Supporting Information

for

Theoretical study on the regioselective photoisomerization of asymmetric N,C-chelate organoboron compound

Fang-Ping Li, Hong-Yang Zhu, Quan-Song Li*, Ze-Sheng Li*

Beijing Key Laboratory of Photoelectronic/Electrophotonic Conversion Materials, Key Laboratory of Cluster Science of Ministry of Education, School of Chemistry and Chemical Engineering, Beijing Institute of Technology, 100081 Beijing, China

E-mail: liquansong@bit.edu.cn, zeshengli@bit.edu.cn

TABLE OF CONTENTS

Table SI1. Absolute and relative energies of the critical points

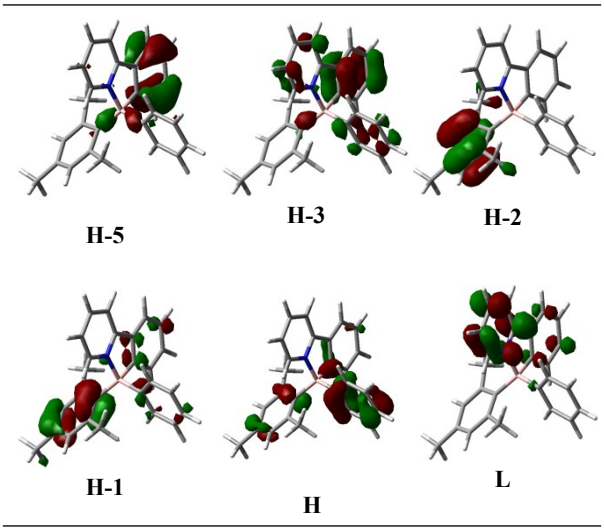
Structure	State	Energy (Hartree)	Energy (eV)
R-S_0	S_0	-1081.58030952	0.00
	S_1	-1081.45712644	3.35
	S_2	-1081.44041857	3.81
	S_3	-1081.43742449	3.89
	S_4	-1081.43378890	3.99
R-S_1	S_0	-1081.56649386	0.38
	S_1	-1081.47744629	2.80
	S_2	-1081.44280884	3.74
	S_3	-1081.44101323	3.79
	S_4	-1081.43783693	3.88
$TS1_{Ph}$-S_0	S_0	-1081.53212049	1.31
	S_1	-1081.44939627	3.56
	S_2	-1081.43038016	4.08
	S_3	-1081.38091658	5.43
	S_4	-1081.36668530	5.81
Int_{Ph}-S_0	S_0	-1081.53393459	1.26
	S_1	-1081.43719493	3.89
	S_2	-1081.40862910	4.67
	S_3	-1081.39959509	4.92
	S_4	-1081.36990245	5.73
$TS2_{Ph}$-S_0	S_0	-1081.49011837	2.45
	S_1	-1081.38410048	5.34
	S_2	-1081.38071460	5.43
	S_3	-1081.33696840	6.62
	S_4	-1081.32675588	6.90
A_{Ph}-S_0	S_0	-1081.53641016	1.19
	S_1	-1081.45160478	3.50
	S_2	-1081.43441171	3.97
	S_3	-1081.40861674	4.67
	S_4	-1081.39330982	5.09
TS_{HT}-S_0	S_0	-1081.49741847	2.26
	S_1	-1081.38832543	5.22
	S_2	-1081.38792678	5.23
	S_3	-1081.36714896	5.80
	S_4	-1081.32470953	6.95
B_{Ph}-S_0	S_0	-1081.57686157	0.09
	S_1	-1081.42793966	4.15
	S_2	-1081.38586904	5.29
	S_3	-1081.36588038	5.83
	S_4	-1081.34714456	6.34

$TS1_{Mes}$-S_0	S_0	-1081.51100611	1.89
	S_1	-1081.41139259	4.60
	S_2	-1081.41123590	4.60
	S_3	-1081.35550241	6.12
	S_4	-1081.34238064	6.47
Int_{Mes}-S_0	S_0	-1081.51333970	1.82
	S_1	-1081.41200528	4.58
	S_2	-1081.38398788	5.34
	S_3	-1081.34887759	6.30
	S_4	-1081.33349405	6.72
$TS2_{Mes}$-S_0	S_0	-1081.48340828	2.64
	S_1	-1081.39683909	4.99
	S_2	-1081.38429970	5.33
	S_3	-1081.34753704	6.33
	S_4	-1081.32375831	6.98
A_{Mes}-S_0	S_0	-1081.53633425	1.20
	S_1	-1081.44586837	3.66
	S_2	-1081.40461515	4.78
	S_3	-1081.39244935	5.11
	S_4	-1081.37028701	5.71
TS_{Ph}-S_1	S_0	-1081.47853320	2.77
	S_1	-1081.46149640	3.23
	S_2	-1081.42348093	4.27
	S_3	-1081.38767315	5.24
	S_4	-1081.38086508	5.43
$(S_1/S_0)_x$-Ph	S_0	-1081.49340534	2.36
	S_1	-1081.47078931	2.98
	S_2	-1081.42974134	4.10
	S_3	-1081.40776930	4.69
	S_4	-1081.40435005	4.79
Int'_{Ph}-S_0	S_0	-1081.52129160	1.61
	S_1	-1081.44711023	3.62
	S_2	-1081.43134033	4.05
	S_3	-1081.41422047	4.52
	S_4	-1081.40961312	4.64
TS_{Mes}-S_1	S_0	-1081.46136782	3.24

	S_1	-1081.44533008	3.67
	S_2	-1081.39592573	5.02
	S_3	-1081.37474635	5.59
	S_4	-1081.36640160	5.82
$(S_1/S_0)_x$-Mes	S_0	-1081.49244223	2.39
	S_1	-1081.48077846	2.71
	S_2	-1081.45145512	3.51
	S_3	-1081.40489075	4.77
	S_4	-1081.38884044	5.21
Int'_{Mes}-S_0	S_0	-1081.52035167	1.63
	S_1	-1081.46067587	3.26
	S_2	-1081.42258553	4.29
	S_3	-1081.40877184	4.67
	S_4	-1081.36808164	5.77

Table SI2. Relative TD-CAM-B3LYP vertical excitation energy (Δ*E*) and wavelength (*λ*) at R-S_0 together with the electronic configuration (weight in the parenthesis, orbitals below the table) and oscillation strength *f*

State	Δ*E*/ (eV)	*λ*/(nm)	Electronic configuration(wight)	*f*
S_0	0	--	--	--
S_1	4.15	299	H→L (43%)	0.1881
			H-1→L (30%)	
			H-3→L(19%)	
S_2	4.45	278	H-1→L (27%)	0.0696
			H→L(50%)	
			H-3→L(15%)	
S_3	4.80	258	H-5→L(19%)	0.0697
			H-2→L(21%)	
			H-3→L(17%)	
S_4	4.90	253	H-2→L(67%)	0.0208



