086	0.984231
42	6	0.139511	3.104284	3.099906	85	1	11.018902	0.676444	0.737108
43	6	-2.168682	2.600176	2.602572					

Table 4. Atomic coordinates oft he optimized geometry of **IV-C2**.

Center Number	Atomic Number	Coordinates (Å)			Center Number	Atomic Number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	7	-2.109431	0.003139	0.005151	59	6	-8.401161	1.224254	0.199792
2	6	-4.815704	0.013297	0.015046	60	1	-6.473468	2.155676	0.340383
3	6	-2.678392	0.806503	-0.802593	61	1	-6.494387	-2.114606	-0.297519
4	6	-2.678432	-0.796407	0.816673	62	1	-8.951964	-2.100130	-0.279944
5	6	-4.080450	-0.822449	0.852522	63	1	-8.930843	2.162893	0.339881
6	6	-4.080308	0.843306	-0.827935	64	6	6.284884	-0.018622	-0.020019
7	1	-4.602228	-1.479923	1.539341	65	6	9.099160	-0.026608	-0.027808
8	1	-4.602137	1.506747	-1.508935	66	6	7.005648	-1.213355	0.150392
9	6	-1.774270	1.639560	-1.653468	67	6	7.011446	1.171997	-0.194504
10	6	0.029440	3.062253	-3.091268	68	6	8.409880	1.170395	-0.199252
11	7	-0.513387	1.474863	-1.489405	69	6	8.404073	-1.219689	0.147411
12	6	-2.221857	2.576728	-2.603487	70	1	6.478981	-2.154136	0.301017
13	6	-1.308845	3.316499	-3.350599	71	1	6.489285	2.115673	-0.342500
14	6	0.372117	2.113629	-2.135418	72	1	8.946478	2.104991	-0.340028
15	1	-3.283211	2.741421	-2.752979	73	1	8.936087	-2.157382	0.285013
16	1	1.414298	1.894720	-1.920554	74	35	10.988911	-0.031926	-0.032959
17	1	0.817447	3.579280	-3.630285	75	6	1.711453	-4.349843	-4.317911
18	6	-1.774133	-1.636359	1.660613	76	7	2.525002	-6.266291	-6.218832
19	6	0.030316	-3.058708	3.097979	77	6	1.237485	-5.665979	-4.268363
20	6	-2.221393	-2.573454	2.610871	78	6	2.602160	-4.018187	-5.345638
21	7	-0.513268	-1.475734	1.492133	79	6	2.971479	-4.994342	-6.258261
22	6	0.372558	-2.115323	2.136879	80	6	1.667561	-6.573432	-5.224176
23	6	-1.307886	-3.312223	3.358301	81	1	0.553030	-5.989260	-3.490589
24	1	-3.282583	-2.717911	2.781108	82	1	2.994657	-3.011615	-5.448421
25	1	1.414627	-1.904045	1.913932	83	1	3.655974	-4.768899	-7.071069
26	1	0.818347	-3.591804	3.621079	84	1	1.323123	-7.603563	-5.211288
27	44	-0.000384	-0.002564	-0.000733	85	6	1.760009	4.339221	4.303869
28	7	2.108660	-0.007516	-0.007466	86	7	2.595292	6.255447	6.196342
29	6	4.815205	-0.014488	-0.015833	87	6	2.673558	4.011451	5.312767
30	6	2.673104	-0.818197	-0.811038	88	6	1.274218	5.651654	4.269533
31	6	2.682229	0.800483	0.792300	89	6	1.715409	6.559012	5.220431
32	6	4.084399	0.828865	0.817949	90	6	3.052906	4.987202	6.221790
33	6	4.074928	-0.853846	-0.845266	91	1	3.076402	3.007929	5.404313
34	1	4.609845	1.495410	1.493083	92	1	0.571539	5.972583	3.507170
35	1	4.592695	-1.523272	-1.523515	93	1	1.361677	7.586078	5.218847
36	7	0.521070	1.485720	1.474243	94	1	3.755239	4.764415	7.019975
37	6	1.326816	3.342394	3.316284	95	35	-10.988909	0.040281	0.036580
38	6	1.782821	1.646629	1.635132	96	6	-1.734618	-4.296497	4.360580
39	6	-0.360898	2.133759	2.115836	97	7	-2.555320	-6.184550	6.286736
40	6	-0.012887	3.090141	3.062037	98	6	-2.633856	-5.318937	4.035770
41	6	2.235607	2.591693	2.574838	99	6	-1.256261	-4.245282	5.675076
42	1	-1.404334	1.916649	1.905049	100	6	-1.690135	-5.194608	6.587516
43	1	-0.798246	3.614880	3.597508	101	6	-3.006459	-6.225248	5.016576
44	1	3.297874	2.753981	2.720346	102	1	-3.030453	-5.422475	3.031026
45	7	0.504206	-1.493947	-1.478333	103	1	-0.565449	-3.471003	5.993334
46	6	1.289339	-3.352770	-3.326426	104	1	-1.342458	-5.180050	7.616551
47	6	-0.384856	-2.139119	-2.113005	105	1	-3.697658	-7.033858	4.796711
48	6	1.764208	-1.659785	-1.648319	106	6	-1.736463	4.304565	-4.349064
49	6	2.206564	-2.605649	-2.592072	107	7	-2.560842	6.203858	-6.262912
50	6	-0.047500	-3.096798	-3.061674	108	6	-1.252845	5.617912	-4.321734
51	1	-1.425759	-1.918253	-1.894146	109	6	-2.642157	3.966968	-5.361728
52	1	3.267027	-2.771423	-2.746653	110	6	-3.016319	4.934660	-6.281411
53	1	-0.838157	-3.619545	-3.591158	111	6	-1.688590	6.516792	-5.283103
54	6	-6.285169	0.019595	0.020623	112	1	-0.556144	5.945895	-3.556907
55	6	-9.099159	0.032031	0.030337	113	1	-3.042638	2.961984	-5.447861
56	6	-7.002788	1.215720	0.194022	114	1	-3.712399	4.704185	-7.082893
57	6	-7.014437	-1.170167	-0.147729	115	1	-1.336568	7.544430	-5.287294
58	6	-8.412845	-1.166331	-0.143845					

Table 5. Atomic coordinates oft he optimized geometry of **V-C1**.

