Electronic Supplementary Information

Theoretical study and design of multifunctional phosphorescent platinum(II) complexes containing triarylboron moieties for efficient OLED emitters

Yong Wu, Guo-Gang Shan, Hai-Bin Li, Shui-Xing Wu, Xin-Yao Ren, Yun Geng,* and Zhong-Min Su*

Institute of Functional Material Chemistry, Faculty of Chemistry, Northeast Normal University, Changchun 130024, China.

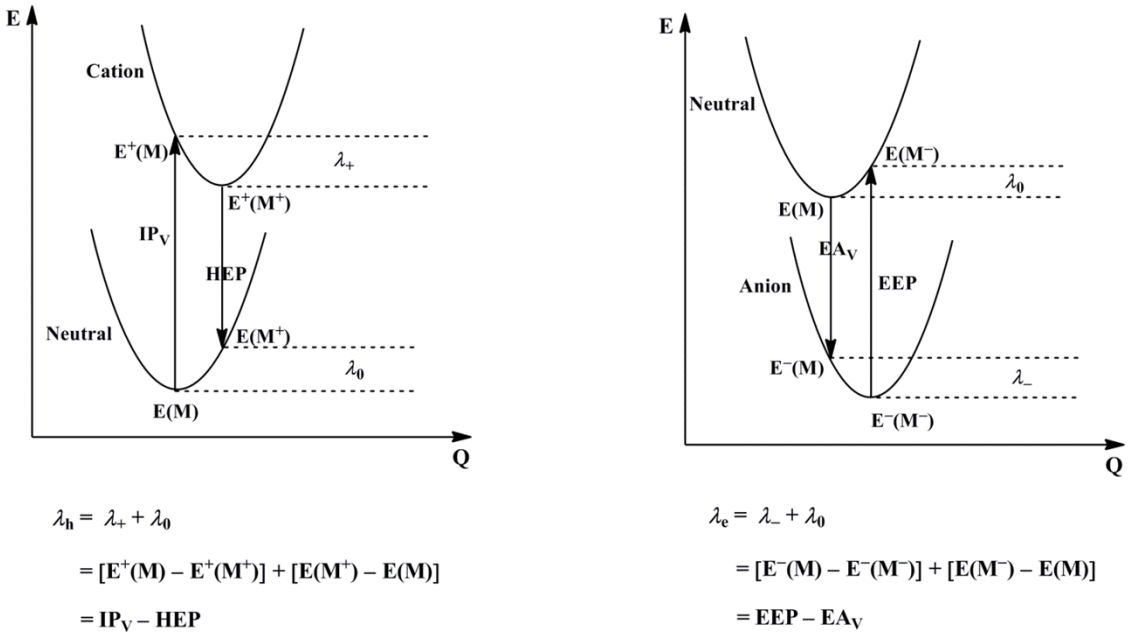
E-mail: gengy575@nenu.edu.cn; zmsu@nenu.edu.cn

Table S1 Optimized bond lengths [Å] and angles [°] for complex **1** obtained by different level of theories compared to experimental values.

	TPSS	TPSSh	B3LYP	PBE0	Expt.
Pt-C	1.980	1.975	1.983	1.964	1.967
Pt-N	2.009	2.005	2.019	1.994	1.995
Pt-O1	2.014	2.010	2.025	2.006	1.997
Pt-O2	2.097	2.093	2.114	2.091	2.081
C-Pt-O2	174.4	174.6	174.9	174.7	174.3
N-Pt-O1	175.3	175.4	175.7	175.7	174.5

Table S2 The calculated emission wavelengths and the first singlet (S_1) excitation energies of **1** and **2** in CH_2Cl_2 solutions with different methods, together with their experimental values.

	TD-TPSS	TD-TPSSh	TD-B3LYP	TD-PBE0	TD-PBE0/TDA	TD-M062X	Expt.
S_1 excitation energy (λ_{abs}, nm)							
1	566	493	448	428	422	360	426
2	637	556	505	481	470	406	474
Emission wavelength (λ_{em}, nm)							
1	691	644	613	615	579	531	527
2	811	744	695	690	655	597	596



$\lambda_h = \lambda_+ + \lambda_0$

$= [E^+(M) - E^+(M^+)] + [E(M^+) - E(M)]$

$= IP_V - HEP$

$\lambda_e = \lambda_- + \lambda_0$

$= [E^-(M) - E^-(M^-)] + [E(M^-) - E(M)]$

$= EEP - EA_V$

Fig. S1 The potential energy surfaces of the corresponding ground and ionic states, as well as the formulas of hole/electron reorganization energies (λ_h/λ_e). $E^+(M)/E^-(M)$ and $E(M^+)/E(M^-)$ represent the energies of cation/anion and neutral species with the geometries of neutral and cation/anion respectively, while $E^+(M^+)/E^-(M^-)$ and E(M) represent the energies of the cation/anion and neutral species in their optimized geometries, respectively.

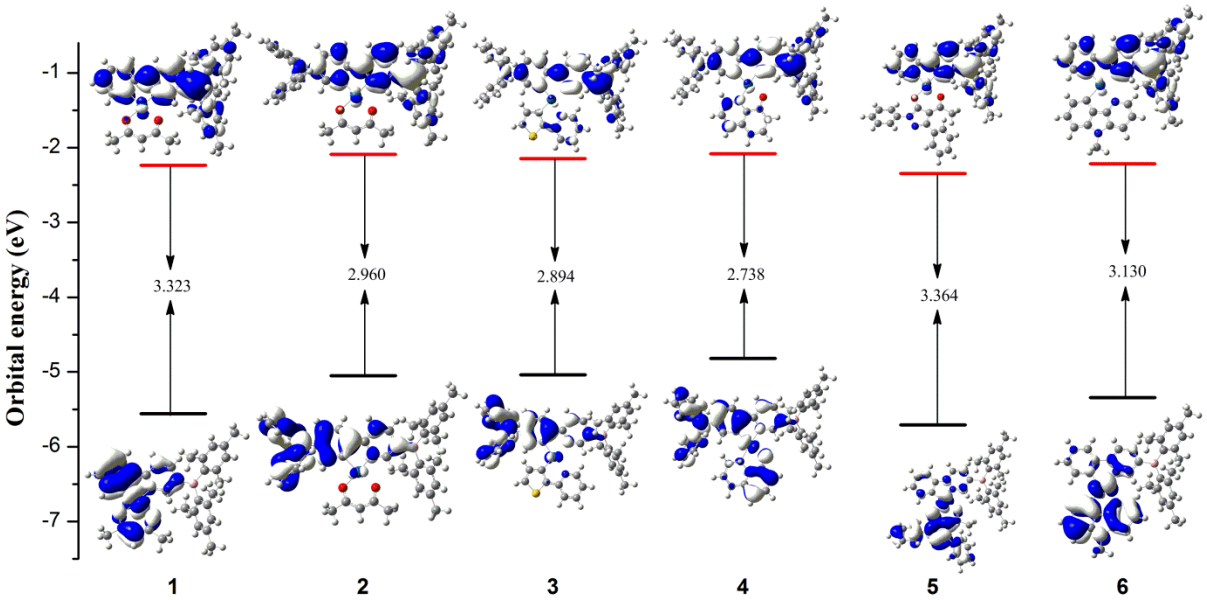


Fig. S2 Calculated electronic structures and isodensity surface plots of HOMO (bottom) and LUMO (top) for **1**–**6** at their T_1 optimized geometries.

Table S3 MO composition of 5d(Pt), h (NPh_2, pzl, NCaz), B in their corresponding frontier molecular orbitals.

