Semiempirical Configuration Interaction Calculations for Ru–Centered Dyes
Supporting Information

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Contents

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1 Effect of Geometry on CI

Previously we showed that small changes in molecular structure changed the calculated TDDFT absorption spectrum.[40] To investigate this further, we have explored the calculated PM6scCI transitions (Figure S1) and the Boltzmann weighted sum (Figure S2) of the breathing mode of a complex which has been shown to be one of the dominant modes in the deactivation of the initial photoexcited state.

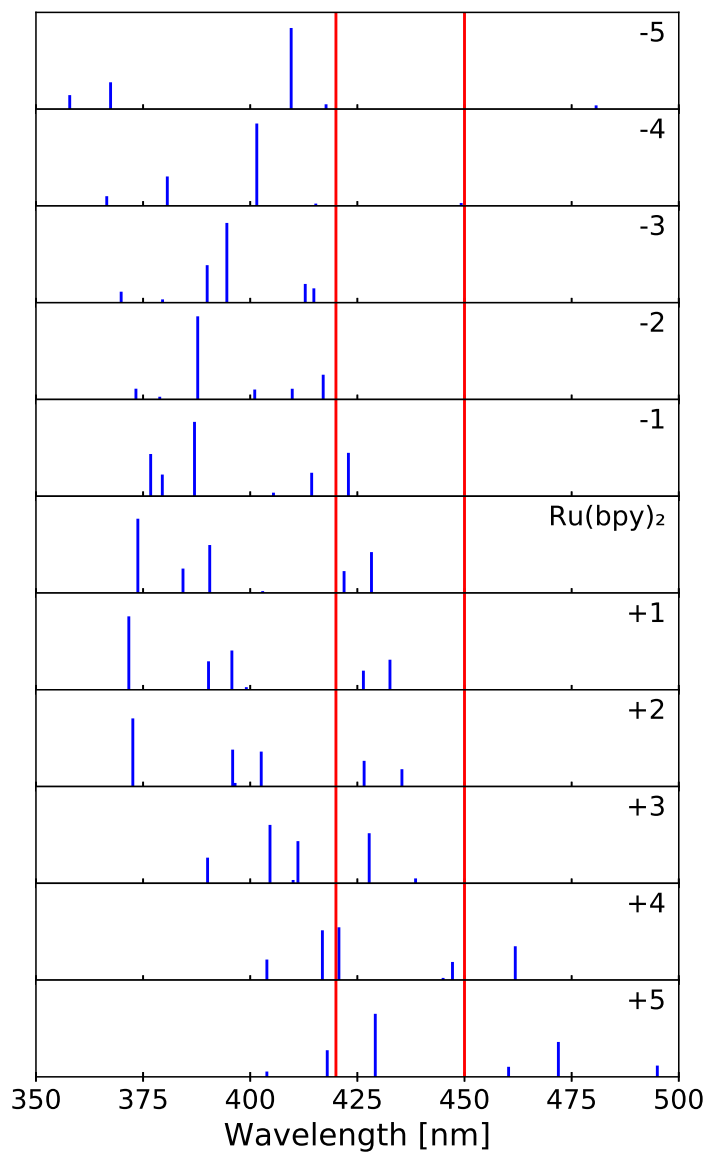Figure S1: Comparison of calculated PM6scCI transitions at $+/-$ the number of steps indicated along the breathing mode of Ru(BPy)$_2$ as calculated at the PBE0/6-31G(d,p)[C,N,H]SDD[Ru]—PCM(MeCN) level of theory. The experimental maxima are shown in red for reference.
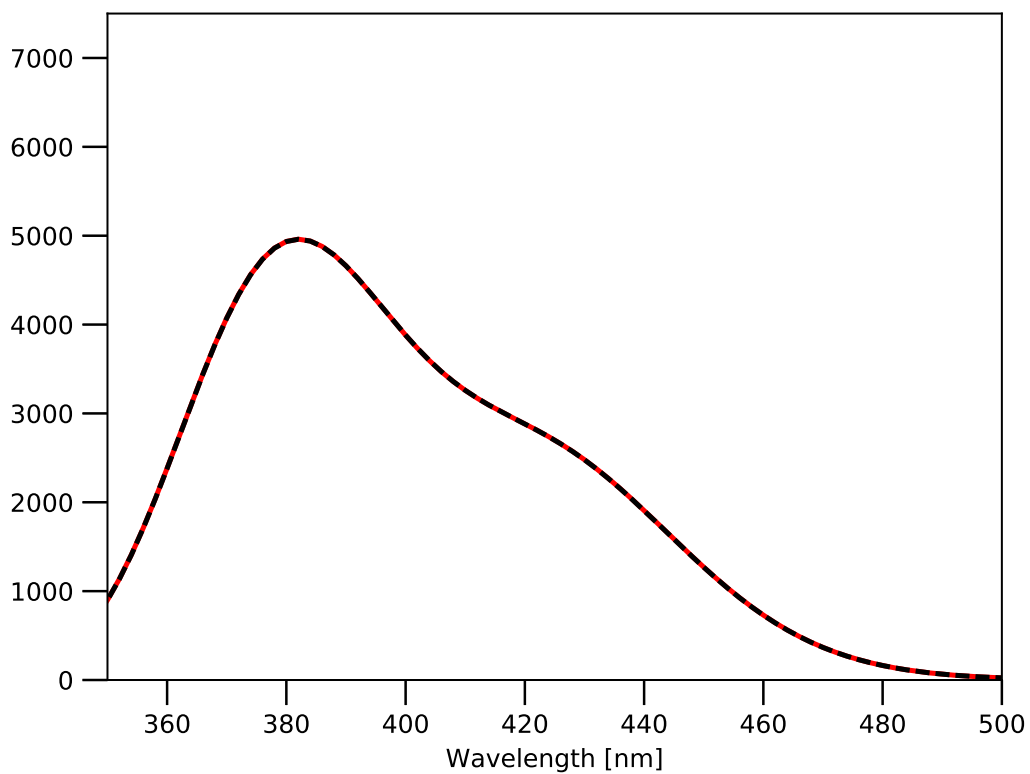
Figure S2: Comparison of PM6scCI calculated UV/Vis spectrum of the DFT optimized geometry minimum (red) and the Boltzmann weighted sum (dashed black line) at 10 steps along the breathing mode of Ru(BPy)$_2$ as calculated at the PBE0/6-31G(d,p)[C,N,H]SDD[Ru]—PCM(MeCN) level of theory.

2   CI Active Space

An active space of 5 molecular orbitals with 2 doubly occupied orbitals was used for parameterization of the CI model and for subsequent calculations. In MOPAC, this active space is specified using the keyword `c.i.=(5,2)`. This is a somewhat small active space, and while it is consistent with the semiempirical philosophy to use a smaller active space, there is a legitimate question as to whether a larger active space would have a significant impact on the results. To assess the effect of larger active spaces on the results, calculations of the UV/Vis spectra were made using a number of different active spaces for two compounds, ru(BPy)$_2$ and Ru(TPy)$_2$. The same set of CI parameters was used for all calculations as described in the section on MOPAC headers below. The results of these calculations are depicted in figures S3 and S4 below. It is clearly seen that the results from the many different active spaces are quite similar. Larger active spaces tend to add some higher energy states, but the energies seen up to 3.5 eV are quite similar. This is an indication that the size of the active space does not strongly affect the results and that the (5,2) active space used for parameterization and calculation is adequate for the intended purpose.
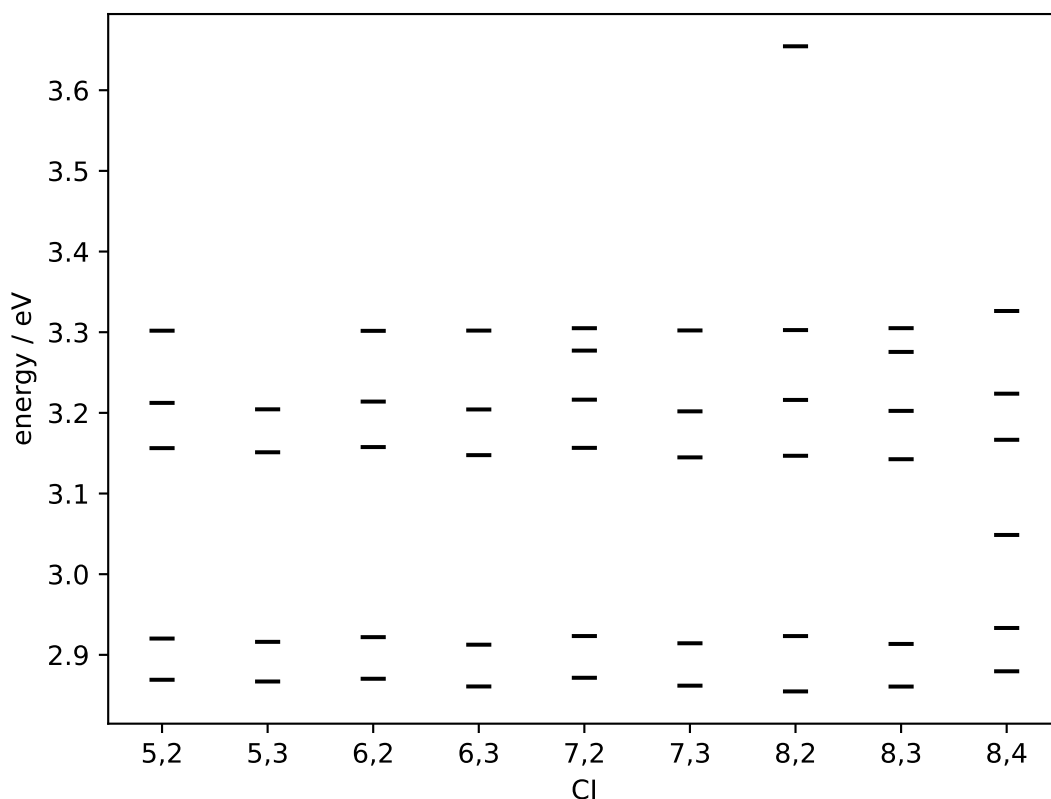
Figure S3: Plot of CI energies for the indicated active spaces for Ru(BPy)$_2$.
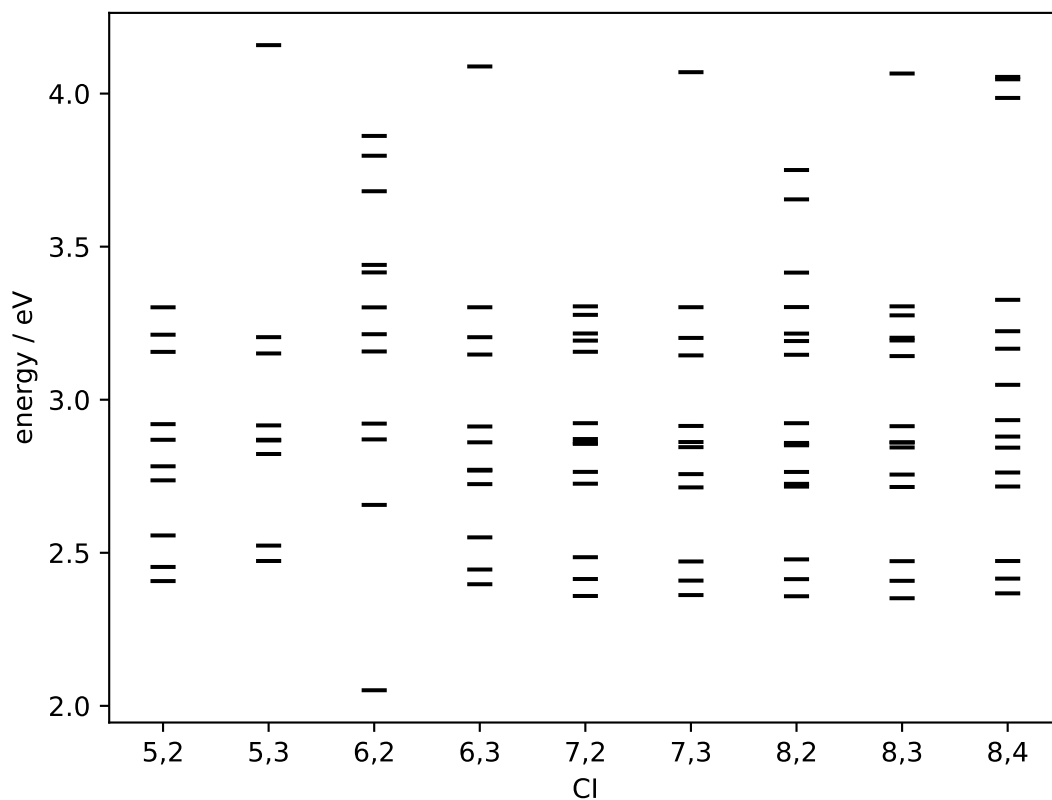
Figure S4: Plot of CI energies for the indicated active spaces for Ru(TPy)$_2$.

