

Supporting Information:

Controlling Electron Transfer through the Manipulation of Structure and Ligand-Based Torsional Motions: A Computational Exploration of Ruthenium Donor-Bridge-Acceptor Systems using Density Functional Theory

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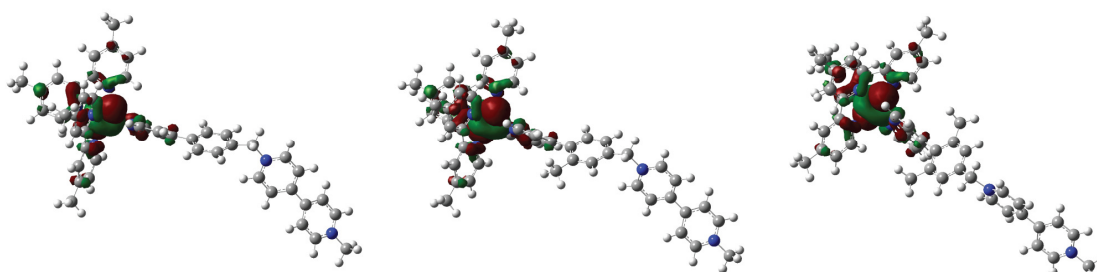
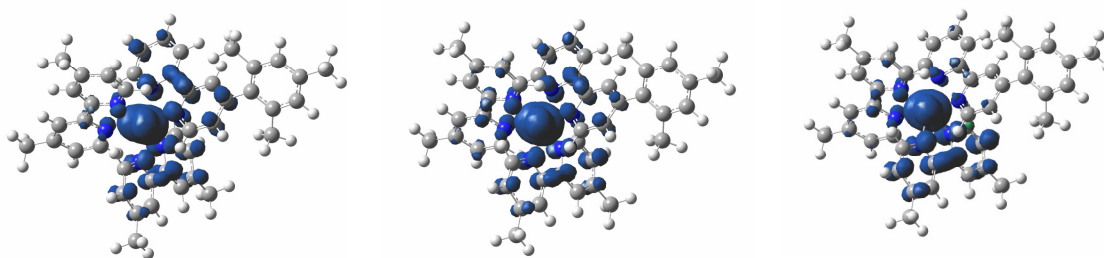


Figure S1. Kohn-Sham HOMO orbitals calculated in vacuo for the ground state dmb-based DA species DA1, DA2, and DA3 (from left to right).

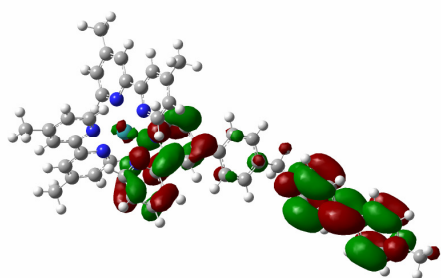


D3* B3LYP

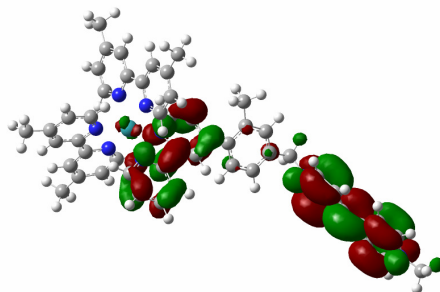
D3* B3PW91

D3* PBE1PBE

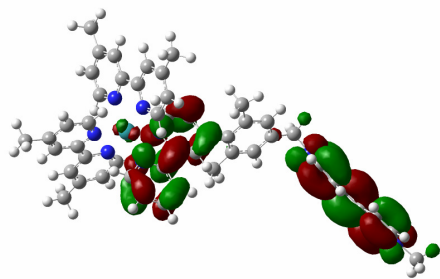
Figure S2. Spin density distributions (contour value = 0.0025) for the optimized ³MLCT state of D3* using various functional models.



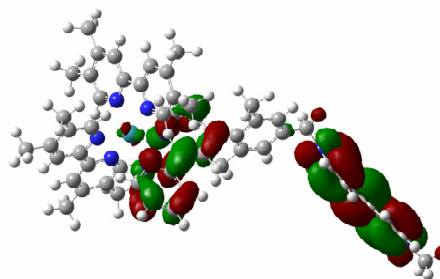
${}^3\text{DA1}$ (L = dmb)



${}^3\text{DA2}$ (L = dmb)



${}^3\text{DA3}$ (L = dmb)



${}^3\text{DA3}'$ (L = tmb)

Figure S3. Kohn-Sham HOMO orbitals (contour value=0.02) calculated in vacuo for the triplet state **DA** species.

TABLE S1. Energy and Structural Properties of Ground State Singlet for [Ru(dmb)₂(bpy- ϕ -MV)]⁴⁺ (**DA1**), [Ru(dmb)₂(bpy-*o*-tolyl-MV)]⁴⁺ (**DA2**), [Ru(dmb)₂(bpy-2,6-Me₂- ϕ -MV)]⁴⁺ (**DA3**) and [Ru(tmb)₂(bpy-2,6-Me₂- ϕ -MV)]⁴⁺ (**DA3'**)

Method	DA1 (L=dmb)	DA2 (L=dmb)	DA3 (L=dmb)	DA3' (L=tmb)
B3LYP				
Energy (hartrees)	-2540.8162	-2580.1222	-2619.4297	-2776.6763
θ_1 (av)	34.6°	49.9°	85.5	85.9°
θ_2 (av)	39.5°	38.7°	38.7°	39.0°
C ₁	1.489 Å	1.495 Å	1.501 Å	1.505 Å
C ₂	1.472 Å	1.472 Å	1.471 Å	1.471 Å
C ₃	1.474 Å	1.474 Å	1.474 Å	1.471 Å
C ₄	1.490 Å	1.490 Å	1.490 Å	1.490 Å
RuN ₁	2.104 Å	2.110 Å	2.110 Å	2.110 Å
RuN ₂	2.105 Å	2.106 Å	2.106 Å	2.103 Å
B3PW91				
Energy (hartrees)	-2539.9363	-2579.2295	-2618.5240	-2775.7182
θ_1 (av)	35.8°	50.8°	86.3°	88.0°
θ_2 (av)	42.6°	40.6°	41.2°	41.3°
C ₁	1.485 Å	1.491 Å	1.500 Å	1.500 Å
C ₂	1.467 Å	1.467 Å	1.467 Å	1.466 Å
C ₃	1.469 Å	1.469 Å	1.469 Å	1.466 Å
C ₄	1.486 Å	1.486 Å	1.486 Å	1.486 Å
RuN ₁	2.079 Å	2.082 Å	2.086 Å	2.082 Å
RuN ₂	2.082 Å	2.082 Å	2.083 Å	2.080 Å
PBE1PBE				
Energy (hartrees)	-2537.9378	-2577.1962	-2616.4558	-2773.5108
θ_1 (av)	35.6°	49.4°	85.3	88.8°
θ_2 (av)	40.5°	40.2°	40.2°	40.4°
C ₁	1.483 Å	1.488 Å	1.497 Å	1.498 Å
C ₂	1.466 Å	1.466 Å	1.466 Å	1.466 Å
C ₃	1.468 Å	1.468 Å	1.468 Å	1.464 Å
C ₄	1.484 Å	1.484 Å	1.484 Å	1.484 Å
RuN ₁	2.074 Å	2.076 Å	2.080 Å	2.076 Å
RuN ₂	2.076 Å	2.078 Å	2.077 Å	2.074 Å

For all calculations the basis set for Ru was LANL2DZ with an ECP and 631-G for all N, C and H atoms,

TABLE S2: Energy and Structural Properties of Lowest Energy Triplet for [Ru(dmb)₂(4-*p*-tolyl-2,2'-bipyridine)]²⁺ (**D1***), [Ru(dmb)₂(4-(2,6-dimethylphenyl)-2,2'-bipyridine)]²⁺ (**D2***), [Ru(dmb)₂(4-mesityl-2,2'-bipyridine)]²⁺ (**D3***), and [Ru(tmb)₂(4-mesityl-2,2'-bipyridine)]²⁺ (**D3'***).

Method	D1* (L=dmb)	D2* (L=dmb)	D3* (L=dmb)	D3'* (L=tmb)
B3LYP				
Energy (hartrees)	-2006.8796	-2046.1826	-2085.4849	-2242.7317
<S ² >	2.0193	2.0176	2.0060	2.0135
θ ₁ (av)	21.3°	34.9°	54.8°	55.9°
C ₁	1.460 Å	1.466 Å	1.483 Å	1.482 Å
C ₂	1.426 Å	1.425 Å	1.451 Å	1.420 Å
C ₃	1.474 Å	1.474 Å	1.449 Å	1.471 Å
RuN ₁	2.016 Å	2.018 Å	2.066 Å	2.031 Å
RuN ₂	2.093 Å	2.092 Å	2.101 Å	2.084 Å
B3PW91				
Energy (hartrees)	-2006.2046	-2045.4947	-2084.7846	-2241.9788
<S ² >	2.0193	2.0173	2.0055	2.0132
θ ₁ (av)	23.2°	36.2°	56.8°	56.4°
C ₁	1.457 Å	1.464 Å	1.480 Å	1.479 Å
C ₂	1.423 Å	1.423 Å	1.451 Å	1.417 Å
C ₃	1.469 Å	1.469 Å	1.446 Å	1.466 Å
RuN ₁	2.004 Å	2.006 Å	2.064 Å	2.021 Å
RuN ₂	2.073 Å	2.071 Å	2.082 Å	2.063 Å
PBE1PBE				
Energy (hartrees)	-2004.6231	-2043.8785	-2083.1335	-2240.1895
<S ² >	2.0214	2.0193	2.0071	2.0127
θ ₁ (av)	24.5°	36.6°	54.5°	59.8°
C ₁	1.459 Å	1.464 Å	1.476 Å	1.481 Å
C ₂	1.419 Å	1.418 Å	1.459 Å	1.415 Å
C ₃	1.469 Å	1.469 Å	1.433 Å	1.465 Å
RuN ₁	1.998 Å	2.001 Å	2.066 Å	2.025 Å
RuN ₂	2.063 Å	2.062 Å	2.087 Å	2.049 Å

For all calculations the basis set for the Ru was LANL2DZ with an ECP and 631-G for the H, N, C atoms.

