

Supporting information for:

Rational design of novel star-shaped organic molecules as hole-transporting materials in perovskite solar cells

Ming Qin,^a Wenjing Zhu,^a Yue Liu^a and Xin Zhou^{*a,b}

^a *College of Environment and Chemical Engineering, Dalian University, Dalian 116622, Liaoning, China*

^b *Interdisciplinary Research Center for Biology and Chemistry, Liaoning Normal University, Dalian 116029, Liaoning, China*

* Corresponding authors.

Email addresses: zhouxin@dlu.edu.cn

Table S1 The centroid to centroid distance (r , Å), hole transfer integral (v , eV), hole hopping rate (k , s⁻¹), hole reorganization energy (λ , eV) and hole mobility (μ , cm² V⁻¹ s⁻¹) of all the molecules.

Molecules	pathway	r	v	k	λ	μ
A1	1	24.15	2.13×10^{-5}	1.33×10^6	0.25	4.17×10^{-4}
	2	12.07	-5.61×10^{-5}	9.27×10^6		
	3	25.47	5.85×10^{-4}	1.01×10^9		
	4	29.84	-4.30×10^{-5}	5.45×10^6		
B1	1	18.96	-7.75×10^{-7}	2.52×10^3	0.22	1.43×10^{-4}
	2	21.39	-9.98×10^{-6}	4.19×10^5		
	3	22.15	-3.32×10^{-5}	4.63×10^6		
	4	13.68	-5.30×10^{-4}	1.18×10^9		
C1	1	29.09	-1.29×10^{-14}	5.40×10^{-13}	0.24	5.32×10^{-3}
	2	5.79	-3.49×10^{-3}	3.96×10^{10}		
	3	40.98	-6.73×10^{-11}	1.47×10^{-5}		
	4	24.44	9.63×10^{-7}	3.01×10^3		
D1	1	27.09	4.11×10^{-9}	7.11×10^{-2}	0.22	8.59×10^{-2}
	2	6.03	2.95×10^{-2}	3.65×10^{12}		
	3	37.31	1.37×10^{-18}	7.91×10^{-21}		
	4	23.96	-1.16×10^{-4}	5.61×10^7		
E1	1	19.44	2.42×10^{-3}	1.75×10^{10}	0.25	3.97×10^{-3}
	2	32.35	-3.19×10^{-13}	3.05×10^{-10}		
	3	17.34	1.35×10^{-11}	5.43×10^{-7}		
	4	8.23	6.82×10^{-4}	1.39×10^9		
F1	1	30.49	1.59×10^{-11}	1.09×10^{-6}	0.22	7.22×10^{-2}
	2	11.00	-1.45×10^{-2}	9.21×10^{11}		
	3	24.55	3.14×10^{-8}	4.28×10^0		
	4	19.43	1.58×10^{-4}	1.08×10^8		
A2	1	35.29	9.15×10^{-19}	3.29×10^{-21}	0.23	1.21×10^{-4}
	2	25.79	-2.67×10^{-4}	2.80×10^8		
	3	28.18	5.48×10^{-6}	1.18×10^5		
	4	15.09	-1.90×10^{-6}	1.42×10^4		
B2	1	23.57	1.06×10^{-8}	6.04×10^{-1}	0.20	1.09×10^{-4}
	2	24.34	2.30×10^{-4}	2.85×10^8		
	3	29.25	6.88×10^{-16}	2.56×10^{-15}		
	4	13.57	-2.42×10^{-5}	3.16×10^6		
C2	1	19.42	3.50×10^{-9}	6.01×10^{-2}	0.21	1.84×10^{-1}
	2	8.78	2.74×10^{-2}	3.68×10^{12}		
	3	28.38	-4.21×10^{-10}	8.70×10^{-4}		
	4	31.41	-9.24×10^{-4}	4.19×10^9		
D2	1	5.75	-9.52×10^{-4}	4.74×10^9	0.20	3.51×10^{-2}
	2	19.37	5.33×10^{-3}	1.49×10^{11}		
	3	11.16	-1.54×10^{-5}	1.24×10^6		
	4	24.47	1.45×10^{-4}	1.10×10^8		

E2	1	24.84	2.88×10^{-6}	3.44×10^4	0.22	1.29×10^{-1}
	2	6.00	3.64×10^{-2}	5.51×10^{12}		
	3	22.09	6.71×10^{-5}	1.88×10^7		
	4	41.59	1.38×10^{-13}	7.95×10^{-11}		
F2	1	18.79	9.56×10^{-5}	5.56×10^7	0.19	1.19×10^{-1}
	2	33.93	1.52×10^{-5}	1.40×10^6		
	3	5.77	-3.01×10^{-2}	5.53×10^{12}		
	4	38.75	-3.51×10^{-14}	7.50×10^{-12}		