Center Number	Atomic Number	Coordinates (Å)			Center Number	Atomic Number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	7	3.105283	-0.000536	0.000600	55	1	1.840474	5.081138	-0.022141
2	6	5.812917	-0.001672	0.000979	56	6	7.283121	-0.002552	0.001584
3	6	3.675205	0.001324	-1.138368	57	6	10.116947	-0.010974	0.012218
4	6	3.674877	-0.002724	1.139733	58	6	8.008061	-0.942573	-0.748072
5	6	5.076661	-0.003591	1.183737	59	6	8.008083	0.939323	0.748933
6	6	5.077017	0.001048	-1.181986	60	6	9.406853	0.939756	0.750570
7	1	5.599005	-0.018700	2.134456	61	6	9.406842	-0.944759	-0.747463
8	1	5.599582	0.015717	-2.132569	62	1	7.487484	-1.695139	-1.336570
9	6	2.771519	0.003785	-2.329743	63	1	7.487411	1.697777	1.329762
10	6	0.967826	0.002673	-4.356172	64	1	9.938097	1.690196	1.332300
11	7	1.508088	0.000869	-2.098167	65	1	9.938088	-1.684604	-1.342606
12	6	3.221482	0.007829	-3.662937	66	6	-5.280556	0.000574	-0.000433
13	6	2.302825	0.007347	-4.697672	67	6	-8.091247	0.000737	-0.000755
14	6	0.623908	-0.000363	-3.010247	68	6	-6.001272	0.596116	1.048331
15	1	4.278676	0.012142	-3.902461	69	6	-6.001105	-0.594874	-1.049368
16	1	2.621135	0.010972	-5.734203	70	6	-7.399201	-0.594528	-1.051979
17	1	-0.418488	-0.003207	-2.705570	71	6	-7.399369	0.595930	1.050622
18	1	0.196674	0.002146	-5.118986	72	1	-5.475630	1.055509	1.883498
19	6	2.770862	-0.004580	2.330864	73	1	-5.475325	-1.054346	-1.884406
20	6	0.966634	-0.002359	4.356807	74	1	-7.935644	-1.056203	-1.877234
21	6	3.220470	-0.008636	3.664180	75	1	-7.935948	1.057658	1.875758
22	7	1.507493	-0.001099	2.098942	76	6	11.616845	0.009091	-0.013082
23	6	0.623077	0.000650	3.010792	77	1	11.968667	0.653210	-0.824774
24	6	2.301537	-0.007586	4.698666	78	1	12.018432	-0.998895	-0.161106
25	1	4.277608	-0.013390	3.903978	79	1	12.018465	0.382286	0.934890
26	1	-0.419232	0.003924	2.705840	80	35	-9.980558	0.000834	-0.000964
27	1	2.619581	-0.011214	5.735277	81	6	-0.707456	6.126504	-0.034103
28	1	0.195286	-0.001383	5.119416	82	6	-0.226018	7.031155	0.917363
29	44	0.998475	-0.000104	0.000315	83	6	-1.579813	6.617150	-1.010050
30	7	-1.111754	0.000145	0.000071	84	6	-1.940213	7.961482	-1.017494
31	6	-3.813808	0.000441	-0.000248	85	6	-0.614289	8.366655	0.876890
32	6	-1.680000	1.140344	0.001424	86	1	0.452594	6.697600	1.701799
33	6	-1.680253	-1.139924	-0.001400	87	1	-1.967274	5.957740	-1.785672
34	6	-3.081647	-1.183903	-0.006800	88	1	-2.604857	8.369528	-1.774016
35	6	-3.081391	1.184629	0.006487	89	1	-0.249969	9.088757	1.602478
36	1	-3.607827	-2.131826	-0.003722	90	6	-0.708874	-6.126263	0.034349
37	1	-3.607367	2.132665	0.003288	91	6	-1.580527	-6.616951	1.010897
38	7	0.483990	-2.097099	0.002248	92	6	-0.228440	-7.030735	-0.917782
39	6	-0.296967	-4.716896	0.018584	93	6	-0.617031	-8.366132	-0.877360
40	6	-0.775365	-2.331519	0.004902	94	6	-1.941251	-7.961199	1.018276
41	6	1.375270	-2.998740	0.002751	95	1	-1.967158	-5.957639	1.787018
42	6	1.040062	-4.346709	0.009267	96	1	0.449617	-6.697104	-1.702665
43	6	-1.216964	-3.669732	0.016117	97	1	-0.253564	-9.088170	-1.603444
44	1	2.416039	-2.684581	0.002402	98	1	-2.605346	-8.369233	1.775281
45	1	1.839276	-5.081572	0.022754	99	7	-1.464012	-8.806514	0.078560
46	1	-2.278764	-3.889014	0.011385	100	7	-1.461964	8.806964	-0.078436
47	7	0.484470	2.097008	-0.001783	101	6	-1.847104	-10.228842	0.113263
48	6	-0.295876	4.717013	-0.018270	102	1	-2.845530	-10.320946	0.548426
49	6	1.375962	2.998432	-0.002146	103	1	-1.106388	-10.752117	0.722875
50	6	-0.774830	2.331726	-0.004668	104	1	-1.860004	-10.620467	-0.907159
51	6	-1.216108	3.670046	-0.015936	105	6	-1.844915	10.229322	-0.113542

52	6	1.041067	4.346484	-0.008757	106	1	-1.108800	10.750921	-0.730125
53	1	2.416652	2.684009	-0.001599	107	1	-1.849970	10.623720	0.905868
54	1	-2.277862	3.889550	-0.011334	108	1	-2.846662	10.320296	-0.541277

Table 6. Atomic coordinates oft he optimized geometry of **V-C2**.