TABLE S3: Energy and Structural Properties of the lowest triplet state for [Ru(dmb)₂(bpy- ϕ -MV)]⁴⁺ (**³DA1**), [Ru(dmb)₂(bpy-*o*-tolyl-MV)]⁴⁺ (**³DA2**), [Ru(dmb)₂(bpy-2,6-Me₂- ϕ -MV)]⁴⁺ (**³DA3**), and [Ru(tmb)₂(bpy-2,6-Me₂- ϕ -MV)]⁴⁺ (**³DA3'**)

Method	³DA1 (L = dmb)	³DA2 (L = dmb)	³DA3 (L = dmb)	³DA3' (L = tmb)
B3LYP				
Energy (hartrees)	-2540.7628	-2580.0670	-2619.3726	-2776.6256
<S ² >	2.0081	2.0078	2.0072	2.0075
ΔE (eV)	1.450	1.500	1.555	1.380
θ_1 (av)	28.0°	43.9°	73.8°	81.3°
θ_2 (av)	14.8°	12.7°	15.8°	13.7°
C ₁	1.479 Å	1.485 Å	1.500 Å	1.501 Å
C ₂	1.457 Å	1.456 Å	1.452 Å	1.456 Å
C ₃	1.473 Å	1.474 Å	1.473 Å	1.469 Å
C ₄	1.456 Å	1.455 Å	1.457 Å	1.453 Å
RuN ₁	2.092 Å	2.095 Å	2.101 Å	2.108 Å
RuN ₂	2.106 Å	2.103 Å	2.098 Å	2.104 Å
B3PW91				
Energy (hartrees)	-2539.8834	-2579.1753	-2618.4675	-2775.6685
<S ² >	2.0083	2.0080	2.0074	2.0076
ΔE (eV)	1.439	1.474	1.536	1.354
θ_1 (av)	29.3°	44.6°	74.9°	82.1°
θ_2 (av)	17.2°	16.5°	17.9°	15.9°
C ₁	1.476 Å	1.482 Å	1.496 Å	1.497 Å
C ₂	1.453 Å	1.452 Å	1.448 Å	1.452 Å
C ₃	1.469 Å	1.469 Å	1.469 Å	1.465 Å
C ₄	1.452 Å	1.452 Å	1.454 Å	1.450 Å
RuN ₁	2.076 Å	2.078 Å	2.085 Å	2.089 Å
RuN ₂	2.085 Å	2.083 Å	2.080 Å	2.084 Å
PBE1PBE				
Energy (hartrees)	-2537.8840	-2577.1413	-2616.3984	-2773.4603
<S ² >	2.0099	2.0095	2.0088	2.0094
ΔE (eV)	1.463	1.496	1.561	1.375
θ_1 (av)	28.4°	43.1°	70.2°	78.4°
θ_2 (av)	15.1°	14.5°	16.0°	13.3°
C ₁	1.473 Å	1.479 Å	1.491 Å	1.493 Å
C ₂	1.454 Å	1.452 Å	1.450 Å	1.454 Å
C ₃	1.467 Å	1.468 Å	1.468 Å	1.464 Å
C ₄	1.448 Å	1.447 Å	1.450 Å	1.445 Å
RuN ₁	2.071 Å	2.074 Å	2.078 Å	2.084 Å
RuN ₂	2.080 Å	2.078 Å	2.075 Å	2.080 Å

For all calculations the basis set for the Ru was LANL2DZ with an ECP and 631G for H, N, and C.

All Geometries reported here were optimized with a B3LYP functional and a Basis of LANL2DZ for the Ruthenium atom and 631G for C, N, and H atoms, in the gas phase unless otherwise noted.

**[Ru(dmb)₂(bpy- ϕ -MV)]⁴⁺ ground state (DA1)
Energy -2540.8162185 Hartrees**

Atom Type	Coordinates (Angstroms)						
	X	Y	Z				
1 C	4.987428	-4.552982	0.932151	44 C	-6.702302	-1.254183	2.438634
2 C	3.674408	-4.132015	1.206454	45 N	-7.960634	-0.911687	1.619111
3 C	3.271754	-2.842786	0.871641	46 C	-9.109622	-1.581708	1.919463
4 N	4.101489	-1.946936	0.281380	47 C	-10.304569	-1.265582	1.291179
5 C	5.391735	-2.332222	0.000985	48 C	-10.348160	-0.233944	0.330868
6 C	5.838374	-3.618371	0.318016	49 C	-9.141212	0.430144	0.033850
7 C	4.748467	0.308281	2.584250	50 C	-7.963889	0.074455	0.684917
8 C	5.269842	0.980228	3.683847	51 C	-11.632610	0.138735	-0.326211
9 C	5.348282	2.386087	3.679480	52 C	-11.962685	1.485368	-0.574689
10 C	4.869649	3.045239	2.536330	53 C	-13.179161	1.809784	-1.162098
11 C	4.351243	2.327574	1.452144	54 N	-14.065050	0.836245	-1.511005
12 N	4.294959	0.955985	1.480131	55 C	-13.771328	-0.475905	-1.292099
13 C	6.232509	-1.306736	-0.641103	56 C	-12.569927	-0.844672	-0.701492
14 C	3.836206	2.953243	0.221413	57 C	-15.390439	1.209334	-2.111350
15 N	5.605764	-0.114807	-0.906600	58 H	2.969893	-4.806365	1.678944
16 C	6.318318	0.874041	-1.506843	59 H	2.266592	-2.500717	1.076655
17 C	7.653845	0.724873	-1.861187	60 H	6.855807	-3.909441	0.088544
18 C	8.323683	-0.485296	-1.596318	61 H	4.686379	-0.770796	2.563795
19 C	7.577414	-1.500218	-0.977622	62 H	5.619590	0.412361	4.538462
20 C	3.792012	4.336040	0.007895	63 H	4.912972	4.126429	2.500376
21 C	3.300257	4.869171	-1.193539	64 H	5.788571	1.795806	-1.701133
22 C	2.845555	3.950907	-2.159542	65 H	8.172538	1.547382	-2.340397
23 C	2.905575	2.585877	-1.904582	66 H	8.060391	-2.444098	-0.759703
24 N	3.394018	2.079936	-0.742627	67 H	4.145520	5.013526	0.774754
25 C	3.407754	-1.090809	-3.155659	68 H	2.452175	4.299361	-3.107688
26 C	1.013603	0.354324	1.404532	69 H	2.569337	1.863970	-2.636076
27 C	-0.343396	0.253720	1.687380	70 H	4.472004	-0.903882	-3.138298
28 C	-1.227393	-0.288971	0.731543	71 H	1.708094	0.753212	2.130663
29 C	-0.667582	-0.692001	-0.492879	72 H	-0.698215	0.563725	2.662458
30 C	0.708340	-0.570390	-0.733267	73 H	-1.309673	-1.087409	-1.269296
31 N	1.550616	-0.055539	0.225621	74 H	-0.374340	-1.696289	-3.048612
32 C	1.364004	-0.969050	-1.989236	75 H	0.893947	-2.302627	-5.089529
33 N	2.721836	-0.754175	-2.033167	76 H	3.373637	-1.899443	-5.145909
34 C	0.693931	-1.526725	-3.086421	77 H	-2.837803	1.349231	2.221870
35 C	1.404912	-1.869721	-4.237824	78 H	-5.143583	0.940560	2.942221
36 C	2.785725	-1.646745	-4.272098	79 H	-5.216204	-2.707883	0.631492
37 Ru	3.590528	0.028875	-0.282654	80 H	-2.896731	-2.320370	-0.048480
38 C	-2.674695	-0.458709	1.038848	81 H	-6.838066	-0.734737	3.392393
39 C	-3.348639	0.460793	1.868033	82 H	-6.773826	-2.329234	2.619720
40 C	-4.670621	0.238780	2.260867	83 H	-9.043978	-2.353103	2.675918
41 C	-5.366340	-0.906186	1.828977	84 H	-11.197230	-1.806248	1.580726
42 C	-4.713607	-1.803172	0.961067	85 H	-9.099677	1.212131	-0.714426
43 C	-3.391943	-1.580141	0.570256	86 H	-7.015148	0.553719	0.484520
				87 H	-11.299550	2.292875	-0.290319
				88 H	-13.473931	2.832621	-1.356090
				89 H	-14.513334	-1.201576	-1.598739

90 H	-12.369947	-1.900089	-0.563813	100 H	10.107930	-1.697535	-1.772602
91 H	-15.296736	2.171703	-2.613008	101 H	9.950786	-0.441824	-3.012064
92 H	-16.137245	1.273030	-1.315959	102 C	5.935115	3.142965	4.840571
93 H	-15.679523	0.449546	-2.837329	103 H	7.026042	3.024502	4.867317
94 C	5.471649	-5.934884	1.281678	104 H	5.720426	4.212590	4.779616
95 H	5.915636	-6.431625	0.411620	105 H	5.550615	2.769478	5.795385
96 H	6.246734	-5.894016	2.057076	106 C	3.278696	6.352676	-1.448013
97 H	4.660808	-6.564761	1.654186	107 H	3.399462	6.925232	-0.525116
98 C	9.772547	-0.674238	-1.956129	108 H	4.094051	6.640704	-2.124425
99 H	10.410699	-0.001529	-1.369848	109 H	2.343616	6.662594	-1.925410

[Ru(dmb)₂(bpy- ϕ -MV)]⁴⁺ triplet state (³DA1)
Energy -2540.762787 Hartrees

Atom Type	Coordinates (Angstroms)						
	X	Y	Z				
1 C	-4.661636	-4.432002	-1.757227	38 C	2.616768	0.285648	-1.304361
2 C	-3.392109	-3.855775	-1.968818	39 C	3.148628	1.396879	-1.992158
3 C	-3.080210	-2.626297	-1.403088	40 C	4.477279	1.407880	-2.418549
4 N	-3.970375	-1.932795	-0.645736	41 C	5.320481	0.308506	-2.185131
5 C	-5.215268	-2.467694	-0.417204	42 C	4.809236	-0.787228	-1.464677
6 C	-5.566447	-3.705417	-0.963731	43 C	3.484242	-0.797741	-1.029625
7 C	-4.987628	0.774880	-2.347939	44 C	6.701654	0.283898	-2.817865
8 C	-5.583608	1.656881	-3.240479	45 N	7.850202	0.099045	-1.879885
9 C	-5.657733	3.031456	-2.934159	46 C	8.713709	-0.965210	-2.037038
10 C	-5.103428	3.442581	-1.708857	47 C	9.863216	-1.071338	-1.291370
11 C	-4.509009	2.522118	-0.840727	48 C	10.226108	-0.074047	-0.337220
12 N	-4.451704	1.189553	-1.170357	49 C	9.290931	0.996622	-0.182967
13 C	-6.107606	-1.654879	0.426920	50 C	8.144901	1.063072	-0.936681
14 C	-3.919144	2.874143	0.462387	51 C	11.479612	-0.128423	0.398893
15 N	-5.570185	-0.476968	0.887986	52 C	12.005949	1.004350	1.084052
16 C	-6.335206	0.341900	1.657777	53 C	13.213758	0.942215	1.744144
17 C	-7.640130	0.022087	2.008947	54 N	13.948301	-0.214223	1.773560
18 C	-8.220034	-1.181575	1.557331	55 C	13.472903	-1.331032	1.136878
19 C	-7.418926	-2.011921	0.753194	56 C	12.273273	-1.310428	0.460112
20 C	-3.863013	4.173523	0.973601	57 C	15.274827	-0.245874	2.450399
21 C	-3.281224	4.436708	2.226698	58 H	-2.651182	-4.366531	-2.572867
22 C	-2.749081	3.335930	2.929954	59 H	-2.112302	-2.168233	-1.552509
23 C	-2.819304	2.060665	2.385159	60 H	-6.548021	-4.121248	-0.776655
24 N	-3.401330	1.820898	1.179929	61 H	-4.924774	-0.283193	-2.562365
25 C	-3.198940	-1.871142	2.767177	62 H	-5.992129	1.277942	-4.170219
26 C	-1.130158	0.874208	-1.352259	63 H	-5.146815	4.490684	-1.441840
27 C	0.206898	0.951248	-1.691110	64 H	-5.874721	1.259925	1.994978
28 C	1.185699	0.243344	-0.934399	65 H	-8.206322	0.705696	2.631021
29 C	0.709898	-0.502365	0.158739	66 H	-7.836251	-2.939855	0.383986
30 C	-0.655307	-0.561009	0.471418	67 H	-4.271467	4.998142	0.403661
31 N	-1.582567	0.122757	-0.306727	68 H	-2.283693	3.475482	3.898788
32 C	-1.212329	-1.294078	1.601106	69 H	-2.417123	1.203544	2.907314
33 N	-2.584898	-1.205135	1.752055	70 H	-4.273876	-1.771704	2.830532
34 C	-0.460630	-2.062523	2.508776	71 H	-1.881214	1.396329	-1.929213
35 C	-1.093498	-2.732205	3.551944	72 H	0.491003	1.527354	-2.561689
36 C	-2.490175	-2.635758	3.685543	73 H	1.415999	-1.024613	0.790595
37 Ru	-3.580532	-0.072963	0.282262	74 H	0.613215	-2.136604	2.398328
				75 H	-0.515368	-3.323299	4.252303
				76 H	-3.014296	-3.143699	4.485255
				77 H	2.532754	2.267317	-2.188321