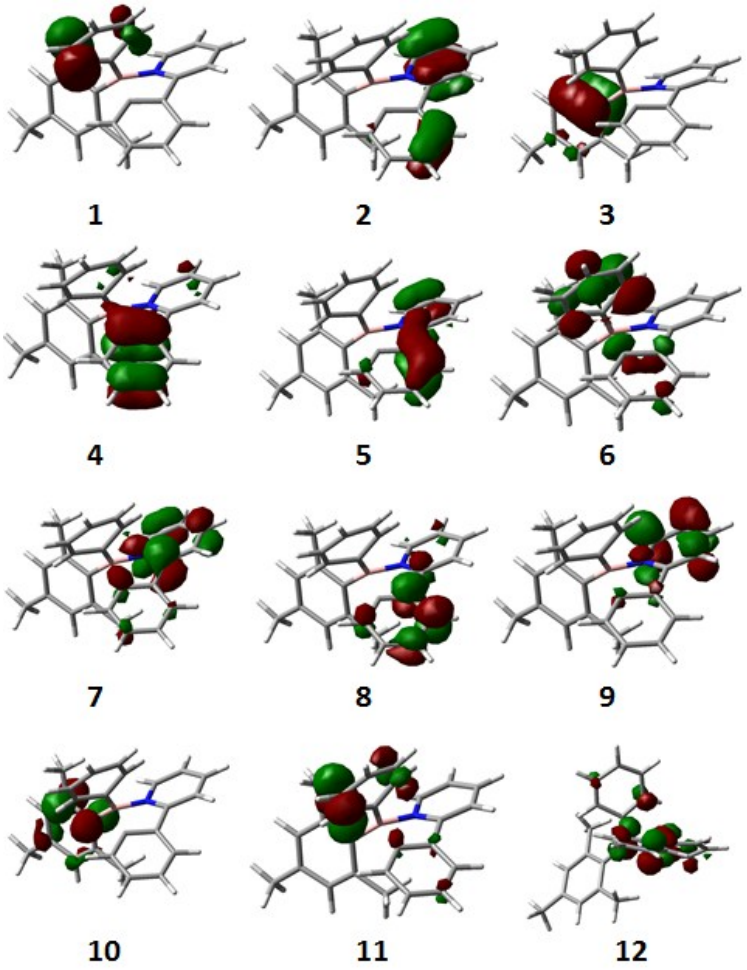


Fig. SI1 The (12,12) active space at TS_{Ph}-S1.

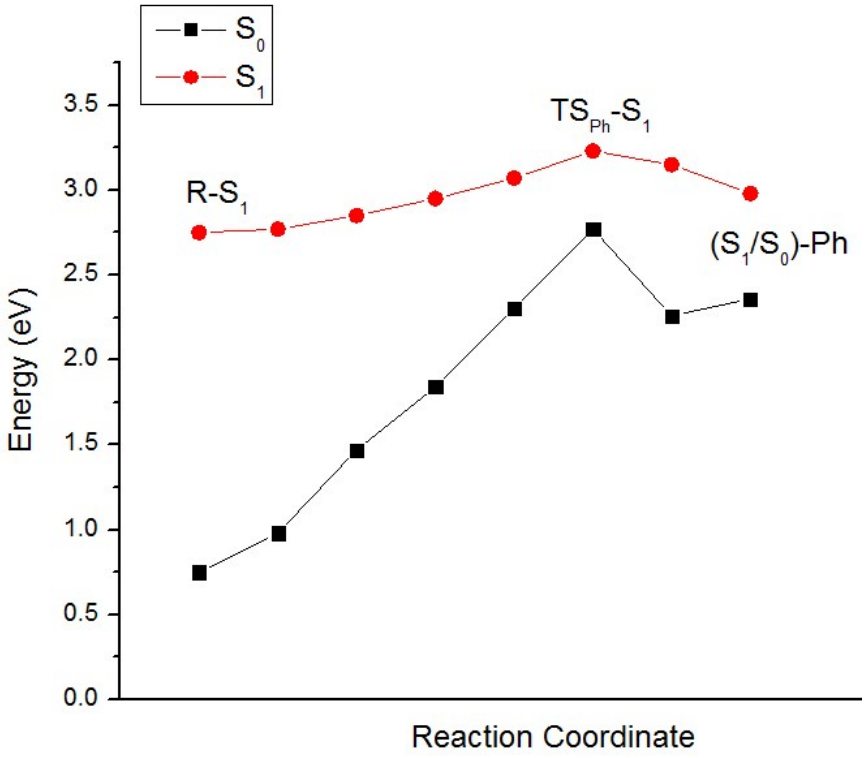
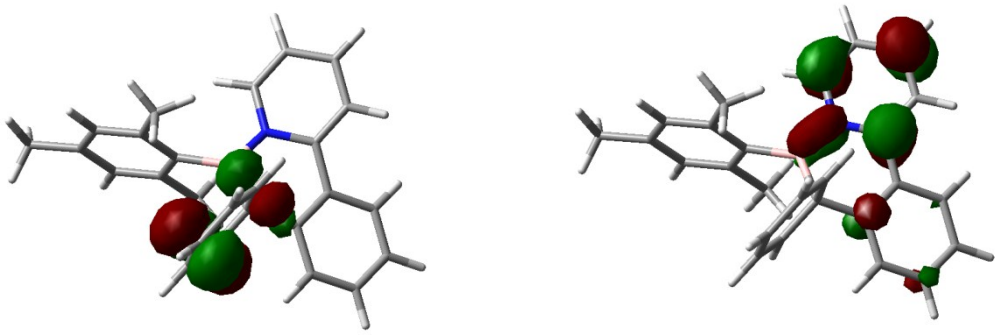


Fig. SI2 CASPT2 energy profile from R-S_1 to $(S_1/S_0)_x$-Ph via TS_{Ph}-S_1.



SOMO-1 SOMO-2

Fig. SI3 Plots of the two singly occupied molecular orbitals (SOMO-1 and SOMO-2) at Int'$_{Ph}$-S_0.

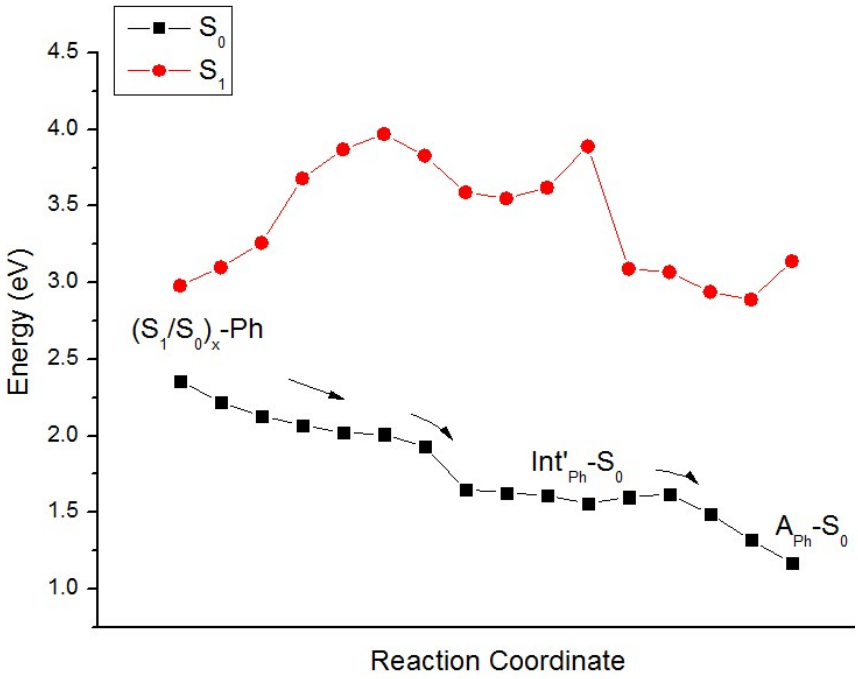


Fig. SI4 CASPT2 energy profile in S_0 state from $(S_1/S_0)_x$-Ph to A_{Ph}-S_0 via Int'$_{Ph}$-S_0.