3 Basis Set

The PM6 basis set parameters for Ru are presented in a format suitable for use in MOPAC below (called rRu.basis in headers).

```
USS        Ru      -44.90152100
UPP        Ru      -41.42440900
UDD        Ru      -37.93451400
ZS         Ru        1.45919500
ZP         Ru        5.53720100
ZD         Ru        2.09316400
BETAS      Ru      -12.85950800
BETAP      Ru       -8.47551800
BETAD      Ru       -3.83079700
GSS        Ru        4.41364279
GPP        Ru       22.49044761
GSP        Ru        5.35699582
```

```
GP2       Ru      19.59995666
HSP       Ru       0.00805809
ZSN       Ru       0.98444900
ZPN       Ru       4.58661300
ZDN       Ru       0.76533200
FOSD      Ru       5.91740400
G2SD      Ru       5.85973800
ALPB_H    Ru       2.89201896
XFAC_H    Ru       7.14609528
ALPB_C    Ru       2.78870566
XFAC_C    Ru       1.09168381
ALPB_N    Ru       3.10082239
XFAC_N    Ru       2.32425209
ALPB_RU   Ru       0.57205600
XFAC_RU   Ru       0.09780500
```

4 MOPAC headers

The MOPAC keywords used for PM6 structural optimization using basis set rRu where the molecular charge replaces XX:

```
pm6 opt bfgs gnorm=1.0 scfcrt=1e-8 charge=XX external=rRu.basis
```

The MOPAC keywords used for PM6scCI using basis set rRu where the molecular charge replaces XX:

```
pm6 1scf charge=XX c.i.=(5,2) cisd meci external=rRu.basis jscale +
fss=1.0097  fsp=1.0182  fsd=1.0009  fpp=1.0082  fpd=1.0090  fdd=0.9844
```

Note that the input keywords jscale, fss, fsp, fsd, fpp, fpd, and fdd are enabled by our modifications to the MOPAC source code and will not work with the default version of MOPAC.

5 Optimized Structures

Cartesian coordinates of optimized geometries at the PM6/rRu level of theory for 13 Ru-containing light harvesting dyes are presented below.

$[Ru(DQPz)_2]^{2+}$

```
1    C        2.894912   -0.914317   -3.145804
2    C        3.909967   -0.007076   -2.994490
3    C        3.741208    1.097759   -2.096879
4    C        2.501522    1.237132   -1.400377
5    C        1.727648   -0.786597   -2.335866
6    H        5.736776    1.907163   -2.433357
```

7	H	2.963330	-1.743015	-3.857189
8	H	4.845661	-0.097193	-3.558068
9	C	4.785755	2.051409	-1.908524
10	C	2.283767	2.466347	-0.669447
11	H	0.925563	-1.541986	-2.415273
12	C	3.333860	3.351800	-0.473381
13	C	4.595505	3.131975	-1.083140
14	H	3.211140	4.256660	0.132207
15	H	5.400416	3.855235	-0.905032
16	C	-4.703966	2.758596	1.609451
17	C	-4.807915	1.569281	2.285728
18	C	-3.706624	0.660140	2.312375
19	C	-2.511306	0.959771	1.589315
20	C	-2.377482	2.275481	1.005933
21	C	-3.477770	3.120743	0.994361
22	H	-4.687199	-0.763758	3.650281
23	H	-5.547674	3.455598	1.561457
24	H	-5.727854	1.302082	2.816147
25	C	-3.780110	-0.548972	3.074462
26	H	-3.414690	4.108903	0.525375
27	C	-1.584466	-1.106128	2.261584
28	C	-2.708327	-1.403480	3.084544
29	H	-0.738972	-1.814413	2.234462
30	H	-2.702345	-2.313243	3.690843
31	C	-0.746865	4.198309	0.389196
32	C	0.556390	4.232282	-0.073003
33	H	-1.376358	5.042743	0.618934
34	H	1.184198	5.076761	-0.320112
35	N	1.538063	0.212712	-1.456600
36	N	-1.486727	-0.003079	1.496704
37	C	-2.709560	1.404128	-3.082190
38	C	-3.783248	0.552173	-3.070823
39	C	-3.710115	-0.657635	-2.309518
40	C	-2.513790	-0.959707	-1.588946
41	C	-1.585336	1.105275	-2.259956
42	H	-5.731245	-1.299482	-2.812931
43	H	-2.702162	2.313596	-3.688921
44	H	-4.690708	0.768609	-3.645325
45	C	-4.811029	-1.567065	-2.283832
46	C	-2.378793	-2.276346	-1.008764
47	H	-0.739512	1.813133	-2.233387
48	C	-3.478985	-3.121461	-0.997479
49	C	-4.705711	-2.758144	-1.610820
50	H	-3.415521	-4.110367	-0.530234
51	H	-5.548739	-3.456107	-1.564502

52	C	4.598428	-3.131932	1.066461
53	C	4.788385	-2.054181	1.895851
54	C	3.742304	-1.103853	2.090756
55	C	2.502563	-1.242052	1.394218
56	C	2.284525	-2.469402	0.660587
57	C	3.335598	-3.352651	0.459665
58	H	4.843952	0.082231	3.561112
59	H	5.404354	-3.852777	0.883445
60	H	5.740303	-1.910345	2.419533
61	C	3.908828	-0.004811	2.996191
62	H	3.212736	-4.256362	-0.147443
63	C	1.726520	0.776377	2.339777
64	C	2.892365	0.899527	3.153078
65	H	0.924113	1.531759	2.420782
66	H	2.958178	1.723056	3.870822
67	C	0.557717	-4.235769	0.057598
68	C	-0.745698	-4.200043	-0.403997
69	H	1.185553	-5.081812	0.299634
70	H	-1.374813	-5.043230	-0.639170
71	N	-1.487622	0.001458	-1.496512
72	N	1.538111	-0.218244	1.455320
73	Ru	0.030722	-0.001540	-0.000098
74	N	-0.036979	-2.033609	-0.153614
75	N	-0.035873	2.030916	0.151959
76	C	-1.105933	2.810540	0.521478
77	C	-1.106159	-2.811837	-0.527590
78	N	0.981951	2.888621	-0.211474
79	N	0.982154	-2.892415	0.204289

$[Ru(BPy)_3]^{2+}$

1	C	-0.726717	-2.907606	2.544753
2	C	-2.068705	-2.671772	2.861258
3	C	-2.776172	-1.694873	2.154599
4	C	-2.125707	-0.968878	1.142481
5	C	-0.122256	-2.157228	1.527036
6	H	-0.151882	-3.668137	3.084753
7	H	0.930051	-2.311920	1.245992
8	C	-3.856891	2.086018	-1.252535
9	C	-4.134875	0.450220	0.499475
10	H	-4.255364	2.880750	-1.892771
11	H	-4.761778	-0.047759	1.246095
12	N	-0.796344	-1.197132	0.826001
13	C	0.669884	2.952971	2.509700
14	C	2.009574	2.722980	2.840189

15	C	2.723330	1.737093	2.152777
16	C	2.081566	0.996609	1.145350
17	C	0.074028	2.187758	1.498350
18	H	0.089993	3.719985	3.034898
19	H	-0.976270	2.336513	1.207496
20	C	3.834457	-2.090585	-1.191340
21	C	4.097795	-0.427313	0.536902
22	H	4.238693	-2.894702	-1.816323
23	H	4.718693	0.083509	1.279902
24	N	0.754333	1.218758	0.815794
25	Ru	-0.014215	0.000013	-0.691814
26	C	2.751740	-0.064900	0.359276
27	C	2.498812	-1.691135	-1.333170
28	C	-2.788509	0.082254	0.336251
29	C	-2.521005	1.682099	-1.379100
30	C	4.642264	-1.449224	-0.246316
31	C	-4.672198	1.460746	-0.303355
32	N	-1.977709	0.695647	-0.604951
33	N	1.948445	-0.693986	-0.577990
34	H	1.829925	-2.168590	-2.064388
35	H	3.772242	1.545836	2.401205
36	H	-3.827050	-1.499701	2.391912
37	H	-1.846322	2.147172	-2.113274
38	H	2.495660	3.308818	3.630212
39	H	5.691474	-1.743836	-0.120405
40	H	-2.561501	-3.246335	3.655251
41	H	-5.721688	1.758956	-0.189275
42	N	-0.617232	-1.186748	-2.296230
43	C	-1.247295	-2.396554	-2.213882
44	C	-0.347762	-0.674968	-3.555233
45	C	-1.625846	-3.125031	-3.349516
46	H	-1.442129	-2.771954	-1.198380
47	C	-0.707421	-1.367285	-4.723913
48	C	-1.352857	-2.602758	-4.618151
49	H	-2.130997	-4.091210	-3.241285
50	H	-0.487585	-0.946503	-5.710279
51	H	-1.641832	-3.155376	-5.520596
52	N	0.603018	1.164238	-2.307782
53	C	0.341946	0.635740	-3.561622
54	C	1.234162	2.374282	-2.237373
55	C	0.709916	1.312099	-4.737014
56	C	1.621318	3.087014	-3.380152
57	H	1.422524	2.763036	-1.225684
58	C	1.356009	2.548259	-4.643543
59	H	0.496181	0.878344	-5.719260