Complex	5d(Pt)% in HOMO	h% in HOMO	B% in LUMO
1	36.55	—	27.05
2	1.35	61.43	26.90
3	2.05	61.30	24.44
4	9.18	33.34	22.28
5	21.50	70.07	26.90
6	31.37	54.22	20.61

Table S4 Vertical excitation energies (λ/nm), oscillator strengths (f), dominant configurations and corresponding assignments of the most relevant singlet excited states of **1-6** at their respective S_0 optimized geometries obtained from TD-PBE0 calculations in CH_2Cl_2 solution.

Complex	State	λ/nm	f	Configuration[a]	Nature	Exp./nm
1	S_1	428	0.1783	H→L (81%)	MLCT/LLCT	426
	S_5	352	0.1111	H-4→L (92%)	LC	
	S_6	341	0.1090	H-5→L (92%)	LC	339
	S_{13}	300	0.2258	H-1→L+1 (70%)	LC/MLCT	
	S_{42}	238	0.2055	H-8→L+1 (33%)	LLCT/MLCT	231
				H-7→L+2 (22%)	LLCT	
2	S_1	481	0.8308	H→L (95%)	LC	474
	S_5	359	0.0748	H-4→L (90%)	LC/MLCT	
	S_{15}	299	0.1950	H→L+4 (86%)	LC	302
	S_{46}	246	0.1423	H-1→L+4 (39%)	LC/LLCT/MLCT	241
				H-1→L+5 (26%)	LLCT/MLCT	
3	S_1	496	0.6504	H→L (92%)	LC	
	S_7	363	0.0940	H-5→L (58%)	LC/LLCT/MLCT	
				H-4→L (34%)	LC/LLCT/MLCT	
	S_{22}	299	0.2482	H-4→L+1 (32%)	LC/MLCT	
				H-1→L+3 (16%)	LC/MLCT	
				H→L+5 (19%)	LC	
	S_{31}	277	0.1167	H-2→L+3 (77%)	LLCT/MLCT	
4	S_1	503	0.3034	H-1→L (36%)	LLCT/MLCT	
				H→L (57%)	LC/LLCT/MLCT	
	S_2	480	0.4905	H-1→L (55%)	LLCT/MLCT	
				H→L (39%)	LC/LLCT/MLCT	

	S_{15}	329	0.0977	H-8→L (75%)	LLCT/MLCT
	S_{20}	300	0.1731	H-9→L (20%)	LC/MLCT
				H→L +5(19%)	LLCT/MLCT
				H→L+6 (44%)	LLCT/MLCT
5	S_1	422	0.1933	H-1→L (92%)	LC/LLCT/MLCT
	S_{13}	306	0.3043	H→L+2 (66%)	LC
	S_{24}	269	0.1495	H→L+4 (52%)	LC/MLCT
6	S_1	453	0.0316	H→L (75%)	LLCT/MLCT
	S_2	427	0.1772	H-1→L (74%)	LC/LLCT/MLCT
				H→L (19%)	LLCT/MLCT
	S_7	352	0.1972	H-5→L (84%)	LC/MLCT
	S_{15}	315	0.3079	H-9→L (38%)	LC/MLCT
				H-1→L+2 (21%)	LC/LLCT/MLCT
	S_{34}	259	0.1690	H-4→L+2 (14%)	LC/LLCT
				H-3→L+3 (14%)	MLCT
				H→L+4 (29%)	MLCT

[a] H and L denote HOMO and LUMO respectively.

Table S5 Cartesian coordinates of complex **1** at the S_0 and T_1 optimized geometries.

S_0				T_1			
C	-4.847167	-3.823157	0.480342	C	-4.909298	-3.771695	0.375285
C	-4.589160	-2.478312	0.232559	C	-4.627152	-2.433717	0.182467
H	-5.409540	-1.787567	0.058209	H	-5.426346	-1.711746	0.041882
C	-3.276439	-1.995449	0.205302	C	-3.298238	-1.973406	0.162368
C	-2.227524	-2.921784	0.438544	C	-2.207388	-2.942282	0.354465
C	-2.492167	-4.275100	0.687814	C	-2.527341	-4.308749	0.551097
H	-1.679995	-4.976396	0.865475	H	-1.740906	-5.043932	0.694279
C	-3.802977	-4.725489	0.708407	C	-3.844874	-4.701301	0.558957
H	-4.016742	-5.773066	0.900964	H	-4.084725	-5.751162	0.709713
C	-0.898149	-2.342598	0.394967	C	-0.911346	-2.394416	0.323718
C	0.318322	-3.003480	0.593123	C	0.328369	-3.066016	0.486403
H	0.316224	-4.066704	0.808714	H	0.322569	-4.137516	0.663581
C	1.507123	-2.301136	0.512772	C	1.508791	-2.375796	0.430488
H	2.453243	-2.816357	0.662330	H	2.452789	-2.895706	0.569742
C	1.512459	-0.917985	0.248779	C	1.526490	-0.958419	0.207960
C	0.258965	-0.326443	0.068007	C	0.253364	-0.354818	0.058526
H	0.155497	0.734142	-0.141540	H	0.169777	0.713668	-0.117488
C	-6.316907	2.041433	-0.654764	C	-6.305486	2.102724	-0.512955
H	-6.724024	1.445609	-1.479076	H	-6.735289	1.535277	-1.345609
H	-6.553255	3.094185	-0.823341	H	-6.524546	3.163395	-0.650801
H	-6.811859	1.703146	0.261995	H	-6.792325	1.750127	0.402797
C	-4.836165	1.793756	-0.543928	C	-4.829070	1.825577	-0.431011
C	-3.950433	2.867257	-0.678113	C	-3.925155	2.888855	-0.539405
H	-4.389582	3.842498	-0.855228	H	-4.348568	3.876868	-0.678090
C	-2.548828	2.801150	-0.616814	C	-2.526492	2.795902	-0.500415
C	-1.739612	4.055486	-0.818487	C	-1.691285	4.033345	-0.674392
H	-0.958803	4.112609	-0.053048	H	-0.901391	4.051574	0.083555
H	-2.352727	4.959425	-0.790884	H	-2.282915	4.950022	-0.620666
H	-1.232613	4.004338	-1.789527	H	-1.190801	3.992212	-1.649266
N	-0.893696	-1.001482	0.130291	N	-0.891204	-1.009376	0.107695
O	-4.541326	0.567782	-0.329516	O	-4.551392	0.589179	-0.264891
O	-1.865569	1.749788	-0.417622	O	-1.859922	1.721745	-0.342365
Pt	-2.680805	-0.151737	-0.113291	Pt	-2.683917	-0.166856	-0.089224
B	2.822023	-0.064931	0.154653	B	2.803650	-0.096667	0.122837
C	2.717918	1.500037	0.323706	C	2.669344	1.482999	0.227624
C	4.182878	-0.817764	-0.108352	C	4.204144	-0.817139	-0.060097
C	2.085889	2.079968	1.448254	C	2.070900	2.099087	1.351990
C	1.975628	3.469353	1.553052	C	1.963088	3.492034	1.421814
C	2.450928	4.323166	0.562910	C	2.416220	4.319369	0.399205
C	3.080055	3.748562	-0.542637	C	2.998483	3.711057	-0.713601
C	3.234365	2.370527	-0.671709	C	3.140181	2.328217	-0.810047

