

A Definitive Example of a Geometric "Entatic State" Effect: Electron-Transfer Kinetics for a Copper(II/I) Complex Involving a Quinquedentate Macrocyclic Trithiaether-bipyridine Ligand

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SUPPORTING INFORMATION

Ref. 44 [Complete Reference]: Frisch, M. J.; Trucks, G. W.; Schelegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Scalmani, G.; Kudin, K. N.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Li, X.; Hratchian, H. P.; Peralta, J. P.; Izmaylov, A. G.; Brothers, E.; Staroverov, V.; Kobayashi, R.; Normand, J.; Burant, J. C.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Chen, W.; Wong, M. W.; Pople, J. A. *Gaussian DV*, Revision E.05; Gaussian, Inc.; Wallingford, CT, 2006.

A. TABULATION OF EXPERIMENTAL RATE CONSTANTS

Table S-1. Experimental Rate Constant Data for the Reduction of $[\text{Cu}^{\text{II}}([\text{15}]ane\text{S}_3\text{bpy})]^{2+}$ with $[\text{Ru}^{\text{II}}(\text{NH}_3)_5\text{py}]^{2+}$ under Second-Order Conditions in Acetonitrile at 25 °C, $\mu = 0.10$ M (NaClO_4).

Table S-2. Experimental Rate Constant Data for the Reduction of $[\text{Cu}^{\text{II}}([\text{15}]ane\text{S}_3\text{bpy})]^{2+}$ with $[\text{Co}^{\text{II}}(\text{dmg})_3(\text{BC}_6\text{H}_5)_2]$ under Pseudo-First-Order Conditions in Acetonitrile at 25 °C, $\mu = 0.10$ M (NaClO_4).

Table S-3. Experimental Rate Constant Data for the Oxidation of $[\text{Cu}^{\text{I}}([\text{15}] \text{aneS}_3 \text{bpy})]^{2+}$ with $[\text{Ru}^{\text{III}}(\text{NH}_3)_4 \text{bpy}]^{3+}$ under Second-Order Conditions in Acetonitrile at 25 °C, $\mu = 0.10 \text{ M}$ (NaClO_4).

Table S-4. Experimental Rate Constant Data for the Oxidation of $[\text{Cu}^{\text{I}}([\text{15}] \text{aneS}_3 \text{bpy})]^{2+}$ with $[\text{Ru}^{\text{III}}(\text{NH}_3)_5 \text{isn}]^{3+}$ under Second-Order Conditions in Acetonitrile at 25 °C, $\mu = 0.10 \text{ M}$ (NaClO_4).

Table S-5. Experimental Rate Constant Data for the Oxidation of $[\text{Cu}^{\text{I}}([\text{15}] \text{aneS}_3 \text{bpy})]^{2+}$ with $[\text{Co}^{\text{III}}(\text{phen})_3]^{3+}$ under Pseudo-First-Order Conditions in Acetonitrile at 25 °C, $\mu = 0.10 \text{ M}$ (NaClO_4).

Table S-6. Experimental Rate Constant Data for the Oxidation of $[\text{Cu}^{\text{I}}([\text{15}] \text{aneS}_3 \text{bpy})]^{2+}$ with $[\text{Co}^{\text{III}}(\text{phen})_3]^{3+}$ under Pseudo-First-Order Conditions in Acetonitrile at 25 °C, $\mu = 0.10 \text{ M}$ (NaClO_4).

Table S-7. NMR Line-Broadening Measurements for $[\text{Cu}^{\text{II/I}}([\text{15}] \text{aneS}_3 \text{bpy})]^{2+/+}$ Electron Self Exchange in Acetonitrile at 25 °C.

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Table S-1. Experimental Rate Constant Data for the Reduction of $[\text{Cu}^{\text{II}}([\text{15}]\text{aneS}_3\text{bpy})]^{2+}$ with $[\text{Ru}^{\text{II}}(\text{NH}_3)_5\text{py}]^{2+}$ under Second-Order Conditions in Acetonitrile at 25 °C, $\mu = 0.10$ M (NaClO_4).

$[\text{Cu}^{\text{II}}([\text{15}]\text{aneS}_3\text{bpy})], \mu\text{M}$	$[\text{Ru}^{\text{II}}], \mu\text{M}$	Mean $k_{21} \times 10^{-5}, \text{M}^{-1}\text{s}^{-1}$
33.1	46.1	2.5(4)
33.1	7.25	1.9(3)
44.2	7.25	2.0(1)
66.5	7.25	1.9(2)

Table S-2. Experimental Rate Constant Data for the Reduction of $[\text{Cu}^{\text{II}}([\text{15}]\text{aneS}_3\text{bpy})]^{2+}$ with $[\text{Co}^{\text{II}}(\text{dmg})_3(\text{BC}_6\text{H}_5)_2]$ under Pseudo-First-Order Conditions in Acetonitrile at 25 M (ClO_4^-). $[\text{Co}^{\text{II}}(\text{dmg})_3(\text{BC}_6\text{H}_5)_2] = 7.75 \mu\text{M}$.

$[\text{Cu}^{\text{II}}([\text{15}]\text{aneS}_3\text{bpy})], \mu\text{M}$	Mean $k_{\text{obs}}, \text{s}^{-1}$
110	1.25(4)
166	2.15(13)
220	2.89(12)
386	6.03(19)
552	8.51(28)

Table S-3. Experimental Rate Constant Data for the Oxidation of $[\text{Cu}^{\text{I}}([\text{15}] \text{aneS}_3 \text{bpy})]^{2+}$ with $[\text{Ru}^{\text{III}}(\text{NH}_3)_4 \text{bpy}]^{3+}$ under Second-Order Conditions in Acetonitrile at 25 °C, $\mu = 0.10 \text{ M}$ (NaClO_4).

$[\text{Cu}^{\text{II}}([\text{15}] \text{aneS}_3 \text{bpy})], \mu\text{M}$	$[\text{Ru}^{\text{III}}], \mu\text{M}$	Mean $k_{12} \times 10^{-6}, \text{M}^{-1}\text{s}^{-1}$
3.39	3.08	9.6(6)
3.39	4.31	7.9(5)
4.85	4.31	11.9(13)
4.85	6.16	8.1(6)
7.76	6.16	10.3(4)

Table S-4. Experimental Rate Constant Data for the Oxidation of $[\text{Cu}^{\text{I}}([\text{15}] \text{aneS}_3 \text{bpy})]^{2+}$ with $[\text{Ru}^{\text{III}}(\text{NH}_3)_5 \text{isn}]^{3+}$ under Second-Order Conditions in Acetonitrile at 25 °C, $\mu = 0.10 \text{ M}$ (NaClO_4).

$[\text{Cu}^{\text{II}}([\text{15}] \text{aneS}_3 \text{bpy})], \mu\text{M}$	$[\text{Ru}^{\text{III}}], \mu\text{M}$	Mean $k_{21} \times 10^{-5}, \text{M}^{-1}\text{s}^{-1}$
55.5	19.5	3.01(9)
76.5	19.5	3.62(12)
115	19.5	3.38(16)
153	19.5	3.39(29)
192	19.5	2.66(33)

Table S-5. Experimental Rate Constant Data for the Oxidation of $[\text{Cu}^{\text{I}}([\text{15}]\text{aneS}_3\text{bpy})]^{2+}$ with $[\text{Co}^{\text{III}}(\text{phen})_3]^{3+}$ under Pseudo-First-Order Conditions in Acetonitrile at 25 °C, $\mu = 0.10 \text{ M}$ (NaClO_4). $[\text{Cu}^{\text{I}}([\text{15}]\text{aneS}_3\text{bpy})]^{2+} = 21.6 \text{ }\mu\text{M}$

$[\text{Co}^{\text{III}}], \mu\text{M}$	Mean $k_{\text{obs}}, \text{s}^{-1}$
72.2	0.159(1)
144	0.278(3)
289	0.520(7)
432	0.776(20)
575	0.945(20)

Table S-6. Experimental Rate Constant Data for the Oxidation of $[\text{Cu}^{\text{I}}([\text{15}]\text{aneS}_3\text{bpy})]^{2+}$ with $[\text{Co}^{\text{III}}(\text{phen})_3]^{3+}$ under Pseudo-First-Order Conditions in Acetonitrile at 25 °C, $\mu = 0.10 \text{ M}$ (NaClO_4). $[\text{Cu}^{\text{I}}([\text{15}]\text{aneS}_3\text{bpy})]^{2+} = 20.4 \text{ }\mu\text{M}$

$[\text{Co}^{\text{III}}], \mu\text{M}$	Mean $k_{\text{obs}}, \text{s}^{-1}$
289	0.181(6)
385	0.225(7)
482	0.276(7)
725	0.414(14)
965	0.549(19)

Table S-7. NMR Line-Broadening Measurements for $[\text{Cu}^{\text{II/I}}([\text{15}]\text{aneS}_3\text{bpy})]^{2+/+}$ Electron Self Exchange in Acetonitrile at 25 °C. $[\text{Cu}^{\text{I}}\text{L}] = 1.16 \text{ mM}$, $Q_{\text{calc}} = 1.97$

$[\text{Cu}^{\text{II}}([\text{15}]\text{aneS}_3\text{bpy})]$, mM	Linewidth (4.2 ppm), Hz	Linewidth (7.6 ppm), Hz
0.00	7.44	16.83
0.172	15.52	21.80
0.344	26.70	35.98
0.516	41.17	50.60

B. DFT CALCULATIONS

All gas-phase and NCMsolvated data for the calculations described in the text are presented with the exception of the geometries for the linearly interpolated structures. The linearly interpolated geometries are easily regenerated by running an OPT(QST2, PATH) job in Gaussian with the appropriate ground state geometries passed as the reactant and product structures.

