

Table SX. Cartesian coordinates of optimized **1** in their singlet ground state.

Atom	X	Y	Z	Re	-0.62449	-0.814919	-0.255718
C	-2.92284	1.425007	-0.005665	Cl	-1.466378	-0.687782	-2.667229
C	-4.06625	2.029411	0.501879	C	-1.477318	-2.558925	-0.136359
C	-4.377475	0.151288	1.928029	C	0.948845	-1.695708	-0.869348
C	-3.227699	-0.386691	1.383894	C	0.000123	-0.94707	1.521419
H	-4.359935	3.002006	0.126629	O	-1.984854	-3.587911	-0.075471
H	-4.911629	-0.397445	2.693128	O	1.867326	-2.280142	-1.247794
H	-2.857679	-1.345027	1.723053	O	0.377126	-1.063185	2.609274
C	-2.153223	2.109197	-1.095554	C	-4.811273	1.388744	1.4775
H	-2.55889	3.106094	-1.255215	H	-5.705542	1.848887	1.881364
H	-2.254416	1.533957	-2.018778				
C	-0.056122	3.444068	-0.818861				
C	0.069723	1.209744	-0.48916				
C	1.229225	3.152134	-0.523542				
H	-0.538068	4.380238	-1.045283				
H	2.100931	3.778421	-0.437602				
C	2.486364	1.090185	0.017897				
C	3.253558	0.542761	-1.011729				
C	2.86963	1.023795	1.357899				
C	4.421844	-0.126015	-0.6615				
C	4.042904	0.336576	1.659577				
C	4.825072	-0.249969	0.666968				
H	5.027712	-0.568013	-1.447098				
H	4.354146	0.263177	2.697716				
C	2.829207	0.678516	-2.44294				
H	1.806733	0.320371	-2.592112				
H	2.850187	1.725988	-2.760334				
H	3.492874	0.111022	-3.096239				
C	2.076026	1.705852	2.431537				
H	2.309417	2.775633	2.459201				
H	1.001489	1.612869	2.266239				
H	2.311646	1.285591	3.410037				
C	6.063829	-1.019174	1.021185				
H	5.831986	-2.081584	1.153275				
H	6.816505	-0.94496	0.233087				
H	6.501964	-0.660355	1.954945				
N	-2.505188	0.22195	0.427147				
N	-0.740752	2.247019	-0.793753				
N	1.286053	1.786042	-0.322936				

Table SX. Cartesian coordinates of optimized **2** in their singlet ground state.

Atom	X	Y	Z	N	1.28966	1.784801	-0.314092
C	-2.908567	1.397076	0.010118	Re	-0.610474	-0.821874	-0.219598
C	-4.066815	1.968755	0.533289	Cl	-1.458501	-0.700523	-2.622735
C	-4.383012	0.199414	1.888971	C	-1.450155	-2.572239	-0.088252
C	-3.231685	-0.389192	1.396337	C	0.969365	-1.698574	-0.829926
H	-4.389794	2.941333	0.175057	C	0.016718	-0.940953	1.559737
H	-4.966192	-0.305359	2.651514	O	-1.950371	-3.603665	-0.019599
H	-2.893906	-1.347383	1.766636	O	1.887927	-2.282209	-1.205666
C	-2.152817	2.1034	-1.07049	O	0.394609	-1.048363	2.647307
H	-2.56751	3.100198	-1.209306	N	-4.810863	1.384155	1.461801
H	-2.259946	1.543285	-2.002595				
C	-0.056466	3.439551	-0.810932				
C	0.073318	1.206451	-0.467871				
C	1.230721	3.149504	-0.523071				
H	-0.54053	4.374104	-1.0394				
H	2.102761	3.776589	-0.447127				
C	2.494219	1.091709	0.018229				
C	3.25359	0.544936	-1.017722				
C	2.88906	1.028411	1.354858				
C	4.426376	-0.120373	-0.676864				
C	4.066277	0.343637	1.647052				
C	4.841085	-0.242148	0.648393				
H	5.026444	-0.561994	-1.467094				
H	4.386666	0.272094	2.682505				
C	2.81548	0.676318	-2.445213				
H	1.793008	0.31393	-2.58461				
H	2.829356	1.723126	-2.765093				
H	3.475276	0.110069	-3.103458				
C	2.104983	1.712121	2.434388				
H	2.345016	2.780418	2.462995				
H	1.028978	1.626226	2.275187				
H	2.343646	1.28843	3.410645				
C	6.084563	-1.008385	0.9921				
H	5.860257	-2.074738	1.1037				
H	6.838629	-0.914315	0.207382				
H	6.51763	-0.663326	1.93329				
N	-2.48875	0.200634	0.448476				
N	-0.740296	2.242064	-0.772973				

Table SX. Cartesian coordinates of optimized **3** in their singlet ground state.