C	4.349048	-1.663423	-1.228853	C	4.444094	-1.686873	-1.151314
C	5.562820	-2.324589	-1.433516	C	5.686512	-2.309106	-1.297975
C	6.626573	-2.203914	-0.544954	C	6.717896	-2.123144	-0.382157
C	6.457023	-1.372137	0.563012	C	6.480847	-1.266747	0.692448
C	5.272791	-0.673976	0.787337	C	5.261741	-0.611941	0.861298
C	1.538593	1.263859	2.595902	C	1.538756	1.311397	2.525338
H	1.507689	3.893188	2.440781	H	1.520325	3.940715	2.310770
C	2.290557	5.813687	0.670681	C	2.314616	5.816354	0.497404
H	3.471108	4.396818	-1.325523	H	3.360534	4.334557	-1.530367
C	3.935339	1.850802	-1.901261	C	3.761640	1.766577	-2.062473
C	3.267546	-1.867847	-2.263821	C	3.403510	-1.959652	-2.210278
H	5.678645	-2.949986	-2.317802	H	5.852591	-2.954423	-2.160005
C	7.915506	-2.945915	-0.761354	C	8.036809	-2.827709	-0.536268
H	7.277882	-1.256863	1.269413	H	7.274111	-1.096489	1.419398
H	0.453162	1.127531	2.507319	H	0.467676	1.097002	2.411955
H	1.721755	1.775115	3.547543	H	1.655206	1.879087	3.455300
H	1.982614	0.267671	2.662723	H	2.043089	0.349966	2.651032
H	2.050768	6.118473	1.694173	H	1.666638	6.120581	1.325770
H	1.480443	6.170952	0.021668	H	1.913472	6.253092	-0.424654
H	3.202543	6.337857	0.364026	H	3.299468	6.270905	0.664828
H	4.250757	2.678467	-2.544313	H	4.169429	2.566454	-2.689024
H	3.285671	1.202614	-2.501382	H	3.022662	1.224828	-2.666690
H	4.822541	1.263614	-1.644069	H	4.568893	1.063415	-1.836637
H	2.578145	-1.022334	-2.333150	H	2.769575	-1.090423	-2.407439
H	2.659340	-2.753624	-2.041609	H	2.732102	-2.776901	-1.917548
H	3.709398	-2.019754	-3.254493	H	3.879199	-2.251187	-3.152892
H	8.017092	-3.777082	-0.051862	H	8.083034	-3.725797	0.093752
H	8.782892	-2.292052	-0.616125	H	8.872472	-2.183752	-0.240727
H	7.972258	-3.364962	-1.770766	H	8.202675	-3.145812	-1.570712
C	5.184353	0.205817	2.008864	C	5.101768	0.287312	2.059996
H	4.981134	1.248119	1.742511	H	4.814932	1.303203	1.770711
H	4.382271	-0.112615	2.685984	H	4.325254	-0.082040	2.741097
H	6.119857	0.176100	2.576250	H	6.034381	0.345781	2.630561
H	-5.875005	-4.179278	0.497534	H	-5.935462	-4.126798	0.388577

Table S6 Cartesian coordinates of complex **2** at the S_0 and T_1 optimized geometries.

S_0				T_1			
C	-4.192064	-1.387805	-0.003886	C	-4.210172	-1.378549	-0.044340
C	-3.409010	-0.225429	-0.041976	C	-3.419758	-0.206115	-0.065730
H	-3.890904	0.746995	-0.069227	H	-3.902670	0.766671	-0.056115
C	-2.018642	-0.293889	-0.035335	C	-2.044341	-0.272167	-0.059367
C	-1.402112	-1.572384	0.024164	C	-1.402230	-1.582916	-0.038867
C	-2.185493	-2.734420	0.064422	C	-2.208775	-2.759634	-0.029705
H	-1.721071	-3.717558	0.094035	H	-1.746989	-3.742484	-0.042458
C	-3.563748	-2.649464	0.045427	C	-3.573269	-2.657521	-0.032821
H	-4.168282	-3.550320	0.057615	H	-4.187388	-3.552361	-0.063386
C	0.040149	-1.544436	0.040600	C	0.006680	-1.561369	-0.026792
C	0.909597	-2.641103	0.106233	C	0.892683	-2.667901	0.004633
H	0.496567	-3.643208	0.155442	H	0.478136	-3.671661	0.022180
C	2.276077	-2.439691	0.109458	C	2.248977	-2.476002	0.023828
H	2.949988	-3.292093	0.157113	H	2.920979	-3.329170	0.063242
C	2.817960	-1.138906	0.062824	C	2.807675	-1.158295	0.012774
C	1.889283	-0.095304	0.004326	C	1.860566	-0.102500	-0.019328
H	2.204212	0.943302	-0.037192	H	2.190275	0.932092	-0.037962
C	-3.288082	4.661526	-0.186129	C	-3.280491	4.687948	0.009127
H	-3.924676	4.307109	-1.003612	H	-3.914919	4.395831	-0.834517
H	-3.108784	5.732584	-0.302442	H	-3.089057	5.762180	-0.037003
H	-3.839423	4.491114	0.745561	H	-3.839849	4.464030	0.924538
C	-2.012243	3.863186	-0.163088	C	-2.013107	3.875078	-0.012638
C	-0.783419	4.531077	-0.170413	C	-0.779442	4.531670	-0.001200
H	-0.817523	5.614298	-0.198859	H	-0.803423	5.615375	0.017371
C	0.487553	3.933961	-0.147587	C	0.487930	3.923563	-0.020197
C	1.715438	4.805843	-0.181682	C	1.721802	4.785687	-0.043973
H	2.416780	4.476847	0.592240	H	2.463497	4.382240	0.652782
H	1.483281	5.864550	-0.044215	H	1.508660	5.829499	0.198882
H	2.221527	4.677603	-1.145891	H	2.169387	4.742438	-1.044304
N	0.565889	-0.280708	-0.011900	N	0.552024	-0.273215	-0.037931
O	-2.205018	2.599638	-0.129617	O	-2.219700	2.613144	-0.035347
O	0.720373	2.686034	-0.113943	O	0.709738	2.674137	-0.039120
Pt	-0.758658	1.210283	-0.076693	Pt	-0.773359	1.208324	-0.042168
B	4.352426	-0.845093	0.075082	B	4.319689	-0.852947	0.036469
C	4.842767	0.601447	0.476891	C	4.805671	0.622502	0.370333
C	5.337394	-2.016455	-0.313814	C	5.340687	-2.029655	-0.264697
C	4.453003	1.193550	1.700609	C	4.424656	1.275540	1.565820
C	4.883997	2.482836	2.025690	C	4.859930	2.578793	1.831286
C	5.676714	3.234437	1.164366	C	5.658737	3.285749	0.939461
C	6.059864	2.647781	-0.042604	C	6.036588	2.641119	-0.239633
C	5.673066	1.356019	-0.391800	C	5.638143	1.338365	-0.529638

