Supplementary Material: Probing ground and low-lying excited states for indole derived compounds of potential herbicide action

Rafael M. Motta[1] and Gabriel L. C. de Souza[1,2*]

[1]*Departamento de Química, Universidade Federal de Mato Grosso, Cuiabá, Mato Grosso, 78060-900 Brazil*

[2]*Instituto de Física, Universidade Federal de Mato Grosso, Cuiabá, Mato Grosso, 78060-900 Brazil*

TABLE I. Cartesians coordinates of indole optimized at the M06-2X/aug-cc-pVTZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
C	-0.245982	-0.666243	-0.000029
C	-0.247953	0.745109	0.000050
C	0.977559	1.421505	0.000038
C	2.146257	0.690051	-0.000066
C	2.123568	-0.714900	-0.000037
C	0.932668	-1.410401	-0.000093
C	-2.376377	0.028448	0.000243
C	-1.620766	1.160270	0.000011
H	1.004987	2.503115	0.000060
H	3.098841	1.201623	-0.000112
H	3.057184	-1.260421	-0.000105
H	0.914932	-2.492247	-0.000161
H	-3.446824	-0.087373	0.000358
H	-1.995333	2.169066	-0.000036
N	-1.556894	-1.075460	-0.000125
H	-1.869376	-2.028578	0.000174

TABLE II. Cartesians coordinates of indole optimized at the M06-2X/aug-cc-pVTZ level of theory in water. Values are given in Å

Atom	X	Y	Z
C	-0.248669	-0.665886	0.000019
C	-0.247231	0.747565	0.000040
C	0.980613	1.422923	-0.000041
C	2.148791	0.688212	-0.000110
C	2.122760	-0.718269	-0.000129
C	0.929769	-1.412647	-0.000060
C	-2.375469	0.028303	-0.000053
C	-1.619820	1.163415	0.000233
H	1.010173	2.504802	-0.000003
H	3.102685	1.197984	-0.000143
H	3.055469	-1.265734	-0.000173
H	0.907574	-2.494132	-0.000054
H	-3.445668	-0.090670	-0.000132
H	-1.994414	2.172694	0.000350
N	-1.558112	-1.074023	0.000056
H	-1.873501	-2.028474	0.000370

TABLE III. Cartesians coordinates of indole optimized at the M06-2X/aug-cc-pVTZ level of theory in DMSO. Values are given in Å

Atom	X	Y	Z
C	-0.248624	-0.665879	0.000019
C	-0.247233	0.747528	0.000040
C	0.980567	1.422893	-0.000041
C	2.148738	0.688230	-0.000110
C	2.122752	-0.718219	-0.000129
C	0.929798	-1.412609	-0.000060
C	-2.375471	0.028316	-0.000053
C	-1.619818	1.163364	0.000233
H	1.010096	2.504768	-0.000003
H	3.102615	1.198026	-0.000143
H	3.055477	-1.265652	-0.000173
H	0.907661	-2.494098	-0.000055
H	-3.445673	-0.090614	-0.000132
H	-1.994408	2.172636	0.000349
N	-1.558086	-1.074047	0.000056
H	-1.873422	-2.028480	0.000370

TABLE IV. Cartesians coordinates of indole optimized at the CAM-B3LYP/aug-cc-pVTZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
C	-0.245763	-0.665342	0.000017
C	-0.246197	0.742581	0.000037
C	0.976584	1.417691	-0.000042
C	2.142756	0.688072	-0.000111
C	2.119480	-0.713411	-0.000125
C	0.930495	-1.406908	-0.000058
C	-2.372696	0.030853	-0.000065
C	-1.616740	1.157865	0.000247
H	1.005205	2.498755	-0.000004
H	3.095117	1.199118	-0.000143
H	3.052797	-1.258507	-0.000167
H	0.914929	-2.488286	-0.000061
H	-3.443078	-0.080632	-0.000155
H	-1.989630	2.167061	0.000373
N	-1.556167	-1.074289	0.000051
H	-1.869686	-2.025889	0.000403

TABLE V. Cartesians coordinates of indole optimized at the CAM-B3LYP/aug-cc-pVTZ level of theory in water. Values are given in Å