Cartesian coordinates of optimized structures

	R-S_0				R-S_1		
C	-1.88073	-1.362609	0.926061	C	-1.966348	-1.184198	0.976459
C	-0.373216	-0.58544	2.521524	C	-0.263555	-0.771971	2.568905
C	-1.028987	-1.242903	3.532424	C	-1.012030	-1.296633	3.569538
C	-2.160843	-1.985092	3.209649	C	-2.322718	-1.774913	3.271045
C	-2.590459	-2.051038	1.901667	C	-2.765863	-1.723105	1.981203
C	-2.118622	-1.305258	-0.518038	C	-2.182593	-1.102020	-0.437929
C	-1.136025	-0.546872	-1.150919	C	-1.084802	-0.485179	-1.093064
C	-1.235305	-0.391788	-2.531795	C	-1.120100	-0.331479	-2.473799
C	-2.261599	-0.996871	-3.232562	C	-2.191290	-0.815202	-3.210487
C	-3.227951	-1.760107	-2.577897	C	-3.248376	-1.447306	-2.561074
C	-3.162228	-1.914365	-1.210296	C	-3.249558	-1.603052	-1.186487
H	0.509899	-0.005618	2.697108	H	0.734010	-0.424380	2.741744
H	-2.696549	-2.512397	3.978015	H	-2.935550	-2.191464	4.040985
H	-3.454471	-2.626608	1.632779	H	-3.733961	-2.106286	1.723747
H	-0.510057	0.197953	-3.06386	H	-0.299892	0.139835	-2.987723
H	-2.321008	-0.876001	-4.300236	H	-2.203441	-0.713901	-4.279249
H	-4.021971	-2.220299	-3.137821	H	-4.073544	-1.831573	-3.136117
H	-3.909882	-2.494598	-0.698229	H	-4.062565	-2.117681	-0.707187
B	-0.135791	0.15491	-0.060276	B	-0.024342	0.025601	0.064548
N	-0.79564	-0.641525	1.25786	N	-0.705665	-0.669634	1.299546
C	1.490201	-0.141667	-0.080366	C	1.589706	-0.190784	-0.046202
C	2.033831	-1.355931	-0.647806	C	2.135010	-1.391838	-0.625786
C	2.430855	0.746035	0.462481	C	2.510992	0.734113	0.452108
C	3.38365	-1.548491	-0.743025	C	3.484532	-1.542715	-0.774279
C	3.824095	0.503176	0.337561	C	3.905410	0.537927	0.277233
C	4.316641	-0.604828	-0.274584	C	4.403599	-0.563643	-0.345529
H	3.753299	-2.463274	-1.176119	H	3.866719	-2.451366	-1.210042
H	4.505841	1.229489	0.747992	H	4.582125	1.282296	0.663415
C	-0.614796	1.723511	-0.038593	C	-0.598192	1.545839	-0.062643
C	-1.58221	2.251801	0.824176	C	-1.727040	1.972540	0.725145
C	-0.130831	2.590514	-1.034888	C	-0.107486	2.474501	-1.052212
C	-2.02757	3.572303	0.716387	C	-2.264621	3.251311	0.593846
C	-0.565146	3.891459	-1.155075	C	-0.640618	3.708256	-1.180162
C	-1.519839	4.400457	-0.275509	C	-1.734878	4.124228	-0.351184
H	-2.768772	3.943957	1.403083	H	-3.090477	3.553349	1.215413
H	-0.163291	4.520246	-1.931182	H	-0.243633	4.400222	-1.905405
C	2.111396	2.011661	1.245806	C	2.141044	1.969983	1.255989
H	2.137745	2.891965	0.613007	H	2.125979	2.867798	0.646725
H	1.144437	2.000425	1.721412	H	1.183897	1.884782	1.750851
H	2.858665	2.148183	2.021757	H	2.883606	2.128123	2.032776
C	1.166674	-2.505954	-1.124605	C	1.252280	-2.550448	-1.043544
H	0.398015	-2.761896	-0.405568	H	0.490168	-2.757274	-0.300368
H	0.670019	-2.2929	-2.061934	H	0.741085	-2.365001	-1.979789
H	1.777483	-3.389691	-1.270219	H	1.848095	-3.448433	-1.162968
C	5.796627	-0.857984	-0.426672	C	5.884494	-0.778194	-0.543998
H	6.085986	-1.792561	0.046093	H	6.212777	-1.699340	-0.070328
H	6.074701	-0.927793	-1.474735	H	6.130915	-0.853860	-1.599507
H	6.381459	-0.062245	0.020482	H	6.462460	0.037127	-0.124086
H	-0.666129	-1.180923	4.540011	H	-0.607698	-1.366918	4.557454
H	-2.008638	1.639914	1.600678	H	-2.140976	1.287607	1.449576
H	0.616924	2.232033	-1.722336	H	0.721414	2.172031	-1.669152
H	-1.858222	5.417567	-0.366218	H	-2.146846	5.114355	-0.471298