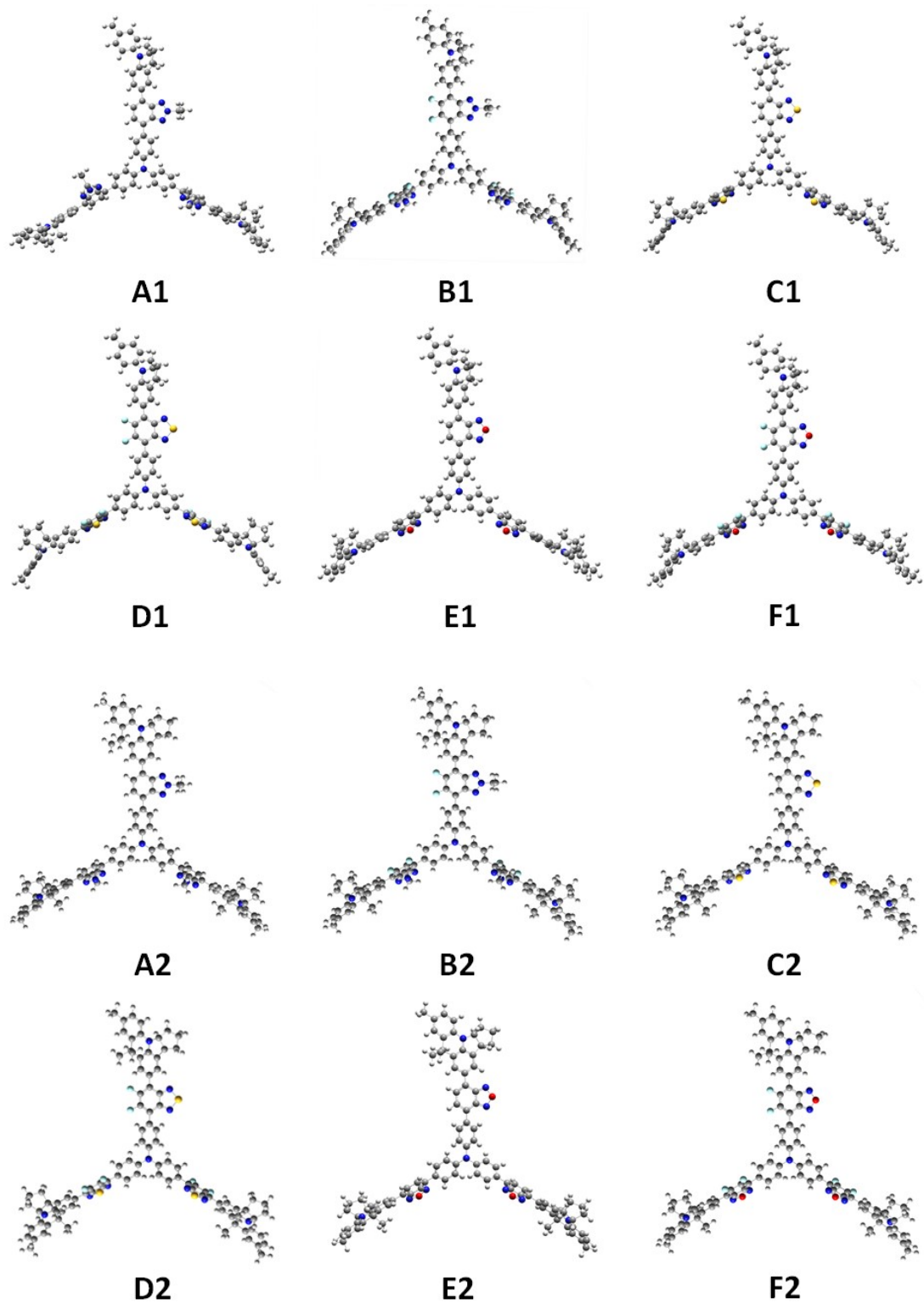


Fig. S1. The optimized structures of all the designed molecules

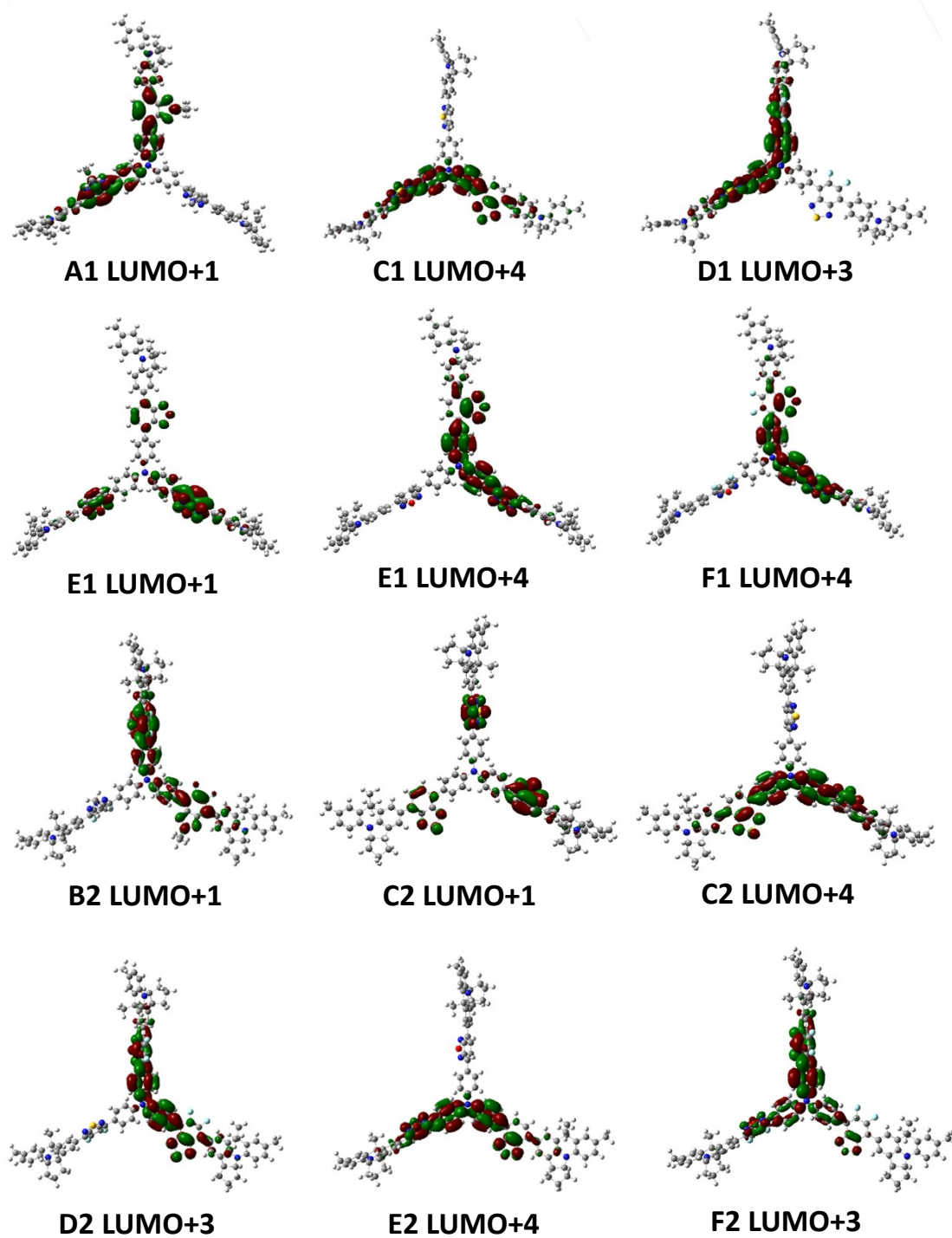


Fig. S2. The electron cloud distributions of molecular orbitals

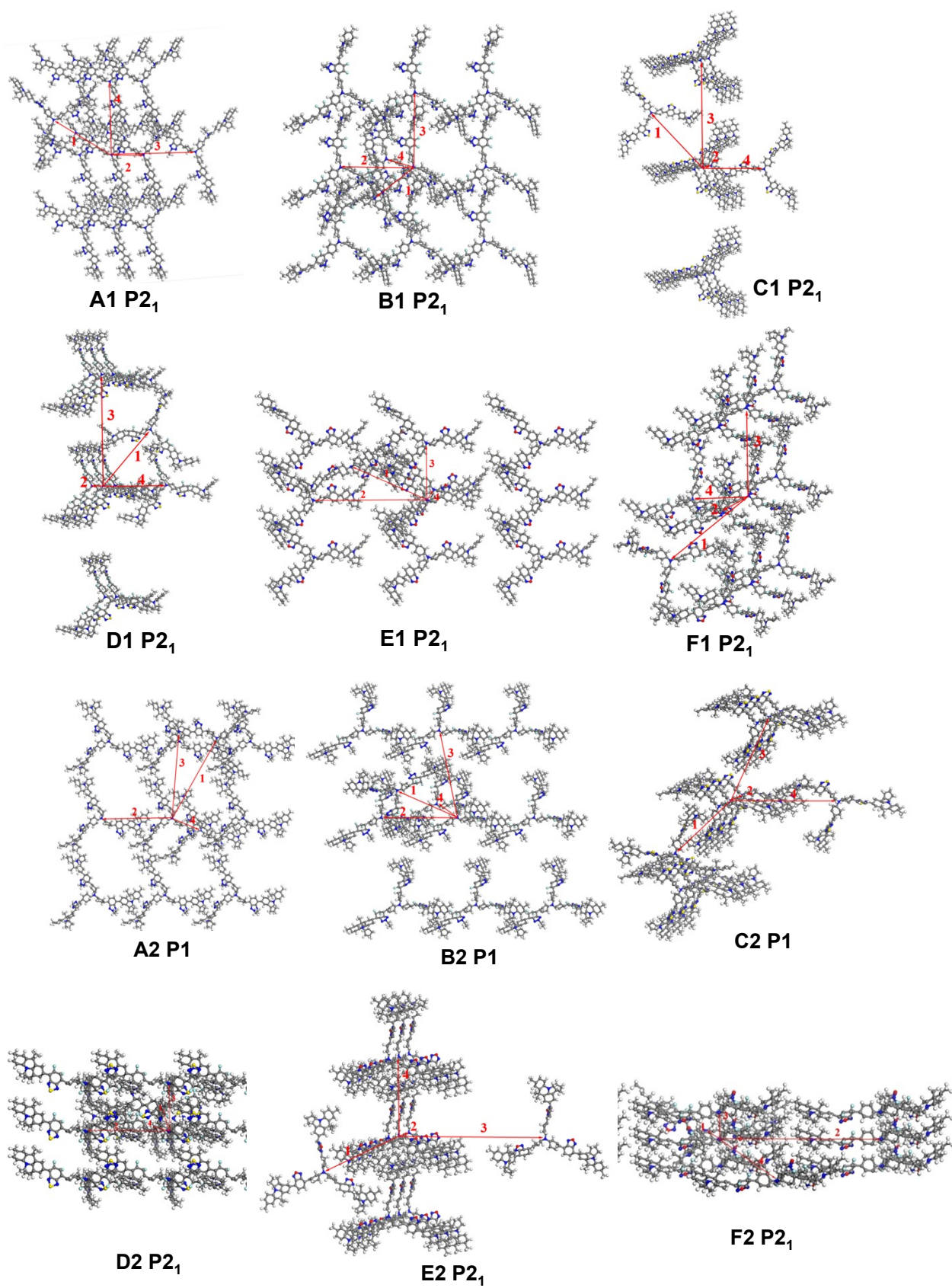


Fig. S3. The main hole hopping pathways selected on basis of the molecular crystal structures.

The cartesian coordinates of all the molecules in their ground state and first-excited state

CS-53: ground state

N	-0.14036500	-0.08663600	-0.07140500
C	-1.54572600	-0.28164900	-0.08279300
C	-2.12499300	-1.30083400	-0.85701100
C	-2.39253000	0.53879500	0.68096500
C	-3.50211400	-1.49366300	-0.85708400
H	-1.49185400	-1.93465900	-1.46852800
C	-3.76962000	0.34770600	0.66131300
H	-1.96556900	1.31999900	1.30054000
C	-4.36174100	-0.67404700	-0.10314700
H	-3.91993700	-2.27291800	-1.48721300
H	-4.39307500	0.98113100	1.28484100
C	0.39717300	1.22827500	-0.05733300
C	1.49053200	1.54724400	0.76424200
C	-0.14903000	2.23866600	-0.86550800
