

Electronic Supplementary Information

Halogen atom effect on the photophysical properties of substituted aza-BODIPY derivatives

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Table S1

1a

Atomic Number	S ₀			S ₁		
	X	Y	Z	X	Y	Z
6	0.683437	1.645267	-1.987281	0.545036	1.827086	-1.985439
6	-0.274319	0.723168	-1.437262	-0.356978	0.843968	-1.441777
6	0.6276	2.0183	0.199715	0.380581	2.2362	0.192278
6	-0.268828	0.964787	-0.076143	-0.414179	1.113503	-0.080431
1	-0.861815	0.457161	0.675387	-1.045395	0.61604	0.64786
7	1.178712	2.451648	-0.959309	0.951404	2.679562	-0.990635
6	-1.125963	-0.243321	-2.124786	-1.027999	-0.203103	-2.182014
6	-2.281481	-0.679354	-1.45745	-1.42828	-1.373413	-1.510191
6	-0.812896	-0.743399	-3.39385	-1.304567	-0.050904	-3.553096
6	-3.113595	-1.620851	-2.05617	-2.07408	-2.381606	-2.214716
1	-2.534649	-0.250149	-0.492913	-1.185601	-1.485947	-0.457298
6	-1.658783	-1.691899	-3.974677	-1.971328	-1.063044	-4.238406
1	0.074551	-0.38273	-3.90549	-0.999501	0.861769	-4.053463
6	-2.800669	-2.130897	-3.311233	-2.346706	-2.231637	-3.578851
1	-3.448737	-2.869058	-3.776907	-2.863936	-3.022356	-4.116591
6	0.896489	2.517992	1.545772	0.551261	2.827691	1.505014
6	1.1883	3.859117	1.827678	0.83487	4.188409	1.7153
6	0.805528	1.610433	2.613943	0.379745	2.001681	2.633411
6	1.381386	4.271507	3.138518	0.936754	4.692062	3.003459
1	1.250755	4.577968	1.017497	0.962733	4.849164	0.863583
6	1.008566	2.027136	3.920414	0.485734	2.511381	3.915525
1	0.606679	0.55969	2.408491	0.196503	0.9379	2.491668
6	1.29432	3.362816	4.187998	0.763736	3.863426	4.108309
1	1.6002	5.318394	3.340934	1.150994	5.750041	3.145276
1	0.947664	1.304959	4.732532	0.362076	1.849787	4.771175
1	1.450584	3.693589	5.213346	0.849968	4.267502	5.115563
7	1.085448	1.720809	-3.238276	0.996195	1.838242	-3.236079
6	2.006737	2.60041	-3.58851	1.965841	2.687266	-3.562343
6	2.427559	2.897446	-4.921554	2.505658	2.873887	-4.887215
6	3.225396	4.020692	-4.823104	3.389563	3.940741	-4.771152
6	3.337107	4.371077	-3.459212	3.418744	4.364354	-3.436118
1	3.767641	4.495585	-5.633471	4.034204	4.337945	-5.54723
6	2.128425	2.169189	-6.150483	2.203194	2.085588	-6.061622
6	2.162408	0.780332	-6.184001	1.532281	0.856693	-5.95707
6	1.910708	2.903913	-7.329137	2.610576	2.536184	-7.333744
6	2.01964	0.11864	-7.409496	1.27309	0.090585	-7.099861
1	2.362993	0.198689	-5.286342	1.208938	0.477738	-4.991131
6	1.7298	2.229931	-8.528918	2.340535	1.766061	-8.454228
1	1.867678	3.988272	-7.271898	3.108633	3.496619	-7.426508
6	1.791994	0.831888	-8.578056	1.665519	0.534823	-8.352682
1	1.664456	0.353481	-9.544722	1.483932	-0.021632	-9.267783
6	4.137048	5.489217	-2.970482	4.220017	5.468625	-2.942799
6	4.306943	6.598346	-3.81489	4.550307	6.500828	-3.843098
6	4.785772	5.486061	-1.728119	4.72235	5.545968	-1.632316
6	5.093235	7.672737	-3.429213	5.346517	7.56345	-3.453191
1	3.787795	6.626137	-4.771786	4.139844	6.477448	-4.851269
6	5.577251	6.561517	-1.350816	5.522847	6.612267	-1.250422
1	4.674689	4.633751	-1.065511	4.495185	4.758153	-0.921606
6	5.735492	7.65639	-2.194237	5.840188	7.624415	-2.15113
1	5.201499	8.528525	-4.093015	5.575473	8.35549	-4.164179
1	6.079839	6.54005	-0.385567	5.907409	6.649578	-0.232604
1	6.35608	8.497558	-1.890159	6.46537	8.460025	-1.841085
7	2.611794	3.499873	-2.713363	2.563935	3.565376	-2.69325
8	-4.25081	-2.102974	-1.496205	-2.486055	-3.552901	-1.675949
8	-1.451573	-2.255637	-5.185983	-2.315212	-0.994652	-5.545789
8	2.129602	-1.233234	-7.362565	0.617056	-1.07083	-6.868883
8	1.494381	2.832458	-9.718947	2.679881	2.109401	-9.717367
6	-4.61745	-1.61999	-0.229023	-2.261726	-3.760121	-0.302823
1	-3.845647	-1.832775	0.526334	-1.188062	-3.753838	-0.06314
1	-4.809498	-0.536422	-0.246567	-2.769595	-2.998629	0.307656
1	-5.538043	-2.141825	0.044614	-2.676435	-4.743773	-0.069101
6	-0.286508	-1.895583	-5.889465	-2.189077	0.255768	-6.184791
1	-0.29977	-2.480651	-6.81291	-2.576459	0.12012	-7.198797
1	-0.271373	-0.823056	-6.135647	-2.782061	1.025283	-5.668462
1	0.623901	-2.139737	-5.322993	-1.142149	0.587674	-6.2392
6	2.032744	-1.940589	-8.574881	0.187063	-1.816701	-7.980782
1	1.049071	-1.797445	-9.048703	-0.458267	-1.214322	-8.639708
1	2.817629	-1.635719	-9.282414	1.037265	-2.197727	-8.566164
1	2.161563	-2.997329	-8.326193	-0.38771	-2.656454	-7.583177
6	1.419513	4.236999	-9.738587	3.374485	3.318137	-9.911672
1	0.604672	4.606816	-9.098818	2.776783	4.182428	-9.586989
1	2.365588	4.696296	-9.41518	4.333482	3.321155	-9.373394
1	1.218919	4.519683	-10.774979	3.563309	3.394069	-10.985252
5	2.274928	3.551789	-1.181771	2.101069	3.729099	-1.200491
9	1.791748	4.814612	-0.906141	1.655459	5.025071	-1.037884
9	3.363452	3.229924	-0.400091	3.113269	3.418264	-0.314339

Atomic Number	T ₁			T ₂		
	X	Y	Z	X	Y	Z
6	0.554203	1.836454	-1.982831	0.693574	1.618744	-2.017261
6	-0.366171	0.848712	-1.444309	-0.263906	0.722952	-1.48438
6	0.353129	2.251687	0.190354	0.608109	2.054991	0.19595
6	-0.442082	1.125532	-0.092829	-0.28906	1.002666	-0.079821
1	-1.082152	0.628674	0.627815	-0.920479	0.540431	0.66991
7	0.944399	2.69108	-0.996654	1.16476	2.442249	-0.974059
6	-1.025181	-0.212513	-2.186274	-1.112713	-0.208088	-2.15624
6	-1.398331	-1.383214	-1.50668	-2.037065	-0.984763	-1.385644
6	-1.314097	-0.067121	-3.550373	-1.093885	-0.343137	-3.562515
6	-2.041068	-2.404427	-2.200778	-2.928276	-1.836708	-2.012637
1	-1.141141	-1.490099	-0.456436	-2.037193	-0.8986	-0.304538
6	-1.973995	-1.09437	-4.225052	-2.006351	-1.184684	-4.171301
1	-1.021487	0.843891	-4.061222	-0.374489	0.242037	-4.127554
6	-2.330375	-2.262314	-3.557104	-2.931226	-1.940891	-3.408082
1	-2.842592	-3.060695	-4.088155	-3.634399	-2.600714	-3.908834
6	0.50407	2.847952	1.500492	0.839394	2.583616	1.538589
6	0.803883	4.205432	1.709493	1.126369	3.929591	1.804296
6	0.294566	2.029379	2.628373	0.71621	1.69727	2.622139
6	0.886288	4.713153	2.997173	1.281482	4.365072	3.112344
1	0.95714	4.861251	0.858511	1.216813	4.631524	0.98193
6	0.384415	2.543003	3.91017	0.87651	2.138343	3.926502
1	0.094315	0.968622	2.488293	0.527401	0.640812	2.433459
6	0.67927	3.891397	4.101601	1.157487	3.478194	4.17743
1	1.112099	5.768445	3.139293	1.498571	5.414899	3.300768
1	0.231917	1.888006	4.76597	0.789559	1.431257	4.749503
1	0.751198	4.298848	5.108491	1.281852	3.829305	5.200278
7	1.000738	1.840491	-3.235435	1.137465	1.685503	-3.259551
6	1.97267	2.690318	-3.54735	2.061455	2.588305	-3.587924
6	2.527465	2.863507	-4.882828	2.536368	2.845103	-4.902154
6	3.414044	3.918287	-4.767698	3.33482	3.980607	-4.801533
6	3.44186	4.353849	-3.43092	3.383599	4.378372	-3.459655
1	4.064546	4.305501	-5.54367	3.911044	4.43276	-5.601877
6	2.215053	2.073649	-6.061164	2.268565	2.070516	-6.107526
6	1.562817	0.844834	-5.9589	2.153288	0.684329	-6.061312
6	2.603837	2.549553	-7.332086	2.19455	2.735927	-7.345723
6	1.289871	0.097332	-7.109486	1.992534	-0.039933	-7.246226
1	1.249352	0.452464	-4.995637	2.225513	0.146664	-5.118231
6	2.328587	1.793995	-8.46022	2.004563	2.003785	-8.508671
1	3.088563	3.517759	-7.416733	2.262743	3.820487	-7.36378
6	1.664999	0.560952	-8.362061	1.899601	0.606792	-8.471069
1	1.472373	0.013615	-9.280546	1.766268	0.083129	-9.413271
6	4.250725	5.451252	-2.941029	4.137251	5.525566	-2.967431
6	4.608482	6.46506	-3.851823	4.351258	6.601983	-3.846018
6	4.734565	5.538655	-1.624572	4.702845	5.596717	-1.686033
6	5.411592	7.523473	-3.464087	5.102151	7.702171	-3.463628
1	4.215471	6.432119	-4.86653	3.894129	6.579836	-4.83416
6	5.544686	6.598737	-1.246266	5.452014	6.702208	-1.30761
1	4.488295	4.763217	-0.907026	4.566279	4.774803	-0.991051
6	5.887087	7.594581	-2.156226	5.65921	7.758312	-2.188854
1	5.661846	8.302373	-4.182058	5.246022	8.524821	-4.162331
1	5.916885	6.644335	-0.224433	5.88601	6.733628	-0.30945
1	6.519225	8.425605	-1.848389	6.248417	8.621864	-1.884784
7	2.569444	3.56035	-2.683802	2.619236	3.508852	-2.714691
8	-2.42945	-3.579051	-1.645136	-3.840982	-2.606569	-1.378445
8	-2.322627	-1.037418	-5.532751	-2.123995	-1.366546	-5.49407
8	0.63574	-1.068841	-6.890861	1.928811	-1.391659	-7.09542
8	2.652525	2.159153	-9.725536	1.903347	2.546416	-9.74834
6	-2.180585	-3.771394	-0.275812	-3.88631	-2.548698	0.026897
1	-1.1037	-3.744516	-0.050681	-2.937305	-2.881099	0.473468
1	-2.692532	-3.015659	0.339201	-4.115636	-1.532607	0.381027
1	-2.573204	-4.760682	-0.027241	-4.685843	-3.225504	0.336725
6	-2.202898	0.206171	-6.185458	-1.189986	-0.713629	-6.337157
1	-2.59811	0.059224	-7.19502	-1.480176	-0.963181	-7.360924
1	-2.794172	0.981289	-5.675269	-1.222324	0.376464	-6.204714
1	-1.157012	0.536662	-6.252448	-0.172065	-1.075046	-6.14095
6	0.191123	-1.795444	-8.009024	1.777791	-2.174391	-8.252665
1	-0.454776	-1.179555	-8.65486	0.832707	-1.95327	-8.774261
1	1.032794	-2.175767	-8.607244	2.610799	-2.023335	-8.955025
1	-0.387825	-2.635641	-7.618214	1.769453	-3.216419	-7.923022
6	3.332676	3.375984	-9.903836	2.004731	3.943855	-9.85976
1	2.730405	4.230898	-9.56123	1.200986	4.454124	-9.307829
1	4.296434	3.381744	-9.37281	2.97525	4.310129	-9.492689
1	3.513971	3.473321	-10.977287	1.912597	4.175742	-10.924029
5	2.099051	3.736047	-1.196074	2.241209	3.589811	-1.216467
9	1.657388	5.033805	-1.040547	1.680677	4.824098	-0.958382
9	3.10299	3.425445	-0.300917	3.295521	3.310239	-0.372352