78 H	4.850586	2.271186	-2.960651	94 C	-5.025641	-5.762809	-2.352425
79 H	5.435578	-1.652696	-1.272198	95 H	-4.343873	-6.547225	-2.001955
80 H	3.109360	-1.683658	-0.528323	96 H	-6.044033	-6.061839	-2.096187
81 H	6.876279	1.213776	-3.368395	97 H	-4.944212	-5.738144	-3.445827
82 H	6.764663	-0.532082	-3.543789	98 C	-9.627852	-1.556685	1.923309
83 H	8.452939	-1.690560	-2.795705	99 H	-9.955344	-2.465743	1.414882
84 H	10.509071	-1.914993	-1.493958	100 H	-9.716398	-1.724337	3.004359
85 H	9.457151	1.782574	0.541658	101 H	-10.328269	-0.752206	1.671110
86 H	7.430781	1.868817	-0.834623	102 C	-6.310005	4.007072	-3.872525
87 H	11.491846	1.955731	1.078141	103 H	-7.383545	3.798368	-3.964182
88 H	13.638158	1.796492	2.253943	104 H	-6.197492	5.039146	-3.534069
89 H	14.086731	-2.219515	1.198546	105 H	-5.886604	3.928829	-4.880376
90 H	11.948051	-2.232836	-0.001297	106 C	-3.235721	5.825377	2.798122
91 H	15.280810	0.478116	3.265100	107 H	-3.519585	6.580909	2.062489
92 H	16.062257	0.000304	1.733015	108 H	-3.922707	5.914426	3.650137
93 H	15.447353	-1.241919	2.858653	109 H	-2.235501	6.067683	3.17314

[Ru(dmb)₂(*p*-tolyl-2,2'-bipyridine)]²⁺ triplet state (D1*)
Energy –2006.879592 Hartrees

Atom Type	Coordinates (Angstroms)						
	X	Y	Z				
1 C	1.761333	-4.355346	1.990169	26 C	-1.826582	0.725507	1.045957
2 C	0.461000	-3.816799	1.999697	27 C	-3.187674	0.700315	1.153124
3 C	0.212513	-2.583158	1.409398	28 C	-3.982590	-0.112220	0.242853
4 N	1.193012	-1.857249	0.814474	29 C	-3.278257	-0.813139	-0.739876
5 C	2.469870	-2.355059	0.787751	30 C	-1.877711	-0.763939	-0.849523
6 C	2.763134	-3.592815	1.370987	31 N	-1.126522	0.005272	0.098312
7 C	1.645190	0.953669	2.681613	32 C	-1.107827	-1.396602	-1.869949
8 C	1.975281	1.883565	3.660969	33 N	0.269144	-1.163986	-1.821985
9 C	2.014848	3.255144	3.344604	34 C	-1.630158	-2.217870	-2.907596
10 C	1.710054	3.615149	2.022952	35 C	-0.789124	-2.777803	-3.848463
11 C	1.380968	2.643575	1.070586	36 C	0.605682	-2.533461	-3.775345
12 N	1.350502	1.314959	1.408622	37 Ru	0.870039	-0.013271	-0.179607
13 C	3.467370	-1.502922	0.117560	38 C	-5.436657	-0.168935	0.355998
14 C	1.044624	2.944251	-0.332566	39 C	-6.163196	0.852651	1.022110
15 N	2.980342	-0.338723	-0.416410	40 C	-7.549740	0.805520	1.116265
16 C	3.837546	0.506440	-1.042838	41 C	-8.284923	-0.262974	0.564757
17 C	5.193331	0.230934	-1.170816	42 C	-7.565732	-1.290168	-0.088783
18 C	5.722947	-0.959225	-0.635379	43 C	-6.183408	-1.246104	-0.194418
19 C	4.826760	-1.820886	0.014486	44 H	-0.356458	-4.357542	2.462409
20 C	0.973801	4.236049	-0.864124	45 H	-0.776461	-2.147858	1.398788
21 C	0.632339	4.446197	-2.209670	46 H	3.774484	-3.977823	1.345275
22 C	0.369179	3.305383	-2.993375	47 H	1.604719	-0.104890	2.900032
23 C	0.450820	2.039677	-2.427869	48 H	2.199730	1.543240	4.665350
24 N	0.785624	1.852690	-1.124979	49 H	1.732315	4.661573	1.746280
25 C	1.084565	-1.733271	-2.752512	50 H	3.408748	1.411794	-1.450241
				51 H	5.834625	0.936978	-1.685785
				52 H	5.201135	-2.743361	0.439316
				53 H	1.176299	5.093189	-0.234797

54 H	0.096096	3.405018	-4.037466	71 C	2.058027	-5.694792	2.609785
55 H	0.246105	1.145226	-2.999495	72 H	1.546418	-6.497063	2.063896
56 H	2.141158	-1.519263	-2.655027	73 H	3.127782	-5.916644	2.605869
57 H	-1.224311	1.305386	1.732386	74 H	1.704696	-5.737266	3.646138
58 H	-3.661730	1.254881	1.950960	75 C	7.187834	-1.284824	-0.753471
59 H	-3.827798	-1.381864	-1.478376	76 H	7.796092	-0.548711	-0.213845
60 H	-2.695611	-2.403598	-2.957355	77 H	7.418435	-2.272862	-0.348450
61 H	-1.191963	-3.401242	-4.638164	78 H	7.512446	-1.262185	-1.800003
62 H	1.289061	-2.958704	-4.499054	79 C	0.538835	5.830353	-2.792315
63 H	-5.642856	1.707639	1.437813	80 H	-0.489794	6.051900	-3.102504
64 H	-8.078748	1.607792	1.620276	81 H	0.845945	6.595756	-2.075932
65 H	-8.107585	-2.133980	-0.504295	82 H	1.168160	5.925538	-3.684525
66 H	-5.669429	-2.072728	-0.672412	83 C	2.367228	4.286565	4.383216
67 C	-9.787027	-0.310749	0.654659	84 H	2.373426	5.296627	3.967003
68 H	-10.139486	-1.309167	0.936917	85 H	1.650536	4.267304	5.212877
69 H	-10.172136	0.407109	1.383613	86 H	3.357129	4.090249	4.811403
70 H	-10.244432	-0.074563	-0.316070				

[Ru(dmb)₂(bpy-*o*-tolyl-MV)]⁴⁺ ground state (DA2)
Energy -2580.122230 Hartrees

Atom Type	Coordinates (Angstroms)			26 C	1.122293	0.606938	1.381988
	X	Y	Z				
1 C	4.833899	-4.521883	1.493295	27 C	-0.233240	0.650182	1.688664
2 C	3.550997	-3.995881	1.740888	28 C	-1.174902	0.068982	0.814701
3 C	3.201981	-2.747985	1.239023	29 C	-0.671490	-0.534498	-0.349736
4 N	4.056898	-1.987301	0.507508	30 C	0.705225	-0.550429	-0.619333
5 C	5.314690	-2.475542	0.251684	31 N	1.601615	0.018741	0.255198
6 C	5.708293	-3.729099	0.735070	32 C	1.303536	-1.152873	-1.821600
7 C	4.891757	0.515078	2.471078	33 N	2.670213	-1.032748	-1.916826
8 C	5.477975	1.298721	3.458623	34 C	0.573080	-1.805639	-2.823714
9 C	5.621426	2.685940	3.266127	35 C	1.232600	-2.339898	-3.932168
10 C	5.138290	3.212371	2.057723	36 C	2.622967	-2.209798	-4.020257
11 C	4.553499	2.385564	1.091705	37 Ru	3.630251	-0.080325	-0.302345
12 N	4.434350	1.033699	1.302281	38 C	-2.631306	0.030121	1.151507
13 C	6.186308	-1.593503	-0.543507	39 C	-3.349906	1.180892	1.572337
14 C	4.029937	2.869885	-0.197842	40 C	-4.680715	1.017430	1.997574
15 N	5.614245	-0.413567	-0.949742	41 C	-5.318529	-0.234435	2.011945
16 C	6.358337	0.447879	-1.691201	42 C	-4.616110	-1.354842	1.533430
17 C	7.673513	0.180674	-2.052740	43 C	-3.295636	-1.214194	1.106971
18 C	8.286962	-1.020486	-1.647460	44 C	-6.655658	-0.394116	2.692740
19 C	7.508282	-1.903512	-0.883480	45 N	-7.909978	-0.369330	1.797461
20 C	4.044284	4.212917	-0.592828	46 C	-9.062701	-0.878830	2.317943
21 C	3.541944	4.606944	-1.842574	47 C	-10.253350	-0.816576	1.610350
22 C	3.015537	3.593366	-2.666537	48 C	-10.288301	-0.215966	0.334826
23 C	3.018513	2.272855	-2.232713	49 C	-9.077697	0.289332	-0.179420
24 N	3.517426	1.900982	-1.025583	50 C	-7.905004	0.200321	0.564951
25 C	3.305691	-1.553958	-2.997483	51 C	-11.567437	-0.113949	-0.422513
				52 C	-11.886539	1.038985	-1.166434
				53 C	-13.097557	1.122257	-1.841716

54 N	-13.989621	0.094081	-1.800469	84 H	-6.953453	0.571121	0.208595
55 C	-13.706894	-1.037763	-1.097177	85 H	-11.218569	1.890406	-1.205694
56 C	-12.510657	-1.160992	-0.402679	86 H	-13.383644	1.995962	-2.412262
57 C	-15.308971	0.219816	-2.507215	87 H	-14.452902	-1.821636	-1.110065
58 H	2.830394	-4.557668	2.324233	88 H	-12.319470	-2.086315	0.126441
59 H	2.223080	-2.325327	1.419517	89 H	-15.195988	0.892603	-3.356603
60 H	6.702814	-4.101763	0.525989	90 H	-16.050849	0.617556	-1.810174
61 H	4.778791	-0.552716	2.596687	91 H	-15.617958	-0.762862	-2.862866
62 H	5.826952	0.831122	4.372237	92 C	5.241922	-5.874792	2.011650
63 H	5.230059	4.276040	1.877609	93 H	4.697401	-6.672124	1.490122
64 H	5.870758	1.364232	-1.992393	94 H	6.310161	-6.057261	1.873806
65 H	8.220348	0.904806	-2.645844	95 H	5.014234	-5.976205	3.078328
66 H	7.948590	-2.836247	-0.554918	96 C	9.709558	-1.339532	-2.020393
67 H	4.453262	4.966818	0.067752	97 H	10.391265	-0.550904	-1.681528
68 H	2.611548	3.832866	-3.643589	98 H	10.042395	-2.284131	-1.584401
69 H	2.626940	1.477745	-2.852042	99 H	9.822758	-1.412028	-3.108911
70 H	4.379125	-1.431825	-3.022770	100 C	6.280911	3.558787	4.299787
71 H	1.860891	1.036307	2.044537	101 H	7.371591	3.437212	4.267740
72 H	-0.546258	1.110332	2.616953	102 H	6.063120	4.617312	4.137536
73 H	-1.360809	-0.981386	-1.054963	103 H	5.959692	3.292582	5.311735
74 H	-0.502064	-1.901186	-2.744143	104 C	3.582753	6.043041	-2.292040
75 H	0.675070	-2.847410	-4.710302	105 H	3.764736	6.724986	-1.457780
76 H	3.171894	-2.609815	-4.863879	106 H	4.385575	6.196165	-3.025024
77 H	-5.209923	1.892716	2.367062	107 H	2.646774	6.336398	-2.778175
78 H	-5.073041	-2.339848	1.542435	108 C	-2.750739	2.571997	1.594551
79 H	-2.748102	-2.096405	0.792560	109 H	-2.289363	2.801515	2.563299
80 H	-6.816578	0.406835	3.421117	110 H	-1.986039	2.704663	0.825254
81 H	-6.707924	-1.351853	3.215887	111 H	-3.525006	3.326965	1.429613
82 H	-11.149200	-1.209410	2.075223	112 H	-9.002860	-1.315205	3.306728
83 H	-9.029065	0.736839	-1.164535				