Table S-8. Gas-phase electronic and zero-point energies in a.u.

Compound	Symmetry	Saddle-point Order	E(elec)	E(ZPE)
[Cu([15]aneS ₃ bpy)] ⁺	C ₁		-2122.17304059	0.308247
[Cu([15]aneS ₃ bpy)] ⁺	C _s		-2122.17097860	0.308218
[Cu([15]aneS ₃ bpy)] ⁺	C ₁	1	-2122.16613208	0.308235
[Cu([15]aneS ₃ bpy)] ²⁺	C ₁		-2121.84554414	0.310712
[Cu([15]aneS ₃ bpy)] ²⁺	C _s		-2121.84454384	0.310685
[Cu([15]aneS ₃ bpy)] ²⁺	C ₁	1	-2121.83735910	0.310569
[Cu(5-Meimid) ₂ DAP] ⁺	C ₂		-1397.40974778	0.456398
[Cu(5-Meimid) ₂ DAP] ²⁺	C ₂		-1397.11854534	0.459572
[Cu(imidR) ₂ DAP] ⁺	C ₂		-1938.34004170	0.670505
[Cu(imidR) ₂ DAP] ²⁺	C ₂		-1938.05708719	0.673174
[Cu(imidH) ₂ DAP] ⁺	C ₁		-1318.74160796	0.401873
[Cu(imidH) ₂ DAP] ²⁺	C ₁		-1318.44514682	0.405241
[Cu(py) ₂ DAP] ⁺	C ₂		-1362.88971946	0.435771
[Cu(py) ₂ DAP] ²⁺	C ₂		-1362.58418035	0.438546

Table S-9. Solvated electronic and zero-point energies in a.u.

Compound	Symmetry	Saddle-point Order	E(elec)	E(ZPE)
[Cu([15]aneS ₃ bpy)] ⁺	C ₁		-2122.24034312	0.306738
[Cu([15]aneS ₃ bpy)] ⁺	C _s		-2122.23894973	0.306764
[Cu([15]aneS ₃ bpy)] ⁺	C ₁	1	-2122.23347731	0.306753
[Cu([15]aneS ₃ bpy)] ²⁺	C ₁		-2122.07058748	0.310433
[Cu([15]aneS ₃ bpy)] ²⁺	C _s		-2122.07077621	0.310613
[Cu([15]aneS ₃ bpy)] ²⁺	C ₁	1	-2122.06297248	0.310425

Table S-10. Gas-phase electronic energies (a.u.) for Cu([15]aneS₃bpy) linear path geometries

Point	C ₁ Cu(I)	C _s Cu(I)	C ₁ Cu(II)	C _s Cu(II)
1	-2122.17304059	-2122.17097860	-2121.83534113	-2121.83386440
2	-2122.17292711	-2122.17083195	-2121.83765102	-2121.83628000
3	-2122.17239095	-2122.17040920	-2121.83952840	-2121.83838663
4	-2122.17181915	-2122.16972256	-2121.84135762	-2121.84019643
5	-2122.17091452	-2122.16877342	-2121.84283519	-2121.84171102
6	-2122.16971519	-2122.16755174	-2121.84399796	-2121.84292136
7	-2122.16822320	-2122.16603919	-2121.84484736	-2121.84381020
8	-2122.16642565	-2122.16421403	-2121.84536817	-2121.84435730
9	-2122.16430903	-2122.16205549	-2121.84554414	-2121.84454384

Table S-11. Gas-phase electronic energies (a.u.) for Cu(5-Meimid)₂DAP linear path geometries

Point	C ₂ Cu(I)	C ₂ Cu(II)
1	-1397.40974778	-1397.10583434
2	-1397.40957638	-1397.10853904
3	-1397.40906229	-1397.11098340
4	-1397.40818206	-1397.11315857
5	-1397.40692753	-1397.11500503
6	-1397.40525705	-1397.11649856
7	-1397.40314646	-1397.11761019
8	-1397.40041126	-1397.11830474
9	-1397.39696252	-1397.11854534

Table S-12. Gas-phase electronic energies (a.u.) for Cu(imidR)₂DAP linear path geometries

Point	C ₂ Cu(I)	C ₂ Cu(II)
1	-1938.34004170	-1938.04638574
2	-1938.33986786	-1938.04870421
3	-1938.33937034	-1938.05074667
4	-1938.33844294	-1938.05247461
5	-1938.33719511	-1938.05413901
6	-1938.33557401	-1938.05537773
7	-1938.33357120	-1938.05622413
8	-1938.33116608	-1938.05685267
9	-1938.32828644	-1938.05708719

Table S-13. Gas-phase electronic energies (a.u.) for Cu(imidH)₂DAP linear path geometries

Point	C ₁ Cu(I)	C ₁ Cu(II)
1	-1318.74160796	-1318.43238616
2	-1318.74143502	-1318.43512334
3	-1318.74091753	-1318.43757944
4	-1318.74005651	-1318.43975036
5	-1318.73881812	-1318.44159826
6	-1318.73717165	-1318.44308879
7	-1318.73509983	-1318.44420041
8	-1318.73257552	-1318.44490103
9	-1318.72956070	-1318.44514682

Table S-14. Gas-phase electronic energies (a.u.) for Cu(py)₂DAP linear path geometries

Point	C ₂ Cu(I)	C ₂ Cu(II)
1	-1362.88971946	-1362.56948406
2	-1362.88956148	-1362.57254233
3	-1362.88906156	-1362.57531696
4	-1362.88819700	-1362.57777713
5	-1362.88694531	-1362.57989215
6	-1362.88532071	-1362.58166868
7	-1362.88320555	-1362.58297806
8	-1362.88059904	-1362.58380921
9	-1362.87753875	-1362.58418035

Table S-15. Solvated electronic energies (a.u.) for Cu([15]aneS₃bpy) linear path geometries

Point	C ₁ Cu(I)	C _s Cu(I)	C ₁ Cu(II)	C _s Cu(II)
1	-2122.24034312	-2122.23894973	-2122.05989765	-2122.05905781
2	-2122.24007023	-2122.23861445	-2122.06217254	-2122.06133673
3	-2122.23958925	-2122.23812560	-2122.06417582	-2122.06352433
4	-2122.23874946	-2122.23722712	-2122.06581560	-2122.06536270
5	-2122.23779326	-2122.23619608	-2122.06745319	-2122.06713760
6	-2122.23646186	-2122.23477599	-2122.06868985	-2122.06835408
7	-2122.23480540	-2122.23336575	-2122.06951205	-2122.06992018
8	-2122.23293745	-2122.23130531	-2122.07017946	-2122.07056700
9	-2122.23072647	-2122.22882969	-2122.07058748	-2122.07077621

Table S-16. Polynomial fits of Total Distortion Energies and Resulting q_c

Ligand	x^4	x^3	x^2	x	C	q_c
C_1 [15]aneS ₃ bpy		0.017	0.4972	-6.9914	33.184	5.487
C_s [15]aneS ₃ bpy		0.0095	0.6395	-7.8373	35.187	5.463
(5-Meimid) ₂ DAP		0.0403	0.4455	-8.0966	40.911	5.290
(imidR) ₂ DAP		0.0155	0.652	-7.5801	34.965	4.942
(imidH) ₂ DAP		0.0242	0.6309	-8.7481	41.581	5.310
(py) ₂ DAP		0.0299	0.6039	-9.5766	47.507	5.600
C_1 [15]aneS ₃ bpy Solvated		0.0079	0.6031	-7.0895	34.54	5.321
C_s [15]aneS ₃ bpy Solvated	0.0084	-0.123	1.1912	-8.1607	37.89	5.932

