

Theoretical Analyses on Phosphorescent Processes in Pt(thpy)₂ and its Derivatives

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Table S1. Names of Pt complexes.

<i>cis</i> -1	<i>cis</i> -bis[2-(2'-thienyl)pyridinato-N,C _{3'}]platinum(II)	<i>cis</i> -Pt(thpy) ₂
<i>trans</i> -1	<i>trans</i> -bis[2-(2'-thienyl)pyridinato-N,C _{3'}]platinum(II)	<i>trans</i> -Pt(thpy) ₂
2	[2-(2'-thienyl)pyridinato-N,C _{3'}][2,4-pentanedionato-O,O]platinum(II)	<i>thpy</i> Pt(acac)
3	[2-(2'-thienyl)pyridinato-N,C _{3'}] [1,3-bis(phenyl)propane-1,3-dionato-O,O]platinum(II)	<i>thpy</i> Pt(bpp)
4	[2-(2'-thienyl)pyridinato-N,C _{3'}] [1,3-bis(3,4-dimethoxyphenyl)propane-1,3-dionato-O,O]platinum(II)	<i>thpy</i> Pt(bdmp)
5-1	[2-(2'-thienyl)pyridinato-N,C _{3'}] [1,3-bis(2-methoxyphenyl)propane-1,3-dionato-O,O]platinum(II)	<i>thpy</i> Pt(2-bmp)
5-2	[2-(2'-thienyl)pyridinato-N,C _{3'}] [1,3-bis(3-methoxyphenyl)propane-1,3-dionato-O,O]platinum(II)	<i>thpy</i> Pt(3-bmp)
5-3	[2-(2'-thienyl)pyridinato-N,C _{3'}] [1,3-bis(4-methoxyphenyl)propane-1,3-dionato-O,O]platinum(II)	<i>thpy</i> Pt(4-bmp)
5-4	[2-(2'-thienyl)pyridinato-N,C _{3'}] [1,3-bis(5-methoxyphenyl)propane-1,3-dionato-O,O]platinum(II)	<i>thpy</i> Pt(5-bmp)
5-5	[2-(2'-thienyl)pyridinato-N,C _{3'}] [1,3-bis(6-methoxyphenyl)propane-1,3-dionato-O,O]platinum(II)	<i>thpy</i> Pt(6-bmp)
6	[2-2'-(4',5'-benzo)thienyl]pyridinato-N,C _{3'}][2,4-pentanedionato-O,O]platinum(II)	<i>btp</i> Pt(acac)
7-1	[1-(2'-thienyl)isoquinolyl-N,C _{3'}][2,4-pentanedionato-O,O]platinum(II)	<i>ltiq</i> Pt(acac)
7-2	[3-(2'-thienyl)isoquinolyl-N,C _{3'}][2,4-pentanedionato-O,O]platinum(II)	<i>3tiq</i> Pt(acac)
7-3	[2-(2'-thienyl)quinolyl-N,C _{3'}][2,4-pentanedionato-O,O]platinum(II)	<i>thq</i> Pt(acac)
	[2-(2'-thienyl)pyridinato-N,C _{3'}] [1,3-bis(3,4-dibutoxyphenyl)propane-1,3-dionato-O,O]platinum(II)	<i>thpy</i> Pt(bdbp)
	[2-2'-(4',5'-benzo)thienyl]pyridinato-N,C _{3'}] [1,3-bis(3,4-dibutoxyphenyl)propane-1,3-dionato-O,O]platinum(II)	<i>btp</i> Pt(bdbp)
	[1-(2'-thienyl)isoquinolyl-N,C _{3'}] [1,3-bis(3,4-dibutoxyphenyl)propane-1,3-dionato-O,O]platinum(II)	<i>ltiq</i> Pt(bdbp)

Table S2. Cartesian coordinates [Å] optimized at the DFT (B3LYP/SBKJC+p) level of theory.

<i>cis</i> -1	Ground state (C ₂)			
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Hydrogen	1.0	-0.6833742493	-0.6790985273	3.1289906312
Hydrogen	1.0	0.6833742493	0.6790985273	3.1289906312
Carbon	6.0	-1.6773513350	-0.5396186158	2.6792282381
Carbon	6.0	1.6773513350	0.5396186158	2.6792282381
Carbon	6.0	-2.8369483910	-0.7312508370	3.4580253389
Carbon	6.0	2.8369483910	0.7312508370	3.4580253389
Hydrogen	1.0	-2.7457175288	-0.9996609941	4.5230158987
Hydrogen	1.0	2.7457175288	0.9996609941	4.5230158987
Hydrogen	1.0	-5.0348753146	-0.6980427422	3.3956563188
Hydrogen	1.0	5.0348753146	0.6980427422	3.3956563188
Carbon	6.0	-4.0965118085	-0.5692355837	2.8271234656
Carbon	6.0	4.0965118085	0.5692355837	2.8271234656
Carbon	6.0	-4.1361850521	-0.2626622133	1.4552423189
Carbon	6.0	4.1361850521	0.2626622133	1.4552423189
Hydrogen	1.0	-5.0957057711	-0.1605657619	0.9222579556
Hydrogen	1.0	5.0957057711	0.1605657619	0.9222579556
Carbon	6.0	-2.9165850830	-0.1057798957	0.7355825138
Carbon	6.0	2.9165850830	0.1057798957	0.7355825138
Carbon	6.0	-2.7945019115	0.1352132064	-0.6927632294
Carbon	6.0	2.7945019115	-0.1352132064	-0.6927632294
Nitrogen	7.0	-1.6959428803	-0.2023996186	1.3709160217
Nitrogen	7.0	1.6959428803	0.2023996186	1.3709160217
Carbon	6.0	-1.5181058703	0.1569858910	-1.2920307595
Carbon	6.0	1.5181058703	-0.1569858910	-1.2920307595
Hydrogen	1.0	-0.8161513023	0.5589545648	-3.4066999894
Hydrogen	1.0	0.8161513023	-0.5589545648	-3.4066999894
Carbon	6.0	-1.6562019012	0.4413726913	-2.7077373451
Carbon	6.0	1.6562019012	-0.4413726913	-2.7077373451
Hydrogen	1.0	-3.3402497153	0.8216281713	-4.1383474706
Hydrogen	1.0	3.3402497153	-0.8216281713	-4.1383474706
Carbon	6.0	-2.9764732422	0.5991580618	-3.1226348183
Carbon	6.0	2.9764732422	-0.5991580618	-3.1226348183
Sulfur	16.0	-4.1184343691	0.4211744007	-1.8173861459
Sulfur	16.0	4.1184343691	-0.4211744007	-1.8173861459

Table S2 (continued)

<i>cis</i> -1	Lowest triplet state (3A , C_2)			
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Hydrogen	1.0	-0.6362824845	-0.7035845752	3.1107475786
Hydrogen	1.0	0.6362824845	0.7035845752	3.1107475786
Carbon	6.0	-1.6259305350	-0.5291301946	2.6662617617
Carbon	6.0	1.6259305350	0.5291301946	2.6662617617
Carbon	6.0	-2.7774051838	-0.6861469514	3.4492534158
Carbon	6.0	2.7774051838	0.6861469514	3.4492534158
Hydrogen	1.0	-2.6759251227	-0.9600268158	4.5121565049
Hydrogen	1.0	2.6759251227	0.9600268158	4.5121565049
Hydrogen	1.0	-4.9909493439	-0.5959333423	3.4280657237
Hydrogen	1.0	4.9909493439	0.5959333423	3.4280657237
Carbon	6.0	-4.0624943957	-0.4935312322	2.8400217444
Carbon	6.0	4.0624943957	0.4935312322	2.8400217444
Carbon	6.0	-4.1099943150	-0.2012323735	1.4744336968
Carbon	6.0	4.1099943150	0.2012323735	1.4744336968
Hydrogen	1.0	-5.0729599874	-0.0838911586	0.9494253828
Hydrogen	1.0	5.0729599874	0.0838911586	0.9494253828
Carbon	6.0	-2.8952697116	-0.0769641506	0.7255736464
Carbon	6.0	2.8952697116	0.0769641506	0.7255736464
Carbon	6.0	-2.7950083525	0.1337859387	-0.6843800356
Carbon	6.0	2.7950083525	-0.1337859387	-0.6843800356
Nitrogen	7.0	-1.6375584911	-0.1853082163	1.3478160058
Nitrogen	7.0	1.6375584911	0.1853082163	1.3478160058
Carbon	6.0	-1.4880927609	0.1605251383	-1.3005081261
Carbon	6.0	1.4880927609	-0.1605251383	-1.3005081261
Hydrogen	1.0	-0.8020157815	0.5438582078	-3.4191541104
Hydrogen	1.0	0.8020157815	-0.5438582078	-3.4191541104
Carbon	6.0	-1.6365496691	0.4189407040	-2.7158309848
Carbon	6.0	1.6365496691	-0.4189407040	-2.7158309848
Hydrogen	1.0	-3.3213570524	0.7529136043	-4.1536360461
Hydrogen	1.0	3.3213570524	-0.7529136043	-4.1536360461
Carbon	6.0	-2.9567374451	0.5480706629	-3.1345539030
Carbon	6.0	2.9567374451	-0.5480706629	-3.1345539030
Sulfur	16.0	-4.1194771373	0.3665612252	-1.8213073717
Sulfur	16.0	4.1194771373	-0.3665612252	-1.8213073717

Table S2 (continued)

<i>cis</i> -1	Lowest triplet state (C ₁)			
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Hydrogen	1.0	-0.6583911624	-0.7341019450	3.1109438350
Hydrogen	1.0	0.6598092718	0.6666092136	3.1337984316
Carbon	6.0	-1.6465696235	-0.5455993991	2.6655844120
Carbon	6.0	1.6558407916	0.5356201326	2.6873673532
Carbon	6.0	-2.8052505900	-0.6969898555	3.4576963324
Carbon	6.0	2.8088166593	0.7315566898	3.4706389261
Hydrogen	1.0	-2.7024316136	-0.9868155719	4.5161120327
Hydrogen	1.0	2.7096750777	0.9939551213	4.5364304185
Hydrogen	1.0	-5.0175907193	-0.5606310005	3.4511428187
Hydrogen	1.0	5.0095498077	0.7185184889	3.4199664580
Carbon	6.0	-4.0915563932	-0.4710910221	2.8571468639
Carbon	6.0	4.0756269671	0.5843385899	2.8455961701
Carbon	6.0	-4.1418538637	-0.1570526151	1.5004029033
Carbon	6.0	4.1241080884	0.2871569051	1.4732807190
Hydrogen	1.0	-5.1043808141	-0.0030918820	0.9839131023
Hydrogen	1.0	5.0868622337	0.1983161605	0.9436653816
Carbon	6.0	-2.9195405313	-0.0515938792	0.7407555982
Carbon	6.0	2.9099485099	0.1229542834	0.7445023673
Carbon	6.0	-2.8226765753	0.1578235175	-0.6519060831
Carbon	6.0	2.8010449312	-0.1080518910	-0.6835712160
Nitrogen	7.0	-1.6543318437	-0.1936609748	1.3634220837
Nitrogen	7.0	1.6815766849	0.2030442171	1.3744850205
Carbon	6.0	-1.4659655875	0.1797778633	-1.2956084094
Carbon	6.0	1.5284862564	-0.1395108777	-1.2923629985
Hydrogen	1.0	-0.7859079629	0.5920281985	-3.3850217732
Hydrogen	1.0	0.8458478746	-0.5369053110	-3.4149845658
Carbon	6.0	-1.6217167384	0.4648168232	-2.6823474916
Carbon	6.0	1.6792777088	-0.4114906333	-2.7092516379
Hydrogen	1.0	-3.3115131701	0.8509964672	-4.1259765221
Hydrogen	1.0	3.3753711802	-0.7614555287	-4.1322359042
Carbon	6.0	-2.9508165187	0.6141359180	-3.1125413207
Carbon	6.0	3.0034613109	-0.5502652804	-3.1170780820
Sulfur	16.0	-4.1471966445	0.4082286748	-1.7893477720
Sulfur	16.0	4.1359537220	-0.3698722146	-1.8031457967

Table S2 (continued)

<i>trans</i> -1	Ground state (C ₂)			
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Nitrogen	7.0	0.5239158867	1.9925182541	0.1485198644
Nitrogen	7.0	-0.5239158867	-1.9925182541	0.1485198644
Carbon	6.0	1.8725769197	2.2826982468	0.0493605693
Carbon	6.0	-1.8725769197	-2.2826982468	0.0493605693
Carbon	6.0	2.6867750860	1.1009912475	-0.1733784441
Carbon	6.0	-2.6867750860	-1.1009912475	-0.1733784441
Sulfur	16.0	4.4238168297	1.0810152533	-0.4750308764
Sulfur	16.0	-4.4238168297	-1.0810152533	-0.4750308764
Carbon	6.0	4.3684218899	-0.6506549735	-0.6471316054
Carbon	6.0	-4.3684218899	0.6506549735	-0.6471316054
Carbon	6.0	3.0821971136	-1.1638885258	-0.4774765640
Carbon	6.0	-3.0821971136	1.1638885258	-0.4774765640
Carbon	6.0	2.0705050696	-0.1649228760	-0.1805668246
Carbon	6.0	-2.0705050696	0.1649228760	-0.1805668246
Carbon	6.0	2.3401720011	3.6210716511	0.1777543157
Carbon	6.0	-2.3401720011	-3.6210716511	0.1777543157
Carbon	6.0	1.4272158336	4.6535932101	0.4556679089
Carbon	6.0	-1.4272158336	-4.6535932101	0.4556679089
Carbon	6.0	0.0554535456	4.3326152987	0.6144407721
Carbon	6.0	-0.0554535456	-4.3326152987	0.6144407721
Carbon	6.0	-0.3398931550	2.9907452336	0.4524367071
Carbon	6.0	0.3398931550	-2.9907452336	0.4524367071
Hydrogen	1.0	-1.3887329364	2.6946485092	0.5733937422
Hydrogen	1.0	1.3887329364	-2.6946485092	0.5733937422
Hydrogen	1.0	-0.6998370691	5.0976115680	0.8563290277
Hydrogen	1.0	0.6998370691	-5.0976115680	0.8563290277
Hydrogen	1.0	1.7805241856	5.6947266760	0.5616663675
Hydrogen	1.0	-1.7805241856	-5.6947266760	0.5616663675
Hydrogen	1.0	3.4181809365	3.8266857190	0.0747117174
Hydrogen	1.0	-3.4181809365	-3.8266857190	0.0747117174
Hydrogen	1.0	5.2908634648	-1.2082859136	-0.8754178588
Hydrogen	1.0	-5.2908634648	1.2082859136	-0.8754178588
Hydrogen	1.0	2.8947241495	-2.2432834646	-0.5979707670
Hydrogen	1.0	-2.8947241495	2.2432834646	-0.5979707670