[Ru(dmb)₂(bpy-*o*-tolyl-MV)]⁴⁺ triplet state (³DA2)
Energy -2580.066981 Hartrees

Atom Type	Coordinates (Angstroms)						
	X	Y	Z				
1 C	-4.354126	-4.333540	-2.312201	19 C	-7.295801	-2.444090	0.437613
2 C	-3.126034	-3.654783	-2.422090	20 C	-4.226647	3.893880	1.469477
3 C	-2.905002	-2.487675	-1.699066	21 C	-3.668753	4.044784	2.754120
4 N	-3.848801	-1.955048	-0.881936	22 C	-3.049603	2.913464	3.319629
5 C	-5.058460	-2.597156	-0.745976	23 C	-3.014176	1.713610	2.618257
6 C	-5.317242	-3.774352	-1.450127	24 N	-3.573734	1.579952	1.388237
7 C	-5.063836	0.853979	-2.258721	25 C	-3.101800	-2.246366	2.522984
8 C	-5.731426	1.789067	-3.042770	26 C	-1.220935	1.117655	-1.208520
9 C	-5.921382	3.101367	-2.570114	27 C	0.110669	1.358806	-1.494618
10 C	-5.403527	3.402128	-1.295065	28 C	1.135108	0.669219	-0.786179
11 C	-4.734732	2.434960	-0.542554	29 C	0.713038	-0.247947	0.190675
12 N	-4.566505	1.160993	-1.034258	30 C	-0.647971	-0.468303	0.455571
13 C	-6.011998	-1.960379	0.179468	31 N	-1.618633	0.218263	-0.263755
14 C	-4.176352	2.669825	0.800715	32 C	-1.154871	-1.373838	1.476875
15 N	-5.559286	-0.816704	0.796588	33 N	-2.533009	-1.416143	1.607330
16 C	-6.381238	-0.160421	1.655176	34 C	-0.353009	-2.181333	2.305140
17 C	-7.663832	-0.612644	1.944995	35 C	-0.940997	-3.018954	3.247974
18 C	-8.157204	-1.780786	1.333526	36 C	-2.343185	-3.053713	3.360799
				37 Ru	-3.601939	-0.199072	0.266331
				38 C	2.573820	0.864495	-1.099213
				39 C	3.143403	2.146779	-1.323705

40 C	4.491879	2.215992	-1.714806	77 H	4.919823	3.197424	-1.900063
41 C	5.287372	1.077299	-1.899018	78 H	5.318705	-1.086237	-1.745413
42 C	4.730577	-0.182746	-1.619870	79 H	2.970991	-1.263128	-1.060583
43 C	3.399406	-0.278971	-1.221017	80 H	6.884367	2.292135	-2.683712
44 C	6.672984	1.233276	-2.501910	81 H	6.714770	0.727906	-3.471079
45 N	7.806106	0.683938	-1.695714	82 H	10.499242	-1.272667	-2.126995
46 C	8.693513	-0.206811	-2.262173	83 H	9.345875	1.233710	1.236903
47 C	9.836480	-0.595427	-1.605759	84 H	7.336577	1.854874	-0.021284
48 C	10.167346	-0.079491	-0.316636	85 H	11.329870	1.145224	1.892796
49 C	9.206415	0.816191	0.248804	86 H	13.462917	0.544776	2.941061
50 C	8.069183	1.174307	-0.433074	87 H	14.092653	-2.562982	0.222986
51 C	11.412072	-0.416705	0.356289	88 H	11.976731	-2.106741	-0.923208
52 C	11.882802	0.308146	1.489465	89 H	15.137588	-1.050101	3.316177
53 C	13.081942	-0.004810	2.091020	90 H	15.964917	-0.745252	1.763889
54 N	13.863390	-1.030499	1.626618	91 H	15.393874	-2.385906	2.175445
55 C	13.443450	-1.760049	0.545031	92 C	-4.632731	-5.601883	-3.068977
56 C	12.253626	-1.477465	-0.088663	93 H	-4.776195	-6.444185	-2.380570
57 C	15.179236	-1.320414	2.261083	94 H	-5.551379	-5.515589	-3.661140
58 H	-2.345260	-4.035712	-3.069395	95 H	-3.816017	-5.858021	-3.746539
59 H	-1.967194	-1.954003	-1.768154	96 H	-9.536183	-2.305388	1.618558
60 H	-6.270969	-4.274644	-1.337585	97 H	-10.106427	-2.443219	0.692386
61 H	-4.912638	-0.159843	-2.603564	98 H	-9.487668	-3.284937	2.110880
62 H	-6.105250	1.497326	-4.016960	99 H	-10.100245	-1.632767	2.267387
63 H	-5.535660	4.401672	-0.899831	100 C	-6.651507	4.138234	-3.377155
64 H	-5.988917	0.735514	2.116379	101 H	-7.590810	4.423734	-2.886654
65 H	-8.278439	-0.057844	2.643868	102 H	-6.055987	5.052660	-3.480629
66 H	-7.645922	-3.342418	-0.055227	103 H	-6.894922	3.776033	-4.377785
67 H	-4.701201	4.747613	1.002014	104 C	-3.746430	5.355674	3.484845
68 H	-2.598775	2.968628	4.303346	105 H	-3.460662	6.191854	2.837200
69 H	-2.543370	0.833350	3.033709	106 H	-4.773213	5.550604	3.821693
70 H	-4.181938	-2.241489	2.573029	107 H	-3.102288	5.368051	4.366292
71 H	-2.007542	1.627312	-1.748515	108 C	2.389952	3.449165	-1.140627
72 H	0.359478	2.054049	-2.284141	109 H	1.934675	3.794144	-2.078068
73 H	1.459040	-0.777060	0.769730	110 H	1.598002	3.374384	-0.390704
74 H	0.724587	-2.153814	2.210261	111 H	3.074306	4.239390	-0.818844
75 H	-0.324481	-3.639888	3.887090	112 H	8.455841	-0.559013	-3.256774
76 H	-2.832575	-3.694184	4.083628				

[Ru(dmb)₂(4-(2,6-dimethylphenyl)-2,2'-bipyridine)]²⁺ triplet state (D2*)
Energy -2046.182550 Hartrees

Atom Type	Coordinates (Angstroms)						
	X	Y	Z				
1 C	-2.382611	-4.376180	-1.796050	11 C	-1.438995	2.625567	-1.039318
2 C	-1.037661	-3.949042	-1.845996	12 N	-1.578430	1.282810	-1.353585
3 C	-0.680584	-2.717633	-1.315405	13 C	-3.821386	-1.292437	-0.082471
4 N	-1.590728	-1.878573	-0.757012	14 C	-1.037864	2.907226	0.323985
5 C	-2.910885	-2.260233	-0.700724	15 N	-3.220889	-0.190721	0.481183
6 C	-3.309068	-3.505087	-1.208885	16 C	-3.994021	0.756256	1.073144
7 C	-2.009362	0.931187	-2.594979	17 C	-5.375225	0.645849	1.143351
8 C	-2.290900	1.867737	-3.574771	18 C	-6.024582	-0.467974	0.567305
9 C	-2.137792	3.250807	-3.296101	19 C	-5.216350	-1.431179	-0.049964
10 C	-1.711450	3.604297	-2.016145	20 C	-0.812728	4.196757	0.845270
				21 C	-0.456401	4.389577	2.179032
				22 C	-0.316913	3.232520	2.994211
				23 C	-0.526049	1.979273	2.452644

24 N	-0.888865	1.796829	1.149472	59 H	3.438314	0.968222	-2.103913
25 C	-1.300736	-1.847506	2.714024	60 H	3.633405	-1.319889	1.532254
26 C	1.590751	0.509037	-1.145501	61 H	2.498501	-2.338922	3.009729
27 C	2.966047	0.484557	-1.259465	62 H	1.001087	-3.397770	4.668830
28 C	3.757661	-0.194144	-0.287903	63 H	-1.488789	-3.081751	4.457567
29 C	3.066329	-0.819805	0.759025	64 H	7.939791	1.833934	-0.623799
30 C	1.665349	-0.788249	0.842702	65 H	7.832356	-2.449474	-0.517977
31 N	0.927636	-0.114776	-0.127100	66 H	10.010850	0.640264	-0.648899
32 C	0.888245	-1.421731	1.891764	67 H	9.875719	-0.803350	-1.662060
33 N	-0.484135	-1.242778	1.809286	68 C	-2.793965	-5.716711	-2.342494
34 C	1.427553	-2.201240	2.935264	69 H	-2.337055	-6.530450	-1.765768
35 C	0.587585	-2.799415	3.865739	70 H	-3.877641	-5.852675	-2.312912
36 C	-0.806951	-2.625451	3.751197	71 H	-2.463848	-5.836867	-3.380614
37 Ru	-1.109615	-0.035756	0.207201	72 C	-7.522701	-0.603181	0.612396
38 C	5.236590	-0.236092	-0.384761	73 H	-7.861398	-1.532676	0.148960
39 C	5.979596	0.973580	-0.486903	74 H	-7.886874	-0.587325	1.646473
40 C	7.375721	0.907474	-0.571990	75 H	-8.007135	0.231238	0.091094
41 C	8.067002	-0.311284	-0.586148	76 C	-2.438445	4.285740	-4.347088
42 C	7.316192	-1.493900	-0.494361	77 H	-2.238526	5.298519	-3.988909
43 C	5.922406	-1.485845	-0.381843	78 H	-1.836153	4.119351	-5.248055
44 C	9.570817	-0.358838	-0.706155	79 H	-3.490544	4.238140	-4.654207
45 H	-0.276946	-4.577044	-2.294825	80 C	-0.223443	5.761898	2.749115
46 H	0.343595	-2.371151	-1.332781	81 H	-0.327756	6.541018	1.990279
47 H	-4.346702	-3.807142	-1.142934	82 H	-0.936220	5.977458	3.555117
48 H	-2.108443	-0.129559	-2.784472	83 H	0.779944	5.841724	3.184289
49 H	-2.621427	1.537098	-4.552370	84 C	5.331523	2.345517	-0.458030
50 H	-1.596574	4.652639	-1.769997	85 H	4.999722	2.666424	-1.454389
51 H	-3.473131	1.604159	1.495872	86 H	4.463491	2.387409	0.207434
52 H	-5.947471	1.421022	1.639542	87 H	6.050574	3.092973	-0.111232
53 H	-5.683482	-2.290220	-0.514787	88 C	5.205942	-2.822308	-0.310917
54 H	-0.917449	5.058760	0.198228	89 H	4.994956	-3.125162	0.723631
55 H	-0.038469	3.325124	4.037211	90 H	4.255184	-2.819586	-0.853497
56 H	-0.412313	1.082297	3.046177	91 H	5.831770	-3.607226	-0.744592
57 H	-2.362074	-1.678169	2.589515	92 H	10.015117	-0.970561	0.087554
58 H	0.973528	1.016590	-1.874112				