Atom	X	Y	Z
C	-0.248009	-0.665196	0.000022
C	-0.245820	0.744725	0.000037
C	0.978911	1.419164	-0.000023
C	2.145038	0.686778	0.000033
C	2.119254	-0.716305	-0.000279
C	0.928421	-1.408890	-0.000065
C	-2.371888	0.029901	-0.000024
C	-1.616504	1.160665	0.000159
H	1.009207	2.500441	0.000074
H	3.098431	1.196460	0.000069
H	3.051801	-1.263090	-0.000361
H	0.908643	-2.489887	0.000011
H	-3.442050	-0.084955	-0.000092
H	-1.989928	2.170108	0.000227
N	-1.556966	-1.072686	0.000049
H	-1.873761	-2.025311	0.000570

TABLE VI. Cartesians coordinates of indole optimized at the CAM-B3LYP/aug-cc-pVTZ level of theory in DMSO. Values are given in Å

Atom	X	Y	Z
C	-0.247959	-0.665194	0.000022
C	-0.245832	0.744687	0.000037
C	0.978856	1.419138	-0.000023
C	2.144981	0.686805	0.000033
C	2.119255	-0.716248	-0.000279
C	0.928465	-1.408851	-0.000065
C	-2.371896	0.029897	-0.000024
C	-1.616514	1.160607	0.000159
H	1.009116	2.500410	0.000074
H	3.098353	1.196517	0.000068
H	3.051822	-1.262993	-0.000361
H	0.908748	-2.489853	0.000011
H	-3.442063	-0.084925	-0.000091
H	-1.989943	2.170041	0.000227
N	-1.556929	-1.072704	0.000049
H	-1.873675	-2.025314	0.000571

TABLE VII. Cartesians coordinates of the compound 15a optimized at the M06-2X/aug-cc-pVTZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
C	-0.1863780000	0.6780430000	0.0019010000
C	0.2453690000	-0.6748100000	-0.0144790000
C	-0.6930740000	-1.7013560000	-0.0239380000
C	-2.0388190000	-1.3759260000	-0.0176000000
C	-2.4802360000	-0.0586410000	-0.0021270000
C	-1.5495230000	0.9638540000	0.0074310000
C	2.0442620000	0.6643280000	-0.0016050000
C	1.6791000000	-0.6473010000	-0.0133030000
H	-0.3880460000	-2.7390100000	-0.0368760000
Cl	-3.2231030000	-2.6506350000	-0.0296530000
H	-3.5323650000	0.1796070000	0.0029550000
N	-2.0133880000	2.3427320000	0.0245260000
C	3.4409720000	1.1825630000	0.0032230000
C	2.6671740000	-1.7706260000	-0.0100060000
N	0.9212820000	1.4663760000	0.0093150000
H	0.8853860000	2.4711220000	0.0153600000
O	-1.1580480000	3.2139910000	0.0297390000
O	-3.2024820000	2.5564130000	0.0336100000
H	2.3499810000	-2.5553040000	0.6796550000
H	2.7195810000	-2.2309960000	-1.0014020000
C	4.0484820000	-1.2420990000	0.3890650000
H	4.0551410000	-1.0363490000	1.4628480000
H	4.8062880000	-2.0028400000	0.2035930000
C	4.3967950000	0.0424610000	-0.3641000000
H	5.4226040000	0.3416910000	-0.1516460000
H	4.3310560000	-0.1448130000	-1.4388110000
H	3.5425240000	2.0136650000	-0.6975000000
H	3.6848340000	1.5740850000	0.9954810000

TABLE VIII. Cartesians coordinates of the compound 15a optimized at the M06-2X/aug-cc-pVTZ level of theory in water. Values are given in Å

Atom	X	Y	Z
C	-0.1848470000	0.6849430000	0.0019160000
C	0.2486190000	-0.6712710000	-0.0148700000
C	-0.6858440000	-1.6995660000	-0.0239000000
C	-2.0337640000	-1.3753740000	-0.0175190000
C	-2.4806940000	-0.0628520000	-0.0022920000
C	-1.5507510000	0.9642390000	0.0073890000
C	2.0462880000	0.6674490000	-0.0016580000
C	1.6816740000	-0.6446220000	-0.0141290000
H	-0.3749590000	-2.7355960000	-0.0358670000
Cl	-3.2166010000	-2.6567330000	-0.0291390000
H	-3.5339610000	0.1689340000	0.0026820000
N	-2.0208180000	2.3333190000	0.0245000000
C	3.4418720000	1.1868840000	0.0035580000
C	2.6700720000	-1.7682920000	-0.0118950000
N	0.9212390000	1.4701610000	0.0096800000
H	0.9019360000	2.4758690000	0.0152720000
O	-1.1770820000	3.2155380000	0.0304550000
O	-3.2154460000	2.5464480000	0.0321940000
H	2.3508650000	-2.5547340000	0.6743640000
H	2.7232300000	-2.2249580000	-1.0046040000
C	4.0503460000	-1.2383600000	0.3891510000
H	4.0564960000	-1.0335920000	1.4631370000
H	4.8075080000	-1.9990860000	0.2020840000
C	4.3984120000	0.0471200000	-0.3624230000
H	5.4225070000	0.3481180000	-0.1457680000
H	4.3361840000	-0.1396870000	-1.4374430000
H	3.5400200000	2.0190290000	-0.6954100000
H	3.6813670000	1.5781090000	0.9964870000