C	5.214473	-2.693802	-1.548943	C	5.282664	-2.762600	-1.473483
C	6.085569	-3.739447	-1.865459	C	6.194492	-3.793600	-1.719587
C	7.072862	-4.168649	-0.984210	C	7.168331	-4.153613	-0.794273
C	7.190898	-3.498776	0.234357	C	7.223019	-3.433243	0.399539
C	6.360074	-2.433788	0.575386	C	6.344861	-2.386033	0.671112
C	3.596633	0.481784	2.721627	C	3.561753	0.618653	2.616508
H	4.592808	2.907057	2.985897	H	4.569844	3.047699	2.771358
C	6.105391	4.632379	1.512853	C	6.104304	4.692732	1.226926
H	6.687741	3.212410	-0.730526	H	6.667155	3.169627	-0.953841
C	6.132087	0.815169	-1.721917	C	6.089363	0.736133	-1.835230
C	4.185055	-2.314835	-2.587812	C	4.269345	-2.463944	-2.551702
H	5.988549	-4.229516	-2.833455	H	6.141231	-4.327249	-2.668111
C	7.982396	-5.315753	-1.324274	C	8.127713	-5.279783	-1.062025
H	7.962061	-3.809584	0.937949	H	7.979001	-3.691462	1.140411
H	2.539269	0.755984	2.615723	H	2.506464	0.898679	2.498772
H	3.901675	0.760467	3.736315	H	3.867973	0.936270	3.619779
H	3.653460	-0.606838	2.643673	H	3.608535	-0.472391	2.577235
H	5.946369	4.847551	2.574127	H	5.858308	4.989235	2.251672
H	5.538589	5.374939	0.936386	H	5.622837	5.409823	0.549459
H	7.165856	4.793581	1.288786	H	7.186829	4.805198	1.094338
H	6.805574	1.522577	-2.215831	H	6.753688	1.421814	-2.371311
H	5.288795	0.641862	-2.401822	H	5.239202	0.522031	-2.494674
H	6.658462	-0.138144	-1.614587	H	6.622025	-0.208085	-1.684797
H	3.891397	-1.263323	-2.532802	H	3.984792	-1.408509	-2.577059
H	3.266545	-2.905155	-2.479795	H	3.342768	-3.033331	-2.403124
H	4.572116	-2.500784	-3.595509	H	4.662825	-2.733615	-3.537957
H	7.736056	-6.205239	-0.730496	H	7.918042	-6.143563	-0.418018
H	9.030173	-5.070924	-1.115893	H	9.163761	-4.978927	-0.866823
H	7.902450	-5.590988	-2.380488	H	8.065601	-5.619612	-2.100797
C	6.567928	-1.770185	1.913123	C	6.480823	-1.670917	1.991065
H	6.760170	-0.697872	1.807299	H	6.660625	-0.599557	1.855082
H	5.690050	-1.874906	2.562406	H	5.572418	-1.766076	2.598367
H	7.416554	-2.217866	2.439880	H	7.309759	-2.084707	2.574669
C	-6.254301	-0.265440	-0.710700	C	-6.270431	-0.270682	-0.736965
C	-7.359208	0.374116	-0.136541	C	-7.395992	0.337990	-0.166681
H	-7.694483	0.073483	0.851553	H	-7.742652	0.015348	0.810190
C	-8.019287	1.385160	-0.825773	C	-8.050325	1.358228	-0.845080
H	-8.875215	1.871775	-0.365392	H	-8.918700	1.828063	-0.391682
C	-7.581547	1.785790	-2.085877	C	-7.590267	1.789565	-2.088070
C	-6.477278	1.155026	-2.655543	C	-6.467085	1.186711	-2.652183
H	-6.127643	1.451342	-3.641001	H	-6.103124	1.510527	-3.623143
C	-5.822066	0.130769	-1.982253	C	-5.809568	0.159331	-1.988248
H	-4.967261	-0.364361	-2.432747	H	-4.939939	-0.317223	-2.429520
C	-6.369088	-2.251816	0.698070	C	-6.358926	-2.267093	0.662155

C	-6.005298	-2.630377	1.995959	C	-5.933612	-2.689085	1.928979
H	-5.122772	-2.189688	2.450129	H	-5.037349	-2.254209	2.360946
C	-6.768230	-3.560593	2.692692	C	-6.668538	-3.640678	2.625704
H	-6.473319	-3.843930	3.699676	H	-6.333672	-3.956796	3.609649
C	-7.911392	-4.111877	2.117898	C	-7.834092	-4.172741	2.078297
C	-8.281213	-3.727321	0.830787	C	-8.261133	-3.746224	0.820792
H	-9.167570	-4.153215	0.367939	H	-9.164473	-4.161267	0.382514
C	-7.514795	-2.810944	0.119763	C	-7.531013	-2.802631	0.110659
H	-7.796960	-2.520264	-0.887899	H	-7.852942	-2.482211	-0.875514
N	-5.594781	-1.308562	-0.018598	N	-5.602396	-1.313807	-0.055324
H	-8.095790	2.580380	-2.619067	H	-8.102838	2.590443	-2.612976
H	-8.509124	-4.832944	2.668147	H	-8.407714	-4.913475	2.627659

Table S7 Cartesian coordinates of complex **3** at the S_0 and T_1 optimized geometries.

S_0				T_1			
Pt	-0.785298	1.031098	-0.066996	Pt	-0.792107	1.030349	-0.070279
N	0.685038	-0.502445	0.100899	N	0.666764	-0.485132	0.066773
C	2.009677	-0.345236	0.066524	C	1.980127	-0.343812	0.041509
H	2.359663	0.680351	0.051461	H	2.346185	0.676479	0.026014
C	2.943765	-1.386451	0.018393	C	2.930497	-1.394673	-0.000643
C	2.400027	-2.684943	-0.009494	C	2.373243	-2.711008	-0.032581
H	3.068704	-3.542083	-0.048142	H	3.042028	-3.567491	-0.057965
C	1.033113	-2.872489	0.006640	C	1.017038	-2.889390	-0.022921
H	0.616483	-3.873063	-0.031586	H	0.599240	-3.890825	-0.055072
C	0.170497	-1.766235	0.047757	C	0.137151	-1.775435	0.011483
C	-1.273724	-1.825820	0.022056	C	-1.270038	-1.831148	-0.050959
C	-1.989452	-3.027607	0.129739	C	-2.010686	-3.052774	-0.027841
H	-1.466678	-3.978924	0.189416	H	-1.492930	-4.006451	-0.053875
C	-3.369481	-3.031372	0.163809	C	-3.374594	-3.038542	0.039286
H	-3.919262	-3.964391	0.231404	H	-3.937521	-3.966980	0.042451
C	-4.060902	-1.808492	0.121511	C	-4.073864	-1.796347	0.071209
C	-3.343015	-0.609059	0.017989	C	-3.351166	-0.586324	-0.014187
H	-3.903295	0.317329	0.041167	H	-3.911338	0.338917	0.046258
C	-1.949365	-0.576522	-0.072954	C	-1.971566	-0.549695	-0.112650
N	-5.466343	-1.788560	0.179314	N	-5.466069	-1.797798	0.151924
C	-6.193949	-0.834378	-0.571241	C	-6.220006	-0.821278	-0.541155
C	-7.265780	-0.145652	0.007658	C	-7.296602	-0.181388	0.084621
H	-7.525147	-0.340374	1.044003	H	-7.540725	-0.427503	1.113544
C	-7.986531	0.780626	-0.737746	C	-8.031943	0.772450	-0.608033
H	-8.813762	1.310269	-0.272661	H	-8.859950	1.270893	-0.111857