[Ru(dmb)₂(bpy-2,6-Me₂- ϕ -MV)]⁴⁺ ground state (DA3)
Energy -2619.429684 Hartrees

Atom Type	Coordinates (Angstroms)						
	X	Y	Z				
1 C	-4.421280	-4.447746	-2.152236	13 C	-6.105186	-1.919164	0.155269
2 C	-3.174031	-3.801943	-2.252975	14 C	-4.320437	2.697325	0.508798
3 C	-2.954233	-2.604984	-1.581665	15 N	-5.649549	-0.765303	0.743336
4 N	-3.903693	-2.009848	-0.814825	16 C	-6.492886	-0.072119	1.551900
5 C	-5.128688	-2.620089	-0.696235	17 C	-7.795815	-0.485185	1.804430
6 C	-5.393530	-3.827232	-1.353415	18 C	-8.291890	-1.661165	1.209628
7 C	-4.853053	0.660251	-2.487245	19 C	-7.410910	-2.371117	0.378971
8 C	-5.454483	1.521240	-3.398190	20 C	-4.471569	3.969664	1.072808
9 C	-5.722236	2.855551	-3.037266	21 C	-4.066116	4.232006	2.390426
10 C	-5.343338	3.251448	-1.744869	22 C	-3.492938	3.162741	3.105594
11 C	-4.738251	2.350552	-0.861096	23 C	-3.359664	1.916117	2.505330
12 N	-4.496321	1.052202	-1.236881	24 N	-3.765513	1.670030	1.232656
				25 C	-3.337200	-2.003354	2.739685
				26 C	-1.161543	0.907812	-1.188541
				27 C	0.197779	1.122737	-1.394643

28 C	1.142922	0.535159	-0.530261	72 H	0.518381	1.747977	-2.219759
29 C	0.648003	-0.257632	0.515057	73 H	1.342358	-0.724540	1.202361
30 C	-0.733698	-0.447272	0.683138	74 H	0.493787	-1.964709	2.677024
31 N	-1.635177	0.139745	-0.173429	75 H	-0.678388	-3.279630	4.422021
32 C	-1.329660	-1.259791	1.755864	76 H	-3.191213	-3.295628	4.449804
33 N	-2.704828	-1.278393	1.781485	77 H	5.044752	3.021674	0.078738
34 C	-0.588103	-1.977921	2.703663	78 H	5.184263	-0.241141	-2.735205
35 C	-1.244702	-2.720645	3.686688	79 H	6.762595	2.977867	-1.597388
36 C	-2.643696	-2.732068	3.704373	80 H	6.702012	1.813326	-2.934310
37 Ru	-3.673777	-0.199194	0.254193	81 H	11.117778	0.925476	-2.145898
38 C	2.611825	0.781624	-0.744008	82 H	9.003871	-0.477074	1.367496
39 C	3.246848	1.856235	-0.074416	83 H	6.926520	0.520531	0.409307
40 C	4.581030	2.160195	-0.394445	84 H	11.196057	0.181723	2.306486
41 C	5.288317	1.424960	-1.358327	85 H	13.360954	-0.721039	3.114231
42 C	4.658814	0.332275	-1.976345	86 H	14.419503	-1.989020	-0.717798
43 C	3.328646	-0.004720	-1.682594	87 H	12.285667	-1.157689	-1.670706
44 C	6.626110	1.921683	-1.849768	88 H	15.180530	-2.110510	2.807946
45 N	7.881555	1.218129	-1.300174	89 H	16.033468	-1.093895	1.610111
46 C	9.032331	1.323283	-2.023214	90 H	15.567557	-2.773185	1.203642
47 C	10.223319	0.794410	-1.549382	91 C	-4.703022	-5.734790	-2.880151
48 C	10.260054	0.140696	-0.300592	92 H	-5.586850	-6.240114	-2.483329
49 C	9.050851	0.037827	0.415826	93 H	-4.881708	-5.545749	-3.946796
50 C	7.878025	0.579180	-0.101937	94 H	-3.855649	-6.424623	-2.814039
51 C	11.539359	-0.403962	0.234963	95 C	-9.702909	-2.126266	1.448402
52 C	11.861594	-0.302059	1.602473	96 H	-9.874706	-3.128434	1.048774
53 C	13.072678	-0.792857	2.073838	97 H	-9.940484	-2.139688	2.517601
54 N	13.961501	-1.382407	1.227299	98 H	-10.421316	-1.448294	0.970371
55 C	13.675689	-1.504004	-0.099149	99 C	-6.400769	3.805556	-3.987202
56 C	12.479623	-1.021997	-0.613943	100 H	-7.472868	3.580291	-4.058089
57 C	15.281103	-1.874261	1.749334	101 H	-6.303141	4.844420	-3.662754
58 H	-2.379751	-4.232483	-2.851985	102 H	-5.989592	3.721210	-4.998303
59 H	-2.004485	-2.092136	-1.646676	103 C	-4.254393	5.586594	3.019456
60 H	-6.361992	-4.299184	-1.248480	104 H	-4.445578	6.359631	2.271121
61 H	-4.647013	-0.370037	-2.741937	105 H	-5.108228	5.576937	3.709543
62 H	-5.719582	1.153899	-4.383055	106 H	-3.376354	5.881993	3.602636
63 H	-5.532423	4.271236	-1.434314	107 C	2.506602	2.712863	0.930100
64 H	-6.096373	0.828214	1.999502	108 H	1.651902	3.222770	0.470064
65 H	-8.423745	0.106220	2.461019	109 H	2.115229	2.118410	1.763471
66 H	-7.757851	-3.281673	-0.092475	110 H	3.160444	3.481463	1.349399
67 H	-4.913158	4.769762	0.492387	111 H	8.971239	1.848005	-2.967916
68 H	-3.159053	3.301026	4.127649	112 C	2.675596	-1.165260	-2.402055
69 H	-2.931423	1.079631	3.040365	113 H	2.259323	-1.895163	-1.698383
70 H	-4.417447	-1.985815	2.715633	114 H	1.852387	-0.830360	-3.044200
71 H	-1.905143	1.349799	-1.837021	115 H	3.393970	-1.688531	-3.037790

**[Ru(dmb)₂(bpy-2,6-Me₂- ϕ -MV)]⁴⁺ triplet state (³DA3)
Energy -2619.372554 Hartrees**

Atom Type	Coordinates (Angstroms)			X	Y	Z	
1 C	-4.255468	-4.511134	-2.111882	4 N	-3.847608	-2.041469	-0.812284
2 C	-3.021886	-3.832066	-2.188374	5 C	-5.060086	-2.681290	-0.710064
3 C	-2.850837	-2.619950	-1.532593	6 C	-5.270788	-3.905160	-1.351275
				7 C	-4.991782	0.662034	-2.431956
				8 C	-5.602035	1.543323	-3.315420
				9 C	-5.810432	2.887397	-2.943350

10 C	-5.369387	3.270751	-1.664061	63 H	-5.516763	4.294932	-1.346179
11 C	-4.754209	2.353145	-0.807706	64 H	-6.165715	0.804486	1.892602
12 N	-4.565763	1.050295	-1.201422	65 H	-8.479678	0.028542	2.333796
13 C	-6.069187	-1.996410	0.115662	66 H	-7.683311	-3.402337	-0.130349
14 C	-4.278568	2.676766	0.548555	67 H	-4.811181	4.763587	0.579190
15 N	-5.657600	-0.817728	0.689662	68 H	-2.924427	3.209036	4.115509
16 C	-6.530387	-0.117864	1.462013	69 H	-2.795880	0.995777	2.997361
17 C	-7.824362	-0.560691	1.702720	70 H	-4.391302	-2.145671	2.608510
18 C	-8.278538	-1.766815	1.129682	71 H	-1.963990	1.474727	-1.801435
19 C	-7.365930	-2.474031	0.326839	72 H	0.442338	1.944973	-2.163588
20 C	-4.368604	3.944026	1.130721	73 H	1.349209	-0.636890	1.156493
21 C	-3.893387	4.180326	2.433211	74 H	0.527251	-1.958680	2.605055
22 C	-3.312346	3.088830	3.110636	75 H	-0.616027	-3.367699	4.285821
23 C	-3.235597	1.846161	2.494828	76 H	-3.131038	-3.473216	4.297161
24 N	-3.716929	1.630471	1.242105	77 H	4.781831	3.542826	-0.369294
25 C	-3.310579	-2.125596	2.638413	78 H	5.387273	-0.354814	-2.085722
26 C	-1.211187	1.025412	-1.167529	79 H	6.797793	3.132647	-1.407883
27 C	0.135456	1.285382	-1.361374	80 H	6.692005	2.072859	-2.809356
28 C	1.107519	0.681368	-0.517910	81 H	10.586885	-0.121278	-2.425519
29 C	0.638203	-0.171196	0.485731	82 H	9.284545	0.490835	1.678069
30 C	-0.739718	-0.416772	0.655157	83 H	7.245133	1.531117	0.787833
31 N	-1.660360	0.188457	-0.190948	84 H	11.321133	0.302599	2.243094
32 C	-1.305806	-1.265042	1.688961	85 H	13.475366	-0.631179	2.956157
33 N	-2.691764	-1.333167	1.719670	86 H	14.166984	-2.297239	-0.810972
34 C	-0.553777	-2.004712	2.622955	87 H	12.030763	-1.452057	-1.671990
35 C	-1.194268	-2.799564	3.566836	88 H	15.200354	-2.167612	2.640377
36 C	-2.601741	-2.863223	3.576173	89 H	16.006144	-1.259148	1.332172
37 Ru	-3.677763	-0.220785	0.237923	90 H	15.459675	-2.937445	1.061875
38 C	2.564328	0.980256	-0.714108	91 C	-4.473300	-5.820850	-2.815515
39 C	3.064257	2.254552	-0.352556	92 H	-5.427995	-6.276718	-2.545265
40 C	4.407051	2.557313	-0.630463	93 H	-4.463946	-5.682144	-3.904417
41 C	5.250966	1.640588	-1.268624	94 H	-3.674731	-6.533392	-2.580412
42 C	4.749927	0.370352	-1.588066	95 C	-9.675426	-2.266255	1.366186
43 C	3.419143	0.019412	-1.316069	96 H	-9.846783	-3.240750	0.904420
44 C	6.629060	2.096205	-1.717807	97 H	-9.883962	-2.355511	2.438892
45 N	7.789146	1.289098	-1.220213	98 H	-10.414083	-1.564459	0.958936
46 C	8.724147	0.803607	-2.107433	99 C	-6.488085	3.859054	-3.867631
47 C	9.884446	0.207962	-1.671762	100 H	-7.557093	3.624338	-3.956747
48 C	10.178837	0.086923	-0.281687	101 H	-6.402828	4.888728	-3.513718
49 C	9.171483	0.575349	0.605444	102 H	-6.067846	3.805791	-4.877673
50 C	8.017774	1.153982	0.131974	103 C	-4.012926	5.530458	3.081711
51 C	11.436968	-0.470142	0.195700	104 H	-4.241030	6.314683	2.356413
52 C	11.892822	-0.276606	1.530762	105 H	-4.817278	5.526775	3.829761
53 C	13.103275	-0.783307	1.952093	106 H	-3.092774	5.803075	3.608542
54 N	13.906776	-1.499232	1.104058	107 C	2.194870	3.297806	0.319292
55 C	13.500220	-1.718134	-0.186406	108 H	1.453163	3.719225	-0.370899
56 C	12.300702	-1.223616	-0.649969	109 H	1.647989	2.883894	1.174117
57 C	15.233396	-1.996804	1.564498	110 H	2.801316	4.129777	0.685727
58 H	-2.199171	-4.250816	-2.756171	111 H	8.509153	0.939562	-3.158635
59 H	-1.912898	-2.083811	-1.573874	112 C	2.915867	-1.351960	-1.718459
60 H	-6.226575	-4.405507	-1.264036	113 H	2.663121	-1.969284	-0.847417
61 H	-4.827875	-0.373520	-2.697166	114 H	2.018638	-1.287534	-2.345263
62 H	-5.917618	1.187189	-4.289286	115 H	3.675501	-1.893131	-2.287836

[Ru(dmb)₂(4-mesityl-2,2'-bipyridine)]²⁺ triplet state (D3*)