| 60 | H | 2.127220 | 4.053835 | -3.281146 |
| 61 | H | 1.651545 | 3.088516 | -5.551411 |

$[\text{Ru(DQxP)}_2]^{2+}$

1	C	0.014785	5.028136	0.008929
2	C	-1.109641	4.321081	0.425909
3	C	-1.101280	2.911309	0.394012
4	C	1.119785	2.908676	-0.394193
5	C	1.134947	4.318734	-0.414913
6	H	0.017998	6.126326	0.014577
7	H	-1.984835	4.873308	0.785758
8	H	2.013088	4.869005	-0.770623
9	N	0.007631	2.168070	-0.002218
10	C	2.377961	0.999003	-1.508423
11	C	3.558122	2.917395	-1.049887
12	C	3.622777	0.963535	-2.229662
13	C	4.340278	2.176555	-1.889338
14	H	3.764883	3.868212	-0.576313
15	C	3.882613	-0.135765	-3.052537
16	C	1.735707	-1.053279	-2.344318
17	H	5.330139	2.423141	-2.249348
18	C	2.907554	-1.132068	-3.122531
19	H	4.814788	-0.204831	-3.622544
20	H	0.975852	-1.846525	-2.387133
21	H	3.051781	-1.994017	-3.782268
22	C	-2.369341	1.004042	1.500192
23	C	-3.544759	2.923035	1.033088
24	C	-3.619265	0.969033	2.212159
25	C	-4.334253	2.181530	1.865322
26	H	-3.747047	3.874462	0.558827
27	C	-3.883653	-0.129170	3.035054
28	C	-1.732125	-1.047533	2.343178
29	H	-5.327371	2.427438	2.216849
30	C	-2.908995	-1.125332	3.113638
31	H	-4.819217	-0.197872	3.599081
32	H	-0.972313	-1.840494	2.391487
33	H	-3.057845	-1.986051	3.773992
34	N	1.458378	-0.011969	-1.501354
35	N	-1.450415	-0.007612	1.500031
36	N	-2.301778	2.223619	0.754714
37	N	2.316637	2.218790	-0.762623
38	Ru	0.003662	0.000015	-0.001376
39	C	-1.106054	-2.910808	-0.398619
40	C	1.111950	-2.911144	0.398418

41	C	-1.117390	-4.320816	-0.424807
42	C	1.124104	-4.321057	0.423870
43	C	0.003215	-5.029087	-0.000523
44	H	-1.992164	-4.872858	-0.785660
45	H	1.999301	-4.873116	0.784076
46	H	0.003167	-6.127218	-0.000651
47	N	0.002892	-2.168887	-0.000083
48	C	-2.367185	-1.002314	-1.511673
49	C	-3.542256	-2.925859	-1.059821
50	C	-3.611369	-0.969066	-2.234136
51	C	-4.325547	-2.185424	-1.898379
52	H	-3.746325	-3.879191	-0.590083
53	C	-3.872802	0.130413	-3.056006
54	C	-1.728772	1.052570	-2.345324
55	H	-5.313722	-2.434486	-2.261373
56	C	-2.901052	1.130602	-3.122435
57	H	-4.802943	0.197646	-3.629340
58	H	-0.969583	1.846770	-2.386916
59	H	-3.048358	1.994246	-3.779480
60	C	2.369482	-1.002694	1.514272
61	C	3.547350	-2.924791	1.065926
62	C	3.609994	-0.968948	2.242652
63	C	4.327048	-2.183588	1.907236
64	H	3.754018	-3.877678	0.596512
65	C	3.866406	0.129369	3.067938
66	C	1.724821	1.049862	2.349531
67	H	5.314867	-2.430964	2.272265
68	C	2.892341	1.127204	3.133846
69	H	4.793972	0.195670	3.645297
70	H	0.963974	1.842402	2.389415
71	H	3.034532	1.987928	3.795632
72	N	-2.303952	-2.223276	-0.767809
73	N	-1.449167	0.009957	-1.504291
74	N	2.309373	-2.223221	0.769328
75	N	1.451729	0.009595	1.503595

[Ru(DBPzP)$_2$]$^{2+}$

1	C	-1.582329	2.996905	4.072647
2	C	-2.990557	1.412228	5.260010
3	H	-1.196229	4.014936	3.924004
4	H	-3.717426	1.176421	6.049704
5	C	-0.667801	-3.547737	-1.122760
6	C	1.175783	-4.065370	0.392437
7	H	-1.233109	-3.733011	-2.050545

8	H	2.064049	-4.660031	0.660504
9	Ru	-1.019398	-0.753162	2.225486
10	C	0.736423	-3.048572	1.242243
11	C	-1.077525	-2.539171	-0.247744
12	C	-2.540921	0.394164	4.418270
13	C	-1.142479	1.969239	3.238485
14	C	0.465521	-4.308926	-0.794461
15	H	0.800530	-5.108088	-1.475111
16	C	-2.509744	2.715676	5.084528
17	H	-2.858957	3.517852	5.740664
18	N	-1.606090	0.639684	3.384426
19	N	-0.379355	-2.286632	0.924509
20	C	-2.715203	-3.083817	3.530628
21	C	-3.632275	-3.059699	4.646249
22	C	0.936642	1.007828	0.468751
23	C	1.246125	2.416924	0.541694
24	C	-4.002352	-0.498663	-0.864787
25	C	-3.515918	0.034508	0.391705
26	C	2.369974	-2.288814	4.381511
27	C	1.291848	-1.321345	4.353621
28	N	0.576517	-1.508959	3.158817
29	N	-0.004030	0.722404	1.495347
30	N	-2.223092	-1.762761	3.353165
31	N	-2.358949	-0.681328	0.743027
32	N	0.511067	3.014592	1.601133
33	N	-3.717891	-1.740913	5.167792
34	N	2.327140	-3.071639	3.220071
35	N	-3.160509	-1.533700	-1.292087
36	C	1.278353	-2.607493	2.522921
37	C	-2.212230	-1.627410	-0.346464
38	C	-2.904854	-1.009013	4.415813
39	C	-0.199904	2.031270	2.138191
40	C	1.101264	-0.408734	5.406424
41	C	1.989484	-0.478796	6.468354
42	H	1.882668	0.211007	7.313272
43	C	3.050813	-1.426337	6.505081
44	H	3.715803	-1.427320	7.376243
45	C	3.257725	-2.330565	5.482204
46	H	4.071041	-3.062209	5.500185
47	H	0.290749	0.316554	5.382409
48	C	-4.181816	1.087322	1.044677
49	C	-5.320648	1.587451	0.433095
50	H	-5.874825	2.407923	0.903348
51	C	-5.806482	1.069244	-0.800125
52	H	-6.713388	1.511680	-1.227844

```
53      C      -5.169195      0.036934     -1.459220
54      H      -5.533695     -0.368950     -2.407498
55      H      -3.814410      1.486780      1.987515
56      C      -4.279961     -4.231966      5.059233
57      C      -4.003293     -5.401126      4.357514
58      H      -4.491834     -6.335872      4.653886
59      C      -3.106382     -5.418703      3.268004
60      H      -2.926814     -6.366434      2.752161
61      C      -2.448896     -4.266664      2.835292
62      H      -1.764372     -4.296543      1.997000
63      C       2.154056      2.992211     -0.357385
64      C       2.734792      2.157964     -1.308094
65      H       3.448708      2.575398     -2.026620
66      C       2.429186      0.782276     -1.374004
67      H       2.915494      0.173434     -2.141496
68      C       1.529147      0.183360     -0.491325
69      H       1.306588     -0.874122     -0.554844
70      H       2.388078      4.059611     -0.301245
71      H      -4.974689     -4.211945      5.904584
```

Ru[BPy–2COOH)$_2$(NCS)$_2$

```
 1      C      -0.862075     -2.963056      2.334633
 2      C      -2.247885     -2.762335      2.546173
 3      C      -2.914856     -1.765728      1.841538
 4      C      -2.194677     -0.971572      0.922193
 5      C      -0.199744     -2.164974      1.417033
 6      H      -0.339023     -3.749037      2.888979
 7      H       0.870742     -2.291129      1.203841
 8      C      -3.602938      2.286500     -1.381399
 9      C      -4.108290      0.546938      0.234688
10      H      -3.939741      3.128104     -1.997296
11      H      -4.816359      0.018548      0.883511
12      N      -0.834577     -1.172829      0.688639
13      C       0.863317      2.965280      2.332853
14      C       2.248869      2.763948      2.544956
15      C       2.915588      1.766652      1.840926
16      C       2.195237      0.972708      0.921742
17      C       0.200683      2.166762      1.416007
18      H       0.340257      3.751602      2.886770
19      H      -0.869901      2.292942      1.202937
20      C       3.603443     -2.284554     -1.382287
21      C       4.108560     -0.545736      0.234568
22      H       3.940275     -3.126119     -1.998231
23      H       4.816426     -0.017559      0.883782
```

```
24      N           0.835133     1.173870     0.688191
25      Ru          0.000081     0.000713    -0.738595
26      C           2.762698    -0.127235     0.155036
27      C           2.296786    -1.838833    -1.431382
28      C          -2.762501     0.128302     0.155441
29      C          -2.296284     1.840779    -1.430316
30      C           4.527398    -1.632431    -0.524264
31      C          -4.527066     1.633526    -0.524321
32      N          -1.838057     0.767603    -0.676831
33      N           1.838284    -0.766308    -0.677191
34      H           1.545897    -2.303050    -2.093276
35      H           3.988727     1.602174     1.994816
36      C           5.932012    -2.078785    -0.426635
37      O           6.819338    -1.641220     0.269968
38      O           6.178753    -3.145267    -1.261411
39      H           7.127860    -3.449425    -1.213214
40      C           3.013587     3.596490     3.501378
41      O           4.175488     3.506762     3.822311
42      O           2.219317     4.573608     4.057613
43      H           2.724789     5.150289     4.697180
44      H          -3.988218    -1.601865     1.994562
45      H          -1.545367     2.305195    -2.092023
46      C          -3.013232    -3.595689     3.501477
47      O          -4.175176    -3.504972     3.822059
48      O          -2.220656    -4.575217     4.055732
49      H          -2.727119    -5.152901     4.693494
50      C          -5.932213     2.078453    -0.428245
51      O          -6.819694     1.641365     0.268424
52      O          -6.179849     3.142472    -1.266015
53      H          -7.129722     3.444814    -1.219647
54      N           0.700770     1.247760    -2.175994
55      C           1.106326     1.991580    -2.999059
56      S           1.644409     3.037891    -4.090026
57      N          -0.700664    -1.245671    -2.176651
58      C          -1.105956    -1.992972    -2.996613
59      S          -1.643802    -3.042496    -4.084551
```

[Ru(TPy)$_2$]$^{2+}$

```
1       C           2.663330     0.830354     0.851045
2       C           4.065762     0.838738     0.853982
3       C           4.753145    -0.006099    -0.027153
4       C           4.054935    -0.849653    -0.900629
5       C           2.652647    -0.839185    -0.882827
6       H           4.620153     1.493860     1.532659
```