C_1 [Cu([15]aneS₃bpy)]⁺

1	29	0	-0.483397	-0.023365	-0.357487
2	16	0	-1.567461	-2.128897	-1.101514
3	16	0	-1.752012	-0.021805	1.618603
4	16	0	-1.555340	1.937823	-1.249626
5	7	0	1.144258	1.356830	-0.124343
6	7	0	1.242509	-1.257574	-0.306859
7	6	0	-2.314974	-2.519463	0.552844
8	6	0	-3.013414	-1.292978	1.143366
9	6	0	-2.649526	1.574776	1.398622
10	6	0	-2.951153	2.000268	-0.042250
11	6	0	-0.385713	3.217164	-0.589471
12	6	0	0.996728	2.682166	-0.229431
13	6	0	2.073325	3.554506	-0.020028
14	6	0	3.320444	3.010886	0.296992
15	6	0	3.469303	1.624452	0.386822
16	6	0	2.348302	0.814055	0.169573
17	6	0	2.363589	-0.673726	0.187426
18	6	0	3.435160	-1.443002	0.657025
19	6	0	3.339275	-2.834703	0.604469
20	6	0	2.191862	-3.423944	0.066619
21	6	0	1.160904	-2.595196	-0.390742
22	6	0	-0.057736	-3.180975	-1.090554
23	1	0	-1.519970	-2.874934	1.215957
24	1	0	-3.043465	-3.323984	0.415314
25	1	0	-3.714742	-0.854254	0.427156
26	1	0	-3.564893	-1.580539	2.043445
27	1	0	-1.999557	2.298809	1.900373
28	1	0	-3.581412	1.528941	1.973029
29	1	0	-3.699777	1.348796	-0.504421

30	1	0	-3.364551	3.014847	-0.043419
31	1	0	-0.297069	3.993432	-1.354695
32	1	0	-0.857940	3.679170	0.284865
33	1	0	1.940920	4.630287	-0.106204
34	1	0	4.175563	3.662492	0.456064
35	1	0	4.443788	1.193894	0.596921
36	1	0	4.321683	-0.972180	1.071225
37	1	0	4.150973	-3.453698	0.977633
38	1	0	2.104305	-4.505251	-0.006571
39	1	0	-0.313568	-4.167384	-0.693243
40	1	0	0.169626	-3.315277	-2.154979

C_s [Cu([15]aneS₃bpy)]⁺

1	29	0	-0.416367	-0.000163	-0.068001
2	16	0	-1.336861	-1.987157	-1.234530
3	16	0	-2.055872	-0.000001	1.525818
4	16	0	-1.337574	1.986450	-1.235216
5	7	0	1.246646	1.300802	0.048497
6	7	0	1.247196	-1.300394	0.048855
7	6	0	-2.987785	-1.964230	-0.413615
8	1	0	-3.566475	-1.312163	-1.075750
9	1	0	-3.431770	-2.963622	-0.476317
10	6	0	-3.054469	-1.480491	1.042469
11	1	0	-2.681321	-2.249884	1.726016
12	1	0	-4.096997	-1.291685	1.321976
13	6	0	-3.055348	1.479625	1.041646
14	1	0	-4.097825	1.290162	1.320911
15	1	0	-2.682989	2.249535	1.725034
16	6	0	-2.988618	1.962889	-0.414590
17	1	0	-3.433177	2.962001	-0.477709
18	1	0	-3.566794	1.310259	-1.076621
19	6	0	-0.325120	3.142142	-0.187931
20	1	0	-0.345427	4.141936	-0.627527
21	1	0	-0.791650	3.189566	0.802943
22	6	0	1.100839	2.631491	-0.052089
23	6	0	2.203795	3.489752	-0.004680
24	1	0	2.075017	4.565105	-0.097935
25	6	0	3.475372	2.932587	0.168470
26	1	0	4.350926	3.575007	0.213605
27	6	0	3.618534	1.547493	0.264563
28	1	0	4.605617	1.109016	0.377986
29	6	0	2.471842	0.744997	0.189074
30	6	0	2.472179	-0.744049	0.189092
31	6	0	3.619255	-1.546036	0.264241
32	1	0	4.606183	-1.107113	0.377292
33	6	0	3.476678	-2.931196	0.168233

34	1	0	4.352532	-3.573225	0.213116
35	6	0	2.205300	-3.488922	-0.004556
36	1	0	2.076970	-4.564334	-0.097753
37	6	0	1.101961	-2.631145	-0.051720
38	6	0	-0.323788	-3.142423	-0.187351
39	1	0	-0.790182	-3.190066	0.803573
40	1	0	-0.343724	-4.142217	-0.626961

[Cu([15]aneS₃bpy)]⁺ TS

1	29	0	0.422821	-0.037844	-0.097815
2	16	0	1.482979	1.891312	-1.278599
3	16	0	2.120558	-0.006163	1.453658
4	16	0	1.185637	-2.160668	-1.115623
5	7	0	-1.139816	1.390285	0.023086
6	7	0	-1.379367	-1.204219	0.063820
7	6	0	3.164591	1.916448	-0.525010
8	6	0	3.502395	0.958496	0.656865
9	6	0	2.727324	-1.742738	1.278769
10	6	0	2.738580	-2.328026	-0.137829
11	6	0	-0.012161	-3.204440	-0.154280
12	6	0	-1.374244	-2.539936	-0.073625
13	6	0	-2.561245	-3.278120	-0.113183
14	6	0	-3.776375	-2.595744	0.002970
15	6	0	-3.776686	-1.206770	0.133980
16	6	0	-2.548959	-0.530145	0.154285
17	6	0	-2.404733	0.948405	0.208970
18	6	0	-3.462745	1.849171	0.391418
19	6	0	-3.193571	3.218152	0.351645
20	6	0	-1.884763	3.660718	0.135537
21	6	0	-0.873390	2.706126	-0.011587
22	6	0	0.584684	3.086920	-0.171381
23	1	0	3.364052	2.951264	-0.236078
24	1	0	3.822308	1.693262	-1.369386
25	1	0	3.957136	1.529318	1.469464
26	1	0	2.066325	-2.307238	1.944108
27	1	0	3.733483	-1.795594	1.709343
28	1	0	3.481718	-1.827521	-0.767752
29	1	0	3.017612	-3.386429	-0.093466
30	1	0	-0.082223	-4.189901	-0.620298
31	1	0	0.395982	-3.329522	0.854950
32	1	0	-2.537637	-4.358505	-0.231056
33	1	0	4.233960	0.215029	0.330846
34	1	0	-4.715718	-3.141657	-0.027366
35	1	0	-4.716413	-0.665622	0.192035
36	1	0	-4.477344	1.498316	0.555185
37	1	0	-3.999060	3.936307	0.481132

38	1	0	-1.655818	4.722290	0.088669
39	1	0	1.077831	3.051554	0.807794
40	1	0	0.687268	4.096855	-0.576070

C_1 [Cu([15]aneS₃bpy)]²⁺

1	29	0	-0.257094	-0.237133	-0.404316
2	16	0	-0.129867	-2.542529	-0.962795
3	16	0	-1.497316	-0.889007	1.699193
4	16	0	-2.285779	0.545023	-1.367703
5	7	0	0.134150	1.698289	-0.125183
6	7	0	1.725463	-0.345935	-0.230655
7	6	0	-0.404637	-3.254953	0.734626
8	6	0	-1.685738	-2.699545	1.349660
9	6	0	-3.153931	-0.212310	1.271030
10	6	0	-3.523345	-0.198815	-0.215702
11	6	0	-2.162718	2.296792	-0.755312
12	6	0	-0.779824	2.675944	-0.265041
13	6	0	-0.444111	4.006161	0.018545
14	6	0	0.848521	4.298081	0.456745
15	6	0	1.794085	3.273769	0.572621
16	6	0	1.415346	1.967296	0.259620
17	6	0	2.315041	0.793215	0.230761
18	6	0	3.668857	0.793469	0.574946
19	6	0	4.404267	-0.386492	0.426108
20	6	0	3.789815	-1.532350	-0.086265
21	6	0	2.431481	-1.478295	-0.418132
22	6	0	1.714785	-2.629281	-1.090646
23	1	0	0.470735	-3.027186	1.350162
24	1	0	-0.482584	-4.339403	0.610383
25	1	0	-2.549219	-2.858632	0.697287
26	1	0	-1.875920	-3.203051	2.301673
27	1	0	-3.144200	0.794613	1.699003
28	1	0	-3.907786	-0.781224	1.825561
29	1	0	-3.663561	-1.206868	-0.618590
30	1	0	-4.466584	0.338425	-0.363697
31	1	0	-2.456693	2.934894	-1.594129
32	1	0	-2.911497	2.431365	0.032049
33	1	0	-1.180268	4.795564	-0.106797
34	1	0	1.126506	5.322539	0.688620
35	1	0	2.808883	3.500948	0.883878
36	1	0	4.148560	1.691217	0.952131
37	1	0	5.456651	-0.407696	0.695594
38	1	0	4.356878	-2.446739	-0.237427
39	1	0	2.034097	-3.604052	-0.711422
40	1	0	1.914476	-2.616227	-2.168742