C	2.02144300	2.83233900	0.76772800
H	1.91562800	0.78551900	1.40907900
C	0.38017900	3.52463900	-0.84413100
H	-0.98290900	2.00873700	-1.52023100
C	1.48021700	3.85556300	-0.03193300
H	2.84879600	3.05384100	1.43489600
H	-0.04645900	4.27625600	-1.50126000
C	0.73610800	-1.20554800	-0.06015800
C	1.89519300	-1.21436200	-0.85268600
C	0.46802700	-2.32454300	0.74459100
C	2.76051300	-2.30270600	-0.82835300
H	2.12114700	-0.35917800	-1.48061600
C	1.33035700	-3.41610400	0.74800800
H	-0.42307200	-2.33939400	1.36301500
C	2.50065900	-3.43295400	-0.03217900
H	3.66138400	-2.26745400	-1.43308200
H	1.08321100	-4.27493400	1.36443100
C	2.04642600	5.22475400	-0.01693400
C	1.23104100	6.35812400	-0.18746700
C	3.42299800	5.44455300	0.17139000
C	1.76364000	7.64337300	-0.16593600
H	0.15817500	6.23472600	-0.30152800
C	3.95572400	6.72945300	0.18875400
H	4.09289300	4.59558700	0.27007400
C	3.14066000	7.86522300	0.02375300
H	1.09267700	8.49147300	-0.26357100
H	5.02884700	6.85224800	0.29919400