7	H	5.850234	−0.007076	−0.033119
8	H	4.601029	−1.505803	−1.585244
9	N	1.970247	−0.003813	−0.012096
10	C	1.757567	1.640343	1.695379
11	C	2.201648	2.566930	2.653683
12	C	−0.500190	2.135640	2.218800
13	C	1.263890	3.284515	3.401332
14	H	3.271806	2.727561	2.815411
15	C	−0.102328	3.068523	3.183577
16	H	−1.561054	1.930450	2.011059
17	H	1.596210	4.011538	4.153148
18	H	−0.852165	3.621547	3.759824
19	C	1.736530	−1.647463	−1.717261
20	C	2.168642	−2.573696	−2.681433
21	C	−0.527176	−2.139681	−2.215462
22	C	1.222048	−3.289138	−3.419693
23	H	3.236869	−2.735719	−2.855151
24	C	−0.141432	−3.071529	−3.186215
25	H	−1.585611	−1.934322	−1.995215
26	H	1.544845	−4.015373	−4.176168
27	H	−0.898369	−3.622573	−3.755078
28	N	0.400005	1.423296	1.476531
29	N	0.381877	−1.428740	−1.482695
30	C	−4.754096	0.005191	0.027158
31	C	−4.057639	−0.873427	0.866815
32	C	−2.655166	−0.865572	0.848825
33	C	−2.662373	0.868427	−0.820188
34	C	−4.064639	0.881431	−0.821241
35	H	−5.851065	0.006860	0.033533
36	H	−4.604844	−1.554245	1.525940
37	H	−4.617572	1.564251	−1.473511
38	N	−1.970918	−0.000134	0.009999
39	C	−1.740499	−1.706113	1.652439
40	C	−2.174573	−2.667263	2.580715
41	C	0.522109	−2.218294	2.134339
42	C	−1.229431	−3.411277	3.292365
43	H	−3.243121	−2.834331	2.747061
44	C	0.134409	−3.185918	3.068786
45	H	1.580895	−2.005004	1.923691
46	H	−1.553610	−4.165635	4.020121
47	H	0.890298	−3.758663	3.616988
48	C	−1.754541	1.706590	−1.634230
49	C	−2.196478	2.668618	−2.557804
50	C	0.504018	2.215093	−2.139391
51	C	−1.257432	3.410980	−3.279001

52	H	-3.266469	2.837462	-2.713418
53	C	0.108314	3.183932	-3.069098
54	H	1.564543	2.000066	-1.939497
55	H	-1.587949	4.165448	-4.003653
56	H	0.859409	3.756295	-3.624643
57	N	-0.385455	-1.480395	1.426960
58	N	-0.397554	1.477719	-1.423874
59	Ru	-0.000242	-0.002177	-0.001049

$[Ru(PzPyPz)_2]^{2+}$
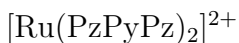
1	C	-1.518291	2.866626	3.994998
2	C	-2.977218	1.277594	5.161149
3	H	-1.125023	3.882602	3.886487
4	H	-3.706943	1.070227	5.950505
5	C	-0.689479	-3.625730	-1.205720
6	C	1.131529	-4.169817	0.343816
7	H	-1.221859	-3.821254	-2.142166
8	H	1.999146	-4.785778	0.602080
9	Ru	-1.011660	-0.906413	2.066561
10	C	0.687770	-3.137662	1.181092
11	C	-1.091682	-2.608534	-0.330113
12	C	-2.535484	0.275402	4.287231
13	C	-1.111067	1.826586	3.149133
14	C	0.427414	-4.397337	-0.848797
15	H	0.759408	-5.202291	-1.522055
16	C	-2.455451	2.570261	4.997065
17	H	-2.789438	3.372696	5.672496
18	N	-1.614747	0.547350	3.292755
19	N	-0.409475	-2.365849	0.847399
20	N	-2.922561	-1.105858	4.261931
21	C	-3.823001	-1.823629	5.084196
22	C	-2.909287	-3.178445	3.511642
23	C	-3.821586	-3.127786	4.620454
24	H	-4.367101	-1.362574	5.897695
25	H	-2.661704	-4.043853	2.907366
26	H	-4.391043	-3.963253	5.005334
27	N	-0.172306	1.886468	2.065628
28	C	0.586757	2.970504	1.565047
29	C	1.004132	1.079541	0.385113
30	C	1.329685	2.473465	0.508285
31	H	0.535000	3.965123	1.987437
32	H	1.400645	0.376340	-0.338600
33	H	2.027033	3.014337	-0.117329
34	N	-2.194759	-1.703028	-0.477859

35	C	-3.160794	-1.590887	-1.505457
36	C	-3.998323	-0.549794	-1.143782
37	H	-3.169147	-2.236287	-2.373490
38	C	-3.519885	-0.043387	0.112734
39	H	-4.854017	-0.174251	-1.688886
40	H	-3.936295	0.775419	0.688968
41	N	1.241883	-2.722960	2.437964
42	C	2.352104	-3.217718	3.162526
43	C	2.450402	-2.442413	4.304876
44	H	2.953252	-4.047896	2.816888
45	C	1.386301	-1.478582	4.251565
46	H	3.180714	-2.529889	5.098314
47	H	1.162672	-0.710016	4.982753
48	N	0.653347	-1.646854	3.121969
49	N	0.094600	0.722191	1.326495
50	N	-2.363150	-1.955488	3.293378
51	N	-2.429553	-0.741748	0.519118

$[Ru(DQP)_2]^{2+}$

1	C	-1.149112	-2.794727	0.292082
2	C	-1.147114	-4.205739	0.341862
3	C	0.001422	-4.916423	0.001868
4	C	1.149364	-4.205171	-0.339121
5	C	1.151117	-2.794121	-0.289092
6	N	0.000792	-2.085671	0.001636
7	H	-2.044680	-4.752402	0.650574
8	H	0.001812	-6.012539	0.002345
9	C	-3.612251	-2.769426	0.245377
10	C	3.614338	-2.766523	-0.244100
11	H	2.046370	-4.751410	-0.649892
12	C	4.874943	-2.373039	-0.768988
13	C	-4.873810	-2.376577	0.768214
14	C	4.955424	-1.358832	-1.689903
15	H	5.769244	-2.924789	-0.460642
16	C	2.439575	-2.116429	-0.595186
17	C	-4.956369	-1.360449	1.686845
18	H	-5.767307	-2.929794	0.459840
19	C	-2.438416	-2.117707	0.596896
20	C	3.786363	-0.609575	-2.025378
21	H	5.905061	-1.106099	-2.172001
22	C	2.550347	-0.911213	-1.379690
23	C	-2.551000	-0.911669	1.379805
24	C	-3.788288	-0.609717	2.022750
25	H	-5.907020	-1.107461	2.166799

26	N	1.460299	-0.036760	-1.505187
27	C	3.820774	0.449865	-2.986891
28	N	-1.461536	-0.036513	1.506605
29	C	-3.825305	0.451518	2.982047
30	C	2.688428	1.190790	-3.215310
31	H	4.750085	0.645782	-3.531868
32	C	1.531798	0.948858	-2.418984
33	C	-1.535248	0.950371	2.418868
34	C	-2.693906	1.193533	3.211777
35	H	-4.756215	0.648165	3.524200
36	H	2.659794	1.976865	-3.974695
37	H	0.645046	1.595993	-2.524122
38	H	-0.648803	1.597758	2.525144
39	H	-2.667211	1.981391	3.969701
40	C	1.150526	2.794370	0.290898
41	C	3.613637	2.767602	0.245759
42	C	2.439196	2.116766	0.597130
43	C	2.550553	0.911363	1.381091
44	N	1.460809	0.036437	1.507089
45	C	1.533731	-0.950725	2.419007
46	H	0.647414	-1.598319	2.524230
47	C	2.691557	-1.193816	3.213509
48	H	2.664502	-1.982148	3.970700
49	C	3.822896	-0.451197	2.985515
50	H	4.752752	-0.647109	3.529875
51	C	3.787023	0.609662	2.025928
52	C	4.955301	1.360816	1.691432
53	H	5.904924	1.109165	2.174023
54	C	4.874151	2.375497	0.771044
55	H	5.768486	2.928076	0.463358
56	N	0.000168	2.086090	0.000959
57	C	-1.149468	2.795161	-0.290356
58	C	-3.612725	2.769793	-0.244722
59	C	-2.438648	2.118394	-0.595829
60	C	-2.550295	0.912732	-1.379349
61	N	-1.460984	0.037153	-1.504890
62	C	-1.533990	-0.949760	-2.417044
63	H	-0.648097	-1.598023	-2.521842
64	C	-2.691587	-1.192047	-3.211967
65	C	-3.822987	-0.449592	-2.983660
66	H	-4.753128	-0.645596	-3.527350
67	C	-3.786810	0.611363	-2.023974
68	C	-4.955252	1.361645	-1.688595
69	H	-5.905388	1.108959	-2.169606
70	C	-4.873643	2.377018	-0.768930

71	H	−5.767718	2.929687	−0.461117
72	C	−1.146982	4.206129	−0.340985
73	H	−2.043919	4.752845	−0.651269
74	C	0.001569	4.916859	−0.000622
75	H	0.001946	6.012954	−0.000728
76	C	1.149476	4.205497	0.339957
77	H	2.047317	4.751504	0.649216
78	Ru	−0.000049	0.000172	0.001253
79	H	−2.663751	−1.979724	−3.969796
80	H	3.594914	−3.634741	0.424119
81	H	−3.591325	−3.638227	−0.421998
82	H	3.593580	3.635162	−0.423554
83	H	−3.592329	3.638181	0.423288

$[Ru(DCpP)_2]^{2+}$

1	C	2.510960	−0.834267	−3.504241
2	C	3.543534	0.103524	−3.429302
3	C	3.528403	1.044053	−2.392644
4	C	2.477901	1.017145	−1.461417
5	C	1.501542	−0.823642	−2.528363
6	H	2.490709	−1.580186	−4.307725
7	H	4.357219	0.101548	−4.166275
8	H	0.681539	−1.558004	−2.552152
9	C	−3.522917	1.049231	2.402446
10	C	−2.476938	1.017981	1.466095
11	H	−4.346209	0.111589	4.181045
12	C	−3.536371	0.109328	3.439720
13	C	−1.502892	−0.826281	2.528314
14	C	−2.507658	−0.833119	3.509082
15	H	−0.686289	−1.564426	2.547765
16	H	−2.486720	−1.579743	4.311953
17	C	−1.192519	4.214812	0.161724
18	C	1.192922	4.214083	−0.155350
19	H	−2.150710	4.742002	0.269539
20	H	2.151702	4.740332	−0.262710
21	N	1.474887	0.079466	−1.500243
22	N	−1.477187	0.076813	1.500268
23	C	−2.508726	0.835539	−3.507239
24	C	−3.540084	−0.103786	−3.435529
25	C	−3.525862	−1.045598	−2.399955
26	C	−2.477565	−1.017938	−1.466015
27	C	−1.501770	0.825553	−2.528720
28	H	−2.487518	1.582076	−4.310169
29	H	−4.352300	−0.102409	−4.174151

```
30      H        -0.683037     1.561658     -2.549256
31      C         3.527591    -1.041620      2.394299
32      C         2.477557    -1.015688      1.462413
33      H         4.354420    -0.098591      4.168660
34      C         3.541171    -0.101210      3.431194
35      C         1.498673     0.823747      2.528696
36      C         2.507291     0.835280      3.505497
37      H         0.678241     1.557563      2.551306
38      H         2.485455     1.581103      4.309140
39      C         1.194045    -4.213860      0.155666
40      C        -1.190659    -4.215707     -0.164561
41      H         2.152724    -4.739826      0.264974
42      H        -2.148654    -4.743006     -0.273603
43      N        -1.475980    -0.078693     -1.501733
44      N         1.473552    -0.079037      1.500528
45      Ru       -0.001404    -0.000459     -0.000485
46      C        -1.154438    -2.809311     -0.177136
47      C         1.155381    -2.807545      0.171932
48      C         1.154371     2.807765     -0.171197
49      C        -1.155718     2.808601      0.175101
50      C         0.002411    -4.925489     -0.006164
51      H         0.003610    -6.024101     -0.008784
52      C         0.000772     4.925158      0.003784
53      H         0.000625     6.023785      0.005049
54      N        -0.000963     2.090978      0.001074
55      N        -0.000089    -2.091291     -0.002056
56      H         4.331900     1.786757     -2.298093
57      H        -4.324308     1.793852      2.311065
58      H        -4.328229    -1.789395     -2.308248
59      H         4.331798    -1.783509      2.300249
60      C        -2.456709    -2.060335     -0.376106
61      O        -3.439185    -2.347055      0.255178
62      C        -2.456821     2.057602      0.373524
63      O        -3.439035     2.339784     -0.260310
64      C         2.456228     2.058224     -0.370351
65      O         3.438199     2.343763      0.262521
66      C         2.456636    -2.056870      0.371656
67      O         3.438709    -2.341154     -0.261565
```