C	-7.643648	1.045099	-2.061831	C	-7.702853	1.102376	-1.921625
H	-8.206011	1.773293	-2.639384	H	-8.279530	1.850539	-2.457675
C	-6.573856	0.363279	-2.638893	C	-6.629905	0.465361	-2.543469
H	-6.300782	0.551441	-3.673975	H	-6.370640	0.707989	-3.570252
C	-5.857467	-0.576814	-1.905957	C	-5.890784	-0.494427	-1.862746
H	-5.030910	-1.116071	-2.359447	H	-5.060323	-1.001004	-2.345246
C	-6.167939	-2.713542	0.984798	C	-6.133557	-2.755871	0.943504
C	-5.694911	-3.051198	2.259269	C	-5.591145	-3.152060	2.174020
H	-4.782770	-2.591078	2.627258	H	-4.671254	-2.692444	2.522418
C	-6.390294	-3.963718	3.044237	C	-6.243071	-4.108116	2.943386
H	-6.010178	-4.213476	4.031392	H	-5.817324	-4.403314	3.898304
C	-7.573062	-4.539190	2.584700	C	-7.441176	-4.670226	2.507362
H	-8.117294	-5.245807	3.204705	H	-7.949660	-5.413468	3.114422
C	-8.050594	-4.196126	1.321779	C	-7.984573	-4.269452	1.286955
H	-8.968796	-4.640656	0.946748	H	-8.914438	-4.707317	0.934728
C	-7.353497	-3.298259	0.521842	C	-7.338553	-3.322596	0.503971
H	-7.722251	-3.041939	-0.466788	H	-7.752560	-3.022570	-0.453682
N	0.338463	2.857010	0.328639	N	4.441630	-1.090895	-0.003262
C	-2.098549	2.410172	-0.651759	C	5.452869	-2.213040	-0.486834
C	-3.360697	2.396415	-1.324575	C	4.936290	0.332672	0.502000
H	-3.926479	1.503235	-1.560959	H	5.320944	-2.800691	-1.769555
C	-3.811995	3.636349	-1.685791	C	6.220148	-3.782454	-2.192659
H	-4.737292	3.881131	-2.192489	H	7.255744	-4.235099	-1.380166
S	-2.718598	4.890504	-1.250036	S	7.386401	-3.656236	-0.118700
C	-1.634727	3.716531	-0.571147	C	6.520339	-2.660298	0.331701
C	-0.349679	3.987667	0.002003	C	4.630055	0.786889	1.806980
C	0.187376	5.256654	0.255307	C	5.098964	2.028280	2.251148
H	-0.377897	6.138893	-0.028819	H	5.856325	2.865425	1.436509
C	1.417425	5.367919	0.879839	C	6.145950	2.422324	0.145471
H	1.842555	6.347654	1.080025	H	5.712984	1.183536	-0.324040
C	2.088317	4.208805	1.265146	C	4.243135	-2.383231	-2.740133
H	3.046420	4.234636	1.772026	H	6.109233	-4.200845	-3.192461
C	1.502723	2.986208	0.973496	C	8.192822	-5.317616	-1.838292
H	1.991457	2.067987	1.276988	H	8.193367	-3.985791	0.534851
B	4.475882	-1.093784	0.010526	B	6.740156	-2.110576	1.717505
C	5.458947	-2.199851	-0.536075	C	3.822567	-0.037500	2.781978
C	4.972645	0.299020	0.568846	C	4.877101	2.340098	3.271692
C	5.284607	-2.755551	-1.826286	C	6.365892	4.191406	1.930570
C	6.161186	-3.739179	-2.289860	C	6.734286	3.058504	-0.514774
C	7.204289	-4.225911	-1.507518	C	3.282556	-2.860656	-2.510347
C	7.373773	-3.675965	-0.236895	C	4.514241	-2.666533	-3.762789
C	6.539118	-2.672742	0.251918	C	4.065330	-1.303608	-2.726001
C	4.655525	0.710390	1.883273	C	8.201255	-5.404481	-2.929708
C	5.106921	1.945702	2.359851	C	7.898095	-6.295225	-1.434451

C	5.850820	2.814049	1.566655	C	9.219107	-5.127773	-1.504876
C	6.151025	2.409228	0.264530	C	7.651478	-2.524977	2.160832
C	5.741873	1.176295	-0.237375	C	5.908690	-2.363316	2.387306
C	4.196266	-2.301647	-2.770704	C	6.828002	-1.019931	1.714327
H	6.024770	-4.132670	-3.296327	H	3.997818	-1.110408	2.665187
C	8.112767	-5.314024	-2.006582	C	2.742270	0.114239	2.654801
H	8.189715	-4.033056	0.389840	H	4.067303	0.236384	3.814039
C	6.812073	-2.138598	1.635272	C	6.068812	5.009602	1.263156
C	3.864415	-0.149353	2.842235	C	7.461785	4.203346	1.980978
H	4.878037	2.228468	3.386953	H	5.986917	4.418075	2.932532
C	6.338585	4.135007	2.093565	C	6.059079	0.795986	-1.738029
H	6.729658	3.072205	-0.377064	H	6.531944	-0.190072	-1.783664
H	3.279621	-2.891182	-2.645968	H	5.162448	0.751683	-2.369214
H	4.518998	-2.421587	-3.810344	H	6.740096	1.524499	-2.189806
H	3.917882	-1.254058	-2.627757	H	0.339294	2.840255	0.348014
H	8.095999	-5.380996	-3.098996	H	-2.111642	2.427533	-0.614984
H	7.808546	-6.292686	-1.613142	H	-3.379791	2.438227	-1.277631
H	9.148492	-5.147544	-1.691136	H	-3.949238	1.553411	-1.535405
H	7.681368	-2.635990	2.076671	H	-3.829222	3.688150	-1.604457
H	5.965611	-2.301679	2.313063	H	-4.756599	3.950564	-2.098412
H	7.007805	-1.061752	1.622645	H	-2.725127	4.925582	-1.148079
H	3.893748	-1.211142	2.586307	H	-1.640782	3.729742	-0.509009
H	2.805323	0.139370	2.867546	H	-0.346612	3.981502	0.051184
H	4.250288	-0.039575	3.861739	H	0.200339	5.243442	0.316082
H	6.054380	4.959883	1.429391	H	-0.365809	6.132399	0.055388
H	7.432705	4.150816	2.171982	H	1.441590	5.339233	0.919823
H	5.932655	4.345109	3.088222	H	1.876034	6.313166	1.127784
C	6.105847	0.826218	-1.657450	C	2.112538	4.169827	1.273395
H	6.632568	-0.131450	-1.716660	H	3.081562	4.180080	1.759330
H	5.216047	0.743781	-2.294073	H	1.516563	2.954775	0.975104
H	6.747665	1.596287	-2.096570	H	2.007216	2.031763	1.256798

Table S8 Cartesian coordinates of complex **4** at the S_0 and T_1 optimized geometries.

S_0				T_1			
Pt	-0.674369	0.945498	-0.151152	Pt	-0.673453	0.928988	-0.169790
N	0.672900	-0.531928	-0.041321	N	0.688960	-0.540543	-0.047381
C	1.986958	-0.295379	0.041106	C	2.004380	-0.306709	0.026235
H	2.258262	0.754857	0.105678	H	2.284304	0.741833	0.066744
C	2.951330	-1.308325	0.027827	C	2.970554	-1.316246	0.037457
C	2.457613	-2.624146	-0.076764	C	2.479234	-2.637153	-0.028572
H	3.161741	-3.452847	-0.096270	H	3.184092	-3.465361	-0.025205
C	1.100247	-2.874181	-0.146707	C	1.121806	-2.887694	-0.087952
H	0.727434	-3.890585	-0.215923	H	0.748260	-3.905606	-0.126451
C	0.194934	-1.806484	-0.132564	C	0.214995	-1.820790	-0.101016
C	-1.247906	-1.875475	-0.170745	C	-1.226241	-1.890972	-0.135038
C	-1.968473	-3.076709	-0.171118	C	-1.952563	-3.088715	-0.109533
H	-1.449657	-4.030646	-0.230683	H	-1.437610	-4.045952	-0.143432
C	-3.349414	-3.074386	-0.108367	C	-3.333296	-3.077990	-0.053820
H	-3.907018	-4.004698	-0.135450	H	-3.893556	-4.007144	-0.058903
C	-4.028206	-1.849698	0.005346	C	-4.012456	-1.849260	0.019500
C	-3.298781	-0.652030	0.020502	C	-3.281779	-0.652181	0.002367
H	-3.858747	0.261536	0.183177	H	-3.833735	0.273297	0.116226
C	-1.912166	-0.613951	-0.124024	C	-1.893429	-0.630740	-0.123291
N	-5.431474	-1.816702	0.097408	N	-5.415591	-1.815463	0.100250
C	-6.153949	-0.753766	-0.493389	C	-6.136162	-0.773652	-0.531386
C	-7.210552	-0.142893	0.192136	C	-7.192505	-0.137830	0.130729
H	-7.470363	-0.490345	1.187618	H	-7.451577	-0.446702	1.139073
C	-7.916089	0.901418	-0.395991	C	-7.898272	0.882606	-0.497295
H	-8.732238	1.365948	0.151080	H	-8.713960	1.368694	0.031375
C	-7.573857	1.362958	-1.665143	C	-7.555356	1.294690	-1.783093
H	-8.126412	2.180315	-2.119876	H	-8.106132	2.095666	-2.268037
C	-6.521440	0.756090	-2.349845	C	-6.502229	0.663594	-2.443629
H	-6.252870	1.092919	-3.347809	H	-6.230752	0.965369	-3.451813
C	-5.821652	-0.299765	-1.776834	C	-5.802550	-0.369487	-1.830337
H	-5.010477	-0.779454	-2.316429	H	-4.989774	-0.868195	-2.350002
C	-6.131625	-2.827560	0.795957	C	-6.120948	-2.808084	0.818449
C	-5.647174	-3.314070	2.016262	C	-5.645090	-3.266448	2.053170
H	-4.729344	-2.903299	2.426352	H	-4.729258	-2.847503	2.459435
C	-6.336633	-4.313209	2.693711	C	-6.341128	-4.247181	2.750443
H	-5.947419	-4.680070	3.639827	H	-5.958496	-4.591598	3.707644
C	-7.524663	-4.828376	2.179651	C	-7.527594	-4.771770	2.242266
H	-8.064109	-5.604027	2.715562	H	-8.072306	-5.532675	2.793771
C	-8.013869	-4.336892	0.971344	C	-8.008388	-4.308133	1.019681
H	-8.936134	-4.733258	0.554757	H	-8.929518	-4.711719	0.607485
C	-7.322324	-3.350624	0.277375	C	-7.310321	-3.340703	0.306134
H	-7.698686	-2.979850	-0.671520	H	-7.680760	-2.991424	-0.653135

