Structural and electronic properties of luminescent copper(I) halide complexes of bis[2-(diphenylphosphano)phenyl] ether (DPEphos). Crystal structure of [CuCl(DPEphos)(dmpymtH]

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Table S1. Selected structural parameters of complexes **1-9** in their S_0 and T_1 states calculated at the PEB0/Def2-TZVP level of theory.[a]

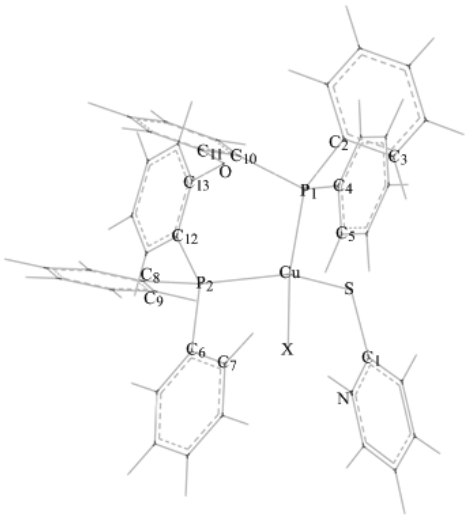
Parameter	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
R_e(Cu-X)	2.390 (2.312)	2.514 (2.427)	2.702 (2.606)	2.392 (2.280)	2.520 (2.408)	2.707 (2.591)	2.416 (2.377)	2.517 (2.405)	2.697 (2.589)
R_e(Cu-S)	2.383 (2.252)	2.384 (2.260)	2.391 (2.269)	2.376 (2.264)	2.382 (2.267)	2.388 (2.273)	2.371 (2.290)	2.378 (2.267)	2.382 (2.271)
R_e(Cu-P1)	2.306 (2.405)	2.312 (2.428)	2.331 (2.444)	2.295 (2.429)	2.310 (2.442)	2.329 (2.458)	2.364 (2.424)	2.314 (2.444)	2.330 (2.458)
R_e(Cu-P2)	2.354 (2.329)	2.360 (2.331)	2.362 (2.338)	2.357 (2.342)	2.360 (2.343)	2.363 (2.347)	2.317 (2.356)	2.362 (2.347)	2.369 (2.347)
R_e(S-C1)	1.697 (1.745)	1.696 (1.746)	1.695 (1.744)	1.688 (1.767)	1.687 (1.766)	1.686 (1.764)	1.697 (1.816)	1.693 (1.767)	1.691 (1.764)
R_e(C1-N)	1.360 (1.389)	1.360 (1.389)	1.360 (1.390)	1.371 (1.376)	1.371 (1.376)	1.371 (1.376)	1.371 (1.377)	1.369 (1.374)	1.369 (1.375)
R_e(P1-C2)	1.834 (1.834)	1.836 (1.834)	1.837 (1.833)	1.836 (1.830)	1.835 (1.831)	1.836 (1.832)	1.834 (1.861)	1.836 (1.831)	1.836 (1.831)
R_e(P1-C4)	1.837 (1.832)	1.837 (1.833)	1.838 (1.834)	1.836 (1.831)	1.837 (1.832)	1.838 (1.833)	1.836 (1.865)	1.837 (1.832)	1.838 (1.833)
R_e(P2-C6)	1.834 (1.823)	1.833 (1.824)	1.833 (1.824)	1.833 (1.820)	1.833 (1.820)	1.833 (1.821)	1.843 (1.863)	1.834 (1.820)	1.833 (1.821)
R_e(P2-C8)	1.844 (1.834)	1.840 (1.834)	1.838 (1.835)	1.840 (1.837)	1.839 (1.837)	1.838 (1.837)	1.837 (1.867)	1.839 (1.837)	1.839 (1.837)
<(X-Cu-S)	111.8 (121.1)	114.0 (124.0)	115.9 (126.0)	111.8 (127.5)	113.6 (128.0)	115.7 (129.2)	111.0 (118.1)	113.8 (129.2)	115.9 (130.2)
<(S-Cu-P1)	111.0 (108.5)	110.3 (103.9)	107.1 (100.5)	112.9 (106.2)	110.9 (104.5)	107.6 (102.3)	111.8 (112.7)	110.0 (103.1)	107.6 (100.6)
<(P1-Cu-P2)	112.7 (112.5)	112.6 (113.3)	113.0 (114.1)	112.8 (117.8)	113.1 (116.5)	113.3 (116.1)	113.0 (116.0)	112.8 (116.9)	112.9 (116.7)
<(P2-Cu-X)	98.3 (96.9)	98.6 (99.8)	99.9 (101.1)	97.3 (100.5)	98.5 (101.4)	99.8 (102.1)	99.2 (102.3)	98.9 (100.8)	99.6 (101.8)
<(Cu-P1-C10)	109.4 (110.1)	108.6 (110.0)	108.5 (110.1)	109.2 (106.6)	108.6 (107.7)	108.5 (108.2)	109.5 (110.7)	109.2 (107.3)	108.7 (108.0)
<(Cu-P2-C12)	119.0 (116.8)	119.3 (116.1)	117.9 (115.2)	119.7 (116.1)	119.6 (116.4)	118.5 (116.4)	118.0 (116.2)	118.5 (116.2)	118.4 (116.1)
<(Cu-S-C1-N)	4.7 (20.4)	5.9 (24.6)	3.8 (31.0)	7.6 (15.8)	7.4 (18.7)	4.9 (22.9)	7.1 (18.0)	3.5 (14.7)	2.7 (19.6)
<(Cu-P1-C2-C3)	48.2 (50.1)	48.4 (53.6)	52.2 (55.9)	45.6 (49.5)	48.3 (50.9)	51.7 (51.9)	52.9 (45.9)	47.8 (51.8)	50.3 (53.7)
<(Cu-P1-C4-C5)	15.1 (15.9)	15.7 (18.6)	17.3 (22.9)	15.2 (16.3)	16.2 (19.0)	18.0 (24.4)	17.7 (24.0)	17.4 (19.6)	19.2 (24.1)
<(Cu-P2-C6-C7)	62.0 (68.5)	70.8 (67.0)	67.8 (67.8)	73.1 (76.4)	73.5 (76.2)	70.9 (74.7)	65.6 (66.2)	69.2 (75.1)	69.8 (75.3)
<(Cu-P2-C8-C9)	20.2 (21.2)	9.4 (20.8)	9.2 (18.6)	13.9 (20.2)	6.6 (16.1)	6.1 (11.1)	38.5 (33.8)	13.1 (15.3)	6.6 (10.6)
<(P1-C12-C13-O)	9.7 (7.8)	10.4 (7.6)	10.2 (7.3)	10.0 (7.2)	10.4 (7.0)	10.1 (7.0)	9.4 (47.9)	9.6 (7.0)	9.9 (7.0)

[a] Numbers in parenthesis refer to the T_1 state.

Table S2 Differences between selected structural parameters of S_0 and T_1 states of complexes **1-9** calculated at the PEB1PBE/Def2-TZVP level of theory.[a]

Parameter	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
ΔR_e(Cu-X)	-0.078	-0.087	-0.096	-0.112	-0.112	-0.116	-0.146	-0.112	-0.078
ΔR_e(Cu-S)	-0.131	-0.124	-0.122	-0.112	-0.115	-0.115	-0.138	-0.111	-0.131
ΔR_e(Cu-P1)	0.099	0.116	0.113	0.134	0.132	0.129	0.090	0.130	0.099
ΔR_e(Cu-P2)	-0.025	-0.029	-0.024	-0.015	-0.017	-0.016	-0.017	-0.015	-0.025
ΔR_e(S-C1)	0.048	0.050	0.049	0.079	0.079	0.078	0.079	0.074	0.048
ΔR_e(C1-N)	0.029	0.029	0.030	0.005	0.005	0.005	0.004	0.005	0.029
ΔR_e(P1-C2)	0.000	-0.002	-0.004	-0.006	-0.004	-0.004	-0.005	-0.005	0.000
ΔR_e(P1-C4)	-0.005	-0.004	-0.004	-0.005	-0.005	-0.005	-0.006	-0.005	-0.005
ΔR_e(P2-C6)	-0.011	-0.009	-0.009	-0.013	-0.013	-0.012	-0.010	-0.014	-0.011
ΔR_e(P2-C8)	-0.010	-0.006	-0.003	-0.003	-0.002	-0.001	-0.003	-0.002	-0.010
Δ<(X-Cu-S)	9.3	10.0	10.1	15.7	14.4	13.5	10.3	15.4	9.3
Δ<(S-Cu-P1)	-2.5	-6.4	-6.6	-6.7	-6.4	-5.3	0.4	-6.9	-2.5
Δ<(P1-Cu-P2)	-0.2	0.7	1.1	5.0	3.4	2.8	0.7	4.1	-0.2
Δ<(P2-Cu-X)	-1.4	1.2	1.2	3.2	2.9	2.3	3.4	1.9	-1.4
Δ<(Cu-P1-C10)	0.7	1.4	1.6	-2.6	-0.9	-0.3	0.8	-1.9	0.7
Δ<(Cu-P2-C12)	-2.2	-3.2	-2.7	-3.6	-3.2	-2.1	-0.6	-2.3	-2.2
Δ<(Cu-S-C1-N)	4.7	20.4	5.9	24.6	3.8	31.0	7.6	15.8	7.4
Δ<(Cu-P1-C2-C3)	48.2	50.1	48.4	53.6	52.2	55.9	45.6	49.5	48.3
Δ<(Cu-P1-C4-C5)	15.1	15.9	15.7	18.6	17.3	22.9	15.2	16.3	16.2
Δ<(Cu-P2-C6-C7)	62.0	68.5	70.8	67.0	67.8	67.8	73.1	76.4	73.5
Δ<(Cu-P2-C8-C9)	20.2	21.2	9.4	20.8	9.2	18.6	13.9	20.2	6.6
Δ<(P1-C12-C13-O)	9.7	7.8	10.4	7.6	10.2	7.3	10.0	7.2	10.4

[a] The minus sign indicates a shortening of the corresponding bond length upon going from the S_0 to T_1 state while for the bond angles indicates that they become more acute.



Numbering Scheme

Table S3 Principal singlet-singlet optical transitions ($f > 0.01$) for the absorptions of **1**, calculated in the gas phase using the PBE/Def2-TZVP method.

Excitation (% composition)	E (eV)	λ (nm)	OS, f	μ	% CT
H→L (85.0%), H-1→L (10.0%)	2.983	415.6	0.032	0.670	14
H→L+1 (94%)	3.477	356.6	0.019	0.265	14
H→L+2 (30%), H→L+3 (56%)	3.688	336.2	0.029	0.047	13
H→L+4 (78%)	3.779	328.1	0.058	0.466	11
H-3→L (19%), H→L+2 (25%), H→L+3 (11%), H→L+5 (11%)	3.807	325.7	0.081	0.171	9
H→L+5 (73%)	3.874	320.1	0.043	0.562	11
H-1→L+2 (31%), H-1→L+3 (54%)	3.970	312.3	0.035	0.249	14
H-1→L+5 (18%), H→L+6 (72%)	4.062	305.3	0.013	0.792	13
H→L+7 (84%)	4.128	300.3	0.065	0.930	12
H-3→L+1 (14%), H-2→L+4 (26%), H→L+9 (35%)	4.318	287.1	0.018	0.292	10
H-3→L+1 (51%), H→L+10 (23%)	4.332	286.2	0.016	0.673	9
H-3→L+1 (13%), H→L+10 (60%)	4.345	285.4	0.025	0.600	11
H-2→L+5 (28%), H-1→L+6 (51%)	4.360	284.4	0.015	0.268	13
H-1→L+7 (74%)	4.392	282.3	0.015	0.115	12
H-6→L (24%), H-5→L (15%), H-2→L+5 (28%), H-1→L+7 (11%)	4.410	281.2	0.016	0.358	7

Table S4 Principal singlet-singlet optical transitions ($f > 0.01$) for the absorptions of **2**, calculated in the gas phase using the PBE/Def2-TZVP method.

Excitation (% composition)	E (eV)	λ (nm)	OS, f	μ	% CT
H-1→L (19%), H→L (75%)	2.951	420.2	0.018	0.504	16
H-1→L (70%), H→L (20%)	3.060	405.2	0.011	0.388	17
H→L+1 (94%)	3.445	359.9	0.016	0.428	16
H→L+2 (39%), H→L+3 (40%)	3.692	335.9	0.035	0.621	13
H→L+3 (10%), H→L+4 (10%)	3.767	329.2	0.048	0.721	3
H→L+3 (15%), H→L+4 (61%), H→L+5 (12%)	3.783	327.8	0.053	0.759	15
H-1→L+1 (12%), H-1→L+2 (25%), H-1→L+3 (24%), H→L+2 (13%)	3.840	322.9	0.018	0.439	14
H→L+4 (17%), H→L+5 (60%)	3.885	319.2	0.029	0.553	13
H-1→L+2 (29%), H-1→L+3 (53%)	3.954	313.6	0.039	0.636	16
H-2→L+1 (73%), H-1→L+4 (14%)	4.004	309.7	0.004	0.396	18
H-1→L+5 (25%), H→L+6 (41%), H→L+7 (22%)	4.099	302.4	0.014	0.368	15
H→L+6 (20%), H→L+7 (64%)	4.108	301.8	0.051	0.710	14
H-2→L+3 (86%)	4.200	295.2	0.010	0.318	16
H-5→L (16%), H-3→L+1 (72%)	4.273	290.1	0.022	0.453	10
H→L+9 (52%), H→L+10 (-30%)	4.314	287.4	0.010	0.133	14
H-2→L+5 (-20%), H-1→L+6 (40%), H-1→L+7 (32%)	4.350	285.0	0.020	0.309	18
H-2→L+5 (12%), H-1→L+6 (20%), H-1→L+7 (57%)	4.367	283.9	0.019	0.199	18
H-2→L+5 (55%), H-1→L+6 (32%)	4.373	283.5	0.010	0.432	17
H-3→L+2 (18%), H-1→L+8 (70%)	4.450	278.7	0.030	0.418	16

Table S5 Singlet-singlet optical transitions ($f > 0.01$) for the absorptions of **3**, calculated in the gas phase using the PBE/Def2-TZVP method.

Excitation (% composition)	E (eV)	λ (nm)	OS, f	μ	% *CT*
H→L (76%), H-1→L (17%)	2.864	432.9	0.010	0.360	13
H-1→L (68%), H→L (20%)	2.987	415.1	0.010	0.348	14
H-3→L (18%), H→L+1 (76%)	3.436	360.8	0.019	0.533	13
H-3→L (69%), H→L+1 (19%)	3.452	359.2	0.024	0.359	10
H-4→L (11%), H-1→L+1 (15%), H-1→L+2 (17%), H→L+2 (41%)	3.623	342.2	0.012	0.451	12
H→L+3 (80%)	3.677	337.2	0.018	0.568	11
H-1→L+1 (59%), H→L+2 (30%)	3.690	336.1	0.029	0.359	14
H-4→L (11%), H→L+4 (65%)	3.768	329.1	0.012	0.493	11
H-4→L (14%), H-1→L+1 (14%), H-1→L+2 (19%), H→L+2 (12%), H→L+4 (12%)	3.774	328.5	0.023	0.354	11
H-1→L+3 (28%), H→L+5 (49%)	3.874	320.0	0.012	0.399	11
H-2→L+1 (67%), H-1→L+2 (10%)	3.893	318.5	0.015	0.461	10
H-2→L+1 (19%), H-1→L+3 (43%), H→L+5 (27%)	3.916	316.6	0.020	0.393	13
H-5→L (64%), H-1→L+4 (13%)	3.969	312.4	0.015	0.421	6
H-2→L+2 (52%), H-1→L+5 (24%)	4.016	308.8	0.018	0.345	10
H-2→L+2 (20%), H-1→L+5 (57%)	4.038	307.1	0.012	0.508	12
H→L+7 (73%)	4.079	303.9	0.026	0.458	10
H→L+6 (73%)	4.090	303.2	0.021	0.639	10
H-3→L+1 (86%)	4.139	299.5	0.041	0.453	10
H-3→L+2 (11%), H-2→L+5 (50%), H→L+9 (12%)	4.271	290.3	0.022	0.637	9
H-3→L+2 (30%), H-2→L+5 (31%), H→L+9 (19%)	4.286	289.3	0.043	0.410	10
H-1→L+7 (57%), H→L+10 (22%)	4.300	288.4	0.018	0.443	12
H-1→L+6 (44%), H-1→L+7 (14%), H→L+10 (27%)	4.310	287.6	0.021	0.335	13
H-1→L+6 (39%), H-1→L+7 (12%), H→L+10 (27%)	4.322	286.9	0.012	0.622	12
H-3→L+2 (29%), H-3→L+3 (19%), H→L+9 (28%)	4.335	286.0	0.041	0.533	9

Table S6 Principal singlet-singlet optical transitions ($f > 0.01$) for the absorptions of **4**, calculated in the gas phase using the PBE/Def2-TZVP method.

Excitation (% composition)	E (eV)	λ (nm)	OS, f	μ	% CT
H→L (91%)	2.732	453.9	0.010	0.382	17
H-3→L (15%), H→L+1 (72%)	3.400	364.7	0.024	0.534	15
H-3→L (20%), H→L+2 (53%)	3.613	343.2	0.068	0.873	12
H→L+3 (91%)	3.722	333.1	0.042	0.680	16
H-1→L+1 (28%), H-1→L+2 (57%)	3.809	325.5	0.005	0.219	17
H→L+4 (75%), H→L+5 (13%)	3.815	325.0	0.028	0.549	16
H-1→L+3 (82%)	4.016	308.7	0.041	0.648	17
H-2→L+2 (13%), H-1→L+4 (70%)	4.073	304.4	0.015	0.387	18
H-2→L+2 (18%), H-1→L+5 (16%), H→L+6 (56%)	4.103	302.2	0.014	0.378	18
H→L+7 (75%)	4.123	300.7	0.052	0.716	13
H-6→L (20%), H-1→L+5 (36%)	4.154	298.5	0.017	0.405	9
H-2→L+3 (86%)	4.244	292.2	0.014	0.372	21
H-21→L (14%), H-15→L (11%), H-14→L (11%), H-6→L (14%), H-3→L+1 (20%)	4.316	287.2	0.047	0.665	5
H-3→L+1 (15%), H→L+9 (26%), H→L+10 (26%)	4.368	283.8	0.021	0.439	11
H-3→L+1 (26%), H-1→L+6 (25%), H→L+9 (23%)	4.386	282.7	0.059	0.738	13
H-2→L+5 (44%), H-1→L+6 (24%), H-1→L+7 (15%)	4.412	281.0	0.023	0.458	19

Table S7 Principal singlet-singlet optical transitions ($f > 0.01$) for the absorptions of **5**, calculated in the gas phase using the PBE/Def2-TZVP method.