Table S2 (continued)

<i>trans</i> -1	Lowest triplet state (3B , C_2)			
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Nitrogen	7.0	0.5072185297	1.9862621488	0.1215281963
Nitrogen	7.0	-0.5072185297	-1.9862621488	0.1215281963
Carbon	6.0	1.8138726822	2.3021786368	-0.2602902588
Carbon	6.0	-1.8138726822	-2.3021786368	-0.2602902588
Carbon	6.0	2.5658936690	1.1276178153	-0.6447764804
Carbon	6.0	-2.5658936690	-1.1276178153	-0.6447764804
Sulfur	16.0	4.2473916392	1.0284440304	-1.1524412987
Sulfur	16.0	-4.2473916392	-1.0284440304	-1.1524412987
Carbon	6.0	4.0740109277	-0.6946251822	-1.4588078696
Carbon	6.0	-4.0740109277	0.6946251822	-1.4588078696
Carbon	6.0	2.7997212277	-1.1674267409	-1.1679836572
Carbon	6.0	-2.7997212277	1.1674267409	-1.1679836572
Carbon	6.0	1.9159364483	-0.1345252894	-0.6648350999
Carbon	6.0	-1.9159364483	0.1345252894	-0.6648350999
Carbon	6.0	2.2662113174	3.6507274183	-0.2505106954
Carbon	6.0	-2.2662113174	-3.6507274183	-0.2505106954
Carbon	6.0	1.3940930981	4.6793355828	0.1430632946
Carbon	6.0	-1.3940930981	-4.6793355828	0.1430632946
Carbon	6.0	0.0605056510	4.3397155624	0.5306484858
Carbon	6.0	-0.0605056510	-4.3397155624	0.5306484858
Carbon	6.0	-0.3287432093	2.9933134624	0.5037525524
Carbon	6.0	0.3287432093	-2.9933134624	0.5037525524
Hydrogen	1.0	-1.3382860182	2.6845858672	0.8150284673
Hydrogen	1.0	1.3382860182	-2.6845858672	0.8150284673
Hydrogen	1.0	-0.6590772081	5.1059036701	0.8622521715
Hydrogen	1.0	0.6590772081	-5.1059036701	0.8622521715
Hydrogen	1.0	1.7367069585	5.7286425360	0.1538419509
Hydrogen	1.0	-1.7367069585	-5.7286425360	0.1538419509
Hydrogen	1.0	3.3031983331	3.8687607327	-0.5564509312
Hydrogen	1.0	-3.3031983331	-3.8687607327	-0.5564509312
Hydrogen	1.0	4.9374885408	-1.2652116930	-1.8362500535
Hydrogen	1.0	-4.9374885408	1.2652116930	-1.8362500535
Hydrogen	1.0	2.5101784092	-2.2199196135	-1.3165860974
Hydrogen	1.0	-2.5101784092	2.2199196135	-1.3165860974

Table S2 (continued)

2	Ground state				
	Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
	Carbon	6.0	2.9417152494	-2.1506368660	-2.4860200032
	Carbon	6.0	2.0869691071	-1.7578451067	-1.2820302966
	Oxygen	8.0	1.3173762331	-0.7426798229	-1.4672806220
	Carbon	6.0	2.1930879026	-2.5218062386	-0.0793024855
	Carbon	6.0	1.4687234091	-2.3041423197	1.1274412889
	Oxygen	8.0	0.5856160021	-1.3851111139	1.3489991310
	Carbon	6.0	1.7172404696	-3.2164092394	2.3261980799
	Carbon	6.0	-1.7764462589	3.5412893791	-2.7927027231
	Carbon	6.0	-0.8033823713	2.6626470029	-3.3363411777
	Carbon	6.0	-0.2945410633	1.6364365723	-2.5170147270
	Nitrogen	7.0	-0.7004102299	1.4591916625	-1.2379441483
	Carbon	6.0	-1.6516454882	2.3034681730	-0.6892556713
	Carbon	6.0	-2.2024581807	3.3618352058	-1.4636548132
	Carbon	6.0	-1.9615246468	1.9507285174	0.6848965995
	Sulfur	16.0	-3.0932915878	2.7087333472	1.7970076753
	Carbon	6.0	-2.6678980046	1.5439859251	3.0304695266
	Carbon	6.0	-1.7088958946	0.6250354273	2.6063933071
	Carbon	6.0	-1.2857303724	0.8480078804	1.2427279193
	Hydrogen	1.0	3.6465512022	-2.9734265924	-2.2551568578
	Hydrogen	1.0	3.5102968962	-1.2645459681	-2.8401629270
	Hydrogen	1.0	2.2746634564	-2.4667918938	-3.3175116783
	Hydrogen	1.0	2.9044131111	-3.3622604824	-0.0833537887
	Hydrogen	1.0	2.4424317046	-4.0210387243	2.0957619827
	Hydrogen	1.0	2.0988151739	-2.6091158975	3.1748967915
	Hydrogen	1.0	0.7542563403	-3.6648536289	2.6506688131
	Hydrogen	1.0	-2.1981827893	4.3596579147	-3.4031023322
	Hydrogen	1.0	-0.4409172025	2.7656478764	-4.3718621900
	Hydrogen	1.0	0.4650232891	0.9240051573	-2.8755098243
	Hydrogen	1.0	-2.9563302309	4.0259444079	-1.0101716681
	Hydrogen	1.0	-1.3175243563	-0.1830849006	3.2444011642
	Hydrogen	1.0	-3.1564044895	1.6021916635	4.0164308086

Table S2 (continued)

2	Lowest triplet state			
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Carbon	6.0	2.9425932181	-2.1350700632	-2.5023048818
Carbon	6.0	2.0785074263	-1.7608989417	-1.2992551012
Oxygen	8.0	1.3138123786	-0.7396593314	-1.4760609679
Carbon	6.0	2.1830431676	-2.5364773165	-0.1046719546
Carbon	6.0	1.4702380604	-2.3210175213	1.1108293147
Oxygen	8.0	0.5968351961	-1.3990207714	1.3470819544
Carbon	6.0	1.7243600034	-3.2442533452	2.3001480891
Carbon	6.0	-1.7999682014	3.5485667786	-2.8066261933
Carbon	6.0	-0.8092740842	2.6526731925	-3.3412397993
Carbon	6.0	-0.2934546876	1.6270851089	-2.5189617734
Nitrogen	7.0	-0.6882567120	1.4415105943	-1.2436067512
Carbon	6.0	-1.6701885269	2.3108036231	-0.6909395826
Carbon	6.0	-2.2242931455	3.3758365616	-1.4899467649
Carbon	6.0	-1.9787875227	1.9787554890	0.6450190266
Sulfur	16.0	-3.1131312720	2.7361760792	1.7576894030
Carbon	6.0	-2.6569920053	1.5323371561	3.0257594591
Carbon	6.0	-1.6822928952	0.6108372104	2.5860769971
Carbon	6.0	-1.2586912076	0.8114104322	1.2521466576
Hydrogen	1.0	3.5329346585	-3.0561937623	-2.3301518457
Hydrogen	1.0	3.6346564604	-1.2946781561	-2.7272008237
Hydrogen	1.0	2.2922000923	-2.2712366916	-3.3924358054
Hydrogen	1.0	2.8871709126	-3.3827426514	-0.1198350428
Hydrogen	1.0	2.4478773685	-4.0475643353	2.0602159972
Hydrogen	1.0	2.1095239177	-2.6437788497	3.1520063791
Hydrogen	1.0	0.7623648766	-3.6946641951	2.6249459681
Hydrogen	1.0	-2.2168760706	4.3597153124	-3.4284701228
Hydrogen	1.0	-0.4427174843	2.7491537665	-4.3759426219
Hydrogen	1.0	0.4693378797	0.9224964315	-2.8871907773
Hydrogen	1.0	-2.9813648486	4.0391898306	-1.0389186208
Hydrogen	1.0	-1.2906309192	-0.1921568680	3.2309680127
Hydrogen	1.0	-3.1448788170	1.5926785654	4.0114319699

Table S2 (continued)

3	Ground state				
	Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
	Carbon	6.0	2.1007498183	-1.7098763753	-1.3284829675
	Oxygen	8.0	1.3186146886	-0.6931256511	-1.4741577094
	Carbon	6.0	2.2262586194	-2.4943732815	-0.1431307378
	Hydrogen	1.0	2.9720122315	-3.2953646613	-0.1693852367
	Carbon	6.0	1.5107373250	-2.3185288029	1.0752758523
	Oxygen	8.0	0.6040616804	-1.4179535412	1.2984650117
	Hydrogen	1.0	-2.2617244891	4.4382113722	-3.2526334283
	Carbon	6.0	-1.8308739351	3.6044094746	-2.6701335576
	Carbon	6.0	-0.8614800253	2.7439264518	-3.2485465827
	Hydrogen	1.0	-0.5125602211	2.8751871945	-4.2854799763
	Carbon	6.0	-0.3403985768	1.6972537902	-2.4635707845
	Hydrogen	1.0	0.4121491484	0.9928173350	-2.8513615422
	Nitrogen	7.0	-0.7307624510	1.4844947278	-1.1850988949
	Carbon	6.0	-1.6818736698	2.3074455527	-0.6048715864
	Carbon	6.0	-2.2438177676	3.3854115359	-1.3429473879
	Hydrogen	1.0	-2.9957356242	4.0329688011	-0.8631920306
	Carbon	6.0	-1.9801035525	1.9092317091	0.7589231609
	Sulfur	16.0	-3.1181165654	2.6141939164	1.8992101153
	Carbon	6.0	-2.6776753018	1.4104686126	3.0885941313
	Carbon	6.0	-1.7098098041	0.5188712493	2.6292169661
	Carbon	6.0	-1.2911916133	0.7945608347	1.2738180862
	Hydrogen	1.0	-1.3130347275	-0.3069776883	3.2395742781
	Hydrogen	1.0	-3.1645495427	1.4261634610	4.0768974589
	Carbon	6.0	4.0294000975	-1.2994715409	-4.6158353435
	Carbon	6.0	3.2355469675	-1.0245029888	-3.4787053053
	Carbon	6.0	4.5355629526	-2.6059579822	-4.8336810938
	Hydrogen	1.0	2.8399100599	-0.0115235515	-3.3005450029
	Hydrogen	1.0	5.1516815914	-2.8225269710	-5.7249243368
	Carbon	6.0	2.9513521349	-2.0488014508	-2.5304400200
	Carbon	6.0	4.2425960030	-3.6352621536	-3.9038698688
	Hydrogen	1.0	4.6195600215	-4.6598406082	-4.0734919047
	Carbon	6.0	3.4599014881	-3.3599057504	-2.7581057258
	Hydrogen	1.0	3.2218571072	-4.1771784331	-2.0581830410
	Hydrogen	1.0	4.2535546494	-0.4909197941	-5.3347518705
	Carbon	6.0	2.9848383149	-5.0636052863	3.3723012210
	Carbon	6.0	2.7670423155	-4.2542265099	2.2342152218
	Carbon	6.0	2.2259436735	-4.8609108060	4.5525260458
	Hydrogen	1.0	3.3751407657	-4.4338602088	1.3341807130
	Hydrogen	1.0	2.3995674149	-5.4954504727	5.4403331030
	Carbon	6.0	1.7834827300	-3.2224276883	2.2583053171
	Carbon	6.0	1.2451071036	-3.8387081535	4.5840113245
	Hydrogen	1.0	0.6476393688	-3.6709159337	5.4980399025
	Carbon	6.0	1.0256309594	-3.0262788003	3.4484688666
	Hydrogen	1.0	0.2676304076	-2.2284075510	3.4644929298
	Hydrogen	1.0	3.7536380296	-5.8560604928	3.3352856350

Table S2 (continued)

3	Lowest triplet state			
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Carbon	6.0	2.1030534060	-1.7070323994	-1.3339236944
Oxygen	8.0	1.3204333004	-0.6895086395	-1.4774844657
Carbon	6.0	2.2331225998	-2.4933427544	-0.1511739790
Hydrogen	1.0	2.9812818307	-3.2916935998	-0.1822666044
Carbon	6.0	1.5187797815	-2.3246821688	1.0706648271
Oxygen	8.0	0.6090645537	-1.4313474369	1.2998804568
Hydrogen	1.0	-2.2357570249	4.4517654834	-3.2909233154
Carbon	6.0	-1.8197485764	3.6211708676	-2.6946949782
Carbon	6.0	-0.8376280650	2.7347733755	-3.2603662430
Hydrogen	1.0	-0.4796212829	2.8558313081	-4.2954411768
Carbon	6.0	-0.3211110903	1.6851477354	-2.4695572695
Hydrogen	1.0	0.4308769789	0.9828793334	-2.8633807446
Nitrogen	7.0	-0.7072872209	1.4685752621	-1.1965952367
Carbon	6.0	-1.6863280128	2.3226353414	-0.6164899197
Carbon	6.0	-2.2392284963	3.4126541199	-1.3816946864
Hydrogen	1.0	-2.9912665442	4.0658637181	-0.9081452323
Carbon	6.0	-1.9937998348	1.9472310172	0.7076050900
Sulfur	16.0	-3.1350773567	2.6609112437	1.8422444818
Carbon	6.0	-2.6799611574	1.4136154286	3.0668943168
Carbon	6.0	-1.6997254825	0.5132353422	2.5977846375
Carbon	6.0	-1.2698596477	0.7626044428	1.2740595796
Hydrogen	1.0	-1.3126356945	-0.3096646345	3.2190525456
Hydrogen	1.0	-3.1713588043	1.4351848624	4.0523828756
Carbon	6.0	4.0268984425	-1.2891933331	-4.6225752909
Carbon	6.0	3.2368137587	-1.0156742452	-3.4825190169
Carbon	6.0	4.5253788738	-2.5973646019	-4.8480399651
Hydrogen	1.0	2.8469200979	-0.0015533748	-3.2985219776
Hydrogen	1.0	5.1383140577	-2.8126992979	-5.7417651231
Carbon	6.0	2.9496331256	-2.0435470959	-2.5389083652
Carbon	6.0	4.2288875179	-3.6300486977	-3.9230310793
Hydrogen	1.0	4.5996363371	-4.6557840002	-4.0991300740
Carbon	6.0	3.4503223627	-3.3563593628	-2.7741296048
Hydrogen	1.0	3.2086664364	-4.1757087716	-2.0778574022
Hydrogen	1.0	4.2538689569	-0.4783197910	-5.3379294072
Carbon	6.0	3.0257213210	-5.0681714640	3.3480065643
Carbon	6.0	2.7974043320	-4.2536352343	2.2157104288
Carbon	6.0	2.2651095667	-4.8827163346	4.5298471742
Hydrogen	1.0	3.4071612073	-4.4197028787	1.3143268043
Hydrogen	1.0	2.4467114552	-5.5213900190	5.4130758398
Carbon	6.0	1.8017284016	-3.2336549477	2.2476933500
Carbon	6.0	1.2721439722	-3.8724609135	4.5692235893
Hydrogen	1.0	0.6734617054	-3.7184441967	5.4848554058
Carbon	6.0	1.0425336089	-3.0545191607	3.4396084702
Hydrogen	1.0	0.2752923367	-2.2656257853	3.4619035125
Hydrogen	1.0	3.8041911985	-5.8507624540	3.3049428767