Atom	X	Y	Z
C	-2.923412	1.427058	0.083719
C	-4.041942	2.038965	0.633396
C	-4.297226	0.173905	2.088275
C	-3.174478	-0.374026	1.499895
H	-4.349198	3.009177	0.263297
H	-4.799626	-0.366165	2.880409
H	-2.795882	-1.33195	1.830275
C	-2.192999	2.108801	-1.036626
H	-2.604935	3.105503	-1.179275
H	-2.339073	1.556533	-1.965406
C	-0.090868	3.448342	-0.816819
C	0.046852	1.215723	-0.489576
C	1.199031	3.158577	-0.539742
H	-0.578522	4.383621	-1.03428
H	2.069969	3.787183	-0.463856
C	2.46609	1.098306	-0.003165
C	3.236332	0.556838	-1.033906
C	2.845099	1.025724	1.337808
C	4.400746	-0.117815	-0.682954
C	4.015236	0.333141	1.639433
C	4.798258	-0.251291	0.64654
H	5.008946	-0.555873	-1.46884
H	4.323005	0.253875	2.678066
C	2.825548	0.709963	-2.467421
H	1.794255	0.384892	-2.628393
H	2.882252	1.757384	-2.780524
H	3.47613	0.124876	-3.118148
C	2.054978	1.709001	2.413515
H	2.323993	2.769281	2.468385
H	0.980333	1.658059	2.230783
H	2.260525	1.260342	3.386077
C	6.032692	-1.02707	1.000504
H	5.797379	-2.090504	1.116917
H	6.791446	-0.944314	0.219173
H	6.463981	-0.681047	1.942126
N	-2.491624	0.225731	0.508693
N	-0.771829	2.249037	-0.783153
N	1.26318	1.792764	-0.341416

Re	-0.650959	-0.810375	-0.254359
C	-1.493334	-2.562443	-0.083938
C	0.913224	-1.684017	-0.921381
C	0.052042	-0.958527	1.517444
O	-1.98741	-3.592345	0.015973
O	1.82664	-2.25661	-1.32169
O	0.466386	-1.084504	2.58281
N	-1.432562	-0.668575	-2.241767
C	-1.796065	-0.702914	-3.331169
C	-2.256331	-0.7302	-4.69514
H	-2.857646	0.15903	-4.895283
H	-1.398224	-0.745501	-5.36978
H	-2.863575	-1.622278	-4.859643
C	-4.745925	1.408566	1.645888
H	-5.620562	1.875211	2.083519

Table SX. Cartesian coordinates of optimized **4** in their singlet ground state.