Center Number	Atomic Number	Coordinates (Å)			Center Number	Atomic Number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	7	-1.991198	-0.000187	-0.000795	67	6	6.967402	1.177848	0.275263
2	6	-4.768057	-0.007592	0.004005	68	6	8.366868	1.183563	0.275218
3	6	-2.654298	0.852605	-0.826920	69	6	8.363348	-1.189737	-0.287780
4	6	-2.646886	-0.856663	0.827450	70	1	6.441092	-2.111073	-0.482888
5	6	-4.042213	-0.875195	0.848011	71	1	6.447331	2.110885	0.468977
6	6	-4.049796	0.863770	-0.842524	72	1	8.905346	2.101459	0.483555
7	1	-4.570065	-1.535134	1.525040	73	1	8.899097	-2.109296	-0.495817
8	1	-4.583712	1.520783	-1.517643	74	35	11.001421	-0.007217	-0.005433
9	6	-1.746144	1.683570	-1.636947	75	6	1.670509	-4.275610	-4.400349
10	6	0.117479	3.141642	-3.068934	76	6	0.894602	-5.415055	-4.696849
11	7	-0.401251	1.462684	-1.425268	77	6	2.878943	-4.110320	-5.103728
12	6	-2.180810	2.634019	-2.561326	78	6	3.271944	-5.048401	-6.048396
13	6	-1.248681	3.384832	-3.297654	79	6	1.327528	-6.324826	-5.648431
14	6	0.498921	2.183102	-2.132155	80	1	-0.034379	-5.620885	-4.181107
15	1	-3.243072	2.769051	-2.722533	81	1	3.516476	-3.249528	-4.948992
16	1	1.545011	1.987490	-1.936916	82	1	4.191110	-4.946344	-6.608572
17	1	0.890301	3.699158	-3.584069	83	1	0.760784	-7.212432	-5.896478
18	6	-1.731579	-1.682310	1.634791	84	6	1.678720	4.280366	4.392787
19	6	0.144333	-3.127612	3.063985	85	6	2.883754	4.107401	5.099992
20	6	-2.158371	-2.633600	2.562032	86	6	0.907473	5.423219	4.687891
21	7	-0.388626	-1.455211	1.418143	87	6	1.342669	6.329998	5.641408
22	6	0.517707	-2.169577	2.123464	88	6	3.279017	5.042669	6.046598
23	6	-1.219895	-3.377393	3.297136	89	1	3.516722	3.243213	4.945588
24	1	-3.219317	-2.775486	2.726112	90	1	-0.019073	5.633730	4.169533
25	1	1.562137	-1.969417	1.923978	91	1	0.780148	7.220565	5.888481
26	1	0.921214	-3.680023	3.578538	92	1	4.195412	4.934865	6.610274
27	44	-0.001189	0.003883	-0.004804	93	35	-11.004083	-0.024141	0.015229
28	7	1.988780	0.005552	-0.007337	94	6	-1.655877	-4.389423	4.283118
29	6	4.765546	0.002421	-0.007414	95	6	-2.858838	-5.101808	4.116437
30	6	2.647284	-0.827030	-0.857344	96	6	-0.880922	-4.676406	5.425436
31	6	2.649076	0.836451	0.842980	97	6	-1.311198	-5.626092	6.338592
32	6	4.044557	0.848523	0.862083	98	6	-3.248734	-6.044736	5.057518
33	6	4.042662	-0.842214	-0.876692	99	1	-3.493961	-4.954514	3.252555
34	1	4.576523	1.486235	1.556920	100	1	0.044864	-4.154699	5.631006
35	1	4.572996	-1.482071	-1.570832	101	1	-0.745957	-5.866158	7.229297
36	7	0.394202	1.426274	1.455240	102	1	-4.163075	-6.612704	4.954994
37	6	1.236567	3.299370	3.378310	103	6	-1.691585	4.398563	-4.278738
38	6	1.738435	1.641495	1.675962	104	6	-2.899446	5.101860	-4.109781
39	6	-0.507963	2.130477	2.175923	105	6	-0.917139	4.698239	-5.418300
40	6	-0.129094	3.067678	3.135164	106	6	-1.349921	5.654136	-6.323447
41	6	2.170735	2.566548	2.626888	107	6	-3.292758	6.050741	-5.043677
42	1	-1.553514	1.932389	1.980290	108	1	-3.536585	4.943867	-3.249333
43	1	-0.902718	3.581094	3.693131	109	1	0.010859	4.181980	-5.627657
44	1	3.232393	2.731430	2.762355	110	1	-0.784110	5.905102	-7.210812
45	7	0.391047	-1.416761	-1.464553	111	1	-4.211853	6.610269	-4.937837
46	6	1.229900	-3.291817	-3.387972	112	7	-2.480452	-6.295988	6.149666
47	6	-0.512436	-2.121150	-2.183536	113	7	-2.522624	6.317530	-6.130799
48	6	1.734779	-1.631929	-1.688231	114	7	2.501470	-6.136343	-6.310650
49	6	2.165144	-2.557552	-2.639309	115	7	2.513648	6.134732	6.306801
50	6	-0.135370	-3.059275	-3.142533	116	6	2.937637	7.129294	7.323447
51	1	-1.557548	-1.922468	-1.986176	117	1	3.010104	8.112500	6.855984
52	1	3.226656	-2.721875	-2.776120	118	1	3.909622	6.845906	7.724071
53	1	-0.910558	-3.572318	-3.698696	119	1	2.203588	7.153010	8.130643
54	6	-6.247882	-0.011460	0.006650	120	6	-2.937740	7.343255	-7.119655
55	6	-9.054518	-0.018977	0.011742	121	1	-2.215798	8.161700	-7.112216
56	6	-6.971964	1.171797	-0.245170	122	1	-3.922949	7.724530	-6.856054

57	6	-6.964723	-1.198595	0.261019	123	1	-2.977584	6.890745	-8.111575
58	6	-8.364132	-1.210257	0.262920	124	6	2.923962	-7.133690	-7.325031
59	6	-8.371406	1.175974	-0.241946	125	1	2.185605	-7.164198	-8.128071
60	1	-6.453548	2.109927	-0.417301	126	1	3.002830	-8.114615	-6.853763
61	1	-6.440671	-2.133937	0.431215	127	1	3.892352	-6.847805	-7.732672
62	1	-8.898327	-2.135271	0.449697	128	6	-2.902343	-7.305034	7.152697
63	1	-8.911246	2.098109	-0.426726	129	1	-2.151492	-8.095177	7.205235
64	6	6.245371	0.000209	-0.006960	130	1	-3.859122	-7.731608	6.856030
65	6	9.051779	-0.004161	-0.006051	131	1	-3.004953	-6.823122	8.126273
66	6	6.963914	-1.179665	-0.288724					

Table 7. Atomic coordinates oft he optimized geometry of **VI-C1**.