TABLE IX. Cartesians coordinates of the compound 15a optimized at the M06-2X/aug-cc-pVTZ level of theory in DMSO. Values are given in Å

Atom	X	Y	Z
C	-0.1848980000	0.6848850000	0.0020020000
C	0.2485790000	-0.6713150000	-0.0147180000
C	-0.6858730000	-1.6995730000	-0.0236210000
C	-2.0338420000	-1.3753790000	-0.0171880000
C	-2.4806970000	-0.0628620000	-0.0020120000
C	-1.5507660000	0.9642940000	0.0075560000
C	2.0462730000	0.6674420000	-0.0016380000
C	1.6816690000	-0.6446020000	-0.0140570000
H	-0.3751060000	-2.7356420000	-0.0355510000
Cl	-3.2165750000	-2.6567530000	-0.0286690000
H	-3.5339510000	0.1690220000	0.0030090000
N	-2.0207720000	2.3333780000	0.0246250000
C	3.4418890000	1.1868670000	0.0032180000
C	2.6700090000	-1.7683200000	-0.0120180000
N	0.9211910000	1.4701470000	0.0096820000
H	0.9016070000	2.4758430000	0.0154250000
O	-1.1769240000	3.2155390000	0.0305330000
O	-3.2153230000	2.5465740000	0.0323040000
H	2.3511240000	-2.5545140000	0.6746840000
H	2.7225930000	-2.2252770000	-1.0046260000
C	4.0505180000	-1.2383750000	0.3882610000
H	4.0572020000	-1.0335920000	1.4622420000
H	4.8076010000	-1.9990890000	0.2008390000
C	4.3981990000	0.0471200000	-0.3634750000
H	5.4224560000	0.3480290000	-0.1474590000
H	4.3352240000	-0.1395820000	-1.4384680000
H	3.5398330000	2.0191750000	-0.6955920000
H	3.6818750000	1.5777610000	0.9961640000

TABLE X. Cartesians coordinates of the compound 15b optimized at the M06-2X/aug-cc-pVTZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
C	0.4959360000	0.4924980000	-0.0000150000
C	0.5684200000	-0.9218020000	0.0000060000
C	-0.5977890000	-1.6785580000	0.0000240000
C	-1.8177030000	-1.0233370000	0.0000090000
C	-1.9095800000	0.3629950000	-0.0000180000
C	-0.7491340000	1.1158190000	-0.0000320000
C	2.6565970000	-0.1006320000	-0.0000010000
C	1.9609790000	-1.2749520000	0.0000090000
H	-0.5645390000	-2.7596510000	0.0000530000
H	-2.8660520000	0.8621760000	-0.0000310000
H	1.9982760000	1.9419470000	-0.0000650000
N	1.7688270000	0.9627650000	-0.0000170000
Cl	-3.2844410000	-1.9570510000	0.0000300000
C	4.1199080000	0.1661810000	-0.0000090000
H	4.4120150000	0.7385250000	-0.8817520000
H	4.4120150000	0.7385300000	0.8817300000
H	4.6784430000	-0.7655120000	0.0000000000
C	2.4868120000	-2.6711240000	0.0000440000
H	2.1455230000	-3.2191540000	0.8799410000
H	2.1446580000	-3.2194670000	-0.8793180000
H	3.5745420000	-2.6897900000	-0.0005040000
N	-0.8443750000	2.5669020000	-0.0000650000
O	-1.9389510000	3.0782650000	-0.0000080000
O	0.2067970000	3.1882430000	-0.0000060000

TABLE XI. Cartesians coordinates of the compound 15b optimized at the M06-2X/aug-cc-pVTZ level of theory in water. Values are given in Å