Table S2 (continued)

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Ground state

Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Carbon	6.0	2.8170634636	-1.0785923839	-0.1528815162
Oxygen	8.0	1.5650838183	-1.3943281008	-0.1141981876
Carbon	6.0	3.3311037640	0.2536389055	-0.1414473871
Hydrogen	1.0	4.4145805590	0.3609911628	-0.2615824548
Carbon	6.0	2.5772114456	1.4596268943	-0.0660671159
Oxygen	8.0	1.2837247687	1.5528039131	0.0021913853
Hydrogen	1.0	-4.3998016857	-4.0055187837	0.0289727521
Carbon	6.0	-3.5653680612	-3.2816935175	0.0245804810
Carbon	6.0	-2.2199541462	-3.7305819486	-0.0258397288
Hydrogen	1.0	-1.9652559011	-4.8021766184	-0.0590955758
Carbon	6.0	-1.1925686303	-2.7674461249	-0.0302185857
Hydrogen	1.0	-0.1269736358	-3.0432076323	-0.0635108396
Nitrogen	7.0	-1.4406707929	-1.4375532947	0.0104388170
Carbon	6.0	-2.7473482434	-0.9789058915	0.0659782847
Carbon	6.0	-3.8309086071	-1.9006573418	0.0715918524
Hydrogen	1.0	-4.8633833833	-1.5171868774	0.1150568710
Carbon	6.0	-2.8105121871	0.4703156263	0.1175614693
Sulfur	16.0	-4.2186177625	1.5208619780	0.2075197822
Carbon	6.0	-3.1744103196	2.9237628459	0.2349312131
Carbon	6.0	-1.8204264663	2.5980003760	0.1778539280
Carbon	6.0	-1.5905945881	1.1728164681	0.1075152479
Hydrogen	1.0	-1.0171653743	3.3513616633	0.1930742754
Hydrogen	1.0	-3.6242342504	3.9278538200	0.2955372348
Carbon	6.0	4.1638205903	-4.6113657284	-0.7992100474
Carbon	6.0	3.2981947240	-3.4979247993	-0.6907750623
Carbon	6.0	5.5331724393	-4.4932975706	-0.4418030307
Hydrogen	1.0	2.2394293281	-3.5971103218	-0.9772859369
Carbon	6.0	3.7751075466	-2.2399129236	-0.2389203652
Carbon	6.0	6.0193200167	-3.2341776603	0.0424400542
Carbon	6.0	5.1484796788	-2.1309433779	0.1310939473
Hydrogen	1.0	5.5683411982	-1.1885506903	0.5158451303
Hydrogen	1.0	3.7657083693	-5.5663164355	-1.1754019004
Carbon	6.0	5.3083607058	4.1745000895	0.2306026717
Carbon	6.0	4.6695233543	2.9129406589	0.2504288241
Carbon	6.0	4.5642145736	5.3409898454	-0.1467214849
Hydrogen	1.0	5.2364375390	2.0248975124	0.5586060946
Carbon	6.0	3.2864462473	2.7913657310	-0.0829240129
Carbon	6.0	3.1924342529	5.2135125148	-0.4634546487
Hydrogen	1.0	2.6386065460	6.1284139243	-0.7364218270
Carbon	6.0	2.5490845910	3.9551604908	-0.4245271123
Hydrogen	1.0	1.4813875901	3.8602275422	-0.6741416873
Oxygen	8.0	6.6269487247	4.3855063607	0.5733985587
Carbon	6.0	7.3932145220	3.2552566382	0.9986080381
Hydrogen	1.0	6.9552629826	2.7830280884	1.9069655186
Hydrogen	1.0	7.4774876120	2.4890233761	0.1946521808
Hydrogen	1.0	8.4025478999	3.6463029564	1.2398414031
Oxygen	8.0	5.1302274999	6.6019071200	-0.1294171856
Carbon	6.0	6.1364390181	6.8409046034	-1.1377164558
Hydrogen	1.0	7.0090945211	6.1665641004	-1.0075577020
Hydrogen	1.0	5.7083785322	6.7076480379	-2.1583021552
Hydrogen	1.0	6.4559701898	7.8956648842	-1.0076769830
Oxygen	8.0	7.3570248862	-3.0600689458	0.3618609098
Carbon	6.0	7.7714936707	-3.7025332538	1.5860832375
Hydrogen	1.0	7.2078699793	-3.2930459975	2.4566159740
Hydrogen	1.0	7.6276600564	-4.8031469985	1.5352576567
Hydrogen	1.0	8.8510941419	-3.4748330356	1.7058941437
Oxygen	8.0	6.4554909222	-5.5075676697	-0.5275917316
Carbon	6.0	6.0112660149	-6.7677230488	-1.0428450482
Hydrogen	1.0	5.2208853001	-7.2163234818	-0.3995010891
Hydrogen	1.0	5.6241456047	-6.6679020729	-2.0817649337
Hydrogen	1.0	6.9030826491	-7.4265908004	-1.0445394722

Table S2 (continued)

4

Lowest triplet state

Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Carbon	6.0	2.8190330202	-1.0795846011	-0.1552322032
Oxygen	8.0	1.5662560510	-1.3958055931	-0.1152982012
Carbon	6.0	3.3358808436	0.2508472328	-0.1444478980
Hydrogen	1.0	4.4193835003	0.3545576809	-0.2668297833
Carbon	6.0	2.5853571463	1.4604696891	-0.0673748079
Oxygen	8.0	1.2941593987	1.5589642299	0.0024563497
Hydrogen	1.0	-4.3826666836	-4.0551634169	0.0274486883
Carbon	6.0	-3.5626781359	-3.3161343120	0.0245719020
Carbon	6.0	-2.1901077383	-3.7457595949	-0.0198704915
Hydrogen	1.0	-1.9208293762	-4.8139085360	-0.0485449658
Carbon	6.0	-1.1654250804	-2.7745002034	-0.0241151532
Hydrogen	1.0	-0.1008241866	-3.0563348273	-0.0525953439
Nitrogen	7.0	-1.4096308280	-1.4493842330	0.0107530872
Carbon	6.0	-2.7585803153	-0.9972235367	0.0638520275
Carbon	6.0	-3.8405599944	-1.9506377589	0.0669528122
Hydrogen	1.0	-4.8772214263	-1.5759901532	0.1059986705
Carbon	6.0	-2.8412070000	0.4102851063	0.1132384600
Sulfur	16.0	-4.2583426805	1.4509207533	0.1932142023
Carbon	6.0	-3.1797451638	2.8995140463	0.2297888000
Carbon	6.0	-1.8097263851	2.5673097531	0.1773952517
Carbon	6.0	-1.5541831453	1.1776165910	0.1062645169
Hydrogen	1.0	-1.0167140283	3.3319365382	0.1972082352
Hydrogen	1.0	-3.6386875975	3.8988711708	0.2922087632
Carbon	6.0	4.1581427559	-4.6125578434	-0.8108230398
Carbon	6.0	3.2951128115	-3.4973861164	-0.7012486875
Carbon	6.0	5.5264237776	-4.4995854654	-0.4473836981
Hydrogen	1.0	2.2373381888	-3.5923013064	-0.9925826990
Carbon	6.0	3.7741680662	-2.2424578624	-0.2427071626
Carbon	6.0	6.0144584793	-3.2435756929	0.0435412858
Carbon	6.0	5.1464227192	-2.1382875879	0.1329525047
Hydrogen	1.0	5.5668032741	-1.1984308800	0.5233224223
Hydrogen	1.0	3.7588980355	-5.5648997908	-1.1923024777
Carbon	6.0	5.3304021616	4.1621566950	0.2247279936
Carbon	6.0	4.6859030875	2.9035306027	0.2448792300
Carbon	6.0	4.5905070608	5.3324150267	-0.1497250198
Hydrogen	1.0	5.2496459245	2.0126518295	0.5505357449
Carbon	6.0	3.3013614312	2.7886122949	-0.0849137450
Carbon	6.0	3.2172443482	5.2114126495	-0.4631703518
Hydrogen	1.0	2.6669989130	6.1290203276	-0.7342542333
Carbon	6.0	2.5683897384	3.9560563505	-0.4236567298
Hydrogen	1.0	1.4997061463	3.8659186322	-0.6708792324
Oxygen	8.0	6.6506448614	4.3667103630	0.5645001009
Carbon	6.0	7.4137487942	3.2319097730	0.9837106479
Hydrogen	1.0	6.9772218155	2.7591456962	1.8924414210
Hydrogen	1.0	7.4915579425	2.4677524256	0.1771757705
Hydrogen	1.0	8.4256187897	3.6180202814	1.2221326333
Oxygen	8.0	5.1617414703	6.5906476225	-0.1329375112
Carbon	6.0	6.1688377015	6.8259988735	-1.1414572669
Hydrogen	1.0	7.0381523541	6.1472224067	-1.0125272107
Hydrogen	1.0	5.7394633784	6.6962137830	-2.1619089446
Hydrogen	1.0	6.4934415783	7.8790024864	-1.0100843404
Oxygen	8.0	7.3512617736	-3.0746848502	0.3689260670
Carbon	6.0	7.7589791639	-3.7222887710	1.5927955074
Hydrogen	1.0	7.1932927524	-3.3136662231	2.4623720788
Hydrogen	1.0	7.6118642695	-4.8222599759	1.5380140844
Hydrogen	1.0	8.8388174791	-3.4983698448	1.7173749099
Oxygen	8.0	6.4459274231	-5.5159454224	-0.5331326464
Carbon	6.0	5.9998961084	-6.7738515763	-1.0529225261
Hydrogen	1.0	5.2058327899	-7.2213373376	-0.4134444535
Hydrogen	1.0	5.6171007747	-6.6705135125	-2.0930554314
Hydrogen	1.0	6.8898510695	-7.4351895120	-1.0526285662

Table S2 (continued)

5-1	Ground state			
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Carbon	6.0	2.7330266280	1.2728055508	0.1075786955
Oxygen	8.0	1.4632795082	1.4987666011	0.0083264140
Carbon	6.0	3.3445277022	-0.0139239531	0.1665531139
Carbon	6.0	2.6708540538	-1.2657650856	0.1514874322
Oxygen	8.0	1.3840985464	-1.4549239157	0.1083880653
Carbon	6.0	-3.7798378459	3.0272005010	-0.1979705213
Carbon	6.0	-2.4690181609	3.5698974520	-0.1487197324
Carbon	6.0	-1.3775203664	2.6812083057	-0.0934724730
Nitrogen	7.0	-1.5344259215	1.3368877906	-0.0869973892
Carbon	6.0	-2.8059754197	0.7872002369	-0.1284007111
Carbon	6.0	-3.9497815562	1.6307385867	-0.1870118685
Carbon	6.0	-2.7714901413	-0.6637895242	-0.1014925849
Sulfur	16.0	-4.1056215208	-1.8100692643	-0.1421642826
Carbon	6.0	-2.9703471539	-3.1395811218	-0.0729784164
Carbon	6.0	-1.6422203834	-2.7204300349	-0.0214624654
Carbon	6.0	-1.5079707325	-1.2808152385	-0.0358176819
Carbon	6.0	3.8483642354	4.8162306517	-0.8177602147
Carbon	6.0	3.1300490454	3.6032538688	-0.7166297107
Carbon	6.0	5.0471113329	4.9675204166	-0.0829907989
Carbon	6.0	3.5886870376	2.5205487461	0.0841897058
Carbon	6.0	5.5192456449	3.9181997004	0.7436806433
Carbon	6.0	4.8006345813	2.6943324680	0.8354777970
Carbon	6.0	5.3745473849	-4.0452010834	-0.1747222186
Carbon	6.0	4.7314874668	-2.7879736115	-0.3428074600
Carbon	6.0	4.7595277482	-5.0702151781	0.5853736958
Carbon	6.0	3.4504181350	-2.5553883111	0.2635378219
Carbon	6.0	3.4913362592	-4.8608761486	1.1749374297
Carbon	6.0	2.8479786447	-3.6150640563	0.9982942773
Oxygen	8.0	5.1969929852	1.6564061408	1.6457111473
Carbon	6.0	6.3679074300	1.8280360864	2.4486603040
Oxygen	8.0	5.2729932659	-1.7710925055	-1.0949117820
Carbon	6.0	6.5065845627	-2.0109278167	-1.7773928438
Hydrogen	1.0	4.4355478030	-0.0413950142	0.2291535543
Hydrogen	1.0	-4.6617288351	3.6909561614	-0.2426746691
Hydrogen	1.0	-2.2889033246	4.6570597641	-0.1513171935
Hydrogen	1.0	-0.3334653026	3.0298063998	-0.0494909226
Hydrogen	1.0	-4.9531103520	1.1755682826	-0.2210547171
Hydrogen	1.0	-3.3511058957	-4.1735735296	-0.0767702546
Hydrogen	1.0	-0.7890174503	-3.4162624007	0.0180038006
Hydrogen	1.0	3.4753980146	5.6311012634	-1.4626662682
Hydrogen	1.0	2.1921749552	3.4591407633	-1.2774733640
Hydrogen	1.0	5.6257020342	5.9072009207	-0.1413744329
Hydrogen	1.0	6.4455881440	4.0659627304	1.3193159505
Hydrogen	1.0	6.3524935308	-4.2356311300	-0.6417866167
Hydrogen	1.0	5.2802675372	-6.0371086615	0.7073197811
Hydrogen	1.0	3.0057988487	-5.6575872196	1.7652075713
Hydrogen	1.0	1.8570923828	-3.4293978410	1.4434265482
Hydrogen	1.0	7.2758391191	1.9866290365	1.8236759245
Hydrogen	1.0	6.2594396695	2.6804940810	3.1566623697
Hydrogen	1.0	6.4774243586	0.8860841927	3.0231925672
Hydrogen	1.0	7.3360441880	-2.2260564366	-1.0661837581
Hydrogen	1.0	6.4180956015	-2.8539206973	-2.4992957644
Hydrogen	1.0	6.7298458517	-1.0758320952	-2.3298651569