Atom	X	Y	Z	Re	-0.599393	-0.895752	-0.239137
C	-2.971666	1.447857	0.088463	C	-1.440864	-2.643869	-0.050847
C	-4.074725	2.084693	0.650735	C	0.981042	-1.761283	-0.838727
C	-4.420876	0.341493	2.043	C	0.054562	-0.998931	1.553842
C	-3.321086	-0.31226	1.507608	O	-1.94875	-3.665108	0.065956
H	-4.368697	3.067815	0.296671	O	1.916262	-2.32508	-1.201335
H	-4.99843	-0.122996	2.834859	O	0.442545	-1.088308	2.632495
H	-3.014874	-1.285795	1.867752	N	-4.801639	1.542089	1.619821
C	-2.210086	2.081496	-1.036355	N	-1.35174	-0.757237	-2.285027
H	-2.610909	3.073694	-1.23464	C	-1.683138	-0.776267	-3.384984
H	-2.339251	1.486086	-1.941149	C	-2.100227	-0.788026	-4.762754
C	-0.126038	3.429982	-0.762604	H	-3.127381	-0.425562	-4.836076
C	0.043211	1.192772	-0.475611	H	-1.444011	-0.140901	-5.347725
C	1.166145	3.154171	-0.483395	H	-2.046942	-1.806707	-5.15142
H	-0.625277	4.362172	-0.966429				
H	2.027631	3.793811	-0.393303				
C	2.462504	1.10049	0.008286				
C	3.218575	0.56646	-1.037063				
C	2.862472	1.02553	1.342725				
C	4.39425	-0.098713	-0.707429				
C	4.042858	0.340818	1.62257				
C	4.814662	-0.232966	0.615061				
H	4.992675	-0.529869	-1.504501				
H	4.367523	0.259569	2.655855				
C	2.776979	0.710736	-2.462301				
H	1.769067	0.313811	-2.61278				
H	2.75236	1.763094	-2.761919				
H	3.457075	0.181461	-3.130323				
C	2.08304	1.695476	2.434438				
H	2.344148	2.757501	2.493053				
H	1.006199	1.636884	2.267616				
H	2.306834	1.241984	3.40071				
C	6.061205	-0.999609	0.945345				
H	5.840916	-2.068676	1.036733				
H	6.815036	-0.887861	0.16278				
H	6.4921	-0.67014	1.892966				
N	-2.600366	0.240458	0.52862				
N	-0.791596	2.221457	-0.756834				
N	1.248621	1.786734	-0.309927				

Table SX. Cartesian coordinates of optimized $\mathbf{1}^+$ in their doublet ground state.

Atom	X	Y	Z	Re	-0.655479	-0.790006	-0.263582
C	-2.933715	1.437459	0.002109	Cl	-1.642152	-0.922234	-2.492195
C	-4.087763	2.039641	0.48194	C	-1.604057	-2.572132	0.023861
C	-4.338698	0.242967	2.024085	C	0.948741	-1.649056	-0.969183
C	-3.182507	-0.302253	1.50563	C	0.161828	-1.09204	1.491842
H	-4.40314	2.981675	0.055992	O	-2.13506	-3.56504	0.165065
H	-4.849653	-0.265809	2.828727	O	1.85576	-2.20827	-1.382139
H	-2.789553	-1.220754	1.912673	O	0.640298	-1.360126	2.495781
C	-2.173071	2.101389	-1.109171	C	-4.808985	1.436931	1.498886
H	-2.574144	3.094835	-1.278629	H	-5.709383	1.897493	1.882332
H	-2.280285	1.524888	-2.029019				
C	-0.068217	3.426407	-0.871182				
C	0.063633	1.206604	-0.493339				
C	1.226748	3.135494	-0.570806				
H	-0.547131	4.356992	-1.118667				
H	2.094799	3.765532	-0.498588				
C	2.499107	1.094058	0.0055				
C	3.299012	0.594156	-1.023496				
C	2.847652	0.987769	1.352309				
C	4.465311	-0.074162	-0.664989				
C	4.020456	0.302273	1.660614				
C	4.834581	-0.2411	0.668989				
H	5.095268	-0.479635	-1.447763				
H	4.304154	0.19653	2.700971				
C	2.923444	0.778895	-2.465788				
H	1.895484	0.471008	-2.662531				
H	3.001208	1.829762	-2.756393				
H	3.584432	0.19968	-3.108527				
C	2.02378	1.627661	2.433218				
H	2.22739	2.701166	2.480077				
H	0.953608	1.514893	2.263101				
H	2.267144	1.199088	3.404254				
C	6.073676	-1.011518	1.02822				
H	5.858884	-2.083409	1.074294				
H	6.858116	-0.869336	0.283534				
H	6.458862	-0.711267	2.003149				
N	-2.488834	0.264731	0.498341				
N	-0.754152	2.242692	-0.813156				
N	1.288056	1.783459	-0.342582				

Table SX. Cartesian coordinates of optimized $\mathbf{1}^0$ in their doublet ground state.