Energy -2085.484922 Hartrees

Atom Type	Coordinates (Angstroms)						
	X	Y	Z				
1 C	-2.382611	-4.376180	-1.796050	46 H	0.343595	-2.371151	-1.332781
2 C	-1.037661	-3.949042	-1.845996	47 H	-4.346702	-3.807142	-1.142934
3 C	-0.680584	-2.717633	-1.315405	48 H	-2.108443	-0.129559	-2.784472
4 N	-1.590728	-1.878573	-0.757012	49 H	-2.621427	1.537098	-4.552370
5 C	-2.910885	-2.260233	-0.700724	50 H	-1.596574	4.652639	-1.769997
6 C	-3.309068	-3.505087	-1.208885	51 H	-3.473131	1.604159	1.495872
7 C	-2.009362	0.931187	-2.594979	52 H	-5.947471	1.421022	1.639542
8 C	-2.290900	1.867737	-3.574771	53 H	-5.683482	-2.290220	-0.514787
9 C	-2.137792	3.250807	-3.296101	54 H	-0.917449	5.058760	0.198228
10 C	-1.711450	3.604297	-2.016145	55 H	-0.038469	3.325124	4.037211
11 C	-1.438995	2.625567	-1.039318	56 H	-0.412313	1.082297	3.046177
12 N	-1.578430	1.282810	-1.353585	57 H	-2.362074	-1.678169	2.589515
13 C	-3.821386	-1.292437	-0.082471	58 H	0.973528	1.016590	-1.874112
14 C	-1.037864	2.907226	0.323985	59 H	3.438314	0.968222	-2.103913
15 N	-3.220889	-0.190721	0.481183	60 H	3.633405	-1.319889	1.532254
16 C	-3.994021	0.756256	1.073144	61 H	2.498501	-2.338922	3.009729
17 C	-5.375225	0.645849	1.143351	62 H	1.001087	-3.397770	4.668830
18 C	-6.024582	-0.467974	0.567305	63 H	-1.488789	-3.081751	4.457567
19 C	-5.216350	-1.431179	-0.049964	64 H	7.939791	1.833934	-0.623799
20 C	-0.812728	4.196757	0.845270	65 H	7.832356	-2.449474	-0.517977
21 C	-0.456401	4.389577	2.179032	66 H	10.010850	0.640264	-0.648899
22 C	-0.316913	3.232520	2.994211	67 H	9.875719	-0.803350	-1.662060
23 C	-0.526049	1.979273	2.452644	68 C	-2.793965	-5.716711	-2.342494
24 N	-0.888865	1.796829	1.149472	69 H	-2.337055	-6.530450	-1.765768
25 C	-1.300736	-1.847506	2.714024	70 H	-3.877641	-5.852675	-2.312912
26 C	1.590751	0.509037	-1.145501	71 H	-2.463848	-5.836867	-3.380614
27 C	2.966047	0.484557	-1.259465	72 C	-7.522701	-0.603181	0.612396
28 C	3.757661	-0.194144	-0.287903	73 H	-7.861398	-1.532676	0.148960
29 C	3.066329	-0.819805	0.759025	74 H	-7.886874	-0.587325	1.646473
30 C	1.665349	-0.788249	0.842702	75 H	-8.007135	0.231238	0.091094
31 N	0.927636	-0.114776	-0.127100	76 C	-2.438445	4.285740	-4.347088
32 C	0.888245	-1.421731	1.891764	77 H	-2.238526	5.298519	-3.988909
33 N	-0.484135	-1.242778	1.809286	78 H	-1.836153	4.119351	-5.248055
34 C	1.427553	-2.201240	2.935264	79 H	-3.490544	4.238140	-4.654207
35 C	0.587585	-2.799415	3.865739	80 C	-0.223443	5.761898	2.749115
36 C	-0.806951	-2.625451	3.751197	81 H	-0.327756	6.541018	1.990279
37 Ru	-1.109615	-0.035756	0.207201	82 H	-0.936220	5.977458	3.555117
38 C	5.236590	-0.236092	-0.384761	83 H	0.779944	5.841724	3.184289
39 C	5.979596	0.973580	-0.486903	84 C	5.331523	2.345517	-0.458030
40 C	7.375721	0.907474	-0.571990	85 H	4.999722	2.666424	-1.454389
41 C	8.067002	-0.311284	-0.586148	86 H	4.463491	2.387409	0.207434
42 C	7.316192	-1.493900	-0.494361	87 H	6.050574	3.092973	-0.111232
43 C	5.922406	-1.485845	-0.381843	88 C	5.205942	-2.822308	-0.310917
44 C	9.570817	-0.358838	-0.706155	89 H	4.994956	-3.125162	0.723631
45 H	-0.276946	-4.577044	-2.294825	90 H	4.255184	-2.819586	-0.853497
				91 H	5.831770	-3.607226	-0.744592
				92 H	10.015117	-0.970561	0.087554

[Ru(tmb)₂(bpy-2,6-Me₂- ϕ -MV)]⁴⁺ ground state (DA3') Energy -2776.676254 Hartrees

Atom	Coordinates (Angstroms)			Type	X	Y	Z
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1 C	-4.082759	4.931868	0.572123	56 C	12.728831	1.191109	0.221300
2 C	-2.827420	4.361260	0.906493	57 C	15.586020	1.217826	-2.227391
3 C	-2.637129	3.000743	0.652900	58 H	-1.693456	2.527988	0.892512
4 N	-3.583534	2.193607	0.110855	59 H	-6.016057	4.511783	-0.246980
5 C	-4.801752	2.733133	-0.212048	60 H	-4.345052	1.277128	2.454725
6 C	-5.053022	4.091381	0.013554	61 H	-5.208741	-3.528720	2.758350
7 C	-4.546400	0.219204	2.558682	62 H	-5.800486	-1.403390	-1.605837
8 C	-5.151915	-0.272478	3.718743	63 H	-7.429838	3.169066	-1.003017
9 C	-5.401243	-1.666913	3.799960	64 H	-4.598961	-4.638575	1.083235
10 C	-5.021192	-2.463249	2.712021	65 H	-2.652005	-1.986005	-2.536800
11 C	-4.420417	-1.908882	1.576310	66 H	-4.108193	1.033754	-3.210435
12 N	-4.185570	-0.560009	1.508397	67 H	-1.600742	-0.664777	2.166040
13 C	-5.780821	1.799165	-0.786394	68 H	0.820601	-0.953192	2.648955
14 C	-4.009248	-2.683887	0.396047	69 H	1.649657	0.265398	-1.392264
15 N	-5.339935	0.513092	-0.960712	70 H	0.803332	0.990945	-3.183148
16 C	-6.192115	-0.402249	-1.487212	71 H	-0.370020	1.684991	-5.254477
17 C	-7.505905	-0.112664	-1.867404	72 H	-2.882604	1.709887	-5.278608
18 C	-7.973312	1.215076	-1.690103	73 H	5.302751	-2.981183	0.876202
19 C	-7.085812	2.152524	-1.146519	74 H	5.526793	1.022955	2.457477
20 C	-4.162272	-4.069768	0.271979	75 H	7.061765	-2.423590	2.385328
21 C	-3.771590	-4.747382	-0.889692	76 H	7.002855	-0.922290	3.326970
22 C	-3.204661	-3.983899	-1.943240	77 H	11.375091	-0.118897	2.332366
23 C	-3.072696	-2.605523	-1.755636	78 H	9.336329	-0.167744	-1.491144
24 N	-3.461910	-1.956725	-0.629323	79 H	7.258272	-0.826865	-0.277079
25 C	-3.028117	1.035493	-3.244055	80 H	11.580264	-1.052680	-2.074727
26 C	-0.856468	-0.466221	1.407327	81 H	13.746523	-0.429673	-3.110973
27 C	0.501459	-0.623229	1.667134	82 H	14.636712	2.201506	0.003080
28 C	1.447216	-0.361922	0.655758	83 H	12.494805	1.698668	1.148873
29 C	0.954857	0.057599	-0.588106	84 H	15.514205	1.046924	-3.300805
30 C	-0.425633	0.203303	-0.803901	85 H	16.353273	0.570079	-1.795959
31 N	-1.328371	-0.062016	0.199255	86 H	15.831242	2.263747	-2.043292
32 C	-1.020016	0.632355	-2.079417	87 C	-4.369247	6.390857	0.805886
33 N	-2.395073	0.652215	-2.105682	88 H	-5.379541	6.657038	0.487847
34 C	-0.278666	1.002579	-3.209757	89 H	-4.271058	6.653335	1.866519
35 C	-0.935829	1.395336	-4.377039	90 H	-3.665332	7.028302	0.256672
36 C	-2.334965	1.410843	-4.393317	91 C	-9.374868	1.609253	-2.069813
37 R	-3.362801	0.131606	-0.312110	92 H	-9.563881	2.666045	-1.869207
38 C	2.914121	-0.550974	0.931710	93 H	-9.565010	1.429123	-3.135036
39 C	3.524489	-1.797398	0.649808	94 H	-10.117496	1.022784	-1.514863
40 C	4.857969	-2.003675	1.042693	95 C	-6.058703	-2.274801	5.009488
41 C	5.587990	-1.005324	1.705612	96 H	-7.055450	-1.847948	5.175855
42 C	4.983138	0.241326	1.933674	97 H	-6.170812	-3.356296	4.905714
43 C	3.655066	0.487309	1.553462	98 H	-5.478502	-2.081034	5.920049
44 C	6.925540	-1.339508	2.320293	99 C	-3.956676	-6.235935	-1.013975
45 N	8.177747	-0.823718	1.588062	100 H	-4.405572	-6.661880	-0.113975
46 C	9.306697	-0.615289	2.322244	101 H	-4.604206	-6.486854	-1.863196
47 C	10.496737	-0.247554	1.711912	102 H	-3.000425	-6.744624	-1.187587
48 C	10.555079	-0.090608	0.312217	103 C	2.759890	-2.922444	-0.013985
49 C	9.366846	-0.299910	-0.416600	104 H	1.895283	-3.229171	0.586283
50 C	8.194316	-0.660873	0.239332	105 H	2.378738	-2.629919	-0.999059
51 C	11.835748	0.268201	-0.359467	106 H	3.394076	-3.801715	-0.151096
52 C	12.207609	-0.318268	-1.585111	107 H	9.231207	-0.765825	3.391297
53 C	13.420494	0.009890	-2.177610	108 C	3.028960	1.832495	1.852601
54 N	14.263057	0.903576	-1.589657	109 H	2.628038	2.301938	0.946922
55 C	13.928263	1.494688	-0.408829	110 H	2.199047	1.742079	2.563238
				111 H	3.759904	2.518604	2.287489

112 C	-8.384839	-1.191361	-2.443522	120 C	-2.763040	-4.620588	-3.235267
113 H	-9.285951	-1.338466	-1.836059	121 H	-1.999179	-5.388714	-3.064235
114 H	-8.725008	-0.934074	-3.454002	122 H	-3.599230	-5.116987	-3.742590
115 H	-7.860632	-2.148842	-2.501146	123 H	-2.348172	-3.881134	-3.925511
116 C	-1.722818	5.183350	1.517435	124 C	-5.529331	0.666613	4.834129
117 H	-1.430464	6.012124	0.861261	125 H	-6.609388	0.646228	5.024249
118 H	-2.035782	5.630211	2.468811	126 H	-5.039137	0.390128	5.775378
119 H	-0.832928	4.577404	1.709740	127 H	-5.251724	1.698052	4.601628

[Ru(tmb)₂(bpy-2,6-Me₂- ϕ -MV)]⁴⁺ triplet state (³DA3')
Energy -2776.6256215 Hartrees