C	-5.82949900	-0.87830000	-0.11312100
C	-6.71982500	0.20536400	-0.00692900
C	-6.38931400	-2.16331700	-0.23014000
C	-8.09781600	0.01325300	-0.01335400
H	-6.32924900	1.21582200	0.06747200
C	-7.76746100	-2.35426200	-0.24473800
H	-5.73647800	-3.02840700	-0.29772700
C	-8.65887200	-1.27133700	-0.13374000
H	-8.74988800	0.87514700	0.09089000
H	-8.15920900	-3.36057600	-0.35811100
C	3.42685500	-4.59073100	-0.01403400
C	3.63983400	-5.34045700	1.15658900
C	4.13467900	-4.97951800	-1.16545700
C	4.51520300	-6.42189100	1.17482100
H	3.12471800	-5.06454500	2.07186900
C	5.01580000	-6.05593200	-1.14492100
H	3.98665800	-4.43776800	-2.09487800
C	5.23020300	-6.80748500	0.02554100
H	4.63615900	-6.98476900	2.09542000
H	5.56022500	-6.30779400	-2.04993600
C	-10.12739800	-1.47347900	-0.14377800
C	-10.70768000	-2.61503300	0.43327800
C	-10.98798800	-0.51848200	-0.73353100
C	-12.08983300	-2.83163600	0.44640600
H	-10.06857100	-3.34478800	0.92127100
C	-12.35629600	-0.71109900	-0.72209300
H	-10.57226100	0.36239900	-1.21398500
C	-12.92093400	-1.87593000	-0.13851600
H	-12.49352300	-3.71223300	0.93187500
C	-13.50833900	0.04520700	-1.32845100
C	-14.65963300	-0.41643200	-0.43512700
C	3.70828300	9.23312200	0.04968400
C	4.81400400	9.54697200	0.85857400
C	3.15038000	10.27326400	-0.72785200
C	5.37432800	10.82524800	0.90333500
H	5.23495900	8.78008200	1.50182100
C	3.69078500	11.54602300	-0.69350900
H	2.29940500	10.07069100	-1.37227400
C	4.81444600	11.83458900	0.10892200
H	6.20471200	11.02359000	1.56927300
C	3.26808700	12.79150000	-1.43132600
C	4.15325900	13.91584800	-0.79882100
C	6.17207000	-7.95076700	0.04675400
C	6.34915300	-8.77141400	-1.08039000

C	6.92092200	-8.25947200	1.20490000
C	7.23610800	-9.85014800	-1.09304400
H	5.75410600	-8.58680000	-1.96983900
C	7.80325200	-9.32454600	1.21006900
H	6.81887200	-7.64496900	2.09508100
C	7.98264400	-10.12293600	0.06108700
H	7.31045900	-10.47239800	-1.97602800
C	8.69988400	-9.82484300	2.31445800
C	9.28469200	-11.15840100	1.74275500
N	5.16180900	13.18041400	0.00021600
N	-14.33634800	-1.83799400	-0.22416000
N	8.89894800	-11.14354500	0.31151600
C	10.81502300	-11.10914600	1.99281800
C	9.93759900	-8.95499700	2.65150800
C	11.00633400	-9.98938000	3.03413000
C	4.74423800	14.72741700	-1.98128200
C	3.58041500	12.84082900	-2.94873300
C	3.89201700	14.32372800	-3.20017800
C	-15.88121900	0.13162100	-1.16479500
C	-13.78982100	1.54038500	-1.45997900
C	-15.35901300	1.55288500	-1.59540100
H	-13.47202600	2.07987700	-0.56136700
H	-13.29848100	2.00485400	-2.31848500
H	-15.79274000	2.33382700	-0.96490400
H	-15.66182500	1.77145900	-2.62296100
H	-16.10928400	-0.48468100	-2.04087400
H	-16.78350900	0.19331100	-0.55206400
H	-13.69072200	-0.40589200	-2.31986100
H	-14.56915900	0.11290100	0.53181800
H	4.46484900	12.22951000	-3.16530300
H	2.75581400	12.45702600	-3.55654500
H	4.40487200	14.50208600	-4.15032400
H	2.95974400	14.90210100	-3.21757300
H	4.74106500	15.80511700	-1.79733300
H	5.78510400	14.42381500	-2.13624700
H	2.20668700	13.01173000	-1.27664500
H	3.55602400	14.55621800	-0.13850800
H	10.25456400	-8.40094200	1.75964500
H	9.73140100	-8.22449600	3.43927300
H	10.80892400	-10.37348600	4.04284400
H	11.22132000	-12.07008900	2.31943900
H	11.31963600	-10.83912000	1.05891300
H	12.02198600	-9.58189600	3.03254600
H	8.13768000	-10.01977900	3.23371200

H	8.83148800	-12.02604200	2.23729500
C	9.36151400	-12.11138100	-0.59583200
C	9.60172500	-11.80071800	-1.94736400
C	9.64549300	-13.41850800	-0.16033600
C	10.06799100	-12.77437800	-2.82760600
H	9.45382400	-10.78779200	-2.30271400
C	10.12539800	-14.37607600	-1.05159300
H	9.48996700	-13.69061300	0.87780800
C	10.33556900	-14.08366600	-2.40557900
H	10.24605800	-12.50047000	-3.86474900
H	10.33503500	-15.37697000	-0.68210900
C	-15.19636000	-2.72488300	0.45812300
C	-15.05185200	-4.11497100	0.29898300
C	-16.24706500	-2.25368700	1.25997500
C	-15.91408200	-4.99507200	0.94652100
H	-14.27769300	-4.50117900	-0.35548600
C	-17.11378000	-3.14919900	1.88816200
H	-16.39021900	-1.18808000	1.39981300
C	-16.96305300	-4.53430200	1.75631800
H	-15.77948500	-6.06445000	0.80318400
H	-17.92136100	-2.75575700	2.50060500
C	6.23923900	13.83211200	0.62375200
C	7.48816500	13.20344200	0.78520200
C	6.11006600	15.16179800	1.06364300
C	8.54546600	13.87202300	1.39752800
H	7.64131800	12.20139800	0.40214800
C	7.18308700	15.82055500	1.66091700
H	5.16808000	15.68513500	0.94164000
C	8.41945300	15.19105600	1.85436300
H	9.49814200	13.35849500	1.50332600
H	7.04955800	16.84860300	1.98880600
C	9.56550500	15.89775000	2.53833000
H	9.57006000	15.70120800	3.61806900
H	10.53147200	15.56421800	2.14675600
H	9.50204800	16.98204400	2.40737500
C	10.81595500	-15.13863300	-3.37354300
H	9.97460800	-15.66978900	-3.83670600
H	11.40467000	-14.69883000	-4.18438600
H	11.43488200	-15.88914000	-2.87284200
C	-17.88271000	-5.49914700	2.46686200
H	-18.12514700	-6.36016900	1.83567600
H	-17.42065700	-5.89185600	3.38136000
H	-18.82035500	-5.01655000	2.75669300