[Ru(DNinP)₂]²⁺

```
 1      C        -4.877735    -2.355007     -0.791905
 2      C        -3.620792    -2.768598     -0.269726
 3      C        -2.436241    -2.122187     -0.596753
 4      C        -3.771584    -0.585743     -2.007120
```

5	C	-4.956833	-1.320250	-1.689417
6	H	-5.778257	-2.908132	-0.494922
7	H	-3.616079	-3.651174	0.381438
8	H	-5.898975	-1.035146	-2.177827
9	C	-1.150956	-2.804935	-0.287431
10	C	-1.150883	-4.215465	-0.334378
11	C	-0.000916	-4.927037	0.000315
12	H	-2.051043	-4.762806	-0.638130
13	C	1.150857	-2.805280	0.288228
14	C	1.149157	-4.215950	0.335617
15	H	-0.001247	-6.024445	0.000306
16	H	2.048472	-4.764142	0.640448
17	N	0.000157	-2.095530	0.000162
18	C	-2.531871	-0.908501	-1.362958
19	C	-1.551263	0.952825	-2.405133
20	C	-2.755460	1.150281	-3.174534
21	H	-0.695391	1.631520	-2.536053
22	H	-2.793649	1.925872	-3.958564
23	N	-1.450152	-0.022275	-1.486784
24	C	2.436651	-2.123324	0.597651
25	C	3.620756	-2.771183	0.272346
26	C	3.772085	-0.585268	2.006225
27	C	4.877793	-2.357179	0.794202
28	H	3.615847	-3.654878	-0.377236
29	C	4.957041	-1.320695	1.689704
30	H	5.778269	-2.910758	0.498099
31	H	5.899212	-1.034528	2.177550
32	C	2.532469	-0.908473	1.362115
33	C	1.551704	0.953947	2.402291
34	C	2.756176	1.152871	3.170913
35	H	0.694883	1.631531	2.533364
36	H	2.794346	1.930013	3.953384
37	N	1.450806	-0.022188	1.485027
38	Ru	0.000094	0.000339	-0.000617
39	H	-2.788950	-1.923312	3.959610
40	C	-2.752212	-1.148157	3.175121
41	C	-1.548855	-0.950016	2.404776
42	H	-0.691522	-1.626787	2.536237
43	C	-3.770929	0.586439	2.007898
44	N	-1.449952	0.023839	1.484826
45	C	-2.532160	0.909340	1.361887
46	C	-2.437205	2.122947	0.595512
47	C	-4.956694	1.320508	1.690842
48	C	-3.622250	2.768583	0.269061
49	C	-4.878719	2.354335	0.792150

50	H	−5.898336	1.035431	2.180198
51	H	−3.618448	3.650789	−0.382574
52	H	−5.780145	2.905684	0.494550
53	C	−1.151384	2.805313	0.286282
54	C	−1.150331	4.215860	0.334028
55	C	1.151063	2.805508	−0.287419
56	C	0.000449	4.927283	0.001720
57	H	−2.050744	4.763286	0.637014
58	C	1.150826	4.216156	−0.332416
59	H	0.000688	6.024699	0.003023
60	H	2.051215	4.764091	−0.634587
61	N	−0.000180	2.095803	−0.001048
62	C	2.436609	2.123232	−0.597648
63	C	2.532285	0.908620	−1.362364
64	C	3.621404	2.770171	−0.272378
65	C	4.878063	2.356233	−0.794974
66	H	3.617202	3.653449	0.377821
67	C	4.956846	1.320174	−1.690947
68	H	5.778804	2.909912	−0.499297
69	H	5.898673	1.034434	−2.179761
70	C	3.771611	0.584884	−2.006659
71	C	2.755328	−1.153069	−3.171336
72	C	1.550713	−0.953057	−2.403519
73	H	2.793804	−1.930437	−3.953510
74	H	0.693626	−1.630117	−2.534879
75	N	1.450409	0.022594	−1.485552
76	N	3.852316	0.447283	2.934455
77	N	−3.851768	0.445489	−2.936823
78	N	3.851974	−0.448386	−2.934010
79	N	−3.849447	−0.444544	2.937953

$[Ru(DQPCOOH)_2]^{2+}$

1	C	−2.708204	−1.192110	3.194249
2	C	−3.841615	−0.457707	2.948127
3	C	−3.798957	0.601970	1.987303
4	C	−2.555065	0.908216	1.359726
5	C	−1.541609	−0.945800	2.414289
6	H	−5.921334	1.094359	2.102629
7	H	−2.686725	−1.976469	3.956292
8	H	−4.777798	−0.658657	3.480272
9	C	−4.964274	1.350264	1.636374
10	C	−2.434900	2.114027	0.578471
11	H	−0.652734	−1.587199	2.533977
12	C	−3.604470	2.767873	0.216638

13	C	-4.871460	2.370130	0.722519
14	H	-3.577236	3.641673	-0.445104
15	H	-5.762125	2.924342	0.405889
16	C	4.886656	2.361878	-0.770998
17	C	4.965443	1.347481	-1.691917
18	C	3.794985	0.600616	-2.028096
19	C	2.558698	0.905177	-1.384461
20	C	2.450909	2.108157	-0.596606
21	C	3.627051	2.756652	-0.245238
22	H	4.758103	-0.658160	-3.532649
23	H	5.782301	2.912659	-0.462837
24	H	5.915102	1.093420	-2.174103
25	C	3.827829	-0.458470	-2.989681
26	H	3.610228	3.624898	0.424020
27	C	1.535173	-0.948831	-2.429316
28	C	2.693149	-1.194996	-3.221853
29	H	0.645591	-1.591249	-2.539095
30	H	2.664040	-1.980698	-3.982270
31	C	1.170577	4.195163	-0.320666
32	C	-1.135660	4.195202	0.356866
33	H	2.070865	4.753323	-0.619508
34	H	-2.032376	4.753588	0.667225
35	N	-1.462838	0.038818	1.499879
36	N	1.464716	0.036328	-1.514555
37	C	2.712065	1.196792	3.188319
38	C	3.845052	0.461832	2.942034
39	C	3.801045	-0.600447	1.984266
40	C	2.556378	-0.908025	1.358945
41	C	1.543989	0.947940	2.411465
42	H	5.923263	-1.093640	2.099129
43	H	2.691581	1.982915	3.948586
44	H	4.782056	0.664286	3.472324
45	C	4.965587	-1.350559	1.634745
46	C	2.435025	-2.115521	0.580486
47	H	0.654529	1.588500	2.531876
48	C	3.603848	-2.771664	0.220347
49	C	4.871352	-2.373616	0.724745
50	H	3.575785	-3.647432	-0.438671
51	H	5.761220	-2.930047	0.409699
52	C	-4.886303	-2.360219	-0.770496
53	C	-4.964572	-1.346769	-1.692512
54	C	-3.793755	-0.600415	-2.028953
55	C	-2.557810	-0.904715	-1.384509
56	C	-2.450629	-2.107296	-0.596074
57	C	-3.626977	-2.754987	-0.244252

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58      H        -4.755973     0.656961    -3.535362
59      H        -5.782221    -2.910339    -0.462092
60      H        -5.914061    -1.092928    -2.175056
61      C        -3.826115     0.457737    -2.991552
62      H        -3.610513    -3.623001     0.425212
63      C        -1.533649     0.948494    -2.430268
64      C        -2.691284     1.194146    -3.223503
65      H        -0.644118     1.590889    -2.540161
66      H        -2.661790     1.979158    -3.984682
67      C        -1.171470    -4.194682    -0.319888
68      C         1.134439    -4.196078     0.359248
69      H        -2.071543    -4.752347    -0.620103
70      H         2.030445    -4.754985     0.670475
71      N         1.464124    -0.038630     1.499234
72      N        -1.463489    -0.036294    -1.515075
73      Ru        0.000353    -0.000124    -0.007738
74      C         1.140136    -2.786532     0.290698
75      C        -1.163150    -2.782574    -0.284853
76      C        -1.140397     2.785803     0.288528
77      C         1.163031     2.782888    -0.285779
78      C        -0.023080    -4.902241     0.029469
79      C         0.021842     4.902074     0.027818
80      N         0.008940     2.074779    -0.005479
81      N        -0.008788    -2.075050    -0.004311
82      C         0.012737    -6.398493     0.058328
83      O         0.969784    -7.101098     0.258102
84      O        -1.232631    -6.909198    -0.179457
85      H        -1.244197    -7.917083    -0.171419
86      C        -0.016188     6.398334     0.057158
87      O        -0.974691     7.098338     0.259139
88      O         1.227534     6.911485    -0.183164
89      H         1.237141     7.919465    -0.175004
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$[Ru(DQPNH_2)_2]^{2+}$

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1       C        -2.691547    -1.186999     3.205852
2       C        -3.823535    -0.447556     2.973131
3       C        -3.787283     0.610914     2.010758
4       C        -2.549027     0.916713     1.371313
5       C        -1.533480    -0.945906     2.410440
6       H        -5.909855     1.093797     2.141361
7       H        -2.663682    -1.972444     3.965102
8       H        -4.754120    -0.643423     3.514774
9       C        -4.958531     1.352970     1.666860
10      C        -2.439177     2.124730     0.591343
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11	H	-0.648737	-1.596941	2.511185
12	C	-3.615045	2.768018	0.231921
13	C	-4.877715	2.366883	0.745892
14	H	-3.592996	3.636369	-0.435962
15	H	-5.772591	2.911152	0.428644
16	C	4.876197	2.371562	-0.747580
17	C	4.959825	1.353866	-1.664060
18	C	3.789618	0.610079	-2.007978
19	C	2.549668	0.917480	-1.372476
20	C	2.437430	2.127171	-0.595175
21	C	3.612445	2.772528	-0.236222
22	H	4.761485	-0.650079	-3.503960
23	H	5.770068	2.918704	-0.431796
24	H	5.912306	1.093127	-2.135074
25	C	3.829029	-0.451982	-2.966277
26	H	3.589036	3.642441	0.429629
27	C	1.536964	-0.947777	-2.410048
28	C	2.697727	-1.192077	-3.200467
29	H	0.651961	-1.598044	-2.512688
30	H	2.672387	-1.979860	-3.957319
31	C	1.158990	4.214321	-0.349668
32	C	-1.162883	4.212914	0.346614
33	H	2.054155	4.751105	-0.667853
34	H	-2.058358	4.748585	0.665773
35	N	-1.459914	0.040251	1.498143
36	N	1.461108	0.040523	-1.500191
37	C	2.695203	1.192594	3.199121
38	C	3.826994	0.452528	2.966426
39	C	3.788995	-0.609109	2.007743
40	C	2.549967	-0.916608	1.370602
41	C	1.535317	0.947865	2.407544
42	H	5.911574	-1.092207	2.137741
43	H	2.668434	1.980393	3.955959
44	H	4.758500	0.650477	3.505891
45	C	4.959656	-1.352886	1.665426
46	C	2.439097	-2.126527	0.593558
47	H	0.649878	1.597625	2.509522
48	C	3.614395	-2.771980	0.236067
49	C	4.877485	-2.370402	0.748685
50	H	3.591756	-3.642292	-0.429143
51	H	5.771766	-2.916956	0.433399
52	C	-4.875651	-2.370303	-0.746254
53	C	-4.959207	-1.353755	-1.664029
54	C	-3.789057	-0.610261	-2.008905
55	C	-2.549261	-0.917139	-1.372962