Atom	X	Y	Z	Re	-0.628766	-0.870994	-0.294423
C	-2.892665	1.462883	0.074701	Cl	-1.582731	-0.779892	-2.867429
C	-3.887736	2.137594	0.738439	C	-1.45447	-2.634718	-0.15874
C	-4.236567	0.214523	2.125773	C	0.939348	-1.755648	-0.973642
C	-3.226428	-0.410089	1.452063	C	0.045327	-1.071956	1.457536
H	-4.123699	3.143921	0.411773	O	-1.924882	-3.688328	-0.093178
H	-4.744668	-0.32816	2.914193	O	1.858494	-2.348775	-1.360735
H	-2.936044	-1.417506	1.715827	O	0.443357	-1.257283	2.535442
C	-2.202065	2.092544	-1.090296	C	-4.605309	1.544229	1.797878
H	-2.608084	3.082879	-1.276216	H	-5.396024	2.067459	2.315938
H	-2.319093	1.477745	-1.984325				
C	-0.07864	3.449931	-0.904799				
C	0.062779	1.217242	-0.567849				
C	1.214012	3.1699	-0.622429				
H	-0.570846	4.379277	-1.129907				
H	2.080578	3.801651	-0.548005				
C	2.481548	1.117217	-0.033153				
C	3.297766	0.571708	-1.024969				
C	2.804354	1.042175	1.322902				
C	4.453391	-0.092548	-0.623564				
C	3.966344	0.360783	1.678287				
C	4.797458	-0.218215	0.72124				
H	5.094154	-0.529787	-1.38046				
H	4.226601	0.283162	2.727539				
C	2.940936	0.696968	-2.477878				
H	1.952649	0.283684	-2.683549				
H	2.919564	1.744125	-2.789691				
H	3.667355	0.171487	-3.09644				
C	1.947336	1.701898	2.36511				
H	2.085939	2.786506	2.34798				
H	0.887682	1.51165	2.199806				
H	2.211177	1.3455	3.35987				
C	6.02394	-0.985697	1.13019				
H	5.797039	-2.051788	1.227239				
H	6.818202	-0.888995	0.388378				
H	6.404195	-0.643038	2.093331				
N	-2.503455	0.167855	0.416878				
N	-0.758208	2.248496	-0.866825				
N	1.28388	1.80163	-0.41697				

Table SX. Cartesian coordinates of optimized 2^+ in their doublet ground state.

Atom	X	Y	Z	Re	-0.6103	-0.886629	-0.28075
C	-2.897554	1.436495	0.070353	Cl	-1.562415	-0.781463	-2.82976
C	-3.927867	2.073339	0.709659	C	-1.434993	-2.649159	-0.13207
C	-4.274119	0.274166	2.053199	C	0.96372	-1.767458	-0.948387
C	-3.243707	-0.387261	1.453599	C	0.058611	-1.079054	1.478441
H	-4.191791	3.076054	0.388054	O	-1.910375	-3.698173	-0.050988
H	-4.823211	-0.220564	2.847745	O	1.882053	-2.357993	-1.33674
H	-2.972096	-1.38324	1.774174	O	0.455002	-1.257834	2.556877
C	-2.197263	2.095182	-1.073645	N	-4.670606	1.540618	1.721685
H	-2.606119	3.088059	-1.239765				
H	-2.313083	1.50039	-1.980355				
C	-0.079722	3.450518	-0.874142				
C	0.068593	1.217001	-0.5475				
C	1.214511	3.171713	-0.598991				
H	-0.575192	4.379606	-1.092913				
H	2.080103	3.804749	-0.524819				
C	2.489331	1.117543	-0.028804				
C	3.297335	0.576534	-1.029761				
C	2.822587	1.037068	1.324277				
C	4.456165	-0.089137	-0.640332				
C	3.987332	0.353974	1.667289				
C	4.810777	-0.220743	0.70116				
H	5.090906	-0.522943	-1.404207				
H	4.255909	0.271836	2.714069				
C	2.928046	0.70601	-2.479174				
H	1.944541	0.279069	-2.680515				
H	2.888397	1.754526	-2.784233				
H	3.657559	0.195168	-3.10625				
C	1.974825	1.693003	2.376416				
H	2.119216	2.776961	2.366714				
H	0.913177	1.509806	2.216195				
H	2.242751	1.327733	3.366827				
C	6.040484	-0.989932	1.096819				
H	5.81528	-2.057025	1.186424				
H	6.830248	-0.886317	0.351153				
H	6.425832	-0.654544	2.060458				
N	-2.494648	0.159276	0.427167				
N	-0.756906	2.247464	-0.838017				
N	1.287646	1.802733	-0.400356				

Table SX. Cartesian coordinates of optimized 2^0 in their doublet ground state.