Excitation (% composition)	E (eV)	λ (nm)	OS, f	μ	% CT
H→L (88%)	2.719	456.0	0.010	0.336	15
H-3→L (37%), H→L+1 (48%)	3.389	365.9	0.013	0.400	12
H-3→L (45%), H-1→L+1 (21%), H→L+1 (15%)	3.452	359.2	0.012	0.370	12
H-1→L+1 (18%), H→L+2 (57%)	3.602	344.2	0.055	0.786	13
H→L+3 (88%)	3.751	330.5	0.042	0.675	15
H→L+4 (81%)	3.834	323.4	0.028	0.542	14
H→L+5 (73%)	3.940	314.6	0.011	0.333	13
H-1→L+3 (79%)	4.015	308.8	0.043	0.659	15
H-2→L+2 (43%), H-1→L+4 (-43%)	4.067	304.8	0.013	0.366	17
H-1→L+5 (56%), H→L+6 (28%)	4.122	300.8	0.017	0.406	16
H→L+7 (80%)	4.133	300.0	0.044	0.658	13
H-1→L+5 (31%), H→L+6 (60%)	4.164	297.7	0.014	0.371	16
H-2→L+3 (89%)	4.236	292.7	0.014	0.365	19
H→L+8 (77%)	4.284	289.4	0.013	0.356	13
H-22→L (12%), H-3→L+1 (42%)	4.300	288.3	0.067	0.795	5
H-22→L (19%), H-9→L (18%), H-3→L+1 (25%)	4.311	287.6	0.036	0.584	4
H-1→L+7 (83%)	4.392	282.3	0.018	0.403	16
H-2→L+5 (54%), H-1→L+6 (28%)	4.412	281.0	0.017	0.396	16

Table S8 Principal singlet-singlet optical transitions (f > 0.01) for the absorptions of **6**, calculated in the gas phase using the PBE/Def2-TZVP method.

Excitation (% composition)	E (eV)	λ (nm)	OS, f	μ	% CT
H→L (89%)	2.630	471.5	0.004	0.253	13
H-1→L+1 (19%), H→L+1 (59%)	3.334	371.9	0.017	0.459	12
H-4→L (12%), H-1→L+1 (-30%), H→L+1 (31%), H→L+2 (13%)	3.454	358.9	0.012	0.373	13
H→L+2 (78%)	3.537	350.6	0.021	0.488	12
H-5→L (13%), H→L+3 (71%)	3.728	332.6	0.019	0.450	11
H-5→L (71%), H→L+3 (13%)	3.731	332.3	0.017	0.433	7
H→L+4 (82%)	3.823	324.3	0.023	0.494	12
H-1→L+3 (32%), H→L+5 (48%)	3.935	315.1	0.019	0.444	20
H-2→L+2 (23%), H-1→L+3 (43%), H→L+5 (25%)	3.972	312.1	0.021	0.462	14
H-2→L+2 (64%), H-1→L+3 (10%), H→L+5 (13%)	3.983	311.3	0.014	0.381	13
H-3→L+1 (73%)	4.067	304.8	0.067	0.822	9
H-1→L+5 (78%)	4.097	302.6	0.027	0.517	13
H→L+7 (77%)	4.106	302.0	0.040	0.633	11
H-2→L+3 (89%)	4.145	299.1	0.002	0.361	13
H-8→L (13%), H-4→L+1 (45%), H-3→L+2 (11%)	4.239	292.5	0.014	0.327	9
H-3→L+2 (59%)	4.273	290.2	0.011	0.337	7
H-22→L (-21%), H-8→L (19%), H-4→L+1 (34%)	4.290	289.0	0.012	0.367	9
H-2→L+5 (62%), H-1→L+7 (19%)	4.348	285.2	0.014	0.459	12

Table S9 Principal singlet-singlet optical transitions ($f > 0.01$) for the absorptions of **7**, calculated in the gas phase using the PBE/Def2-TZVP method.

Excitation (% composition)	E (eV)	λ (nm)	OS, f	μ	% CT
H→L (90%)	2.895	428.3	0.022	0.554	16
H→L+1 (71%)	3.774	328.5	0.079	0.922	13
H→L+2 (77%)	3.878	319.7	0.083	0.936	14
H→L+3 (90%)	3.963	312.9	0.014	0.380	16
H→L+4 (89%)	4.085	303.5	0.029	0.541	16
H→L+5 (59%), H-1→L+3 (32%)	4.178	296.8	0.032	0.556	17
H-1→L+3 (58%), H→L+5 (31%)	4.219	293.9	0.031	0.549	17
H→L+6 (79%)	4.335	286.0	0.018	0.411	14
H→L+7 (80%)	4.367	283.9	0.030	0.526	14
H-2→L+3 (74%)	4.392	282.3	0.021	0.440	19
H-1→L+5 (70%)	4.418	280.6	0.030	0.522	13
H-3→L+1 (48%), H→L+8 (21%)	4.482	276.6	0.111	1.003	10
H→L+8 (61%)	4.496	275.7	0.038	0.588	11
H-1→L+6 (46%), H→L+9 (19%)	4.563	271.7	0.011	0.316	12
H-8→L (31%), H-3→L+2 (20%), H-11→L (18%),	4.645	266.9	0.028	0.491	9
H-3→L+2 (63%)	4.689	264.4	0.022	0.435	8

Table S10 Principal singlet-singlet optical transitions ($f > 0.01$) for the absorptions of **8**, calculated in the gas phase using the PBE/Def2-TZVP method.

Excitation (% composition)	E (eV)	λ (nm)	OS, f	μ	% CT
H→L (82%)	2.905	426.8	0.010	0.342	15
H-1→L (76%)	3.056	405.8	0.010	0.350	16
H→L+1 (93%)	3.447	359.7	0.018	0.456	17
H-3→L (27%), H-1→L+1 (19%), H-1→L+2 (30%)	3.625	342.1	0.013	0.384	13
H→L+2 (21%), H→L+3 (67%)	3.679	337.0	0.039	0.655	15
H-1→L+1 (59%), H→L+2 (18%)	3.729	332.5	0.049	0.729	15
H→L+3 (10%), H→L+4 (76%)	3.790	327.1	0.034	0.602	15
H-1→L+1 (15%), H-1→L+2 (30%), H→L+2 (18%), H→L+4 (12%)	3.798	326.4	0.024	0.502	14
H-1→L+3 (12%), H→L+5 (68%)	3.907	317.3	0.018	0.431	14
H-1→L+2 (17%), H-1→L+3 (53%), H→L+5 (14%)	3.932	315.3	0.023	0.486	16
H-4→L (34%), H-1→L+4 (51%)	4.006	309.5	0.011	0.331	15
H-4→L (52%), H-1→L+4 (29%)	4.010	309.2	0.014	0.378	13
H-1→L+5 (51%), H→L+6 (30%)	4.062	305.2	0.016	0.396	16
H→L+6 (23%), H→L+7 (62%)	4.077	304.1	0.044	0.665	15
H-2→L+2 (45%), H→L+6 (24%), H→L+7 (13%)	4.097	302.6	0.019	0.430	16
H-5→L (11%), H-2→L+3 (72%)	4.169	297.4	0.012	0.345	16
H-5→L (56%), H-2→L+3 (14%)	4.176	296.9	0.002	0.125	6
H-3→L+1 (50%), H-1→L+7 (40%)	4.310	287.6	0.063	0.770	14
H-2→L+5 (16%), H-1→L+6 (60%), H-1→L+7 (12%)	4.336	286.0	0.015	0.374	18
H-2→L+5 (37%), H→L+10 (40%)	4.373	283.5	0.010	0.303	15
H-3→L+2 (10%), H-1→L+8 (78%)	4.446	278.9	0.022	0.447	17

Table S11 Principal singlet-singlet optical transitions ($f > 0.01$) for the absorptions of **9**, calculated in the gas phase using the PBE/Def2-TZVP method.

Excitation (% composition)	E (eV)	λ (nm)	OS, f	μ	% CT
H-2→L (20%), H-1→L (60%), H→L (27%)	2.999	413.5	0.010	0.351	15
H→L+1 (87%)	3.429	361.6	0.016	0.434	13
H-3→L (82%)	3.463	358.1	0.017	0.452	9
H-1→L+1 (10%), H-1→L+2 (24%), H→L+2 (38%)	3.549	349.4	0.013	0.381	11
H→L+3 (80%)	3.654	339.3	0.014	0.400	12
H-1→L+1 (41%), H→L+2 (-36%)	3.668	338.0	0.050	0.749	12
H→L+4 (87%)	3.784	327.7	0.019	0.455	13
H-1→L+3 (67%), H→L+5 (12%)	3.885	319.1	0.018	0.438	13
H-5→L (62%), H-1→L+4 (12%), H→L+5 (13%)	3.957	313.4	0.021	0.463	8
H-5→L (14%), H-1→L+4 (65%)	3.971	312.3	0.023	0.484	11
H→L+6 (74%), H→L+7 (14%)	4.033	307.4	0.034	0.584	13
H-1→L+5 (76%)	4.048	306.3	0.017	0.410	13
H-3→L+1 (87%)	4.159	298.1	0.043	0.650	10
H-3→L+2 (41%), H-2→L+5 (22%)	4.272	290.2	0.035	0.575	8
H-3→L+2 (20%), H-2→L+5 (64%)	4.286	289.3	0.035	0.575	12
H-3→L+3 (81%)	4.341	285.6	0.023	0.460	9

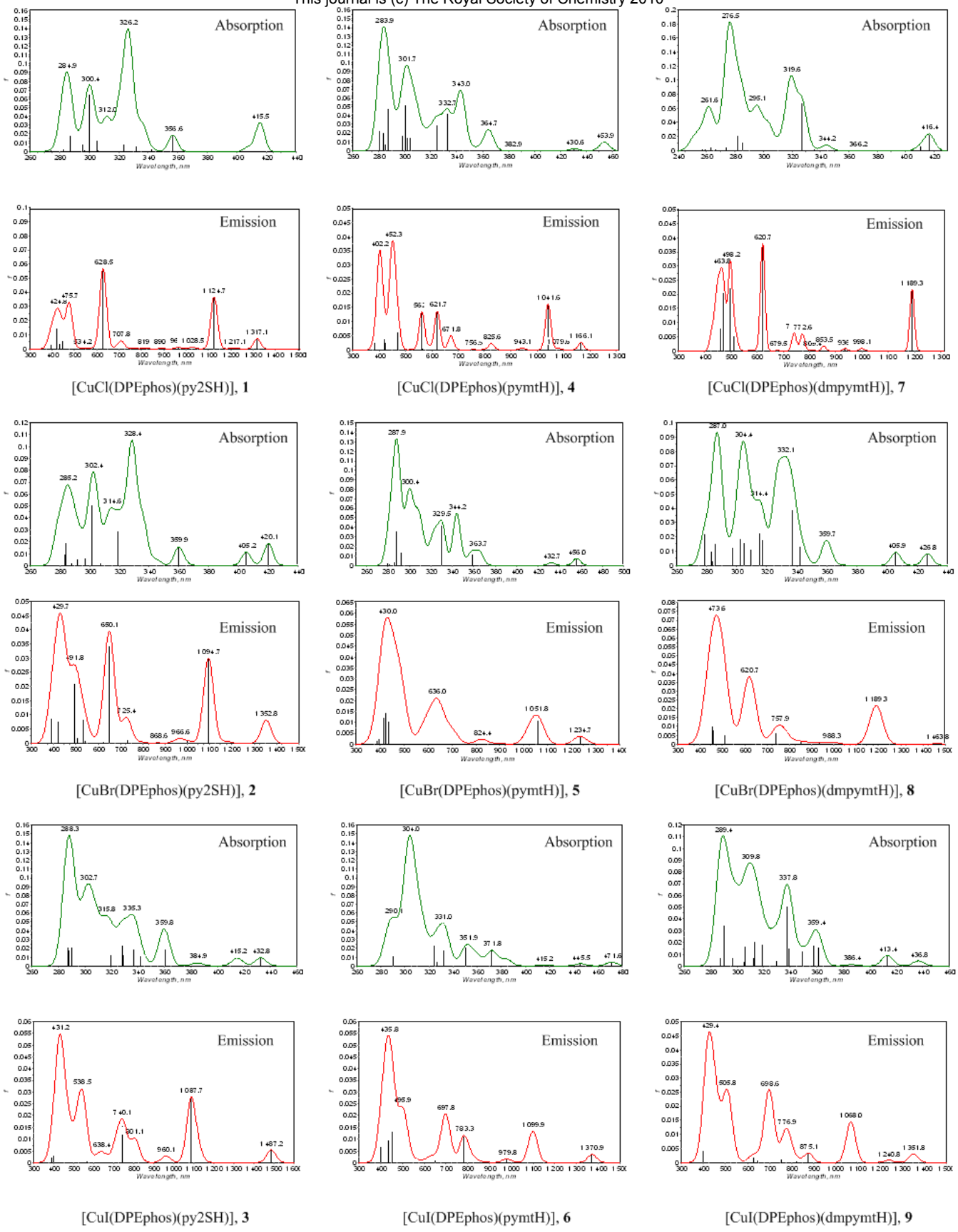


Fig. S1. Absorption and emission spectra of complexes **1-9** computed with TD-DFT calculations at the PEB0/Def2-TZVP levels in the gas phase.

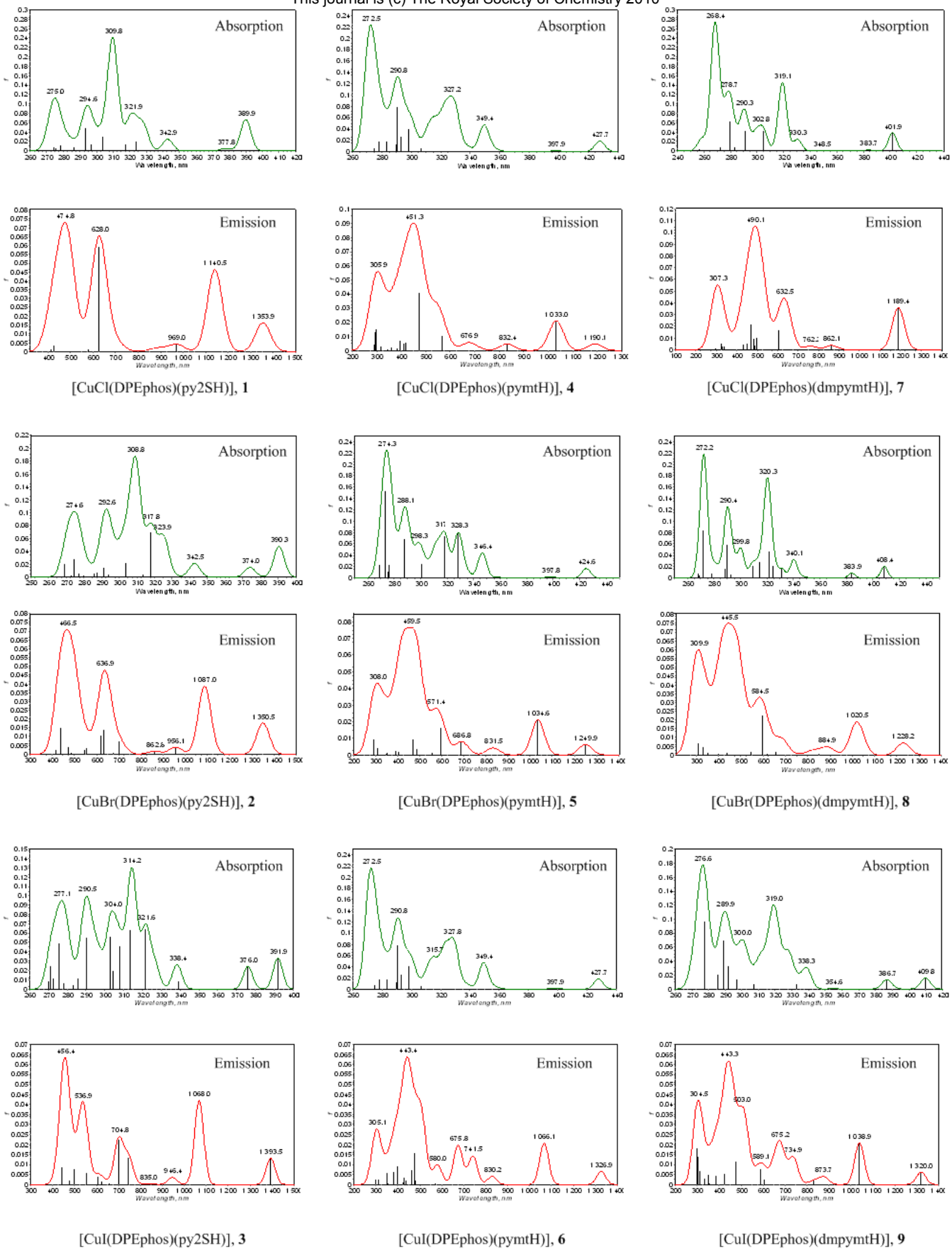


Fig. S2. Absorption and emission spectra of complexes **1-9** computed with TD-DFT calculations at the PEB0/Def2-TZVP levels in CH_2Cl_2 solution.

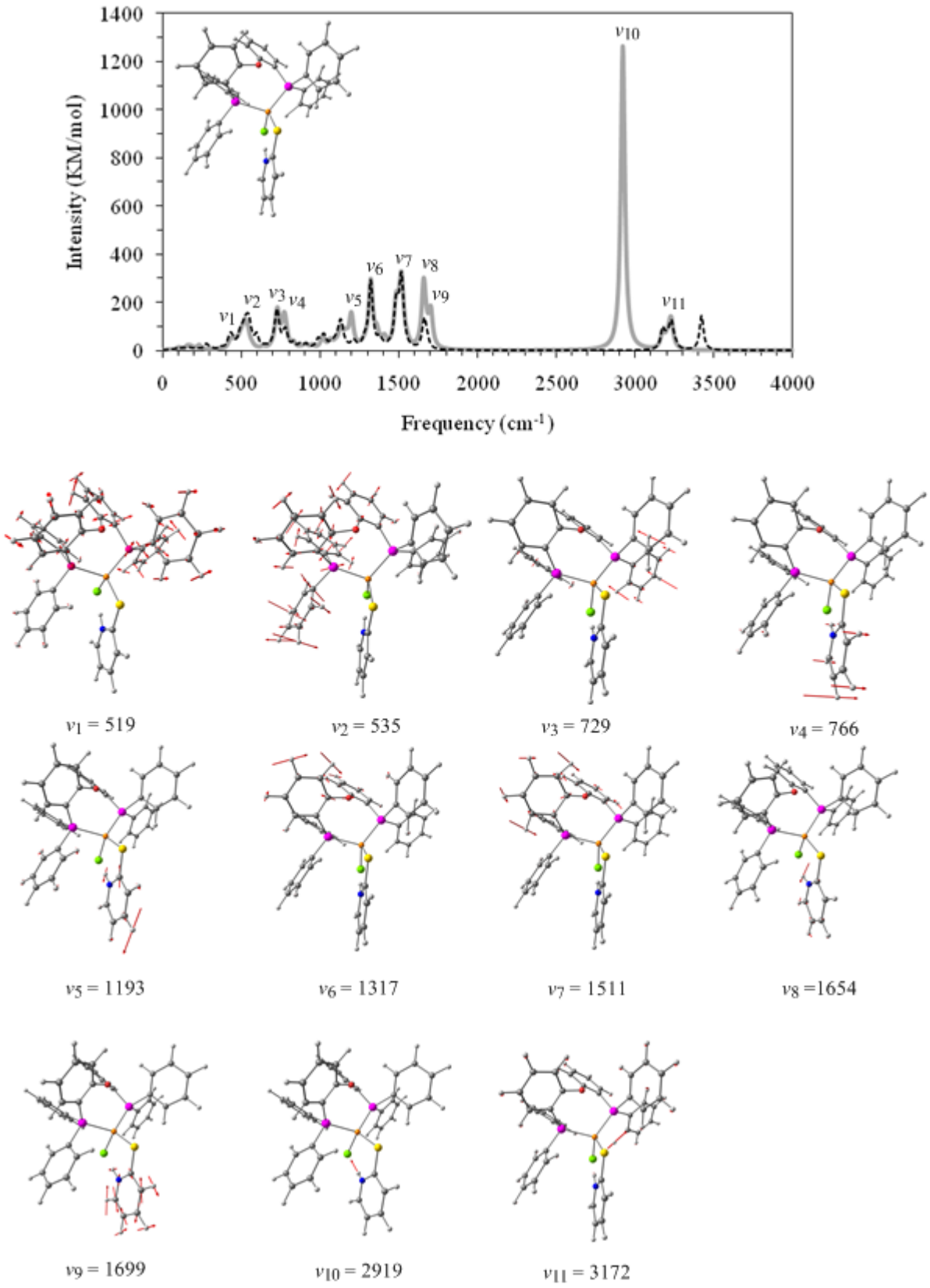


Fig. S3 Infrared spectra along with the normal modes of the most intense absorption bands of complex **1** in both the S_0 and T_1 states computed at the PEB0/Def2-TZVP level of theory (S_0 grey line, T_1 black/dashed line).