Atom	X	Y	Z
C	0.498538	0.500360	-0.000007
C	0.575273	-0.917485	-0.000010
C	-0.585455	-1.679833	-0.000012
C	-1.809470	-1.028379	-0.000014
C	-1.911365	0.354385	-0.000014
C	-0.752453	1.115034	-0.000006
C	2.660423	-0.091585	-0.000017
C	1.967872	-1.268088	0.000014
H	-0.543330	-2.760727	-0.000002
H	-2.871865	0.845200	-0.000023
H	2.012700	1.946603	-0.000032
N	1.767953	0.970762	-0.000011
Cl	-3.274197	-1.972356	-0.000008
C	4.121718	0.181379	-0.000032
H	4.407053	0.757617	-0.880929
H	4.407082	0.757566	0.880889
H	4.684088	-0.747758	-0.000065
C	2.497620	-2.663203	0.000057
H	2.155973	-3.211858	0.879182
H	2.155582	-3.212039	-0.878802
H	3.585143	-2.675955	-0.000188
N	-0.860607	2.557943	-0.000002
O	-1.961980	3.067338	0.000041
O	0.179641	3.197031	0.000014

TABLE XII. Cartesians coordinates of the compound 15b optimized at the M06-2X/aug-cc-pVTZ level of theory in DMSO. Values are given in Å

Atom	X	Y	Z
C	0.4984430000	0.5002150000	0.0000880000
C	0.5751500000	-0.9175890000	0.0001620000
C	-0.5857020000	-1.6797860000	0.0000660000
C	-1.8096580000	-1.0282740000	-0.0001390000
C	-1.9114100000	0.3545310000	-0.0002570000
C	-0.7524410000	1.1150120000	-0.0001430000
C	2.6602890000	-0.0916390000	0.0001080000
C	1.9677690000	-1.2681690000	0.0003240000
H	-0.5437390000	-2.7606810000	0.0001330000
H	-2.8718110000	0.8455170000	-0.0004130000
H	2.0123340000	1.9465750000	0.0005420000
N	1.7678780000	0.9706840000	0.0003810000
Cl	-3.2743400000	-1.9721680000	-0.0002670000
C	4.1216750000	0.1810830000	0.0000950000
H	4.4071340000	0.7572430000	-0.8808050000
H	4.4071810000	0.7570990000	0.8810730000
H	4.6837740000	-0.7481900000	0.0000060000
C	2.4976490000	-2.6633230000	0.0004970000
H	2.1558160000	-3.2118840000	0.8795770000
H	2.1558700000	-3.2120580000	-0.8784940000
H	3.5851500000	-2.6759090000	0.0005320000
N	-0.8603140000	2.5580950000	-0.0002120000
O	-1.9615790000	3.0675440000	-0.0003180000
O	0.1801470000	3.1968710000	-0.0001300000

TABLE XIII. Cartesians coordinates of the compound 3a optimized at the M06-2X/aug-cc-pVTZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
C	-1.2666770000	-0.8642830000	-0.0253010000
C	-0.8388970000	0.4810850000	0.0225520000
C	-1.7996750000	1.4956060000	0.0566690000
C	-3.1377070000	1.1533830000	0.0435370000
C	-3.5397800000	-0.1894260000	-0.0030180000
C	-2.6131260000	-1.2139260000	-0.0379560000
C	0.9768350000	-0.8437710000	-0.0222780000
C	0.5966190000	0.4634120000	0.0205490000
H	-1.4975830000	2.5346050000	0.0939860000
H	-4.5946650000	-0.4272910000	-0.0119410000
C	2.3798820000	-1.3471420000	-0.0388970000
C	1.5755660000	1.5946200000	0.0452070000
N	-0.1394560000	-1.6524200000	-0.0519770000
H	-0.1287000000	-2.6554920000	-0.0796580000
H	1.2523890000	2.3923090000	-0.6269480000
H	1.6220640000	2.0350990000	1.0464540000
C	2.9634790000	1.0915620000	-0.3622180000
H	2.9749690000	0.9104220000	-1.4406280000
H	3.7144230000	1.8547940000	-0.1571750000
C	3.3232010000	-0.2073330000	0.3604580000
H	4.3538440000	-0.4899600000	0.1462660000
H	3.2490790000	-0.0461910000	1.4390430000
H	2.4930650000	-2.1941850000	0.6418050000
H	2.6351300000	-1.7097890000	-1.0397570000
H	-2.9256670000	-2.2493140000	-0.0742750000
H	-3.8904700000	1.9292080000	0.0708400000