Atom	X	Y	Z	Re	-0.6103	-0.886629	-0.28075
C	-2.897554	1.436495	0.070353	Cl	-1.562415	-0.781463	-2.82976
C	-3.927867	2.073339	0.709659	C	-1.434993	-2.649159	-0.13207
C	-4.274119	0.274166	2.053199	C	0.96372	-1.767458	-0.948387
C	-3.243707	-0.387261	1.453599	C	0.058611	-1.079054	1.478441
H	-4.191791	3.076054	0.388054	O	-1.910375	-3.698173	-0.050988
H	-4.823211	-0.220564	2.847745	O	1.882053	-2.357993	-1.33674
H	-2.972096	-1.38324	1.774174	O	0.455002	-1.257834	2.556877
C	-2.197263	2.095182	-1.073645	N	-4.670606	1.540618	1.721685
H	-2.606119	3.088059	-1.239765				
H	-2.313083	1.50039	-1.980355				
C	-0.079722	3.450518	-0.874142				
C	0.068593	1.217001	-0.5475				
C	1.214511	3.171713	-0.598991				
H	-0.575192	4.379606	-1.092913				
H	2.080103	3.804749	-0.524819				
C	2.489331	1.117543	-0.028804				
C	3.297335	0.576534	-1.029761				
C	2.822587	1.037068	1.324277				
C	4.456165	-0.089137	-0.640332				
C	3.987332	0.353974	1.667289				
C	4.810777	-0.220743	0.70116				
H	5.090906	-0.522943	-1.404207				
H	4.255909	0.271836	2.714069				
C	2.928046	0.70601	-2.479174				
H	1.944541	0.279069	-2.680515				
H	2.888397	1.754526	-2.784233				
H	3.657559	0.195168	-3.10625				
C	1.974825	1.693003	2.376416				
H	2.119216	2.776961	2.366714				
H	0.913177	1.509806	2.216195				
H	2.242751	1.327733	3.366827				
C	6.040484	-0.989932	1.096819				
H	5.81528	-2.057025	1.186424				
H	6.830248	-0.886317	0.351153				
H	6.425832	-0.654544	2.060458				
N	-2.494648	0.159276	0.427167				
N	-0.756906	2.247464	-0.838017				
N	1.287646	1.802733	-0.400356				

Table SX. Cartesian coordinates of optimized 3^+ in their doublet ground state.

Atom	X	Y	Z	Re	-0.636426	-0.712052	-0.342218
C	-2.905767	1.456719	0.021931	C	-1.581376	-2.518492	-0.127909
C	-4.050444	2.038444	0.542746	C	0.952443	-1.561425	-1.077678
C	-4.234329	0.214872	2.063423	C	0.201945	-1.003678	1.390931
C	-3.086671	-0.306187	1.501735	O	-2.102699	-3.513703	-0.01866
H	-4.390842	2.986166	0.145401	O	1.857237	-2.106504	-1.501239
H	-4.713285	-0.313007	2.877548	O	0.693259	-1.242917	2.389221
H	-2.666287	-1.226788	1.883903	N	-1.525035	-0.649183	-2.256384
C	-2.171208	2.148168	-1.088801	C	-1.956402	-0.779563	-3.313931
H	-2.577612	3.146691	-1.229241	C	-2.500053	-0.930176	-4.633633
H	-2.289939	1.606427	-2.027671	H	-3.49685	-0.486105	-4.6697
C	-0.071081	3.45217	-0.814753	H	-1.847669	-0.433499	-5.354432
C	0.064501	1.22763	-0.510694	H	-2.566043	-1.993832	-4.87335
C	1.23379	3.146259	-0.509763	C	-4.73542	1.408755	1.569609
H	-0.534988	4.401003	-1.028676	H	-5.631475	1.8525	1.986604
H	2.09785	3.782655	-0.411936				
C	2.490542	1.100559	0.030386				
C	3.296233	0.601567	-0.994777				
C	2.820735	0.996106	1.382589				
C	4.446343	-0.084887	-0.621825				
C	3.979639	0.294051	1.700301				
C	4.794926	-0.261548	0.716512				
H	5.084767	-0.493809	-1.398877				
H	4.252739	0.184754	2.745388				
C	2.956359	0.82233	-2.438197				
H	1.899573	0.641726	-2.650226				
H	3.167992	1.856297	-2.729368				
H	3.549425	0.166089	-3.075322				
C	2.001531	1.654668	2.45227				
H	2.289117	2.706247	2.554591				
H	0.930981	1.635193	2.238095				
H	2.165995	1.169193	3.414631				
C	6.014676	-1.0494	1.089296				
H	5.767833	-2.112706	1.178668				
H	6.794365	-0.956724	0.330508				
H	6.420255	-0.723949	2.049204				
N	-2.433975	0.282857	0.482713				
N	-0.75124	2.282714	-0.807013				
N	1.292407	1.804392	-0.326655				