CS-53: the first excited state

N	0.11830900	-0.08207200	-0.02703000
C	1.51598000	-0.29777000	-0.01318400
C	2.07608000	-1.30202900	0.78420400
C	2.36669400	0.49773400	-0.78844000
C	3.44559700	-1.50402900	0.79619200
H	1.43265000	-1.91348500	1.40633000
C	3.73553200	0.29290400	-0.76048600
H	1.94489300	1.26709400	-1.42475500
C	4.30915100	-0.71126800	0.02962300
H	3.85590300	-2.27162800	1.44377400
H	4.36941100	0.90442200	-1.39383400
C	-0.39565100	1.22084100	-0.04519800
C	-1.55675600	1.53727700	-0.78394200
C	0.22665400	2.26299000	0.67634600
C	-2.06397700	2.81143400	-0.79623700
H	-2.04320500	0.76139400	-1.36465600
C	-0.27860600	3.53791600	0.65792600
H	1.10784200	2.04455400	1.26927400
C	-1.45459500	3.88658000	-0.07697400
H	-2.93743400	3.00033700	-1.40801800
H	0.22257100	4.28735600	1.25788500
C	-0.76035500	-1.19215000	-0.01938200
C	-1.91871900	-1.17614200	0.76429700
C	-0.49416900	-2.31940400	-0.80371900
C	-2.78454100	-2.25658900	0.75614800
H	-2.13720400	-0.30903900	1.37674700
C	-1.36113400	-3.39909800	-0.79444500
H	0.39839900	-2.34628700	-1.41825400
C	-2.52804600	-3.39371800	-0.01995800
H	-3.68535400	-2.20992900	1.35872500
H	-1.12049100	-4.26895500	-1.39631600
C	-1.98337400	5.21245800	-0.09083200
C	-1.29107600	6.32594900	0.48783500
C	-3.24878700	5.53193800	-0.68278200
C	-1.79697000	7.59370300	0.47321600
H	-0.31470700	6.17672600	0.93336200
C	-3.75453700	6.79961900	-0.69679000
H	-3.85277200	4.74239300	-1.11374700
C	-3.06044400	7.91360700	-0.12176300
H	-1.19518900	8.38150700	0.91028400
H	-4.73323200	6.94644100	-1.13782100
C	5.77312200	-0.92551100	0.05547300
C	6.66493900	0.14712400	-0.05618600

C	6.31683600	-2.20740400	0.19519000
C	8.03663500	-0.05358500	-0.03099900
H	6.28052700	1.15755200	-0.14954000
C	7.68860300	-2.40651300	0.22695100
H	5.65646100	-3.06532400	0.26844400
C	8.58105100	-1.33464800	0.11281100
H	8.69764800	0.80045800	-0.13648200
H	8.07453900	-3.41238700	0.35612600
C	-3.45854500	-4.54528500	-0.02313600
C	-3.67074800	-5.30415900	-1.17945400
C	-4.16265200	-4.91256000	1.12900700
C	-4.54537300	-6.38005700	-1.18286400
H	-3.15452500	-5.04088300	-2.09688600
C	-5.04299100	-5.98357600	1.12269200
H	-4.01267700	-4.35815300	2.04966500
C	-5.25529100	-6.74448600	-0.03285200
H	-4.67051300	-6.95496300	-2.09456100
H	-5.58731900	-6.22507300	2.02971600
C	10.04710900	-1.54678800	0.14596300
C	10.62408800	-2.67833300	-0.43391100
C	10.89592700	-0.61016700	0.76423100
C	12.00045800	-2.90541400	-0.42198700
H	9.98730600	-3.39573400	-0.94145400
C	12.25720000	-0.81414800	0.77829700
H	10.47605700	0.26750600	1.24569800
C	12.82079100	-1.96975200	0.19233200
H	12.40766600	-3.78249900	-0.90917700
C	13.40108500	-0.07809800	1.41349100
C	14.55609800	-0.53654800	0.53722100
C	-3.58810000	9.24254400	-0.13718700
C	-4.76667700	9.57890100	-0.87293300
C	-2.96142100	10.32094700	0.56770400
C	-5.30634300	10.84440100	-0.89858900
H	-5.25248600	8.81925800	-1.47202300
C	-3.49377900	11.57903800	0.54995100
H	-2.05575600	10.14828100	1.13661500
C	-4.68183000	11.86622800	-0.16069400
H	-6.18049200	11.04310700	-1.50467800
C	-3.00365800	12.83490000	1.21509000
C	-3.94545800	13.94211400	0.66041100
C	-6.19749700	-7.88702500	-0.03863700
C	-6.35267700	-8.70227000	1.08522800
C	-6.96018100	-8.19129700	-1.18009300
C	-7.23620700	-9.77861900	1.11200000

H	-5.74494700	-8.51421300	1.96453100
C	-7.83697900	-9.25375600	-1.17118600
H	-6.87071200	-7.57696900	-2.07108600
C	-7.99622400	-10.04821200	-0.02471900
H	-7.29803200	-10.39985500	1.99570800
C	-8.75148700	-9.75398000	-2.25485900
C	-9.30072800	-11.09334000	-1.68431900
N	-5.00574100	13.19969900	-0.05297900
N	14.23143900	-1.94627900	0.31092600
N	-8.91779100	-11.06284600	-0.26165700
C	-10.82589700	-11.07897500	-1.92833100
C	-10.00370800	-8.90212900	-2.54087800
C	-11.05207800	-9.94317700	-2.93593500
C	-4.44662800	14.74311500	1.88001100
C	-3.16094200	12.90672900	2.74766800
C	-3.46640600	14.38350300	3.00369000
C	15.76484500	-0.00806600	1.28941300
C	13.69043600	1.40749000	1.56324500
C	15.24932900	1.40527400	1.72519400
H	13.39259700	1.95524300	0.66420600
H	13.18783200	1.86860500	2.41551600
H	15.70012300	2.18914800	1.11259400
H	15.53526200	1.61042700	2.75909100
H	15.97104100	-0.63738200	2.16020800
H	16.67715100	0.05139900	0.69330900
H	13.56298000	-0.54315600	2.39986600
H	14.48280100	0.00521300	-0.42322100
H	-4.01023500	12.28998200	3.06108500
H	-2.27531600	12.54362400	3.27417200
H	-3.87804700	14.57391700	3.99790500
H	-2.54936200	14.97575100	2.90834100
H	-4.50467200	15.81604300	1.68683900
H	-5.45278000	14.40102700	2.14092500
H	-1.96550500	13.04898000	0.94636300
H	-3.41837700	14.58591200	-0.05094800
H	-10.31544600	-8.38626200	-1.62584100
H	-9.82722800	-8.14250300	-3.30634500
H	-10.85678800	-10.29780000	-3.95440400
H	-11.20745900	-12.04079000	-2.27777700
H	-11.33234300	-10.84777200	-0.98643500
H	-12.07458300	-9.55766100	-2.91417400
H	-8.21336800	-9.92983300	-3.19063800
H	-8.82766400	-11.95028600	-2.17763700
C	-9.35189700	-12.03799500	0.64573900