56	C	-2.436983	-2.126621	-0.595504
57	C	-3.611759	-2.771837	-0.235671
58	H	-4.759562	0.647562	-3.507701
59	H	-5.769625	-2.916289	-0.429049
60	H	-5.911947	-1.093553	-2.135009
61	C	-3.827676	0.450444	-2.968698
62	H	-3.588107	-3.642026	0.429771
63	C	-1.535985	0.947407	-2.411485
64	C	-2.696284	1.190432	-3.203016
65	H	-0.651046	1.597724	-2.513901
66	H	-2.670171	1.977009	-3.961132
67	C	-1.159095	-4.213893	-0.352538
68	C	1.160785	-4.214043	0.349238
69	H	-2.053516	-4.749618	-0.674304
70	H	2.055088	-4.750441	0.670486
71	N	1.460668	-0.040319	1.497512
72	N	-1.460511	-0.040445	-1.501104
73	Ru	0.000019	-0.000135	-0.001757
74	C	1.152072	-2.817398	0.293324
75	C	-1.149559	-2.817300	-0.296733
76	C	-1.152631	2.816377	0.291350
77	C	1.149817	2.817632	-0.295801
78	C	0.000418	-4.951623	-0.000624
79	C	-0.002462	4.951032	-0.001745
80	N	-0.001107	2.104615	-0.002543
81	N	0.001183	-2.104862	-0.001404
82	N	0.000221	-6.322273	0.000582
83	N	-0.004015	6.321644	-0.003196
84	H	0.819223	-6.853839	0.253923
85	H	0.815449	6.853103	-0.254877
86	H	-0.822403	6.852432	0.253413
87	H	-0.819318	-6.853165	-0.251883

[Ru(TPy–COOH)(NCS)₃]³⁻

1	C	1.234402	1.636459	0.001409
2	C	1.271141	3.021394	-0.040836
3	C	0.055498	3.749993	-0.060519
4	C	-1.185647	3.063198	-0.035408
5	C	-1.195183	1.677680	0.007056
6	H	2.222613	3.560067	-0.059618
7	H	-2.117908	3.633894	-0.049819
8	N	0.007907	0.952481	0.025447
9	C	2.389883	0.710420	0.026402
10	C	3.731712	1.124171	0.014022

11	C	3.057571	-1.558951	0.090131
12	C	4.750065	0.166530	0.039743
13	H	4.006643	2.182162	-0.016107
14	C	4.409794	-1.188501	0.078017
15	H	2.731424	-2.608606	0.120116
16	H	5.206002	-1.936382	0.098358
17	C	-2.379285	0.788202	0.037975
18	C	-3.705507	1.248113	0.033001
19	C	-3.123442	-1.457234	0.105269
20	C	-4.755739	0.325839	0.064451
21	H	-3.944707	2.314856	0.004531
22	C	-4.462269	-1.039993	0.101158
23	H	-2.834393	-2.517571	0.133807
24	H	-5.283805	-1.759730	0.125808
25	N	2.052654	-0.639351	0.064718
26	N	-2.087788	-0.572475	0.074623
27	Ru	-0.023830	-0.953103	0.078721
28	C	0.051262	5.198033	-0.106268
29	O	-0.863627	6.002425	-0.129926
30	O	1.342020	5.732824	-0.125316
31	H	1.322493	6.716961	-0.156443
32	C	-6.233139	0.817663	0.059395
33	O	-7.097807	-0.074984	0.090599
34	O	-6.390427	2.049707	0.024381
35	C	6.244437	0.604157	0.025252
36	O	7.076078	-0.319495	0.051847
37	O	6.447076	1.829825	-0.011807
38	N	-0.017398	-0.964946	2.130919
39	N	-0.029462	-1.072553	-1.970402
40	N	-0.059622	-3.015887	0.135974
41	C	-0.028493	-1.152954	-3.138294
42	C	-0.008926	-0.989533	3.301321
43	C	-0.078462	-4.185600	0.172500
44	S	-0.027361	-1.244606	-4.774113
45	S	-0.104120	-5.825405	0.222746
46	S	0.002927	-1.001903	4.939509

6   Additional Structures

Cartesian coordinates of optimized geometries at the PM6/rRu level of theory for 7 additional light-harvesting dyes. Structures in this section were used in the fitting and/or testing of the basis set for Ru, but were not used to evaluate the performance of the CI model for UV/Vis spectra.

Ru(NCN)$_2$

1	C	2.646055	0.855320	0.876826
2	C	4.044467	0.847514	0.862813
3	C	4.724524	-0.004210	-0.023425
4	C	4.033880	-0.854721	-0.902429
5	C	2.635329	-0.859954	-0.901896
6	H	4.613651	1.492384	1.529215
7	H	5.810155	-0.005069	-0.029022
8	H	4.594856	-1.500648	-1.574643
9	C	1.945034	-0.001807	-0.008917
10	C	1.749802	1.659511	1.714766
11	C	2.159791	2.594777	2.682875
12	C	-0.526467	2.130700	2.213168
13	C	1.204349	3.299509	3.417822
14	H	3.221163	2.761833	2.851616
15	C	-0.155018	3.070158	3.185968
16	H	-1.581018	1.907848	1.986447
17	H	1.518062	4.024450	4.168134
18	H	-0.916469	3.606461	3.745640
19	C	1.729993	-1.663102	-1.730871
20	C	2.129546	-2.598914	-2.702813
21	C	-0.551544	-2.131666	-2.207638
22	C	1.166471	-3.302420	-3.428623
23	H	3.189200	-2.767180	-2.881557
24	C	-0.190481	-3.071495	-3.183830
25	H	-1.603436	-1.907417	-1.970922
26	H	1.472114	-4.027640	-4.182042
27	H	-0.957639	-3.607126	-3.736116
28	N	0.388358	1.432999	1.485569
29	N	0.371129	-1.434985	-1.488740
30	C	-4.724894	0.004970	0.025135
31	C	-4.036221	-0.878994	0.872204
32	C	-2.637667	-0.887279	0.871186
33	C	-2.644652	0.891433	-0.844250
34	C	-4.043130	0.886384	-0.830217
35	H	-5.810489	0.006767	0.031380
36	H	-4.598781	-1.547791	1.520246
37	H	-4.611085	1.556034	-1.472678
38	C	-1.945416	0.001319	0.009904
39	C	-1.733640	-1.722295	1.669763
40	C	-2.134894	-2.693423	2.605560
41	C	0.546986	-2.212091	2.129003
42	C	-1.173228	-3.425962	3.304339

43	H	−3.194849	−2.866773	2.777296
44	C	0.184079	−3.187968	3.068583
45	H	1.599093	−1.980629	1.901330
46	H	−1.480497	−4.178956	4.029136
47	H	0.950310	−3.745497	3.600289
48	C	−1.746917	1.723427	−1.653072
49	C	−2.155503	2.692319	−2.587947
50	C	0.530149	2.209095	−2.133570
51	C	−1.198996	3.421084	−3.297737
52	H	−3.216686	2.866433	−2.750926
53	C	0.160040	3.182213	−3.073166
54	H	1.584297	1.977201	−1.914217
55	H	−1.511585	4.171780	−4.022815
56	H	0.922208	3.736934	−3.613591
57	N	−0.374393	−1.487416	1.436542
58	N	−0.385922	1.487043	−1.431564
59	Ru	−0.000164	−0.000474	0.000529

[Ru(DQB)$_2$]

1	C	−2.632893	−1.272834	3.192486
2	C	−3.769669	−0.525783	3.025436
3	C	−3.761896	0.568399	2.102102
4	C	−2.548276	0.889077	1.422179
5	C	−1.500927	−1.003078	2.367384
6	H	−5.866271	1.051465	2.339330
7	H	−2.579885	−2.092291	3.906499
8	H	−4.681081	−0.742117	3.579860
9	C	−4.939402	1.329107	1.843678
10	C	−2.458161	2.128670	0.678924
11	H	−0.621909	−1.669030	2.408391
12	C	−3.649343	2.789531	0.404711
13	C	−4.886220	2.383351	0.965089
14	H	−3.645794	3.670405	−0.238648
15	H	−5.785625	2.943667	0.711008
16	C	4.885197	2.387111	−0.964849
17	C	4.940272	1.330658	−1.840640
18	C	3.763610	0.568767	−2.099078
19	C	2.548794	0.889855	−1.421504
20	C	2.457151	2.130712	−0.680140
21	C	3.647428	2.793501	−0.406628
22	H	4.685644	−0.744464	−3.572626
23	H	5.783812	2.948923	−0.711004
24	H	5.868178	1.052223	−2.334080
25	C	3.773220	−0.527287	−3.020141

26	H	3.642591	3.675914	0.234573
27	C	1.503501	-1.004038	-2.365462
28	C	2.637097	-1.274992	-3.187820
29	H	0.624298	-1.669980	-2.406731
30	H	2.585933	-2.095611	-3.900609
31	C	1.151110	4.179339	-0.349539
32	C	-1.154184	4.178251	0.346724
33	H	2.035156	4.742463	-0.648665
34	H	-2.039021	4.740518	0.645018
35	N	-1.458137	0.005961	1.479369
36	N	1.458929	0.006564	-1.479231
37	C	2.636357	1.275930	3.187255
38	C	3.772746	0.528408	3.019808
39	C	3.763546	-0.567837	2.099072
40	C	2.549003	-0.889463	1.421088
41	C	1.502727	1.004268	2.365012
42	H	5.867706	-1.051924	2.335781
43	H	2.584998	2.096698	3.899939
44	H	4.684969	0.745940	3.572562
45	C	4.940108	-1.330222	1.841838
46	C	2.457765	-2.130250	0.680100
47	H	0.623262	1.669541	2.407076
48	C	3.648012	-2.793191	0.407463
49	C	4.885532	-2.387120	0.966604
50	H	3.643483	-3.675718	-0.233427
51	H	5.784072	-2.949524	0.713961
52	C	-4.885364	-2.386161	-0.965768
53	C	-4.940022	-1.330063	-1.842154
54	C	-3.763195	-0.568296	-2.100416
55	C	-2.548753	-0.889432	-1.422098
56	C	-2.457398	-2.129931	-0.680652
57	C	-3.647704	-2.792651	-0.407237
58	H	-4.684265	0.743828	-3.575694
59	H	-5.784068	-2.947770	-0.712006
60	H	-5.867996	-1.051743	-2.335771
61	C	-3.772330	0.527074	-3.022189
62	H	-3.643064	-3.675339	0.233615
63	C	-1.502884	1.004300	-2.366329
64	C	-2.636009	1.275022	-3.189421
65	H	-0.623652	1.670291	-2.407485
66	H	-2.584233	2.095148	-3.902731
67	C	-1.151912	-4.178923	-0.350948
68	C	1.152610	-4.179102	0.347653
69	H	-2.035851	-4.741484	-0.651241
70	H	2.036681	-4.742129	0.646877