TABLE XIV. Cartesians coordinates of the compound 3a optimized at the M06-2X/aug-cc-pVTZ level of theory in water. Values are given in Å

Atom	X	Y	Z
C	-1.5628450000	-0.9364450000	-0.0268040000
C	-1.1358280000	0.4127720000	0.0200990000
C	-2.0985840000	1.4272730000	0.0542680000
C	-3.4384150000	1.0836400000	0.0428650000
C	-3.8386480000	-0.2612640000	-0.0020810000
C	-2.9104720000	-1.2867620000	-0.0378440000
C	0.6779690000	-0.9149020000	-0.0244550000
C	0.2992640000	0.3954840000	0.0180800000
H	-1.7974310000	2.4670350000	0.0897980000
H	-4.8935940000	-0.5010250000	-0.0094990000
C	2.0810010000	-1.4188630000	-0.0395710000
C	1.2807380000	1.5260630000	0.0446420000
N	-0.4372330000	-1.7227840000	-0.0534160000
H	-0.4239480000	-2.7279040000	-0.0808580000
H	0.9595620000	2.3265100000	-0.6253250000
H	1.3288150000	1.9650270000	1.0464280000
C	2.6682360000	1.0199160000	-0.3615830000
H	2.6815020000	0.8392970000	-1.4401480000
H	3.4189230000	1.7825130000	-0.1542200000
C	3.0248610000	-0.2800650000	0.3605860000
H	4.0543580000	-0.5645740000	0.1450890000
H	2.9524370000	-0.1189760000	1.4394390000
H	2.1890250000	-2.2680220000	0.6379050000
H	2.3336080000	-1.7807050000	-1.0407090000
H	-3.2213780000	-2.3225460000	-0.0729560000
H	-4.1919200000	1.8593080000	0.0702770000

TABLE XV. Cartesians coordinates of the compound 3a optimized at the M06-2X/aug-cc-pVTZ level of theory in DMSO. Values are given in Å

Atom	X	Y	Z
C	-1.2651900000	-0.8657600000	-0.0259020000
C	-0.8381550000	0.4833900000	0.0210270000
C	-1.8008550000	1.4978950000	0.0551620000
C	-3.1406700000	1.1543200000	0.0436910000
C	-3.5409360000	-0.1905370000	-0.0012890000
C	-2.6128000000	-1.2160400000	-0.0369980000
C	0.9756780000	-0.8442250000	-0.0235420000
C	0.5969400000	0.4660940000	0.0190110000
H	-1.4996590000	2.5376380000	0.0907310000
H	-4.5958860000	-0.4302640000	-0.0087650000
C	2.3787210000	-1.3481590000	-0.0387390000
C	1.5783510000	1.5966970000	0.0455430000
N	-0.1395500000	-1.6521360000	-0.0525030000
H	-0.1263070000	-2.6572250000	-0.0799510000
H	1.2571050000	2.3970980000	-0.6244450000
H	1.6264070000	2.0356460000	1.0473360000
C	2.9658500000	1.0906380000	-0.3607630000
H	2.9790460000	0.9100450000	-1.4393300000
H	3.7165370000	1.8532510000	-0.1534350000
C	3.3225770000	-0.2093340000	0.3613720000
H	4.3520890000	-0.4937940000	0.1458450000
H	3.2501610000	-0.0482700000	1.4402250000
H	2.4869030000	-2.1972610000	0.6388070000
H	2.6313320000	-1.7100010000	-1.0398880000
H	-2.9237960000	-2.2518010000	-0.0721320000
H	-3.8941490000	1.9300070000	0.0710770000

TABLE XVI. Cartesians coordinates of the compound 3b optimized at the M06-2X/aug-cc-pVTZ level of theory in the gas-phase. Values are given in Å