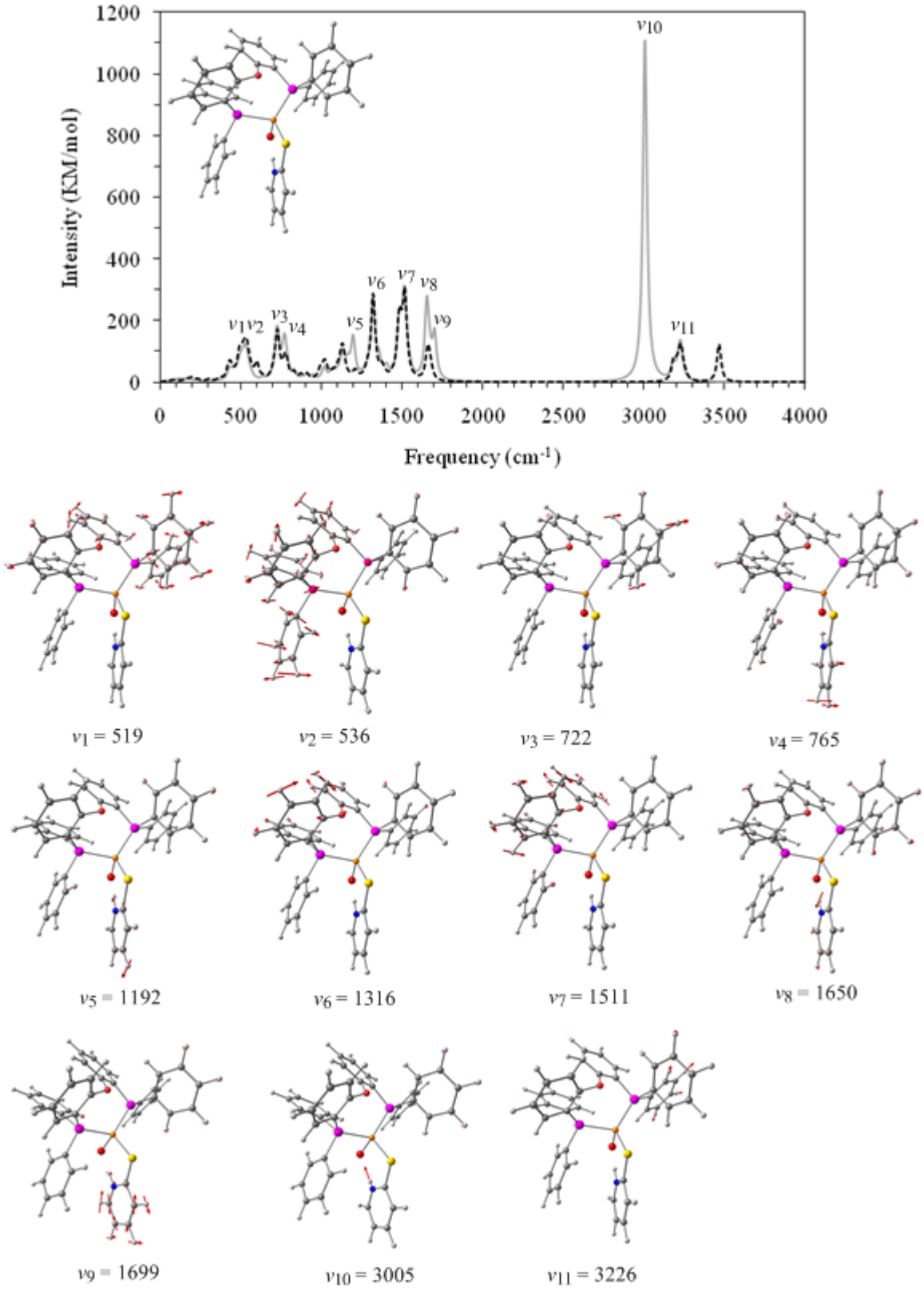


Fig. S4 Infrared spectra along with the normal modes of the most intense absorption bands of complex **2** in both the S_0 and T_1 states computed at the PEB0/Def2-TZVP level of theory (S_0 grey line, T_1 black/dashed line).

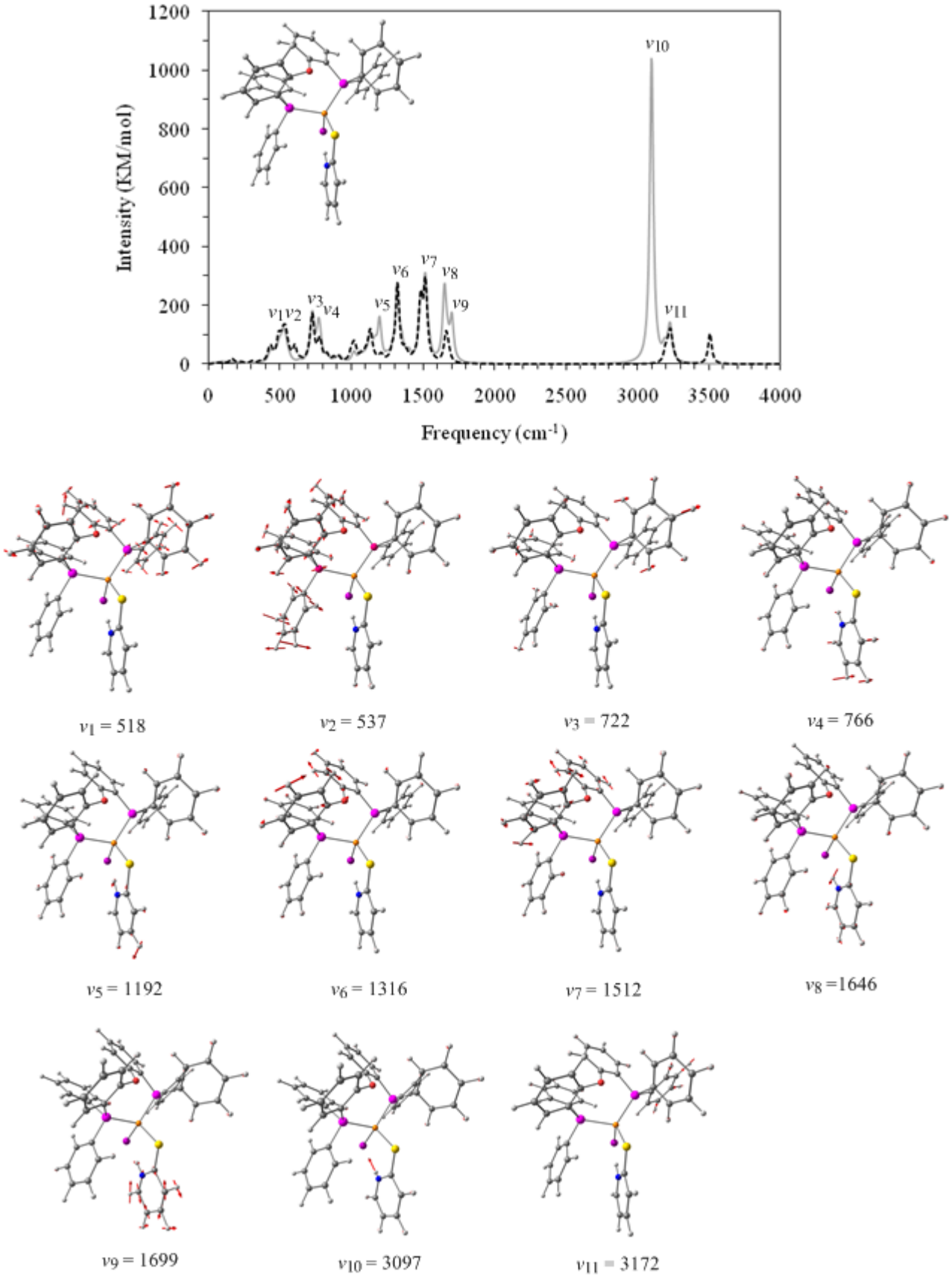


Fig. S5 Infrared spectra along with the normal modes of the most intense absorption bands of complex **3** in both the S_0 and T_1 states computed at the PEB0/Def2-TZVP level of theory (S_0 grey line, T_1 black/dashed line).

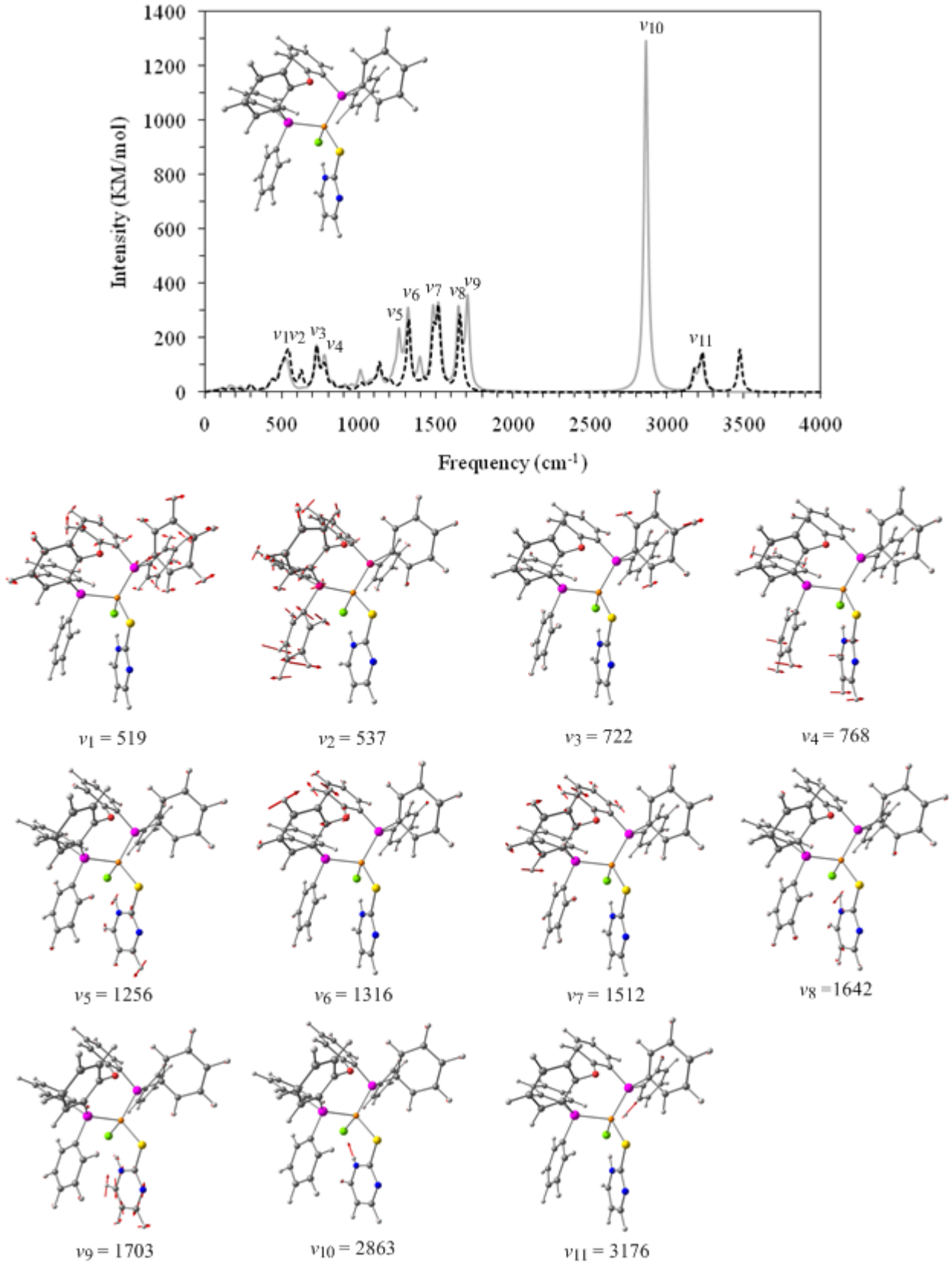


Fig. S6 Infrared spectra along with the normal modes of the most intense absorption bands of complex **4** in both the S_0 and T_1 states computed at the PEB0/Def2-TZVP level of theory (S_0 grey line, T_1 black/dashed line).

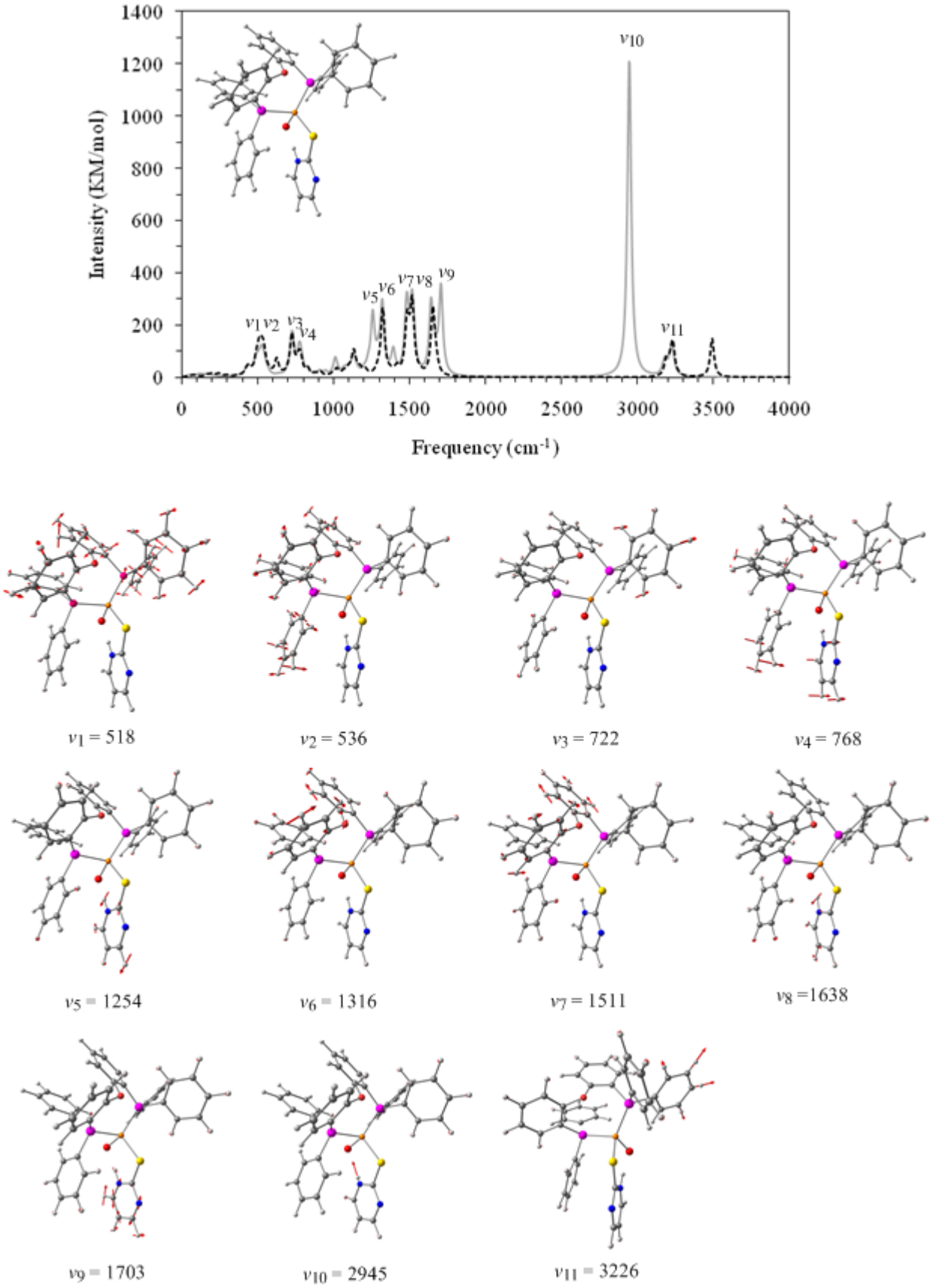


Fig. S7 Infrared spectra along with the normal modes of the most intense absorption bands of complex **5** in both the S_0 and T_1 states computed at the PEB0/Def2-TZVP level of theory (S_0 grey line, T_1 black/dashed line).