	$TS1_{Ph}$-S_0				Int_{Ph}-S_0		
C	-1.971283	-1.209625	1.046228	C	-2.023542	-1.182984	1.101654
C	-0.145307	-0.982648	2.575142	C	-0.091910	-1.528782	2.562685
C	-0.880035	-1.469946	3.599025	C	-0.861078	-2.117574	3.494319
C	-2.258062	-1.834674	3.353972	C	-2.296845	-2.271428	3.246460
C	-2.784409	-1.709337	2.128735	C	-2.843691	-1.833753	2.114965
C	-2.281453	-1.022869	-0.279736	C	-2.349238	-0.692276	-0.098797
C	-1.124699	-0.473071	-0.972603	C	-1.139875	-0.082768	-0.790413
C	-1.202768	-0.484097	-2.439747	C	-1.120597	-0.539597	-2.239646
C	-2.363690	-0.808751	-3.055577	C	-2.271569	-0.843605	-2.869883
C	-3.562138	-1.170765	-2.309480	C	-3.563711	-0.860928	-2.161033
C	-3.513203	-1.283547	-0.975994	C	-3.604601	-0.810640	-0.831252
H	0.883333	-0.703995	2.677504	H	0.964525	-1.388233	2.673790
H	-2.853681	-2.214644	4.164466	H	-2.903367	-2.749073	3.994674
H	-3.801451	-1.985776	1.925345	H	-3.893529	-1.947499	1.920210
H	-0.337695	-0.220438	-3.019454	H	-0.195049	-0.521668	-2.787002
H	-2.408166	-0.818007	-4.130708	H	-2.262854	-1.101475	-3.914633
H	-4.471395	-1.365038	-2.848727	H	-4.465508	-0.958827	-2.738820
H	-4.387740	-1.581578	-0.423328	H	-4.540144	-0.889924	-0.304309
B	-0.008329	-0.324112	0.072457	B	0.038564	-0.510224	0.233336
N	-0.681657	-0.824100	1.314771	N	-0.632992	-1.053292	1.366697
C	1.588232	-0.293662	-0.023099	C	1.612692	-0.400342	0.099701
C	2.246073	-1.376662	-0.702218	C	2.315201	-1.454997	-0.571144
C	2.394068	0.677049	0.567760	C	2.348276	0.663949	0.606322
C	3.606840	-1.396690	-0.813552	C	3.665446	-1.371038	-0.747013
C	3.803184	0.620740	0.425114	C	3.749289	0.713273	0.401168
C	4.416876	-0.381923	-0.261581	C	4.411096	-0.269879	-0.270872
H	4.083163	-2.216643	-1.325232	H	4.184562	-2.169308	-1.251188
H	4.396445	1.395932	0.881516	H	4.296651	1.554613	0.792520
C	-0.903463	1.324888	-0.452368	C	-1.152948	1.472243	-0.751611
C	-1.889057	1.933377	0.353752	C	-1.972175	2.187861	0.149051
C	-0.151456	2.125027	-1.277097	C	-0.329492	2.199705	-1.581199
C	-2.065960	3.299084	0.338094	C	-1.952077	3.567477	0.185905
C	-0.336377	3.517207	-1.307905	C	-0.310261	3.601719	-1.547892
C	-1.279254	4.102125	-0.509348	C	-1.111252	4.287924	-0.675934
H	-2.816174	3.752243	0.961655	H	-2.590586	4.091044	0.875558
H	0.271499	4.116302	-1.962733	H	0.342727	4.132830	-2.218160
C	1.860815	1.831865	1.393715	C	1.724471	1.802866	1.386522
H	1.949947	2.770459	0.855683	H	1.684529	2.709449	0.792135
H	0.822510	1.715463	1.664817	H	0.714914	1.583633	1.707865
H	2.437055	1.929342	2.309533	H	2.312828	2.017405	2.273653
C	1.454709	-2.534400	-1.275195	C	1.574274	-2.693223	-1.030853
H	0.753522	-2.935496	-0.550810	H	1.197354	-3.257337	-0.181655
H	0.879354	-2.244854	-2.146752	H	0.722991	-2.456949	-1.659611
H	2.118872	-3.338447	-1.570834	H	2.227109	-3.349126	-1.594725
C	5.916442	-0.445397	-0.423684	C	5.902472	-0.220684	-0.500516
H	6.316671	-1.364787	-0.005682	H	6.393952	-1.085984	-0.064906
H	6.196471	-0.419672	-1.473104	H	6.133264	-0.218584	-1.562054
H	6.403224	0.386693	0.071727	H	6.340535	0.668328	-0.062179
H	-0.445672	-1.590236	4.572400	H	-0.429135	-2.474383	4.409231
H	-2.512714	1.328432	0.984190	H	-2.625467	1.653453	0.811015
H	0.607196	1.694551	-1.904255	H	0.318467	1.697585	-2.275217
H	-1.427550	5.167141	-0.530149	H	-1.101029	5.363065	-0.650275

	$TS2_{Ph}$-S_0				A_{Ph}-S_0		
C	-2.194352	-1.053987	1.024774	C	-1.991404	-1.288175	0.858726
C	-0.260028	-1.166044	2.439880	C	-0.174216	-1.123398	2.318490
C	-0.946461	-1.777383	3.424793	C	-0.744429	-1.932362	3.252981
C	-2.372959	-1.983141	3.256342	C	-2.025332	-2.414071	2.996694
C	-2.963644	-1.639004	2.110939	C	-2.634744	-2.092375	1.814960
C	-2.603881	-0.843011	-0.254453	C	-2.616952	-1.011543	-0.456076
C	-1.608864	-0.257884	-1.180453	C	-2.091488	-0.075959	-1.336839
C	-1.655281	-0.855335	-2.538164	C	-2.743750	0.101901	-2.587883
C	-2.762195	-1.494579	-2.974229	C	-3.849720	-0.627697	-2.939786
C	-3.924908	-1.677176	-2.113027	C	-4.359124	-1.595048	-2.050999
C	-3.833520	-1.379432	-0.816058	C	-3.754106	-1.771416	-0.848169
H	0.791699	-0.984530	2.501332	H	0.795979	-0.700259	2.463213
H	-2.943139	-2.423915	4.054111	H	-2.536148	-3.027922	3.715872
H	-4.013307	-1.801819	1.962223	H	-3.624575	-2.447820	1.630260
H	-0.831432	-0.727990	-3.210321	H	-2.368682	0.851404	-3.256958
H	-2.792516	-1.880333	-3.978098	H	-4.328069	-0.458679	-3.888045
H	-4.827526	-2.089869	-2.525978	H	-5.212085	-2.190288	-2.321576
H	-4.665174	-1.571136	-0.161377	H	-4.143236	-2.534041	-0.204560
B	-0.173383	0.035299	0.224073	B	-0.037626	0.353581	0.283496
N	-0.874393	-0.729153	1.272531	N	-0.775110	-0.791033	1.154815
C	1.427420	0.059821	0.138481	C	1.569330	0.234770	0.325508
C	2.144380	-0.795332	-0.768463	C	2.226741	-0.759139	-0.482831
C	2.196929	0.858971	0.989153	C	2.385088	1.043760	1.114665
C	3.506570	-0.736741	-0.848742	C	3.588457	-0.850064	-0.507440
C	3.608137	0.892194	0.866881	C	3.798005	0.922715	1.056679
C	4.271098	0.132570	-0.046311	C	4.408652	0.007793	0.256639
H	4.019388	-1.390130	-1.535303	H	4.058598	-1.600731	-1.121518
H	4.162605	1.535720	1.529883	H	4.395286	1.577117	1.670448
C	-1.116765	1.075215	-1.037131	C	-0.887545	0.728233	-1.018376
C	-1.143072	1.726830	0.224584	C	-0.954016	1.649273	0.236851
C	-0.362635	1.735168	-2.094104	C	-0.174876	1.330535	-2.185454
C	-0.576016	3.050984	0.353855	C	-0.504994	3.049063	0.046500
C	0.192497	2.942508	-1.904990	C	0.327873	2.577973	-2.182741
C	0.091024	3.635439	-0.651080	C	0.111787	3.481042	-1.044503
H	-0.712501	3.562533	1.289455	H	-0.716041	3.736172	0.849874
H	0.705063	3.418424	-2.722361	H	0.870777	2.942306	-3.037271
C	1.649283	1.675535	2.145309	C	1.857473	2.074624	2.094219
H	1.837026	2.733558	1.997413	H	1.966225	3.078662	1.697942
H	0.590915	1.542993	2.302479	H	0.812671	1.929533	2.326037
H	2.154201	1.385511	3.062812	H	2.419781	2.029256	3.023219
C	1.441038	-1.810360	-1.643024	C	1.428846	-1.749961	-1.304437
H	0.558804	-2.222001	-1.171709	H	0.735987	-2.316415	-0.689504
H	1.135283	-1.373106	-2.586501	H	0.843802	-1.260369	-2.072028
H	2.110095	-2.631547	-1.873716	H	2.087834	-2.460977	-1.790136
C	5.772873	0.170906	-0.190948	C	5.910836	-0.122360	0.181246
H	6.205817	-0.813455	-0.037417	H	6.233031	-1.123001	0.456561
H	6.059559	0.497871	-1.186496	H	6.268471	0.064701	-0.827567
H	6.221829	0.849496	0.525058	H	6.402161	0.580788	0.844083
H	-0.442343	-2.104529	4.313434	H	-0.218916	-2.160047	4.159974
H	-1.927854	1.467779	0.911763	H	-1.890919	1.587141	0.774553
H	-0.304740	1.275165	-3.058649	H	-0.033785	0.709277	-3.053988
H	0.521010	4.614463	-0.545807	H	0.429853	4.505559	-1.129171