1b

Atomic Number	S ₀			S ₁		
	X	Y	Z	X	Y	Z
6	0.684012	1.644699	-1.98983	0.545215	1.832157	-1.990953
6	-0.273479	0.722435	-1.437888	-0.353729	0.84536	-1.450305
6	0.629579	2.01929	0.196591	0.376541	2.239147	0.185597
6	-0.266906	0.965897	-0.07594	-0.413935	1.111735	-0.088957
1	-0.860342	0.458951	0.675822	-1.044848	0.60997	0.637001
7	1.18002	2.452125	-0.963258	0.947236	2.686607	-0.993606
6	-1.124259	-0.245067	-2.12358	-1.016102	-0.205229	-2.196833
6	-2.277792	-0.683847	-1.453644	-1.382229	-1.392426	-1.53602
6	-0.811985	-0.743146	-3.394127	-1.314583	-0.038752	-3.560888
6	-3.110061	-1.626147	-2.051863	-2.016755	-2.405508	-2.245827
1	-2.530414	-0.255945	-0.48826	-1.122025	-1.513418	-0.488101
6	-1.656968	-1.693229	-3.974449	-1.969241	-1.055495	-4.251987
1	0.073855	-0.380321	-3.907161	-1.036852	0.887684	-4.052186
6	-2.797262	-2.134141	-3.308463	-2.310655	-2.24136	-3.603685
1	-3.444875	-2.873156	-3.773653	-2.818851	-3.035127	-4.14576
6	0.902032	2.522559	1.539985	0.541513	2.832605	1.497024
6	1.207759	3.862082	1.816375	0.827828	4.193595	1.705088
6	0.802929	1.622112	2.613149	0.365227	2.01169	2.628449
6	1.404022	4.288883	3.122164	0.92791	4.710423	2.987808
1	1.279862	4.578854	1.004595	0.959741	4.855225	0.854357
6	1.006417	2.035108	3.920964	0.466074	2.51698	3.913059
1	0.595741	0.571328	2.417121	0.180332	0.947338	2.494398
6	1.301093	3.371219	4.157999	0.745231	3.869152	4.077284
1	1.632174	5.33133	3.330891	1.141765	5.765889	3.138339
1	0.942236	1.327385	4.743925	0.342023	1.868704	4.777364
7	1.084812	1.721068	-3.241328	0.999332	1.84458	-3.237871
6	2.004686	2.602424	-3.592235	1.966068	2.700548	-3.563906
6	2.424347	2.901651	-4.925587	2.509201	2.887144	-4.883957
6	3.221646	4.026644	-4.826107	3.393652	3.954883	-4.766577
6	3.334038	4.373213	-3.462005	3.416877	4.378437	-3.431665
1	3.76321	4.502192	-5.636739	4.040098	4.351876	-5.541614
6	2.12547	2.173079	-6.153977	2.207298	2.094483	-6.057491
6	2.160196	0.783737	-6.184772	1.517473	0.874868	-5.944288
6	1.907945	2.906803	-7.333645	2.624701	2.523855	-7.330579
6	2.017913	0.11953	-7.409556	1.246289	0.099377	-7.080357
1	2.361379	0.203417	-5.286272	1.182373	0.511914	-4.976309
6	1.726618	2.230656	-8.532796	2.347146	1.742638	-8.445581
1	1.8641	3.991369	-7.278259	3.13851	3.475066	-7.433982
6	1.789841	0.832023	-8.578883	1.651557	0.521991	-8.335501
1	1.662384	0.352391	-9.545087	1.46831	-0.042388	-9.245581
6	4.133179	5.488585	-2.967246	4.216467	5.480059	-2.931191
6	4.306238	6.602898	-3.803815	4.553608	6.515282	-3.825058
6	4.778395	5.479364	-1.722809	4.712531	5.553399	-1.617811
6	5.089242	7.679954	-3.417169	5.351797	7.577642	-3.437085
1	3.792358	6.639667	-4.763128	4.148995	6.50057	-4.835658
6	5.570546	6.548009	-1.328244	5.516258	6.611278	-1.219858
1	4.669018	4.624858	-1.062477	4.482469	4.765545	-0.907635
6	5.716113	7.634793	-2.178584	5.828613	7.610426	-2.13147
1	5.206421	8.544326	-4.066288	5.591551	8.377145	-4.134119
1	6.075493	6.530783	-0.365546	5.902887	6.653597	-0.204373
7	2.610157	3.500299	-2.716048	2.557916	3.579922	-2.693201
8	-4.244709	-2.110345	-1.491222	-2.395053	-3.592091	-1.717629
8	-1.450736	-2.255661	-5.185548	-2.334191	-0.975863	-5.553262
8	2.128232	-1.231358	-7.360886	0.566252	-1.041677	-6.832784
8	1.490502	2.830312	-9.722974	2.69801	2.066523	-9.707264
6	-4.611803	-1.630007	-0.223365	-2.144622	-3.814546	-0.351776
1	-3.838975	-1.842344	0.531256	-1.067562	-3.786065	-0.128705
1	-4.806297	-0.546734	-0.239596	-2.660696	-3.074556	0.2782
1	-5.531122	-2.154176	0.050233	-2.532088	-4.811249	-0.126531
6	-0.287112	-1.895493	-5.890626	-2.231936	0.282287	-6.179526
1	-0.301413	-2.480887	-6.813923	-2.636653	0.15509	-7.187977
1	-0.272815	-0.822859	-6.137205	-2.822506	1.040463	-5.643876
1	0.624212	-2.139139	-5.325081	-1.188609	0.62469	-6.248096
6	2.033857	-1.941138	-8.571902	0.09112	-1.783277	-7.929896
1	1.050529	-1.799795	-9.047208	-0.494641	-1.149657	-8.614526
1	2.819427	-1.636411	-9.278848	0.915181	-2.249358	-8.490454
1	2.163681	-2.99735	-8.321189	-0.558055	-2.557695	-7.514193
6	1.414048	4.234421	-9.747186	3.412843	3.261901	-9.917463
1	0.600034	4.605387	-9.106816	2.82678	4.139154	-9.60734
1	2.360563	4.695772	-9.427606	4.369899	3.256378	-9.376241
1	1.210866	4.513621	-10.784081	3.605541	3.318183	-10.991419
5	2.272823	3.552621	-1.186405	2.09498	3.736845	-1.200927
9	1.78836	4.816646	-0.909954	1.650388	5.03395	-1.031392
9	3.362069	3.236297	-0.400828	3.109571	3.426419	-0.314858
35	1.576205	3.965486	5.97886	0.888541	4.593628	5.865885
35	6.818205	9.126178	-1.624441	6.950458	9.085472	-1.573575