C	-9.56788700	-11.73682000	1.99640600
C	-9.63248000	-13.33767500	0.20907900
C	-10.00783700	-12.71514700	2.87669500
H	-9.41993900	-10.72509800	2.35325300
C	-10.08687300	-14.30067400	1.10033200
H	-9.49555900	-13.60092500	-0.83324800
C	-10.27209800	-14.01795700	2.45309900
H	-10.16792100	-12.45010600	3.91819400
H	-10.29733700	-15.30032600	0.73041600
C	15.08523900	-2.81001600	-0.40321400
C	14.94192000	-4.19702100	-0.28115500
C	16.12072300	-2.31717700	-1.19879700
C	15.79198300	-5.05553400	-0.96117800
H	14.17425400	-4.59890800	0.37061400
C	16.97688200	-3.19123000	-1.86025600
H	16.26292000	-1.24838800	-1.30738200
C	16.82660900	-4.57270700	-1.76616800
H	15.65962100	-6.12801500	-0.84837100
H	17.77780300	-2.78218500	-2.46966100
C	-6.15712700	13.83660900	-0.52886900
C	-7.39897200	13.18612500	-0.55730000
C	-6.09678800	15.17161600	-0.95297000
C	-8.52466000	13.84430900	-1.02875100
H	-7.48986500	12.17708900	-0.17532900
C	-7.23556900	15.81516000	-1.41165400
H	-5.15441200	15.70612700	-0.93252700
C	-8.47066700	15.16676900	-1.47242800
H	-9.47548000	13.31890900	-1.03351500
H	-7.15955500	16.84902300	-1.73624100
C	-9.69303300	15.86216000	-2.00829200
H	-9.78337200	15.72674400	-3.09186200
H	-10.60598600	15.46788400	-1.55534400
H	-9.65522700	16.93760800	-1.81840900
C	-10.72632600	-15.07811700	3.42136700
H	-9.87301200	-15.58744900	3.88254800
H	-11.32275200	-14.64922400	4.23059000
H	-11.32898600	-15.84113200	2.92286500
C	17.73539200	-5.51505800	-2.51081500
H	18.01012600	-6.37517800	-1.89424100
H	17.24984500	-5.90607900	-3.41138800
H	18.65467800	-5.01552700	-2.82460200

CS-54: ground state

N	0.74629600	-0.97817000	0.04881600
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C	2.08875900	-1.43646800	0.10116800
C	3.11622600	-0.72381700	-0.53838600
C	2.42362100	-2.60910400	0.80015400
C	4.43179300	-1.16596800	-0.47256500
H	2.87813000	0.17544300	-1.09601400
C	3.73964600	-3.04842500	0.85753200
H	1.64811500	-3.16603400	1.31477700
C	4.78009600	-2.33921400	0.22404500
H	5.19802100	-0.60339600	-0.99792200
H	3.97017700	-3.93833500	1.43436900
C	-0.31490200	-1.90593000	-0.11520000
C	-1.50546300	-1.77666000	0.61844500
C	-0.19867400	-2.97784400	-1.01720600
C	-2.54006000	-2.68990700	0.45548200
H	-1.61202800	-0.96406800	1.32879300
C	-1.23403700	-3.89029200	-1.17102700
H	0.70428300	-3.08460900	-1.60867900
C	-2.43156400	-3.77386100	-0.43669500
H	-3.43557100	-2.57658400	1.05946700
H	-1.12516800	-4.69007100	-1.89653400
C	0.46580400	0.40561500	0.19687500
C	-0.51010100	1.03182100	-0.59536500
C	1.15794000	1.18129500	1.14298200
C	-0.78110100	2.38667800	-0.44515700
H	-1.04822500	0.45441600	-1.33935800
C	0.88648100	2.53547900	1.28406000
H	1.90143800	0.71288900	1.77876300
C	-0.08761700	3.17635600	0.49210100
H	-1.52328400	2.84515600	-1.09211100
H	1.41635800	3.10007400	2.04445300
C	6.16200700	-2.81473400	0.30351600
C	6.62594100	-4.08554900	0.56711000
S	7.52275300	-1.72339700	0.07854400
C	8.04145900	-4.19425300	0.57646500
H	5.96647400	-4.93283700	0.71691200
C	8.69750000	-3.00902900	0.31939200
H	8.56268700	-5.13143400	0.73472800
C	-0.34969500	4.60742100	0.65112500
C	0.47333900	5.58036000	1.17608600
S	-1.87922500	5.32631800	0.16384200
C	-0.09595500	6.88046000	1.17761400
H	1.48071800	5.37507100	1.51987000
C	-1.37009700	6.93663400	0.65341400
H	0.43582600	7.75944500	1.52328100

C	-3.50538100	-4.75443300	-0.60195000
C	-3.42628100	-6.05321900	-1.05627000
S	-5.17553400	-4.36473200	-0.21282500
C	-4.67115900	-6.73494900	-1.07839600
H	-2.48918600	-6.52338000	-1.33201700
C	-5.73617400	-5.97536500	-0.64188500
H	-4.77166800	-7.77287100	-1.37414000
C	-7.14672100	-6.35157300	-0.52720100
C	-8.02720300	-5.67402800	0.33427200
C	-7.65897800	-7.43020500	-1.29026200
C	-9.37269200	-6.02984400	0.46305000
H	-7.65046000	-4.86147000	0.94885300
C	-8.98015400	-7.80620300	-1.15900100
H	-7.01391500	-7.95553300	-1.98779800
C	-9.85534500	-7.10264100	-0.28722900
H	-10.00683700	-5.49430000	1.15925000
C	-9.83600500	-8.82324500	-1.86617600
C	-10.93923500	-9.04380700	-0.83098500
C	10.13736800	-2.74866900	0.26005000
C	10.66666700	-1.67292300	-0.47401300
C	11.04012800	-3.58980500	0.95650500
C	12.03836500	-1.41226500	-0.53847500
H	9.99474800	-1.03206300	-1.03774700
C	12.39840400	-3.35586900	0.88821300
H	10.66117000	-4.41069800	1.55756100
C	12.91243700	-2.25598900	0.14812300
H	12.40150200	-0.58543700	-1.13697500
C	13.58579000	-3.98081400	1.57112400
C	14.71084100	-3.59679100	0.61022300
C	-2.24754600	8.09910400	0.50143100
C	-3.27822700	8.13283500	-0.45395200
C	-2.06520400	9.23631600	1.32676300
C	-4.11351000	9.24189100	-0.61683200
H	-3.41908900	7.28211700	-1.11457400
C	-2.86934800	10.34575600	1.16507900
H	-1.29898000	9.23015300	2.09588200
C	-3.90982000	10.35746500	0.19626000
H	-4.87808300	9.23201100	-1.38437000
C	-2.99334600	11.64439300	1.91614100
C	-3.63870500	12.53376100	0.85377900
N	-11.14673200	-7.68328500	-0.30587600
N	14.32588800	-2.23109000	0.21495800
N	-4.57939100	11.60509500	0.20367000
C	-11.95427500	-9.87571900	-1.60702500