	TS_{HT}-S_0				B_{Ph}-S_0		
C	-2.024632	-0.456187	0.926481	C	-2.096778	-0.131403	0.988248
C	-0.191172	-1.736174	1.907210	C	-0.220198	-1.443009	1.916305
C	-0.954514	-2.167700	2.901344	C	-0.984885	-2.006932	2.839615
C	-2.258538	-1.537030	3.123152	C	-2.346501	-1.505156	3.056000
C	-2.766731	-0.714867	2.184331	C	-2.859865	-0.609753	2.201640
C	-2.628823	-0.748694	-0.333309	C	-2.607420	-0.692186	-0.331745
C	-2.094329	-0.234887	-1.542256	C	-2.267971	-0.002848	-1.530442
C	-2.662231	-0.716497	-2.783627	C	-2.670372	-0.535243	-2.732283
C	-3.761164	-1.515157	-2.802326	C	-3.410468	-1.725841	-2.796216
C	-4.393666	-1.881093	-1.571479	C	-3.740599	-2.384566	-1.647044
C	-3.854184	-1.501601	-0.398216	C	-3.331900	-1.864552	-0.406572
H	0.798504	-2.109659	1.728742	H	0.790140	-1.760367	1.755484
H	-2.790946	-1.730270	4.037161	H	-2.904454	-1.837279	3.913125
H	-3.725861	-0.246969	2.314123	H	-3.849892	-0.209373	2.329779
H	-2.199544	-0.448384	-3.713224	H	-2.399868	-0.040124	-3.647118
H	-4.162019	-1.867769	-3.735464	H	-3.705972	-2.114328	-3.754647
H	-5.277787	-2.493201	-1.588919	H	-4.302899	-3.300635	-1.681778
H	-4.299733	-1.828119	0.521862	H	-3.586908	-2.390161	0.494150
B	0.246832	0.210063	0.412307	B	0.254668	0.346847	0.284056
N	-0.602110	-0.702983	1.052694	N	-0.643209	-0.390093	1.093727
C	1.831889	0.128127	0.418674	C	1.829856	0.129193	0.406906
C	2.553715	-0.492406	-0.651393	C	2.538700	-0.574584	-0.615345
C	2.555182	0.659862	1.478804	C	2.550188	0.634316	1.483851
C	3.916522	-0.546458	-0.611432	C	3.890356	-0.744756	-0.514728
C	3.969989	0.591276	1.479469	C	3.951318	0.448241	1.546569
C	4.655371	0.002453	0.460323	C	4.625956	-0.229686	0.573467
H	4.450814	-1.020854	-1.417906	H	4.415355	-1.282996	-1.286569
H	4.507034	1.012874	2.313068	H	4.490736	0.852942	2.386351
C	-1.243099	0.904937	-1.508285	C	-1.498943	1.279928	-1.508172
C	-0.661280	1.346753	-0.260414	C	-0.315343	1.440027	-0.720253
C	-1.131053	1.771951	-2.661529	C	-1.921610	2.317079	-2.307747
C	-0.169350	2.731743	-0.215025	C	0.382380	2.636885	-0.838696
C	-0.626102	3.012624	-2.566220	C	-1.215155	3.525925	-2.377771
C	-0.164249	3.533646	-1.303307	C	-0.068512	3.687522	-1.653270
H	0.221683	3.092812	0.719373	H	1.297194	2.768102	-0.289501
H	-0.586023	3.640820	-3.438361	H	-1.583006	4.317897	-3.005978
C	1.898169	1.333352	2.667396	C	1.875140	1.364737	2.629503
H	2.149247	2.390246	2.699292	H	2.577245	2.014793	3.139931
H	0.818684	1.248869	2.655027	H	1.046116	1.978789	2.296266
H	2.244121	0.892741	3.597428	H	1.483518	0.665375	3.362726
C	1.815022	-1.086119	-1.830478	C	1.791860	-1.139645	-1.804141
H	1.021185	-1.755203	-1.513282	H	0.982275	-1.794769	-1.494179
H	1.357849	-0.310338	-2.436818	H	1.352692	-0.349461	-2.405123
H	2.489076	-1.648426	-2.466152	H	2.452973	-1.714049	-2.442490
C	6.162767	-0.081028	0.449806	C	6.120511	-0.436989	0.632441
H	6.496421	-1.113973	0.407388	H	6.367895	-1.494734	0.643422
H	6.575489	0.427526	-0.416877	H	6.610096	0.000191	-0.233145
H	6.589843	0.371669	1.337070	H	6.547300	0.014451	1.520515
H	-0.608825	-2.949852	3.550401	H	-0.600023	-2.812123	3.436029
H	-1.648873	1.017098	0.549731	H	-2.216138	0.943051	0.947590
H	-1.510617	1.443698	-3.608217	H	-2.822711	2.207404	-2.883410
H	0.213709	4.538792	-1.251487	H	0.488797	4.605978	-1.702674

	$TS1_{Mes}$-S_0				Int_{Mes}-S_0		
C	-1.998585	-1.489225	-0.157582	C	-1.941892	-1.500106	-0.794518
C	-2.378446	0.229761	-1.780954	C	-3.440380	0.146615	0.218522
C	-3.303604	-0.492577	-2.419783	C	-4.474395	-0.709191	0.152361
C	-3.614660	-1.820367	-1.929165	C	-4.275987	-2.034374	-0.441587
C	-2.983732	-2.306429	-0.833718	C	-3.080186	-2.404813	-0.891599
C	-1.231276	-1.757611	0.935092	C	-0.665532	-1.680997	-1.132574
C	-0.388448	-0.596777	1.256345	C	0.152297	-0.406424	-0.932413
C	0.102219	-0.606883	2.649616	C	0.587408	-0.063100	-2.364981
C	0.021733	-1.704938	3.403994	C	0.915660	-1.038520	-3.235122
C	-0.567373	-2.949807	2.928740	C	0.735920	-2.462990	-2.901098
C	-1.207289	-2.960617	1.737730	C	-0.079555	-2.783695	-1.902151
H	-2.105711	1.219261	-2.087938	H	-3.517148	1.127655	0.641415
H	-4.354373	-2.412271	-2.437023	H	-5.114992	-2.703302	-0.508021
H	-3.205038	-3.281633	-0.444371	H	-2.920295	-3.370878	-1.332305
H	0.502399	0.282366	3.085515	H	0.652756	0.961882	-2.674207
H	0.377093	-1.667467	4.419603	H	1.252715	-0.784632	-4.225649
H	-0.529844	-3.823486	3.553393	H	1.212784	-3.212543	-3.507293
H	-1.702474	-3.850032	1.388300	H	-0.312412	-3.809062	-1.669411
B	-0.704859	0.455408	0.173837	B	-0.982538	0.572716	-0.334876
N	-1.708037	-0.249718	-0.680871	N	-2.175789	-0.201033	-0.264739
C	1.103592	-0.397622	0.107737	C	1.372030	-0.539044	0.046749
C	2.142244	0.472957	0.602233	C	2.560080	0.261274	-0.118226
C	1.461695	-1.337247	-0.859741	C	1.341184	-1.400606	1.150797
C	3.430305	0.350926	0.123546	C	3.638741	0.060981	0.700348
C	2.800567	-1.416066	-1.306479	C	2.493153	-1.566396	1.958206
C	3.789891	-0.606897	-0.835968	C	3.646583	-0.881221	1.740411
H	3.039819	-2.153462	-2.051886	H	4.517503	0.665357	0.551077
H	4.187210	1.016928	0.503486	H	2.439562	-2.264419	2.775654
C	-0.656451	2.042340	0.040229	C	-0.912581	2.092159	0.083356
C	0.088215	2.713807	-0.960644	C	-1.728408	3.042594	-0.579999
C	-1.463165	2.819714	0.861156	C	-0.083531	2.546428	1.086767
C	0.027202	4.073625	-1.102279	C	-1.696224	4.369053	-0.247805
C	-1.524130	4.218181	0.719007	C	-0.054062	3.905126	1.447812
C	-0.786885	4.839358	-0.250889	C	-0.851273	4.813476	0.784474
H	0.605141	4.562386	-1.867300	H	-2.317888	5.073288	-0.771996
H	-2.153866	4.793153	1.375177	H	0.596507	4.230429	2.240041
C	0.541109	-2.329545	-1.540952	C	0.134287	-2.193622	1.626444
H	0.127821	-3.041795	-0.841554	H	-0.780148	-1.618924	1.603515
H	-0.278545	-1.844718	-2.051387	H	-0.024485	-3.094914	1.047691
H	1.099063	-2.884517	-2.284455	H	0.293895	-2.493396	2.656013
C	1.991335	1.571599	1.646051	C	2.717114	1.388916	-1.124688
H	2.495068	2.465166	1.295829	H	2.929372	1.025428	-2.121991
H	2.470310	1.268820	2.572161	H	1.841742	2.021492	-1.174522
H	0.979023	1.851726	1.864627	H	3.545921	2.018380	-0.823567
C	5.215226	-0.711230	-1.315553	C	4.879800	-1.075335	2.588168
H	5.549071	0.227267	-1.748751	H	5.711099	-1.437943	1.990051
H	5.884690	-0.943247	-0.492252	H	5.193941	-0.141089	3.045010
H	5.325104	-1.485466	-2.065485	H	4.703643	-1.792358	3.381756
H	-3.809867	-0.092174	-3.276571	H	-5.436894	-0.426264	0.532682
H	0.723004	2.142815	-1.615616	H	-2.384284	2.715604	-1.369145
H	-2.054429	2.350114	1.628950	H	0.555992	1.859219	1.610752
H	-0.827391	5.908185	-0.366535	H	-0.829142	5.855154	1.051058