B	4.477934	-0.971944	0.100887	B	4.492114	-0.964493	0.095792
C	5.501254	-2.073109	-0.381794	C	5.528298	-2.065548	-0.360893
C	4.929019	0.436668	0.646231	C	4.922671	0.468003	0.601815
C	5.429672	-2.626508	-1.679633	C	5.453714	-2.649333	-1.646521
C	6.342635	-3.608399	-2.075300	C	6.375420	-3.628229	-2.027083
C	7.322703	-4.091872	-1.215340	C	7.367926	-4.081550	-1.164069
C	7.386998	-3.547105	0.068741	C	7.436098	-3.506507	0.105737
C	6.513838	-2.548011	0.491026	C	6.553484	-2.508644	0.512908
C	4.495672	0.913887	1.904729	C	4.504798	0.955178	1.862724
C	4.899807	2.173504	2.355149	C	4.886193	2.231298	2.283573
C	5.706963	3.006070	1.588373	C	5.659462	3.070091	1.486910
C	6.134782	2.532618	0.346694	C	6.062839	2.590841	0.240390
C	5.776486	1.273630	-0.126615	C	5.724098	1.315079	-0.205466
C	4.413822	-2.178948	-2.704531	C	4.422725	-2.236655	-2.670826
H	6.284708	-4.002130	-3.089388	H	6.315025	-4.044483	-3.031888
C	8.285064	-5.163315	-1.645401	C	8.337557	-5.152839	-1.577653
H	8.148733	-3.906353	0.759458	H	8.208769	-3.838797	0.797769
C	6.663601	-2.015696	1.893800	C	6.705777	-1.948700	1.904199
C	3.622278	0.106726	2.836306	C	3.665178	0.140140	2.818357
H	4.569139	2.511137	3.336474	H	4.568059	2.577197	3.266293
C	6.102443	4.373908	2.069119	C	6.077958	4.432792	1.963570
H	6.772576	3.164111	-0.270198	H	6.665274	3.229513	-0.404006
H	3.558123	-2.864919	-2.747623	H	3.530112	-2.872855	-2.622700
H	4.861405	-2.160057	-3.704391	H	4.830884	-2.327928	-3.683190
H	4.010579	-1.183864	-2.501528	H	4.081776	-1.206136	-2.541486
H	8.180633	-5.391441	-2.710621	H	8.248107	-5.384199	-2.643548
H	8.118479	-6.093361	-1.087577	H	8.163362	-6.081712	-1.020041
H	9.323812	-4.862916	-1.464542	H	9.373275	-4.851290	-1.382647
H	7.487757	-2.515765	2.412295	H	7.584758	-2.373213	2.399392
H	5.757629	-2.174539	2.491332	H	5.836364	-2.178084	2.532971
H	6.861908	-0.939172	1.897885	H	6.813228	-0.859740	1.892523
H	3.642705	-0.964628	2.623348	H	3.779714	-0.937428	2.674806
H	2.574648	0.428417	2.775878	H	2.597289	0.366691	2.705806
H	3.942028	0.246917	3.874981	H	3.935448	0.369165	3.854975
H	5.559784	5.155607	1.522248	H	6.049641	5.167444	1.151343
H	7.171913	4.558670	1.916444	H	7.105816	4.418002	2.348776
H	5.883592	4.503695	3.133538	H	5.431169	4.791581	2.770650
C	6.289188	0.857417	-1.482313	C	6.194923	0.896888	-1.575141
H	6.899138	-0.049816	-1.426216	H	6.736633	-0.053444	-1.548418
H	5.471592	0.651436	-2.183247	H	5.355228	0.769920	-2.269777
H	6.901309	1.650702	-1.922855	H	6.857517	1.654493	-2.005242
O	0.759624	2.438488	-0.010435	O	0.730802	2.478348	-0.003977
N	-1.863994	2.582791	-0.412830	N	-1.877387	2.537104	-0.421381
C	-3.140905	2.639185	-0.762237	C	-3.192170	2.618816	-0.842263

H	-3.638471	1.699205	-0.956757	H	-3.649465	1.688291	-1.147952
C	-3.834736	3.854155	-0.890923	C	-3.875295	3.799968	-0.907751
H	-4.883857	3.824594	-1.166801	H	-4.909541	3.780591	-1.237334
C	-3.179467	5.038360	-0.657152	C	-3.242344	5.023892	-0.577106
H	-3.700882	5.989309	-0.736690	H	-3.775559	5.967937	-0.618965
C	-1.802700	5.028064	-0.333917	C	-1.872437	4.986936	-0.255724
C	-1.026592	6.188611	-0.125883	C	-1.077179	6.131587	0.010678
H	-1.497933	7.165228	-0.183812	H	-1.558701	7.106171	-0.001000
C	0.324227	6.056875	0.132305	C	0.309418	6.045336	0.282020
H	0.924335	6.950357	0.287944	H	0.866385	6.956219	0.481617
C	0.958057	4.806541	0.185500	C	0.942180	4.830794	0.289614
H	2.025776	4.727927	0.366866	H	2.003432	4.717770	0.487327
C	0.232742	3.629883	-0.007832	C	0.173242	3.638048	0.028935
C	-1.172992	3.757480	-0.240571	C	-1.225651	3.723880	-0.208199

Table S9 Cartesian coordinates of complex **5** at the S_0 and T_1 optimized geometries.