Table S2 (continued)

5-1	Lowest triplet state			
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Carbon	6.0	2.7347760499	1.2785287348	0.1103215120
Oxygen	8.0	1.4633537098	1.5028288702	0.0144309131
Carbon	6.0	3.3506776921	-0.0054041209	0.1679977859
Carbon	6.0	2.6817410354	-1.2612805893	0.1529084494
Oxygen	8.0	1.3982745048	-1.4573023413	0.1087010530
Carbon	6.0	-3.7876877618	3.0524821700	-0.1962946730
Carbon	6.0	-2.4508894491	3.5815574918	-0.1316636016
Carbon	6.0	-1.3590907433	2.6869776635	-0.0770566327
Nitrogen	7.0	-1.5077763075	1.3476482150	-0.0826939111
Carbon	6.0	-2.8197413350	0.7979981843	-0.1370754637
Carbon	6.0	-3.9664061703	1.6700269380	-0.1981439506
Carbon	6.0	-2.8035276048	-0.6125880811	-0.1186874043
Sulfur	16.0	-4.1434940445	-1.7533668800	-0.1693425930
Carbon	6.0	-2.9668069947	-3.1233924384	-0.1075796841
Carbon	6.0	-1.6246561646	-2.6929915586	-0.0477604401
Carbon	6.0	-1.4672133318	-1.2868719582	-0.0474855060
Carbon	6.0	3.8287155350	4.8260531492	-0.8199278437
Carbon	6.0	3.1151887441	3.6111293336	-0.7116897032
Carbon	6.0	5.0348245075	4.9805058957	-0.0978687652
Carbon	6.0	3.5857619139	2.5290107044	0.0833739755
Carbon	6.0	5.5188948874	3.9322521633	0.7231992184
Carbon	6.0	4.8053535523	2.7059954656	0.8219264057
Carbon	6.0	5.3992784769	-4.0275431281	-0.1703244169
Carbon	6.0	4.7490275725	-2.7744984897	-0.3422147462
Carbon	6.0	4.7923611598	-5.0517746671	0.5973004241
Carbon	6.0	3.4690288732	-2.5460646682	0.2678165983
Carbon	6.0	3.5251541875	-4.8464020737	1.1905928949
Carbon	6.0	2.8744582206	-3.6051012227	1.0098722883
Oxygen	8.0	5.2140271116	1.6690899355	1.6271090441
Carbon	6.0	6.3908249390	1.8452925883	2.4206203376
Oxygen	8.0	5.2814285828	-1.7584011346	-1.1013440289
Carbon	6.0	6.5134279420	-1.9944602107	-1.7883142079
Hydrogen	1.0	4.4417985269	-0.0290265587	0.2292918826
Hydrogen	1.0	-4.6581740798	3.7298280419	-0.2419187186
Hydrogen	1.0	-2.2592063882	4.6667045976	-0.1227011177
Hydrogen	1.0	-0.3176629366	3.0432301421	-0.0240314506
Hydrogen	1.0	-4.9724998019	1.2202075714	-0.2434950726
Hydrogen	1.0	-3.3536653239	-4.1544950573	-0.1253489539
Hydrogen	1.0	-0.7788927216	-3.3987022747	-0.0120910023
Hydrogen	1.0	3.4463169690	5.6400784833	-1.4602912538
Hydrogen	1.0	2.1720930911	3.4643237976	-1.2627434624
Hydrogen	1.0	5.6098221482	5.9219952462	-0.1619274559
Hydrogen	1.0	6.4507280400	4.0826448466	1.2891901760
Hydrogen	1.0	6.3764525783	-4.2153297341	-0.6400776454
Hydrogen	1.0	5.3186551160	-6.0152607204	0.7222321673
Hydrogen	1.0	3.0463266112	-5.6426964423	1.7868471686
Hydrogen	1.0	1.8841189514	-3.4222619741	1.4575063544
Hydrogen	1.0	7.2928915436	2.0080992298	1.7883344912
Hydrogen	1.0	6.2842810636	2.6969097707	3.1298614626
Hydrogen	1.0	6.5089245229	0.9034768817	2.9936525304
Hydrogen	1.0	7.3471788783	-2.2018746666	-1.0799202813
Hydrogen	1.0	6.4261671303	-2.8410722661	-2.5061078549
Hydrogen	1.0	6.7288790979	-1.0605948966	-2.3459041369

Table S2 (continued)

5-2	Ground state			
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Carbon	6.0	2.7244861761	-0.0431238715	-1.2895620739
Oxygen	8.0	1.4534575870	-0.0284001465	-1.5131394128
Carbon	6.0	3.3436503264	-0.0998260592	-0.0056614232
Carbon	6.0	2.6855109642	-0.1121668447	1.2565356386
Oxygen	8.0	1.4022085142	-0.0698794016	1.4429086220
Carbon	6.0	-3.7886166084	0.1999727483	-3.0124844117
Carbon	6.0	-2.4787129311	0.1762486259	-3.5587971193
Carbon	6.0	-1.3845453303	0.1178283721	-2.6738019846
Nitrogen	7.0	-1.5388192851	0.0825150443	-1.3295823941
Carbon	6.0	-2.8085747168	0.1100667955	-0.7763451785
Carbon	6.0	-3.9550136185	0.1675065950	-1.6159278380
Carbon	6.0	-2.7691118689	0.0771775076	0.6743918964
Sulfur	16.0	-4.1015605615	0.0968637259	1.8221821747
Carbon	6.0	-2.9643336429	0.0392290729	3.1493231168
Carbon	6.0	-1.6363718523	0.0069397290	2.7276649977
Carbon	6.0	-1.5034073122	0.0287041392	1.2883429791
Carbon	6.0	3.8781640756	-0.5177550004	-4.9076639670
Carbon	6.0	3.0774130396	-0.5367533126	-3.7473796418
Carbon	6.0	5.1908895987	0.0240515390	-4.8873416805
Carbon	6.0	3.5971886430	-0.0183536073	-2.5240926402
Carbon	6.0	5.6994048607	0.5533302657	-3.6715216565
Carbon	6.0	4.9042971882	0.5288881734	-2.4946841202
Carbon	6.0	5.6227100213	-0.2903266172	3.7670117754
Carbon	6.0	4.9068953515	-0.2330884888	2.5433644491
Carbon	6.0	4.9257758820	-0.2933269771	5.0042086060
Carbon	6.0	3.4886343197	-0.1791741860	2.5392528663
Carbon	6.0	3.5070669756	-0.2405648662	4.9912180610
Carbon	6.0	2.7870249790	-0.1845175488	3.7815044249
Oxygen	8.0	6.9487729531	1.1175505023	-3.5267776861
Carbon	6.0	7.7941455519	1.1658286887	-4.6785116033
Oxygen	8.0	6.9954468196	-0.3408416516	3.6417945756
Carbon	6.0	7.7701157177	-0.3775966549	4.8424853526
Hydrogen	1.0	4.4366764086	-0.1563200952	0.0002776940
Hydrogen	1.0	-4.6724944625	0.2453546894	-3.6734588520
Hydrogen	1.0	-2.3012182275	0.2037543907	-4.6459911547
Hydrogen	1.0	-0.3407830097	0.1009855908	-3.0249529798
Hydrogen	1.0	-4.9574419877	0.1874465813	-1.1580527500
Hydrogen	1.0	-3.3426551323	0.0320330244	4.1840876894
Hydrogen	1.0	-0.7849603192	-0.0308276237	3.4248492964
Hydrogen	1.0	3.4843583086	-0.9322178212	-5.8531627860
Hydrogen	1.0	2.0613230419	-0.9609702746	-3.7647153796
Hydrogen	1.0	5.7923001013	0.0313904048	-5.8095096341
Hydrogen	1.0	5.3233623723	0.9726096721	-1.5784312627
Hydrogen	1.0	5.4967920310	-0.2335486598	1.6150817727
Hydrogen	1.0	5.4616104834	-0.3354461431	5.9649263241
Hydrogen	1.0	2.9617451122	-0.2437104340	5.9519920843
Hydrogen	1.0	1.6881024736	-0.1430620529	3.7758206176
Hydrogen	1.0	8.0206838666	0.1455283431	-5.0641270930
Hydrogen	1.0	7.3406898311	1.7710930432	-5.4965396012
Hydrogen	1.0	8.7355701790	1.6483275693	-4.3457262246
Hydrogen	1.0	8.8310443494	-0.4068530526	4.5208659026
Hydrogen	1.0	7.5998409432	0.5287894804	5.4673028900
Hydrogen	1.0	7.5450647773	-1.2843874581	5.4492367263

Table S2 (continued)

5-2	Lowest triplet state			
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Carbon	6.0	2.7266069686	-0.0463168287	-1.2932723847
Oxygen	8.0	1.4547060937	-0.0327720180	-1.5169197687
Carbon	6.0	3.3492593343	-0.1028867414	-0.0117627960
Carbon	6.0	2.6955658227	-0.1124502658	1.2542254220
Oxygen	8.0	1.4152854929	-0.0667884409	1.4459604957
Carbon	6.0	-3.7964394494	0.1812422040	-3.0388930265
Carbon	6.0	-2.4596033586	0.1601035018	-3.5708773959
Carbon	6.0	-1.3652539296	0.1078751582	-2.6795346623
Nitrogen	7.0	-1.5120098880	0.0754527775	-1.3402611240
Carbon	6.0	-2.8230293415	0.1027339540	-0.7875548807
Carbon	6.0	-3.9725999840	0.1533565987	-1.6565033812
Carbon	6.0	-2.8030347945	0.0783247900	0.6222743340
Sulfur	16.0	-4.1423669292	0.0999810521	1.7647863009
Carbon	6.0	-2.9630867789	0.0473850198	3.1316662659
Carbon	6.0	-1.6203019006	0.0153398712	2.6989271916
Carbon	6.0	-1.4634198103	0.0307946121	1.2934967344
Carbon	6.0	3.8757460755	-0.5210104351	-4.9124420008
Carbon	6.0	3.0762445465	-0.5404751903	-3.7512955188
Carbon	6.0	5.1877009539	0.0227118469	-4.8938271660
Carbon	6.0	3.5971534546	-0.0208278322	-2.5290311585
Carbon	6.0	5.6971430751	0.5535187967	-3.6790033831
Carbon	6.0	4.9035138476	0.5284946556	-2.5012698526
Carbon	6.0	5.6458844848	-0.2985310056	3.7488576513
Carbon	6.0	4.9236626009	-0.2395858877	2.5289704369
Carbon	6.0	4.9554379191	-0.2976619304	4.9896693015
Carbon	6.0	3.5056320132	-0.1803880294	2.5327273667
Carbon	6.0	3.5368365560	-0.2393883836	4.9845129130
Carbon	6.0	2.8105565778	-0.1817736142	3.7786528876
Oxygen	8.0	6.9457349100	1.1196847527	-3.5361191946
Carbon	6.0	7.7897262039	1.1686595910	-4.6889395528
Oxygen	8.0	7.0174759459	-0.3546512402	3.6162902611
Carbon	6.0	7.7986566844	-0.3940450848	4.8128267650
Hydrogen	1.0	4.4420753994	-0.1607595645	-0.0095769404
Hydrogen	1.0	-4.6688755461	0.2208940782	-3.7140146873
Hydrogen	1.0	-2.2696104740	0.1853877715	-4.6560193262
Hydrogen	1.0	-0.3235316946	0.0943164905	-3.0379254278
Hydrogen	1.0	-4.9784685819	0.1708924969	-1.2043665588
Hydrogen	1.0	-3.3474953613	0.0436933338	4.1637633064
Hydrogen	1.0	-0.7768572250	-0.0185219450	3.4065971120
Hydrogen	1.0	3.4813760425	-0.9363464310	-5.8572791141
Hydrogen	1.0	2.0607144775	-0.9659413328	-3.7671554652
Hydrogen	1.0	5.7879249770	0.0305089729	-5.8167683271
Hydrogen	1.0	5.3227649638	0.9736493829	-1.5858274096
Hydrogen	1.0	5.5084436983	-0.2433201807	1.5975197044
Hydrogen	1.0	5.4963938925	-0.3410887550	5.9474512874
Hydrogen	1.0	2.9969556292	-0.2395725802	5.9483380423
Hydrogen	1.0	1.7117717330	-0.1362283246	3.7782711368
Hydrogen	1.0	8.0172492825	0.1484959061	-5.0743008976
Hydrogen	1.0	7.3344325541	1.7729441402	-5.5066405318
Hydrogen	1.0	8.7308328841	1.6526183376	-4.3574061217
Hydrogen	1.0	8.8576010158	-0.4282790656	4.4853034629
Hydrogen	1.0	7.6359145102	0.5135870918	5.4378175022
Hydrogen	1.0	7.5728373557	-1.2994457869	5.4213224372