71	N	1.458680	-0.006245	1.478789
72	N	-1.458711	-0.006131	-1.479899
73	Ru	-0.000082	-0.000133	-0.000318
74	C	1.172725	-2.769519	0.321934
75	C	-1.172239	-2.769509	-0.323030
76	C	-1.173429	2.768799	0.320737
77	C	1.171810	2.769881	-0.322617
78	C	0.000537	-4.882531	-0.002273
79	H	0.000029	-5.967650	-0.003354
80	C	-0.001965	4.882347	-0.001703
81	H	-0.002606	5.967473	-0.001986
82	C	0.000143	-2.044534	-0.000216
83	C	-0.000400	2.044293	-0.000772

[Ru(DQIm)₂]²⁺

1	C	2.837585	1.154444	-3.095231
2	C	3.876095	0.265671	-3.017650
3	C	3.740847	-0.905944	-2.202871
4	C	2.515617	-1.123835	-1.501040
5	C	1.683284	0.938591	-2.284981
6	H	5.746925	-1.640147	-2.629730
7	H	2.876855	2.032754	-3.746069
8	H	4.803766	0.418905	-3.580402
9	C	4.805264	-1.851305	-2.111877
10	C	2.337134	-2.415574	-0.869052
11	H	0.864369	1.677933	-2.312546
12	C	3.396365	-3.304040	-0.785650
13	C	4.644310	-3.008969	-1.392192
14	H	3.293253	-4.264416	-0.270322
15	H	5.461466	-3.733331	-1.296663
16	C	-4.644932	-3.008762	1.390167
17	C	-4.804912	-1.852222	2.111938
18	C	-3.740135	-0.907238	2.203285
19	C	-2.515483	-1.124566	1.500215
20	C	-2.337553	-2.415663	0.866820
21	C	-3.397481	-3.303385	0.782568
22	H	-4.802203	0.416439	3.582827
23	H	-5.462586	-3.732362	1.293856
24	H	-5.746106	-1.641516	2.630987
25	C	-3.874790	0.263734	3.019147
26	H	-3.294689	-4.263199	0.266057
27	C	-1.682600	0.937357	2.285218
28	C	-2.836361	1.152551	3.096377
29	H	-0.863880	1.676884	2.312354

30	H	-2.875359	2.030697	3.747498
31	C	-0.643693	-4.200592	0.231348
32	C	0.642375	-4.200483	-0.235768
33	H	-1.286357	-5.031686	0.482628
34	H	1.284324	-5.031414	-0.488397
35	N	1.525311	-0.120750	-1.472487
36	N	-1.525233	-0.121295	1.471758
37	C	2.836576	-1.153740	3.096691
38	C	3.875098	-0.264871	3.020096
39	C	3.740776	0.906039	2.204181
40	C	2.516279	1.123300	1.500750
41	C	1.683324	-0.938573	2.285002
42	H	5.746320	1.640755	2.632989
43	H	2.875331	-2.032194	3.747495
44	H	4.802222	-0.417778	3.583988
45	C	4.805534	1.851160	2.113188
46	C	2.338720	2.414562	0.867294
47	H	0.864574	-1.678299	2.311689
48	C	3.398795	3.302086	0.782626
49	C	4.646125	3.007234	1.390630
50	H	3.296769	4.261354	0.264872
51	H	5.463983	3.730660	1.294177
52	C	-4.643857	3.009856	-1.389160
53	C	-4.804124	1.853709	-2.111306
54	C	-3.739704	0.908385	-2.203424
55	C	-2.514736	1.124946	-1.500541
56	C	-2.336363	2.416187	-0.866844
57	C	-3.395940	3.304264	-0.782060
58	H	-4.802951	-0.414428	-3.582860
59	H	-5.461433	3.733505	-1.292188
60	H	-5.745449	1.643440	-2.630158
61	C	-3.875239	-0.262218	-3.019328
62	H	-3.293224	4.263830	-0.264807
63	C	-1.683565	-0.937443	-2.285704
64	C	-2.837398	-1.151931	-3.096608
65	H	-0.865474	-1.677582	-2.312665
66	H	-2.877256	-2.030019	-3.747661
67	C	-0.641346	4.200474	-0.232944
68	C	0.645062	4.199941	0.233341
69	H	-1.283723	5.031572	-0.484380
70	H	1.288627	5.030951	0.484107
71	N	1.526037	0.120210	1.471587
72	N	-1.525383	0.121090	-1.471929
73	Ru	0.000141	-0.000239	-0.000352
74	N	-1.051362	-2.828838	0.372562

75	N	-1.049716	2.828856	-0.373106
76	N	1.050366	-2.828684	-0.375597
77	N	1.052374	2.827944	0.373457
78	C	0.001032	1.980163	0.000259
79	C	-0.000299	-1.980501	-0.000858

[Ru(DQPFur)$_2$]$^{2+}$

1	C	1.308302	-2.640952	3.219688
2	C	0.614976	-3.802697	2.990868
3	C	-0.445736	-3.811351	2.030072
4	C	-0.802539	-2.587831	1.388994
5	C	1.016314	-1.494132	2.425199
6	H	-0.844417	-5.950949	2.165338
7	H	2.094948	-2.580215	3.976691
8	C	-1.140666	-5.011768	1.688249
9	C	-2.012141	-2.528262	0.605672
10	H	1.628722	-0.582766	2.527587
11	C	-2.606979	-3.729662	0.247492
12	C	-2.156064	-4.973493	0.765989
13	H	-3.473198	-3.745653	-0.423246
14	H	-2.664044	-5.890756	0.451211
15	C	-2.581406	4.768329	-0.747713
16	C	-1.568001	4.896383	-1.664041
17	C	-0.770196	3.761022	-2.003543
18	C	-1.020785	2.510153	-1.364544
19	C	-2.222300	2.344839	-0.584256
20	C	-2.923861	3.489259	-0.231541
21	H	-3.171780	5.636526	-0.436826
22	H	-1.353396	5.858195	-2.139921
23	C	0.287539	3.843811	-2.963782
24	H	-3.795275	3.428849	0.431036
25	C	0.883920	1.576366	-2.403588
26	C	1.076363	2.745216	-3.196156
27	H	1.570500	0.719860	-2.509284
28	H	1.863308	2.752424	-3.954947
29	C	-2.747598	-1.269635	0.302126
30	C	-2.846208	1.027609	-0.279940
31	C	-4.248850	0.967464	-0.330707
32	C	-4.928106	-0.214204	0.011609
33	C	-4.153161	-1.333028	0.353349
34	H	-4.840709	1.838382	-0.641452
35	H	-4.654149	-2.254169	0.665854
36	N	0.025785	-1.461948	1.514945
37	N	-2.086406	-0.091719	0.011787

38	N	-0.099819	1.458894	-1.492972
39	C	-1.083767	-2.746832	-3.192285
40	C	-0.295909	-3.845922	-2.959468
41	C	0.763996	-3.762066	-2.001504
42	C	1.017010	-2.511011	-1.363881
43	C	-0.888815	-1.577181	-2.401649
44	H	1.345528	-5.859527	-2.137614
45	H	-1.872063	-2.754230	-3.949665
46	C	1.561938	-4.897689	-1.663098
47	C	2.219990	-2.346095	-0.585383
48	H	-1.574849	-0.720008	-2.507579
49	C	2.921028	-3.491014	-0.233370
50	C	2.577535	-4.769845	-0.749033
51	H	3.793033	-3.430623	0.428271
52	H	3.167819	-5.638447	-0.439324
53	C	2.153662	4.974250	0.757049
54	C	1.137339	5.013646	1.678318
55	C	0.443203	3.813366	2.022163
56	C	0.801291	2.588687	1.383957
57	C	2.010040	2.528584	0.599597
58	C	2.605014	3.729762	0.240421
59	H	2.661468	5.891035	0.440942
60	H	0.840364	5.953811	2.153272
61	C	-0.617616	3.805379	2.982782
62	H	3.471812	3.745460	-0.429531
63	C	-1.013496	1.493630	2.426368
64	C	-1.307216	2.642467	3.217076
65	H	-1.623060	0.580740	2.532914
66	H	-2.092862	2.582421	3.975102
67	C	2.844846	-1.028980	-0.282036
68	C	2.745249	1.269315	0.297077
69	C	4.150791	1.333173	0.348231
70	C	4.926191	0.213948	0.008951
71	C	4.247491	-0.968475	-0.331883
72	H	4.651499	2.255044	0.659278
73	H	4.839948	-1.839628	-0.640725
74	N	0.095904	-1.459770	-1.491947
75	N	2.084763	0.090657	0.008590
76	N	-0.024791	1.461844	1.513986
77	Ru	-0.000693	-0.000487	0.010568
78	C	-6.370626	-0.274859	0.011785
79	C	-7.313395	-1.249126	0.276620
80	C	-8.602472	-0.648871	0.089715
81	C	-8.384797	0.656703	-0.278742
82	O	-7.022488	0.932709	-0.339292

83	H	-7.146515	-2.270643	0.570282
84	H	-9.549876	-1.147410	0.218787
85	H	-8.998189	1.500876	-0.527162
86	C	8.383486	-0.656065	-0.276180
87	C	8.600013	0.651940	0.084374
88	C	7.310522	1.251939	0.268696
89	C	6.368630	0.275263	0.009794
90	O	7.021511	-0.933752	-0.334348
91	H	8.997305	-1.501108	-0.519994
92	H	9.547242	1.151599	0.210983
93	H	7.142713	2.274944	0.556344
94	H	-0.453867	-4.785240	-3.499016
95	H	0.443722	4.782431	-3.505324
96	H	0.850211	-4.723616	3.533779
97	H	-0.855765	4.727946	3.522013

$[\text{Ru(DQPl)}_2]^{2+}$

1	C	2.754639	-1.219827	-3.112484
2	C	3.835411	-0.378678	-3.011952
3	C	3.751089	0.777408	-2.174669
4	C	2.535786	1.038959	-1.472105
5	C	1.603476	-0.964188	-2.319285
6	H	5.787153	1.449539	-2.566633
7	H	2.764425	-2.090726	-3.775130
8	H	4.757758	-0.567517	-3.573206
9	C	4.852491	1.676604	-2.044517
10	C	2.380674	2.300569	-0.786764
11	H	0.749623	-1.666416	-2.362965
12	C	3.485791	3.130742	-0.672125
13	C	4.727912	2.810000	-1.280410
14	H	3.409742	4.077192	-0.124926
15	H	5.570979	3.498501	-1.154790
16	C	-4.725572	2.816689	1.294180
17	C	-4.848913	1.683319	2.058540
18	C	-3.748762	0.782053	2.184075
19	C	-2.535511	1.041714	1.477288
20	C	-2.380738	2.303279	0.791788
21	C	-3.485066	3.135192	0.681462
22	H	-4.753507	-0.561326	3.585440
23	H	-5.568169	3.506134	1.171754
24	H	-5.781885	1.457741	2.584223
25	C	-3.832757	-0.374431	3.020861
26	H	-3.409323	4.081835	0.134606
27	C	-1.604894	-0.964408	2.319810