$C_s [\text{Cu}([15]\text{aneS}_3\text{bpy})]^{2+}$

1	29	0	-0.294355	-0.000083	-0.299577
2	16	0	-1.429401	-1.866405	-1.216635
3	16	0	-1.861735	-0.000051	1.659266
4	16	0	-1.429816	1.866089	-1.216715
5	7	0	1.196752	1.297068	-0.042854
6	7	0	1.197195	-1.296729	-0.043100
7	6	0	-2.995345	-1.876511	-0.236656
8	1	0	-3.643363	-1.204371	-0.806655
9	1	0	-3.425088	-2.880679	-0.320345
10	6	0	-2.889185	-1.470395	1.238671
11	1	0	-2.436682	-2.266103	1.838764
12	1	0	-3.894497	-1.311228	1.643114
13	6	0	-2.890215	1.469437	1.238153
14	1	0	-3.895570	1.309439	1.642157
15	1	0	-2.438664	2.265548	1.838421
16	6	0	-2.996077	1.875470	-0.237243
17	1	0	-3.426250	2.879443	-0.321059
18	1	0	-3.643612	1.203034	-0.807442
19	6	0	-0.371465	3.141942	-0.365390
20	1	0	-0.374217	4.037984	-0.990751
21	1	0	-0.846210	3.392167	0.589493
22	6	0	1.034670	2.631234	-0.135370
23	6	0	2.128531	3.491443	0.009989
24	1	0	1.998210	4.566223	-0.080080
25	6	0	3.386281	2.942739	0.272861
26	1	0	4.248378	3.592678	0.394759
27	6	0	3.538778	1.555982	0.364121
28	1	0	4.517069	1.126413	0.555593
29	6	0	2.418446	0.740060	0.188394
30	6	0	2.418676	-0.739346	0.188393
31	6	0	3.539215	-1.554920	0.364388
32	1	0	4.517329	-1.125042	0.556067
33	6	0	3.387148	-2.941731	0.273183
34	1	0	4.249405	-3.591412	0.395325
35	6	0	2.129620	-3.490819	0.010058
36	1	0	1.999644	-4.565645	-0.079983
37	6	0	1.035533	-2.630944	-0.135609
38	6	0	-0.370344	-3.142192	-0.366108
39	1	0	-0.845048	-3.393479	0.588518
40	1	0	-0.372528	-4.037750	-0.992173

$[\text{Cu}([\text{15}] \text{aneS}_3 \text{bpy})]^{2+}$ TS

1	29	0	0.298887	-0.009729	-0.276378
2	16	0	1.526790	1.827373	-1.213675
3	16	0	1.986407	0.020368	1.588992
4	16	0	1.330111	-1.976750	-1.156039
5	7	0	-1.300046	-1.213612	-0.068943
6	7	0	-1.120884	1.376509	-0.008163
7	6	0	3.139853	1.925519	-0.306343
8	1	0	3.898120	1.833491	-1.088151
9	1	0	3.192382	2.948762	0.072097
10	6	0	3.430473	0.897459	0.819026
11	1	0	3.945152	1.408664	1.635697
12	1	0	4.101655	0.122163	0.445067
13	6	0	2.531020	-1.734325	1.435144
14	1	0	1.757141	-2.298947	1.964517
15	1	0	3.460256	-1.854363	2.001851
16	6	0	2.740023	-2.239036	0.005897
17	1	0	3.579384	-1.744670	-0.491557
18	1	0	2.962540	-3.311810	0.005811
19	6	0	0.081772	-3.189877	-0.505358
20	1	0	-0.017762	-3.976307	-1.258487
21	1	0	0.501069	-3.645024	0.398687
22	6	0	-1.256112	-2.552985	-0.209464
23	6	0	-2.414503	-3.327442	-0.073581
24	1	0	-2.369530	-4.405335	-0.202713
25	6	0	-3.620614	-2.692845	0.226245
26	1	0	-4.530397	-3.275195	0.342902
27	6	0	-3.657347	-1.301684	0.355566
28	1	0	-4.595155	-0.798693	0.568709
29	6	0	-2.477372	-0.573887	0.188893
30	6	0	-2.375315	0.898647	0.218435
31	6	0	-3.441552	1.781461	0.411087
32	1	0	-4.443788	1.411016	0.601607
33	6	0	-3.204837	3.156610	0.337082
34	1	0	-4.024199	3.857473	0.470899
35	6	0	-1.915525	3.626695	0.076480
36	1	0	-1.714845	4.691539	-0.000137
37	6	0	-0.879719	2.700156	-0.080804
38	6	0	0.554815	3.116131	-0.278967
39	1	0	1.040749	3.244032	0.694939
40	1	0	0.632702	4.055635	-0.831504

$C_2 [Cu(5\text{-Meimid})_2DAP]^+$

1	6	0	0.044871	1.170959	2.807155
2	6	0	0.068207	1.202408	4.209941
3	6	0	0.000000	0.000000	4.916458
4	6	0	-0.068207	-1.202408	4.209941
5	6	0	-0.044871	-1.170959	2.807155
6	7	0	0.000000	0.000000	2.127854
7	1	0	0.000000	0.000000	6.003400
8	1	0	0.140120	2.145824	4.743522
9	1	0	-0.140120	-2.145824	4.743522
10	6	0	0.000000	-2.391117	1.954245
11	6	0	0.000000	2.391117	1.954245
12	6	0	-0.236740	3.718274	2.640861
13	1	0	-1.169290	3.696096	3.217941
14	1	0	0.574924	3.933315	3.347068
15	1	0	-0.292560	4.552413	1.940019
16	6	0	0.236740	-3.718274	2.640861
17	1	0	1.169290	-3.696096	3.217941
18	1	0	-0.574924	-3.933315	3.347068
19	1	0	0.292560	-4.552413	1.940019
20	7	0	0.124402	2.173319	0.684213
21	7	0	-0.124402	-2.173319	0.684213
22	6	0	-0.114646	3.210271	-0.311379
23	1	0	0.070115	4.227658	0.058269
24	1	0	0.567365	3.036779	-1.151558
25	6	0	0.114646	-3.210271	-0.311379
26	1	0	-0.567365	-3.036779	-1.151558
27	1	0	-0.070115	-4.227658	0.058269
28	6	0	1.580064	-3.119883	-0.803595
29	1	0	2.234310	-3.214473	0.075536
30	1	0	1.780126	-3.996364	-1.432118
31	6	0	-1.580064	3.119883	-0.803595
32	1	0	-2.234310	3.214473	0.075536
33	1	0	-1.780126	3.996364	-1.432118
34	6	0	-1.938361	1.880844	-1.577822
35	6	0	1.938361	-1.880844	-1.577822
36	7	0	-1.486008	0.598477	-1.253181
37	7	0	1.486008	-0.598477	-1.253181
38	6	0	2.799828	-1.806359	-2.657361
39	6	0	-2.799828	1.806359	-2.657361
40	6	0	2.065292	0.227142	-2.115333
41	1	0	1.930729	1.297935	-2.153029
42	6	0	-2.065292	-0.227142	-2.115333
43	1	0	-1.930729	-1.297935	-2.153029
44	29	0	0.000000	0.000000	0.071744
45	7	0	-2.864311	0.456589	-2.975822

46	7	0	2.864311	-0.456589	-2.975822
47	6	0	-3.588232	2.835913	-3.404609
48	1	0	-4.665044	2.740501	-3.214288
49	1	0	-3.290237	3.842301	-3.099771
50	1	0	-3.431256	2.758595	-4.487709
51	6	0	3.588232	-2.835913	-3.404609
52	1	0	4.665044	-2.740501	-3.214288
53	1	0	3.290237	-3.842301	-3.099771
54	1	0	3.431256	-2.758595	-4.487709
55	1	0	3.417155	-0.051725	-3.721833
56	1	0	-3.417155	0.051725	-3.721833

 $C_2 [Cu(5\text{-Meimid})_2\text{DAP}]^{2+}$

1	6	0	-0.983903	-0.655092	2.684847
2	6	0	-1.014960	-0.668662	4.086043
3	6	0	0.000000	0.000000	4.781616
4	6	0	1.014960	0.668662	4.086043
5	6	0	0.983903	0.655092	2.684847
6	7	0	0.000000	0.000000	2.042782
7	1	0	0.000000	0.000000	5.868030
8	1	0	-1.801076	-1.187174	4.626714
9	1	0	1.801076	1.187174	4.626714
10	6	0	1.912247	1.353668	1.751412
11	6	0	-1.912247	-1.353668	1.751412
12	6	0	-2.997653	-2.222571	2.321378
13	1	0	-2.557975	-3.063205	2.873489
14	1	0	-3.600996	-1.647687	3.034029
15	1	0	-3.666356	-2.627440	1.562314
16	6	0	2.997653	2.222571	2.321378
17	1	0	2.557975	3.063205	2.873489
18	1	0	3.600996	1.647687	3.034029
19	1	0	3.666356	2.627440	1.562314
20	7	0	-1.643532	-1.161685	0.492519
21	7	0	1.643532	1.161685	0.492519
22	6	0	-2.260941	-1.912089	-0.604802
23	1	0	-3.257277	-2.279323	-0.340409
24	1	0	-2.360828	-1.235597	-1.457680
25	6	0	2.260941	1.912089	-0.604802
26	1	0	2.360828	1.235597	-1.457680
27	1	0	3.257277	2.279323	-0.340409
28	6	0	1.351802	3.098746	-0.989004
29	1	0	1.242274	3.747959	-0.108493
30	1	0	1.885901	3.689299	-1.742183
31	6	0	-1.351802	-3.098746	-0.989004
32	1	0	-1.242274	-3.747959	-0.108493
33	1	0	-1.885901	-3.689299	-1.742183