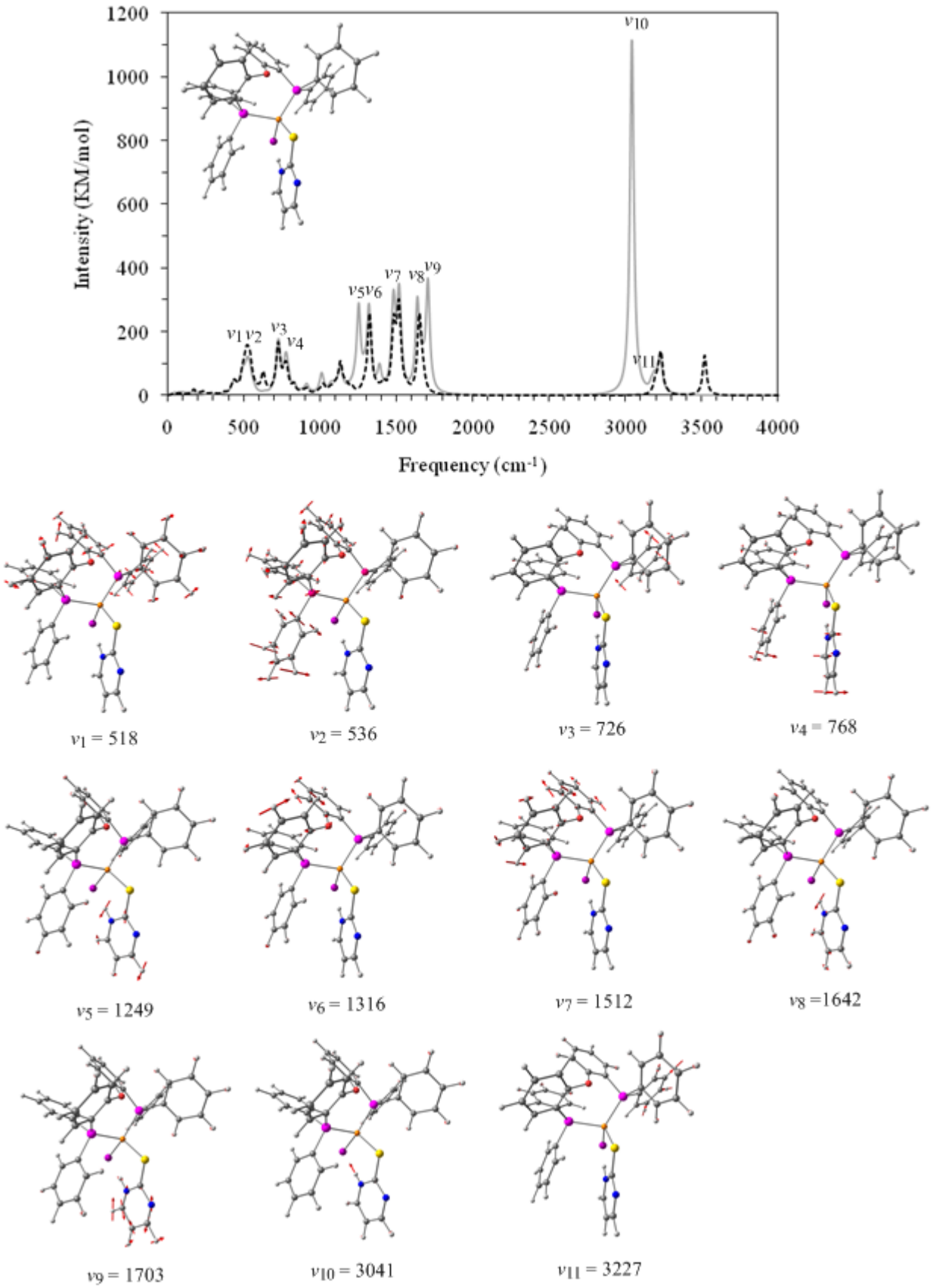


Fig. S8 Infrared spectra along with the normal modes of the most intense absorption bands of complex **6** in both the S_0 and T_1 states computed at the PEB0/Def2-TZVP level of theory (S_0 grey line, T_1 black/dashed line).

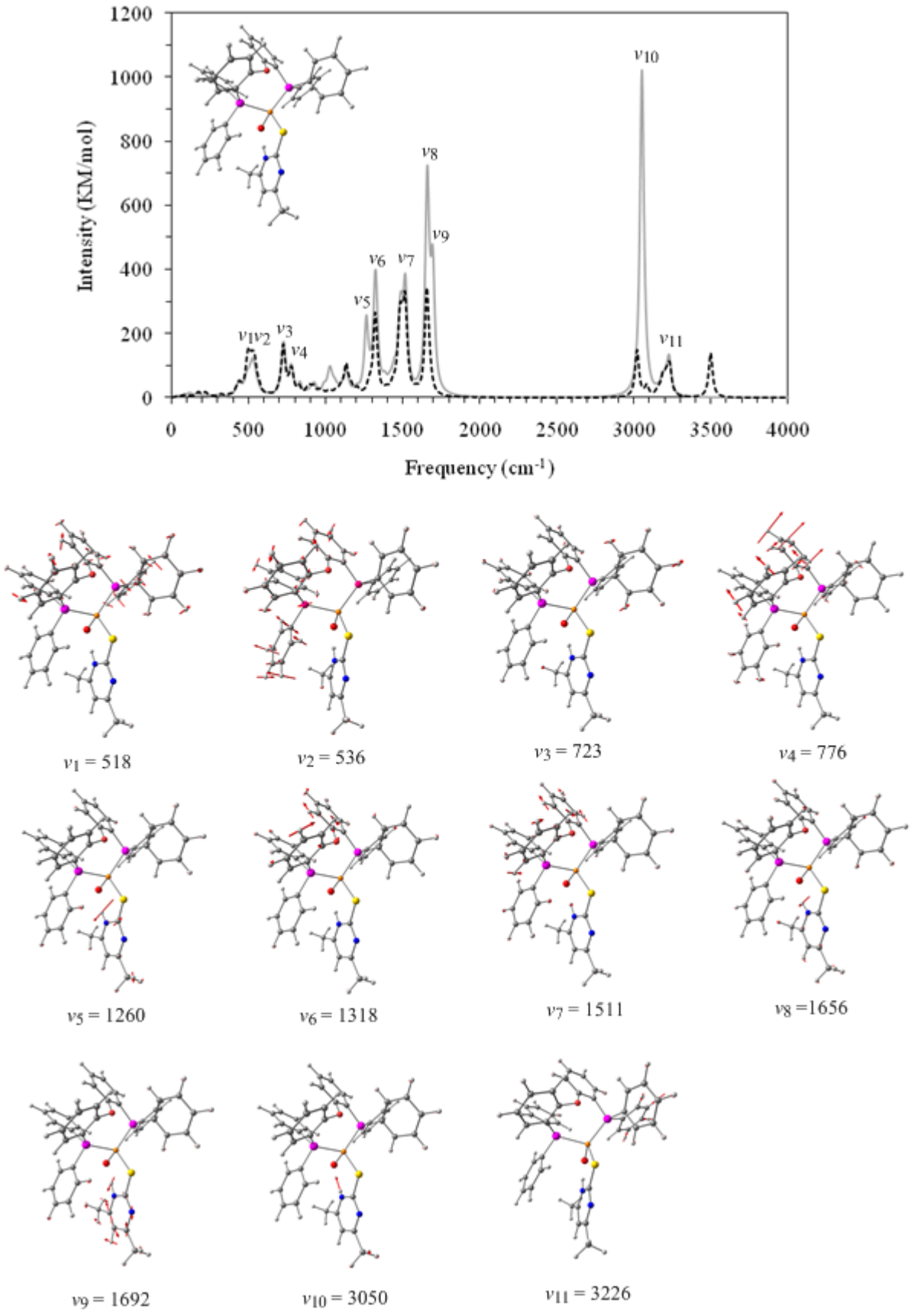


Fig. S9 Infrared spectra along with the normal modes of the most intense absorption bands of complex **8** in both the S_0 and T_1 states computed at the PEB0/Def2-TZVP level of theory (S_0 grey line, T_1 black/dashed line).

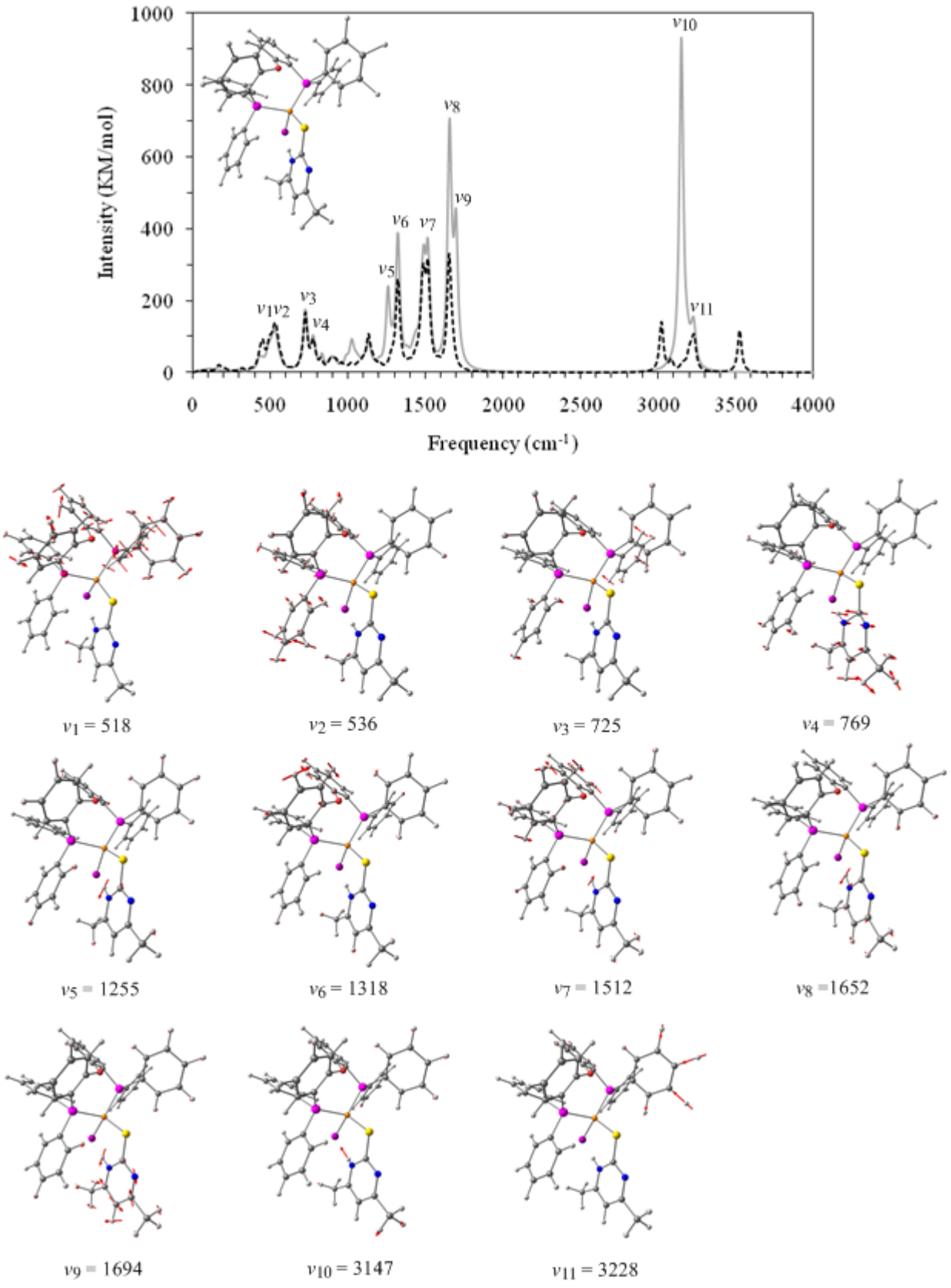


Fig. S10 Infrared spectra along with the normal modes of the most intense absorption bands of complex **9** in both the S_0 and T_1 states computed at the PEB0/Def2-TZVP level of theory (S_0 grey line, T_1 black/dashed line).

Table S12 Cartesian Coordinates and energy data of the Stationary Points on the Potential Energy Surface of the [CuCl(DPEphos)(thione)] complexes (**1**-**9**) in both the S_0 and T_1 states.

[CuCl(DPEphos)(py2SH)], **1** (S_0)

Charge = 0 Multiplicity = 1
Cu,0,-0.1830273491,-0.8449222159,-0.2944533809
P,0,-1.30237054,1.2054154955,-0.0039825262
P,0,2.1030386712,-0.6519291947,-0.0593733433
O,0,1.1689696112,1.4392153614,1.6715188696
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C,0,2.4666158641,-2.4792839726,1.9963105728
C,0,3.0092932507,-2.9806218949,3.17726946
C,0,3.9295015715,-2.2242121177,3.9026091596
C,0,4.3062008199,-0.9639639151,3.4405407884
C,0,3.7701345931,-0.4625654164,2.2547139434
C,0,3.1835907858,-1.4564872188,-1.3080636353
C,0,4.5517524228,-1.6742582564,-1.0898533701
C,0,5.3307204579,-2.2850048737,-2.0694322236
C,0,4.750850571,-2.6877274686,-3.2737952274
C,0,3.3900381326,-2.4830728049,-3.4913350089
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C,0,3.4143203641,1.6412693102,-1.1622581655
C,0,-1.1397371261,2.0932188175,1.6042400416
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C,0,-5.2309586509,1.2193231536,-1.3026689596
C,0,-5.8559481363,0.4019247572,-0.3635248285
C,0,-5.1103415117,-0.1397623406,0.6850276903
C,0,-3.7491845777,0.1330610883,0.7911750024
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H,0,5.3628789734,-3.1702696281,-4.0403772415
H,0,2.9279821031,-2.8070992632,-4.42729722

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H,0,-5.5902833208,-0.7879694223,1.4228180835
H,0,-3.1652487848,-0.3167466182,1.5995058339
Cl,0,-0.9463536863,-1.345781468,-2.5029394503
S,0,-1.0844782034,-2.3510053079,1.3171883535
C,0,-3.1823059266,-4.1213310343,1.328413368
N,0,-2.6735230127,-3.060335238,-0.7114986058
C,0,-2.364430075,-3.2083769374,0.6046922928
C,0,-4.2143757375,-4.7863238734,0.7073374194
C,0,-4.4829970164,-4.5791372832,-0.6637756696
C,0,-3.6757637239,-3.6988990864,-1.3398722187
H,0,-2.960050433,-4.268502731,2.385944671
H,0,-2.0705377657,-2.4134023499,-1.2880181384
H,0,-4.8316121339,-5.4817729604,1.2823811264
H,0,-5.2948591314,-5.0941902222,-1.1768383186
H,0,-3.7833329113,-3.462103463,-2.4006626499

Sum of electronic and zero-point Energies= -4888.627379
Sum of electronic and thermal Energies= -4888.583650
Sum of electronic and thermal Enthalpies= -4888.582706
Sum of electronic and thermal Free Energies= -4888.709910

[CuCl(DPEphos)(py2SH)], **1** (T_1)

Charge=0 Multiplicity=3
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P -1.32872 1.10108 -0.05588
P 2.17792 -0.68261 -0.1541
O 1.07705 1.17984 1.70359
C 2.89441 -1.4334 1.35795
C 2.5448 -2.75911 1.64759
C 3.0733 -3.39721 2.76697
C 3.94586 -2.71552 3.61501
C 4.2895 -1.39325 3.33806
C 3.76785 -0.75347 2.2141
C 3.2644 -1.32677 -1.4817
C 4.63613 -1.54183 -1.28249
C 5.42754 -2.02284 -2.32212
C 4.85596 -2.29881 -3.56572

C	3.49155	-2.09905	-3.76399
C	2.69157	-1.61813	-2.72627
C	2.63291	1.08739	-0.04222
C	1.91853	1.87177	0.87923
C	2.09131	3.25167	0.94607
C	2.99478	3.86489	0.07909
C	3.71943	3.10791	-0.83808
C	3.53504	1.72684	-0.89687
C	-1.22494	1.83595	1.62469
C	-2.31716	2.41085	2.28756
C	-2.18898	2.90793	3.58328
C	-0.96464	2.82722	4.24436
C	0.13517	2.26102	3.60435
C	0.00379	1.78257	2.30339
C	-0.82182	2.48021	-1.15381
C	-1.08758	3.81464	-0.81533
C	-0.71665	4.84296	-1.67755
C	-0.07575	4.54915	-2.88185
C	0.18863	3.22438	-3.22235
C	-0.18009	2.18883	-2.36353
C	-3.11536	0.89858	-0.35912
C	-3.71798	1.40583	-1.51623
C	-5.06613	1.15585	-1.76746
C	-5.81862	0.39457	-0.87508
C	-5.21927	-0.12517	0.27249
C	-3.8729	0.11867	0.52693
H	1.84498	-3.29202	0.99794
H	2.79236	-4.43086	2.9826
H	4.35526	-3.21494	4.49665
H	4.97072	-0.85341	4.00082
H	4.0444	0.28231	2.001
H	5.08444	-1.33886	-0.30628
H	6.49539	-2.18963	-2.15962
H	5.47795	-2.68087	-4.37938
H	3.03691	-2.32829	-4.73092
H	1.61387	-1.48771	-2.87636
H	1.51744	3.83918	1.66497
H	3.12841	4.9483	0.12493
H	4.42495	3.59156	-1.51688
H	4.09015	1.13375	-1.62724
H	-3.28537	2.45589	1.78374
H	-3.05469	3.35047	4.08102
H	-0.86426	3.20102	5.26602
H	1.10283	2.16993	4.10159
H	-1.58509	4.05317	0.12791
H	-0.92928	5.88028	-1.40695
H	0.21692	5.35766	-3.55665
H	0.68701	2.9881	-4.16557
H	0.00003	1.14607	-2.64103
H	-3.13312	1.99515	-2.22525
H	-5.52833	1.55703	-2.67271
H	-6.8735	0.19521	-1.07927
H	-5.79189	-0.74679	0.9644
H	-3.40758	-0.31567	1.41521
Cl	-0.87666	-1.24028	-2.5808

S	-0.96468	-2.22773	1.26658
C	-3.40786	-3.36276	1.71816
N	-2.85792	-2.84902	-0.55089
C	-2.52702	-2.84883	0.79783
C	-4.67379	-3.8993	1.3106
C	-4.96687	-3.87169	-0.06741
C	-4.0745	-3.34982	-0.97536
H	-3.10976	-3.35301	2.76814
H	-2.22645	-2.40332	-1.22405
H	-5.36764	-4.31911	2.03797
H	-5.91369	-4.26741	-0.44335
H	-4.26119	-3.301	-2.04781

Sum of electronic and zero-point Energies= -4888.546238
Sum of electronic and thermal Energies= -4888.501901
Sum of electronic and thermal Enthalpies= -4888.500957
Sum of electronic and thermal Free Energies= -4888.630062

[CuBr(DPEphos)(py2SH)], **2** (S_0)

Charge = 0 Multiplicity = 1
Cu,0,-0.138823,-0.812055,-0.220311
P,0,-1.193335,1.282063,0.051865
P,0,2.15633,-0.690886,0.032454
O,0,1.266091,1.443957,1.742265
C,0,2.859455,-1.251827,1.633116
C,0,2.429735,-2.490472,2.126568
C,0,2.94285,-2.987961,3.322384
C,0,3.879601,-2.249192,4.04452
C,0,4.302712,-1.01023,3.565043
C,0,3.796393,-0.513083,2.364625
C,0,3.249125,-1.529617,-1.183432
C,0,4.604565,-1.78172,-0.92608
C,0,5.39522,-2.413543,-1.882698
C,0,4.840441,-2.803719,-3.102891
C,0,3.492212,-2.564787,-3.35992
C,0,2.694572,-1.934501,-2.403849
C,0,2.668228,1.065128,-0.098483
C,0,2.03644,1.986908,0.754537
C,0,2.22227,3.359152,0.606283
C,0,3.056207,3.827057,-0.407906
C,0,3.704962,2.933063,-1.256049
C,0,3.508516,1.561225,-1.099419
C,0,-1.018115,2.178188,1.655133
C,0,-2.062472,2.855746,2.298927
C,0,-1.873009,3.469759,3.535684
C,0,-0.629551,3.407372,4.162414
C,0,0.424403,2.739935,3.54431
C,0,0.229271,2.142489,2.300941
C,0,-0.799848,2.601875,-1.167657
C,0,-1.201992,3.933746,-0.995901
C,0,-0.872374,4.8957,-1.946961
C,0,-0.136895,4.537324,-3.078335
C,0,0.266071,3.215612,-3.254407