28	C	-2.753895	-1.218520	3.116540
29	H	-0.752573	-1.668768	2.359581
30	H	-2.763498	-2.090413	3.777917
31	C	-0.683231	4.127771	0.205454
32	C	0.681747	4.126997	-0.210824
33	H	-1.268688	5.009179	0.400927
34	H	1.266937	5.007625	-0.410425
35	N	1.493861	0.092737	-1.485182
36	N	-1.495522	0.093153	1.486506
37	C	-2.755733	1.221607	-3.112421
38	C	-3.835779	0.379343	-3.014449
39	C	-3.751565	-0.777959	-2.178732
40	C	-2.537260	-1.039481	-1.474530
41	C	-1.605709	0.966001	-2.317622
42	H	-5.786433	-1.450696	-2.574556
43	H	-2.765136	2.093134	-3.774287
44	H	-4.757637	0.567898	-3.576635
45	C	-4.852419	-1.678083	-2.051485
46	C	-2.382100	-2.301934	-0.790878
47	H	-0.752269	1.668953	-2.359061
48	C	-3.486470	-3.133597	-0.680136
49	C	-4.728004	-2.813176	-1.289819
50	H	-3.410225	-4.081366	-0.135202
51	H	-5.570421	-3.502785	-1.167184
52	C	4.726479	-2.813100	1.282211
53	C	4.850710	-1.679915	2.046852
54	C	3.749418	-0.780678	2.177025
55	C	2.534783	-1.041570	1.473236
56	C	2.379498	-2.302862	0.787524
57	C	3.484381	-3.133473	0.673642
58	H	4.754960	0.562374	3.578232
59	H	5.569429	-3.501566	1.156935
60	H	5.785100	-1.453252	2.569569
61	C	3.833103	0.374576	3.015823
62	H	3.408004	-4.080402	0.127413
63	C	1.602125	0.961200	2.321271
64	C	2.752380	1.215694	3.116304
65	H	0.748386	1.663662	2.364253
66	H	2.761402	2.085787	3.780104
67	C	0.680603	-4.128097	0.206903
68	C	-0.684525	-4.127592	-0.209028
69	H	1.265460	-5.009365	0.404369
70	H	-1.269454	-5.008728	-0.406439
71	N	-1.496213	-0.092142	-1.485082
72	N	1.493093	-0.094935	1.486304

73	Ru	-0.001288	-0.000218	0.000497
74	N	-0.001421	-1.940888	-0.000836
75	N	-0.000514	1.940317	0.001735
76	C	-1.088703	2.796554	0.322234
77	C	1.087515	2.795430	-0.321734
78	C	1.086609	-2.796776	0.320941
79	C	-1.089666	-2.796135	-0.323328

$[\text{Ru}(\text{PzbPybPz})_2]^{2+}$
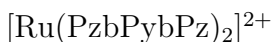
1	C	-1.924819	3.083188	3.884591
2	C	-2.843641	1.456470	5.376211
3	H	-1.707753	4.126198	3.625437
4	H	-3.392317	1.202194	6.290856
5	C	-0.732531	-3.933301	-1.210113
6	C	1.311192	-4.084788	0.018822
7	H	-1.372422	-4.252216	-2.041458
8	H	2.287690	-4.551746	0.193917
9	Ru	-1.053554	-0.870705	2.019903
10	C	0.864110	-3.032893	0.841059
11	C	-1.165627	-2.934932	-0.317490
12	C	-2.373786	0.442904	4.520148
13	C	-1.530481	2.037747	3.029447
14	C	0.514059	-4.531870	-1.033278
15	H	0.856919	-5.331503	-1.702372
16	C	-2.604461	2.794585	5.067075
17	H	-2.941604	3.597580	5.735137
18	N	-1.726579	0.705330	3.330175
19	N	-0.378974	-2.449597	0.707367
20	N	-3.005497	-1.964973	4.062355
21	C	-3.832607	-3.059085	4.429198
22	C	-2.520516	-3.600172	2.676169
23	C	-3.562684	-4.081129	3.536401
24	H	-4.548719	-3.005214	5.236957
25	H	-2.039783	-4.152904	1.882395
26	H	-4.029940	-5.052448	3.484126
27	N	0.245760	1.757049	1.252632
28	C	1.273053	2.385952	0.501262
29	C	1.134412	0.193184	-0.009516
30	C	1.865813	1.399940	-0.267456
31	H	1.515584	3.433998	0.605890
32	H	1.304051	-0.768495	-0.470934
33	H	2.707880	1.500181	-0.934933
34	N	-2.864119	-1.054010	-0.399321
35	C	-3.916487	-0.437180	-1.130583

36	C	-4.349560	0.639662	-0.379504
37	H	-4.223983	-0.778593	-2.108833
38	C	-3.586514	0.616321	0.836281
39	H	-5.109238	1.361963	-0.636493
40	H	-3.692187	1.295488	1.669916
41	N	1.400332	-2.208435	3.180326
42	C	2.237099	-2.341634	4.322129
43	C	1.808658	-1.405203	5.244775
44	H	3.008387	-3.095424	4.394554
45	C	0.750479	-0.670403	4.612028
46	H	2.184059	-1.241540	6.243358
47	H	0.211084	0.164660	5.035077
48	N	0.535639	-1.139295	3.351282
49	N	0.132331	0.427363	0.883897
50	N	-2.164307	-2.331880	3.025587
51	N	-2.717191	-0.432150	0.830454
52	C	-0.977796	2.463958	1.685411
53	C	-2.514119	-0.972279	5.041307
54	H	-0.747201	3.565162	1.705326
55	H	-1.783646	2.342163	0.907203
56	H	-1.520189	-1.305683	5.454671
57	H	-3.219647	-0.980798	5.918093
58	C	-2.610847	-2.509637	-0.470000
59	C	1.890185	-2.490577	1.813662
60	H	-3.005703	-2.874367	-1.458799
61	H	-3.224701	-3.040753	0.312093
62	H	2.740576	-3.222555	1.904482
63	H	2.343087	-1.557373	1.372734

[Ru(CPyC)(TPy)]$^{2+}$

1	C	0.333095	2.929722	0.520744
2	C	0.172292	4.315290	0.667966
3	C	-1.121091	4.839754	0.786899
4	C	-2.240664	3.998284	0.759045
5	C	-2.050166	2.616633	0.610931
6	H	1.040005	4.978222	0.689769
7	H	-3.245678	4.415740	0.851860
8	N	-0.772353	2.097327	0.495391
9	C	1.599427	2.179202	0.376712
10	C	2.868730	2.782898	0.364637
11	C	2.581347	0.040412	0.106907
12	C	4.006482	1.986348	0.220001
13	H	2.964159	3.866830	0.467511
14	C	3.864168	0.599492	0.089126

15	H	2.417035	-1.042631	0.008042
16	H	4.743403	-0.041035	-0.025491
17	C	-3.088810	1.564277	0.557569
18	C	-4.467327	1.821918	0.652158
19	C	-3.508957	-0.757701	0.348970
20	C	-5.371375	0.759123	0.592816
21	H	-4.829140	2.846414	0.771365
22	C	-4.889527	-0.546594	0.439454
23	H	-3.081887	-1.763901	0.227830
24	H	-5.581402	-1.392382	0.390568
25	N	1.453620	0.799973	0.247653
26	N	-2.605658	0.266767	0.404950
27	Ru	-0.529182	0.165832	0.288362
28	C	-0.375362	-0.411837	2.262448
29	C	-0.578197	0.003536	-1.766988
30	N	-0.295278	-1.867444	0.068311
31	H	-1.258819	5.919118	0.902628
32	H	-6.448430	0.945194	0.665992
33	H	5.002407	2.442364	0.209040
34	C	-0.209666	-1.843518	2.376173
35	N	-0.353180	0.015030	3.584723
36	N	-0.105541	-2.141504	3.740007
37	N	-0.191775	-1.028793	4.464249
38	C	-0.437082	-1.373768	-2.183349
39	N	-0.681052	0.689354	-2.971430
40	N	-0.615451	-0.153346	-4.055194
41	N	-0.468958	-1.388405	-3.582849
42	C	-0.288656	-2.429908	-1.198761
43	C	-0.169842	-2.675676	1.187679
44	C	-0.034288	-4.063876	1.056087
45	C	-0.027538	-4.623113	-0.228470
46	C	-0.154342	-3.814477	-1.365606
47	H	0.063570	-4.705613	1.930426
48	H	-0.148953	-4.264203	-2.357352
49	H	0.077095	-5.707560	-0.345377
50	C	-0.361084	-2.531946	-4.498438
51	H	-0.424468	-2.207387	-5.563652
52	H	-1.184164	-3.254595	-4.327279
53	H	0.611525	-3.048856	-4.371221
54	C	0.074704	-3.446711	4.389346
55	H	-0.769920	-4.125031	4.153537
56	H	0.116493	-3.346742	5.499407
57	H	1.024500	-3.919724	4.067464
58	C	-0.835841	2.105312	-3.238242
59	C	-0.464554	1.347189	4.143408

60	C	-1.741280	1.850325	4.494044
61	C	0.314935	2.900931	-3.460154
62	C	-2.137140	2.652745	-3.354213
63	C	0.711883	2.092395	4.404077
64	C	-1.825655	3.119769	5.070357
65	C	-2.974590	1.041382	4.274479
66	C	0.145123	4.253979	-3.761653
67	C	-1.137763	4.815359	-3.879282
68	H	1.020460	4.880390	-3.942099
69	C	-2.267640	4.009666	-3.656797
70	C	-3.348961	1.801916	-3.177401
71	C	-0.670582	3.876139	5.331361
72	H	-2.800979	3.519638	5.353138
73	C	0.588062	3.358207	4.980505
74	C	2.060844	1.538380	4.092034
75	C	-0.776075	5.214378	5.971437
76	H	1.484033	3.943994	5.193602
77	H	-3.262677	4.447114	-3.755361
78	C	-1.300082	6.250117	-4.234846
79	C	1.683374	2.311682	-3.396433
80	H	1.838581	1.692850	-2.503734
81	H	2.474417	3.078050	-3.402760
82	H	1.873157	1.677117	-4.280547
83	H	-3.302770	1.182371	-2.272585
84	H	-3.477889	1.125014	-4.040582
85	H	-4.276044	2.393731	-3.120096
86	H	-3.020070	0.601189	3.270070
87	H	-3.896201	1.627517	4.415641
88	H	-3.029869	0.214112	5.004291
89	H	2.116389	1.091486	3.091531
90	H	2.337373	0.757742	4.823366
91	H	2.854966	2.299135	4.152602
92	H	-1.686623	5.330431	6.580529
93	H	-0.792393	6.022064	5.222752
94	H	0.069496	5.428931	6.645505
95	H	-0.466233	6.638541	-4.841485
96	H	-1.359255	6.885792	-3.337156
97	H	-2.215300	6.444012	-4.817574