Table SX. Cartesian coordinates of optimized 3^0 in their doublet ground state.

Atom	X	Y	Z	Re	-0.677468	-0.83132	-0.282125
C	-2.90294	1.449308	0.108211	C	-1.506078	-2.583208	-0.119509
C	-3.888248	2.118878	0.791929	C	0.901615	-1.695355	-0.939453
C	-4.207658	0.18926	2.166981	C	-0.004635	-0.973351	1.491678
C	-3.208297	-0.427387	1.472446	O	-1.985102	-3.626894	-0.039093
H	-4.129776	3.129372	0.474038	O	1.831369	-2.26818	-1.319765
H	-4.700391	-0.364584	2.960155	O	0.391136	-1.094527	2.568815
H	-2.914711	-1.439765	1.723647	N	-1.441996	-0.689408	-2.296813
C	-2.232005	2.097668	-1.052517	C	-1.790485	-0.708237	-3.391606
H	-2.634462	3.098122	-1.204101	C	-2.226396	-0.721429	-4.765427
H	-2.382389	1.528944	-1.973776	H	-3.252352	-0.353846	-4.828955
C	-0.101355	3.427547	-0.896065	H	-1.575512	-0.079615	-5.362216
C	0.019382	1.200835	-0.536739	H	-2.183842	-1.740413	-5.154803
C	1.187356	3.138121	-0.608408	C	-4.587069	1.520223	1.85735
H	-0.583651	4.36231	-1.128274	H	-5.368418	2.040452	2.395834
H	2.061347	3.763272	-0.537109				
C	2.439643	1.087658	-0.023605				
C	3.235901	0.542389	-1.031912				
C	2.79317	1.027533	1.325225				
C	4.399396	-0.118837	-0.652376				
C	3.962564	0.347797	1.657362				
C	4.771466	-0.237464	0.685617				
H	5.026396	-0.559415	-1.422146				
H	4.249424	0.279488	2.702924				
C	2.848453	0.675744	-2.473653				
H	1.822606	0.338477	-2.643099				
H	2.89977	1.720099	-2.798018				
H	3.51442	0.089044	-3.107446				
C	1.972164	1.711061	2.377352				
H	2.213032	2.778885	2.4159				
H	0.902491	1.627971	2.178275				
H	2.174302	1.285336	3.36097				
C	6.005343	-0.999388	1.071677				
H	5.774983	-2.061663	1.207638				
H	6.77422	-0.928486	0.299032				
H	6.422719	-0.631557	2.011485				
N	-2.502693	0.15535	0.429148				
N	-0.789511	2.235295	-0.848745				
N	1.243119	1.774956	-0.390665				

Table SX. Cartesian coordinates of optimized 4⁺ in their doublet ground state.