C,0,-0.060815,2.249662,-2.302445
C,0,-3.00731,1.071719,-0.104033
C,0,-3.681774,1.414364,-1.282171
C,0,-5.038425,1.125256,-1.428393
C,0,-5.737177,0.489135,-0.404408
C,0,-5.06915,0.132491,0.768062
C,0,-3.712842,0.41229,0.915495
Br,0,-1.005935,-1.373726,-2.511781
S,0,-1.094064,-2.127007,1.523892
C,0,-3.372911,-3.633437,1.789671
N,0,-2.876349,-2.793576,-0.352532
C,0,-2.503359,-2.878745,0.952709
C,0,-4.511415,-4.213917,1.280044
C,0,-4.84124,-4.076176,-0.086552
C,0,-3.983125,-3.350785,-0.874196
H,0,1.675905,-3.061565,1.57732
H,0,2.598725,-3.95504,3.697295
H,0,4.276551,-2.637255,4.986034
H,0,5.033541,-0.424515,4.128747
H,0,4.132054,0.458922,1.993502
H,0,5.042322,-1.489742,0.032016
H,0,6.450108,-2.607816,-1.672437
H,0,5.461762,-3.303236,-3.85085
H,0,3.04785,-2.878626,-4.307754
H,0,1.629706,-1.768861,-2.599657
H,0,1.709649,4.05274,1.275374
H,0,3.196464,4.903488,-0.5317
H,0,4.359341,3.301417,-2.049035
H,0,4.001668,0.859629,-1.776101
H,0,-3.04762,2.88786,1.827562
H,0,-2.704894,3.991307,4.014706
H,0,-0.478781,3.875106,5.138271
H,0,1.406884,2.659877,4.013692
H,0,-1.772246,4.223808,-0.109779
H,0,-1.189854,5.931889,-1.804336
H,0,0.122559,5.293627,-3.823751
H,0,0.842088,2.92877,-4.137517
H,0,0.241678,1.208427,-2.440487
H,0,-3.142534,1.9061,-2.094565
H,0,-5.550601,1.401317,-2.353576
H,0,-6.801264,0.267733,-0.51963
H,0,-5.605949,-0.374816,1.573853
H,0,-3.192639,0.105872,1.827041
H,0,-3.102425,-3.728918,2.841884
H,0,-2.244015,-2.265131,-1.004432
H,0,-5.166336,-4.787842,1.941125
H,0,-5.737895,-4.526478,-0.511742
H,0,-4.129117,-3.179118,-1.942887

Sum of electronic and zero-point Energies= -7002.271931
Sum of electronic and thermal Energies= -7002.227884
Sum of electronic and thermal Enthalpies= -7002.226940
Sum of electronic and thermal Free Energies= -7002.355100

[CuBr(DPEphos)(py2SH)], **2** (T_1)

Charge = 0 Multiplicity = 3
Cu,0,-0.3285472227,-0.688362186,-0.4129730587
P,0,-0.6368621073,1.6060743803,-0.1373676619
P,0,1.9976246378,-1.3686073505,-0.2670919202
O,0,1.7012808582,0.8253522388,1.5291104743
C,0,2.4178364563,-2.2928365707,1.2599592256
C,0,1.6425044348,-3.4202112923,1.5639344745
C,0,1.9229636273,-4.1820468337,2.6954098917
C,0,2.9710710688,-3.8201451747,3.5413027882
C,0,3.7397044517,-2.6943984404,3.2497798374
C,0,3.4664177655,-1.9333493365,2.1134939785
C,0,2.7536485567,-2.4022195212,-1.578769295
C,0,3.9361978736,-3.1253029945,-1.3633591961
C,0,4.4897303216,-3.8856583356,-2.3901114553
C,0,3.8660779827,-3.9354805934,-3.6381457067
C,0,2.6850005676,-3.228635523,-3.8535571723
C,0,2.1244450663,-2.4658690901,-2.8281201943
C,0,3.0801399039,0.1086835262,-0.2181565293
C,0,2.7262381957,1.1299948303,0.6799674779
C,0,3.4031306717,2.3465890074,0.6991406494
C,0,4.4555585928,2.550909808,-0.1923816821
C,0,4.8297784379,1.5511384487,-1.0866711808
C,0,4.1412995648,0.338412587,-1.0981764674
C,0,-0.1897506524,2.2908404568,1.5084171348
C,0,-0.958798028,3.2454334145,2.1862526101
C,0,-0.5935071944,3.6889002438,3.4561601362
C,0,0.5433672813,3.1737123178,4.0761541278
C,0,1.3226240261,2.2233788671,3.4206866027
C,0,0.9613127384,1.7989863129,2.1450619956
C,0,0.3240456647,2.6485732409,-1.3006631178
C,0,0.5799699166,3.9993774598,-1.0252509483
C,0,1.2900359816,4.7771062919,-1.9358850645
C,0,1.7533585587,4.2135240329,-3.1256787826
C,0,1.5018010262,2.8717091915,-3.4029556381
C,0,0.7908519239,2.087334802,-2.4946861909
C,0,-2.3709127738,2.1139223883,-0.384718061
C,0,-2.7688982946,2.8270853654,-1.5217908409
C,0,-4.1154665544,3.1282411901,-1.7202811436
C,0,-5.072057289,2.7166126034,-0.7941615996
C,0,-4.6819482449,1.9946347474,0.3340369001
C,0,-3.3392987683,1.6875991792,0.5358797616
Br,0,-1.3045654355,-0.9732082495,-2.6163051295
S,0,-1.2495270021,-1.4874345701,1.4897225149
C,0,-3.8429425349,-1.5227686,2.3550234357
N,0,-3.4896414709,-1.6026900711,-0.0064604844
C,0,-2.9826305747,-1.5223496562,1.2843554385
C,0,-5.2618306799,-1.6043326354,2.1637142399
C,0,-5.7274600458,-1.6789377873,0.8357421221
C,0,-4.8535897283,-1.670337622,-0.226601144
H,0,0.8085269488,-3.6997194348,0.9145751109
H,0,1.3112144719,-5.0585862683,2.9218625979
H,0,3.186588225,-4.4151595448,4.4322691187
H,0,4.561450687,-2.4055927328,3.9100890298

H,0,4.0772064033,-1.0558229937,1.8867325761
H,0,4.4219305006,-3.0977634336,-0.3844417253
H,0,5.4104014039,-4.4475878841,-2.2137586295
H,0,4.2994809417,-4.5366734095,-4.4415848893
H,0,2.1835994414,-3.2767047625,-4.8232923204
H,0,1.1798808398,-1.9366541573,-2.991801367
H,0,3.1029159979,3.1273827771,1.4001173691
H,0,4.9852834803,3.5064792269,-0.1833741776
H,0,5.6541018067,1.7153340596,-1.7837860562
H,0,4.422244296,-0.4413495326,-1.8097288753
H,0,-1.8646834282,3.6352339542,1.7164908214
H,0,-1.2089051889,4.4328885383,3.9668510664
H,0,0.8232873903,3.5066919867,5.0783251082
H,0,2.2088807835,1.7890641268,3.8874223036
H,0,0.2244524786,4.4463220926,-0.09346327
H,0,1.4836978569,5.8297084247,-1.7146507647
H,0,2.3129936911,4.8248456291,-3.8382133477
H,0,1.8611034009,2.4252375997,-4.3331468192
H,0,0.5753287237,1.0386988539,-2.7189320579
H,0,-2.0274748399,3.144497996,-2.2578999208
H,0,-4.4168570575,3.6855173518,-2.6105579829
H,0,-6.127149924,2.9506925679,-0.9562933537
H,0,-5.4239784984,1.6469978828,1.0562901624
H,0,-3.049494515,1.1056835694,1.414500364
H,0,-3.4098270849,-1.4669414542,3.3553306522
H,0,-2.8489400877,-1.5206044886,-0.7991592814
H,0,-5.9438437033,-1.6168760781,3.0130965566
H,0,-6.7974013672,-1.74593871,0.6234697313
H,0,-5.1662016258,-1.7184112509,-1.2692748819
Sum of electronic and zero-point Energies= -7002.191140
Sum of electronic and thermal Energies= -7002.146541
Sum of electronic and thermal Enthalpies= -7002.145597
Sum of electronic and thermal Free Energies= -7002.275539

[CuI(DPEphos)(py2SH)], **3** (S_0)

Charge = 0 Multiplicity = 1
Cu,0,-0.2834097518,-0.6073560104,-0.4139754154
P,0,-0.4865707269,1.7225255278,-0.0859803896
P,0,1.9138083158,-1.3640504559,-0.2346303686
O,0,1.8501698106,0.870372961,1.5737443002
C,0,2.3543351918,-2.2211487962,1.3288729918
C,0,1.5343486079,-3.2818832102,1.7353997717
C,0,1.8253427441,-3.9912359369,2.8983263764
C,0,2.9296049683,-3.6417281156,3.6749908838
C,0,3.7442305748,-2.5809724867,3.2815968386
C,0,3.4596037294,-1.873931346,2.1138798459
C,0,2.6455206689,-2.4855587713,-1.4934925522
C,0,3.8068597007,-3.231283884,-1.2427834701
C,0,4.3363880492,-4.0593931318,-2.2292250112
C,0,3.7107835136,-4.1556433543,-3.4735086788
C,0,2.5520089763,-3.4244868085,-3.725261893
C,0,2.0167691042,-2.5950216916,-2.7390717652
C,0,3.0346422035,0.0866471807,-0.2904172423

C,0,2.7773204161,1.1365271227,0.6079313777
C,0,3.4574361556,2.3489920357,0.5225265707
C,0,4.4163360499,2.5219833516,-0.4741559701
C,0,4.6997142849,1.491205084,-1.3667558496
C,0,4.0102337083,0.2826563907,-1.2723408897
C,0,0.0115838462,2.4120376551,1.5530332887
C,0,-0.7033949665,3.4020394427,2.2407730531
C,0,-0.3020749555,3.8404374151,3.5014112533
C,0,0.8225365831,3.2840648818,4.1085115376
C,0,1.5497915132,2.2984501379,3.4467356831
C,0,1.149626981,1.87887166,2.1800716752
C,0,0.3840171357,2.8456001333,-1.2524472399
C,0,0.4946580063,4.2258356127,-1.033868028
C,0,1.1718894703,5.029424152,-1.9470935934
C,0,1.745642148,4.4628304804,-3.0870451867
C,0,1.6405868188,3.0917713429,-3.3092124908
C,0,0.9645925905,2.2841928849,-2.3945633714
C,0,-2.2417457207,2.2353636107,-0.2129457604
C,0,-2.7325727135,2.9147020504,-1.3338850966
C,0,-4.0951969128,3.1888983793,-1.4518831549
C,0,-4.9828275794,2.7875243935,-0.4561729363
C,0,-4.5030127878,2.0986741913,0.6591088566
C,0,-3.1447391232,1.8153137344,0.776967125
I,0,-1.496831072,-0.8478754309,-2.8161596271
H,0,0.6537415227,-3.5448438312,1.1431428795
H,0,1.1773166617,-4.8161174189,3.204569211
H,0,3.1531774065,-4.1944926328,4.5909731208
H,0,4.6102447906,-2.3007045049,3.8868758242
H,0,4.1051972824,-1.0461410943,1.8095621636
H,0,4.2956392393,-3.1693299631,-0.267090009
H,0,5.2407010422,-4.6378892899,-2.0236193196
H,0,4.1255428776,-4.8099432935,-4.2447372246
H,0,2.0483203559,-3.5036773486,-4.6918285084
H,0,1.0927094369,-2.0412602099,-2.9321243537
H,0,3.2290041877,3.1514900847,1.2262659373
H,0,4.944665932,3.475381964,-0.5488343801
H,0,5.4528707706,1.6278710676,-2.1457073867
H,0,4.2188753728,-0.520064335,-1.9831682481
H,0,-1.6019587946,3.8247197263,1.7851261094
H,0,-0.8780790127,4.6139999193,4.0145357908
H,0,1.133586928,3.6136786064,5.1026861848
H,0,2.4271432358,1.8316604259,3.8987798223
H,0,0.0532618661,4.6761408131,-0.1410980643
H,0,1.2537075934,6.1046750917,-1.768438838
H,0,2.2775403968,5.0949853437,-3.8028223192
H,0,2.0880519763,2.6417587084,-4.1986191096
H,0,0.8721425828,1.2087480336,-2.5652942904
H,0,-2.0475973505,3.2284306915,-2.1244240723
H,0,-4.4626850244,3.7198818933,-2.3335183936
H,0,-6.0493450285,3.0075733641,-0.549212016
H,0,-5.1924235769,1.7728946376,1.4424101356
H,0,-2.7785079741,1.2576164296,1.6435181875
S,0,-1.4848934969,-1.4899919519,1.4558132481
C,0,-4.074357399,-2.2163079488,2.004490403
N,0,-3.5780267397,-1.5723377213,-0.2032664513

C,0,-3.1090279453,-1.7678218339,1.0587175051
C,0,-5.3832614367,-2.4177899468,1.6325348937
C,0,-5.7996291042,-2.1876398859,0.3018332996
C,0,-4.8509677941,-1.7631117411,-0.593472603
H,0,-3.7355252278,-2.3898898433,3.026464061
H,0,-2.8892079324,-1.2688331974,-0.928181605
H,0,-6.1079670928,-2.7610594263,2.3758375526
H,0,-6.8309883683,-2.3414381814,-0.0145947606
H,0,-5.048442716,-1.5580685833,-1.6481708244
Sum of electronic and zero-point Energies= -4726.436347
Sum of electronic and thermal Energies= -4726.392131
Sum of electronic and thermal Enthalpies= -4726.391186
Sum of electronic and thermal Free Energies= -4726.520483

[CuI(DPEphos)(py2SH)], **3** (T_1)

Charge = 0 Multiplicity = 3
Cu,0,-0.3449991026,-0.7146116768,-0.4916774628
P,0,-0.7009141311,1.5784166972,-0.2059987587
P,0,2.0013505872,-1.3846954103,-0.3491930989
O,0,1.6031629799,0.7784444143,1.4676025887
C,0,2.3753411712,-2.3558897993,1.159933559
C,0,1.621475044,-3.5170119719,1.380705622
C,0,1.8662234996,-4.3120453101,2.4973976769
C,0,2.85503008,-3.9498747213,3.4118043372
C,0,3.601152197,-2.7911375402,3.2031349973
C,0,3.3644479526,-1.9967618028,2.0815183826
C,0,2.8187873555,-2.3674548287,-1.6643265876
C,0,3.9636383579,-3.1372157132,-1.4107477149
C,0,4.5696585527,-3.853382119,-2.4400164471
C,0,4.0374590264,-3.8122805898,-3.7297568003
C,0,2.8946375679,-3.057536068,-3.9854664811
C,0,2.2829293105,-2.3397817347,-2.9574823506
C,0,3.0740805842,0.0962395095,-0.2151475516
C,0,2.6722654394,1.1000962965,0.6833282175
C,0,3.345783125,2.3165183321,0.7603238223
C,0,4.4444941667,2.5370523731,-0.0691900695
C,0,4.8680228913,1.5539574666,-0.9600690204
C,0,4.1812201265,0.3423927628,-1.0319006561
C,0,-0.2923710355,2.2310255992,1.4629458604
C,0,-1.0746918699,3.1669757166,2.1506543536
C,0,-0.7266284785,3.5844731893,3.4343273314
C,0,0.4053576893,3.0619815953,4.0569877485
C,0,1.1978362447,2.1298193029,3.3911248139
C,0,0.8538477471,1.7326411689,2.1023545463
C,0,0.3100321256,2.6336804975,-1.3152719722
C,0,0.5060748993,3.9949908841,-1.0423244054
C,0,1.2579593477,4.7815751185,-1.9104904498
C,0,1.8230259827,4.2166502446,-3.0551199871
C,0,1.6332044197,2.8642490287,-3.3292025475
C,0,0.8812014133,2.0720796244,-2.4617565363
C,0,-2.4193281552,2.1151006452,-0.5002610928
C,0,-2.7701661274,2.8344506317,-1.6491235716
C,0,-4.1042096601,3.1583729675,-1.8902592473
C,0,-5.0962475877,2.764181558,-0.994489595

C,0,-4.753642323,2.0347928181,0.1441545744
C,0,-3.4234510514,1.7039367536,0.3884168812
I,0,-1.4454009351,-1.1061144444,-2.8216550785
H,0,0.8338680349,-3.798413796,0.6766064899
H,0,1.2724675257,-5.2149501172,2.6585682504
H,0,3.0417975919,-4.5709220307,4.2914125071
H,0,4.3768432772,-2.5023746211,3.916965574
H,0,3.9589509563,-1.0942979788,1.919193566
H,0,4.3786955469,-3.1805446592,-0.4005672319
H,0,5.4602166491,-4.4520354595,-2.2327164713
H,0,4.511417371,-4.3795597249,-4.5349012031
H,0,2.4623564826,-3.0342430825,-4.9887579776
H,0,1.3660424937,-1.7774721459,-3.1571887868
H,0,3.0076941983,3.0848921616,1.4576088919
H,0,4.9716352414,3.4925380652,-0.014141982
H,0,5.7292516475,1.7305676129,-1.6077766289
H,0,4.5002954636,-0.4235459767,-1.7423452448
H,0,-1.9763024065,3.5635026151,1.6784964821
H,0,-1.3518282388,4.3143602809,3.9533966122
H,0,0.6711109757,3.3747933756,5.0694568254
H,0,2.0805290147,1.6903332005,3.859783671
H,0,0.0703791491,4.4431265546,-0.1457938588
H,0,1.404392373,5.8423393863,-1.6921044068
H,0,2.414399202,4.8354300123,-3.7347739332
H,0,2.0733542335,2.4162617484,-4.2231247552
H,0,0.7200834028,1.0131559245,-2.679730464
H,0,-2.0017026611,3.1386120258,-2.3627321222
H,0,-4.3676082382,3.7194387599,-2.790096841
H,0,-6.1414125062,3.0176372374,-1.1886696959
H,0,-5.5227097101,1.7022587363,0.8448363077
H,0,-3.1729697509,1.1174891745,1.2763835655
S,0,-1.1187505563,-1.4922955491,1.4946453783
C,0,-3.6220635646,-1.3193638478,2.5914205807
N,0,-3.4903319206,-1.6491293147,0.2298306029
C,0,-2.8625088559,-1.4602231804,1.4557475848
C,0,-5.0537926287,-1.3577221098,2.5331048135
C,0,-5.6421438628,-1.5484649314,1.2663462693
C,0,-4.8701329874,-1.6838790629,0.1363657732
H,0,-3.0980584096,-1.1852016637,3.5393573722
H,0,-2.9204674427,-1.657169603,-0.6161667555
H,0,-5.6556799097,-1.2540807661,3.4352392531
H,0,-6.7286000149,-1.5944267281,1.1579568274
H,0,-5.2778115934,-1.8265969875,-0.8640036695
Sum of electronic and zero-point Energies= -4726.356645
Sum of electronic and thermal Energies= -4726.311958
Sum of electronic and thermal Enthalpies= -4726.311014
Sum of electronic and thermal Free Energies= -4726.441304

[CuCl(DPEphos)(pymtH)], **4** (S_0)

Charge = 0 Multiplicity = 1
Cu,0,-0.238140438,-0.6400171063,-0.3456689189
P,0,-0.4654645487,1.6818664213,0.0084588055
P,0,1.9438090211,-1.3742001086,-0.1591339544
O,0,1.9339574661,0.898147435,1.6030528686