S_0				T_1			
C	-2.044462	-5.517616	-0.012965	C	-2.132659	-5.467767	-0.123142
C	-2.188507	-4.133015	-0.014618	C	-2.250231	-4.091170	-0.081841
H	-3.179307	-3.690375	-0.064438	H	-3.228378	-3.619830	-0.106495
C	-1.066043	-3.300310	0.036819	C	-1.108167	-3.276977	-0.011293
C	0.212206	-3.912795	0.076277	C	0.218928	-3.911593	-0.005638
C	0.351349	-5.306726	0.080049	C	0.307301	-5.328172	-0.038247
H	1.336433	-5.766381	0.112534	H	1.275432	-5.819935	-0.024733
C	-0.778479	-6.109078	0.038148	C	-0.842952	-6.075187	-0.095690
H	-0.679299	-7.190829	0.040192	H	-0.772222	-7.159744	-0.125684
C	1.320747	-2.977814	0.096506	C	1.302325	-3.020042	0.029243
C	2.683591	-3.285243	0.142150	C	2.689929	-3.326953	0.044611
H	2.992616	-4.324655	0.174867	H	2.993330	-4.369674	0.035318
C	3.621746	-2.268876	0.146652	C	3.624561	-2.330526	0.078447
H	4.681918	-2.508714	0.181107	H	4.683269	-2.573300	0.103977
C	3.222876	-0.919484	0.120369	C	3.231542	-0.949507	0.101085
C	1.844484	-0.690322	0.082062	C	1.834357	-0.715738	0.088406
H	1.438309	0.316296	0.064952	H	1.448700	0.299263	0.102380
N	0.931240	-1.667619	0.063664	N	0.919902	-1.667243	0.053202
B	4.230006	0.280071	0.148441	B	4.215406	0.241292	0.137552
C	3.698384	1.695347	0.600144	C	3.666046	1.676991	0.533119
C	5.726763	0.010343	-0.267721	C	5.738610	-0.017274	-0.211949
C	3.039922	1.872118	1.839386	C	2.996456	1.898140	1.759470
C	2.559800	3.132465	2.205002	C	2.517335	3.171782	2.084252

C	2.685715	4.239871	1.371375	C	2.661391	4.255385	1.223757
C	3.328325	4.059967	0.145564	C	3.316491	4.035192	0.010904
C	3.845461	2.826256	-0.243380	C	3.824715	2.785919	-0.338234
C	6.048494	-0.577986	-1.512874	C	6.120259	-0.601567	-1.443421
C	7.382212	-0.823965	-1.848433	C	7.469667	-0.822509	-1.731232
C	8.427171	-0.531891	-0.977548	C	8.478448	-0.504485	-0.826994
C	8.106417	0.049299	0.250092	C	8.101555	0.072153	0.385935
C	6.792007	0.336371	0.610753	C	6.767992	0.327897	0.699993
C	2.844324	0.751034	2.832921	C	2.779460	0.805898	2.779635
H	2.076320	3.249594	3.174131	H	2.026152	3.319205	3.045739
C	2.180976	5.592891	1.788086	C	2.159664	5.623633	1.593456
H	3.436855	4.910748	-0.525591	H	3.441421	4.866371	-0.682128
C	4.521369	2.733314	-1.587996	C	4.505307	2.647453	-1.675649
C	5.002166	-0.930539	-2.544261	C	5.114993	-0.983924	-2.502590
H	7.608421	-1.253704	-2.823425	H	7.738284	-1.251919	-2.695838
C	9.854481	-0.834337	-1.337755	C	9.923126	-0.781169	-1.136509
H	8.908004	0.295877	0.944858	H	8.872167	0.338569	1.108350
H	1.844384	0.307667	2.743304	H	1.785754	0.350141	2.674568
H	2.937881	1.128517	3.857093	H	2.839328	1.211056	3.795999
H	3.566391	-0.060242	2.711095	H	3.511029	-0.001409	2.694664
H	1.427823	5.514557	2.578485	H	1.496874	5.586078	2.463848
H	1.734861	6.131188	0.944809	H	1.607133	6.085177	0.766827
H	2.997962	6.216616	2.173387	H	2.990208	6.297591	1.839491
H	4.550856	3.713269	-2.074379	H	4.586216	3.618736	-2.174194
H	3.992742	2.050809	-2.264688	H	3.945929	1.982454	-2.345519
H	5.548730	2.365798	-1.501572	H	5.511737	2.228772	-1.577969
H	4.100657	-0.317503	-2.464609	H	4.245429	-0.320577	-2.513951
H	4.682946	-1.976457	-2.454751	H	4.731666	-2.000717	-2.348481
H	5.403588	-0.801588	-3.555156	H	5.572790	-0.956703	-3.497292
H	10.229465	-1.697158	-0.772615	H	10.270899	-1.688555	-0.625617
H	10.513105	0.010847	-1.108027	H	10.568573	0.040643	-0.806852
H	9.958964	-1.066220	-2.402174	H	10.082097	-0.927932	-2.209657
C	6.548439	0.973518	1.955495	C	6.462723	0.953109	2.037215
H	6.049623	1.943108	1.859008	H	5.934880	1.906026	1.928628
H	5.913544	0.350659	2.597013	H	5.826807	0.305443	2.652737
H	7.492938	1.129205	2.486214	H	7.383751	1.136586	2.599933
Pt	-1.031386	-1.339867	0.050404	Pt	-1.038009	-1.355244	0.071246
N	-5.351772	1.426941	-0.240845	N	-5.334518	1.452409	-0.217023
N	-4.961012	0.132275	-0.033007	N	-4.958847	0.153260	0.001526
O	-3.039798	-1.142672	0.096241	O	-3.055458	-1.143843	0.147851
O	-0.809931	0.760013	0.070930	O	-0.803242	0.730398	0.126723
C	-1.710002	1.641641	-0.032839	C	-1.695594	1.624921	0.018336
C	-1.216994	3.059070	0.058674	C	-1.182363	3.031925	0.120388
H	-0.319601	3.068508	0.683438	H	-0.302404	3.029667	0.769842

H	-1.967612	3.742822	0.457796	H	-1.932868	3.731191	0.490981
C	-3.079745	1.317916	-0.191018	C	-3.064643	1.316435	-0.153788
C	-3.600925	-0.002977	-0.034297	C	-3.603483	0.002040	0.006686
C	-4.255449	2.139363	-0.336300	C	-4.230611	2.151961	-0.310192
C	-4.393965	3.580688	-0.612627	C	-4.347915	3.592814	-0.596091
C	-5.302389	4.343595	0.129689	C	-5.257316	4.370213	0.129730
H	-5.861609	3.862712	0.926621	H	-5.832875	3.901108	0.922003
C	-5.486087	5.693042	-0.152919	C	-5.420116	5.720075	-0.163034
H	-6.190791	6.275418	0.434660	H	-6.125074	6.314770	0.411600
C	-4.770262	6.296625	-1.184271	C	-4.682729	6.308367	-1.188012
H	-4.913955	7.351057	-1.404409	H	-4.810119	7.363192	-1.415850
C	-3.874710	5.540967	-1.938123	C	-3.785953	5.537915	-1.925270
H	-3.326460	6.001056	-2.755968	H	-3.220417	5.986803	-2.737398
C	-3.689114	4.191819	-1.655990	C	-3.620428	4.188447	-1.632836
H	-3.011387	3.596717	-2.262351	H	-2.940629	3.582111	-2.225605
C	-5.949590	-0.872547	0.067903	C	-5.959112	-0.840805	0.101245
C	-7.197050	-0.644204	-0.517602	C	-7.192397	-0.611498	-0.512493
H	-7.371010	0.292335	-1.034892	H	-7.348456	0.317643	-1.048553
C	-8.190177	-1.610814	-0.417271	C	-8.195181	-1.568469	-0.415567
H	-9.158145	-1.427230	-0.875800	H	-9.152526	-1.385203	-0.895751
C	-7.950786	-2.805648	0.257687	C	-7.978580	-2.753524	0.283943
H	-8.729035	-3.560216	0.329663	H	-8.764536	-3.500192	0.353518
C	-6.707163	-3.020869	0.844582	C	-6.748965	-2.969078	0.899624
H	-6.511415	-3.942651	1.385859	H	-6.572807	-3.882342	1.461576
C	-5.703875	-2.060205	0.761394	C	-5.736564	-2.017686	0.820093
H	-4.742645	-2.224734	1.231712	H	-4.787138	-2.180103	1.314853
H	-0.929040	3.420152	-0.935536	H	-0.854801	3.378954	-0.866751
H	-2.929225	-6.149061	-0.054009	H	-3.016433	-6.096516	-0.177147

Table S10 Cartesian coordinates of complex **6** at the S_0 and T_1 optimized geometries.