34	6	0	0.000000	-2.714851	-1.527071
35	6	0	0.000000	2.714851	-1.527071
36	7	0	0.697269	-1.561450	-1.150121
37	7	0	-0.697269	1.561450	-1.150121
38	6	0	-0.779802	3.459298	-2.392192
39	6	0	0.779802	-3.459298	-2.392192
40	6	0	-1.874748	1.618837	-1.769884
41	1	0	-2.672362	0.895172	-1.701014
42	6	0	1.874748	-1.618837	-1.769884
43	1	0	2.672362	-0.895172	-1.701014
44	29	0	0.000000	0.000000	0.075081
45	7	0	1.958688	-2.740635	-2.520321
46	7	0	-1.958688	2.740635	-2.520321
47	6	0	0.560854	-4.767888	-3.083194
48	1	0	1.190493	-5.557969	-2.656210
49	1	0	-0.479709	-5.086584	-2.985259
50	1	0	0.787005	-4.697529	-4.153298
51	6	0	-0.560854	4.767888	-3.083194
52	1	0	-1.190493	5.557969	-2.656210
53	1	0	0.479709	5.086584	-2.985259
54	1	0	-0.787005	4.697529	-4.153298
55	1	0	-2.753867	3.011467	-3.089002
56	1	0	2.753867	-3.011467	-3.089002

 $C_2 [Cu(imidR)_2DAP]^+$

1	6	0	1.108510	0.380948	4.127141
2	6	0	1.145462	0.370354	5.529781
3	6	0	0.000000	0.000000	6.236815
4	6	0	-1.145462	-0.370354	5.529781
5	6	0	-1.108510	-0.380948	4.127141
6	7	0	0.000000	0.000000	3.446468
7	1	0	0.000000	0.000000	7.323782
8	1	0	2.050627	0.645537	6.063226
9	1	0	-2.050627	-0.645537	6.063226
10	6	0	-2.232456	-0.865943	3.278777
11	6	0	2.232456	0.865943	3.278777
12	6	0	3.391551	1.547845	3.973076
13	1	0	3.047342	2.423033	4.537874
14	1	0	3.862743	0.864609	4.690320
15	1	0	4.164026	1.877489	3.277044
16	6	0	-3.391551	-1.547845	3.973076
17	1	0	-3.047342	-2.423033	4.537874
18	1	0	-3.862743	-0.864609	4.690320
19	1	0	-4.164026	-1.877489	3.277044
20	7	0	2.071908	0.690591	2.006504
21	7	0	-2.071908	-0.690591	2.006504

22	6	0	2.950324	1.298687	1.015290
23	1	0	3.959498	1.515945	1.390012
24	1	0	3.052468	0.598619	0.178076
25	6	0	-2.950324	-1.298687	1.015290
26	1	0	-3.052468	-0.598619	0.178076
27	1	0	-3.959498	-1.515945	1.390012
28	6	0	-2.311371	-2.617780	0.514810
29	1	0	-2.143892	-3.261003	1.390921
30	1	0	-3.041998	-3.137244	-0.117337
31	6	0	2.311371	2.617780	0.514810
32	1	0	2.143892	3.261003	1.390921
33	1	0	3.041998	3.137244	-0.117337
34	6	0	1.032699	2.470320	-0.262464
35	6	0	-1.032699	-2.470320	-0.262464
36	7	0	0.000000	1.594115	0.069392
37	7	0	0.000000	-1.594115	0.069392
38	6	0	-0.650894	-3.210945	-1.359371
39	6	0	0.650894	3.210945	-1.359371
40	6	0	0.968959	-1.822664	-0.814683
41	1	0	1.917086	-1.305611	-0.854213
42	6	0	-0.968959	1.822664	-0.814683
43	1	0	-1.917086	1.305611	-0.854213
44	29	0	0.000000	0.000000	1.393792
45	7	0	-0.624747	2.797186	-1.697606
46	7	0	0.624747	-2.797186	-1.697606
47	1	0	-1.145917	-4.004230	-1.900988
48	1	0	1.145917	4.004230	-1.900988
49	6	0	1.437582	-3.280774	-2.838930
50	1	0	1.011801	-2.870756	-3.761409
51	1	0	2.432882	-2.842564	-2.707573
52	6	0	-1.437582	3.280774	-2.838930
53	1	0	-2.432882	2.842564	-2.707573
54	1	0	-1.011801	2.870756	-3.761409
55	6	0	1.505672	-4.791361	-2.914064
56	6	0	0.954783	-5.471877	-4.006344
57	6	0	2.130999	-5.537148	-1.900912
58	6	0	1.029148	-6.866756	-4.088328
59	1	0	0.469016	-4.912247	-4.805453
60	6	0	2.199545	-6.926340	-1.985433
61	1	0	2.564938	-5.028470	-1.040607
62	6	0	1.651660	-7.618047	-3.082270
63	1	0	0.596864	-7.374980	-4.948738
64	1	0	2.690611	-7.486394	-1.190762
65	6	0	-1.505672	4.791361	-2.914064
66	6	0	-2.130999	5.537148	-1.900912
67	6	0	-0.954783	5.471877	-4.006344

68	6	0	-2.199545	6.926340	-1.985433
69	1	0	-2.564938	5.028470	-1.040607
70	6	0	-1.029148	6.866756	-4.088328
71	1	0	-0.469016	4.912247	-4.805453
72	6	0	-1.651660	7.618047	-3.082270
73	1	0	-2.690611	7.486394	-1.190762
74	1	0	-0.596864	7.374980	-4.948738
75	6	0	1.751032	-9.124230	-3.171901
76	1	0	2.789918	-9.439451	-3.333133
77	1	0	1.408247	-9.601919	-2.246464
78	1	0	1.151608	-9.517017	-3.998822
79	6	0	-1.751032	9.124230	-3.171901
80	1	0	-2.789918	9.439451	-3.333133
81	1	0	-1.408247	9.601919	-2.246464
82	1	0	-1.151608	9.517017	-3.998822

C_2 [Cu(imidR)₂DAP]²⁺

1	6	0	1.162919	0.203786	3.819433
2	6	0	1.197464	0.203687	5.220716
3	6	0	0.000000	0.000000	5.917026
4	6	0	-1.197464	-0.203687	5.220716
5	6	0	-1.162919	-0.203786	3.819433
6	7	0	0.000000	0.000000	3.175458
7	1	0	0.000000	0.000000	7.003442
8	1	0	2.126219	0.361835	5.760712
9	1	0	-2.126219	-0.361835	5.760712
10	6	0	-2.297498	-0.468992	2.890382
11	6	0	2.297498	0.468992	2.890382
12	6	0	3.636387	0.830718	3.470867
13	1	0	3.564213	1.773982	4.027182
14	1	0	3.956493	0.059361	4.181459
15	1	0	4.416012	0.940339	2.717556
16	6	0	-3.636387	-0.830718	3.470867
17	1	0	-3.564213	-1.773982	4.027182
18	1	0	-3.956493	-0.059361	4.181459
19	1	0	-4.416012	-0.940339	2.717556
20	7	0	1.982213	0.399289	1.630290
21	7	0	-1.982213	-0.399289	1.630290
22	6	0	2.861088	0.833232	0.541261
23	1	0	3.918546	0.780677	0.818545
24	1	0	2.696863	0.163764	-0.307343
25	6	0	-2.861088	-0.833232	0.541261
26	1	0	-2.696863	-0.163764	-0.307343
27	1	0	-3.918546	-0.780677	0.818545
28	6	0	-2.495414	-2.279091	0.142081
29	1	0	-2.629526	-2.922699	1.023210

30	1	0	-3.225705	-2.616723	-0.601998
31	6	0	2.495414	2.279091	0.142081
32	1	0	2.629526	2.922699	1.023210
33	1	0	3.225705	2.616723	-0.601998
34	6	0	1.110015	2.448654	-0.419157
35	6	0	-1.110015	-2.448654	-0.419157
36	7	0	0.000000	1.694401	-0.037960
37	7	0	0.000000	-1.694401	-0.037960
38	6	0	-0.699181	-3.411256	-1.312867
39	6	0	0.699181	3.411256	-1.312867
40	6	0	1.041618	-2.219057	-0.693062
41	1	0	2.065585	-1.882654	-0.627612
42	6	0	-1.041618	2.219057	-0.693062
43	1	0	-2.065585	1.882654	-0.627612
44	29	0	0.000000	0.000000	1.198698
45	7	0	-0.663039	3.258948	-1.470310
46	7	0	0.663039	-3.258948	-1.470310
47	1	0	-1.236873	-4.200169	-1.818763
48	1	0	1.236873	4.200169	-1.818763
49	6	0	1.544442	-4.043811	-2.394634
50	1	0	1.492754	-3.566171	-3.378265
51	1	0	2.562071	-3.925775	-2.009577
52	6	0	-1.544442	4.043811	-2.394634
53	1	0	-2.562071	3.925775	-2.009577
54	1	0	-1.492754	3.566171	-3.378265
55	6	0	1.144727	-5.496217	-2.479849
56	6	0	0.471080	-5.979134	-3.612036
57	6	0	1.447043	-6.390080	-1.438548
58	6	0	0.108022	-7.325152	-3.700600
59	1	0	0.241306	-5.305409	-4.437101
60	6	0	1.080659	-7.731490	-1.531905
61	1	0	1.979863	-6.039148	-0.555072
62	6	0	0.406819	-8.226083	-2.665201
63	1	0	-0.406120	-7.682290	-4.590869
64	1	0	1.330481	-8.412186	-0.719945
65	6	0	-1.144727	5.496217	-2.479849
66	6	0	-1.447043	6.390080	-1.438548
67	6	0	-0.471080	5.979134	-3.612036
68	6	0	-1.080659	7.731490	-1.531905
69	1	0	-1.979863	6.039148	-0.555072
70	6	0	-0.108022	7.325152	-3.700600
71	1	0	-0.241306	5.305409	-4.437101
72	6	0	-0.406819	8.226083	-2.665201
73	1	0	-1.330481	8.412186	-0.719945
74	1	0	0.406120	7.682290	-4.590869
75	6	0	0.052895	-9.689734	-2.778529