Atomic Number	T ₁			T ₂		
	X	Y	Z	X	Y	Z
6	0.551255	1.835897	-1.983688	0.695642	1.622321	-2.015673
6	-0.363845	0.844537	-1.441681	-0.259552	0.723675	-1.479817
6	0.351015	2.253455	0.18894	0.610421	2.055494	0.193551
6	-0.438415	1.122821	-0.089137	-0.284979	0.999908	-0.082146
1	-1.076383	0.624263	0.632423	-0.91527	0.535984	0.667817
7	0.939405	2.69358	-0.999426	1.167351	2.445853	-0.976717
6	-1.018344	-0.219151	-2.182615	-1.105624	-0.211667	-2.156758
6	-1.382163	-1.393646	-1.503585	-2.030264	-0.990741	-1.384711
6	-1.31179	-0.07204	-3.546223	-1.084137	-0.348309	-3.558186
6	-2.019319	-2.418348	-2.198383	-2.921739	-1.848832	-2.007201
1	-1.121413	-1.500902	-0.45414	-2.030288	-0.90104	-0.303784
6	-1.96774	-1.101665	-4.221659	-1.994893	-1.196089	-4.164899
1	-1.026482	0.842202	-4.055601	-0.367206	0.237982	-4.125296
6	-2.313484	-2.273781	-3.554205	-2.922101	-1.955795	-3.400661
1	-2.821816	-3.0746	-4.085547	-3.621604	-2.617844	-3.903665
6	0.499776	2.859623	1.494084	0.841249	2.587378	1.532946
6	0.795749	4.219949	1.69198	1.144244	3.931777	1.794131
6	0.293496	2.051764	2.630086	0.705486	1.709802	2.622498
6	0.877602	4.748716	2.970988	1.299963	4.382398	3.096849
1	0.947469	4.872499	0.837876	1.246742	4.631287	0.970534
6	0.378742	2.569331	3.910995	0.86334	2.148256	3.928099
1	0.097047	0.988596	2.504322	0.50758	0.653556	2.443851
6	0.668423	3.920287	4.06587	1.156128	3.487677	4.148617
1	1.098061	5.803607	3.114784	1.527073	5.427793	3.29149
1	0.231633	1.931822	4.779519	0.769975	1.45675	4.762075
7	0.996095	1.840855	-3.236748	1.134247	1.687948	-3.261194
6	1.967837	2.690573	-3.549222	2.057051	2.591765	-3.591088
6	2.520457	2.86797	-4.885446	2.528569	2.852456	-4.906869
6	3.410539	3.920926	-4.768085	3.327933	3.987613	-4.805206
6	3.441877	4.349455	-3.429573	3.381068	4.379218	-3.461452
1	4.061419	4.306966	-5.544468	3.902526	4.441028	-5.606241
6	2.204506	2.082176	-6.064914	2.258699	2.079143	-6.112603
6	1.554055	0.851721	-5.962358	2.145845	0.692378	-6.065766
6	2.588797	2.561937	-7.33606	2.181911	2.745029	-7.350511
6	1.278633	0.105222	-7.113614	1.98477	-0.032503	-7.250811
1	1.244685	0.45651	-4.998894	2.222182	0.154761	-5.122833
6	2.310499	1.808304	-8.465269	1.991724	2.012536	-8.513949
1	3.071866	3.531129	-7.420375	2.248349	3.829828	-7.368837
6	1.649125	0.573288	-8.366271	1.889269	0.614853	-8.475421
1	1.45467	0.027679	-9.285548	1.756237	0.091162	-9.417789
6	4.256961	5.437877	-2.93221	4.137835	5.520509	-2.963939
6	4.629635	6.45224	-3.836199	4.355364	6.602342	-3.834968
6	4.734392	5.517247	-1.612445	4.704079	5.582778	-1.681793
6	5.442564	7.503727	-3.449356	5.108806	7.702081	-3.454429
1	4.243192	6.43125	-4.853593	3.89927	6.59183	-4.823599
6	5.555208	6.562782	-1.217375	5.459306	6.678858	-1.287958
1	4.477852	4.743963	-0.89559	4.568236	4.758721	-0.988943
6	5.90103	7.543447	-2.137482	5.655241	7.724263	-2.178188
1	5.710093	8.288222	-4.153082	5.260756	8.53465	-4.13742
1	5.92877	6.610552	-0.197408	5.899946	6.712789	-0.294334
7	2.568333	3.566095	-2.683735	2.618468	3.507932	-2.716757
8	-2.396623	-3.596566	-1.645684	-3.830875	-2.61707	-1.368893
8	-2.321558	-1.043622	-5.526962	-2.111463	-1.382675	-5.483239
8	0.628195	-1.062088	-6.895482	1.92266	-1.38396	-7.100329
8	2.628582	2.176013	-9.730013	1.888339	2.554451	-9.752554
6	-2.140854	-3.793329	-0.278397	-3.879626	-2.550541	0.0362
1	-1.063144	-3.758121	-0.057827	-2.931298	-2.879329	0.487012
1	-2.657016	-3.044766	0.342001	-4.111692	-1.532513	0.383072
1	-2.523913	-4.787127	-0.032836	-4.678948	-3.226594	0.348152
6	-2.208144	0.200487	-6.179162	-1.184609	-0.72788	-6.335115
1	-2.606346	0.053199	-7.187585	-1.481364	-0.981735	-7.355756
1	-2.800506	0.973267	-5.666418	-1.221498	0.361804	-6.203074
1	-1.163373	0.534426	-6.249278	-0.165197	-1.086598	-6.142938
6	0.183706	-1.789547	-8.013042	1.778557	-2.167465	-8.257832
1	-0.465227	-1.175065	-8.657341	0.833959	-1.950168	-8.782261
1	1.025662	-2.166858	-8.612874	2.613051	-2.012417	-8.957591
1	-0.392135	-2.631696	-7.621593	1.773935	-3.209679	-7.928402
6	3.305188	3.394397	-9.910238	1.990907	3.951435	-9.866317
1	2.70201	4.247515	-9.564439	1.187469	4.463175	-9.315057
1	4.271113	3.401627	-9.382973	2.962	4.317159	-9.499911
1	3.481983	3.49314	-10.984338	1.898869	4.181864	-10.930948
5	2.097362	3.732991	-1.198077	2.243643	3.586202	-1.217623
9	1.663725	5.034765	-1.041524	1.693287	4.826947	-0.956032
9	3.099261	3.419381	-0.299363	3.302313	3.307001	-0.375457
35	0.787132	4.66192	5.847873	1.371202	4.118758	5.96501
35	7.045113	9.000761	-1.582764	6.712919	9.25432	-1.627848

1c

Atomic Number	S ₀			S ₁		
	X	Y	Z	X	Y	Z
6	0.683495	1.647325	-1.991522	1.478251	-1.21818	-0.169302
6	-0.276018	0.726775	-1.440203	2.01824	-2.553505	-0.145116
6	0.629918	2.02068	0.195213	-0.250559	-2.609793	-0.135397
6	-0.2694	0.969785	-0.078302	0.913482	-3.393352	-0.093527
1	-0.863959	0.463386	0.672884	0.926706	-4.47752	-0.126745
7	1.181021	2.453013	-0.964556	0.107576	-1.273747	-0.203378
6	-1.12763	-0.239888	-2.126001	3.424323	-2.902795	-0.158586
6	-2.281467	-0.677831	-1.456075	3.834978	-4.128746	0.397162
6	-0.815371	-0.738689	-3.396274	4.370733	-2.039156	-0.738869
6	-3.113987	-1.620124	-2.05388	5.183584	-4.466556	0.390282
1	-2.533971	-0.249474	-0.490856	3.093389	-4.772657	0.862173
6	-1.660641	-1.688753	-3.97616	5.714844	-2.403873	-0.757312
1	0.070756	-0.376469	-3.909309	4.032824	-1.098372	-1.161785
6	-2.801239	-2.128884	-3.310186	6.12551	-3.607227	-0.18527
1	-3.448949	-2.868039	-3.775012	7.176471	-3.885901	-0.194384
6	0.906111	2.519247	1.539617	-1.599927	-3.13577	-0.132094
6	1.226197	3.854024	1.8208	-2.688214	-2.480949	-0.734457
6	0.798675	1.61767	2.610608	-1.829277	-4.390934	0.464184
6	1.4292	4.273472	3.12835	-3.948757	-3.058745	-0.74539
1	1.304395	4.57364	1.01199	-2.539375	-1.517096	-1.212093
6	1.008326	2.02539	3.91924	-3.08532	-4.97234	0.462564
1	0.580539	0.569351	2.412739	-1.010858	-4.901631	0.969269
6	1.31928	3.357843	4.168046	-4.141288	-4.300308	-0.148546
1	1.669807	5.314705	3.33041	-4.77573	-2.540897	-1.22652
1	0.934161	1.308563	4.733778	-3.242604	-5.93608	0.942146
7	1.084851	1.72355	-3.242851	2.196734	-0.106464	-0.065215
6	2.005434	2.604357	-3.593465	1.567837	1.057732	0.072815
6	2.426789	2.901488	-4.926725	2.201112	2.351213	0.113941
6	3.224481	4.026162	-4.827933	1.155303	3.268048	0.125559
6	3.335121	4.37513	-3.464155	-0.05955	2.569227	0.133547
1	3.766661	4.500467	-5.638864	1.238354	4.345929	0.212049
6	2.128329	2.171156	-6.154232	3.625015	2.608551	0.168725
6	2.163637	0.781773	-6.183206	4.530533	1.575218	0.459788
6	1.910009	2.903179	-7.334806	4.120701	3.909284	-0.04431
6	2.021416	0.115852	-7.407059	5.905684	1.831611	0.533403
1	2.365078	0.202668	-5.283984	4.183101	0.561612	0.637411
6	1.728515	2.225297	-8.532954	5.486502	4.146262	0.036115
1	1.865584	3.987797	-7.280803	3.431595	4.710914	-0.293566
6	1.792684	0.826658	-8.577273	6.397094	3.109537	0.321057
1	1.665255	0.345802	-9.542864	7.453527	3.358785	0.367469
6	4.131679	5.492605	-2.969913	-1.368748	3.19119	0.139883
6	4.311354	6.603147	-3.809632	-1.500395	4.474692	-0.42514
6	4.766269	5.491635	-1.720448	-2.508928	2.602919	0.714484
6	5.087885	7.684224	-3.419738	-2.710746	5.14659	-0.422453
1	3.807173	6.634923	-4.774397	-0.641661	4.935837	-0.910506
6	5.550093	6.565748	-1.323612	-3.723761	3.271274	0.7268
1	4.656139	4.639659	-1.057042	-2.437074	1.620091	1.169911
6	5.704556	7.654709	-2.173291	-3.820094	4.537322	0.15893
1	5.204498	8.541007	-4.079629	-2.793307	6.129519	-0.881038
1	6.040249	6.545812	-0.352825	-4.592179	2.802085	1.184462
7	2.609976	3.503235	-2.717827	0.205072	1.20861	0.133129
8	-4.248787	-2.103756	-1.492949	5.692595	-5.605028	0.914775
8	-1.454308	-2.252058	-5.186871	6.695478	-1.662513	-1.322807
8	2.132367	-1.234957	-7.356559	6.667066	0.747154	0.803593
8	1.491239	2.823146	-9.723863	6.062489	5.352831	-0.152794
6	-4.614977	-1.623608	-0.224778	4.797405	-6.515483	1.504002
1	-3.841751	-1.83631	0.529341	4.277933	-6.069982	2.365617
1	-4.809205	-0.540279	-0.240584	4.049896	-6.87258	0.779639
1	-5.534268	-2.147599	0.049292	5.399073	-7.361647	1.8452
6	-0.289558	-1.894134	-5.891185	6.307779	-0.547148	-2.091695
1	-0.303922	-2.480879	-6.81365	7.228371	-0.133656	-2.514015
1	-0.273652	-0.821826	-6.13917	5.634589	-0.844785	-2.909431
1	0.620875	-2.138132	-5.324349	5.811662	0.221708	-1.480327
6	2.038261	-1.946374	-8.566587	8.064983	0.892202	0.753516
1	1.055139	-1.805497	-9.042458	8.390852	1.294753	-0.218546
1	2.824127	-1.642775	-9.273707	8.431269	1.553049	1.553461
1	2.167693	-3.002281	-8.31438	8.481269	-0.109871	0.883599
6	1.412371	4.227069	-9.749793	5.229634	6.449692	-0.446147
1	0.598417	4.597475	-9.109013	4.702575	6.307765	-1.40107
1	2.358413	4.69055	-9.43192	4.491216	6.617393	0.35133
1	1.207539	4.504554	-10.786834	5.884632	7.320947	-0.521154
5	2.272878	3.554341	-1.187874	-0.788806	0.003962	-0.033457
9	1.786448	4.817164	-0.909785	-1.562587	0.245136	-1.152084
9	3.362845	3.238133	-0.403351	-1.566651	-0.178787	1.094252
53	1.636231	4.000374	6.17665	-6.077928	-5.188411	-0.156635
53	6.898887	9.307587	-1.548016	-5.695541	5.548048	0.156682