Atom Type	Coordinates (Angstroms)						
	X	Y	Z				
1 C	-3.701704	4.947056	0.967546	40 C	4.660360	-2.652431	0.745361
2 C	-2.471353	4.268806	1.186054	41 C	5.547632	-1.691170	1.243992
3 C	-2.394960	2.919458	0.833441	42 C	5.089697	-0.378872	1.426958
4 N	-3.435516	2.226166	0.304568	43 C	3.759229	-0.025054	1.155269
5 C	-4.627558	2.868259	0.080154	44 C	6.928881	-2.136398	1.697606
6 C	-4.763012	4.219792	0.409261	45 N	8.081353	-1.326963	1.199083
7 C	-4.591939	0.064014	2.577834	46 C	8.985428	-0.783550	2.087427
8 C	-5.192455	-0.522337	3.694905	47 C	10.143876	-0.184757	1.655608
9 C	-5.444673	-1.921250	3.658160	48 C	10.475091	-0.118032	0.268079
10 C	-5.073720	-2.626663	2.503705	49 C	9.498493	-0.666326	-0.621383
11 C	-4.472120	-1.984273	1.418070	50 C	8.345163	-1.246668	-0.153110
12 N	-4.231098	-0.634142	1.470368	51 C	11.731863	0.440935	-0.200423
13 C	-5.689180	2.047152	-0.516980	52 C	12.208285	0.234054	-1.528055
14 C	-4.074279	-2.652346	0.171487	53 C	13.418826	0.744525	-1.940839
15 N	-5.348780	0.745505	-0.789539	54 N	14.207295	1.478990	-1.093004
16 C	-6.278821	-0.086280	-1.325857	55 C	13.781838	1.711262	0.189766
17 C	-7.580633	0.313614	-1.638020	56 C	12.581373	1.213858	0.644739
18 C	-7.946765	1.660881	-1.367483	57 C	15.535141	1.978370	-1.544153
19 C	-6.978122	2.504662	-0.803392	58 H	-1.477760	2.364740	0.980597
20 C	-4.229105	-4.018595	-0.079443	59 H	-5.702850	4.726437	0.230857
21 C	-3.829954	-4.588901	-1.297321	60 H	-4.386525	1.126286	2.563260
22 C	-3.248085	-3.735821	-2.274808	61 H	-5.266696	-3.691097	2.461628
23 C	-3.110759	-2.380914	-1.963031	62 H	-5.960665	-1.102416	-1.516547
24 N	-3.517509	-1.840968	-0.785246	63 H	-7.246502	3.531074	-0.587970
25 C	-3.056886	1.442719	-3.079096	64 H	-4.668888	-4.659027	0.674550
26 C	-0.883759	-0.773681	1.297826	65 H	-2.672578	-1.696901	-2.677703
27 C	0.462825	-1.038487	1.498694	66 H	-4.133406	1.517195	-3.010914
28 C	1.409969	-0.706162	0.495752	67 H	-1.622222	-1.023465	2.047872
29 C	0.921993	-0.104350	-0.669283	68 H	0.785358	-1.500824	2.423563
30 C	-0.452532	0.154103	-0.838142	69 H	1.616297	0.150898	-1.459937
31 N	-1.348493	-0.184025	0.163324	70 H	0.769182	1.116193	-3.155954
32 C	-1.040505	0.752545	-2.027828	71 H	-0.406059	2.122497	-5.086294
33 N	-2.420551	0.874398	-2.019337	72 H	-2.912775	2.334825	-5.025279
34 C	-0.309226	1.205461	-3.141939	73 H	5.002526	-3.671457	0.589655
35 C	-0.968025	1.774033	-4.227845	74 H	5.762656	0.382249	1.810802
36 C	-2.369665	1.896202	-4.197758	75 H	7.101710	-3.175015	1.396939
37 Ru	-3.375884	0.198311	-0.271309	76 H	6.987569	-2.106923	2.789767
38 C	2.863763	-1.023958	0.694125	77 H	10.817986	0.192764	2.412420
39 C	3.317556	-2.345777	0.472955	78 H	9.638041	-0.629102	-1.693499
				79 H	7.598836	-1.669859	-0.811445
				80 H	11.650314	-0.357570	-2.240889
				81 H	13.804407	0.582353	-2.938235

82 H	14.436273	2.303403	0.815086	105 H	1.903887	-3.142945	-0.975688
83 H	12.299146	1.452803	1.660887	106 H	2.949064	-4.355188	-0.228942
84 H	15.505468	2.162152	-2.618164	107 H	8.745237	-0.877403	3.137791
85 H	16.306780	1.237349	-1.318628	108 C	3.299056	1.397265	1.400202
86 H	15.762425	2.912674	-1.030367	109 H	2.954998	1.881448	0.477832
87 C	-3.864559	6.399237	1.317269	110 H	2.471118	1.437165	2.118728
88 H	-4.874847	6.755735	1.107292	111 H	4.111888	2.005821	1.803878
89 H	-3.656339	6.578396	2.379282	112 C	-8.551275	-0.665109	-2.241652
90 H	-3.162447	7.024373	0.751216	113 H	-9.441793	-0.782482	-1.612553
91 C	-9.326724	2.169706	-1.672430	114 H	-8.902620	-0.324669	-3.223186
92 H	-9.439030	3.222541	-1.406386	115 H	-8.101200	-1.652353	-2.372247
93 H	-9.562216	2.063304	-2.738779	116 C	-1.276944	4.968075	1.777447
94 H	-10.089397	1.600013	-1.126893	117 H	-0.965400	5.817265	1.157304
95 C	-6.093606	-2.626954	4.814897	118 H	-1.502064	5.370956	2.772225
96 H	-7.086636	-2.211019	5.026538	119 H	-0.423106	4.292826	1.875408
97 H	-6.210759	-3.695433	4.623778	120 C	-2.793518	-4.256852	-3.611688
98 H	-5.504790	-2.509717	5.733190	121 H	-2.036009	-5.041587	-3.498365
99 C	-4.015506	-6.057560	-1.555283	122 H	-3.625937	-4.702513	-4.169698
100 H	-4.465258	-6.565564	-0.699960	123 H	-2.365543	-3.463843	-4.230050
101 H	-4.660046	-6.228913	-2.426657	124 C	-5.557628	0.317381	4.889165
102 H	-3.058575	-6.546837	-1.775028	125 H	-6.634636	0.274574	5.091769
103 C	2.395083	-3.432759	-0.039127	126 H	-5.053119	-0.036882	5.796149
104 H	1.604860	-3.670570	0.683853	127 H	-5.286555	1.366040	4.743920

[Ru(tmb)₂(4-mesityl-2,2'-bipyridine)]²⁺ triplet state (D3^h)
Energy -2242.731703 Hartrees

Atom Type	Coordinates (Angstroms)						
	X	Y	Z				
1 C	-1.742786	4.767316	0.870089	25 C	-1.135700	1.183807	-3.083891
2 C	-0.431461	4.242626	0.997560	26 C	1.736443	-0.475367	1.153700
3 C	-0.234886	2.888183	0.713753	27 C	3.102672	-0.485976	1.243093
4 N	-1.233157	2.057202	0.327630	28 C	3.907819	0.052831	0.165698
5 C	-2.503609	2.549053	0.195320	29 C	3.230605	0.546843	-0.940610
6 C	-2.763308	3.895987	0.466890	30 C	1.816747	0.535703	-1.031270
7 C	-1.790527	-0.294421	2.769538	31 N	1.059675	0.034836	0.068063
8 C	-2.136862	-0.969945	3.943487	32 C	1.060866	0.954186	-2.158639
9 C	-2.147937	-2.388491	3.914810	33 N	-0.329521	0.783722	-2.059312
10 C	-1.812387	-3.025459	2.712877	34 C	1.597350	1.518487	-3.352846
11 C	-1.472287	-2.290449	1.572336	35 C	0.765923	1.899311	-4.383758
12 N	-1.463102	-0.921977	1.615556	36 C	-0.640661	1.732107	-4.251852
13 C	-3.518059	1.581575	-0.248846	37 Ru	-0.950872	0.029691	-0.218964
14 C	-1.108604	-2.886643	0.277696	38 C	5.386523	0.077146	0.266330
15 N	-3.057394	0.320221	-0.511746	39 C	6.106186	-1.128517	0.509288
16 C	-3.931247	-0.632251	-0.918416	40 C	7.501467	-1.084033	0.603829
17 C	-5.296791	-0.399037	-1.100941	41 C	8.219776	0.114874	0.488524
18 C	-5.788424	0.905285	-0.835504	42 C	7.495549	1.295047	0.253682
19 C	-4.875924	1.877871	-0.407206	43 C	6.102942	1.303346	0.129456
20 C	-1.010327	-4.260154	0.037402	44 C	9.722700	0.144210	0.620251
21 C	-0.643467	-4.755205	-1.221896	45 H	0.747685	2.443575	0.791089
22 C	-0.370469	-3.821037	-2.255332	46 H	-3.767955	4.284673	0.357998
23 C	-0.485426	-2.461776	-1.955757	47 H	-1.765995	0.787540	2.745455
24 N	-0.846674	-1.998413	-0.733545	48 H	-1.819391	-4.107665	2.677006
				49 H	-3.513953	-1.612386	-1.109660
				50 H	-5.239019	2.876136	-0.197784
				51 H	-1.212173	-4.963801	0.835184

52 H	-0.280373	-1.708197	-2.704264	79 H	0.476649	-6.513061	-1.779581
53 H	-2.198204	1.036243	-2.937565	80 C	5.421714	-2.478225	0.612170
54 H	1.118447	-0.849871	1.958954	81 H	5.024367	-2.665735	1.618260
55 H	3.579553	-0.861172	2.138566	82 H	4.588805	-2.574301	-0.091572
56 H	3.801383	0.922332	-1.780248	83 H	6.134639	-3.279818	0.398872
57 H	2.668360	1.649544	-3.443686	84 C	5.414425	2.635781	-0.100248
58 H	1.179457	2.327231	-5.289527	85 H	5.195695	2.810617	-1.161846
59 H	-1.316615	2.023632	-5.045402	86 H	4.467945	2.712805	0.444133
60 H	8.045137	-2.010726	0.762519	87 H	6.060149	3.455134	0.228472
61 H	8.033207	2.235656	0.172704	88 H	10.187315	0.669068	-0.222628
62 H	10.142682	-0.864296	0.664043	89 C	-6.201669	-1.509232	-1.566529
63 H	10.028231	0.671968	1.533061	90 H	-6.999396	-1.706277	-0.840216
64 C	-2.033637	6.216681	1.150877	91 H	-6.691629	-1.254513	-2.514036
65 H	-1.452285	6.872042	0.490590	92 H	-5.648949	-2.440197	-1.717062
66 H	-3.091353	6.449608	1.009399	93 C	0.731037	5.102809	1.417693
67 H	-1.762370	6.485268	2.179235	94 H	0.884520	5.933384	0.718066
68 C	-7.245723	1.239815	-1.006203	95 H	0.564763	5.547344	2.406504
69 H	-7.451331	2.281001	-0.748357	96 H	1.658895	4.527062	1.461207
70 H	-7.572017	1.077713	-2.040976	97 C	0.040718	-4.259387	-3.636059
71 H	-7.876844	0.603640	-0.373634	98 H	0.970680	-4.840294	-3.609273
72 C	-2.508355	-3.190025	5.136600	99 H	-0.720720	-4.900123	-4.097002
73 H	-2.470902	-4.263464	4.938368	100 H	0.201775	-3.403017	-4.295477
74 H	-1.824937	-2.976324	5.967644	101 C	-2.481486	-0.198281	5.189872
75 H	-3.518174	-2.946140	5.488721	102 H	-3.496863	-0.428103	5.534846
76 C	-0.536633	-6.236062	-1.463687	103 H	-1.802914	-0.447453	6.014725
77 H	-0.778596	-6.809396	-0.566154	104 H	-2.420845	0.880184	5.022714
78 H	-1.213812	-6.558008	-2.264477				