C,0,2.4198913664,-2.1897736312,1.4146091581
C,0,1.5707025394,-3.1914005036,1.9023472864
C,0,1.8837372528,-3.8685838982,3.0787839707
C,0,3.0406618429,-3.544663296,3.7867348467
C,0,3.8847216598,-2.5412817063,3.3126774265
C,0,3.5773917781,-1.8663421037,2.1317536979
C,0,2.6262218314,-2.5264401729,-1.4167320385
C,0,3.7950547308,-3.2698519717,-1.1976564762
C,0,4.2788461665,-4.1244992433,-2.1851069935
C,0,3.5994300684,-4.2486562165,-3.3982716605
C,0,2.432466495,-3.5199515347,-3.6175468988
C,0,1.9415106624,-2.6644838368,-2.6303782414
C,0,3.0604940975,0.0755776146,-0.2808281811
C,0,2.8284753588,1.1449777356,0.6020073702
C,0,3.5000633535,2.3575289197,0.4661304702
C,0,4.4254175817,2.5106840162,-0.56504158
C,0,4.683976696,1.4606795803,-1.4425843381
C,0,4.0023679505,0.252411224,-1.2984980461
C,0,0.0760324292,2.4169501956,1.6113465139
C,0,-0.6245909466,3.4176334933,2.2986684482
C,0,-0.1819509115,3.8944650992,3.5310094123
C,0,0.9719527246,3.3680836163,4.1093374629
C,0,1.6866410751,2.3738898078,3.4469798982
C,0,1.2446648743,1.9148783506,2.2080081188
C,0,0.3180509384,2.810230738,-1.214785286
C,0,0.3795294702,4.1983631042,-1.0291136598
C,0,0.9954807847,5.0078351935,-1.9796306688
C,0,1.5575132789,4.4387604785,-3.1241213898
C,0,1.500263602,3.0601019158,-3.3140574468
C,0,0.8847856531,2.246122779,-2.3628434409
C,0,-2.2445252319,2.1153039316,-0.0644922681
C,0,-2.8113977687,2.6439938921,-1.2307914448
C,0,-4.1900696259,2.8355443082,-1.3214243494
C,0,-5.0194650511,2.5000865956,-0.2527881649
C,0,-4.4636522915,1.9616759397,0.9089180784
C,0,-3.0882883166,1.7609753338,1.0009815374
H,0,0.6496092431,-3.4328387594,1.3644272874
H,0,1.2112924346,-4.6457411396,3.4500826566
H,0,3.2818937801,-4.0711989067,4.7136184584
H,0,4.7907486262,-2.2802591904,3.8657624348
H,0,4.2430614003,-1.0804577159,1.764985266
H,0,4.3252750991,-3.1864169452,-0.245431076
H,0,5.1892779686,-4.7017554715,-2.00458416
H,0,3.9786555083,-4.9231363873,-4.1704297456
H,0,1.8882948646,-3.6214602529,-4.5598378666
H,0,1.0115854593,-2.1105076903,-2.7966258977
H,0,3.292045926,3.1752888664,1.1585551925
H,0,4.9474156854,3.4637730371,-0.6784515371
H,0,5.4111207744,1.5818696425,-2.2483742108
H,0,4.1900367963,-0.5656113624,-1.9977751813
H,0,-1.544546294,3.8187260588,1.8668020818
H,0,-0.7481977576,4.6745275014,4.0451103929
H,0,1.315591297,3.7278875814,5.0820594978
H,0,2.5861367355,1.9300248122,3.8780741436
H,0,-0.0516968703,4.6506400136,-0.1325080477

H,0,1.0392693247,6.0892032174,-1.8263630594
H,0,2.042392134,5.0751583195,-3.8690001346
H,0,1.9384909694,2.6087325487,-4.2074320169
H,0,0.8252677124,1.165118938,-2.5116043397
H,0,-2.1710590993,2.902265397,-2.0769173339
H,0,-4.6161275054,3.252789982,-2.2373819804
H,0,-6.0987643912,2.6574847578,-0.3237011768
H,0,-5.1048530551,1.6904915825,1.7516429434
H,0,-2.6682380542,1.315230918,1.9065014189
Br,0,-1.2934832635,-0.772906957,-2.630563194
S,0,-1.5927896122,-1.5560501118,1.3869063276
N,0,-4.1890683016,-2.0208842272,1.691732061
N,0,-3.5045230544,-1.4048938051,-0.4573045638
C,0,-3.1884948442,-1.6683179642,0.8502030505
C,0,-5.4171181143,-2.0824886169,1.2332209808
C,0,-5.7847391723,-1.8028553946,-0.1008050524
C,0,-4.7510402372,-1.458696244,-0.9373050346
H,0,-2.7231866081,-1.1588785957,-1.1210365716
H,0,-6.1889690678,-2.37443888,1.9575102671
H,0,-6.8154696586,-1.8597878612,-0.4478182993
H,0,-4.8604573974,-1.2186790848,-1.9980859047
Sum of electronic and zero-point Energies= -7018.290516
Sum of electronic and thermal Energies= -7018.246585
Sum of electronic and thermal Enthalpies= -7018.245641
Sum of electronic and thermal Free Energies= -7018.373689

[CuCl(DPEphos)(pymtH)], **4** (T_1)

Charge = 0 Multiplicity = 3
Cu,0,-0.2888910784,-0.6474392193,-0.4835895654
P,0,-0.6683219975,1.6332286004,-0.1039000308
P,0,2.0211502925,-1.4138581716,-0.2837893772
O,0,1.7188418927,0.8151951349,1.4416458794
C,0,2.4201261442,-2.2745311052,1.2823878047
C,0,1.5785208205,-3.3223080091,1.6783677763
C,0,1.8452293529,-4.0333376279,2.8460741876
C,0,2.9450267849,-3.697717859,3.6347160692
C,0,3.7796968031,-2.6485958028,3.2516188926
C,0,3.520103004,-1.9388165363,2.0800704316
C,0,2.7775739935,-2.4899816116,-1.559121292
C,0,3.927372567,-3.2507208405,-1.3018518417
C,0,4.4826641146,-4.0419934112,-2.3043635971
C,0,3.8941236868,-4.0848547009,-3.5692676047
C,0,2.7453667038,-3.3394794796,-3.8265678329
C,0,2.1828856135,-2.5464598588,-2.8259363793
C,0,3.0997644897,0.0662769189,-0.2831588405
C,0,2.7451423973,1.1077396346,0.5918733118
C,0,3.4168461864,2.3271045488,0.5786876032
C,0,4.4645981443,2.5123075405,-0.3229983433
C,0,4.8394180552,1.4924431876,-1.194302584
C,0,4.155810131,0.2768196917,-1.1734511408
C,0,-0.1624023532,2.2812643273,1.5364480066
C,0,-0.8926303793,3.2346912488,2.2566456744
C,0,-0.4601092733,3.6692056579,3.5082473764
C,0,0.7064957479,3.1483222357,4.0648144228

C,0,1.4495812938,2.201558396,3.3640795488
C,0,1.0201566,1.7862084552,2.1071192851
C,0,0.2449369333,2.7216378611,-1.2677635144
C,0,0.4134105669,4.085761582,-0.9884626763
C,0,1.1093192169,4.9011782311,-1.8760848837
C,0,1.646581405,4.363171104,-3.0467158147
C,0,1.4810005589,3.009447894,-3.328478632
C,0,0.7841278039,2.1870072519,-2.4428332026
C,0,-2.4181446983,2.0983904437,-0.2933535384
C,0,-2.8683409261,2.6641481378,-1.4929942944
C,0,-4.2237674333,2.9328706236,-1.672011438
C,0,-5.1381920283,2.6335807115,-0.6637875279
C,0,-4.6962758265,2.0566685532,0.5267012205
C,0,-3.3438413234,1.782915733,0.7127283227
H,0,0.7007249062,-3.5740308662,1.0776880443
H,0,1.1803789332,-4.8463867749,3.1469594753
H,0,3.1487899931,-4.2517797568,4.5543677114
H,0,4.640976653,-2.3796707982,3.8684664032
H,0,4.1793281193,-1.1189053441,1.7830498044
H,0,4.3857174427,-3.2299784823,-0.3097349432
H,0,5.3774843509,-4.6335117968,-2.095036212
H,0,4.3289004492,-4.7102004519,-4.3532311829
H,0,2.270933007,-3.3808844951,-4.8100618525
H,0,1.2637286786,-1.9856288061,-3.0235852917
H,0,3.1166885123,3.1246522269,1.2604827431
H,0,4.9902713633,3.4699861415,-0.3403186912
H,0,5.6609978998,1.6426816926,-1.8977666363
H,0,4.4369420106,-0.5204416097,-1.8655004541
H,0,-1.8196557167,3.6321297599,1.8377274198
H,0,-1.0468908487,4.4103170997,4.0553075927
H,0,1.0378936871,3.4736863227,5.0536312978
H,0,2.3577701687,1.7631218272,3.7821705668
H,0,0.0027125607,4.5134990496,-0.0706695924
H,0,1.2339888264,5.9634883924,-1.6518341085
H,0,2.1954973002,5.0045138987,-3.7409395788
H,0,1.8976031912,2.582545506,-4.2437605994
H,0,0.6392769803,1.1282228215,-2.6737702345
H,0,-2.159181238,2.8931850888,-2.291185872
H,0,-4.5654635342,3.3753005429,-2.6108182514
H,0,-6.2011870859,2.8408210171,-0.8096125227
H,0,-5.4066049426,1.7949611989,1.3139672629
H,0,-3.0179709295,1.3075246372,1.6411655223
Br,0,-1.1873903916,-0.9146949715,-2.701513493
S,0,-1.2479869192,-1.2164872433,1.4904476883
N,0,-3.7760570888,-1.3198734903,2.2234119894
N,0,-3.4198169938,-1.472622339,-0.0945338616
C,0,-2.9862707937,-1.3327487829,1.2036675053
C,0,-5.1365343809,-1.4700584363,2.0087853224
C,0,-5.6506939235,-1.56003006,0.7100457297
C,0,-4.7879808576,-1.5457352757,-0.363035565
H,0,-2.7509044868,-1.4383653165,-0.8649448226
H,0,-5.7739067785,-1.4893305182,2.894279491
H,0,-6.7268485302,-1.635038514,0.5375671155
H,0,-5.0790065809,-1.5957085653,-1.4106087811
Sum of electronic and zero-point Energies= -7018.218410

Sum of electronic and thermal Energies= -7018.173899
Sum of electronic and thermal Enthalpies= -7018.172955
Sum of electronic and thermal Free Energies= -7018.303141

[CuBr(DPEphos)(pymtH)], **5** (S_0)

Charge = 0 Multiplicity = 3
Cu,0,-0.2888910784,-0.6474392193,-0.4835895654
P,0,-0.6683219975,1.6332286004,-0.1039000308
P,0,2.0211502925,-1.4138581716,-0.2837893772
O,0,1.7188418927,0.8151951349,1.4416458794
C,0,2.4201261442,-2.2745311052,1.2823878047
C,0,1.5785208205,-3.3223080091,1.6783677763
C,0,1.8452293529,-4.0333376279,2.8460741876
C,0,2.9450267849,-3.697717859,3.6347160692
C,0,3.7796968031,-2.6485958028,3.2516188926
C,0,3.520103004,-1.9388165363,2.0800704316
C,0,2.7775739935,-2.4899816116,-1.559121292
C,0,3.927372567,-3.2507208405,-1.3018518417
C,0,4.4826641146,-4.0419934112,-2.3043635971
C,0,3.8941236868,-4.0848547009,-3.5692676047
C,0,2.7453667038,-3.3394794796,-3.8265678329
C,0,2.1828856135,-2.5464598588,-2.8259363793
C,0,3.0997644897,0.0662769189,-0.2831588405
C,0,2.7451423973,1.1077396346,0.5918733118
C,0,3.4168461864,2.3271045488,0.5786876032
C,0,4.4645981443,2.5123075405,-0.3229983433
C,0,4.8394180552,1.4924431876,-1.194302584
C,0,4.155810131,0.2768196917,-1.1734511408
C,0,-0.1624023532,2.2812643273,1.5364480066
C,0,-0.8926303793,3.2346912488,2.2566456744
C,0,-0.4601092733,3.6692056579,3.5082473764
C,0,0.7064957479,3.1483222357,4.0648144228
C,0,1.4495812938,2.201558396,3.3640795488
C,0,1.0201566,1.7862084552,2.1071192851
C,0,0.2449369333,2.7216378611,-1.2677635144
C,0,0.4134105669,4.085761582,-0.9884626763
C,0,1.1093192169,4.9011782311,-1.8760848837
C,0,1.646581405,4.363171104,-3.0467158147
C,0,1.4810005589,3.009447894,-3.328478632
C,0,0.7841278039,2.1870072519,-2.4428332026
C,0,-2.4181446983,2.0983904437,-0.2933535384
C,0,-2.8683409261,2.6641481378,-1.4929942944
C,0,-4.2237674333,2.9328706236,-1.672011438
C,0,-5.1381920283,2.6335807115,-0.6637875279
C,0,-4.6962758265,2.0566685532,0.5267012205
C,0,-3.3438413234,1.782915733,0.7127283227
H,0,0.7007249062,-3.5740308662,1.0776880443
H,0,1.1803789332,-4.8463867749,3.1469594753
H,0,3.1487899931,-4.2517797568,4.5543677114
H,0,4.640976653,-2.3796707982,3.8684664032
H,0,4.1793281193,-1.1189053441,1.7830498044
H,0,4.3857174427,-3.2299784823,-0.3097349432
H,0,5.3774843509,-4.6335117968,-2.095036212
H,0,4.3289004492,-4.7102004519,-4.3532311829

H,0,2.270933007,-3.3808844951,-4.8100618525
H,0,1.2637286786,-1.9856288061,-3.0235852917
H,0,3.1166885123,3.1246522269,1.2604827431
H,0,4.9902713633,3.4699861415,-0.3403186912
H,0,5.6609978998,1.6426816926,-1.8977666363
H,0,4.4369420106,-0.5204416097,-1.8655004541
H,0,-1.8196557167,3.6321297599,1.8377274198
H,0,-1.0468908487,4.4103170997,4.0553075927
H,0,1.0378936871,3.4736863227,5.0536312978
H,0,2.3577701687,1.7631218272,3.7821705668
H,0,0.0027125607,4.5134990496,-0.0706695924
H,0,1.2339888264,5.9634883924,-1.6518341085
H,0,2.1954973002,5.0045138987,-3.7409395788
H,0,1.8976031912,2.582545506,-4.2437605994
H,0,0.6392769803,1.1282228215,-2.6737702345
H,0,-2.159181238,2.8931850888,-2.291185872
H,0,-4.5654635342,3.3753005429,-2.6108182514
H,0,-6.2011870859,2.8408210171,-0.8096125227
H,0,-5.4066049426,1.7949611989,1.3139672629
H,0,-3.0179709295,1.3075246372,1.6411655223
Br,0,-1.1873903916,-0.9146949715,-2.701513493
S,0,-1.2479869192,-1.2164872433,1.4904476883
N,0,-3.7760570888,-1.3198734903,2.2234119894
N,0,-3.4198169938,-1.472622339,-0.0945338616
C,0,-2.9862707937,-1.3327487829,1.2036675053
C,0,-5.1365343809,-1.4700584363,2.0087853224
C,0,-5.6506939235,-1.56003006,0.7100457297
C,0,-4.7879808576,-1.5457352757,-0.363035565
H,0,-2.7509044868,-1.4383653165,-0.8649448226
H,0,-5.7739067785,-1.4893305182,2.894279491
H,0,-6.7268485302,-1.635038514,0.5375671155
H,0,-5.0790065809,-1.5957085653,-1.4106087811

[CuBr(DPEphos)(pymtH)], **5** (T_1)

Charge = 0 Multiplicity = 3
Cu,0,-0.2888910784,-0.6474392193,-0.4835895654
P,0,-0.6683219975,1.6332286004,-0.1039000308
P,0,2.0211502925,-1.4138581716,-0.2837893772
O,0,1.7188418927,0.8151951349,1.4416458794
C,0,2.4201261442,-2.2745311052,1.2823878047
C,0,1.5785208205,-3.3223080091,1.6783677763
C,0,1.8452293529,-4.0333376279,2.8460741876
C,0,2.9450267849,-3.697717859,3.6347160692
C,0,3.7796968031,-2.6485958028,3.2516188926
C,0,3.520103004,-1.9388165363,2.0800704316
C,0,2.7775739935,-2.4899816116,-1.559121292
C,0,3.927372567,-3.2507208405,-1.3018518417
C,0,4.4826641146,-4.0419934112,-2.3043635971
C,0,3.8941236868,-4.0848547009,-3.5692676047
C,0,2.7453667038,-3.3394794796,-3.8265678329
C,0,2.1828856135,-2.5464598588,-2.8259363793
C,0,3.0997644897,0.0662769189,-0.2831588405
C,0,2.7451423973,1.1077396346,0.5918733118
C,0,3.4168461864,2.3271045488,0.5786876032

C,0,4.4645981443,2.5123075405,-0.3229983433
C,0,4.8394180552,1.4924431876,-1.194302584
C,0,4.155810131,0.2768196917,-1.1734511408
C,0,-0.1624023532,2.2812643273,1.5364480066
C,0,-0.8926303793,3.2346912488,2.2566456744
C,0,-0.4601092733,3.6692056579,3.5082473764
C,0,0.7064957479,3.1483222357,4.0648144228
C,0,1.4495812938,2.201558396,3.3640795488
C,0,1.0201566,1.7862084552,2.1071192851
C,0,0.2449369333,2.7216378611,-1.2677635144
C,0,0.4134105669,4.085761582,-0.9884626763
C,0,1.1093192169,4.9011782311,-1.8760848837
C,0,1.646581405,4.363171104,-3.0467158147
C,0,1.4810005589,3.009447894,-3.328478632
C,0,0.7841278039,2.1870072519,-2.4428332026
C,0,-2.4181446983,2.0983904437,-0.2933535384
C,0,-2.8683409261,2.6641481378,-1.4929942944
C,0,-4.2237674333,2.9328706236,-1.672011438
C,0,-5.1381920283,2.6335807115,-0.6637875279
C,0,-4.6962758265,2.0566685532,0.5267012205
C,0,-3.3438413234,1.782915733,0.7127283227
H,0,0.7007249062,-3.5740308662,1.0776880443
H,0,1.1803789332,-4.8463867749,3.1469594753
H,0,3.1487899931,-4.2517797568,4.5543677114
H,0,4.640976653,-2.3796707982,3.8684664032
H,0,4.1793281193,-1.1189053441,1.7830498044
H,0,4.3857174427,-3.2299784823,-0.3097349432
H,0,5.3774843509,-4.6335117968,-2.095036212
H,0,4.3289004492,-4.7102004519,-4.3532311829
H,0,2.270933007,-3.3808844951,-4.8100618525
H,0,1.2637286786,-1.9856288061,-3.0235852917
H,0,3.1166885123,3.1246522269,1.2604827431
H,0,4.9902713633,3.4699861415,-0.3403186912
H,0,5.6609978998,1.6426816926,-1.8977666363
H,0,4.4369420106,-0.5204416097,-1.8655004541
H,0,-1.8196557167,3.6321297599,1.8377274198
H,0,-1.0468908487,4.4103170997,4.0553075927
H,0,1.0378936871,3.4736863227,5.0536312978
H,0,2.3577701687,1.7631218272,3.7821705668
H,0,0.0027125607,4.5134990496,-0.0706695924
H,0,1.2339888264,5.9634883924,-1.6518341085
H,0,2.1954973002,5.0045138987,-3.7409395788
H,0,1.8976031912,2.582545506,-4.2437605994
H,0,0.6392769803,1.1282228215,-2.6737702345
H,0,-2.159181238,2.8931850888,-2.291185872
H,0,-4.5654635342,3.3753005429,-2.6108182514
H,0,-6.2011870859,2.8408210171,-0.8096125227
H,0,-5.4066049426,1.7949611989,1.3139672629
H,0,-3.0179709295,1.3075246372,1.6411655223
Br,0,-1.1873903916,-0.9146949715,-2.701513493
S,0,-1.2479869192,-1.2164872433,1.4904476883
N,0,-3.7760570888,-1.3198734903,2.2234119894
N,0,-3.4198169938,-1.472622339,-0.0945338616
C,0,-2.9862707937,-1.3327487829,1.2036675053
C,0,-5.1365343809,-1.4700584363,2.0087853224