Atomic Number	T ₁			T ₂		
	X	Y	Z	X	Y	Z
6	0.559129	1.833685	-1.982578	0.692853	1.627046	-2.018271
6	-0.354997	0.842001	-1.440118	-0.264554	0.730288	-1.482937
6	0.356632	2.254231	0.189197	0.609932	2.058102	0.191799
6	-0.431195	1.121867	-0.088388	-0.28881	1.005742	-0.084733
1	-1.07021	0.623778	0.632509	-0.920447	0.542785	0.664604
7	0.946165	2.692918	-0.999141	1.166731	2.448285	-0.978758
6	-1.008307	-0.223205	-2.180223	-1.111429	-0.204256	-2.159387
6	-1.366496	-1.399188	-1.501028	-2.03787	-0.980975	-1.387466
6	-1.306501	-0.075581	-3.542636	-1.08791	-0.343254	-3.560963
6	-2.003042	-2.425125	-2.194664	-2.928542	-1.839479	-2.010042
1	-1.101863	-1.506371	-0.452545	-2.039976	-0.889158	-0.306737
6	-1.962453	-1.106161	-4.216644	-1.998023	-1.191436	-4.167723
1	-1.02474	0.839787	-4.052063	-0.369278	0.241308	-4.127724
6	-2.302609	-2.279939	-3.549157	-2.926614	-1.949005	-3.403567
1	-2.810629	-3.081588	-4.079541	-3.62573	-2.611727	-3.906247
6	0.496081	2.864601	1.49309	0.847034	2.583132	1.532746
6	0.79315	4.224495	1.690487	1.167258	3.921693	1.801414
6	0.273236	2.062739	2.629954	0.703619	1.702372	2.618401
6	0.854216	4.758517	2.968939	1.334555	4.361818	3.106749
1	0.958134	4.874111	0.83655	1.274627	4.625734	0.982213
6	0.337407	2.587485	3.909132	0.872609	2.132302	3.925378
1	0.077162	0.999079	2.506974	0.491973	0.649397	2.43564
6	0.623864	3.94058	4.070338	1.185392	3.466962	4.160528
1	1.07361	5.815718	3.10138	1.577423	5.404852	3.296605
1	0.170854	1.9475	4.772611	0.770689	1.429954	4.749537
7	1.002676	1.83841	-3.236022	1.131897	1.692507	-3.263582
6	1.973448	2.688695	-3.549704	2.055462	2.595684	-3.593255
6	2.521393	2.869182	-4.887369	2.528822	2.854166	-4.908784
6	3.411781	3.921905	-4.770668	3.327855	3.989606	-4.807976
6	3.448221	4.346678	-3.430994	3.379237	4.383534	-3.46472
1	4.06022	4.309633	-5.54827	3.902924	4.442012	-5.609232
6	2.201159	2.085785	-6.067372	2.260535	2.07788	-6.113014
6	1.552181	0.854561	-5.964823	2.148896	0.69112	-6.062754
6	2.579666	2.568678	-7.339054	2.183723	2.740475	-7.352679
6	1.272815	0.110235	-7.116503	1.988958	-0.037015	-7.245955
1	1.247127	0.45701	-5.000953	2.225083	0.15595	-5.118422
6	2.297399	1.817184	-8.468726	1.99459	2.004754	-8.514271
1	3.061395	3.538563	-7.423211	2.249246	3.82529	-7.374109
6	1.637739	0.581284	-8.36969	1.893357	0.607087	-8.472289
1	1.44005	0.037413	-9.289311	1.761164	0.080834	-9.413361
6	4.268635	5.430493	-2.93285	4.13328	5.526633	-2.967375
6	4.641522	6.447525	-3.833128	4.356377	6.606161	-3.83939
6	4.753168	5.502076	-1.615737	4.689587	5.595189	-1.681687
6	5.46139	7.493314	-3.444496	5.102229	7.710061	-3.454599
1	4.250348	6.433298	-4.849012	3.90988	6.591587	-4.832518
6	5.581883	6.541843	-1.221145	5.435922	6.696384	-1.285107
1	4.497098	4.726832	-0.900707	4.553725	4.772493	-0.987243
6	5.931768	7.530575	-2.134484	5.638809	7.746108	-2.172229
1	5.724451	8.275371	-4.153257	5.253316	8.53594	-4.146431
1	5.957696	6.573467	-0.200901	5.862869	6.726268	-0.284998
7	2.576899	3.551979	-2.68408	2.615587	3.513195	-2.719635
8	-2.374497	-3.605125	-1.641613	-3.839273	-2.606201	-1.372106
8	-2.321638	-1.047532	-5.520493	-2.112356	-1.380384	-5.486206
8	0.624389	-1.05823	-6.898169	1.927825	-1.388102	-7.091908
8	2.609817	2.188029	-9.734024	1.891138	2.543503	-9.754312
6	-2.112037	-3.802439	-0.2757	-3.889752	-2.537786	0.032808
1	-1.03353	-3.763054	-0.059772	-2.941979	-2.866005	0.485225
1	-2.628455	-3.05667	0.347855	-4.122071	-1.519249	0.378023
1	-2.48994	-4.798072	-0.029563	-4.689531	-3.213314	0.344745
6	-2.211642	0.197059	-6.172316	-1.183125	-0.727851	-6.336949
1	-2.61285	0.049896	-7.179579	-1.478067	-0.982615	-7.357906
1	-2.80333	0.96887	-5.65731	-1.218815	0.362116	-6.206544
1	-1.167469	0.532285	-6.245413	-0.164398	-1.087377	-6.142351
6	0.176938	-1.784291	-8.015419	1.785378	-2.174768	-8.247449
1	-0.474424	-1.169396	-8.656855	0.841119	-1.959547	-8.773334
1	1.017299	-2.160082	-8.618442	2.620405	-2.020921	-8.946847
1	-0.397053	-2.627462	-7.623415	1.781204	-3.216115	-7.915272
6	3.283407	3.408055	-9.914285	1.991688	3.940338	-9.871225
1	2.679918	4.259279	-9.564378	1.187492	4.452157	-9.321142
1	4.25129	3.416087	-9.390632	2.962232	4.30826	-9.505557
1	3.455916	3.509384	-10.98885	1.899372	4.168232	-10.936383
5	2.107073	3.729553	-1.197698	2.242952	3.588663	-1.219603
9	1.677489	5.032539	-1.04136	1.692057	4.828012	-0.953446
9	3.107587	3.412544	-0.29893	3.303283	3.306992	-0.38041
53	0.69553	4.771348	6.031095	1.449167	4.139926	6.166189
53	7.207753	9.124189	-1.521279	6.781481	9.440342	-1.550067

2a

Atomic Number	S ₀			S ₁		
	X	Y	Z	X	Y	Z
6	0.696469	1.607157	-1.960111	0.704566	1.581017	-1.940814
6	-0.25329	0.676092	-1.414647	-0.226104	0.683286	-1.392383
6	0.718435	1.935391	0.230257	0.722087	1.930356	0.268077
6	-0.19711	0.88496	-0.040962	-0.186809	0.905519	-0.00573
7	1.226743	2.382219	-0.931964	1.231672	2.349998	-0.930706
6	-1.113651	-0.21648	-2.189743	-1.112184	-0.195132	-2.167112
6	-2.446415	-0.377583	-1.789898	-2.438735	-0.374795	-1.791804
6	-0.624565	-0.884291	-3.318733	-0.685382	-0.825647	-3.329784
6	-3.28184	-1.233827	-2.504503	-3.301459	-1.287213	-2.488773
1	-2.824297	0.18926	-0.945738	-2.839149	0.206019	-0.967455
6	-1.476624	-1.740881	-4.020114	-1.579643	-1.673374	-4.075909
1	0.40399	-0.725874	-3.628172	0.31947	-0.62748	-3.689594
6	-2.79529	-1.92146	-3.610701	-2.872817	-1.931862	-3.633062
1	-3.446734	-2.590757	-4.167221	-3.526589	-2.600145	-4.183824
6	1.092055	2.487367	1.537032	1.10967	2.490561	1.569968
6	0.857529	3.833098	1.834601	0.895672	3.839793	1.869849
6	1.662931	1.65557	2.506291	1.664653	1.659013	2.548455
6	1.182284	4.333585	3.089088	1.226875	4.34066	3.122715
1	0.423036	4.481207	1.07868	0.478859	4.494055	1.109177
6	2.002673	2.166512	3.751618	1.996519	2.163084	3.800197
1	1.862866	0.611082	2.270567	1.855767	0.612349	2.313078
6	1.755569	3.504264	4.0476	1.774735	3.505416	4.091655
1	0.988677	5.380326	3.316095	1.054498	5.393084	3.342806
1	2.461483	1.516184	4.494069	2.436595	1.5048	4.547779
1	2.014403	3.901817	5.027599	2.034481	3.902161	5.072088
7	1.058503	1.716731	-3.221116	1.058535	1.66117	-3.242352
6	1.970638	2.604987	-3.570199	1.961545	2.570236	-3.582029
6	2.379858	2.903873	-4.905154	2.388782	2.867035	-4.911942
6	3.181255	4.028784	-4.79575	3.181214	4.00793	-4.795679
6	3.30692	4.37041	-3.419341	3.290026	4.361862	-3.43419
6	2.062914	2.121257	-6.099552	2.08565	2.087334	-6.110627
6	2.358914	0.763869	-6.124378	2.333276	0.717363	-6.136321
6	1.550838	2.76224	-7.237355	1.619374	2.733798	-7.265842
6	2.183508	0.041613	-7.31146	2.152137	0.001072	-7.323747
1	2.773852	0.257412	-5.254834	2.727456	0.203359	-5.261221
6	1.355649	2.025691	-8.398739	1.432899	2.006881	-8.434493
1	1.309445	3.819983	-7.188651	1.416518	3.799931	-7.224288
6	1.676707	0.662438	-8.444556	1.696566	0.631287	-8.47359
1	1.522306	0.140785	-9.384709	1.549069	0.114043	-9.417343
6	4.085873	5.466837	-2.845031	4.045123	5.472537	-2.855646
6	3.966274	6.753023	-3.38777	3.932031	6.75062	-3.420547
6	4.964898	5.254118	-1.776319	4.900593	5.292481	-1.760836
6	4.706378	8.065706	-2.868572	4.656345	7.818252	-2.908874
1	3.265384	6.93065	-4.201622	3.245929	6.908935	-4.250834
6	5.715364	6.308331	-1.27327	5.629541	6.362088	-1.258692
1	5.051315	4.261804	-1.342662	4.980862	4.310501	-1.303738
6	5.589474	7.583611	-1.815732	5.513906	7.625979	-1.829644
1	4.592148	8.80358	-3.288156	4.545304	8.80664	-3.352339
1	6.402508	6.130783	-0.448205	6.294212	6.204575	-0.410925
1	6.176954	8.407793	-1.414466	6.08594	8.462087	-1.430033
7	2.583799	3.493861	-2.691671	2.553618	3.468597	-2.707087
8	-4.582871	-1.454843	-2.197654	-4.543557	-1.525394	-2.084687
8	-1.112298	-2.454677	-5.109546	-1.211293	-2.268276	-5.194021
8	2.53836	-1.266574	-7.256967	2.438717	-1.331941	-7.254465
8	0.868697	2.537584	-9.552921	0.997698	2.538913	-9.602269
6	-5.105265	-0.8152	-1.060048	-5.035987	-0.938202	-0.88497
1	-4.550827	-1.091106	-0.149664	-4.394449	-1.187596	-0.030608
1	-5.091705	0.280108	-1.166871	-5.119567	0.15049	-0.987286
1	-6.140978	-1.151814	-0.966273	-6.028699	-1.365994	-0.73764
6	0.126563	-2.159185	-5.708631	0.057226	-1.982999	-5.793896
1	0.181676	-2.783355	-6.604987	0.063623	-2.539085	-6.731709
1	0.187435	-1.097706	-5.990601	0.155603	-0.909683	-5.989256
1	0.977123	-2.402817	-5.054099	0.880169	-2.326806	-5.15751
6	2.42247	-2.025345	-8.435991	2.371828	-2.074828	-8.445458
1	1.380403	-2.063798	-8.790174	1.351068	-2.086072	-8.861903
1	3.058321	-1.622558	-9.23805	3.058366	-1.678906	-9.207871
1	2.754259	-3.036557	-8.185735	2.667559	-3.09692	-8.191698
6	0.572564	3.912851	-9.582831	0.787536	3.929672	-9.646018
1	-0.22519	4.168807	-8.869675	-0.017877	4.23909	-8.96309
1	1.461794	4.521229	-9.357076	1.702886	4.484815	-9.390383
1	0.232025	4.132668	-10.597758	0.497263	4.164745	-10.673431
5	2.372755	3.449754	-1.126765	2.351136	3.427799	-1.149554
9	1.983172	4.685642	-0.69048	1.949448	4.664173	-0.706311
9	3.502106	2.986287	-0.495727	3.496111	2.992114	-0.511193
53	4.313272	4.877528	-6.362112	4.338006	4.843703	-6.359223
53	-1.227912	-0.155169	1.482451	-1.249564	-0.168065	1.482682