Table S2 (continued)**5-3**

Ground state

Carbon	6.0	-2.0075935899	2.2657624409	-0.0223719995
Oxygen	8.0	-1.8514075959	0.9826376408	-0.0208521207
Carbon	6.0	-0.9412910436	3.2132505846	-0.0129856008
Hydrogen	1.0	-1.2194431644	4.2704574447	-0.0168329508
Carbon	6.0	0.4536356350	2.9306606173	-0.0014013484
Oxygen	8.0	0.9947747123	1.7483881383	0.0050445025
Hydrogen	1.0	-2.2200842143	-5.5226235612	-0.0109098041
Carbon	6.0	-1.8330058733	-4.4879982704	-0.0089825829
Carbon	6.0	-2.7240288301	-3.3834686343	-0.0222771540
Hydrogen	1.0	-3.8175255434	-3.5184526184	-0.0347163779
Carbon	6.0	-2.1793080568	-2.0847701847	-0.0192348613
Hydrogen	1.0	-2.8070717869	-1.1808539003	-0.0293962413
Nitrogen	7.0	-0.8464124744	-1.8524306652	-0.0043141476
Carbon	6.0	0.0397046676	-2.9174627310	0.0085385457
Carbon	6.0	-0.4455990727	-4.2542991027	0.0064672733
Hydrogen	1.0	0.2748707066	-5.0884404732	0.0168681588
Carbon	6.0	1.4212648308	-2.4727618481	0.0226833742
Sulfur	16.0	2.8962532222	-3.4322595516	0.0419976663
Carbon	6.0	3.8517423625	-1.9677101139	0.0478962948
Carbon	6.0	3.0755407667	-0.8104169408	0.0356596782
Carbon	6.0	1.6563260776	-1.0848050603	0.0208415518
Hydrogen	1.0	3.5076718664	0.2023702973	0.0371529204
Hydrogen	1.0	4.9510913312	-2.0414164986	0.0603164648
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Carbon	6.0	-5.8449113307	2.1418378600	-0.0789450928
Carbon	6.0	-4.4802563114	1.7722114291	-0.0641862436
Carbon	6.0	-6.1965618911	3.5184386702	-0.0634187558
Hydrogen	1.0	-4.2065499855	0.7063965398	-0.0749150567
Carbon	6.0	-3.4405866593	2.7404190824	-0.0359165462
Carbon	6.0	-5.1686330681	4.5038341069	-0.0341641642
Carbon	6.0	-3.8162683134	4.1189583848	-0.0213947886
Hydrogen	1.0	-3.0509513853	4.9098853979	0.0013105986
Hydrogen	1.0	-6.6153842703	1.3559483232	-0.1017544154
Carbon	6.0	2.0573441446	6.4530947551	0.0056998649
Carbon	6.0	1.0824684134	5.4402089053	0.0006343772
Carbon	6.0	3.4417755826	6.1182648553	0.0139726006
Hydrogen	1.0	0.0229542985	5.7382603325	-0.0059279830
Carbon	6.0	1.4534461839	4.0602096736	0.0039335732
Carbon	6.0	3.8311315370	4.7516374022	0.0173379092
Hydrogen	1.0	4.8928949558	4.4613211996	0.0238146846
Carbon	6.0	2.8392365887	3.7439819165	0.0124462148
Hydrogen	1.0	3.1325072986	2.6833361510	0.0153751232
Hydrogen	1.0	-5.4553068984	5.5690477143	-0.0220152457
Hydrogen	1.0	1.7703015255	7.5183052632	0.0032867713
Oxygen	8.0	-7.4832242902	3.9989003223	-0.0738771198
Carbon	6.0	-8.5520022387	3.0474445441	-0.1132225660
Hydrogen	1.0	-8.5079073479	2.4216005685	-1.0332179016
Hydrogen	1.0	-8.5409760261	2.3829205702	0.7802531073
Hydrogen	1.0	-9.4883966942	3.6412245957	-0.1174667066
Oxygen	8.0	4.3105792145	7.1821671604	0.0182138543
Carbon	6.0	5.7138919082	6.8986300150	0.0270547050
Hydrogen	1.0	6.0088613295	6.3275034325	0.9360942327
Hydrogen	1.0	6.0201719184	6.3269285998	-0.8778852708
Hydrogen	1.0	6.2234276041	7.8835918164	0.0299114651

Table S2 (continued)

5-3

Lowest triplet state

Carbon	6.0	-2.0102985715	2.2672014121	-0.0217538829
Oxygen	8.0	-1.8537713339	0.9829941458	-0.0206077509
Carbon	6.0	-0.9466687023	3.2166837090	-0.0122163218
Hydrogen	1.0	-1.2282343252	4.2728518034	-0.0157471052
Carbon	6.0	0.4505457976	2.9387623155	-0.0011319497
Oxygen	8.0	0.9961252706	1.7605159578	0.0049034263
Hydrogen	1.0	-2.2645416561	-5.5261175519	-0.0101403567
Carbon	6.0	-1.8591104162	-4.4993191261	-0.0082997201
Carbon	6.0	-2.7428465669	-3.3639969423	-0.0219027134
Hydrogen	1.0	-3.8379400985	-3.4851899781	-0.0343876970
Carbon	6.0	-2.1907155918	-2.0644120547	-0.0190980810
Hydrogen	1.0	-2.8249893540	-1.1645072038	-0.0295843582
Nitrogen	7.0	-0.8642623503	-1.8288404491	-0.0042979727
Carbon	6.0	0.0321416882	-2.9342207351	0.0089625320
Carbon	6.0	-0.4823468099	-4.2813613743	0.0070115036
Hydrogen	1.0	0.2318600607	-5.1218300437	0.0175852627
Carbon	6.0	1.3805129538	-2.5201379976	0.0223186125
Sulfur	16.0	2.8520650711	-3.4867032731	0.0413401219
Carbon	6.0	3.8342963237	-1.9712033411	0.0462058911
Carbon	6.0	3.0432953519	-0.8034460450	0.0338296131
Carbon	6.0	1.6492807540	-1.0460905518	0.0201278936
Hydrogen	1.0	3.4868088441	0.2047871274	0.0348897034
Hydrogen	1.0	4.9327011598	-2.0519511793	0.0580641210
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Carbon	6.0	-5.8466741155	2.1358493106	-0.0813125230
Carbon	6.0	-4.4815181859	1.7686630047	-0.0661329383
Carbon	6.0	-6.2008129429	3.5118509860	-0.0632140591
Hydrogen	1.0	-4.2060518180	0.7034339188	-0.0786632799
Carbon	6.0	-3.4436647837	2.7389807520	-0.0352050960
Carbon	6.0	-5.1747117237	4.4993090257	-0.0310288189
Carbon	6.0	-3.8218053311	4.1169879308	-0.0181254096
Hydrogen	1.0	-3.0580469669	4.9093111098	0.0068573407
Hydrogen	1.0	-6.6156271626	1.3485912651	-0.1063757400
Carbon	6.0	2.0370179371	6.4692541492	0.0050020582
Carbon	6.0	1.0668316161	5.4519669200	0.0002587256
Carbon	6.0	3.4230722290	6.1407478864	0.0133417942
Hydrogen	1.0	0.0060133994	5.7451946695	-0.0064260786
Carbon	6.0	1.4442896985	4.0736356465	0.0039525676
Carbon	6.0	3.8188681630	4.7758510517	0.0171437054
Hydrogen	1.0	4.8819883802	4.4905829847	0.0236836973
Carbon	6.0	2.8316287325	3.7638828381	0.0125610356
Hydrogen	1.0	3.1297970378	2.7046100009	0.0157934374
Hydrogen	1.0	-5.4634786071	5.5639103523	-0.0167982775
Hydrogen	1.0	1.7452550916	7.5331505384	0.0022413788
Oxygen	8.0	-7.4879830896	3.9898069331	-0.0736578495
Carbon	6.0	-8.5553207991	3.0365323700	-0.1174107551
Hydrogen	1.0	-8.5085514394	2.4136429524	-1.0392011648
Hydrogen	1.0	-8.5444032294	2.3695696198	0.7741746502
Hydrogen	1.0	-9.4925655949	3.6289100765	-0.1213331179
Oxygen	8.0	4.2866530632	7.2084242351	0.0171846842
Carbon	6.0	5.6915205832	6.9319112562	0.0261135302
Hydrogen	1.0	5.9892017170	6.3627225524	0.9354453929
Hydrogen	1.0	6.0004859919	6.3614248742	-0.8786425101
Hydrogen	1.0	6.1960830933	7.9193978779	0.0285288581

Table S2 (continued)**5-4**

Ground state

Carbon	6.0	2.0542207383	-1.7399426865	-1.3583593780
Oxygen	8.0	1.2829917018	-0.7146833157	-1.4954031418
Carbon	6.0	2.2000697894	-2.5138688287	-0.1684838062
Hydrogen	1.0	2.9361669198	-3.3229327949	-0.2048469252
Carbon	6.0	1.5125715024	-2.3209176874	1.0632806532
Oxygen	8.0	0.6166172086	-1.4132938237	1.2975557217
Hydrogen	1.0	-2.2799988626	4.4417138431	-3.2334396198
Carbon	6.0	-1.8460315410	3.6069134458	-2.6546091044
Carbon	6.0	-0.8893676813	2.7395872306	-3.2437774920
Hydrogen	1.0	-0.5523681514	2.8664333247	-4.2851645246
Carbon	6.0	-0.3639442223	1.6916582504	-2.4632157329
Hydrogen	1.0	0.3795040978	0.9820733878	-2.8591793250
Nitrogen	7.0	-0.7387882535	1.4845543690	-1.1791376228
Carbon	6.0	-1.6760534825	2.3153986902	-0.5875247081
Carbon	6.0	-2.2420944158	3.3942301642	-1.3211653845
Hydrogen	1.0	-2.9831476392	4.0478301949	-0.8327544868
Carbon	6.0	-1.9552548733	1.9246126039	0.7824674706
Sulfur	16.0	-3.0707461028	2.6411196877	1.9381143455
Carbon	6.0	-2.6154376207	1.4414013459	3.1265397455
Carbon	6.0	-1.6596863185	0.5427045938	2.6561679801
Carbon	6.0	-1.2632786076	0.8095652446	1.2921903955
Hydrogen	1.0	-1.2572157407	-0.2813453063	3.2653078157
Hydrogen	1.0	-3.0852872111	1.4644496245	4.1229064337
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Carbon	6.0	3.9075942018	-1.3916868104	-4.6935806367
Carbon	6.0	3.1456707581	-1.0973175625	-3.5329582356
Carbon	6.0	4.3882872064	-2.7103202529	-4.9150219937
Hydrogen	1.0	2.7814038095	-0.0707067549	-3.3739013101
Hydrogen	1.0	4.9775468874	-2.9632388767	-5.8098935432
Carbon	6.0	2.8719897033	-2.1069782218	-2.5765208725
Carbon	6.0	4.0952560811	-3.7195708211	-3.9604555393
Hydrogen	1.0	4.4548568512	-4.7486581213	-4.1399337247
Carbon	6.0	3.3493381565	-3.4337103909	-2.7981544824
Hydrogen	1.0	3.1142129635	-4.2414387549	-2.0877598082
Carbon	6.0	3.0209171066	-5.0434780490	3.3497584955
Carbon	6.0	2.7935026718	-4.2530612299	2.2057336074
Carbon	6.0	2.2894692477	-4.8376786163	4.5492784881
Hydrogen	1.0	3.3854827207	-4.4429578832	1.2983374088
Hydrogen	1.0	2.4914303379	-5.4727905056	5.4255501211
Carbon	6.0	1.8086952665	-3.2190211083	2.2468404422
Carbon	6.0	1.3099678654	-3.8101923301	4.5871129434
Carbon	6.0	1.0746509454	-3.0079888906	3.4406696029
Hydrogen	1.0	0.3148309187	-2.2142025555	3.4838875791
Hydrogen	1.0	3.7850736304	-5.8405786431	3.3166502838
Oxygen	8.0	0.5357430521	-3.5107442098	5.6872324866
Carbon	6.0	0.7401165106	-4.2810877364	6.8737802389
Hydrogen	1.0	0.5217817206	-5.3606211999	6.7059744301
Hydrogen	1.0	1.7809758358	-4.1769613445	7.2569506609
Hydrogen	1.0	0.0314592918	-3.8775481980	7.6252476414
Oxygen	8.0	4.1260259620	-0.3292514091	-5.5447004626
Carbon	6.0	4.8857450822	-0.5729122928	-6.7311556035
Hydrogen	1.0	5.9157401435	-0.9248042413	-6.4942413037
Hydrogen	1.0	4.3887857146	-1.3210787841	-7.3900972833
Hydrogen	1.0	4.9446257960	0.3996600273	-7.2607084020

Table S2 (continued)

5-4	Lowest triplet state			
Carbon	6.0	2.0566081390	-1.7392209213	-1.3612225722
Oxygen	8.0	1.2853014801	-0.7130936732	-1.4978081381
Carbon	6.0	2.2061969372	-2.5139824102	-0.1731731197
Hydrogen	1.0	2.9444306134	-3.3207497489	-0.2131649876
Carbon	6.0	1.5195137043	-2.3264921353	1.0615466474
Oxygen	8.0	0.6212275667	-1.4251248795	1.3005608199
Hydrogen	1.0	-2.2558304329	4.4507090028	-3.2772758297
Carbon	6.0	-1.8362646421	3.6200652445	-2.6835264048
Carbon	6.0	-0.8673607549	2.7256751150	-3.2593631562
Hydrogen	1.0	-0.5220046129	2.8406817509	-4.2993846279
Carbon	6.0	-0.3460767888	1.6759080226	-2.4716341268
Hydrogen	1.0	0.3964134176	0.9679049612	-2.8732382908
Nitrogen	7.0	-0.7161096539	1.4669189852	-1.1926234454
Carbon	6.0	-1.6801942988	2.3304336326	-0.6013581040
Carbon	6.0	-2.2379695187	3.4200557350	-1.3635997266
Hydrogen	1.0	-2.9787324164	4.0801906153	-0.8819176139
Carbon	6.0	-1.9679249745	1.9646127189	0.7298742585
Sulfur	16.0	-3.0855632141	2.6922219407	1.8794127452
Carbon	6.0	-2.6153098018	1.4507164531	3.1045965373
Carbon	6.0	-1.6486457111	0.5413997358	2.6248314541
Carbon	6.0	-1.2412595169	0.7796437798	1.2919032432
Hydrogen	1.0	-1.2560445642	-0.2789929566	3.2460694407
Hydrogen	1.0	-3.0888547797	1.4816551632	4.0985355580
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Carbon	6.0	3.9075182592	-1.3868272914	-4.6968635306
Carbon	6.0	3.1485818138	-1.0929245103	-3.5341159298
Carbon	6.0	4.3805904712	-2.7073037061	-4.9240267138
Hydrogen	1.0	2.7899769576	-0.0650417750	-3.3706383522
Hydrogen	1.0	4.9670824427	-2.9598320119	-5.8208268947
Carbon	6.0	2.8712074955	-2.1051725574	-2.5814299470
Carbon	6.0	4.0834986578	-3.7189240111	-3.9732020462
Hydrogen	1.0	4.4370265406	-4.7492265644	-4.1576262005
Carbon	6.0	3.3409122480	-3.4336987533	-2.8086463119
Hydrogen	1.0	3.1017772064	-4.2427635804	-2.1011027232
Carbon	6.0	3.0526129607	-5.0482834603	3.3326075801
Carbon	6.0	2.8166730488	-4.2545548242	2.1925768420
Carbon	6.0	2.3220399541	-4.8534055748	4.5343741041
Hydrogen	1.0	3.4082755158	-4.4358261721	1.2832780315
Hydrogen	1.0	2.5305317972	-5.4908807151	5.4073875867
Carbon	6.0	1.8241692376	-3.2282011913	2.2405592708
Carbon	6.0	1.3346709062	-3.8336336437	4.5790966292
Carbon	6.0	1.0910775023	-3.0279553466	3.4368071812
Hydrogen	1.0	0.3255492722	-2.2399526481	3.4851936393
Hydrogen	1.0	3.8229873266	-5.8390912982	3.2942888464
Oxygen	8.0	0.5605471751	-3.5451909039	5.6820843398
Carbon	6.0	0.7738404071	-4.3188728242	6.8650583077
Hydrogen	1.0	0.5635358198	-5.3993232936	6.6931439423
Hydrogen	1.0	1.8147867176	-4.2079813850	7.2459738189
Hydrogen	1.0	0.0638452186	-3.9240146993	7.6198385411
Oxygen	8.0	4.1305073011	-0.3224593571	-5.5438887690
Carbon	6.0	4.8865084858	-0.5653551423	-6.7329660900
Hydrogen	1.0	5.9150341208	-0.9237809730	-6.4995096086
Hydrogen	1.0	4.3840479261	-1.3080292785	-7.3939233900
Hydrogen	1.0	4.9495041729	0.4090966008	-7.2585063605