	$TS2_{Mes}$-S_0				A_{Mes}-S_0		
C	-2.058235	1.368841	0.394496	C	-1.759423	-1.322790	-1.014032
C	-0.190207	2.786428	0.888539	C	-2.798621	0.363733	0.218890
C	-0.987323	3.809369	1.263833	C	-4.043869	-0.160605	0.058258
C	-2.422981	3.611410	1.220895	C	-4.149346	-1.379579	-0.639912
C	-2.936019	2.450016	0.804438	C	-3.032312	-1.941480	-1.162228
C	-2.390749	0.139517	-0.074571	C	-0.564407	-1.896678	-1.676920
C	-1.216966	-0.714990	-0.453845	C	0.709021	-1.419098	-1.411488
C	-1.401426	-1.254659	-1.834629	C	1.801020	-1.999373	-2.111996
C	-2.636624	-1.446001	-2.343529	C	1.623167	-3.002018	-3.029158
C	-3.836391	-1.066106	-1.597822	C	0.321961	-3.471516	-3.303408
C	-3.707222	-0.264354	-0.538264	C	-0.733458	-2.925117	-2.647286
H	0.878712	2.859377	0.879001	H	-2.634016	1.264757	0.767951
H	-3.073635	4.412775	1.522827	H	-5.102475	-1.862225	-0.757349
H	-3.996755	2.294683	0.758451	H	-3.109596	-2.873994	-1.676081
H	-0.532839	-1.486874	-2.420233	H	2.784018	-1.610240	-1.923881
H	-2.749291	-1.843586	-3.337517	H	2.467098	-3.409169	-3.556859
H	-4.802716	-1.373263	-1.954895	H	0.164153	-4.241420	-4.036548
H	-4.580697	0.115967	-0.035381	H	-1.712159	-3.276540	-2.903350
B	0.140377	0.383226	0.097449	B	-0.279471	0.467494	0.162082
N	-0.704872	1.578617	0.469915	N	-1.671005	-0.218659	-0.286193
C	-0.315243	-1.404725	0.446948	C	0.969123	-0.297448	-0.470242
C	0.455924	-2.594175	0.021128	C	2.232207	-0.397625	0.336600
C	0.183888	-0.672208	1.590615	C	0.568510	1.134104	-0.996594
C	1.631404	-2.870256	0.606739	C	3.008040	0.659116	0.546663
C	1.484209	-1.064234	2.144091	C	1.597365	2.184708	-0.718764
C	2.231363	-2.072339	1.651401	C	2.729848	1.988824	-0.023673
H	2.137148	-3.780068	0.328326	H	3.868779	0.566700	1.188793
H	1.826635	-0.500759	2.996035	H	1.405852	3.155022	-1.150912
C	1.434605	0.674612	-0.801210	C	-0.352362	0.956136	1.692349
C	1.231911	0.971380	-2.174627	C	-0.312561	2.294889	2.058627
C	2.724746	0.768440	-0.329055	C	-0.498685	0.016413	2.746334
C	2.264909	1.305272	-3.005349	C	-0.400002	2.698851	3.405180
C	3.800189	1.113185	-1.170838	C	-0.586203	0.401739	4.055580
C	3.577574	1.374176	-2.504263	C	-0.534814	1.765019	4.394194
H	2.075483	1.522969	-4.042020	H	-0.360413	3.746365	3.650270
H	4.794612	1.174568	-0.763860	H	-0.691755	-0.336462	4.832098
C	-0.743324	-0.169454	2.701189	C	0.049116	1.285115	-2.423850
H	-1.763700	-0.046137	2.386001	H	-0.321725	2.298004	-2.562424
H	-0.739523	-0.903694	3.501755	H	-0.767059	0.618470	-2.668308
H	-0.388169	0.769646	3.110465	H	0.833904	1.123264	-3.160096
C	-0.154597	-3.656916	-0.879699	C	2.526323	-1.711979	1.024353
H	-1.231148	-3.688571	-0.784220	H	2.671528	-2.531393	0.329088
H	0.077776	-3.518417	-1.927733	H	1.697742	-1.989495	1.670164
H	0.231883	-4.625839	-0.584927	H	3.417028	-1.634516	1.637220
C	3.586401	-2.453644	2.189373	C	3.739231	3.080862	0.223210
H	3.603699	-3.489095	2.518087	H	3.857108	3.270300	1.287815
H	4.351674	-2.342944	1.425897	H	4.718438	2.805303	-0.162059
H	3.863537	-1.831134	3.032286	H	3.443501	4.010713	-0.250168
H	-0.568014	4.746686	1.573662	H	-4.900427	0.334935	0.471547
H	0.233326	0.941033	-2.572457	H	-0.203518	3.048580	1.299575
H	2.935309	0.579844	0.706254	H	-0.541608	-1.033433	2.508110
H	4.392572	1.637836	-3.155060	H	-0.601129	2.065476	5.425479