Atomic Number	T ₁			T ₂		
	X	Y	Z	X	Y	Z
6	0.72481	1.589508	-1.95095	0.700942	1.523911	-1.99745
6	-0.247778	0.650813	-1.395615	-0.283962	0.66311	-1.459645
6	0.692532	1.93057	0.25085	0.672996	1.977621	0.218789
6	-0.201921	0.876419	-0.021117	-0.255622	0.946382	-0.031673
7	1.207505	2.383466	-0.953827	1.202648	2.332372	-0.9638
6	-1.113112	-0.219746	-2.179492	-1.15339	-0.227447	-2.180677
6	-2.437457	-0.423297	-1.759968	-2.450068	-0.517966	-1.677898
6	-0.638444	-0.844044	-3.342924	-0.737523	-0.79002	-3.405606
6	-3.267309	-1.276924	-2.480572	-3.281807	-1.390812	-2.361584
1	-2.814437	0.114792	-0.897433	-2.807822	-0.005161	-0.792653
6	-1.48378	-1.702311	-4.047843	-1.582139	-1.663683	-4.07449
1	0.375159	-0.644068	-3.673912	0.237615	-0.521049	-3.79645
6	-2.789408	-1.925415	-3.615904	-2.850611	-1.980148	-3.553217
1	-3.439234	-2.59143	-4.178243	-3.501385	-2.663484	-4.092752
6	1.07743	2.497691	1.541561	1.040858	2.583282	1.50855
6	0.923386	3.865887	1.7996	0.712616	3.912289	1.787869
6	1.581238	1.663797	2.548814	1.717464	1.824558	2.468155
6	1.253384	4.381112	3.045814	1.043821	4.466477	3.017873
1	0.547147	4.517632	1.016634	0.215697	4.509047	1.027344
6	1.927554	2.188835	3.785728	2.052137	2.384648	3.694235
1	1.728784	0.60441	2.345338	2.002897	0.798131	2.239196
6	1.756452	3.547035	4.039821	1.710407	3.704798	3.972774
1	1.119427	5.443806	3.239318	0.784894	5.502435	3.228515
1	2.335295	1.534054	4.553701	2.589433	1.790623	4.431348
1	2.021012	3.956808	5.013271	1.972175	4.143802	4.934097
7	1.090441	1.6574	-3.233163	1.107784	1.617573	-3.256866
6	1.990707	2.585877	-3.557291	2.018479	2.535804	-3.583161
6	2.401338	2.894445	-4.912873	2.460741	2.831495	-4.900109
6	3.194246	4.020709	-4.80276	3.267989	3.966083	-4.769766
6	3.330074	4.365214	-3.428925	3.356278	4.318727	-3.412093
6	2.079199	2.113376	-6.105475	2.144027	2.075894	-6.11131
6	2.358901	0.751939	-6.135406	2.338238	0.699372	-6.152978
6	1.575442	2.761274	-7.244337	1.709251	2.760188	-7.257748
6	2.174765	0.034978	-7.323706	2.132639	0.007453	-7.351904
1	2.761363	0.235603	-5.265828	2.696447	0.15405	-5.281823
6	1.376104	2.03147	-8.408944	1.495685	2.057825	-8.435833
1	1.341159	3.820436	-7.192416	1.548708	3.832703	-7.200108
6	1.679802	0.664583	-8.457686	1.707637	0.67427	-8.492811
1	1.518935	0.146063	-9.398481	1.540786	0.174996	-9.44296
6	4.091089	5.45847	-2.848931	4.112708	5.418379	-2.810452
6	4.024585	6.734592	-3.433274	3.976903	6.712748	-3.329258
6	4.910119	5.26869	-1.724253	4.996362	5.205399	-1.745642
6	4.756371	7.788843	-2.908985	4.70275	7.768239	-2.794576
1	3.361503	6.904304	-4.279144	3.276962	6.890042	-4.144383
6	5.654043	6.324004	-1.218184	5.725882	6.263475	-1.218858
1	4.957162	4.290024	-1.255817	5.104093	4.206671	-1.332109
6	5.58145	7.584532	-1.805768	5.583747	7.545718	-1.740234
1	4.677722	8.776334	-3.359999	4.576985	8.770044	-3.20223
1	6.294369	6.160306	-0.353617	6.413619	6.082205	-0.394594
7	6.162403	8.410679	-1.399168	6.156189	8.372613	-1.322646
1	2.601377	3.449556	-2.690607	2.598002	3.433391	-2.697352
8	-4.557532	-1.534462	-2.157683	-4.530995	-1.728017	-1.970433
8	-1.126478	-2.373892	-5.165796	-1.28968	-2.281491	-5.2307
8	2.504331	-1.28029	-7.270065	2.371246	-1.331928	-7.304638
8	0.897952	2.552716	-9.56306	1.0841	2.622606	-9.597187
6	-5.073453	-0.93592	-0.995118	-5.014241	-1.177541	-0.769486
1	-4.495668	-1.220745	-0.102173	-4.378453	-1.454748	0.085491
1	-5.087965	0.16166	-1.074739	-5.083096	-0.080768	-0.825615
1	-6.098901	-1.29986	-0.890874	-6.014593	-1.59197	-0.622555
6	0.113742	-2.05527	-5.750699	-0.069669	-1.950655	-5.864463
1	0.17653	-2.637376	-6.674315	-0.044594	-2.522556	-6.79501
1	0.177029	-0.982789	-5.985735	-0.019723	-0.875367	-6.086176
1	0.960353	-2.327298	-5.102225	0.796966	-2.2274	-5.247798
6	2.356442	-2.041289	-8.443535	2.240766	-2.059062	-8.499692
1	1.311783	-2.04597	-8.79284	1.214195	-2.006642	-8.897024
1	3.001257	-1.666024	-9.251882	2.936837	-1.696615	-9.270721
1	2.654417	-3.06199	-8.188873	2.47981	-3.098636	-8.258147
6	0.616083	3.930798	-9.588913	0.913433	4.018549	-9.617569
1	-0.182182	4.192546	-8.878385	0.120334	4.339866	-8.925693
1	1.510364	4.529541	-9.356956	1.845535	4.543884	-9.358257
1	0.28246	4.158178	-10.604524	0.625136	4.278503	-10.639559
5	2.350328	3.441759	-1.138961	2.324721	3.451398	-1.17045
9	1.951766	4.693954	-0.744884	1.833875	4.668512	-0.777691
9	3.464225	3.003735	-0.456672	3.415567	3.049457	-0.43666
53	4.326136	4.855411	-6.376092	4.442733	4.819436	-6.306378
53	-1.238973	-0.163363	1.500925	-1.124423	-0.141025	1.510898

2b

Atomic Number	S ₀			S ₁		
	X	Y	Z	X	Y	Z
6	0.693119	1.605546	-1.96411	0.70438	1.583462	-1.940036
6	-0.25443	0.672975	-1.416973	-0.220042	0.679784	-1.391099
6	0.716962	1.932729	0.225638	0.734819	1.918383	0.270275
6	-0.196186	0.881024	-0.042458	-0.172699	0.890609	-0.004464
7	1.223429	2.381518	-0.936761	1.235203	2.348869	-0.928926
6	-1.115476	-0.220199	-2.189571	-1.107392	-0.196807	-2.168712
6	-2.446624	-0.383206	-1.784706	-2.438442	-0.360905	-1.80403
6	-0.629103	-0.885859	-3.321083	-0.674191	-0.838804	-3.321725
6	-3.283905	-1.238912	-2.49789	-3.304085	-1.267706	-2.505813
1	-2.822582	0.182659	-0.939038	-2.8391	0.225877	-0.983881
6	-1.482544	-1.743053	-4.02008	-1.570287	-1.679384	-4.074513
1	0.398326	-0.726495	-3.633778	0.337909	-0.658403	-3.669948
6	-2.799758	-1.92489	-3.606299	-2.870099	-1.921697	-3.642876
1	-3.452334	-2.594362	-4.161261	-3.526135	-2.58397	-4.198242
6	1.091746	2.488524	1.530563	1.125989	2.472689	1.572301
6	0.857804	3.834048	1.825832	0.960804	3.83044	1.864078
6	1.665618	1.663162	2.502289	1.638655	1.629783	2.563399
6	1.179305	4.346691	3.076448	1.288074	4.333806	3.117383
1	0.421874	4.483535	1.071957	0.585252	4.499782	1.095274
6	2.008345	2.171055	3.748323	1.97078	2.119869	3.820881
1	1.86936	0.617768	2.274411	1.80349	0.576241	2.340922
6	1.751855	3.50922	4.026024	1.784453	3.470423	4.086191
1	0.984438	5.392718	3.301594	1.152919	5.391898	3.330733
1	2.47037	1.526531	4.492453	2.377749	1.453625	4.578132
7	1.054337	1.716265	-3.225237	1.053043	1.666958	-3.241973
6	1.966037	2.605125	-3.574259	1.955219	2.575838	-3.583123
6	2.375274	2.905488	-4.909028	2.380439	2.873117	-4.913447
6	3.176532	4.031236	-4.798981	3.17208	4.014386	-4.799012
6	3.30182	4.370037	-3.422644	3.281795	4.367737	-3.437453
6	2.060199	2.122975	-6.103753	2.078978	2.089648	-6.110585
6	2.355078	0.765183	-6.12658	2.337771	0.721844	-6.133075
6	1.552536	2.764193	-7.243477	1.604027	2.73004	-7.265347
6	2.1837	0.04246	-7.314154	2.158678	0.000642	-7.318042
1	2.767675	0.258728	-5.255943	2.738211	0.212927	-5.257825
6	1.360581	2.02701	-8.405136	1.419255	1.998155	-8.431529
1	1.310922	3.821935	-7.19644	1.391228	3.794347	-7.226221
6	1.681369	0.663548	-8.449067	1.694284	0.624625	-8.467641
1	1.530333	0.141824	-9.389725	1.547337	0.103856	-9.409552
6	4.081069	5.463965	-2.844234	4.033712	5.479903	-2.859216
6	3.972841	6.750591	-3.38632	3.928192	6.755357	-3.430006
6	4.948905	5.251096	-1.767239	4.878481	5.307768	-1.75549
6	4.709315	7.805838	-2.86658	4.647109	7.830268	-2.925131
1	3.280911	6.936433	-4.205787	3.249846	6.915807	-4.265999
6	5.702284	6.297222	-1.251814	5.608167	6.373872	-1.246575
1	5.030903	4.26065	-1.328264	4.95745	4.330447	-1.28827
6	5.576521	7.565462	-1.806622	5.489159	7.625032	-1.838943
1	4.603746	8.804127	-3.285158	4.542854	8.81647	-3.372185
1	6.380784	6.119386	-0.420901	6.26486	6.223451	-0.392832
7	2.579409	3.492772	-2.694689	2.54894	3.4729	-2.708208
8	-4.583319	-1.461036	-2.187864	-4.552192	-1.491142	-2.113912
8	-1.121487	-2.455842	-5.110656	-1.196937	-2.280845	-5.18707
8	2.537732	-1.265391	-7.257808	2.455637	-1.329306	-7.245618
8	0.877489	2.537963	-9.560722	0.975432	2.522821	-9.598659
6	-5.104563	-0.821366	-1.049405	-5.054797	-0.89058	-0.924743
1	-4.548932	-1.097385	-0.139825	-4.430233	-1.144851	-0.059396
1	-5.091482	0.273848	-1.156678	-5.122315	0.19845	-1.03425
1	-6.139956	-1.158331	-0.954402	-6.055162	-1.304359	-0.790379
6	0.116706	-2.162161	-5.712256	0.07732	-2.003395	-5.779104
1	0.169767	-2.788303	-6.607207	0.086138	-2.55857	-6.717396
1	0.177198	-1.101279	-5.996589	0.182919	-0.930538	-5.972846
1	0.968082	-2.404991	-5.05859	0.893328	-2.353714	-5.137311
6	2.428381	-2.024862	-8.437505	2.393801	-2.076375	-8.434794
1	1.388579	-2.062472	-8.798115	1.372406	-2.098812	-8.849068
1	3.069999	-1.623129	-9.235381	3.07516	-1.67584	-9.199286
1	2.757614	-3.03616	-8.184448	2.700187	-3.094606	-8.178521
6	0.582431	3.913603	-9.593879	0.752269	3.911657	-9.646368
1	-0.217806	4.171091	-8.884125	-0.054295	4.215509	-8.962367
1	1.471408	4.521504	-9.366022	1.663263	4.475669	-9.394873
1	0.245899	4.132007	-10.610373	0.457375	4.140696	-10.673718
5	2.369213	3.446382	-1.131332	2.344331	3.434482	-1.15263
9	1.98281	4.682648	-0.690695	1.931708	4.671544	-0.715755
9	3.499393	2.981898	-0.50071	3.492129	3.014255	-0.508977
53	4.30898	4.881975	-6.36362	4.324103	4.849783	-6.365414
53	-1.216605	-0.165039	1.483246	-1.245624	-0.188063	1.472316
53	6.730898	9.173122	-1.014059	6.616086	9.264927	-1.060737
53	2.24753	4.291021	5.948085	2.277485	4.233529	6.021805