C,0,-5.6506939235,-1.56003006,0.7100457297
C,0,-4.7879808576,-1.5457352757,-0.363035565
H,0,-2.7509044868,-1.4383653165,-0.8649448226
H,0,-5.7739067785,-1.4893305182,2.894279491
H,0,-6.7268485302,-1.635038514,0.5375671155
H,0,-5.0790065809,-1.5957085653,-1.4106087811
Sum of electronic and zero-point Energies= -7018.218410
Sum of electronic and thermal Energies= -7018.173899
Sum of electronic and thermal Enthalpies= -7018.172955
Sum of electronic and thermal Free Energies= -7018.303141

[CuI(DPEphos)(pymtH)], **6** (S_0)

Charge = 0 Multiplicity = 1
Cu,0,-0.2673820938,-0.6129770246,-0.4181300246
P,0,-0.4857381963,1.7140015972,-0.0712663236
P,0,1.9264240778,-1.3713162047,-0.2309493915
O,0,1.8630089579,0.8699689858,1.5678560224
C,0,2.3553553679,-2.2224609868,1.3382283154
C,0,1.5229363762,-3.2712870489,1.7499516263
C,0,1.8024160726,-3.9751921569,2.9189266592
C,0,2.9088960994,-3.6325363626,3.6952709938
C,0,3.7372094807,-2.5847060681,3.2957615998
C,0,3.4634542307,-1.8825241304,2.1225267685
C,0,2.6577334313,-2.4985709554,-1.4843842145
C,0,3.8094184785,-3.2558937259,-1.2246972581
C,0,4.3396115286,-4.0874638351,-2.2079489865
C,0,3.7246969021,-4.1751992628,-3.4580945629
C,0,2.5753936901,-3.4323305342,-3.7189379331
C,0,2.0392175533,-2.6000062221,-2.7358054264
C,0,3.0504350104,0.0772385545,-0.2899111834
C,0,2.7933921322,1.131173653,0.6040673187
C,0,3.4761790738,2.3419873697,0.515175027
C,0,4.4384244807,2.5083888622,-0.4794110265
C,0,4.7221018096,1.4733779735,-1.3669844622
C,0,4.0290611258,0.267001485,-1.2700103264
C,0,0.027963182,2.4136355565,1.5582278125
C,0,-0.6760801276,3.4121635394,2.2452726308
C,0,-0.2604311997,3.8582841264,3.4982877373
C,0,0.8679418419,3.3019075671,4.0985381194
C,0,1.5854443208,2.3094317041,3.436776845
C,0,1.1713069083,1.8827395274,2.1769640469
C,0,0.3523352502,2.8445582231,-1.2539680294
C,0,0.4066359367,4.232306544,-1.0635139808
C,0,1.0656284317,5.0420807175,-1.9843462405
C,0,1.6781574575,4.4740970592,-3.1033459947
C,0,1.6295340796,3.0957123279,-3.2973749296
C,0,0.9709079461,2.2822105551,-2.3753090297
C,0,-2.2518470089,2.1956711252,-0.1715955937
C,0,-2.7782956069,2.8042297705,-1.3173126814
C,0,-4.1479239936,3.0470377953,-1.4218234867
C,0,-5.0083195537,2.6844014875,-0.3876856006
C,0,-4.4931778795,2.0670111497,0.7533974135
C,0,-3.1273298793,1.8150432744,0.8585842422
H,0,0.6414041671,-3.5303326885,1.1573243138
H,0,1.1428239419,-4.7886589858,3.2305202295

H,0,3.1232208709,-4.1802358412,4.6164411906
H,0,4.6050212545,-2.3102566506,3.9011004939
H,0,4.1190981264,-1.0643107047,1.8136331728
H,0,4.29004275,-3.2006226156,-0.2445755695
H,0,5.2362305366,-4.6752039387,-1.9951295008
H,0,4.1401058027,-4.8319999748,-4.2267981529
H,0,2.079880509,-3.5048757926,-4.6902253568
H,0,1.1223643824,-2.0372264698,-2.9360525082
H,0,3.2485776583,3.1478652549,1.2152235511
H,0,4.9694977299,3.4600972076,-0.5561686815
H,0,5.4785144351,1.6047977838,-2.1436636861
H,0,4.2380487103,-0.5392384572,-1.9767589218
H,0,-1.5776461536,3.8358024,1.7966473287
H,0,-0.828555549,4.6375653027,4.0114469563
H,0,1.1891902617,3.6369263258,5.0875947674
H,0,2.4654558817,1.8427893413,3.8836899634
H,0,-0.0652372845,4.6838154601,-0.1871627331
H,0,1.1031594346,6.1232294873,-1.8281336408
H,0,2.1959325479,5.1113184229,-3.8249293686
H,0,2.107679375,2.644624403,-4.1700504753
H,0,0.9229733938,1.2007723309,-2.5240451506
H,0,-2.1152125343,3.086133426,-2.137915078
H,0,-4.542274094,3.5237280213,-2.3226735355
H,0,-6.0801941928,2.8818818822,-0.4694816774
H,0,-5.159408356,1.7754709932,1.5696209114
H,0,-2.73707528,1.3154690309,1.7495629489
I,0,-1.4689809425,-0.8325530075,-2.8334526197
S,0,-1.4937798302,-1.4912589756,1.4331882016
N,0,-4.0218952086,-2.1036364859,1.9630865526
N,0,-3.5610194231,-1.4842258839,-0.242476908
C,0,-3.1178064019,-1.7064504874,1.0358395186
C,0,-5.2776223383,-2.2474329404,1.6113771194
C,0,-5.7727944148,-2.0154986679,0.3089537355
C,0,-4.8374091721,-1.6242770676,-0.6168952922
H,0,-2.8575141793,-1.2044557232,-0.9668563302
H,0,-5.966767075,-2.570842301,2.4026324848
H,0,-6.8232478368,-2.1425129337,0.051288385
H,0,-5.0482701983,-1.4118024932,-1.6685651302
Sum of electronic and zero-point Energies= -4742.454595
Sum of electronic and thermal Energies= -4742.410446
Sum of electronic and thermal Enthalpies= -4742.409502
Sum of electronic and thermal Free Energies= -4742.539128

[CuI(DPEphos)(pymtH)], **6** (T_1)

Charge = 0 Multiplicity = 3
Cu,0,-0.3112828948,-0.6450186502,-0.5525955544
P,0,-0.6877929441,1.6359050386,-0.1496145611
P,0,2.0138935898,-1.4135900747,-0.3429913046
O,0,1.6826289991,0.7990641881,1.399009974
C,0,2.3710795714,-2.2941291525,1.222851728
C,0,1.5295698247,-3.3568536065,1.5776909977
C,0,1.7667936381,-4.0807800691,2.7438373667
C,0,2.8362984343,-3.7432979963,3.5721802511
C,0,3.6714060587,-2.6807057268,3.229380301
C,0,3.441814254,-1.9584817957,2.0592204688

C,0,2.8099041992,-2.4758180204,-1.6073665025
C,0,3.898960672,-3.3053454929,-1.3033728976
C,0,4.4900512009,-4.0794679254,-2.2992037228
C,0,3.9996592247,-4.0361060968,-3.6049808028
C,0,2.9120698399,-3.2205531213,-3.9109189303
C,0,2.3144386208,-2.4460474438,-2.9170121153
C,0,3.1023292653,0.0601377448,-0.2967380609
C,0,2.7322945028,1.094711504,0.5803286183
C,0,3.4110289752,2.3102676069,0.5962551361
C,0,4.4866313944,2.4953916761,-0.2718124833
C,0,4.8810512916,1.4800519038,-1.1399252387
C,0,4.1870697741,0.2701576837,-1.1520974463
C,0,-0.1936462164,2.2650794806,1.5035317408
C,0,-0.9264029609,3.2119285553,2.229286761
C,0,-0.4953473052,3.6383876501,3.4841454931
C,0,0.6708009336,3.1146847402,4.0390038627
C,0,1.4141162926,2.1711311031,3.3341164215
C,0,0.9862699668,1.7653705559,2.0736750232
C,0,0.246957448,2.7397525869,-1.2822194977
C,0,0.3331292285,4.115966481,-1.0240778013
C,0,1.0516021735,4.9454452602,-1.8797523438
C,0,1.6955405626,4.4096870316,-2.9966933978
C,0,1.6154740528,3.0439745779,-3.2558399696
C,0,0.8942102923,2.2089358177,-2.4022193779
C,0,-2.4326291538,2.1207514836,-0.3390343355
C,0,-2.8715891569,2.7397286441,-1.5165388868
C,0,-4.2237983877,3.0268804496,-1.6914604517
C,0,-5.1463370314,2.6922991147,-0.7018754108
C,0,-4.71561986,2.0634919186,0.4661819346
C,0,-3.3660003733,1.7729361958,0.6490944136
H,0,0.6753027846,-3.6115410643,0.9454024556
H,0,1.1020294133,-4.905137956,3.0123468328
H,0,3.0160767947,-4.3067389258,4.4911274116
H,0,4.5097636565,-2.4111793458,3.8767730833
H,0,4.1029977284,-1.1297460619,1.7931567669
H,0,4.2819864249,-3.3511290424,-0.2808541865
H,0,5.3366778452,-4.7248879297,-2.0521380178
H,0,4.4622085006,-4.6483324363,-4.3833441659
H,0,2.5120330004,-3.1932685068,-4.9273865323
H,0,1.4408226909,-1.8330783094,-3.1572253081
H,0,3.0952014695,3.1050771805,1.2739745141
H,0,5.0189902985,3.4495206147,-0.2652878458
H,0,5.7258056439,1.6295679248,-1.8155620167
H,0,4.483149453,-0.5227167167,-1.8428164437
H,0,-1.8534651752,3.611084712,1.8123661493
H,0,-1.0833544767,4.3754412469,4.0353605297
H,0,1.0006996417,3.4341360039,5.0302272114
H,0,2.3209288045,1.7289450363,3.7512100158
H,0,-0.1611767741,4.5429565421,-0.1479898515
H,0,1.1104387808,6.0169148172,-1.6729843851
H,0,2.2615626281,5.0622272017,-3.6662763865
H,0,2.1167897581,2.6181079538,-4.1280144692
H,0,0.8208897335,1.1398083033,-2.6148414229
H,0,-2.1567406891,2.9962504742,-2.3012776938
H,0,-4.5565903658,3.5104136229,-2.6129884254

H,0,-6.2068654904,2.9137704397,-0.8448780879
H,0,-5.4315409354,1.7768262391,1.2396506827
H,0,-3.0490459503,1.2652083194,1.5637614889
I,0,-1.312737773,-0.9493057218,-2.9224319831
S,0,-1.1931602745,-1.2148380242,1.4628780498
N,0,-3.6806730701,-1.2540179089,2.3394534567
N,0,-3.4435799315,-1.5796840459,0.0246576866
C,0,-2.9431269117,-1.3433253537,1.2843895092
C,0,-5.0501394278,-1.4162105042,2.2044717996
C,0,-5.62990876,-1.5953963768,0.9432202476
C,0,-4.8232343946,-1.6614584201,-0.1711322395
H,0,-2.8119882631,-1.5934888394,-0.7751488758
H,0,-5.6420344163,-1.3696574495,3.1200282901
H,0,-6.7136055946,-1.6766457291,0.8315498894
H,0,-5.166807374,-1.7828217839,-1.1967091322
Sum of electronic and zero-point Energies= -4742.383266
Sum of electronic and thermal Energies= -4742.338655
Sum of electronic and thermal Enthalpies= -4742.337710
Sum of electronic and thermal Free Energies= -4742.468539

[CuCl(DPEphos)(pymtH)], **7** (S_0)

[CuCl(DPEphos)(pymtH)], **7** (T_1)

Charge = 0 Multiplicity = 3

Cu	-0.22705	-0.7153	-0.39378
Cl	-1.0284	-1.08227	-2.60176
S	-1.4871	-1.49053	1.35473
P	-0.68067	1.57362	-0.06884
P	2.10166	-1.36924	-0.23059
O	1.75559	0.8741	1.48933
N	-4.12483	-1.79926	1.76783
N	-3.48233	-1.73972	-0.50173
H	-2.73261	-1.64198	-1.17998
C	-3.22028	-1.68888	0.8488
C	-5.46591	-2.00822	1.37967
C	-5.78347	-2.01269	0.01524
H	-6.81554	-2.12714	-0.29483
C	-4.81474	-1.86677	-0.95284
C	-6.44921	-2.191	2.48211
H	-6.43836	-1.3405	3.17378
H	-6.2188	-3.07998	3.081
H	-7.46264	-2.30088	2.08994
C	-5.02309	-1.83125	-2.42495
H	-4.68613	-0.88215	-2.85791
H	-6.07979	-1.96035	-2.661
H	-4.45899	-2.62247	-2.9327
C	2.53851	-2.27103	1.34366
C	1.6885	-3.29307	1.76839
H	0.783	-3.51361	1.21651
C	1.99061	-4.01951	2.91623
H	1.32135	-4.80579	3.24289
C	3.1384	-3.72671	3.64795
H	3.36905	-4.28922	4.5446
C	3.985	-2.70445	3.22826

H	4.87831	-2.47013	3.79503
C	3.68792	-1.97855	2.07695
H	4.34942	-1.183	1.75574
C	2.86657	-2.43616	-1.55593
C	3.9889	-3.22902	-1.30432
H	4.42367	-3.25682	-0.31262
C	4.54233	-3.99769	-2.3243
H	5.41042	-4.61355	-2.12178
C	3.97728	-3.97983	-3.59779
H	4.40617	-4.58258	-4.38945
C	2.85289	-3.19849	-3.84614
H	2.39629	-3.19476	-4.82835
C	2.2934	-2.42776	-2.82913
H	1.39215	-1.85639	-3.01777
C	3.20641	0.12826	-0.20041
C	2.85529	1.15833	0.67602
C	3.56743	2.34729	0.72662
H	3.27181	3.13378	1.40788
C	4.66044	2.51192	-0.12122
H	5.21983	3.43895	-0.09164
C	5.0309	1.49967	-0.99967
H	5.87947	1.63201	-1.65859
C	4.30275	0.31144	-1.0374
H	4.58107	-0.47456	-1.72791
C	-0.17846	2.28574	1.57765
C	-0.95204	3.2152	2.27305
H	-1.89458	3.54455	1.85581
C	-0.53069	3.70504	3.50631
H	-1.14481	4.42252	4.03552
C	0.6661	3.26272	4.06246
H	0.98605	3.6282	5.03024
C	1.44838	2.33546	3.38177
H	2.36824	1.9533	3.8048
C	1.02663	1.86893	2.14481
C	0.2073	2.661	-1.29887
C	0.63243	3.94616	-0.95634
H	0.47613	4.32438	0.04607
C	1.25962	4.74714	-1.90604
H	1.58717	5.74354	-1.63444
C	1.4609	4.27154	-3.19946
H	1.95026	4.89646	-3.93687
C	1.03221	2.99274	-3.54162
H	1.18293	2.61667	-4.54609
C	0.40796	2.18314	-2.59559
H	0.06644	1.19066	-2.86833
C	-2.47008	2.05045	-0.2359
C	-2.9134	2.83222	-1.30223
H	-2.21135	3.20349	-2.03722
C	-4.26854	3.12996	-1.42647
H	-4.6077	3.73358	-2.25955
C	-5.18086	2.65068	-0.49159
H	-6.23507	2.87661	-0.59641
C	-4.7372	1.86974	0.57314
H	-5.44007	1.47561	1.29618
C	-3.38618	1.56673	0.70172

H -3.05706 0.94387 1.52473
Sum of electronic and zero-point Energies= -4984.902080
Sum of electronic and thermal Energies= -4984.854488
Sum of electronic and thermal Enthalpies= -4984.853543
Sum of electronic and thermal Free Energies= -4984.991069

[CuBr(DPEphos)(pymtH)], **8** (S_0)

Charge = 0 Multiplicity = 1
Cu,0,-0.2290773496,-0.6936279689,-0.3922973294
Br,0,-1.2684453785,-0.8984890199,-2.6752637327
S,0,-1.547369966,-1.6305742977,1.3516142339
P,0,-0.4935791174,1.632007388,-0.0772149188
P,0,1.969246896,-1.3837595363,-0.1817266481
O,0,1.8558497974,0.8620969047,1.6044622772
N,0,-4.094525624,-2.2724194585,1.6869264652
N,0,-3.5039858054,-1.5334741714,-0.4511871173
H,0,-2.7445444807,-1.2399238729,-1.1102109058
C,0,-3.1476286941,-1.8292250408,0.8374411295
C,0,-5.3403505536,-2.3981490127,1.2697031904
C,0,-5.7377724087,-2.0687614142,-0.0482694814
H,0,-6.773327491,-2.1627355032,-0.3749840664
C,0,-4.7645403123,-1.6244087338,-0.9174698918
C,0,-6.3371822062,-2.9334782009,2.2493767766
H,0,-5.9792515253,-2.7661096173,3.2728917162
H,0,-6.4481941445,-4.0211687997,2.1044262162
H,0,-7.3288958025,-2.4785354595,2.1137514837
C,0,-5.0037735048,-1.2117325934,-2.3281485111
H,0,-4.8948611788,-0.1184428331,-2.4138080409
H,0,-6.0110547773,-1.4983185259,-2.6539547184
H,0,-4.2479197364,-1.652743476,-2.9950925541
C,0,2.4292716972,-2.225811875,1.3837459275
C,0,1.5868379142,-3.2494906394,1.8358222214
H,0,0.6760810873,-3.4891191835,1.2801583983
C,0,1.892226422,-3.949767391,3.0006883931
H,0,1.2244207333,-4.7435192197,3.3441209643
C,0,3.0346604751,-3.6278674777,3.7325555279
H,0,3.2699254224,-4.1728474695,4.6502562911
C,0,3.8716770629,-2.6024364289,3.294320744
H,0,4.7662380088,-2.3425181773,3.866274619
C,0,3.5718643675,-1.9040425371,2.1252407104
H,0,4.2327429645,-1.1020569045,1.7858811121
C,0,2.7026378444,-2.4944978896,-1.4481178951
C,0,3.8748381286,-3.2285690268,-1.2161580475
H,0,4.3744676758,-3.1673510064,-0.2458909724
C,0,4.4019210375,-4.0444312378,-2.2142860928
H,0,5.314933445,-4.6141357093,-2.0231364928
C,0,3.7628531661,-4.1391712777,-3.4516930818
H,0,4.1761608314,-4.7829366837,-4.2325185713
C,0,2.5918867176,-3.4208499621,-3.6839060925
H,0,2.0780090575,-3.5006007526,-4.6451097857
C,0,2.0578382873,-2.6044296483,-2.686234555
H,0,1.1232886444,-2.0617103414,-2.8627183705
C,0,3.0708900191,0.0821542875,-0.2424386461
C,0,2.7925446185,1.1326583618,0.6492118414