Table S2 (continued)

5-5	Ground state			
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Carbon	6.0	2.7232697035	1.2710991457	-0.0492817085
Oxygen	8.0	1.4592882382	1.5067591381	-0.0547612743
Carbon	6.0	3.3334361427	-0.0205243946	-0.0047483126
Carbon	6.0	2.6564198641	-1.2732639522	0.0381767177
Oxygen	8.0	1.3777862008	-1.4701853656	0.0483828447
Carbon	6.0	-3.7632797313	3.0492621963	-0.1025770476
Carbon	6.0	-2.4481743436	3.5827652546	-0.1304223608
Carbon	6.0	-1.3601267279	2.6881131479	-0.1020004103
Nitrogen	7.0	-1.5269890963	1.3459866960	-0.0487287920
Carbon	6.0	-2.8023174665	0.8043051280	-0.0234867397
Carbon	6.0	-3.9421242502	1.6546711055	-0.0495298121
Carbon	6.0	-2.7753609458	-0.6465074824	0.0283862921
Sulfur	16.0	-4.1168106271	-1.7844767422	0.0646989735
Carbon	6.0	-2.9871458632	-3.1204726381	0.1084694420
Carbon	6.0	-1.6553722804	-2.7098528477	0.0952635693
Carbon	6.0	-1.5144238516	-1.2718458709	0.0481911422
Carbon	6.0	4.3160329913	4.6566470903	-1.0111162539
Carbon	6.0	3.4587091840	3.5238631573	-1.0366357493
Carbon	6.0	5.3372302168	4.7551844067	-0.0320946114
Carbon	6.0	3.6339922025	2.4768060213	-0.0721848744
Carbon	6.0	5.5201680557	3.7292009877	0.9225465455
Carbon	6.0	4.6693690978	2.5967091807	0.8895500985
Carbon	6.0	5.2841949522	-3.8760256367	-1.0082510687
Carbon	6.0	4.4919886637	-2.7026756341	-0.9553546591
Carbon	6.0	5.0849687369	-4.8844613086	-0.0380933938
Carbon	6.0	3.5005466151	-2.5252712109	0.0424213976
Carbon	6.0	4.1063105178	-4.7283182524	0.9762601539
Carbon	6.0	3.3083791185	-3.5530857650	1.0234218504
Oxygen	8.0	2.4677494075	3.3450413621	-1.9711056046
Carbon	6.0	2.3244224698	4.3314765921	-2.9954311018
Oxygen	8.0	2.3652991035	-3.3127729515	1.9903781233
Carbon	6.0	2.1727425788	-4.3004342060	3.0052853156
Hydrogen	1.0	4.4317981991	-0.0522971059	-0.0073855704
Hydrogen	1.0	-4.6419830162	3.7185082973	-0.1223468964
Hydrogen	1.0	-2.2618994157	4.6681786345	-0.1713326865
Hydrogen	1.0	-0.3123157332	3.0281139627	-0.1223938652
Hydrogen	1.0	-4.9489737428	1.2065664548	-0.0277686883
Hydrogen	1.0	-3.3747347663	-4.1514804775	0.1407476187
Hydrogen	1.0	-0.8028961313	-3.4071699796	0.1176252142
Hydrogen	1.0	4.1988507808	5.4622325137	-1.7517312881
Hydrogen	1.0	5.9906328769	5.6461872620	-0.0262106461
Hydrogen	1.0	6.3128874715	3.8073837211	1.6869244931
Hydrogen	1.0	4.7932231110	1.7912900190	1.6334162395
Hydrogen	1.0	6.0431710898	-3.9996079651	-1.8003580152
Hydrogen	1.0	4.6259896259	-1.9098545847	-1.7108437852
Hydrogen	1.0	5.6924680228	-5.8071846941	-0.0602932955
Hydrogen	1.0	3.9757379819	-5.5222144851	1.7272585012
Hydrogen	1.0	3.2516821623	4.4297367115	-3.6047420449
Hydrogen	1.0	1.4968777253	3.9765567411	-3.6424568421
Hydrogen	1.0	2.0594184116	5.3276978967	-2.5734842160
Hydrogen	1.0	1.8381279744	-5.2714234726	2.5746084194
Hydrogen	1.0	3.1008410730	-4.4651033215	3.5990213057
Hydrogen	1.0	1.3785081023	-3.9008882370	3.6674382817

Table S2 (continued)

5-5	Lowest triplet state			
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Carbon	6.0	2.7249507740	1.2764830011	-0.0504226004
Oxygen	8.0	1.4599986980	1.5112582247	-0.0567663613
Carbon	6.0	3.3394818092	-0.0123630995	-0.0056968725
Carbon	6.0	2.6676165125	-1.2693223073	0.0387908151
Oxygen	8.0	1.3921417888	-1.4726386100	0.0489789937
Carbon	6.0	-3.7722320792	3.0727534565	-0.1026103715
Carbon	6.0	-2.4306741727	3.5928174815	-0.1316337410
Carbon	6.0	-1.3419525750	2.6927608974	-0.1029334060
Nitrogen	7.0	-1.5005977138	1.3556193201	-0.0483490186
Carbon	6.0	-2.8167627194	0.8138351284	-0.0222199227
Carbon	6.0	-3.9597945600	1.6924369670	-0.0488621627
Carbon	6.0	-2.8077228616	-0.5960669178	0.0282725405
Sulfur	16.0	-4.1549109338	-1.7290291731	0.0676399672
Carbon	6.0	-2.9837135000	-3.1049616802	0.1142332474
Carbon	6.0	-1.6376032601	-2.6827379140	0.0986132952
Carbon	6.0	-1.4735586113	-1.2785607041	0.0504975652
Carbon	6.0	4.3084030700	4.6681488925	-1.0049586909
Carbon	6.0	3.4536525216	3.5334332410	-1.0330531708
Carbon	6.0	5.3297248704	4.7666229198	-0.0261419762
Carbon	6.0	3.6325161398	2.4843156681	-0.0713628255
Carbon	6.0	5.5158679614	3.7386750635	0.9258552517
Carbon	6.0	4.6682029142	2.6040700961	0.8901974451
Carbon	6.0	5.3119713073	-3.8586131701	-0.9995905529
Carbon	6.0	4.5145103923	-2.6888073883	-0.9486754969
Carbon	6.0	5.1145436837	-4.8681106559	-0.0301063341
Carbon	6.0	3.5190780966	-2.5165279437	0.0460911815
Carbon	6.0	4.1323768719	-4.7167147160	0.9815015942
Carbon	6.0	3.3285954689	-3.5453984007	1.0264224539
Oxygen	8.0	2.4631159914	3.3543032378	-1.9673300651
Carbon	6.0	2.3147547525	4.3440473315	-2.9880411524
Oxygen	8.0	2.3814728006	-3.3100592479	1.9905147831
Carbon	6.0	2.1936191930	-4.2971463944	3.0069909025
Hydrogen	1.0	4.4378538207	-0.0396767853	-0.0082476680
Hydrogen	1.0	-4.6397068852	3.7552616109	-0.1225718542
Hydrogen	1.0	-2.2327712120	4.6761454392	-0.1732790331
Hydrogen	1.0	-0.2964342101	3.0408380141	-0.1245412476
Hydrogen	1.0	-4.9696745330	1.2494365230	-0.0259361261
Hydrogen	1.0	-3.3774390630	-4.1331330544	0.1475458789
Hydrogen	1.0	-0.7925389282	-3.3896701193	0.1217857337
Hydrogen	1.0	4.1887762485	5.4754512603	-1.7432813629
Hydrogen	1.0	5.9807589545	5.6593336057	-0.0181448639
Hydrogen	1.0	6.3085742259	3.8170904277	1.6901951624
Hydrogen	1.0	4.7942851998	1.7972035179	1.6320707792
Hydrogen	1.0	6.0738367369	-3.9785892650	-1.7894456044
Hydrogen	1.0	4.6474250492	-1.8951846010	-1.7034962447
Hydrogen	1.0	5.7264494075	-5.7879401374	-0.0506150172
Hydrogen	1.0	4.0034196886	-5.5112347788	1.7320943014
Hydrogen	1.0	3.2406504444	4.4467819983	-3.5986329098
Hydrogen	1.0	1.4868651054	3.9889089253	-3.6344213170
Hydrogen	1.0	2.0476414950	5.3378234718	-2.5618938832
Hydrogen	1.0	1.8651661916	-5.2708329166	2.5776602583
Hydrogen	1.0	3.1219697958	-4.4552813552	3.6020514763
Hydrogen	1.0	1.3963653069	-3.9010197835	3.6675652256

Table S2 (continued)

6	Ground state				
	Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
	Hydrogen	1.0	4.7006608530	2.2888901116	0.1040504022
	Carbon	6.0	3.6201537492	2.5301051261	0.0713141995
	Hydrogen	1.0	3.3526810197	3.1444986255	0.9577057195
	Hydrogen	1.0	3.4089961182	3.1452385365	-0.8300004378
	Carbon	6.0	2.7442206088	1.2791509694	0.0451718439
	Oxygen	8.0	1.4766793748	1.5005865723	0.0257375246
	Carbon	6.0	3.3663985634	-0.0063552470	0.0447028435
	Hydrogen	1.0	4.4668729934	-0.0324353463	0.0614390001
	Carbon	6.0	2.6907185766	-1.2582582336	0.0250790736
	Oxygen	8.0	1.4110415974	-1.4510925332	0.0070520941
	Carbon	6.0	3.5010804449	-2.5525033654	0.0250009202
	Hydrogen	1.0	4.5923379158	-2.3647864510	0.0438920329
	Hydrogen	1.0	3.2148321659	-3.1619213156	0.9082302418
	Hydrogen	1.0	3.2430543040	-3.1438524618	-0.8790365109
	Hydrogen	1.0	-4.5667180742	3.8069429764	-0.0359733627
	Carbon	6.0	-3.7012290245	3.1207516572	-0.0287840882
	Carbon	6.0	-2.3760667766	3.6281628654	-0.0146352340
	Hydrogen	1.0	-2.1675731460	4.7102318461	-0.0103959291
	Carbon	6.0	-1.3059620885	2.7121687120	-0.0060004333
	Hydrogen	1.0	-0.2531765092	3.0348448610	0.0051219233
	Nitrogen	7.0	-1.4978996053	1.3725583889	-0.0106741488
	Carbon	6.0	-2.7817518621	0.8577163403	-0.0243284868
	Carbon	6.0	-3.9056271489	1.7285831872	-0.0336398741
	Hydrogen	1.0	-4.9199135910	1.2977172800	-0.0445594697
	Carbon	6.0	-2.7878481110	-0.5929639960	-0.0265286926
	Sulfur	16.0	-4.2107532578	-1.6492545211	-0.0365719504
	Carbon	6.0	-3.1469612154	-3.0607417921	-0.0274810804
	Carbon	6.0	-1.7507699211	-2.6992107493	-0.0177860856
	Carbon	6.0	-1.5515892643	-1.2513114505	-0.0170318168
	Carbon	6.0	-2.5771444365	-5.4234977775	-0.0192606521
	Carbon	6.0	-3.5665964250	-4.4167830017	-0.0282580770
	Carbon	6.0	-1.1892188276	-5.0861978376	-0.0099975439
	Hydrogen	1.0	-4.6393172802	-4.6762155908	-0.0355238681
	Hydrogen	1.0	-0.4340977371	-5.8929639604	-0.0032370847
	Carbon	6.0	-0.7723193349	-3.7419045276	-0.0093162849
	Hydrogen	1.0	0.2938079236	-3.4703209929	-0.0022684424
	Hydrogen	1.0	-2.8826636045	-6.4855074112	-0.0194813583

Table S2 (continued)

6	Lowest triplet state			
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Hydrogen	1.0	4.6941897779	2.3105274247	0.1062505366
Carbon	6.0	3.6124555455	2.5457389514	0.0711673227
Hydrogen	1.0	3.3390955001	3.1602207264	0.9556313595
Hydrogen	1.0	3.3986851637	3.1577213037	-0.8316328161
Carbon	6.0	2.7426108720	1.2906745223	0.0457424576
Oxygen	8.0	1.4742096244	1.5084973407	0.0253114061
Carbon	6.0	3.3717268475	0.0087798025	0.0467824161
Hydrogen	1.0	4.4722722645	-0.0104532249	0.0646290177
Carbon	6.0	2.7043328342	-1.2486813687	0.0269963637
Oxygen	8.0	1.4279834892	-1.4516297830	0.0077487917
Carbon	6.0	3.5271925834	-2.5354202940	0.0280082577
Hydrogen	1.0	4.6166369445	-2.3379933308	0.0510697355
Hydrogen	1.0	3.2432550369	-3.1486952218	0.9093108426
Hydrogen	1.0	3.2780070241	-3.1276047794	-0.8780192855
Hydrogen	1.0	-4.5645447958	3.8429116333	-0.0332812193
Carbon	6.0	-3.7098695779	3.1442673621	-0.0268545665
Carbon	6.0	-2.3591882697	3.6386436760	-0.0132674098
Hydrogen	1.0	-2.1390421793	4.7183499241	-0.0089717098
Carbon	6.0	-1.2927958151	2.7170336022	-0.0054731642
Hydrogen	1.0	-0.2413532584	3.0449291618	0.0050518665
Nitrogen	7.0	-1.4790086467	1.3793054384	-0.0102268076
Carbon	6.0	-2.7995401319	0.8668008976	-0.0233479421
Carbon	6.0	-3.9238333647	1.7664997676	-0.0317921254
Hydrogen	1.0	-4.9425884590	1.3438941476	-0.0421328244
Carbon	6.0	-2.8163232727	-0.5461747805	-0.0256696843
Sulfur	16.0	-4.2032310533	-1.6110619133	-0.0359376273
Carbon	6.0	-3.1172973538	-3.0528586030	-0.0266857234
Carbon	6.0	-1.7161778437	-2.6827979431	-0.0170828735
Carbon	6.0	-1.5022133387	-1.2620016473	-0.0162622368
Carbon	6.0	-2.5626679825	-5.4206727829	-0.0186947609
Carbon	6.0	-3.5503062216	-4.3843971098	-0.0274684604
Carbon	6.0	-1.1807089950	-5.0910189602	-0.0097301570
Hydrogen	1.0	-4.6255622775	-4.6338788174	-0.0345854101
Hydrogen	1.0	-0.4285814462	-5.9007813483	-0.0032006733
Carbon	6.0	-0.7480475492	-3.7459677882	-0.0089060838
Hydrogen	1.0	0.3209243718	-3.4862931187	-0.0019710850
Hydrogen	1.0	-2.8826537503	-6.4776320393	-0.0190893737