Atom	X	Y	Z
C	2.6012380000	-0.1663720000	-0.0001700000
C	2.6934870000	1.2289900000	-0.0001490000
C	1.5479200000	2.0025240000	-0.0000420000
C	0.3216510000	1.3491920000	0.0000350000
C	0.2259170000	-0.0587910000	0.0000040000
C	1.3920500000	-0.8270040000	-0.0000940000
H	3.6689020000	1.6928170000	-0.0002120000
H	1.6147880000	3.0821630000	-0.0000090000
H	1.3584640000	-1.9077800000	-0.0001250000
C	-1.8513190000	0.7883810000	0.0001620000
C	-3.3216390000	0.9775870000	0.0002120000
C	-4.1140660000	-0.3518710000	-0.0001230000
C	-3.3531430000	-1.7092290000	0.0004000000
C	-1.8047400000	-1.7321730000	0.0001260000
C	-1.1720070000	-0.3860700000	0.0000810000
H	-3.6024010000	1.5740730000	0.8717910000
H	-4.7747540000	-0.3401040000	0.8644670000
H	-3.6928720000	-2.2753960000	0.8655820000
H	-1.4502520000	-2.2915290000	0.8691110000
H	-3.6023830000	1.5744290000	-0.8711300000
H	-4.7738950000	-0.3402130000	-0.8653710000
H	-3.6931590000	-2.2761320000	-0.8641870000
H	-1.4505080000	-2.2915090000	-0.8689770000
N	-0.9612800000	1.8434460000	0.0001880000
H	-1.2148490000	2.8144880000	0.0002790000
Cl	4.0794000000	-1.0947290000	-0.0003040000

TABLE XVII. Cartesians coordinates of the compound 3b optimized at the M06-2X/aug-cc-pVTZ level of theory in water. Values are given in Å

Atom	X	Y	Z
C	2.5989360000	-0.1639650000	-0.0001680000
C	2.6939500000	1.2316630000	-0.0000160000
C	1.5462110000	2.0042220000	0.0000980000
C	0.3195420000	1.3490850000	0.0000580000
C	0.2242450000	-0.0626190000	-0.0000900000
C	1.3924980000	-0.8304670000	-0.0002050000
H	3.6678480000	1.6991410000	-0.0000030000
H	1.6096180000	3.0837250000	0.0001860000
H	1.3582960000	-1.9114930000	-0.0002980000
C	-1.8503630000	0.7887260000	0.0001530000
C	-3.3201530000	0.9795400000	0.0002890000
C	-4.1148670000	-0.3483890000	-0.0001770000
C	-3.3568940000	-1.7087580000	0.0005750000
C	-1.8078150000	-1.7360660000	0.0000430000
C	-1.1724050000	-0.3901530000	-0.0000090000
H	-3.5966440000	1.5778670000	0.8709770000
H	-4.7737870000	-0.3355840000	0.8653370000
H	-3.6965190000	-2.2727280000	0.8669600000
H	-1.4552970000	-2.2971330000	0.8686730000
H	-3.5966910000	1.5783740000	-0.8700330000
H	-4.7725790000	-0.3357540000	-0.8666120000
H	-3.6970830000	-2.2738660000	-0.8648470000
H	-1.4557910000	-2.2970400000	-0.8688480000
N	-0.9604290000	1.8421440000	0.0000570000
H	-1.2148760000	2.8151950000	-0.0000830000
Cl	4.0840710000	-1.0942730000	-0.0003020000

TABLE XVIII. Cartesians coordinates of the compound 3b optimized at the M06-2X/aug-cc-pVTZ level of theory in DMSO. Values are given in Å

Atom	X	Y	Z
C	2.5989440000	-0.1639970000	-0.0001680000
C	2.6939440000	1.2316150000	-0.0000170000
C	1.5462470000	2.0041920000	0.0000970000
C	0.3195770000	1.3491080000	0.0000590000
C	0.2242660000	-0.0625330000	-0.0000890000
C	1.3924680000	-0.8303990000	-0.0002040000
H	3.6678670000	1.6990290000	-0.0000050000
H	1.6097430000	3.0837000000	0.0001850000
H	1.3582510000	-1.9114180000	-0.0002960000
C	-1.8503840000	0.7887280000	0.0001540000
C	-3.3201860000	0.9795010000	0.0002890000
C	-4.1148490000	-0.3484710000	-0.0001780000
C	-3.3568010000	-1.7087940000	0.0005740000
C	-1.8077300000	-1.7359980000	0.0000440000
C	-1.1724010000	-0.3900700000	-0.0000080000
H	-3.5967670000	1.5777620000	0.8710070000
H	-4.7737830000	-0.3357000000	0.8653290000
H	-3.6964130000	-2.2727830000	0.8669530000
H	-1.4551730000	-2.2970150000	0.8686880000
H	-3.5968130000	1.5782690000	-0.8700650000
H	-4.7725740000	-0.3358710000	-0.8666060000
H	-3.6969760000	-2.2739210000	-0.8648400000
H	-1.4556660000	-2.2969210000	-0.8688610000
N	-0.9604420000	1.8421990000	0.0000590000
H	-1.2148800000	2.8152180000	-0.0000770000
Cl	4.0839830000	-1.0942970000	-0.0003020000