	TSPh-S1				(S_1/S_0)x-Ph		
C	-1.87109300	1.50021800	-0.03891600	C	-2.044475	-1.107479	1.016869
C	-0.15815600	2.43582900	-1.39827800	C	-0.131097	-1.161003	2.487828
C	-0.94850800	3.44590600	-1.79728900	C	-0.826681	-1.812551	3.429636
C	-2.29682500	3.51229900	-1.29647500	C	-2.222807	-2.099272	3.215127
C	-2.72139200	2.54884900	-0.40185300	C	-2.795056	-1.761985	2.041821
C	-2.03263000	0.54916300	1.07249800	C	-2.406203	-0.895698	-0.328608
C	-1.19721900	-0.56245300	0.98692300	C	-1.536317	-0.069870	-1.120845
C	-1.16775100	-1.49177700	2.00422700	C	-1.685572	-0.120394	-2.549427
C	-1.97891400	-1.31198800	3.12339800	C	-2.660927	-0.886487	-3.133852
C	-2.80266500	-0.20526400	3.21178400	C	-3.586863	-1.615698	-2.322147
C	-2.82167900	0.74141400	2.19134900	C	-3.466676	-1.607633	-0.976777
H	0.85558200	2.34970200	-1.73390400	H	0.903718	-0.918349	2.600262
H	-2.95130900	4.30137900	-1.60277300	H	-2.789558	-2.584919	3.984266
H	-3.71191000	2.58097800	0.00772500	H	-3.827237	-1.982147	1.856446
H	-0.54230800	-2.36376700	1.93519000	H	-1.057809	0.487686	-3.168363
H	-1.96587300	-2.03710500	3.91756500	H	-2.759730	-0.909358	-4.201866
H	-3.42218900	-0.06230300	4.08043800	H	-4.369016	-2.179641	-2.792857
H	-3.42323400	1.62739000	2.29239300	H	-4.142485	-2.187040	-0.377908
B	0.12585000	0.11901800	-0.37361200	B	0.016060	0.003646	0.282245
N	-0.56881700	1.46950400	-0.53558800	N	-0.714687	-0.734614	1.298819
C	1.69866600	0.05767500	-0.10839900	C	1.586380	-0.106387	0.095239
C	2.30369700	0.57693900	1.08675500	C	2.137924	-1.200734	-0.611505
C	2.54392400	-0.46654400	-1.08719800	C	2.463368	0.845837	0.633481
C	3.65349400	0.47787300	1.26819000	C	3.508719	-1.287884	-0.795061
C	3.93989400	-0.54526700	-0.85832500	C	3.838936	0.723022	0.434645
C	4.50095300	-0.10151500	0.30024000	C	4.378386	-0.325965	-0.287996
H	4.09372500	0.86743800	2.17115400	H	3.911038	-2.123408	-1.338807
H	4.56624600	-0.95955600	-1.63069400	H	4.493885	1.462230	0.860552
C	-0.75370600	-1.04925900	-0.80722000	C	-0.926483	1.218704	-0.478378
C	-1.97890900	-0.80409800	-1.59755800	C	-1.784478	1.984235	0.415082
C	-0.35270600	-2.46829800	-0.74771500	C	-0.081812	2.029148	-1.343977
C	-2.89830400	-1.86750500	-1.82873500	C	-1.726965	3.341949	0.491329
C	-1.22405600	-3.43489100	-1.06496100	C	-0.048511	3.386969	-1.265696
C	-2.56016600	-3.14255500	-1.54005000	C	-0.863044	4.074475	-0.345893
H	-3.85379300	-1.64227500	-2.27407100	H	-2.363605	3.864506	1.180327
H	-0.92385300	-4.46791100	-0.98437600	H	0.608837	3.941802	-1.908239
C	2.06629200	-0.93949300	-2.44908500	C	1.981265	2.013947	1.468070
H	2.79794900	-0.67476000	-3.20600300	H	2.538517	2.068802	2.397536
H	1.94699900	-2.01751100	-2.48000100	H	2.125230	2.953165	0.946717
H	1.12382900	-0.49917600	-2.74488300	H	0.933091	1.938607	1.717463
C	1.47719900	1.24728900	2.16320600	C	1.259391	-2.295996	-1.179072
H	0.80573000	1.98798000	1.74288500	H	1.861199	-3.125934	-1.526330
H	0.86951600	0.53570100	2.70913500	H	0.565689	-2.674890	-0.438587
H	2.12131400	1.74997800	2.87555900	H	0.669721	-1.941583	-2.015781
C	5.98616500	-0.18669600	0.55588900	C	5.865134	-0.434451	-0.525473
H	6.41192000	0.80019600	0.71459700	H	6.417856	0.234358	0.122216
H	6.19595800	-0.77527800	1.44443900	H	6.219292	-1.443162	-0.345267
H	6.50535400	-0.64423500	-0.27824200	H	6.114538	-0.180786	-1.551365
H	-0.56849500	4.19255000	-2.46081200	H	-0.344790	-2.112703	4.337560
H	-2.13143500	0.15130400	-2.06228300	H	-2.478578	1.448221	1.031388
H	0.63666400	-2.71152600	-0.40101200	H	0.564030	1.524661	-2.035761
H	-3.24495300	-3.95375300	-1.71983100	H	-0.834626	5.145604	-0.291657