Atom	X	Y	Z	Re	-0.621055	-0.719944	-0.324018
C	-2.909504	1.429953	-0.002616	C	-1.527744	-2.547241	-0.10989
C	-4.075344	1.980528	0.520887	C	0.977857	-1.565719	-1.033787
C	-4.310398	0.24251	1.937399	C	0.201343	-0.976376	1.426252
C	-3.150742	-0.328588	1.440529	O	-2.022113	-3.555759	-0.000279
H	-4.435187	2.931875	0.143069	O	1.885479	-2.114393	-1.445921
H	-4.860018	-0.25348	2.729436	O	0.682231	-1.194105	2.433607
H	-2.780568	-1.260496	1.844699	N	-4.782051	1.395451	1.477639
C	-2.168694	2.1472	-1.087687	N	-1.499434	-0.672509	-2.240311
H	-2.579987	3.146565	-1.211309	C	-1.930109	-0.804942	-3.297868
H	-2.277846	1.624021	-2.038726	C	-2.472717	-0.958107	-4.617449
C	-0.074464	3.449501	-0.795993	H	-3.469793	-0.514761	-4.65476
C	0.064903	1.223555	-0.493552	H	-1.82005	-0.461722	-5.338262
C	1.232251	3.144009	-0.490724	H	-2.537264	-2.022193	-4.855654
H	-0.537886	4.398476	-1.010827				
H	2.094979	3.782423	-0.393077				
C	2.495194	1.10296	0.041476				
C	3.295086	0.605806	-0.989336				
C	2.836222	1.004025	1.391292				
C	4.450061	-0.075924	-0.623547				
C	3.999406	0.305511	1.701399				
C	4.808663	-0.249785	0.71259				
H	5.084145	-0.483904	-1.404577				
H	4.281096	0.199775	2.744537				
C	2.943847	0.822732	-2.430613				
H	1.888527	0.627627	-2.637497				
H	3.139753	1.859535	-2.722605				
H	3.542202	0.174859	-3.071259				
C	2.027215	1.666966	2.465997				
H	2.326426	2.715121	2.570143				
H	0.955619	1.659454	2.256941				
H	2.190789	1.17717	3.426318				
C	6.033077	-1.033978	1.077321				
H	5.790639	-2.098576	1.163196				
H	6.809169	-0.935234	0.315611				
H	6.44124	-0.710789	2.036845				
N	-2.452041	0.255047	0.4565				
N	-0.75272	2.280663	-0.788724				
N	1.292849	1.803879	-0.30945				

Table SX. Cartesian coordinates of optimized 4^0 in their doublet ground state.

Atom	X	Y	Z	Re	-0.65634	-0.838184	-0.254569
C	-2.905694	1.416351	0.096531	C	-1.48257	-2.589736	-0.07636
C	-3.938887	2.039892	0.746185	C	0.927689	-1.701367	-0.903065
C	-4.257855	0.244989	2.073212	C	0.016254	-0.969334	1.523221
C	-3.224636	-0.407687	1.468548	O	-1.96554	-3.628574	0.023118
H	-4.211215	3.044605	0.426886	O	1.854191	-2.27546	-1.284585
H	-4.797316	-0.261902	2.870194	O	0.414051	-1.083606	2.599445
H	-2.945388	-1.404868	1.78638	N	-4.672826	1.506008	1.756083
C	-2.221455	2.095951	-1.039097	N	-1.414522	-0.702131	-2.26406
H	-2.629842	3.096924	-1.172081	C	-1.765082	-0.720234	-3.358049
H	-2.363765	1.547724	-1.973109	C	-2.204583	-0.731337	-4.730381
C	-0.09871	3.42805	-0.865109	H	-3.229776	-0.361012	-4.790499
C	0.028556	1.200946	-0.508866	H	-1.553493	-0.090887	-5.32839
C	1.191309	3.140515	-0.582658	H	-2.165793	-1.750318	-5.12011
H	-0.583778	4.362062	-1.094314				
H	2.064199	3.767278	-0.512854				
C	2.451315	1.090955	-0.011271				
C	3.238195	0.547661	-1.028066				
C	2.817961	1.031389	1.333925				
C	4.406396	-0.111654	-0.660278				
C	3.991649	0.35311	1.653944				
C	4.791736	-0.23036	0.674001				
H	5.026558	-0.550674	-1.436395				
H	4.289025	0.2849	2.696526				
C	2.836066	0.680221	-2.465888				
H	1.811768	0.334045	-2.627182				
H	2.874803	1.725482	-2.788902				
H	3.501394	0.100666	-3.106815				
C	2.007789	1.71428	2.394837				
H	2.253879	2.780824	2.435526				
H	0.936143	1.636969	2.20446				
H	2.215902	1.284094	3.375245				
C	6.030652	-0.990368	1.047208				
H	5.804664	-2.054283	1.177407				
H	6.794233	-0.911729	0.270073				
H	6.452681	-0.62725	1.986716				
N	-2.483383	0.144321	0.440003				
N	-0.784339	2.234214	-0.816223				
N	1.250266	1.777208	-0.367132				