C	-9.55001300	-10.24895400	-2.33291800
C	-11.00104500	-10.86007300	-2.38114600
C	-1.94662800	12.57935700	2.51787000
C	15.95844300	-3.98868000	1.39435100
C	13.93125300	-5.43175300	1.89926300
C	-4.00892300	13.77989400	1.65102700
C	-2.73377400	13.94280200	2.55970100
C	15.49998600	-5.35897300	2.01903000
C	-5.50945700	12.01721100	-0.77493500
C	-6.63390600	11.22346300	-1.06357700
C	-5.36941300	13.24193600	-1.44504900
C	-7.56728800	11.63706100	-2.00966800
H	-6.78329800	10.29167400	-0.52855100
C	-6.32350500	13.65017300	-2.37804200
H	-4.51083900	13.87488300	-1.25002800
C	-7.43697800	12.85992800	-2.68520000
H	-8.42522700	11.00150900	-2.21502600
H	-6.18896400	14.60306700	-2.88396200
C	-12.17568700	-7.36207100	0.60578900
C	-12.59196800	-6.02778500	0.76194400
C	-12.84047300	-8.35679800	1.33838500
C	-13.61976500	-5.70615100	1.64339400
H	-12.11987900	-5.24728000	0.17478200
C	-13.88130700	-8.01943400	2.20495400
H	-12.54141000	-9.39486000	1.24427800
C	-14.29022400	-6.69296600	2.38218400
H	-13.91786600	-4.66563700	1.74664700
H	-14.37776100	-8.81021500	2.76189000
C	15.15032900	-1.39552100	-0.56811200
C	14.94785900	-0.00324700	-0.57299400
C	16.21841600	-1.91508300	-1.31418200
C	15.77417500	0.82877400	-1.32170800
H	14.15468100	0.42478100	0.03061700
C	17.04912700	-1.06457000	-2.04594200
H	16.39978800	-2.98391300	-1.33446700
C	16.84482700	0.31918800	-2.07277500
H	15.59286000	1.90079300	-1.30790400
H	17.86923600	-1.49425300	-2.61580700
C	17.74957400	1.23753900	-2.85989200
H	17.17448700	1.90945400	-3.50638000
H	18.35179400	1.87078000	-2.19723100
H	18.43893600	0.67108600	-3.49192700
C	-8.47628900	13.31515600	-3.68229700
H	-8.80317800	12.49115400	-4.32473800

H	-9.37052900	13.70347100	-3.17896000
H	-8.09023800	14.11224500	-4.32379200
C	-15.42722000	-6.33453500	3.30969500
H	-15.18908600	-5.45242100	3.91309900
H	-16.34196800	-6.10227600	2.75032300
H	-15.66004600	-7.15760800	3.99104100
H	14.63944000	-4.25437400	-0.27596200
H	16.85933300	-4.09527100	0.78595800
H	16.16395800	-3.24979100	2.17603700
H	15.96415400	-6.19910300	1.49543700
H	15.81643600	-5.42315700	3.06354800
H	13.46407600	-5.79586800	2.81752500
H	13.63316200	-6.10030000	1.08464100
H	13.75656200	-3.39349600	2.49056000
H	-10.52301700	-9.67377400	-0.02307100
H	-10.31104700	-8.29474000	-2.71139300
H	-12.67502600	-10.40721700	-0.98158300
H	-12.51310700	-9.24134200	-2.30309300
H	-11.01388300	-11.85270000	-1.92292700
H	-11.34103100	-10.98341200	-3.41287100
H	-9.04898700	-10.29973900	-3.30269800
H	-8.92712700	-10.78180700	-1.60663700
H	-2.85555200	12.81123300	0.12412400
H	-3.76499300	11.48285600	2.68942900
H	-4.19535600	14.66698700	1.04149500
H	-4.90151200	13.59251200	2.25715300
H	-3.02806600	14.19368500	3.58232400
H	-2.10324800	14.76125900	2.20192900
H	-1.60161400	12.27183000	3.50803600
H	-1.06951100	12.65609000	1.86660100

CS-54: the first excited state

N	-0.72441200	-0.86155300	-0.02568100
C	-2.06837500	-1.29731800	-0.10807200
C	-3.09221300	-0.57534200	0.51290800
C	-2.39663400	-2.46180700	-0.81104300
C	-4.40456700	-1.00677000	0.42848600
H	-2.85257700	0.32070100	1.07371500
C	-3.71038700	-2.88640200	-0.89049300
H	-1.61474800	-3.02117500	-1.31171500
C	-4.74577800	-2.17226300	-0.27032000
H	-5.17528500	-0.43942100	0.94029900
H	-3.94235200	-3.77256900	-1.47096800
C	0.30387200	-1.78861900	0.18834500