Center	Atomic number	Coordinates (Å)			Center	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	7	-2.679614	0.000669	-0.000297	41	6	-0.596622	-3.723303	-2.192498
2	6	-5.457865	-0.102604	-0.052639	42	6	1.668256	-3.001148	-1.774748
3	6	-3.335905	-0.630166	1.010456	43	1	-2.111698	-2.389005	-1.403788
4	6	-3.342493	0.582116	-1.036003	44	1	-1.315611	-4.423080	-2.601380
5	6	-4.736789	0.539685	-1.083515	45	1	2.743138	-3.118202	-1.846214
6	6	-4.730334	-0.691479	1.005353	46	7	-0.360655	1.847014	1.075467
7	1	-5.265395	0.977369	-1.921118	47	6	0.379638	4.182416	2.435926
8	1	-5.256607	-1.169220	1.822371	48	6	-1.301855	2.685595	1.565028
9	6	-2.425038	-1.180257	2.029193	49	6	0.973656	2.158314	1.257050
10	6	-0.544498	-2.136580	3.827892	50	6	1.360088	3.319480	1.931914
11	7	-1.082502	-0.972484	1.790395	51	6	-0.970559	3.858893	2.249249
12	6	-2.851617	-1.868729	3.169351	52	1	-2.334847	2.405601	1.401900
13	6	-1.905636	-2.353379	4.079902	53	1	2.410355	3.550757	2.063005
14	6	-0.172203	-1.442757	2.674111	54	1	-1.760704	4.498859	2.622991
15	1	-3.908126	-2.026639	3.348036	55	6	-6.935887	-0.156540	-0.079347
16	1	-2.225862	-2.888463	4.966622	56	6	-9.785724	-0.260631	-0.130444
17	1	0.869749	-1.255977	2.447016	57	6	-7.632570	-1.245963	0.484140
18	1	0.220170	-2.494517	4.506570	58	6	-7.689439	0.878490	-0.671649
19	6	-2.437821	1.199421	-2.021021	59	6	-9.087115	0.825311	-0.694403
20	6	-0.567843	2.294386	-3.750111	60	6	-9.030347	-1.296226	0.454437
21	6	-2.871810	1.856240	-3.176926	61	1	-7.086444	-2.077733	0.920196
22	7	-1.093418	1.091151	-1.732368	62	1	-7.190020	1.745517	-1.094857
23	6	-0.188176	1.628539	-2.582347	63	1	-9.643653	1.640000	-1.150256
24	6	-1.931073	2.410415	-4.052581	64	1	-9.541407	-2.154248	0.883159
25	1	-3.929867	1.936468	-3.394503	65	6	5.486916	0.076733	0.040896
26	1	0.855350	1.519656	-2.315540	66	6	8.283941	-0.114497	-0.057315
27	1	-2.256839	2.921675	-4.951262	67	6	6.296705	1.126782	0.521420
28	1	0.192751	2.708897	-4.400596	68	6	6.113171	-1.069623	-0.491873
29	44	-0.691206	0.074329	0.036357	69	6	7.506272	-1.173017	-0.543036
30	7	1.284499	0.146677	0.073933	70	6	7.691948	1.037068	0.474536
31	6	4.011836	0.145238	0.077934	71	1	5.864434	2.032904	0.931102
32	6	1.916890	1.185123	0.688106	72	1	5.497507	-1.879818	-0.864696
33	6	2.001315	-0.847757	-0.510069	73	1	7.971178	-2.062628	-0.953419
34	7	3.334663	-0.875694	-0.526708	74	1	8.299854	1.854751	0.845434
35	6	3.311253	1.203642	0.706290	75	6	-11.292960	-0.301585	-0.132713
36	1	3.841196	2.006871	1.197428	76	1	-11.695995	0.188570	0.763542
37	7	-0.203933	-1.675067	-0.991092	77	1	-11.665741	-1.330892	-0.136729
38	6	0.782669	-3.937600	-2.322444	78	1	-11.706663	0.219113	-1.002406
39	6	1.153047	-1.883425	-1.117172	79	35	10.227201	-0.244933	-0.124623
40	6	-1.053265	-2.583813	-1.521887	80	1	1.159653	-4.813396	-2.838137

81	1	0.664926	5.086297	2.961647

Table 8. Atomic coordinates oft he optimized geometry of **VI-C2**.

Center	Atomic number	Coordinates (Å)			Center	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	7	2.931320	-0.554125	0.009133	46	7	0.279050	1.515274	-0.035259
2	6	5.637640	-0.521868	-0.000541	47	6	-0.555261	4.120535	-0.103997
3	6	3.496751	-0.574836	-1.131632	48	6	1.151631	2.435871	-0.058700
4	6	3.504231	-0.518340	1.145784	49	6	-0.985456	1.732007	-0.040543
5	6	4.906135	-0.499772	1.184673	50	6	-1.453843	3.057322	-0.078023
6	6	4.898398	-0.560528	-1.180516	51	6	0.788636	3.777120	-0.091721
7	1	5.430929	-0.481475	2.133566	52	1	2.198051	2.143434	-0.054643
8	1	5.416602	-0.566501	-2.133176	53	1	-2.518798	3.262237	-0.072883
9	6	2.589362	-0.611222	-2.319225	54	1	1.565682	4.534874	-0.121588
10	6	0.777812	-0.683099	-4.337396	55	6	7.106898	-0.505022	-0.005530
11	7	1.327474	-0.623140	-2.082906	56	6	9.939710	-0.478337	-0.006106
12	6	3.033997	-0.633812	-3.654196	57	6	7.839940	-1.479733	-0.700364
13	6	2.111256	-0.670304	-4.684780	58	6	7.821719	0.488895	0.681075
14	6	0.439296	-0.657586	-2.990387	59	6	9.220295	0.506685	0.676691
15	1	4.089833	-0.623206	-3.897268	60	6	9.238555	-1.465110	-0.705202
16	1	2.424147	-0.688771	-5.722273	61	1	7.323571	-2.271595	-1.239483
17	1	-0.602257	-0.667449	-2.681700	62	1	7.290553	1.273430	1.216476
18	1	0.001996	-0.712961	-5.094706	63	1	9.742367	1.298131	1.209870
19	6	2.604681	-0.499789	2.339723	64	1	9.775060	-2.233948	-1.256832
20	6	0.806228	-0.474231	4.370684	65	6	-5.356388	-0.854543	0.049567
21	6	3.058024	-0.461937	3.671418	66	6	-8.163777	-1.164853	0.042016
22	7	1.341283	-0.520982	2.112419	67	6	-6.195119	0.068817	0.702479
23	6	0.458932	-0.510950	3.026165	68	6	-5.973060	-1.943955	-0.596187
24	6	2.141958	-0.448674	4.708514	69	6	-7.363186	-2.099793	-0.604812
25	1	4.115483	-0.444775	3.906946	70	6	-7.587063	-0.081804	0.698306
26	1	-0.584673	-0.534316	2.725067	71	1	-5.773101	0.911967	1.245184
27	1	2.461520	-0.421515	5.743779	72	1	-5.358734	-2.686430	-1.104728
28	1	0.035221	-0.468305	5.133488	73	1	-7.802157	-2.952676	-1.115230
29	44	0.822634	-0.581021	0.016689	74	1	-8.206299	0.646510	1.215422
30	7	-1.273886	-0.582962	0.023346	75	6	11.438656	-0.441476	-0.038965
31	6	-3.885345	-0.710565	0.039723	76	1	11.779675	0.156979	-0.889307
32	6	-1.866102	0.531939	-0.003095	77	1	11.852390	-1.451492	-0.127964
33	6	-1.854968	-1.780865	0.053381	78	1	11.839024	-0.007143	0.883148
34	7	-3.191144	-1.862565	0.056731	79	35	-10.042344	-1.369179	0.035984
35	6	-3.252100	0.518660	0.003354	80	6	-1.002614	5.518157	-0.139926
36	1	-3.822663	1.435636	-0.035846	81	7	-1.866057	8.201004	-0.203947
37	7	0.344613	-2.691548	0.069602	82	6	-0.548641	6.447799	0.802829
38	6	-0.477494	-5.290066	0.139241	83	6	-1.898067	5.967743	-1.117374
39	6	-0.909527	-2.948051	0.079854	84	6	-2.292076	7.296963	-1.109518
40	6	1.224691	-3.607804	0.090032	85	6	-1.002872	7.755678	0.731890
41	6	0.864078	-4.953614	0.125673	86	1	0.139306	6.159860	1.591439
42	6	-1.391167	-4.253589	0.115715	87	1	-2.274611	5.300707	-1.886152
43	1	2.269077	-3.308425	0.079738	88	1	-2.980587	7.679913	-1.857363
44	1	1.630893	-5.721100	0.143513	89	1	-0.674114	8.500684	1.450806
45	1	-2.458504	-4.446509	0.126567	90	1	-0.799611	-6.324620	0.168246