76	1	0	0.902423	-10.259563	-3.177824
77	1	0	-0.196738	-10.119712	-1.803023
78	1	0	-0.793662	-9.848148	-3.453548
79	6	0	-0.052895	9.689734	-2.778529
80	1	0	-0.902423	10.259563	-3.177824
81	1	0	0.196738	10.119712	-1.803023
82	1	0	0.793662	9.848148	-3.453548

C_1 [Cu(imidH)₂DAP]⁺

1	6	0	2.558883	1.059574	-0.492145
2	6	0	3.961537	1.079123	-0.521449
3	6	0	4.666378	-0.004733	0.005591
4	6	0	3.957768	-1.087767	0.528997
5	6	0	2.555237	-1.066506	0.492898
6	7	0	1.877544	-0.003130	-0.001478
7	1	0	5.753272	-0.005241	0.008451
8	1	0	4.496452	1.922791	-0.947570
9	1	0	4.489541	-1.932054	0.957854
10	6	0	1.703094	-2.210488	0.922934
11	6	0	1.710438	2.205300	-0.925635
12	6	0	2.405512	3.511473	-1.240777
13	1	0	2.990284	3.858097	-0.379962
14	1	0	3.105086	3.380516	-2.075649
15	1	0	1.709048	4.304138	-1.516751
16	6	0	2.393467	-3.521468	1.228365
17	1	0	2.977535	-3.863437	0.365234
18	1	0	3.093171	-3.399241	2.064501
19	1	0	1.694332	-4.313913	1.498179
20	7	0	0.438611	1.967203	-0.942438
21	7	0	0.432262	-1.966581	0.945755
22	6	0	-0.551857	3.020134	-1.127600
23	1	0	-0.174621	3.893785	-1.675366
24	1	0	-1.385089	2.604088	-1.705651
25	6	0	-0.561196	-3.017313	1.129096
26	1	0	-1.393884	-2.599619	1.706684
27	1	0	-0.186223	-3.891756	1.677077
28	6	0	-1.068489	-3.480574	-0.258338
29	1	0	-0.195930	-3.808184	-0.841517
30	1	0	-1.700157	-4.366249	-0.118338
31	6	0	-1.059094	3.484583	0.259434
32	1	0	-0.186181	3.810756	0.842871
33	1	0	-1.688994	4.371422	0.118812
34	6	0	-1.841876	2.468599	1.044719
35	6	0	-1.849080	-2.462977	-1.043673
36	7	0	-1.514117	1.114887	1.142733
37	7	0	-1.518254	-1.109990	-1.141850

38	6	0	-2.951845	-2.709482	-1.830283
39	6	0	-2.943738	2.717794	1.831794
40	6	0	-2.402743	-0.570009	-1.974568
41	1	0	-2.439197	0.467861	-2.270358
42	6	0	-2.399472	0.577106	1.975858
43	1	0	-2.438136	-0.460629	2.271871
44	1	0	-3.507031	-3.614002	-2.032538
45	1	0	-3.496713	3.623622	2.034283
46	29	0	-0.178237	-0.000982	-0.001606
47	7	0	-3.280213	1.512505	2.417375
48	7	0	-3.285765	-1.503388	-2.415668
49	1	0	-4.045076	1.355955	3.062105
50	1	0	-4.050614	-1.344988	-3.059957

C_1 [Cu(imidH)₂DAP]²⁺

1	6	0	2.465379	-1.016762	0.606400
2	6	0	3.866499	-1.043617	0.628867
3	6	0	4.563588	-0.004985	-0.000440
4	6	0	3.868678	1.035100	-0.629768
5	6	0	2.467507	1.011201	-0.607302
6	7	0	1.823457	-0.002099	-0.000428
7	1	0	5.649992	-0.006117	-0.000427
8	1	0	4.405740	-1.850315	1.116311
9	1	0	4.409618	1.840676	-1.117187
10	6	0	1.537675	2.043445	-1.145970
11	6	0	1.533401	-2.046993	1.145241
12	6	0	2.107062	-3.295232	1.754020
13	1	0	2.659478	-3.865120	0.995798
14	1	0	2.820222	-3.031400	2.544011
15	1	0	1.351180	-3.950154	2.186182
16	6	0	2.113775	3.290619	-1.754630
17	1	0	2.665090	3.860692	-0.995727
18	1	0	2.828329	3.025536	-2.542914
19	1	0	1.359320	3.945806	-2.188900
20	7	0	0.273804	-1.761571	0.983003
21	7	0	0.277496	1.760744	-0.983484
22	6	0	-0.818436	-2.709737	1.223421
23	1	0	-0.541759	-3.477877	1.951576
24	1	0	-1.667316	-2.150065	1.624908
25	6	0	-0.812691	2.711420	-1.223345
26	1	0	-1.663116	2.153695	-1.624257
27	1	0	-0.534639	3.478868	-1.951713
28	6	0	-1.208826	3.377370	0.111159
29	1	0	-0.327399	3.895696	0.513747
30	1	0	-1.951516	4.152665	-0.107540
31	6	0	-1.216942	-3.374620	-0.110894

32	1	0	-0.336913	-3.894770	-0.514183
33	1	0	-1.961168	-4.148325	0.108202
34	6	0	-1.778507	-2.434871	-1.142983
35	6	0	-1.771696	2.438979	1.143771
36	7	0	-1.400170	-1.097704	-1.292610
37	7	0	-1.396792	1.100777	1.292783
38	6	0	-2.668658	2.757713	2.136289
39	6	0	-2.677318	-2.751365	-2.134535
40	6	0	-2.052602	0.644347	2.361392
41	1	0	-1.990729	-0.351125	2.773120
42	6	0	-2.055846	-0.639682	-2.360625
43	1	0	-1.991681	0.355544	-2.772596
44	1	0	-3.185731	3.676435	2.372038
45	1	0	-3.197083	-3.668739	-2.369614
46	29	0	-0.143261	-0.000045	-0.000365
47	7	0	-2.832516	-1.609898	-2.892455
48	7	0	-2.826123	1.616553	2.894193
49	1	0	-3.429307	-1.514017	-3.706863
50	1	0	-3.422374	1.522120	3.709166

C_2 [Cu(py)₂DAP]⁺

1	6	0	-0.159734	1.161589	-2.530992
2	6	0	-0.180657	1.191930	-3.933788
3	6	0	0.000000	0.000000	-4.639052
4	6	0	0.180657	-1.191930	-3.933788
5	6	0	0.159734	-1.161589	-2.530992
6	7	0	0.000000	0.000000	-1.854982
7	1	0	0.000000	0.000000	-5.725946
8	1	0	-0.343579	2.124372	-4.466789
9	1	0	0.343579	-2.124372	-4.466789
10	6	0	0.262134	-2.377054	-1.672010
11	6	0	-0.262134	2.377054	-1.672010
12	6	0	-0.110550	3.727475	-2.332212
13	1	0	0.796293	3.769803	-2.946827
14	1	0	-0.962581	3.917608	-2.998264
15	1	0	-0.077004	4.542983	-1.607990
16	6	0	0.110550	-3.727475	-2.332212
17	1	0	-0.796293	-3.769803	-2.946827
18	1	0	0.962581	-3.917608	-2.998264
19	1	0	0.077004	-4.542983	-1.607990
20	7	0	-0.455018	2.143001	-0.415096
21	7	0	0.455018	-2.143001	-0.415096
22	6	0	-0.435276	3.191987	0.600257
23	1	0	0.226905	4.029305	0.339839
24	1	0	-1.451019	3.596018	0.714834
25	6	0	0.435276	-3.191987	0.600257