Atomic Number	T ₁			T ₂		
	X	Y	Z	X	Y	Z
6	0.71925	1.590463	-1.953892	0.69821	1.525979	-1.997715
6	-0.251046	0.649618	-1.397822	-0.280661	0.658997	-1.458831
6	0.685665	1.930675	0.247831	0.674406	1.97018	0.21683
6	-0.205318	0.874984	-0.02216	-0.250416	0.934309	-0.035763
7	1.199572	2.385907	-0.957252	1.200722	2.333025	-0.964973
6	-1.114689	-0.221959	-2.180813	-1.146255	-0.235184	-2.183234
6	-2.437446	-0.431434	-1.758035	-2.446883	-0.521714	-1.6835
6	-0.640097	-0.842292	-3.346945	-0.727839	-0.798634	-3.403962
6	-3.265785	-1.286585	-2.478268	-3.279884	-1.395545	-2.365472
1	-2.81507	0.104291	-0.894338	-2.805492	-0.004031	-0.801318
6	-1.483349	-1.703289	-4.050768	-1.573356	-1.671285	-4.073185
1	0.372075	-0.63853	-3.679771	0.248179	-0.531699	-3.793936
6	-2.787319	-1.931542	-3.615831	-2.845947	-1.986748	-3.554208
1	-3.435877	-2.599323	-4.177538	-3.495186	-2.669498	-4.09625
6	1.071057	2.500378	1.537021	1.039438	2.577759	1.505716
6	0.929145	3.870063	1.790559	0.717257	3.908896	1.77997
6	1.566879	1.669908	2.549975	1.710669	1.823912	2.471945
6	1.257427	4.39664	3.032609	1.041305	4.474533	3.006704
1	0.56101	4.5256	1.006961	0.225082	4.508492	1.018648
6	1.915241	2.19011	3.788499	2.04667	2.381313	3.699234
1	1.710303	0.608217	2.356536	1.99757	0.795913	2.253005
6	1.747555	3.55091	4.021131	1.699944	3.702653	3.956569
1	1.131923	5.460354	3.221614	0.785185	5.510924	3.213856
1	2.316529	1.53844	4.561083	2.581412	1.791975	4.440622
7	1.085161	1.659918	-3.235785	1.100962	1.621981	-3.25872
6	1.985958	2.587599	-3.559079	2.010349	2.541574	-3.584572
6	2.39714	2.897288	-4.914221	2.449312	2.840573	-4.902126
6	3.190915	4.023084	-4.803789	3.256421	3.975017	-4.771921
6	3.326781	4.365444	-3.429723	3.348165	4.323352	-3.413078
6	2.075269	2.116572	-6.106958	2.132417	2.084136	-6.112818
6	2.356674	0.755438	-6.136158	2.329498	0.707858	-6.152392
6	1.571281	2.76422	-7.24583	1.69636	2.766316	-7.259832
6	2.174323	0.038051	-7.324602	2.126534	0.014017	-7.350769
1	2.759973	0.239725	-5.266596	2.689754	0.164583	-5.280748
6	1.372861	2.033776	-8.410339	1.484711	2.061874	-8.437286
1	1.335412	3.823056	-7.19436	1.533238	3.838554	-7.204037
6	1.678687	0.667202	-8.458521	1.700231	0.678727	-8.492363
1	1.518796	0.148424	-9.399343	1.535235	0.178185	-9.442163
6	4.09058	5.454695	-2.847746	4.108822	5.417818	-2.809467
6	4.044913	6.728365	-3.438108	3.997456	6.710701	-3.336261
6	4.893839	5.267226	-1.711769	4.973968	5.204268	-1.730098
6	4.779776	7.783073	-2.919214	4.7277	7.765889	-2.806254
1	3.393671	6.905611	-4.291442	3.309925	6.898078	-4.1593
6	5.646215	6.31257	-1.198089	5.714802	6.250801	-1.19592
1	4.9268	4.293701	-1.231067	5.064174	4.20967	-1.302424
6	5.585768	7.562319	-1.806704	5.586851	7.522282	-1.741359
1	4.717047	8.768591	-3.375021	4.621214	8.766471	-3.219486
1	6.27432	6.149987	-0.325386	6.38888	6.069171	-0.362031
7	2.597559	3.449588	-2.691314	2.592394	3.435745	-2.697624
8	-4.553703	-1.549572	-2.154007	-4.529563	-1.729305	-1.97609
8	-1.126706	-2.372352	-5.169702	-1.282236	-2.290291	-5.22654
8	2.505462	-1.276334	-7.270502	2.36882	-1.324455	-7.301822
8	0.894025	2.553544	-9.564181	1.072151	2.623771	-9.599014
6	-5.070892	-0.9555	-0.989261	-5.015957	-1.173402	-0.778224
1	-4.490559	-1.239887	-0.097909	-4.383163	-1.448605	0.079499
1	-5.090476	0.142051	-1.067092	-5.08345	-0.076907	-0.839281
1	-6.094408	-1.324388	-0.884496	-6.017088	-1.586221	-0.633066
6	0.113077	-2.052742	-5.755489	-0.060621	-1.964766	-5.862567
1	0.17591	-2.635396	-6.678668	-0.039456	-2.537866	-6.792233
1	0.174719	-0.980344	-5.991265	-0.007963	-0.889873	-6.084516
1	0.959953	-2.32364	-5.106973	0.804321	-2.244526	-5.245339
6	2.362565	-2.037609	-8.44488	2.244711	-2.053142	-8.497109
1	1.31876	-2.045166	-8.796466	1.218788	-2.005764	-8.896628
1	3.008343	-1.660021	-9.251251	2.940958	-1.687757	-9.266421
1	2.662997	-3.057381	-8.189673	2.488305	-3.091307	-8.254243
6	0.60975	3.931363	-9.591461	0.898809	4.019604	-9.62267
1	-0.188913	4.192225	-8.881126	0.104458	4.340718	-8.932215
1	1.503203	4.531615	-9.360411	1.829849	4.547045	-9.363997
1	0.275662	4.156979	-10.607226	0.61092	4.276581	-10.64544
5	2.34202	3.44251	-1.14205	2.327159	3.442525	-1.169423
9	1.944469	4.696399	-0.748787	1.854523	4.663037	-0.762767
9	3.45404	3.005685	-0.454097	3.421602	3.026887	-0.445362
53	4.323583	4.854628	-6.378155	4.42808	4.826807	-6.311444
53	-1.236753	-0.170731	1.499628	-1.119902	-0.15838	1.504449
53	6.738658	9.168957	-1.015521	6.731478	9.131764	-0.928953
53	2.256509	4.353569	5.930356	2.1996	4.567252	5.842269