Table 9. Atomic coordinates oft he optimized geometry of **VI-C3**.

Center	Atomic number	Coordinates (Å)			Center	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	7	2.991321	-0.468247	0.006544	46	7	0.576233	-2.819932	0.084313
2	6	5.684679	-0.201550	-0.005805	47	6	0.027539	-5.480151	0.172776
3	6	3.559522	-0.377115	1.142451	48	6	1.542687	-3.643508	0.109652
4	6	3.555964	-0.446689	-1.134599	49	6	-0.659469	-3.169987	0.097619
5	6	4.951046	-0.310997	-1.184853	50	6	-0.984684	-4.537015	0.143416
6	6	4.954556	-0.236705	1.179945	51	6	1.325294	-5.015072	0.155051
7	1	5.467464	-0.277536	-2.137929	52	1	2.551769	-3.241091	0.095487
8	1	5.476157	-0.168052	2.128277	53	1	-2.015302	-4.871137	0.157198
9	6	2.662374	-0.430858	2.337105	54	1	2.166183	-5.699734	0.176731
10	6	0.868920	-0.544746	4.369441	55	6	7.146938	-0.057208	-0.012875
11	7	1.405360	-0.561692	2.111053	56	6	9.965514	0.226946	-0.036276
12	6	3.111319	-0.346194	3.668145	57	6	7.774128	0.995855	0.671159
13	6	2.197782	-0.403936	4.705940	58	6	7.961040	-0.970616	-0.700773
14	6	0.525643	-0.620382	3.025519	59	6	9.353113	-0.834883	-0.708220
15	1	4.163506	-0.237109	3.902618	60	6	9.165904	1.134736	0.664161
16	1	2.514129	-0.342174	5.740704	61	1	7.178363	1.729316	1.210928
17	1	-0.512380	-0.733482	2.725509	62	1	7.514896	-1.811704	-1.227922
18	1	0.100273	-0.597639	5.132818	63	1	9.954558	-1.567284	-1.242158
19	6	2.654687	-0.568828	-2.321145	64	1	9.619245	1.960863	1.207527
20	6	0.854672	-0.802472	-4.337385	65	6	-5.280113	-1.060785	0.026350
21	6	3.098990	-0.559828	-3.656384	66	6	-8.104481	-1.047357	0.048258
22	7	1.398549	-0.687427	-2.083651	67	6	-6.020353	-2.071905	-0.615470
23	6	0.515961	-0.800529	-2.990184	68	6	-6.004672	-0.037757	0.668746
24	6	2.182112	-0.678757	-4.685984	69	6	-7.403424	-0.028889	0.684396
25	1	4.149952	-0.460310	-3.900451	70	6	-7.420366	-2.068441	-0.604212
26	1	-0.520951	-0.896264	-2.680560	71	1	-5.514601	-2.870084	-1.154549
27	1	2.494829	-0.674446	-5.723684	72	1	-5.469531	0.768525	1.169601
28	1	0.083615	-0.899478	-5.093931	73	1	-7.927057	0.776499	1.192220
29	44	0.893034	-0.678757	0.016079	74	1	-7.962219	-2.861657	-1.112595
30	7	-1.191881	-0.898561	0.025633	75	6	11.459662	0.355001	-0.016201
31	6	-3.802082	-1.048748	0.027555	76	1	11.871182	-0.197546	0.834015
32	6	-1.662271	-2.069958	0.061862	77	1	11.760693	1.404818	0.064386
33	6	-1.896947	0.230087	-0.005384	78	1	11.897849	-0.038007	-0.939655
34	7	-3.234029	0.170513	-0.001318	79	35	-9.994061	-1.041762	0.063643
35	6	-3.041863	-2.203734	0.066280	80	6	-1.503004	5.229657	-0.151122
36	1	-3.510370	-3.176403	0.115702	81	7	-2.630465	7.815934	-0.223368
37	7	0.191172	1.369304	-0.043201	82	6	-2.521696	5.553142	-1.055784
38	6	-0.916475	3.882462	-0.113260	83	6	-1.065774	6.237305	0.717187
39	6	-1.081624	1.490346	-0.043530	84	6	-1.651166	7.492351	0.645300
40	6	0.966205	2.373679	-0.075756	85	6	-3.043608	6.837839	-1.054862
41	6	0.460292	3.672711	-0.111217	86	1	-2.900426	4.822756	-1.763862
42	6	-1.701678	2.736024	-0.078651	87	1	-0.290131	6.050355	1.452853
43	1	2.037010	2.189364	-0.078302	88	1	-1.337513	8.293241	1.308667
44	1	1.156074	4.505832	-0.151966	89	1	-3.831357	7.120347	-1.747381
45	1	-2.785927	2.793077	-0.066479	90	1	-0.189923	-6.541340	0.208869

Table 10. Atomic coordinates oft he optimized geometry of **VI-C4**.