26	1	0	1.451019	-3.596018	0.714834
27	1	0	-0.226905	-4.029305	0.339839
28	6	0	0.000000	-2.579146	1.954173
29	1	0	0.060587	-3.355903	2.724573
30	1	0	0.710697	-1.785956	2.218579
31	6	0	0.000000	2.579146	1.954173
32	1	0	-0.060587	3.355903	2.724573
33	1	0	-0.710697	1.785956	2.218579
34	6	0	1.392787	1.996348	1.923364
35	6	0	-1.392787	-1.996348	1.923364
36	7	0	1.555490	0.819316	1.257574
37	7	0	-1.555490	-0.819316	1.257574
38	6	0	-2.476320	-2.637386	2.535575
39	6	0	2.476320	2.637386	2.535575
40	6	0	-3.749188	-2.068325	2.474375
41	6	0	3.749188	2.068325	2.474375
42	6	0	-2.794833	-0.277727	1.197974
43	1	0	-2.867199	0.656951	0.647458
44	6	0	2.794833	0.277727	1.197974
45	1	0	2.867199	-0.656951	0.647458
46	1	0	-2.314559	-3.574527	3.062940
47	1	0	-4.595428	-2.555303	2.952560
48	1	0	2.314559	3.574527	3.062940
49	6	0	-3.911070	-0.860903	1.790385
50	6	0	3.911070	0.860903	1.790385
51	1	0	-4.880631	-0.376506	1.715230
52	1	0	4.880631	0.376506	1.715230
53	1	0	4.595428	2.555303	2.952560
54	29	0	0.000000	0.000000	0.205273

$C_2 [Cu(py)_2DAP]^{2+}$

1	6	0	-0.007822	1.182503	-2.602094
2	6	0	-0.010248	1.215677	-4.003331
3	6	0	0.000000	0.000000	-4.699096
4	6	0	0.010248	-1.215677	-4.003331
5	6	0	0.007822	-1.182503	-2.602094
6	7	0	0.000000	0.000000	-1.959436
7	1	0	0.000000	0.000000	-5.785500
8	1	0	-0.017391	2.157495	-4.543991
9	1	0	0.017391	-2.157495	-4.543991
10	6	0	-0.028669	-2.342778	-1.668151
11	6	0	0.028669	2.342778	-1.668151
12	6	0	0.129701	3.736779	-2.216352
13	1	0	1.092054	3.875650	-2.726722
14	1	0	-0.657411	3.907352	-2.960525
15	1	0	0.034631	4.500295	-1.444091

16	6	0	-0.129701	-3.736779	-2.216352
17	1	0	-1.092054	-3.875650	-2.726722
18	1	0	0.657411	-3.907352	-2.960525
19	1	0	-0.034631	-4.500295	-1.444091
20	7	0	0.000000	2.021567	-0.407339
21	7	0	0.000000	-2.021567	-0.407339
22	6	0	0.161588	3.012180	0.672857
23	1	0	0.969215	3.708750	0.420866
24	1	0	-0.766683	3.589821	0.771798
25	6	0	-0.161588	-3.012180	0.672857
26	1	0	0.766683	-3.589821	0.771798
27	1	0	-0.969215	-3.708750	0.420866
28	6	0	-0.463906	-2.308483	2.011380
29	1	0	-0.556866	-3.079297	2.782448
30	1	0	0.390969	-1.679238	2.286606
31	6	0	0.463906	2.308483	2.011380
32	1	0	0.556866	3.079297	2.782448
33	1	0	-0.390969	1.679238	2.286606
34	6	0	1.718570	1.465513	1.977361
35	6	0	-1.718570	-1.465513	1.977361
36	7	0	1.691481	0.345703	1.204096
37	7	0	-1.691481	-0.345703	1.204096
38	6	0	-2.864152	-1.810230	2.702134
39	6	0	2.864152	1.810230	2.702134
40	6	0	-3.999336	-0.999946	2.635632
41	6	0	3.999336	0.999946	2.635632
42	6	0	-2.798289	0.431004	1.134394
43	1	0	-2.726730	1.304992	0.492376
44	6	0	2.798289	-0.431004	1.134394
45	1	0	2.726730	-1.304992	0.492376
46	1	0	-2.859236	-2.704610	3.319441
47	1	0	-4.892327	-1.256775	3.199291
48	1	0	2.859236	2.704610	3.319441
49	6	0	-3.966498	0.143489	1.833435
50	6	0	3.966498	-0.143489	1.833435
51	1	0	-4.826183	0.801256	1.746825
52	1	0	4.826183	-0.801256	1.746825
53	1	0	4.892327	1.256775	3.199291
54	29	0	0.000000	0.000000	0.004335

Solvated C_1 [Cu([15]aneS₃bpy)]⁺

1	29	0	0.465702	-0.014904	-0.323937
2	16	0	1.657893	2.030359	-1.127003
3	16	0	1.818816	-0.072467	1.596633
4	16	0	1.413898	-2.040783	-1.237415
5	7	0	-1.223982	-1.293919	-0.071566

6	7	0	-1.183144	1.318972	-0.297576
7	6	0	2.455496	2.401449	0.507289
8	6	0	3.114849	1.155737	1.099109
9	6	0	2.648695	-1.699298	1.339678
10	6	0	2.875074	-2.126751	-0.111846
11	6	0	0.220206	-3.231962	-0.460408
12	6	0	-1.148992	-2.626391	-0.189992
13	6	0	-2.284180	-3.434785	-0.046977
14	6	0	-3.509294	-2.820440	0.230048
15	6	0	-3.581252	-1.428588	0.341488
16	6	0	-2.405909	-0.684566	0.178852
17	6	0	-2.335264	0.800474	0.202663
18	6	0	-3.358708	1.628055	0.678907
19	6	0	-3.179803	3.013007	0.629433
20	6	0	-2.003908	3.537029	0.083922
21	6	0	-1.026720	2.650444	-0.383950
22	6	0	0.213524	3.169057	-1.096526
23	1	0	1.686928	2.798587	1.179265
24	1	0	3.214386	3.174312	0.347293
25	1	0	3.797911	0.684164	0.384809
26	1	0	3.679290	1.432155	1.995608
27	1	0	1.998184	-2.403745	1.869771
28	1	0	3.609183	-1.680457	1.868189
29	1	0	3.607732	-1.483125	-0.612026
30	1	0	3.267587	-3.150253	-0.128999
31	1	0	0.130256	-4.099845	-1.120122
32	1	0	0.668703	-3.578991	0.478843
33	1	0	-2.211407	-4.518054	-0.148536
34	1	0	-4.410742	-3.423430	0.341913
35	1	0	-4.539066	-0.942508	0.522170
36	1	0	-4.271631	1.207943	1.099138
37	1	0	-3.953171	3.679297	1.012219
38	1	0	-1.850269	4.614432	0.014180
39	1	0	0.531331	4.135886	-0.693353
40	1	0	-0.023280	3.321926	-2.157750

Solvated C_s [Cu([15]aneS₃bpy)]⁺

1	29	0	-0.413594	-0.000572	-0.069972
2	16	0	-1.338728	-1.988626	-1.234184
3	16	0	-2.049418	-0.001210	1.523833
4	16	0	-1.341945	1.985766	-1.235171
5	7	0	1.245525	1.300353	0.043767
6	7	0	1.247366	-1.298957	0.044561
7	6	0	-2.990753	-1.956124	-0.414221
8	1	0	-3.567428	-1.298076	-1.073290
9	1	0	-3.434636	-2.956490	-0.474625

10	6	0	-3.047422	-1.482027	1.043070
11	1	0	-2.669231	-2.255776	1.720369
12	1	0	-4.089715	-1.288047	1.323426
13	6	0	-3.048246	1.479083	1.043806
14	1	0	-4.090230	1.283538	1.324168
15	1	0	-2.669900	2.252879	1.721072
16	6	0	-2.992907	1.954375	-0.413035
17	1	0	-3.434482	2.955893	-0.471118
18	1	0	-3.572382	1.298634	-1.072144
19	6	0	-0.328352	3.141286	-0.188522
20	1	0	-0.349020	4.142388	-0.626855
21	1	0	-0.797465	3.186221	0.802338
22	6	0	1.096619	2.631427	-0.054054
23	6	0	2.198287	3.491893	-0.001879
24	1	0	2.065837	4.570355	-0.092237
25	6	0	3.470797	2.935079	0.172804
26	1	0	4.347884	3.580801	0.222038
27	6	0	3.618245	1.548991	0.266418
28	1	0	4.609026	1.111504	0.382028
29	6	0	2.471914	0.746049	0.186574
30	6	0	2.472992	-0.742813	0.186665
31	6	0	3.620527	-1.544090	0.265937
32	1	0	4.610746	-1.105118	0.380743
33	6	0	3.475037	-2.930409	0.172855
34	1	0	4.353103	-3.574828	0.221698
35	6	0	2.203212	-3.489147	-0.000773
36	1	0	2.072309	-4.567843	-0.090592
37	6	0	1.100313	-2.630266	-0.052625
38	6	0	-0.324126	-3.142177	-0.186232
39	1	0	-0.792126	-3.187172	0.804949
40	1	0	-0.343685	-4.143734	-0.623553