	Int'$_{Ph}$-S_0				TS_{Mes}-S_1		
C	-1.900178	-1.426355	1.043769	C	0.604708	1.985028	0.418740
C	0.145815	-1.709695	2.268905	C	-1.482982	2.577763	-0.559520
C	-0.506109	-2.279169	3.290236	C	-1.137735	3.871107	-0.664834
C	-1.924409	-2.375915	3.267878	C	0.172923	4.273088	-0.216541
C	-2.572794	-1.971060	2.088428	C	1.010170	3.345581	0.333569
C	-2.522432	-1.159063	-0.272457	C	1.090209	0.962379	1.324911
C	-1.987178	-0.213166	-1.140830	C	0.430515	-0.260714	1.107160
C	-2.625999	0.017995	-2.378328	C	0.667444	-1.333767	1.963724
C	-3.734493	-0.689069	-2.746172	C	1.535961	-1.186596	3.027145
C	-4.256254	-1.665817	-1.884124	C	2.200491	0.024707	3.221200
C	-3.660926	-1.895792	-0.678471	C	1.986357	1.101217	2.379398
H	1.210501	-1.610946	2.253074	H	-2.443368	2.226763	-0.875250
H	-2.473062	-2.792486	4.089254	H	0.474373	5.297370	-0.292957
H	-3.631928	-2.117581	1.997110	H	1.974838	3.627178	0.705824
H	-2.231748	0.770074	-3.035468	H	0.179074	-2.279476	1.803423
H	-4.204474	-0.502197	-3.695348	H	1.703007	-2.003230	3.705988
H	-5.115807	-2.241322	-2.178252	H	2.877611	0.131303	4.052889
H	-4.046379	-2.669328	-0.042097	H	2.475567	2.040434	2.567279
B	0.156921	-0.271292	0.262387	B	-0.835858	0.119891	-0.077694
N	-0.516006	-1.149889	1.164386	N	-0.661176	1.631669	-0.048874
C	1.749684	-0.216897	0.230445	C	0.374834	-0.556045	-0.786990
C	2.426560	-1.154847	-0.570717	C	1.476634	0.331811	-1.325368
C	2.504309	0.717142	0.943921	C	0.633720	-2.007521	-1.021754
C	3.807489	-1.123814	-0.662400	C	2.845801	-0.176062	-1.164168
C	3.892784	0.717242	0.837535	C	1.911363	-2.393040	-1.134286
C	4.561704	-0.187470	0.034523	C	3.064267	-1.486061	-1.038484
H	4.309878	-1.848447	-1.281505	H	3.665428	0.525943	-1.201327
H	4.457986	1.441961	1.399034	H	2.127979	-3.440790	-1.288351
C	-0.781228	0.627472	-0.702400	C	-2.320798	-0.469762	0.001256
C	-1.309191	1.777215	0.155384	C	-3.062976	-0.681568	-1.189080
C	-0.003235	1.163880	-1.887953	C	-2.974102	-0.713654	1.200925
C	-1.103364	3.095399	-0.138804	C	-4.356980	-1.125306	-1.161954
C	0.194826	2.491558	-2.129345	C	-4.302738	-1.176860	1.232959
C	-0.344682	3.495974	-1.273156	C	-4.986645	-1.383715	0.066591
H	-1.527156	3.848709	0.502725	H	-4.897190	-1.274784	-2.080776
H	0.774706	2.790820	-2.985121	H	-4.780162	-1.359061	2.179957
C	1.853695	1.751882	1.838759	C	-0.494620	-3.003315	-1.117585
H	2.537299	2.070901	2.617808	H	-1.096931	-3.028983	-0.215733
H	1.565026	2.630741	1.272190	H	-1.170129	-2.761365	-1.931399
H	0.961670	1.370587	2.323247	H	-0.104219	-4.000307	-1.291012
C	1.667993	-2.239541	-1.310888	C	1.180839	1.120396	-2.584176
H	1.295822	-2.994605	-0.624314	H	0.219640	1.618323	-2.528864
H	0.810445	-1.851603	-1.851516	H	1.941189	1.883806	-2.727759
H	2.306706	-2.737388	-2.031093	H	1.184162	0.482313	-3.466658
C	6.067237	-0.167351	-0.091108	C	4.431171	-2.092870	-0.864183
H	6.488210	-1.155324	0.067228	H	4.502534	-2.633397	0.076993
H	6.370815	0.159972	-1.081669	H	4.654600	-2.800972	-1.658996
H	6.514652	0.506047	0.630747	H	5.201852	-1.329825	-0.868232
H	0.060185	-2.661860	4.119226	H	-1.827499	4.582330	-1.063152
H	-1.901548	1.508755	1.011817	H	-2.598397	-0.484613	-2.140886
H	0.419973	0.441148	-2.562814	H	-2.465121	-0.533104	2.131339
H	-0.187119	4.536456	-1.485448	H	-6.003775	-1.734049	0.084292

	(S_1/S_0)x-Mes				Int'_{Mes}-S_0		
C	-1.547764	-0.698962	1.572249	C	2.222901	1.247992	0.128327
C	-2.628916	1.243481	0.697773	C	0.623723	3.026979	0.379678
C	-3.467095	1.325416	1.759993	C	1.582908	3.896608	0.711928
C	-3.278362	0.422196	2.844940	C	2.933058	3.465408	0.812257
C	-2.349110	-0.560626	2.756771	C	3.193753	2.126710	0.500096
C	-0.760023	-1.887907	1.292983	C	2.529595	-0.146322	-0.256463
C	0.221832	-1.924915	0.284670	C	1.548235	-1.144303	-0.262021
C	0.789338	-3.158013	-0.074015	C	1.925414	-2.472484	-0.521295
C	0.487491	-4.309512	0.606551	C	3.233106	-2.809229	-0.821110
C	-0.427181	-4.273062	1.669840	C	4.197129	-1.798859	-0.880731
C	-1.046825	-3.084553	2.001927	C	3.847948	-0.503838	-0.608379
H	-2.648128	1.959342	-0.097782	H	-0.400605	3.319282	0.322987
H	-3.866950	0.533949	3.736536	H	3.719255	4.131312	1.108209
H	-2.186146	-1.225050	3.576316	H	4.204578	1.777223	0.559927
H	1.490533	-3.180927	-0.885448	H	1.170723	-3.236752	-0.493382
H	0.949499	-5.236630	0.330501	H	3.499670	-3.831353	-1.021494
H	-0.669817	-5.170182	2.204777	H	5.212281	-2.033233	-1.147686
H	-1.794114	-3.091675	2.767563	H	4.602056	0.254180	-0.688798
B	-0.237449	0.619061	0.065539	B	-0.222142	0.750001	-0.022962
N	-1.655738	0.300533	0.616605	N	0.865761	1.663657	0.120646
C	0.564896	-0.649098	-0.461524	C	0.068326	-0.841588	0.020395
C	2.079605	-0.458710	-0.541563	C	-0.796293	-1.524604	-1.043574
C	-0.104425	-0.579843	-1.827854	C	-0.274623	-1.330391	1.437775
C	2.701848	-0.192851	-1.691854	C	-1.766839	-2.385995	-0.727202
C	0.678379	-0.267302	-2.996998	C	-1.259173	-2.212071	1.660304
C	2.008341	-0.075994	-2.971039	C	-2.068962	-2.773263	0.623364
H	0.153613	-0.220085	-3.936329	H	-1.452816	-2.526443	2.673242
H	3.768624	-0.049696	-1.689708	H	-2.358154	-2.820086	-1.517336
C	0.321505	2.060228	0.344798	C	-1.705098	1.299419	-0.210867
C	1.034123	2.804146	-0.605793	C	-2.745598	1.011219	0.704459
C	0.162310	2.632371	1.620908	C	-2.026350	2.055211	-1.319645
C	1.572240	4.048068	-0.291725	C	-4.019627	1.468638	0.505158
C	0.714850	3.866052	1.936003	C	-3.335407	2.513752	-1.547062
C	1.423182	4.579688	0.979791	C	-4.329919	2.226185	-0.637252
H	2.113974	4.595403	-1.040783	H	-4.789426	1.243622	1.222163
H	0.594777	4.265977	2.925791	H	-3.552168	3.093324	-2.426908
C	-1.468811	-1.183185	-2.071890	C	0.550758	-0.800513	2.586673
H	-1.911125	-0.762628	-2.969150	H	0.201528	-1.211649	3.526625
H	-2.157148	-1.009995	-1.254588	H	1.598895	-1.060210	2.477608
H	-1.414189	-2.262009	-2.218204	H	0.502179	0.282695	2.662225
C	2.833392	-0.541995	0.762716	C	-0.509490	-1.182036	-2.485177
H	2.756390	-1.530612	1.203852	H	-0.525777	-0.108898	-2.653363
H	2.429545	0.162416	1.483584	H	0.469736	-1.534643	-2.792700
H	3.882743	-0.315945	0.623361	H	-1.248434	-1.627251	-3.140945
C	2.820920	0.229526	-4.201030	C	-3.199367	-3.717810	0.913966
H	3.354915	1.171005	-4.101673	H	-4.163994	-3.269557	0.680335
H	3.567571	-0.541113	-4.378523	H	-3.121752	-4.626946	0.321708
H	2.194856	0.293752	-5.082611	H	-3.217036	-4.005674	1.959456
H	-4.216518	2.083032	1.798213	H	1.309624	4.916231	0.911688
H	1.176155	2.414518	-1.594522	H	-2.533602	0.422153	1.576826
H	-0.378178	2.103202	2.384720	H	-1.263144	2.310280	-2.035759
H	1.852683	5.533273	1.222744	H	-5.333871	2.577908	-0.795962