**[Ru(dmb)₂(bpy- ϕ -MV)]⁴⁺ ground state PCM=acetonitrile (DA1)
Energy -2541.382648 Hartrees**

Atom Type	Coordinates (Angstroms)						
	X	Y	Z				
1 C	-5.112285	-4.325583	-1.398878	21 C	-2.378673	4.494447	1.889471
2 C	-3.851741	-3.881117	-1.827481	22 C	-1.911477	3.395902	2.627635
3 C	-3.348642	-2.668742	-1.363227	23 C	-2.189912	2.101570	2.196337
4 N	-4.035766	-1.879030	-0.501858	24 N	-2.908834	1.847395	1.075639
5 C	-5.275669	-2.290264	-0.072761	25 C	-2.741388	-1.702148	2.850625
6 C	-5.819040	-3.501855	-0.508554	26 C	-1.100570	0.511550	-1.741784
7 C	-4.994508	0.787147	-2.176397	27 C	0.195823	0.494506	-2.240792
8 C	-5.624095	1.680932	-3.038819	28 C	1.215764	-0.163241	-1.524126
9 C	-5.512294	3.062579	-2.817954	29 C	0.856881	-0.784603	-0.315051
10 C	-4.771743	3.480067	-1.700434	30 C	-0.463786	-0.742257	0.143135
11 C	-4.162339	2.546250	-0.857775	31 N	-1.440329	-0.091401	-0.574061
12 N	-4.269792	1.197553	-1.105814	32 C	-0.914039	-1.358463	1.400632
13 C	-5.954990	-1.373035	0.857168	33 N	-2.239978	-1.164861	1.709537
14 C	-3.380747	2.907682	0.337417	34 C	-0.084311	-2.098456	2.253174
15 N	-5.227511	-0.267117	1.228566	35 C	-0.605357	-2.645643	3.427266
16 C	-5.780026	0.619541	2.092314	36 C	-1.956595	-2.444721	3.730318
17 C	-7.064185	0.459291	2.605138	37 Ru	-3.348780	-0.061923	0.306035
18 C	-7.836484	-0.648364	2.221324	38 C	2.610080	-0.191800	-2.024761
19 C	-7.249448	-1.573266	1.342417	39 C	3.122883	0.885645	-2.771719
20 C	-3.121854	4.223787	0.729571	40 C	4.437952	0.860032	-3.243533
				41 C	5.264531	-0.245545	-2.989215
				42 C	4.755222	-1.328288	-2.251088
				43 C	3.447074	-1.298646	-1.768822

44 C	6.675047	-0.274933	-3.533211	77 H	2.507161	1.760734	-2.963253
45 N	7.715518	-0.215699	-2.436078	78 H	4.822253	1.705982	-3.810724
46 C	8.541952	-1.275412	-2.224769	79 H	5.374507	-2.203487	-2.061512
47 C	9.497387	-1.235575	-1.219944	80 H	3.064982	-2.155753	-1.219762
48 C	9.625729	-0.087042	-0.417731	81 H	6.864521	0.576158	-4.193923
49 C	8.757278	0.995039	-0.664416	82 H	6.876170	-1.195086	-4.088776
50 C	7.811133	0.907793	-1.671415	83 H	8.416792	-2.138523	-2.872941
51 C	10.639054	-0.020743	0.660326	84 H	10.148023	-2.096441	-1.091667
52 C	11.317068	1.178687	0.947815	85 H	8.791995	1.900780	-0.065144
53 C	12.261929	1.215368	1.960891	86 H	7.119362	1.716196	-1.888433
54 N	12.540532	0.097770	2.688054	87 H	11.135792	2.086470	0.378975
55 C	11.898308	-1.076452	2.435252	88 H	12.811384	2.119225	2.208959
56 C	10.950041	-1.157991	1.428560	89 H	12.161441	-1.929367	3.054665
57 C	13.586603	0.149120	3.749944	90 H	10.445975	-2.107517	1.270010
58 H	-3.258207	-4.472347	-2.519537	91 H	13.632523	1.160888	4.152394
59 H	-2.379602	-2.311097	-1.683999	92 H	14.551349	-0.124868	3.315355
60 H	-6.795766	-3.818977	-0.155395	93 H	13.321645	-0.550851	4.542447
61 H	-5.063720	-0.280236	-2.337078	94 C	-5.692149	-5.636854	-1.867596
62 H	-6.187766	1.295547	-3.884289	95 H	-5.865191	-6.311612	-1.021278
63 H	-4.677767	4.542097	-1.494992	96 H	-6.658396	-5.484020	-2.361502
64 H	-5.172351	1.470949	2.367166	97 H	-5.023439	-6.137003	-2.571398
65 H	-7.460347	1.205057	3.289099	98 C	-9.246281	-0.841818	2.721239
66 H	-7.819464	-2.443272	1.030810	99 H	-9.954088	-0.882763	1.885587
67 H	-3.496159	5.052660	0.136295	100 H	-9.341164	-1.784983	3.271496
68 H	-1.333165	3.539965	3.536364	101 H	-9.547154	-0.028022	3.384385
69 H	-1.843709	1.242694	2.754460	102 C	-6.157418	4.068298	-3.739074
70 H	-3.788866	-1.522583	3.049556	103 H	-6.879682	4.688097	-3.195486
71 H	-1.896199	1.005841	-2.282121	104 H	-5.408093	4.744506	-4.165938
72 H	0.398546	0.973103	-3.194103	105 H	-6.680955	3.575200	-4.560941
73 H	1.619480	-1.266970	0.284274	106 C	-2.101616	5.914506	2.316638
74 H	0.961572	-2.252539	2.007982	107 H	-1.559394	6.459167	1.535339
75 H	0.033481	-3.220849	4.091914	108 H	-3.036370	6.456926	2.499122
76 H	-2.401430	-2.852886	4.633165	109 H	-1.505533	5.944847	3.231253

**[Ru(dmb)₂(bpy- ϕ -MV)]⁴⁺ triplet state PCM=acetonitrile (³DA1)
Energy -2541.327043 Hartrees**

Atom Type	Coordinates (Angstroms)						
	X	Y	Z				
1 C	-4.829131	-3.963909	-2.482056	14 C	-3.527830	2.666703	1.098395
2 C	-3.584505	-3.360240	-2.743604	15 N	-5.259798	-0.674367	1.032796
3 C	-3.167965	-2.273213	-1.986431	16 C	-5.880033	-0.036836	2.059667
4 N	-3.934555	-1.757465	-0.991534	17 C	-7.150616	-0.400335	2.486732
5 C	-5.154672	-2.324146	-0.714222	18 C	-7.835876	-1.449594	1.844666
6 C	-5.608568	-3.421935	-1.447472	19 C	-7.183808	-2.096420	0.782630
7 C	-5.111020	1.223765	-1.879026	20 C	-3.289828	3.837546	1.820434
8 C	-5.804608	2.281625	-2.452417	21 C	-2.498297	3.815565	2.980557
9 C	-5.777860	3.551884	-1.846113	22 C	-1.958910	2.577450	3.377333
10 C	-5.023437	3.694250	-0.670217	23 C	-2.214320	1.437439	2.627237
11 C	-4.333796	2.606111	-0.130801	24 N	-2.984756	1.472453	1.509575
12 N	-4.386253	1.376293	-0.741154	25 C	-2.728920	-2.498222	2.168232
13 C	-5.902796	-1.704513	0.389594	26 C	-1.152698	1.145155	-1.428554
				27 C	0.145036	1.346375	-1.873356
				28 C	1.194752	0.540634	-1.383292
				29 C	0.857865	-0.455745	-0.444933

30 C	-0.462864	-0.628644	-0.032282	70 H	-3.784802	-2.436505	2.395301
31 N	-1.463391	0.175923	-0.529106	71 H	-1.964630	1.754353	-1.803887
32 C	-0.893079	-1.632561	0.950072	72 H	0.326197	2.114604	-2.618765
33 N	-2.228499	-1.604358	1.278773	73 H	1.638850	-1.070682	-0.014091
34 C	-0.045893	-2.581445	1.530194	74 H	1.007698	-2.615006	1.270774
35 C	-0.560488	-3.498160	2.450459	75 H	0.094123	-4.237093	2.905073
36 C	-1.920130	-3.455241	2.776081	76 H	-2.355305	-4.150743	3.487665
37 Ru	-3.373460	-0.166003	0.258788	77 H	2.400420	2.888676	-2.068396
38 C	2.587597	0.738186	-1.833673	78 H	4.713524	3.217510	-2.837799
39 C	3.052717	2.024805	-2.168718	79 H	5.442739	-1.021868	-2.485279
40 C	4.369576	2.214328	-2.593742	80 H	3.135815	-1.362284	-1.723840
41 C	5.247679	1.125957	-2.712813	81 H	6.823770	2.401932	-3.446686
42 C	4.784476	-0.161353	-2.386336	82 H	6.838209	0.774974	-4.136886
43 C	3.475995	-0.353311	-1.945367	83 H	8.340947	-0.682688	-3.454124
44 C	6.662256	1.343400	-3.218015	84 H	10.064300	-1.445521	-1.899292
45 N	7.705538	0.915577	-2.248618	85 H	8.919089	1.840340	0.741464
46 C	8.508939	-0.175831	-2.509016	86 H	7.237872	2.471338	-0.913520
47 C	9.470328	-0.582228	-1.621002	87 H	10.318217	1.239044	2.088798
48 C	9.687870	0.105878	-0.380385	88 H	12.055293	0.479410	3.626797
49 C	8.832504	1.238313	-0.155963	89 H	13.160003	-2.655665	1.066557
50 C	7.883190	1.613117	-1.068385	90 H	11.466906	-2.024541	-0.576859
51 C	10.691621	-0.304481	0.560800	91 H	13.470367	-1.226870	4.366455
52 C	10.913055	0.379008	1.802916	92 H	14.693050	-0.997080	3.088646
53 C	11.880044	-0.029222	2.684343	93 H	13.907602	-2.583965	3.305115
54 N	12.682635	-1.118058	2.415859	94 C	-5.301796	-5.146495	-3.280651
55 C	12.505095	-1.806690	1.234039	95 H	-4.597608	-5.982275	-3.186974
56 C	11.548231	-1.431849	0.327339	96 H	-6.286327	-5.487479	-2.951811
57 C	13.758539	-1.503760	3.351036	97 H	-5.361258	-4.894611	-4.346459
58 H	-2.936853	-3.732190	-3.533367	98 C	-9.213036	-1.861590	2.284688
59 H	-2.215529	-1.797161	-2.178411	99 H	-9.637543	-2.620785	1.623530
60 H	-6.571495	-3.868650	-1.218015	100 H	-9.183695	-2.270991	3.302471
61 H	-5.120566	0.241758	-2.333272	101 H	-9.889630	-0.999352	2.305082
62 H	-6.364845	2.110465	-3.368031	102 C	-6.538725	4.707721	-2.434070
63 H	-4.984689	4.661904	-0.179096	103 H	-7.618759	4.517935	-2.390047
64 H	-5.341011	0.765830	2.545085	104 H	-6.333976	5.638693	-1.900128
65 H	-7.602524	0.137960	3.316009	105 H	-6.280513	4.847560	-3.490190
66 H	-7.689660	-2.904756	0.263125	106 C	-2.241203	5.065518	3.774839
67 H	-3.711569	4.780107	1.484569	107 H	-2.572656	5.958202	3.238973
68 H	-1.337698	2.496692	4.265773	108 H	-2.776395	5.026016	4.732735
69 H	-1.808052	0.478202	2.919755	109 H	-1.175530	5.170822	4.006460