Solvated [Cu([15]aneS₃bpy)]⁺ TS

1	29	0	0.417319	-0.034436	-0.099353
2	16	0	1.490820	1.898529	-1.268420
3	16	0	2.103247	-0.007187	1.460556
4	16	0	1.203555	-2.149516	-1.128352
5	7	0	-1.142825	1.388533	0.015241
6	7	0	-1.372116	-1.205829	0.042676
7	6	0	3.165056	1.923977	-0.496659
8	6	0	3.492402	0.954125	0.674899
9	6	0	2.709293	-1.743652	1.285165
10	6	0	2.748322	-2.311019	-0.135731
11	6	0	-0.000687	-3.206199	-0.190744
12	6	0	-1.360946	-2.542197	-0.089889
13	6	0	-2.545058	-3.287425	-0.104064

14	6	0	-3.761522	-2.610582	0.034322
15	6	0	-3.769208	-1.219738	0.159925
16	6	0	-2.544670	-0.537369	0.152273
17	6	0	-2.407042	0.942068	0.200485
18	6	0	-3.469712	1.838760	0.377918
19	6	0	-3.202685	3.209395	0.337521
20	6	0	-1.894114	3.657472	0.125686
21	6	0	-0.879461	2.705448	-0.019415
22	6	0	0.576538	3.092650	-0.172325
23	1	0	3.347662	2.957685	-0.190386
24	1	0	3.835067	1.709004	-1.334580
25	1	0	3.947470	1.519010	1.492380
26	1	0	2.037526	-2.315489	1.934810
27	1	0	3.712332	-1.794983	1.725230
28	1	0	3.495938	-1.796103	-0.750168
29	1	0	3.029576	-3.369751	-0.094154
30	1	0	-0.076974	-4.181160	-0.679170
31	1	0	0.410231	-3.358528	0.814380
32	1	0	-2.515870	-4.371293	-0.218549
33	1	0	4.216472	0.205464	0.341966
34	1	0	-4.700994	-3.163641	0.026744
35	1	0	-4.714005	-0.683834	0.239003
36	1	0	-4.487539	1.485380	0.536598
37	1	0	-4.013590	3.927016	0.464032
38	1	0	-1.665918	4.722537	0.080396
39	1	0	1.067144	3.062024	0.809080
40	1	0	0.676816	4.102884	-0.578547

Solvated C_1 [Cu([15]aneS₃bpy)]²⁺

1	29	0	-0.243597	-0.249797	-0.414315
2	16	0	-0.019874	-2.544040	-0.963580
3	16	0	-1.432855	-0.936106	1.704389
4	16	0	-2.308127	0.429764	-1.364195
5	7	0	0.055106	1.695449	-0.135126
6	7	0	1.734792	-0.269985	-0.233808
7	6	0	-0.262984	-3.254697	0.735576
8	6	0	-1.562033	-2.747969	1.349678
9	6	0	-3.114019	-0.326424	1.283798
10	6	0	-3.494497	-0.363492	-0.196499
11	6	0	-2.268821	2.182133	-0.751500
12	6	0	-0.905585	2.625195	-0.270262
13	6	0	-0.635019	3.969425	0.014049
14	6	0	0.643198	4.321676	0.448404
15	6	0	1.639067	3.345969	0.562065
16	6	0	1.320965	2.024557	0.248508
17	6	0	2.272249	0.894760	0.222644

18	6	0	3.623262	0.958784	0.568258
19	6	0	4.406919	-0.190841	0.428645
20	6	0	3.844350	-1.366315	-0.074634
21	6	0	2.486652	-1.371396	-0.410954
22	6	0	1.824092	-2.554602	-1.075376
23	1	0	0.605709	-2.988649	1.347596
24	1	0	-0.298664	-4.342846	0.614688
25	1	0	-2.420674	-2.931917	0.695447
26	1	0	-1.733703	-3.260353	2.301661
27	1	0	-3.139297	0.690793	1.689588
28	1	0	-3.839709	-0.920123	1.852391
29	1	0	-3.584032	-1.386267	-0.580162
30	1	0	-4.463601	0.129645	-0.340768
31	1	0	-2.593142	2.807964	-1.589993
32	1	0	-3.020330	2.283346	0.040238
33	1	0	-1.415423	4.721574	-0.106721
34	1	0	0.872539	5.361635	0.682853
35	1	0	2.645857	3.621256	0.874745
36	1	0	4.063364	1.882721	0.942202
37	1	0	5.462082	-0.165082	0.702591
38	1	0	4.447508	-2.263919	-0.214605
39	1	0	2.181567	-3.511709	-0.680944
40	1	0	2.031912	-2.536678	-2.153359

Solvated C_s [Cu([15]aneS₃bpy)]²⁺

1	29	0	0.293536	-0.000923	-0.340080
2	16	0	1.448322	1.855772	-1.219158
3	16	0	1.798733	0.000576	1.674137
4	16	0	1.444654	-1.863718	-1.213498
5	7	0	-1.188976	-1.292253	-0.057410
6	7	0	-1.183799	1.296146	-0.057906
7	6	0	2.989772	1.848330	-0.206536
8	1	0	3.645186	1.164769	-0.756136
9	1	0	3.425490	2.851977	-0.281483
10	6	0	2.841483	1.461036	1.267660
11	1	0	2.374315	2.268353	1.842903
12	1	0	3.837581	1.293916	1.694518
13	6	0	2.834157	-1.467068	1.276226
14	1	0	3.830792	-1.302407	1.702877
15	1	0	2.363545	-2.268540	1.856797
16	6	0	2.982478	-1.862822	-0.195572
17	1	0	3.413419	-2.868976	-0.265540
18	1	0	3.643545	-1.185607	-0.746327
19	6	0	0.377445	-3.136308	-0.375556
20	1	0	0.375023	-4.028391	-1.008672
21	1	0	0.847579	-3.398907	0.579735

22	6	0	-1.024638	-2.624269	-0.142669
23	6	0	-2.116672	-3.484521	0.014584
24	1	0	-1.981790	-4.563024	-0.069382
25	6	0	-3.372080	-2.933582	0.280635
26	1	0	-4.236278	-3.585087	0.411804
27	6	0	-3.527205	-1.546562	0.366252
28	1	0	-4.507407	-1.113972	0.562710
29	6	0	-2.407330	-0.734221	0.179773
30	6	0	-2.404249	0.743250	0.180111
31	6	0	-3.520400	1.560381	0.368131
32	1	0	-4.502322	1.132041	0.565322
33	6	0	-3.359140	2.946759	0.283152
34	1	0	-4.220360	3.601991	0.415335
35	6	0	-2.101443	3.492400	0.016798
36	1	0	-1.961883	4.570368	-0.066220
37	6	0	-1.013211	2.627555	-0.141674
38	6	0	0.391480	3.132313	-0.373521
39	1	0	0.865909	3.385190	0.582698
40	1	0	0.394514	4.027707	-1.001859

Solvated [Cu([15]aneS₃bpy)]²⁺ TS

1	29	0	0.301335	-0.010431	-0.323460
2	16	0	1.577602	1.803180	-1.210627
3	16	0	1.907020	0.007156	1.615242
4	16	0	1.336115	-1.977891	-1.163387
5	7	0	-1.090484	1.387687	-0.029653
6	7	0	-1.297788	-1.194310	-0.096020
7	6	0	3.154587	1.873465	-0.242088
8	6	0	3.394279	0.827699	0.873787
9	6	0	2.399310	-1.763851	1.483211
10	6	0	2.679253	-2.260648	0.066075
11	6	0	0.054040	-3.180878	-0.572629
12	6	0	-1.264223	-2.531576	-0.232653
13	6	0	-2.423791	-3.298026	-0.063358
14	6	0	-3.617263	-2.652670	0.258621
15	6	0	-3.644942	-1.260189	0.379520
16	6	0	-2.463198	-0.544973	0.184484
17	6	0	-2.346227	0.924476	0.210616
18	6	0	-3.400442	1.817162	0.416276
19	6	0	-3.144785	3.188945	0.341666
20	6	0	-1.853100	3.644755	0.071063
21	6	0	-0.831002	2.705622	-0.099192
22	6	0	0.604226	3.106797	-0.302536
23	1	0	3.196380	2.891097	0.155420
24	1	0	3.942333	1.776825	-0.995170
25	1	0	3.916452	1.319774	1.698904

26	1	0	1.575419	-2.307798	1.958730
27	1	0	3.295303	-1.914072	2.096445
28	1	0	3.553632	-1.777983	-0.382768
29	1	0	2.876391	-3.339635	0.077307
30	1	0	-0.075926	-3.917296	-1.372492
31	1	0	0.464574	-3.705736	0.298863
32	1	0	-2.384447	-4.380568	-0.186424
33	1	0	4.039777	0.029696	0.500701
34	1	0	-4.530982	-3.229933	0.400799
35	1	0	-4.577385	-0.747017	0.610369
36	1	0	-4.408353	1.456844	0.617475
37	1	0	-3.956898	3.901818	0.485508
38	1	0	-1.634969	4.710099	-0.003810
39	1	0	1.088035	3.248097	0.672314
40	1	0	0.687725	4.038875	-0.868967