Center	Atomic number	Coordinates (Å)			Center	Atomic number	Coordinates (Å)		
		X	Y	Z			X	Y	Z
1	7	3.043465	-0.119608	0.003745	51	6	1.232618	4.367508	-0.058080
2	6	5.744169	-0.296651	0.004947	52	1	2.515533	2.632471	-0.033567
3	6	3.611004	-0.172075	-1.134972	53	1	-2.104238	4.102194	-0.057175
4	6	3.612016	-0.141255	1.142971	54	1	2.064362	5.065221	-0.076835
5	6	5.010930	-0.231454	1.187516	55	6	7.210386	-0.392774	0.005918
6	6	5.009765	-0.265417	-1.178276	56	6	10.036841	-0.583937	0.017048
7	1	5.531210	-0.264080	2.138556	57	6	7.869772	-1.413180	-0.697081
8	1	5.530644	-0.300772	-2.128874	58	6	7.996100	0.535597	0.706680
9	6	2.708877	-0.127111	-2.326353	59	6	9.391908	0.445854	0.708128
10	6	0.906549	-0.039724	-4.352109	60	6	9.265387	-1.506065	-0.696106
11	7	1.448707	-0.043432	-2.094939	61	1	7.296916	-2.157023	-1.247344
12	6	3.156550	-0.172286	-3.659697	62	1	7.524308	1.352725	1.248902
13	6	2.238516	-0.127799	-4.694138	63	1	9.970688	1.188842	1.252410
14	6	0.564801	0.000057	-3.006271	64	1	9.744058	-2.307686	-1.254272
15	1	4.211182	-0.241034	-3.898668	65	6	-5.242375	0.206084	0.015720
16	1	2.553843	-0.160611	-5.730588	66	6	-8.064997	0.103661	0.001038
17	1	-0.475813	0.069912	-2.702140	67	6	-6.012161	1.182647	0.676075
18	1	0.134413	-0.001333	-5.112866	68	6	-5.936290	-0.828753	-0.641445
19	6	2.710706	-0.067602	2.333559	69	6	-7.334105	-0.881599	-0.653544
20	6	0.910104	0.074725	4.357734	70	6	-7.411411	1.135060	0.668396
21	6	3.159158	-0.082392	3.667315	71	1	-5.530576	1.987536	1.227219
22	7	1.450542	0.012995	2.101023	72	1	-5.377736	-1.609628	-1.156779
23	6	0.567459	0.082185	3.011553	73	1	-7.833737	-1.694811	-1.172996
24	6	2.241997	-0.009916	4.700951	74	1	-7.976524	1.902262	1.191283
25	1	4.213567	-0.151315	3.907238	75	6	11.534354	-0.662080	-0.009286
26	1	-0.473234	0.146620	2.706467	76	1	11.924539	-0.082210	-0.851325
27	1	2.557826	-0.020620	5.737715	77	1	11.869684	-1.699869	-0.108163
28	1	0.138591	0.133197	5.117844	78	1	11.962351	-0.270087	0.919365
29	44	0.939610	0.018868	0.002857	79	35	-9.953463	0.038490	-0.009546
30	7	-1.150951	0.173623	0.001587	80	6	-0.422813	6.238471	-0.093961
31	6	-3.764749	0.240907	0.010031	81	7	-1.082392	8.978994	-0.131826
32	6	-1.658249	1.329900	-0.014322	82	6	0.095573	7.121441	0.860397
33	6	-1.819953	-0.977302	0.016016	83	6	-1.277838	6.764285	-1.069594
34	7	-3.158092	-0.959741	0.016466	84	6	-1.571115	8.119158	-1.048671
35	6	-3.041513	1.419883	-0.011787	85	6	-0.259006	8.460386	0.802093
36	1	-3.542031	2.377275	-0.042482	86	1	0.756665	6.774516	1.648227
37	7	0.303143	-2.050365	0.029783	87	1	-1.700065	6.135655	-1.846947
38	6	-0.723972	-4.598175	0.060803	88	1	-2.225743	8.560643	-1.794689
39	6	-0.965171	-2.211771	0.031293	89	1	0.121610	9.171060	1.530137
40	6	1.109812	-3.029981	0.043680	90	6	-1.267237	-5.963806	0.077624
41	6	0.645449	-4.344805	0.058796	91	7	-2.311446	-8.585507	0.109489
42	6	-1.545313	-3.476871	0.047281	92	6	-2.272359	-6.334599	0.979314
43	1	2.174303	-2.811958	0.046582	93	6	-0.800721	-6.942443	-0.808472
44	1	1.367368	-5.156058	0.083921	94	6	-1.345579	-8.216551	-0.756083
45	1	-2.627243	-3.568303	0.036936	95	6	-2.753056	-7.635106	0.958252
46	7	0.554614	2.149841	-0.028114	96	1	-2.672052	-5.628631	1.700503
47	6	-0.081705	4.810903	-0.071608	97	1	-0.033611	-6.718770	-1.542831
48	6	1.493931	3.002528	-0.038310	98	1	-1.008563	-8.995964	-1.433437
49	6	-0.690071	2.460960	-0.035672	99	1	-3.529275	-7.954159	1.647924
50	6	-1.057633	3.817920	-0.060518					

Table 11. Atomic coordinates oft he optimized geometry of **VII-C1**.