S_0				T_1			
C	-3.237231	-5.146732	-0.084188	C	-3.368359	-5.054461	-0.166113
C	-3.319954	-3.758817	-0.150945	C	-3.403274	-3.675890	-0.236926
H	-4.273168	-3.303194	-0.388967	H	-4.330821	-3.178269	-0.491247
C	-2.198868	-2.944546	0.057308	C	-2.255875	-2.897645	0.013869
C	-0.957934	-3.611233	0.258948	C	-0.981695	-3.602357	0.215604
C	-0.882602	-5.008609	0.338024	C	-0.988744	-5.015195	0.346476
H	0.073782	-5.499213	0.500979	H	-0.066808	-5.546750	0.561745
C	-2.022646	-5.780134	0.182048	C	-2.153779	-5.716759	0.158532
H	-1.964542	-6.863236	0.241156	H	-2.143468	-6.801226	0.235624
C	0.221041	-2.761855	0.290642	C	0.181257	-2.807213	0.238011
C	1.535773	-3.181920	0.529536	C	1.521156	-3.252494	0.393741
H	1.734284	-4.225327	0.748957	H	1.712214	-4.314390	0.515468
C	2.570844	-2.265986	0.490328	C	2.557154	-2.360274	0.393375
H	3.592869	-2.591657	0.670994	H	3.579866	-2.706663	0.516801
C	2.315030	-0.906489	0.234132	C	2.312892	-0.952799	0.248108
C	0.971746	-0.576863	0.025090	C	0.952118	-0.597173	0.117294
H	0.688956	0.450554	-0.162929	H	0.690839	0.449000	0.026125
N	-0.035370	-1.449267	0.034720	N	-0.063383	-1.439721	0.086917
B	3.422765	0.194780	0.180762	B	3.399851	0.138328	0.190805
C	2.974208	1.699792	0.359934	C	2.950994	1.656287	0.355965
C	4.917849	-0.247114	-0.055678	C	4.909308	-0.283304	-0.043767
C	2.254089	2.114671	1.507647	C	2.267674	2.100288	1.516374
C	1.832018	3.438348	1.630125	C	1.861145	3.430777	1.632906
C	2.070298	4.383915	0.634436	C	2.086250	4.362792	0.622024
C	2.776442	3.972671	-0.494296	C	2.754924	3.926557	-0.520081
C	3.241901	2.664146	-0.641378	C	3.195526	2.608277	-0.663296
C	5.277235	-1.026851	-1.180599	C	5.288512	-1.043600	-1.176798
C	6.606448	-1.411358	-1.370599	C	6.625272	-1.401898	-1.370977
C	7.608025	-1.077674	-0.463718	C	7.622448	-1.053886	-0.465191
C	7.249561	-0.312443	0.646226	C	7.248428	-0.305983	0.651020
C	5.940248	0.115362	0.857085	C	5.928984	0.087368	0.868588
C	1.928510	1.179581	2.648448	C	1.956260	1.181968	2.673922
H	1.298441	3.737993	2.531286	H	1.355376	3.747443	2.544632
C	1.576235	5.796129	0.779098	C	1.620275	5.785522	0.763842
H	2.985881	4.695588	-1.281450	H	2.955350	4.636995	-1.321400
C	3.995304	2.318118	-1.900729	C	3.903343	2.234799	-1.940417
C	4.279849	-1.447451	-2.234476	C	4.297547	-1.477339	-2.229422
H	6.865023	-1.986936	-2.258455	H	6.893349	-1.967152	-2.262980
C	9.026649	-1.531634	-0.663304	C	9.050390	-1.475834	-0.671748
H	8.016590	-0.030536	1.366222	H	8.009951	-0.013402	1.373102
H	0.914388	0.771113	2.553180	H	0.950546	0.750059	2.584772
H	1.971886	1.713302	3.604090	H	1.985720	1.732022	3.621030

H	2.610686	0.327985	2.711568	H	2.654121	0.344194	2.746160
H	1.861585	6.221828	1.747871	H	1.931994	6.214931	1.722969
H	0.480998	5.837523	0.721135	H	0.524977	5.851352	0.725671
H	1.977991	6.444465	-0.005920	H	2.020493	6.419530	-0.033922
H	4.187067	3.216016	-2.496397	H	4.097888	3.121409	-2.552549
H	3.430045	1.624159	-2.535520	H	3.302469	1.545595	-2.547126
H	4.956313	1.842792	-1.681834	H	4.858288	1.737594	-1.744478
H	3.456823	-0.737274	-2.351317	H	3.505862	-0.739737	-2.388939
H	3.826883	-2.418011	-1.997380	H	3.798990	-2.415313	-1.954084
H	4.771866	-1.548972	-3.207637	H	4.800872	-1.644739	-3.187755
H	9.259281	-2.391615	-0.022056	H	9.307531	-2.331856	-0.034205
H	9.740012	-0.739452	-0.410668	H	9.747619	-0.668217	-0.421860
H	9.208664	-1.835583	-1.698886	H	9.234181	-1.773208	-1.709216
C	5.651399	0.934898	2.088929	C	5.623972	0.881914	2.112287
H	5.156994	1.879699	1.842456	H	5.106546	1.818479	1.881176
H	4.994585	0.401367	2.787314	H	4.979129	0.320825	2.800151
H	6.576294	1.165035	2.626880	H	6.543453	1.125517	2.654331
H	-4.132332	-5.742873	-0.247493	H	-4.265449	-5.637214	-0.353129
Pt	-2.085403	-0.987690	-0.048363	Pt	-2.086017	-0.975725	0.011731
C	-4.052635	-0.539643	0.139946	C	-4.066992	-0.507182	0.164728
N	-1.900368	1.348421	-0.491411	N	-1.864547	1.302516	-0.470592
C	-5.251889	-1.143409	0.543675	C	-5.281185	-1.084107	0.558835
C	-4.225800	0.822435	-0.128321	C	-4.205677	0.852561	-0.124376
C	-1.056623	2.345548	-0.799217	C	-0.987022	2.266925	-0.796385
C	-3.181840	1.706197	-0.437255	C	-3.137235	1.700600	-0.436072
C	-6.462925	-0.421134	0.588845	C	-6.476066	-0.333201	0.576080
H	-5.283946	-2.183631	0.853576	H	-5.338593	-2.119156	0.883448
C	-5.403403	1.578743	-0.086420	C	-5.364934	1.637002	-0.112832
C	-1.489160	3.656093	-1.030715	C	-1.384076	3.582706	-1.055762
H	0.001766	2.116601	-0.867108	H	0.064157	2.008012	-0.853752
C	-3.722398	2.996594	-0.619793	C	-3.640246	2.999842	-0.650678
C	-6.587612	0.933821	0.268429	C	-6.566261	1.020003	0.235103
N	-5.085498	2.907699	-0.394776	N	-5.008772	2.950533	-0.440934
C	-2.839152	4.018262	-0.943387	C	-2.723477	3.987491	-0.986581
H	-7.550774	1.433464	0.313472	H	-7.519509	1.539336	0.261527
C	-6.033293	3.981591	-0.521531	C	-5.926177	4.046877	-0.604678
H	-5.533152	4.936461	-0.337412	H	-5.405204	4.990982	-0.423830
H	-6.495932	4.011077	-1.516698	H	-6.365541	4.071730	-1.610142
H	-6.821311	3.864485	0.228405	H	-6.732254	3.961455	0.129817
H	-7.360773	-0.953412	0.896465	H	-7.389681	-0.840052	0.879295
H	-0.743633	4.403979	-1.281019	H	-0.613212	4.302826	-1.309407
H	-3.152527	5.043231	-1.122090	H	-3.002826	5.017866	-1.188130