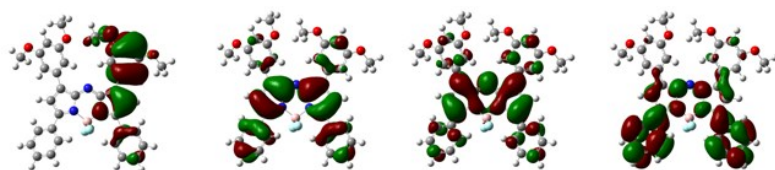
Atomic Number	S ₀			S ₁			S ₂		
	X	Y	X	X	X	Z	X	X	Z
6	0.865451	1.872195	-2.060645	0.878127	1.819662	-2.06977	1.057348	1.862936	-2.158471
6	-0.113975	0.930485	-1.6464	-0.093832	0.892282	-1.629502	0.108945	0.885205	-1.768388
6	0.795413	2.002258	0.145595	0.809331	1.984211	0.154854	0.947946	1.964112	0.062387
6	-0.132932	0.999615	-0.270214	-0.108918	0.991565	-0.243024	0.075561	0.948896	-0.374843
7	1.379968	2.532357	-0.950695	1.395848	2.49037	-0.978144	1.53654	2.523607	-1.041911
6	-0.882314	0.100549	-2.584539	-0.88764	0.055501	-2.535589	-0.540545	-0.065058	-2.677205
6	-1.998194	0.599924	-3.254379	-1.963349	0.566475	-3.26961	-1.367772	0.294344	-3.74511
6	-0.434643	-1.199072	-2.842295	-0.540794	-1.287707	-2.701397	-0.292339	-1.427983	-2.448996
6	-2.646396	-0.190746	-4.21132	-2.655726	-0.239233	-4.183062	-1.923836	-0.688229	-4.582861
6	-1.09245	-1.990218	-3.782546	-1.237053	-2.09913	-3.597444	-0.857729	-2.399878	-3.261942
1	0.440746	-1.560383	-2.307386	0.296083	-1.668586	-2.121269	0.360083	-1.69014	-1.621116
6	-2.193258	-1.475925	-4.468729	-2.289205	-1.565786	-4.345211	-1.664618	-2.030661	-4.341399
1	-2.689658	-2.08565	-5.221558	-2.818263	-2.195335	-5.058352	-2.084029	-2.821085	-4.957882
6	1.095662	2.412947	1.514955	1.118914	2.425263	1.513917	1.214137	2.390535	1.435732
6	1.140199	3.763396	1.880277	1.190775	3.782244	1.851893	1.163101	3.738457	1.80957
6	1.322988	1.435392	2.491965	1.324828	1.473245	2.521023	1.495507	1.432183	2.417576
6	1.392325	4.128874	3.195825	1.446913	4.177424	3.158362	1.378959	4.119179	3.127867
1	0.97769	4.529815	1.128215	1.055124	4.534005	1.080044	0.962943	4.494123	1.056044
6	1.593097	1.792307	3.8052	1.585006	1.855988	3.830208	1.716138	1.8	3.738097
1	1.316527	0.382343	2.21549	1.306466	0.41393	2.26982	1.565877	0.382344	2.137467
6	1.615657	3.140252	4.147025	1.6365	3.210051	4.137169	1.649995	3.144897	4.080446
1	1.412635	5.180382	3.472476	1.494174	5.235395	3.406143	1.333741	5.169892	3.405057
1	1.782874	1.024924	4.551973	1.752168	1.10283	4.596954	1.941982	1.044175	4.486737
7	1.257757	2.058767	-3.301716	1.248431	1.990033	-3.334408	1.44761	2.088153	-3.402412
6	2.222748	2.912295	-3.553762	2.222675	2.877074	-3.576055	2.376735	3.032169	-3.596056
6	2.660026	3.288506	-4.854919	2.656629	3.262963	-4.855325	2.717541	3.535652	-4.858344
6	3.611552	4.26239	-4.656874	3.608566	4.265294	-4.650457	3.641738	4.555774	-4.630553
6	3.752697	4.478463	-3.250799	3.758883	4.46868	-3.271925	3.86961	4.649081	-3.247956
6	2.112594	2.678771	-6.072822	2.124415	2.676002	-6.087691	1.93473	3.055043	-6.002721
6	2.837025	1.680798	-6.712337	2.908893	1.863687	-6.87364	2.139006	1.770204	-6.453622
6	0.830261	3.011117	-6.530036	0.779368	2.883454	-6.502372	0.800498	3.741229	-6.485592
6	2.2868	0.987641	-7.793183	2.390835	1.224819	-8.023459	1.220749	1.131232	-7.333305
1	3.836456	1.418243	-6.369601	3.948402	1.684765	-6.608912	2.974005	1.18551	-6.078718
6	0.259719	2.285443	-7.57345	0.227524	2.182041	-7.608243	-0.128535	3.099709	-7.38205
6	0.988145	1.274166	-8.203941	1.039835	1.362215	-8.370823	0.088006	1.792528	-7.800061
1	0.500634	0.746719	-9.020076	0.593996	0.857703	-9.223014	-0.621982	1.297242	-8.451507
6	4.624786	5.442879	-2.584728	4.627282	5.424261	-2.580495	4.785192	5.537156	-2.531473
6	4.649795	6.771025	-3.029263	4.639816	6.766829	-2.976547	4.865414	6.891523	-2.877493
6	5.441209	5.068752	-1.510985	5.467204	5.02804	-1.533467	5.604921	5.062426	-1.500255
6	5.462705	7.71124	-2.412182	5.467163	7.693183	-2.354856	5.745639	7.749057	-2.230457
1	4.001204	7.080988	-3.846877	3.972788	7.098451	-3.770966	4.208073	7.290509	-3.648461
6	6.271108	5.998966	-0.900415	6.298619	5.94461	-0.902243	6.487037	5.910484	-0.842544
1	5.423804	4.044583	-1.150338	5.457271	3.994391	-1.200908	5.535704	4.020817	-1.198278
6	6.273263	7.31265	-1.354606	6.293417	7.268781	-1.321731	6.554091	7.245997	-1.219139
1	5.457614	8.744391	-2.751604	5.45548	8.735044	-2.667294	5.787631	8.800446	-2.506096
1	6.906812	5.696982	-0.071518	6.943692	5.621715	-0.08822	7.11573	5.524811	-0.042873
7	2.921378	3.639759	-2.596007	2.91677	3.592815	-2.627966	3.078938	3.705486	-2.628431
8	-3.697823	0.303384	-4.922576	-3.665608	0.272641	-4.947568	-2.712443	-0.269758	-5.607247
8	-0.733099	-3.251155	-4.107845	-0.95731	-3.399343	-3.825141	-0.68016	-3.731041	-3.100235
8	3.078654	0.047911	-8.356869	3.262752	0.483278	-8.696911	1.536926	-0.116831	-7.63548
8	-1.001212	2.538636	-8.015209	-1.061104	2.331011	-7.969307	-1.180953	3.815809	-7.738986
6	-4.961601	-0.140848	-4.465301	-4.962452	-0.019481	-4.454868	-3.492762	-1.233072	-6.270416
1	-5.125228	0.15135	-3.41705	-5.115493	0.425775	-3.460005	-4.10307	-1.81342	-5.564031
1	-5.713926	0.33939	-5.096531	-5.676204	0.415922	-5.159587	-4.152767	-0.681193	-6.945927
1	-5.05608	-1.234011	-4.551678	-5.126303	-1.10529	-4.391552	-2.877041	-1.930664	-6.860065
6	0.388605	-3.803862	-3.461334	0.089589	-3.988875	-3.087354	0.064448	-4.158919	-1.982973
1	0.506596	-4.813664	-3.861878	0.145975	-5.029568	-3.415235	0.041358	-5.251323	-1.999226
1	1.299863	-3.224172	-3.670414	1.050539	-3.492491	-3.285958	1.108885	-3.818527	-2.039283
1	0.2395	-3.862333	-2.372966	-0.114282	-3.959234	-2.007411	-0.378494	-3.798768	-1.042322
6	2.571778	-0.661521	-9.460962	2.839608	-0.206734	-9.862211	0.645852	-0.890214	-8.424902
1	1.685081	-1.253828	-9.188676	2.059858	-0.939955	-9.619984	-0.329047	-0.970587	-7.928053
1	2.310446	0.014518	-10.288631	2.469991	0.496984	-10.618833	0.527931	-0.447449	-9.422222
1	3.368036	-1.336145	-9.785101	3.723194	-0.722395	-10.240946	1.101393	-1.877199	-8.511241
6	-1.999989	1.821663	-7.302154	-1.991273	1.503067	-7.265297	-2.244161	3.180742	-8.435983
1	-2.024548	2.105673	-6.23921	-2.064344	1.783093	-6.206633	-2.621147	2.329911	-7.852839
1	-2.9589	2.075229	-7.761313	-2.961583	1.655822	-7.741442	-3.022449	3.937469	-8.541075
1	-1.831337	0.735866	-7.376254	-1.700632	0.445546	-7.339005	-1.914604	2.850646	-9.429543
5	2.577263	3.573133	-1.047009	2.549141	3.557	-1.095808	2.773286	3.507835	-1.090577
9	2.186021	4.823146	-0.647178	2.106036	4.818006	-0.745829	2.467931	4.737665	-0.555019
9	3.627881	3.076151	-0.321219	3.607652	3.146155	-0.320169	3.826552	2.904538	-0.438552
53	4.70134	5.167575	-6.209095	4.703755	5.196155	-6.198484	4.656334	5.564566	-6.1878
53	-1.518253	-0.027062	0.934424	-1.509983	-0.015237	0.973893	-1.313064	-0.095766	0.830047
53	7.533338	8.744436	-0.402033	7.568156	8.683139	-0.348815	7.909852	8.55973	-0.213785
53	2.001235	3.700587	6.16828	2.023848	3.815009	6.151444	1.979007	3.725583	6.11225
53	-0.21812	4.674545	-5.719375	-0.386174	4.315606	-5.572813	0.371841	5.65919	-5.827279
53	-2.751047	2.54153	-2.827984	-2.628802	2.560563	-2.95205	-1.973471	2.314638	-4.052583