Center	Atomic number	Coordinates (Angstroms)			Center	Atomic number	Coordinates (Angstroms)		
		X	Y	Z			X	Y	Z
1	7	9,580	0,002	-0,019	76	1	18,600	0,1703	-0,752
2	6	12,358	-0,113	0,037	77	1	18,559	-1,3714	0,109
3	6	10,237	-0,589	-1,053	78	1	18,605	0,1557	1,014
4	6	10,242	0,537	1,042	79	6	-2,890	-0,0944	0,149
5	6	11,636	0,488	1,091	80	7	-5,616	-0,1102	0,138
6	6	11,632	-0,655	-1,047	81	7	-3,566	0,6206	-0,799
7	1	12,164	0,890	1,948	82	6	-3,588	-0,8372	1,132
8	1	12,159	-1,100	-1,881	83	6	-4,983	-0,8340	1,103
9	6	9,327	-1,096	-2,095	84	6	-4,900	0,5945	-0,776
10	6	7,449	-1,972	-3,936	85	1	-3,056	-1,3841	1,897
11	7	7,985	-0,893	-1,852	86	6	-5,925	-1,5217	1,998
12	6	9,755	-1,740	-3,260	87	6	-7,867	-2,7300	3,554
13	6	8,810	-2,184	-4,192	88	7	-7,260	-1,3129	1,705
14	6	7,076	-1,323	-2,756	89	6	-5,537	-2,3339	3,067
15	1	10,811	-1,896	-3,442	90	6	-6,516	-2,9465	3,857
16	1	9,131	-2,685	-5,099	91	6	-8,200	-1,9094	2,472
17	1	6,034	-1,142	-2,525	92	1	-4,486	-2,4887	3,281
18	1	6,685	-2,299	-4,631	93	1	-9,233	-1,7219	2,209
19	6	9,337	1,116	2,049	94	1	-8,656	-3,1856	4,140
20	6	7,465	2,145	3,817	95	6	-5,750	1,3195	-1,732
21	6	9,769	1,720	3,234	96	6	-7,503	2,6082	-3,426
22	7	7,993	1,025	1,752	97	6	-5,236	2,1103	-2,760
23	6	7,087	1,531	2,621	98	7	-7,106	1,1657	-1,540
24	6	8,828	2,241	4,129	99	6	-7,957	1,8021	-2,377
25	1	10,827	1,785	3,459	100	6	-6,124	2,7664	-3,623
26	1	6,044	1,438	2,347	101	1	-4,162	2,1984	-2,868
27	1	9,153	2,712	5,050	102	1	-9,016	1,6596	-2,197
28	1	6,704	2,536	4,482	103	1	-8,223	3,0982	-4,070
29	44	7,591	0,083	-0,058	104	44	-7,591	-0,0678	0,071
30	7	5,616	0,163	-0,091	105	7	-9,580	-0,0222	0,004
31	6	2,891	0,175	-0,080	106	6	-12,358	0,0444	-0,094
32	6	4,987	1,230	-0,657	107	6	-10,242	0,9422	0,698
33	6	4,897	-0,850	0,460	108	6	-10,237	-0,9551	-0,736
34	7	3,564	-0,873	0,481	109	6	-11,631	-0,9388	-0,801
35	6	3,592	1,258	-0,662	110	6	-11,636	0,9928	0,664
36	1	3,061	2,097	-1,090	111	1	-12,155	-1,6638	-1,411
37	7	7,101	-1,705	0,898	112	1	-12,166	1,7436	1,237
38	6	6,109	-4,017	2,139	113	7	-7,993	1,5636	1,297
39	6	5,743	-1,913	1,022	114	6	-8,831	3,7041	2,892
40	6	7,948	-2,639	1,387	115	6	-7,089	2,3370	1,941
41	6	7,489	-3,804	2,011	116	6	-9,337	1,8406	1,435
42	6	5,225	-3,054	1,635	117	6	-9,772	2,9069	2,229
43	1	9,007	-2,445	1,272	118	6	-7,469	3,4140	2,745
44	1	8,206	-4,523	2,387	119	1	-6,045	2,0825	1,805
45	1	4,150	-3,169	1,706	120	1	-10,830	3,1157	2,332
46	7	7,266	1,897	-1,024	121	1	-6,708	4,0052	3,241
47	6	6,531	4,288	-2,288	122	1	-9,157	4,5331	3,509
48	6	8,209	2,750	-1,484	123	7	-7,984	-1,6804	-1,183
49	6	5,932	2,222	-1,187	124	6	-8,810	-3,7823	-2,834
50	6	5,549	3,411	-1,815	125	6	-9,327	-1,8956	-1,412
51	6	7,881	3,951	-2,119	126	6	-7,074	-2,4955	-1,765
52	1	9,241	2,459	-1,336	127	6	-7,448	-3,5548	-2,595
53	1	4,499	3,651	-1,933	128	6	-9,755	-2,9422	-2,235
54	1	8,673	4,602	-2,471	129	1	-6,032	-2,2895	-1,558
55	6	13,836	-0,174	0,066	130	1	-6,684	-4,1811	-3,040
56	6	16,685	-0,292	0,124	131	1	-10,813	-3,1024	-2,408
57	6	14,530	-1,242	-0,539	132	1	-9,131	-4,5963	-3,474
58	6	14,591	0,833	0,702	133	6	-13,836	0,0802	-0,147
59	6	15,988	0,773	0,728	134	6	-16,685	0,1486	-0,249
60	6	15,927	-1,300	-0,506	135	6	-14,537	1,2995	-0,039
61	1	13,982	-2,053	-1,010	136	6	-14,585	-1,1046	-0,304
62	1	14,094	1,685	1,159	137	6	-15,983	-1,0685	-0,350
63	1	16,547	1,566	1,219	138	6	-15,934	1,3302	-0,090
64	1	16,436	-2,142	-0,967	139	1	-13,994	2,2355	0,059
65	6	1,416	0,117	-0,036	140	1	-14,083	-2,0663	-0,358
66	6	-1,415	-0,040	0,097	141	1	-16,536	-1,9977	-0,458
67	6	0,782	-0,849	0,774	142	1	-16,449	2,2841	-0,011
68	6	0,609	0,997	-0,787	143	6	-18,190	0,1879	-0,330
69	6	-0,782	0,916	-0,724	144	1	-18,636	-0,7374	0,049
70	6	-0,608	-0,925	0,843	145	1	-18,520	0,3070	-1,371
71	1	1,395	-1,537	1,345	146	1	-18,601	1,0278	0,240
72	1	1,051	1,744	-1,439	147	1	6,248	5,2136	-2,776
73	1	-1,395	1,592	-1,309	148	1	-6,230	-3,5785	4,690
74	1	-1,050	-1,690	1,472	149	1	5,730	-4,9113	2,620
75	6	18,192	-0,340	0,130	150	1	-5,748	3,3862	-4,429

Table 12. Atomic coordinates oft he optimized geometry of **VII-C2**.