C,0,3.4648524543,2.3498472278,0.5701322979
H,0,3.2218849112,3.1521587461,1.2692356674
C,0,4.4385322131,2.5267190165,-0.4116059434
H,0,4.9627454977,3.4829289492,-0.4794783344
C,0,4.7418598972,1.4961500832,-1.2977262831
H,0,5.5056753398,1.6362149834,-2.0655918921
C,0,4.0580750811,0.2834730324,-1.2115693232
H,0,4.2822524806,-0.5188652709,-1.9181777386
C,0,-0.0176555208,2.360838225,1.5486590592
C,0,-0.7586737826,3.3457759076,2.2160193603
H,0,-1.6634217062,3.7412107435,1.7484414942
C,0,-0.3756314752,3.8130595563,3.4717761484
H,0,-0.9725836744,4.5807170384,3.9695042831
C,0,0.7573066021,3.2917156364,4.094318549
H,0,1.0538398755,3.6430739347,5.0854246691
C,0,1.5110118724,2.3126510401,3.4527377417
H,0,2.3950563788,1.8723924178,3.918042048
C,0,1.1293397601,1.863940021,2.1902869749
C,0,0.327355521,2.7628729444,-1.2724384665
C,0,0.4720440717,4.138120658,-1.0430558889
H,0,0.0946138814,4.5822650641,-0.118570586
C,0,1.1044007055,4.9449218571,-1.9855380224
H,0,1.2144024378,6.0159699883,-1.7969748043
C,0,1.5978474888,4.3871326825,-3.1662679257
H,0,2.094923213,5.0218167787,-3.9045034432
C,0,1.4569605164,3.0211131374,-3.4003593411
H,0,1.8415103619,2.5780431682,-4.322184247
C,0,0.8282715763,2.2088392729,-2.4563283849
H,0,0.7056603626,1.1376995001,-2.6387965936
C,0,-2.267471705,2.0764097196,-0.2104068304
C,0,-2.7870108057,2.6970465152,-1.3526675806
H,0,-2.1147764757,3.0140447651,-2.1528422543
C,0,-4.1601364521,2.9117443419,-1.4766880274
H,0,-4.5492534287,3.4033162259,-2.372053057
C,0,-5.0303827214,2.5080123817,-0.4653139637
H,0,-6.1048119102,2.6845268335,-0.5610972457
C,0,-4.5209082775,1.8783263435,0.6719055573
H,0,-5.1944760921,1.5536074635,1.4692073501
C,0,-3.1518118174,1.6555747794,0.796344629
H,0,-2.7644489203,1.1409157238,1.6801666285
Sum of electronic and zero-point Energies= -7096.732119
Sum of electronic and thermal Energies= -7096.684480
Sum of electronic and thermal Enthalpies= -7096.683536
Sum of electronic and thermal Free Energies= -7096.820895

[CuBr(DPEphos)(pymtH)], **8** (T_1)

Charge = 0 Multiplicity = 3
Cu,0,-0.2448134772,-0.7180006471,-0.626612276
Br,0,-1.0366349157,-0.9192784116,-2.8890874684
S,0,-1.2342412985,-1.3812925709,1.3023549496
P,0,-0.7027020332,1.5444752195,-0.201600015
P,0,2.0698783648,-1.4490226052,-0.343728602
O,0,1.6257772162,0.7234802006,1.4258740017
N,0,-3.7644893141,-1.6417354957,1.9750132794

N,0,-3.372443549,-1.5554644603,-0.3384686131
H,0,-2.6867003677,-1.4804640604,-1.0903835082
C,0,-2.9631294558,-1.533937386,0.972902021
C,0,-5.1238161741,-1.8169572223,1.7350794181
C,0,-5.6037408176,-1.7569102043,0.4172459161
H,0,-6.6769505108,-1.8210770352,0.2187383334
C,0,-4.7402495314,-1.6024257387,-0.6483690599
C,0,-5.9877465743,-2.0235746706,2.9324473414
H,0,-5.8743876249,-1.1971373058,3.6568198756
H,0,-5.7107130998,-2.9454139997,3.4754068018
H,0,-7.0497463511,-2.0990271808,2.656621348
C,0,-5.1029262281,-1.4647835661,-2.0818091922
H,0,-4.7796339377,-0.4883485511,-2.4870183347
H,0,-6.1895094918,-1.5530544774,-2.2159257847
H,0,-4.6133216087,-2.2365578322,-2.7032028027
C,0,2.4231886971,-2.3478057974,1.212023027
C,0,1.6012612851,-3.435880518,1.5344288424
H,0,0.764571378,-3.7003116022,0.8828548647
C,0,1.834520792,-4.1721034005,2.6936745873
H,0,1.1849774865,-5.016201291,2.9369847669
C,0,2.8804059346,-3.822667536,3.5469589092
H,0,3.0570600629,-4.3965052375,4.4600707857
C,0,3.6955153823,-2.7349206492,3.2364861391
H,0,4.5150262839,-2.4555944519,3.9035774588
C,0,3.4695969101,-1.9994789282,2.0738209681
H,0,4.1136337829,-1.1492208624,1.8345894305
C,0,2.9048609256,-2.4662716711,-1.6178341026
C,0,4.0477889281,-3.2269562414,-1.3318714462
H,0,4.4539712632,-3.2423765737,-0.3172214452
C,0,4.6620609797,-3.9719983838,-2.335500073
H,0,5.5511250643,-4.5640044147,-2.1042116169
C,0,4.1399701328,-3.9679511933,-3.6299135513
H,0,4.6212570265,-4.5570582308,-4.4147840199
C,0,2.9979735288,-3.222716107,-3.9163625195
H,0,2.575033269,-3.2286159422,-4.9238955475
C,0,2.3761014001,-2.476860748,-2.9148981195
H,0,1.4612637642,-1.9178910925,-3.1361102205
C,0,3.1079717635,0.0565929849,-0.2499914689
C,0,2.6842756423,1.0636955676,0.6349477771
C,0,3.3222492147,2.3001776573,0.684917184
H,0,2.9667251962,3.0723670555,1.3691129302
C,0,4.4076725258,2.5364137573,-0.1582078416
H,0,4.9071853141,3.5075859607,-0.1250278196
C,0,4.8522467188,1.5504490872,-1.0357513947
H,0,5.7029428625,1.7405015976,-1.6934971525
C,0,4.200469612,0.3181401917,-1.0808618298
H,0,4.5354355708,-0.4522411708,-1.7792547919
C,0,-0.2837422299,2.1543460022,1.4778391406
C,0,-1.0630427483,3.0732516476,2.1913443611
H,0,-1.9788659566,3.4650155426,1.7435144517
C,0,-0.6933361384,3.4803873424,3.4718975706
H,0,-1.3169016308,4.195686926,4.0126289504
C,0,0.4577580294,2.9647946323,4.0646551608
H,0,0.740227176,3.2687948096,5.0752080143
C,0,1.2472388587,2.0498525636,3.3724361859

H,0,2.1440689583,1.6151906863,3.8180510933
C,0,0.8807403901,1.6627619934,2.0868888183
C,0,0.2284497065,2.6933784796,-1.2913202737
C,0,0.3346832243,4.05497416,-0.9716003083
H,0,-0.137485322,4.4456378434,-0.0669760995
C,0,1.0462538114,4.9157518239,-1.8020348001
H,0,1.1214903085,5.9757462889,-1.5469428849
C,0,1.6621009078,4.4259238792,-2.9551105132
H,0,2.2229906924,5.1027818086,-3.6045997587
C,0,1.5605946611,3.0745563469,-3.2756801038
H,0,2.039683964,2.6849706264,-4.176930339
C,0,0.8474095804,2.2071955864,-2.4477525746
H,0,0.7526647057,1.1501221264,-2.7088544103
C,0,-2.4554337057,1.9707613161,-0.4465242395
C,0,-2.8751405367,2.5751581037,-1.6385065388
H,0,-2.1424554217,2.8625269163,-2.395534072
C,0,-4.2311007327,2.806487265,-1.8629907985
H,0,-4.549718588,3.2803705791,-2.7945737395
C,0,-5.1748715328,2.431638712,-0.9081017246
H,0,-6.2375982259,2.6106405113,-1.0891760311
C,0,-4.7619999556,1.8172014251,0.2742976368
H,0,-5.4947246247,1.5001537846,1.0193463424
C,0,-3.4092578306,1.5814220577,0.505513737
H,0,-3.1027777118,1.0797343984,1.4270374082
Sum of electronic and zero-point Energies= -7096.652298
Sum of electronic and thermal Energies= -7096.604343
Sum of electronic and thermal Enthalpies= -7096.603399
Sum of electronic and thermal Free Energies= -7096.740987

[CuI(DPEphos)(pymtH)], **9** (S_0)

Charge = 0 Multiplicity = 1
Cu,0,-0.0836902128,-0.5912914532,-0.2210817131
I,0,-1.083020632,-0.8371274746,-2.7139057383
S,0,-1.3149032608,-1.6763092135,1.5048579351
P,0,-0.5671130351,1.6939237143,0.1749199032
P,0,2.1676712054,-1.1073489866,0.0874566938
O,0,1.748559393,1.0427707224,1.9459330256
N,0,-3.7672167372,-2.5877667296,1.8961678796
N,0,-3.3267527192,-1.7431220441,-0.2393309469
H,0,-2.6225192645,-1.3600006831,-0.904961421
C,0,-2.898878703,-2.0280890175,1.0297742239
C,0,-5.006991869,-2.8278513587,1.5163621319
C,0,-5.479986713,-2.5095514748,0.2192457696
H,0,-6.5114430757,-2.7012144476,-0.0765481321
C,0,-4.5883399279,-1.9520569735,-0.6697452761
C,0,-5.9205697323,-3.4708608042,2.5120753469
H,0,-5.4300522682,-3.5127372807,3.4917365692
H,0,-6.1659792501,-4.4968758996,2.1928212519
H,0,-6.8703587575,-2.9203970932,2.5923116322
C,0,-4.9178702625,-1.542753415,-2.0625483556
H,0,-4.8751916096,-0.4447777348,-2.1463309886
H,0,-5.9213172029,-1.8862600998,-2.3417501009

H,0,-4.1737757309,-1.9382865886,-2.7706332003
C,0,2.6038743191,-1.9613090079,1.653601768
C,0,1.8580898361,-3.0950443637,2.0006534226
H,0,1.0267274134,-3.4142421838,1.366475168
C,0,2.1583883261,-3.8077138369,3.1593538934
H,0,1.5661905281,-4.6881653242,3.4201934089
C,0,3.1980741017,-3.3900106731,3.9892847041
H,0,3.4284720281,-3.9456405028,4.9018244418
C,0,3.9380981877,-2.2566017274,3.6550051645
H,0,4.7522525318,-1.9222321988,4.3032949366
C,0,3.6437337295,-1.5450019069,2.4926394975
H,0,4.2298795998,-0.6593356364,2.2342423112
C,0,3.0953534338,-2.0965294389,-1.1532056592
C,0,4.2981008505,-2.7476285685,-0.8423121158
H,0,4.7006785807,-2.6956283419,0.1724425206
C,0,4.9797229385,-3.4689754517,-1.8194694227
H,0,5.9151872971,-3.9743304699,-1.5660680125
C,0,4.4673714258,-3.5513383307,-3.1152988038
H,0,5.0020034381,-4.1213884598,-3.8795901684
C,0,3.2682432425,-2.9147480324,-3.4278016037
H,0,2.8523004665,-2.9852219825,-4.4359237453
C,0,2.5805276805,-2.1937185791,-2.4512617696
H,0,1.6257689533,-1.7174629388,-2.6945416638
C,0,3.126605292,0.4561660814,0.1439663167
C,0,2.7019156413,1.4396668267,1.0538791884
C,0,3.2539059975,2.7185462803,1.0517364204
H,0,2.8983827165,3.466201427,1.7630886992
C,0,4.2524168472,3.026301407,0.129330003
H,0,4.6815889217,4.031018084,0.120593055
C,0,4.7014145969,2.0639890133,-0.7717642312
H,0,5.4863729193,2.306254438,-1.4913939379
C,0,4.1387103226,0.7878821092,-0.76168749
H,0,4.4783305687,0.0377681997,-1.47958543
C,0,-0.2383427939,2.3828522698,1.8556511614
C,0,-1.0896900729,3.2746084727,2.522406931
H,0,-1.9993155306,3.6184944215,2.0246779042
C,0,-0.8096128948,3.7126526842,3.8152877901
H,0,-1.4912978489,4.4074023168,4.3113403144
C,0,0.3288569164,3.2544016259,4.4762188517
H,0,0.5451696182,3.5822264828,5.4957488866
C,0,1.1915611538,2.3691726172,3.8357525736
H,0,2.0846867627,1.9802388469,4.3286379675
C,0,0.9114609563,1.9510376253,2.5368222929
C,0,0.23109488,2.9426980871,-0.9133148839
C,0,0.1448103607,4.3217260739,-0.6759526524
H,0,-0.4213679735,4.6961115981,0.1807336025
C,0,0.7856680099,5.2216980347,-1.5232421141
H,0,0.7137121106,6.2951670147,-1.3302522785
C,0,1.520231092,4.7535729921,-2.6145316715
H,0,2.0241367327,5.4614714544,-3.2777590453
C,0,1.6108722282,3.3847884053,-2.8553667471
H,0,2.1847577097,3.0118209189,-3.7069622878
C,0,0.970375249,2.4810429174,-2.0075129929
H,0,1.0311385989,1.4059536853,-2.1949260922
C,0,-2.3611873858,2.0082628143,-0.0320887195

C,0,-2.872308206,2.6302291967,-1.1774978798
H,0,-2.1899387508,3.0238897934,-1.9338360489
C,0,-4.2503183631,2.7486729858,-1.3612923544
H,0,-4.6328350073,3.2410362572,-2.2589370127
C,0,-5.1338000713,2.2458789988,-0.4076775172
H,0,-6.2128084886,2.347829489,-0.5496963499
C,0,-4.6321230972,1.6128956778,0.7313026708
H,0,-5.3161019923,1.2115682538,1.4836974207
C,0,-3.2573951734,1.4860876993,0.9149334086
H,0,-2.8737340953,0.9720887143,1.8009435157
Sum of electronic and zero-point Energies= -4820.895863
Sum of electronic and thermal Energies= -4820.848161
Sum of electronic and thermal Enthalpies= -4820.847217
Sum of electronic and thermal Free Energies= -4820.984544

[CuI(DPEphos)(pymtH)], **9** (T_1)

Charge = 0 Multiplicity = 3

Cu	-0.00104	-0.57503	-0.4498
I	-0.51559	-0.68392	-2.98483
S	-0.94968	-1.68606	1.28897
P	-1.00609	1.45719	0.15682
P	2.3823	-0.83368	0.09327
O	1.20099	0.88417	2.0286
N	-3.42101	-2.45772	1.7711
N	-2.90805	-2.16434	-0.5012
H	-2.20297	-1.90663	-1.18994
C	-2.59349	-2.13893	0.83661
C	-4.70038	-2.88012	1.42301
C	-5.09541	-2.84695	0.07685
H	-6.11774	-3.11463	-0.20337
C	-4.21396	-2.46646	-0.91566
C	-5.58079	-3.31948	2.5432
H	-5.67425	-2.53208	3.31225
H	-5.16429	-4.20315	3.05994
H	-6.58895	-3.57848	2.18797
C	-4.50361	-2.33208	-2.36576
H	-4.35657	-1.29252	-2.71189
H	-5.54	-2.62556	-2.58053
H	-3.83241	-2.96214	-2.97754
C	2.70002	-1.90893	1.54115
C	2.13868	-3.19292	1.52829
H	1.51478	-3.50783	0.68801
C	2.36138	-4.06706	2.58933
H	1.91657	-5.06471	2.56988
C	3.13355	-3.66414	3.67819
H	3.30041	-4.34802	4.51407
C	3.68626	-2.38446	3.70148
H	4.29059	-2.06345	4.55372
C	3.47204	-1.50899	2.6376
H	3.91301	-0.50912	2.65936
C	3.61497	-1.41857	-1.1313
C	4.81935	-2.02249	-0.74189
H	5.03417	-2.17817	0.31831
C	5.74083	-2.43253	-1.7026

H	6.67563	-2.9043	-1.38961
C	5.46902	-2.24758	-3.05882
H	6.19156	-2.57481	-3.8108
C	4.26985	-1.6567	-3.45195
H	4.0425	-1.52369	-4.51241
C	3.34255	-1.24702	-2.49422
H	2.38919	-0.81438	-2.81084
C	3.03373	0.80705	0.58487
C	2.26897	1.5493	1.50201
C	2.6065	2.85911	1.83349
H	1.9895	3.42216	2.53557
C	3.73242	3.43745	1.24827
H	3.99682	4.46639	1.50365
C	4.51288	2.71737	0.34707
H	5.39468	3.17422	-0.10696
C	4.15934	1.40935	0.01665
H	4.75813	0.8462	-0.70272
C	-0.96584	1.8752	1.94421
C	-2.01816	2.49798	2.62614
H	-2.92927	2.76326	2.08557
C	-1.92449	2.76627	3.99054
H	-2.75808	3.24979	4.50453
C	-0.77981	2.40379	4.69788
H	-0.71175	2.59605	5.77109
C	0.27869	1.78365	4.03865
H	1.18005	1.47203	4.56991
C	0.18457	1.53771	2.67231
C	-0.21651	2.92548	-0.61364
C	-0.53466	4.22012	-0.17757
H	-1.2635	4.36661	0.62336
C	0.07794	5.32519	-0.76076
H	-0.17819	6.33071	-0.41784
C	1.01721	5.14902	-1.77871
H	1.49929	6.01817	-2.23333
C	1.33811	3.86576	-2.21355
H	2.07176	3.72063	-3.00985
C	0.72443	2.75531	-1.63356
H	0.96488	1.74913	-1.98473
C	-2.7613	1.55377	-0.31829
C	-3.13964	2.22501	-1.4883
H	-2.39291	2.75811	-2.08049
C	-4.46977	2.20806	-1.90338
H	-4.75573	2.73517	-2.81672
C	-5.42774	1.51816	-1.16206
H	-6.46951	1.50457	-1.49191
C	-5.05308	0.83693	-0.00379
H	-5.79136	0.27748	0.57453
C	-3.7251	0.84723	0.41625
H	-3.44517	0.29324	1.31619

Sum of electronic and zero-point Energies= -4820.817070
Sum of electronic and thermal Energies= -4820.768995
Sum of electronic and thermal Enthalpies= -4820.768051
Sum of electronic and thermal Free Energies= -4820.90628