Atomic Number	T ₁			T ₂		
	X	Y	Z	X	Y	Z
7	0.864245	1.876017	-2.092041	0.868748	1.828029	-2.07907
6	-0.078752	0.872945	-1.665861	-0.110363	0.906594	-1.641398
6	0.742085	2.02195	0.124249	0.778506	2.010527	0.143023
6	-0.118415	0.96318	-0.295344	-0.140559	1.018634	-0.25677
7	1.312824	2.580971	-1.007353	1.377839	2.506257	-0.987576
6	-0.798249	-0.009784	-2.592056	-0.891399	0.057068	-2.547663
6	-1.899548	0.440732	-3.318908	-1.97884	0.546386	-3.277
6	-0.338766	-1.320015	-2.761967	-0.512035	-1.277393	-2.717661
6	-2.525961	-0.410279	-4.23668	-2.655391	-0.275162	-4.187417
6	-0.969364	-2.170078	-3.668647	-1.193092	-2.104081	-3.610744
1	0.523105	-1.640332	-2.181548	0.334871	-1.63889	-2.139625
6	-2.061018	-1.70617	-4.404349	-2.260747	-1.593816	-4.351717
1	-2.541097	-2.364643	-5.12591	-2.779859	-2.234079	-5.06269
6	1.003836	2.484319	1.473515	1.080986	2.457418	1.501566
6	1.057224	3.853493	1.77838	1.158515	3.815988	1.831556
6	1.18354	1.554672	2.511077	1.27564	1.510414	2.515696
6	1.267733	4.280123	3.08106	1.41067	4.217967	3.136692
1	0.926191	4.586459	0.988834	1.029514	4.563839	1.054941
6	1.410662	1.973818	3.812581	1.531911	1.899965	3.823649
1	1.184648	0.489633	2.2877	1.252236	0.44965	2.271138
6	1.44321	3.337399	4.08874	1.590521	3.255624	4.122276
1	1.292814	5.343675	3.306032	1.462714	5.277162	3.378088
1	1.567303	1.242105	4.60158	1.691198	1.150617	4.595787
7	1.244786	2.045432	-3.350559	1.250179	1.990325	-3.341791
6	2.214462	2.929985	-3.565988	2.234136	2.867254	-3.57831
6	2.64861	3.336546	-4.879093	2.680157	3.245512	-4.855229
6	3.642457	4.25945	-4.669292	3.641782	4.238715	-4.647067
6	3.817797	4.441134	-3.262605	3.784109	4.444557	-3.268281
6	2.066911	2.76837	-6.099802	2.134402	2.672762	-6.087004
6	2.761287	1.790091	-6.799926	2.902378	1.856414	-6.883531
6	0.775875	3.129429	-6.507974	0.787999	2.899051	-6.490575
6	2.171214	1.147245	-7.891058	2.364889	1.224185	-8.031128
1	3.766669	1.502849	-6.496835	3.943247	1.666787	-6.631927
6	0.166646	2.459455	-7.565647	0.214758	2.195291	-7.5893
6	0.866197	1.466201	-8.255188	1.010096	1.370154	-8.362055
1	0.353492	0.978386	-9.080629	0.550397	0.866147	-9.206989
6	4.706696	5.357364	-2.575089	4.657589	5.392375	-2.572312
6	4.884235	6.662859	-3.064111	4.684324	6.734572	-2.968569
6	5.401412	4.972236	-1.417052	5.486594	4.989	-1.519485
6	5.725079	7.557741	-2.420657	5.515049	7.653899	-2.340994
1	4.319531	6.996203	-3.932155	4.025653	7.07156	-3.767708
6	6.256948	5.856368	-0.778448	6.321299	5.898501	-0.88228
1	5.264798	3.973129	-1.014122	5.465598	3.955506	-1.1869
6	6.411786	7.143617	-1.283373	6.330137	7.222646	-1.301819
1	5.833474	8.57166	-2.798985	5.514258	8.695845	-2.65335
1	6.796829	5.540842	0.11134	6.957802	5.570229	-0.063646
7	2.947497	3.57713	-2.611454	2.928279	3.579877	-2.627731
8	-3.571339	0.024205	-4.995712	-3.677824	0.213174	-4.951546
8	-0.596467	-3.445937	-3.911033	-0.884908	-3.398522	-3.840687
8	2.933653	0.220998	-8.515257	3.22273	0.479626	-8.714883
8	-1.098395	2.752515	-7.968872	-1.074876	2.354588	-7.933517
6	-4.840833	-0.325791	-4.475492	-4.966105	-0.08824	-4.442854
1	-4.996086	0.11922	-3.480586	-5.112494	0.361516	-3.449158
1	-5.587575	0.070636	-5.168827	-5.69179	0.336014	-5.142287
1	-4.952672	-1.418265	-4.402385	-5.118631	-1.175362	-4.371419
6	0.52014	-3.95092	-3.217978	0.178454	-3.963384	-3.10812
1	0.652942	-4.980178	-3.560056	0.256066	-5.003271	-3.434509
1	1.429274	-3.374593	-3.444947	1.127477	-3.44659	-3.312722
1	0.354633	-3.950357	-2.130402	-0.019364	-3.936455	-2.026893
6	2.385194	-0.43163	-9.633985	2.783982	-0.203363	-9.880299
1	1.491623	-1.014851	-9.364796	2.007207	-0.936923	-9.631013
1	2.121006	0.28328	-10.427463	2.405209	0.506483	-10.62621
1	3.157414	-1.110604	-10.004276	3.662607	-0.71666	-10.273018
6	-2.096228	2.031347	-7.258512	-2.009791	1.550516	-7.204642
1	-2.093703	2.284741	-6.187565	-2.051012	1.832911	-6.144624
1	-3.058786	2.317086	-7.690731	-2.985797	1.726802	-7.66002
1	-1.951825	0.945512	-7.367728	-1.745266	0.487182	-7.287258
5	2.576801	3.525272	-1.076527	2.544079	3.559257	-1.0995
9	2.293845	4.802744	-0.661427	2.112598	4.827782	-0.76312
9	3.573476	2.938692	-0.329064	3.590099	3.141982	-0.310289
53	4.752916	5.118151	-6.233641	4.751755	5.159368	-6.190218
53	-1.48728	-0.107442	0.889697	-1.556574	0.02608	0.952943
53	7.701501	8.511965	-0.28218	7.609399	8.626892	-0.320304
53	1.780095	3.987688	6.089716	1.974328	3.870421	6.134137
53	-0.210986	4.773618	-5.58698	-0.340415	4.372652	-5.583344
53	-2.653294	2.406664	-3.024264	-2.675858	2.533319	-2.968615

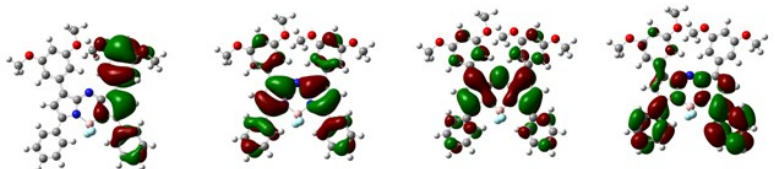
Figure S2

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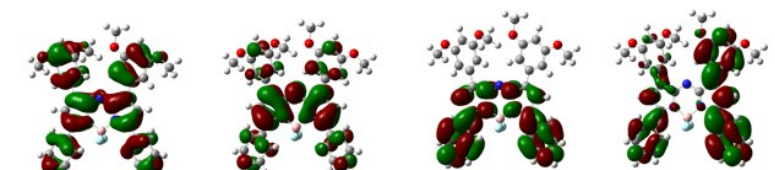
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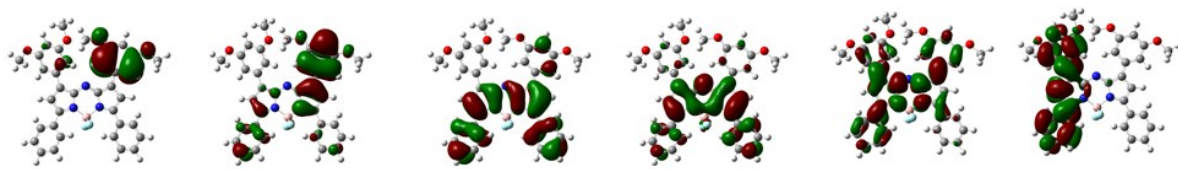
S_1



T_1



T_2



1b

H-3

H-2

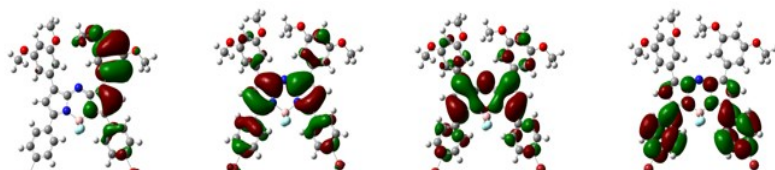
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H

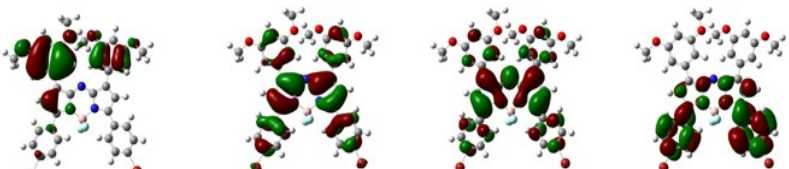
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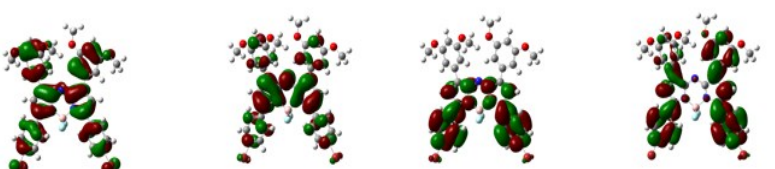
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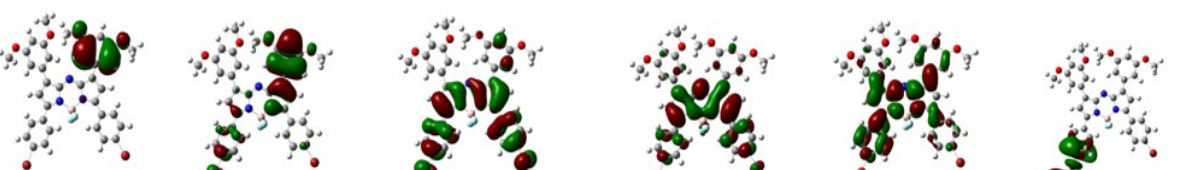
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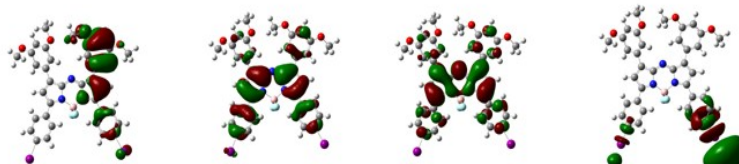
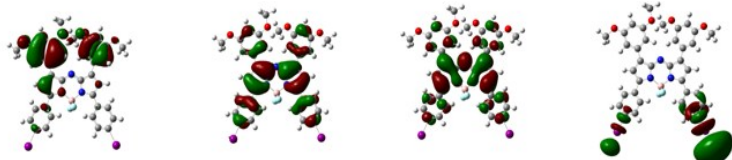
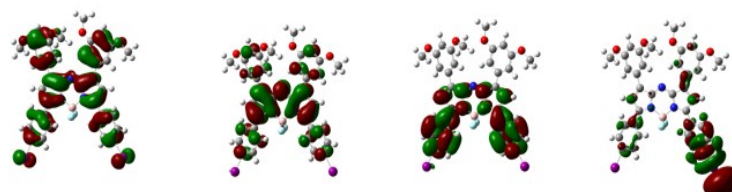
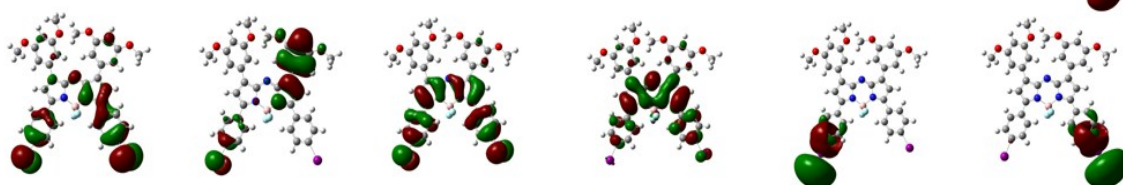


T_1



T_2



1c S_0  S_1  T_1  T_2 **2b**

H-3

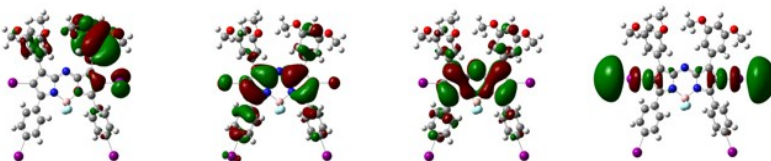
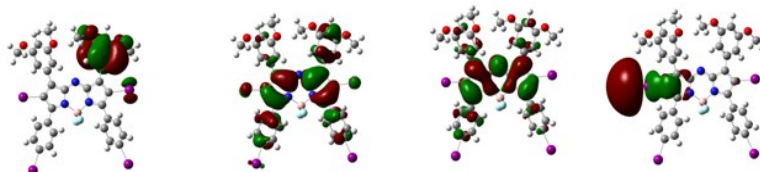
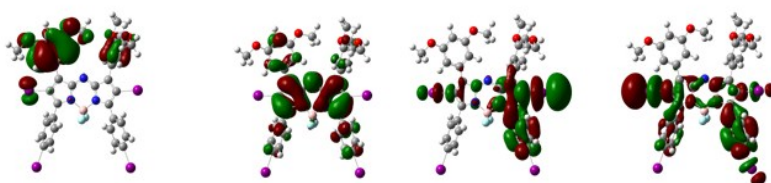
H-2

H-1

H

L

L+1

 S_0  S_1  T_1  T_2 