Center	Atomic number	Coordinates (Angstroms)			Center	Atomic number	Coordinates (Angstroms)		
		X	Y	Z			X	Y	Z
1	7	9.568	0.529	-0.033	85	1	4.057	-5.278	1.261
2	6	12.348	0.545	-0.058	86	1	7.581	-6.452	-0.975
3	6	10.217	0.508	-1.228	87	1	6.768	-8.789	-0.847
4	6	10.238	0.558	1.149	88	1	3.382	-7.662	1.267
5	6	11.634	0.562	1.161	89	6	-2.876	-0.336	0.043
6	6	11.612	0.520	-1.263	90	7	-5.599	-0.485	0.020
7	1	12.169	0.554	2.102	91	7	-3.617	0.812	0.061
8	1	12.131	0.533	-2.214	92	6	-3.507	-1.603	0.010
9	6	9.299	0.482	-2.379	93	6	-4.901	-1.654	-0.001
10	6	7.407	0.431	-4.404	94	6	-4.946	0.706	0.049
11	7	7.957	0.477	-2.061	95	1	-2.925	-2.513	-0.020
12	6	9.720	0.462	-3.712	96	6	-5.780	-2.831	-0.039
13	6	8.768	0.437	-4.738	97	6	-7.612	-4.903	-0.113
14	6	7.041	0.451	-3.056	98	7	-7.133	-2.545	-0.048
15	1	10.776	0.466	-3.951	99	6	-5.320	-4.150	-0.067
16	1	9.083	0.421	-5.775	100	6	-6.243	-5.202	-0.104
17	1	6.000	0.447	-2.760	101	6	-8.018	-3.566	-0.084
18	1	6.638	0.411	-5.166	102	1	-4.256	-4.357	-0.059
19	6	9.341	0.573	2.317	103	1	-9.068	-3.300	-0.090
20	6	7.485	0.608	4.376	104	1	-8.359	-5.687	-0.141
21	6	9.785	0.605	3.642	105	6	-5.860	1.857	0.069
22	7	7.993	0.558	2.023	106	6	-7.709	3.889	0.093
23	6	7.095	0.576	3.035	107	6	-5.414	3.175	0.106
24	6	8.852	0.622	4.685	108	7	-7.200	1.537	0.046
25	1	10.846	0.618	3.862	109	6	-8.097	2.550	0.058
26	1	6.049	0.566	2.758	110	6	-6.342	4.232	0.120
27	1	9.185	0.647	5.716	111	1	-4.344	3.350	0.104
28	1	6.730	0.621	5.151	112	1	-9.144	2.275	0.044
29	44	7.576	0.510	-0.015	113	1	-8.480	4.650	0.123
30	7	5.600	0.487	0.001	114	6	-5.899	5.644	0.162
31	6	2.877	0.343	0.023	115	7	-5.053	8.348	0.246
32	6	4.904	1.659	-0.014	116	6	-4.696	6.014	0.794
33	6	4.945	-0.702	0.032	117	6	-6.666	6.669	-0.425
34	7	3.616	-0.806	0.041	118	6	-6.209	7.990	-0.361
35	6	3.511	1.609	0.001	119	6	-4.317	7.361	0.813
36	1	2.931	2.521	0.005	120	1	-4.067	5.281	1.288
37	7	7.198	-1.537	0.029	121	1	-7.592	6.454	-0.948
38	6	6.335	-4.230	0.097	122	1	-6.784	8.792	-0.813
39	6	5.857	-1.855	0.051	123	1	-3.397	7.666	1.300
40	6	8.093	-2.551	0.040	124	44	-7.575	-0.511	-0.005
41	6	7.702	-3.890	0.072	125	7	-9.566	-0.532	-0.034
42	6	5.408	-3.172	0.085	126	6	-12.347	-0.552	-0.074
43	1	9.140	-2.279	0.028	127	6	-10.243	-0.566	1.145
44	1	8.471	-4.653	0.101	128	6	-10.209	-0.509	-1.232
45	1	4.338	-3.345	0.081	129	6	-11.604	-0.522	-1.275
46	7	7.138	2.545	-0.052	130	6	-11.639	-0.572	1.148
47	6	6.253	5.204	-0.098	131	1	-12.117	-0.533	-2.229
48	6	8.025	3.565	-0.081	132	1	-12.179	-0.568	2.087
49	6	5.786	2.834	-0.044	133	7	-8.003	-0.566	2.030
50	6	5.327	4.154	-0.067	134	6	-8.875	-0.642	4.688
51	6	7.621	4.903	-0.105	135	6	-7.110	-0.587	3.047
52	1	9.074	3.297	-0.086	136	6	-9.352	-0.585	2.317
53	1	4.264	4.362	-0.063	137	6	-9.803	-0.623	3.640
54	1	8.370	5.685	-0.128	138	6	-7.507	-0.624	4.385
55	6	13.828	0.554	-0.072	139	1	-6.062	-0.573	2.776
56	6	16.680	0.568	-0.097	140	1	-10.865	-0.639	3.853
57	6	14.547	-0.083	-1.104	141	1	-6.756	-0.639	5.165
58	6	14.559	1.196	0.950	142	1	-9.214	-0.672	5.717
59	6	15.958	1.202	0.934	143	7	-7.945	-0.471	-2.053
60	6	15.946	-0.077	-1.112	144	6	-8.741	-0.423	-4.734
61	1	14.020	-0.616	-1.891	145	6	-9.285	-0.478	-2.378
62	1	14.041	1.718	1.749	146	6	-7.024	-0.441	-3.043
63	1	16.497	1.710	1.729	147	6	-7.382	-0.416	-4.393
64	1	16.476	-0.588	-1.912	148	6	-9.699	-0.454	-3.714
65	6	1.408	0.188	0.031	149	1	-5.984	-0.436	-2.742
66	6	-1.408	-0.178	0.047	150	1	-6.609	-0.393	-5.151
67	6	0.846	-1.092	0.220	151	1	-10.754	-0.459	-3.958
68	6	0.537	1.283	-0.148	152	1	-9.051	-0.405	-5.773
69	6	-0.845	1.102	-0.138	153	6	-13.826	-0.561	-0.095
70	6	-0.537	-1.274	0.229	154	6	-16.678	-0.581	-0.136
71	1	1.507	-1.938	0.363	155	6	-14.562	-1.210	0.919
72	1	0.921	2.284	-0.312	156	6	-14.541	0.075	-1.131
73	1	-1.507	1.948	-0.280	157	6	-15.940	0.064	-1.148
74	1	-0.921	-2.274	0.392	158	6	-15.960	-1.221	0.895
75	6	18.187	0.600	-0.126	159	1	-14.047	-1.739	1.716
76	1	18.546	1.477	-0.680	160	1	-14.011	0.606	-1.916
77	1	18.596	-0.288	-0.619	161	1	-16.467	0.568	-1.954
78	1	18.606	0.658	0.884	162	1	-16.502	-1.741	1.680
79	6	5.890	-5.642	0.136	163	6	-18.185	-0.569	-0.142
80	7	5.037	-8.344	0.213	164	1	-18.581	-0.511	-1.161
81	6	4.685	-6.011	0.766	165	1	-18.569	0.301	0.407
82	6	6.655	-6.667	-0.453	166	1	-18.595	-1.463	0.338
83	6	6.195	-7.987	-0.393	167	1	5.912	6.233	-0.116

84	6	4.304	-7.358	0.781	168	1	-5.900	-6.230	-0.126