Table S2 (continued)

7-1	Ground state			
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Hydrogen	1.0	3.4991147706	-3.1028468057	-2.3241188921
Carbon	6.0	2.9165799569	-2.1774008407	-2.5000137091
Hydrogen	1.0	3.6158257543	-1.3455464849	-2.7344259712
Hydrogen	1.0	2.2609615827	-2.3139931823	-3.3862400879
Carbon	6.0	2.0619921521	-1.7873757096	-1.2948913628
Oxygen	8.0	1.3033377772	-0.7626537310	-1.4725315927
Carbon	6.0	2.1676538769	-2.5544545397	-0.0941838727
Hydrogen	1.0	2.8646082798	-3.4067996370	-0.1054459208
Carbon	6.0	1.4627909141	-2.3204830528	1.1207189210
Oxygen	8.0	0.5988233587	-1.3849949387	1.3480343070
Carbon	6.0	1.7093378325	-3.2332358823	2.3195304311
Hydrogen	1.0	2.4291267048	-4.0423005477	2.0877949687
Hydrogen	1.0	2.0959644452	-2.6277596803	3.1671484371
Hydrogen	1.0	0.7446058549	-3.6765049514	2.6463237317
Carbon	6.0	-0.7889454464	2.5723783963	-3.3621679959
Hydrogen	1.0	-0.4224099387	2.6411866182	-4.3991523892
Carbon	6.0	-0.3058831608	1.5854985253	-2.5167998264
Hydrogen	1.0	0.4470788616	0.8518758291	-2.8407551902
Nitrogen	7.0	-0.7287550491	1.4543896568	-1.2194016298
Carbon	6.0	-1.6630848247	2.3060147292	-0.6864224607
Carbon	6.0	-1.9570911865	1.9638024639	0.6991549188
Sulfur	16.0	-3.0627254611	2.6908209066	1.8687773061
Carbon	6.0	-2.5954431180	1.5207836710	3.0760600573
Carbon	6.0	-1.6431370801	0.6164783391	2.6134235467
Carbon	6.0	-1.2627254434	0.8580608125	1.2429312373
Hydrogen	1.0	-1.2239772760	-0.1976317620	3.2250949739
Hydrogen	1.0	-3.0576158254	1.5664782675	4.0747348064
Carbon	6.0	-1.7673002593	3.5035113550	-2.8697461246
Carbon	6.0	-2.2994425291	4.5504078903	-3.6981729324
Carbon	6.0	-2.2206357246	3.3774800574	-1.4998837718
Carbon	6.0	-3.2466624990	5.4463915989	-3.1933637340
Carbon	6.0	-3.1959753891	4.3139944207	-1.0087251834
Carbon	6.0	-3.6963350161	5.3250527682	-1.8375681008
Hydrogen	1.0	-1.9433890051	4.6335262139	-4.7403201529
Hydrogen	1.0	-3.6488841630	6.2489674271	-3.8370949504
Hydrogen	1.0	-3.5578882682	4.2455959731	0.0269301045
Hydrogen	1.0	-4.4442471010	6.0341502898	-1.4410064290

Table S2 (continued)

7-1	Lowest triplet state			
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Hydrogen	1.0	3.4895233244	-3.1095062502	-2.3357176001
Carbon	6.0	2.9081921222	-2.1830790251	-2.5098067883
Hydrogen	1.0	3.6076382261	-1.3519497266	-2.7459981476
Hydrogen	1.0	2.2493508707	-2.3179843712	-3.3938714606
Carbon	6.0	2.0576691789	-1.7911252675	-1.3027740091
Oxygen	8.0	1.3036767205	-0.7625585829	-1.4796116279
Carbon	6.0	2.1631713982	-2.5612341227	-0.1041337181
Hydrogen	1.0	2.8573098685	-3.4156615916	-0.1201178304
Carbon	6.0	1.4636976902	-2.3294057781	1.1152371946
Oxygen	8.0	0.6034417276	-1.3943040306	1.3513104355
Carbon	6.0	1.7147804664	-3.2481448966	2.3084903023
Hydrogen	1.0	2.4346307452	-4.0555411943	2.0715180686
Hydrogen	1.0	2.1024143475	-2.6457578833	3.1578068636
Hydrogen	1.0	0.7509845206	-3.6934481641	2.6353020139
Carbon	6.0	-0.8050995421	2.5873847254	-3.3460600266
Hydrogen	1.0	-0.4342410321	2.6542723269	-4.3819665626
Carbon	6.0	-0.3058130851	1.5810091035	-2.4998443904
Hydrogen	1.0	0.4499538970	0.8616600292	-2.8517718479
Nitrogen	7.0	-0.7071739150	1.4326086788	-1.2252638241
Carbon	6.0	-1.6899242208	2.3275897522	-0.6744258358
Carbon	6.0	-1.9664686099	1.9838360286	0.6659718660
Sulfur	16.0	-3.0713246329	2.7110851566	1.8322055511
Carbon	6.0	-2.5922516057	1.5159764861	3.0660404560
Carbon	6.0	-1.6323569394	0.6080315400	2.5982643285
Carbon	6.0	-1.2451934405	0.8322989109	1.2472534258
Hydrogen	1.0	-1.2162029596	-0.2035005247	3.2157229244
Hydrogen	1.0	-3.0569684824	1.5658677497	4.0630307070
Carbon	6.0	-1.7937362801	3.5309031792	-2.8645970930
Carbon	6.0	-2.3109116018	4.5623415723	-3.7019377059
Carbon	6.0	-2.2524213606	3.4067042322	-1.4946658684
Carbon	6.0	-3.2724844064	5.4760874842	-3.2147872854
Carbon	6.0	-3.2233183108	4.3402339806	-1.0247287271
Carbon	6.0	-3.7228801528	5.3580601890	-1.8756009820
Hydrogen	1.0	-1.9443897850	4.6354284771	-4.7415753179
Hydrogen	1.0	-3.6665741124	6.2724047539	-3.8702796806
Hydrogen	1.0	-3.5996893001	4.2859716506	0.0068194553
Hydrogen	1.0	-4.4743320111	6.0651234963	-1.4808155444

Table S2 (continued)

7-2	Ground state			
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Hydrogen	1.0	3.5438202570	-3.0518054392	-2.3194882588
Carbon	6.0	2.8623212287	-2.2057206173	-2.5351191795
Hydrogen	1.0	3.4540561674	-1.3412479008	-2.9054948319
Hydrogen	1.0	2.1638760327	-2.4981045256	-3.3490970378
Carbon	6.0	2.0528060978	-1.7788061591	-1.3113980481
Oxygen	8.0	1.2663650130	-0.7775962385	-1.4999803526
Carbon	6.0	2.2184191904	-2.4972833077	-0.0875187097
Hydrogen	1.0	2.9366977580	-3.3317877455	-0.0932433105
Carbon	6.0	1.5480789735	-2.2420669135	1.1434348210
Oxygen	8.0	0.6662276640	-1.3247754200	1.3747661032
Carbon	6.0	1.8618083252	-3.1097118038	2.3600871339
Hydrogen	1.0	2.5847050248	-3.9151634926	2.1252136115
Hydrogen	1.0	2.2741083336	-2.4691776785	3.1690123655
Hydrogen	1.0	0.9196265060	-3.5558621476	2.7435359464
Carbon	6.0	-0.9994890830	2.5098172776	-3.4032229444
Carbon	6.0	-0.4415222077	1.5167598082	-2.5375133637
Hydrogen	1.0	0.3123210062	0.8031122517	-2.9090012484
Nitrogen	7.0	-0.7831617894	1.3928482868	-1.2563114202
Carbon	6.0	-1.7369139919	2.2621081170	-0.6902108572
Carbon	6.0	-1.9659123379	1.9425255793	0.7104252030
Sulfur	16.0	-3.0561208395	2.7142446617	1.8529076710
Carbon	6.0	-2.5478084076	1.5987646058	3.1027771537
Carbon	6.0	-1.5931710126	0.6857237804	2.6596136804
Carbon	6.0	-1.2426480488	0.8724119515	1.2695495482
Hydrogen	1.0	-1.1542664631	-0.0950653640	3.3006882891
Hydrogen	1.0	-2.9888088083	1.6803233479	4.1091589104
Carbon	6.0	-1.9771315632	3.4231905035	-2.8469301669
Carbon	6.0	-2.3275280193	3.2685412986	-1.4675112640
Hydrogen	1.0	-3.0681098449	3.9435057374	-1.0078992951
Carbon	6.0	-2.5411103629	4.4314700248	-3.7079404348
Carbon	6.0	-0.6106530156	2.6132159546	-4.7838855041
Carbon	6.0	-2.1463290461	4.5135039669	-5.0473149030
Carbon	6.0	-1.1765256520	3.6011022950	-5.5945889261
Hydrogen	1.0	-3.2869390032	5.1344414537	-3.2969144088
Hydrogen	1.0	0.1355457541	1.9052173463	-5.1857742512
Hydrogen	1.0	-2.5844861068	5.2905704162	-5.6992358538
Hydrogen	1.0	-0.8829815633	3.6870741920	-6.6555611089

Table S2 (continued)

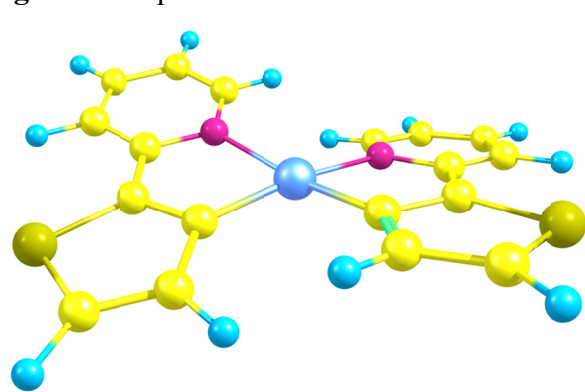
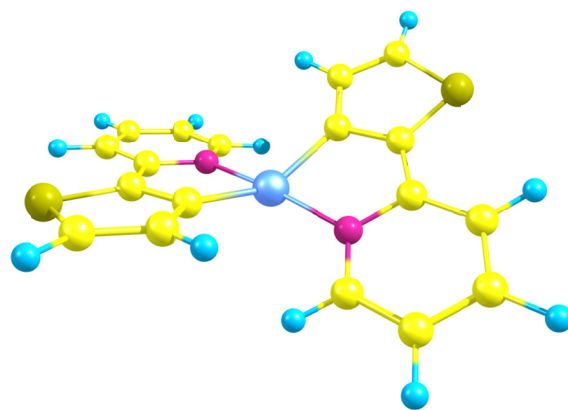
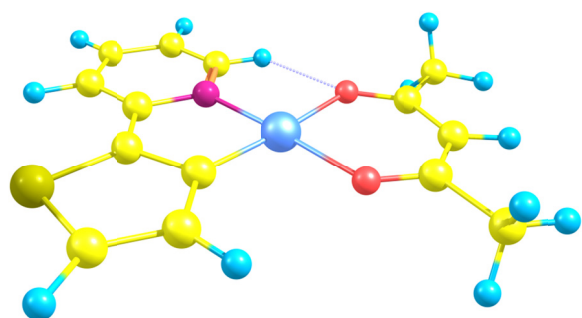
7-2	Lowest triplet state			
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Hydrogen	1.0	3.5237785582	-3.0394173303	-2.3631567659
Carbon	6.0	2.8445513034	-2.1880153131	-2.5641880201
Hydrogen	1.0	3.4370740201	-1.3213764648	-2.9281102802
Hydrogen	1.0	2.1388713543	-2.4668113390	-3.3766033931
Carbon	6.0	2.0452266975	-1.7722578618	-1.3308409152
Oxygen	8.0	1.2569691835	-0.7688288586	-1.5062068183
Carbon	6.0	2.2186841426	-2.4992880927	-0.1137588702
Hydrogen	1.0	2.9367688685	-3.3337176981	-0.1295574648
Carbon	6.0	1.5553082067	-2.2519710972	1.1228088285
Oxygen	8.0	0.6747526814	-1.3366637636	1.3653262531
Carbon	6.0	1.8756528148	-3.1275898800	2.3317902754
Hydrogen	1.0	2.6004177205	-3.9290065054	2.0891757822
Hydrogen	1.0	2.2877781585	-2.4913252387	3.1440982175
Hydrogen	1.0	0.9359680254	-3.5796637317	2.7143982818
Carbon	6.0	-1.0130801016	2.5287540282	-3.4116693447
Carbon	6.0	-0.4439223036	1.5212556391	-2.5276852111
Hydrogen	1.0	0.3119673171	0.8148282690	-2.9082305656
Nitrogen	7.0	-0.7816398092	1.3947793984	-1.2589400467
Carbon	6.0	-1.7446040517	2.2638980489	-0.6834232643
Carbon	6.0	-1.9774614359	1.9666466006	0.6683197577
Sulfur	16.0	-3.0783289805	2.7509895314	1.8044998396
Carbon	6.0	-2.5558522088	1.6072843946	3.0833902502
Carbon	6.0	-1.5841376521	0.6799621037	2.6358156435
Carbon	6.0	-1.2206852116	0.8399436977	1.2812433462
Hydrogen	1.0	-1.1561973150	-0.0941566754	3.2928552585
Hydrogen	1.0	-3.0003518860	1.6916822846	4.0876950125
Carbon	6.0	-1.9999968922	3.4474355358	-2.8608234576
Carbon	6.0	-2.3561587010	3.3026847959	-1.4908643248
Hydrogen	1.0	-3.0974376939	3.9746196502	-1.0288685569
Carbon	6.0	-2.5565968536	4.4479948984	-3.7390875729
Carbon	6.0	-0.6197565208	2.6196009813	-4.7717995290
Carbon	6.0	-2.1499206756	4.5195052744	-5.0843052453
Carbon	6.0	-1.1833925885	3.6110036362	-5.6136314631
Hydrogen	1.0	-3.3061492055	5.1542918051	-3.3408327788
Hydrogen	1.0	0.1301332533	1.9100311673	-5.1648714474
Hydrogen	1.0	-2.5863996056	5.2924390906	-5.7426592892
Hydrogen	1.0	-0.8772364199	3.6819015656	-6.6717653723

Table S2 (continued)

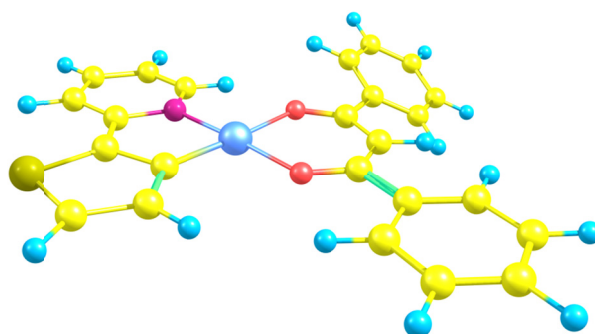
7-3	Ground state				
	Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
	Hydrogen	1.0	3.6561844699	-3.3517651235	-1.7504903735
	Carbon	6.0	2.9966382392	-2.5306122814	-2.0932826557
	Hydrogen	1.0	3.6155226927	-1.7011596703	-2.4966951843
	Hydrogen	1.0	2.3562058623	-2.8978082792	-2.9240131842
	Carbon	6.0	2.1055728841	-1.9979106532	-0.9721538197
	Oxygen	8.0	1.3592454196	-1.0014649133	-1.2920627988
	Carbon	6.0	2.1525856048	-2.6227825122	0.3096750193
	Hydrogen	1.0	2.8451868410	-3.4681892757	0.4412179162
	Carbon	6.0	1.3702251409	-2.2376494669	1.4314227013
	Oxygen	8.0	0.5077277919	-1.2746381885	1.4802838119
	Carbon	6.0	1.5105563258	-2.9992601203	2.7473708545
	Hydrogen	1.0	2.2911216425	-3.7831535991	2.6952678224
	Hydrogen	1.0	1.7564110652	-2.2835573739	3.5604877786
	Hydrogen	1.0	0.5363631691	-3.4675235436	3.0055910982
	Carbon	6.0	-1.0402926230	2.8557601587	-3.3617208508
	Nitrogen	7.0	-0.7444574619	1.5030160479	-1.3034516415
	Carbon	6.0	-1.6747477152	2.3030884675	-0.6938340595
	Carbon	6.0	-1.9461161351	1.9638499354	0.6851508405
	Sulfur	16.0	-3.0530137227	2.7304563162	1.8211849738
	Carbon	6.0	-2.5749838575	1.5891082227	3.0564697163
	Carbon	6.0	-1.6202381032	0.6731444894	2.6179513754
	Carbon	6.0	-1.2469986476	0.8830144366	1.2373528497
	Hydrogen	1.0	-1.2005545648	-0.1198698720	3.2555919538
	Hydrogen	1.0	-3.0323180651	1.6566049106	4.0566443736
	Carbon	6.0	-2.0159971380	3.6667166065	-2.6871097334
	Carbon	6.0	-2.3284103513	3.3928407506	-1.3680615448
	Hydrogen	1.0	-2.5033491023	4.4975886451	-3.2279474364
	Hydrogen	1.0	-3.0681801817	3.9885962514	-0.8099735846
	Carbon	6.0	-0.4145574221	1.7662042677	-2.6338364176
	Carbon	6.0	0.5546555223	0.9701655443	-3.3296012704
	Carbon	6.0	0.8808206886	1.2489688853	-4.6650971122
	Carbon	6.0	-0.6863805662	3.1136447366	-4.7290670295
	Carbon	6.0	0.2649349535	2.3238411801	-5.3809372115
	Hydrogen	1.0	1.0379327329	0.1364925092	-2.8064638371
	Hydrogen	1.0	1.6322553965	0.6168277404	-5.1720106206
	Hydrogen	1.0	-1.1850460436	3.9511352212	-5.2493005855
	Hydrogen	1.0	0.5373354190	2.5237446188	-6.4321998192

Table S2 (continued)

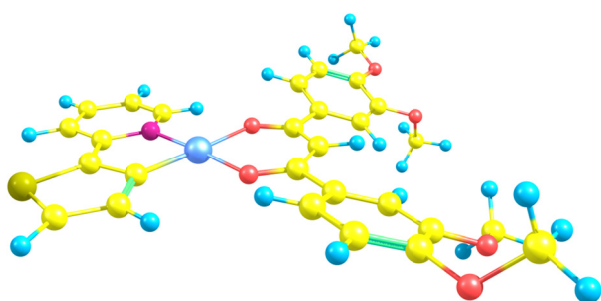
7-3	Lowest triplet state			
Platinum	78.0	0.0000000000	0.0000000000	0.0000000000
Hydrogen	1.0	3.6439368813	-3.3557081698	-1.7810698553
Carbon	6.0	2.9839257378	-2.5315185175	-2.1153088125
Hydrogen	1.0	3.6012463455	-1.7013159948	-2.5193758438
Hydrogen	1.0	2.3359967950	-2.8925281355	-2.9427868052
Carbon	6.0	2.1026325260	-2.0017549997	-0.9856074715
Oxygen	8.0	1.3528495105	-1.0049984205	-1.2997133549
Carbon	6.0	2.1626706180	-2.6288031980	0.2936686225
Hydrogen	1.0	2.8576368579	-3.4733480099	0.4168631525
Carbon	6.0	1.3891821038	-2.2470911106	1.4239426943
Oxygen	8.0	0.5269738973	-1.2866838452	1.4827276554
Carbon	6.0	1.5434710058	-3.0140955222	2.7352222380
Hydrogen	1.0	2.3309345513	-3.7903125950	2.6749878380
Hydrogen	1.0	1.7861632536	-2.3000329416	3.5506424841
Hydrogen	1.0	0.5747080264	-3.4927790620	2.9949326098
Carbon	6.0	-1.0310567072	2.8429231555	-3.3584304698
Nitrogen	7.0	-0.7177514877	1.4722218963	-1.3038055302
Carbon	6.0	-1.6945633103	2.3174050673	-0.6856214482
Carbon	6.0	-1.9539440071	1.9852971015	0.6593744242
Sulfur	16.0	-3.0590930100	2.7408522740	1.8023144260
Carbon	6.0	-2.5524852182	1.5673997267	3.0605716590
Carbon	6.0	-1.5891533476	0.6558711922	2.6043353927
Carbon	6.0	-1.2210167692	0.8569545689	1.2428660730
Hydrogen	1.0	-1.1633151847	-0.1369192316	3.2383197592
Hydrogen	1.0	-3.0081921860	1.6325820831	4.0612874239
Carbon	6.0	-2.0269069895	3.6703146212	-2.6935894769
Carbon	6.0	-2.3398295428	3.3978541462	-1.3785584247
Hydrogen	1.0	-2.5092857926	4.4940423678	-3.2465179763
Hydrogen	1.0	-3.0840445083	3.9954214099	-0.8258714586
Carbon	6.0	-0.3952617302	1.7472146001	-2.6302338609
Carbon	6.0	0.5787131115	0.9606436012	-3.3334284604
Carbon	6.0	0.9115359440	1.2395782430	-4.6729021814
Carbon	6.0	-0.6728706407	3.0954459697	-4.7124318419
Carbon	6.0	0.2913183996	2.3082976847	-5.3765828416
Hydrogen	1.0	1.0652317262	0.1275269913	-2.8137365029
Hydrogen	1.0	1.6668362978	0.6106730020	-5.1775448297
Hydrogen	1.0	-1.1718531763	3.9305438758	-5.2361083666
Hydrogen	1.0	0.5575924040	2.5200566882	-6.4272803249

Figure S1. Optimized structures of the lowest triplet states.*cis-1**trans-1*

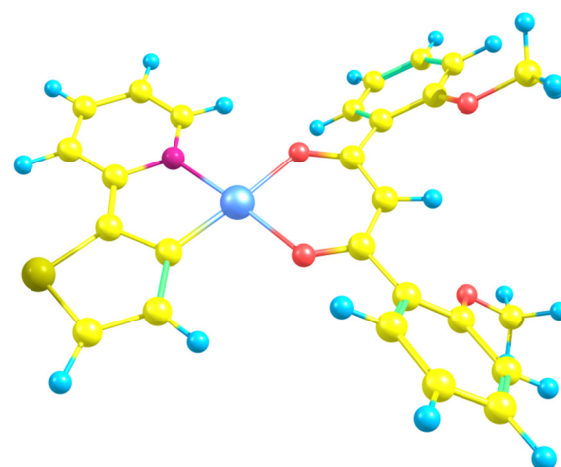
2



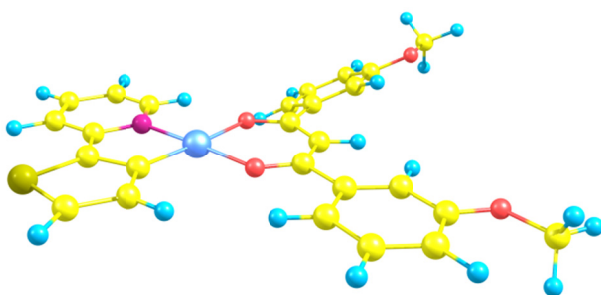
3



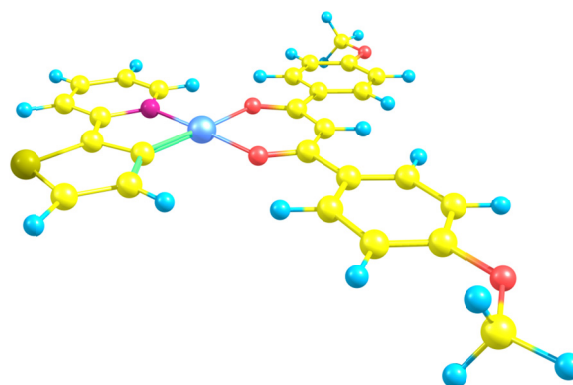
4



5-1

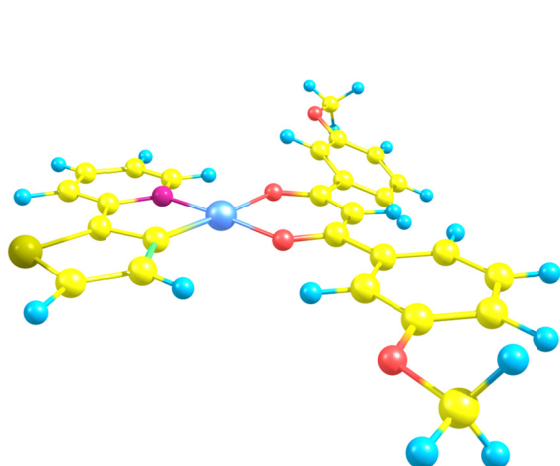


5-2

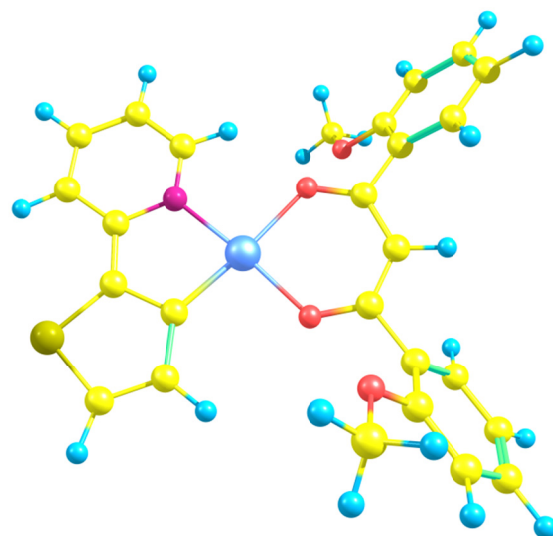


5-3

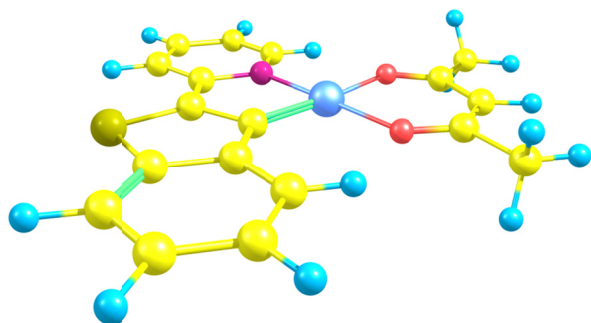
Figure S1 (continued)



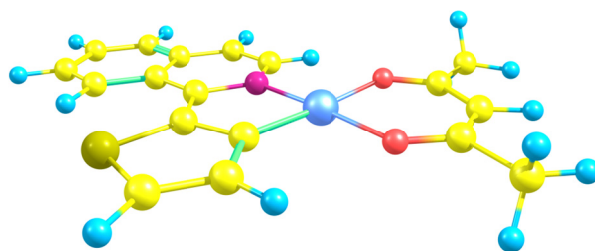
5-4



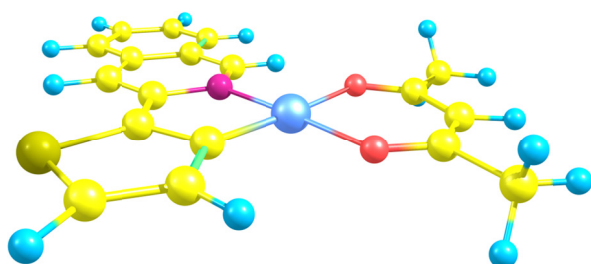
5-5



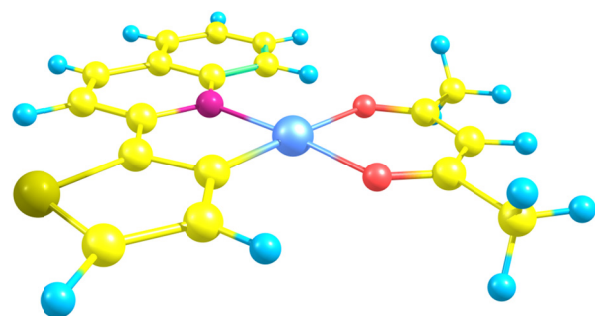
6



7-1



7-2



7-3

Figure S2. Transition-state geometries for the rotation of a *bmp* ligand in **5-2** and **5-3**.