C	1.55823400	-1.64359300	-0.44072200
C	0.11372300	-2.89903700	1.04158400
C	2.56474100	-2.55134600	-0.22958600
H	1.72244600	-0.80692300	-1.11037800
C	1.11512000	-3.81004800	1.25238100
H	-0.83780000	-3.02251700	1.54640900
C	2.39475300	-3.68238100	0.62674600
H	3.50894900	-2.40991100	-0.74545600
H	0.93062800	-4.63791500	1.92713400
C	-0.42997500	0.51429000	-0.17052800
C	0.53503700	1.12646500	0.63551500
C	-1.09299000	1.28716500	-1.13099000
C	0.82317100	2.47183400	0.48522500
H	1.04760300	0.54355000	1.39191900
C	-0.80068300	2.63123900	-1.27331500
H	-1.82860100	0.82283800	-1.77756100
C	0.16138900	3.25716600	-0.46788100
H	1.55658900	2.92663100	1.14335600
H	-1.30675300	3.20132600	-2.04468400
C	-6.12955000	-2.64219100	-0.36084700
C	-6.58435600	-3.90947600	-0.61000800
S	-7.47786500	-1.55368500	-0.16159900
C	-7.99988300	-4.01447500	-0.62868800
H	-5.92412200	-4.75775100	-0.74345100
C	-8.64282200	-2.82891600	-0.39333000
H	-8.52603500	-4.94925000	-0.77902100
C	0.44742400	4.68390700	-0.62935800
C	-0.36540700	5.66140700	-1.13770600
S	1.98456200	5.36664700	-0.16780700
C	0.22901000	6.95026500	-1.14615300
H	-1.38002900	5.47218200	-1.46647900
C	1.50299700	6.97248600	-0.64496000
H	-0.28629600	7.84124500	-1.48347900
C	3.42012700	-4.61945000	0.84721600
C	3.39598400	-5.79210300	1.64885500
S	5.01652800	-4.45693300	0.09776800
C	4.57177700	-6.50077800	1.65608600
H	2.51812800	-6.09714400	2.20360800
C	5.60595600	-5.94041500	0.86385700
H	4.70554500	-7.41577200	2.21893900
C	6.91952200	-6.41532200	0.66501500
C	7.84668700	-5.73017600	-0.17386100
C	7.37996700	-7.61311200	1.30424600
C	9.13476500	-6.17790300	-0.38726800

H	7.52770400	-4.82595500	-0.68178300
C	8.65011200	-8.06094500	1.09286700
H	6.71746600	-8.16705500	1.95947900
C	9.55423700	-7.35209100	0.24741500
H	9.79129700	-5.63520800	-1.05580500
C	9.44753200	-9.19563900	1.66570200
C	10.48668500	-9.41066900	0.57420900
C	-10.08505400	-2.56680300	-0.34270300
C	-10.61468200	-1.52625200	0.42408500
C	-10.97285200	-3.37874400	-1.07557000
C	-11.98399000	-1.27290800	0.49050400
H	-9.94635500	-0.90605500	1.01329100
C	-12.32717300	-3.15156700	-1.00656200
H	-10.58580000	-4.17519700	-1.70280700
C	-12.84510800	-2.08963000	-0.22893400
H	-12.35419100	-0.47067900	1.11619000
C	-13.50805100	-3.75648600	-1.70863500
C	-14.62373300	-3.41900100	-0.73233600
C	2.40891800	8.11775000	-0.50778300
C	3.41535700	8.14619800	0.46047400
C	2.27005000	9.22886100	-1.36275700
C	4.27551200	9.23336400	0.60880800
H	3.52113600	7.30860900	1.14293900
C	3.09881500	10.31597200	-1.21624200
H	1.51584600	9.22133800	-2.14289800
C	4.11681400	10.32425200	-0.23433500
H	5.02711700	9.22400200	1.38799300
C	3.26776500	11.59082800	-1.99025000
C	3.91215300	12.47959600	-0.93822000
N	10.76423900	-8.03676300	0.14176100
N	-14.25679100	-2.06915700	-0.29911600
N	4.82054300	11.54999600	-0.26359000
C	11.46372100	-10.36167400	1.24297300
C	9.07398100	-10.62427600	2.02711900
C	10.47377400	-11.32762300	1.97942600
C	2.25471800	12.53384100	-2.62073800
C	-15.86775500	-3.79670300	-1.51701500
C	-13.83935700	-5.19339700	-2.08087000
C	4.32007500	13.69784900	-1.74795100
C	3.06828200	13.87240800	-2.67293600
C	-15.40177600	-5.13304700	-2.18792000
C	5.70424600	11.96387200	0.75329200
C	6.80213300	11.16604800	1.09589000
C	5.54427700	13.18849700	1.40254900

C	7.68886000	11.57434300	2.07997400
H	6.96944400	10.23345700	0.56864800
C	6.45287400	13.59282100	2.37521800
H	4.70810300	13.83189600	1.15495200
C	7.53394100	12.79519000	2.74176500
H	8.53321500	10.93660100	2.32665200
H	6.30833000	14.55248200	2.86330200
C	11.85565000	-7.66766800	-0.65617400
C	12.32699500	-6.34831000	-0.65144000
C	12.52384500	-8.61390600	-1.43832300
C	13.41829000	-5.99241000	-1.42750700
H	11.85256100	-5.61123100	-0.01397800
C	13.62441400	-8.24131200	-2.19974200
H	12.17863700	-9.64081400	-1.46263600
C	14.08968000	-6.92743900	-2.21976200
H	13.76842300	-4.96427600	-1.40327100
H	14.12757100	-8.99431900	-2.79946700
C	-15.06736700	-1.30924900	0.56828300
C	-14.90104200	0.07823400	0.64702100
C	-16.08053900	-1.90116800	1.32322100
C	-15.70680800	0.83737700	1.48127000
H	-14.15083700	0.56165600	0.03122400
C	-16.89304800	-1.12365800	2.14198100
H	-16.23892700	-2.97232900	1.27846400
C	-16.71924700	0.25407800	2.24740400
H	-15.55745500	1.91272400	1.52370900
H	-17.67727400	-1.60791600	2.71687900
C	-17.58167200	1.08948900	3.15658500
H	-17.03345200	1.39392500	4.05442900
H	-17.91641900	2.00397200	2.65912800
H	-18.46636100	0.53795600	3.48215100
C	8.50010200	13.22265000	3.81506400
H	8.34666000	12.65241900	4.73731900
H	9.53664300	13.06090900	3.50623900
H	8.38063100	14.28071400	4.05800900
C	15.26358600	-6.52204300	-3.07075600
H	14.93523900	-6.00778700	-3.98044900
H	15.92603100	-5.83656400	-2.53531100
H	15.85031400	-7.39046300	-3.37822900
H	-14.53564000	-4.10662400	0.12811500
H	-16.76246500	-3.93177400	-0.90684800
H	-16.08452200	-3.03292800	-2.26963100
H	-15.85388100	-5.99480900	-1.69210700
H	-15.72346400	-5.16539300	-3.23108400

H	-13.37436100	-5.52336700	-3.01166800
H	-13.52896900	-5.88268200	-1.29001000
H	-13.68814400	-3.13772300	-2.60298700
H	10.00124300	-9.94289000	-0.26145900
H	9.99630500	-8.77829800	2.52546000
H	12.11999300	-10.89453600	0.55339600
H	12.09121800	-9.82117900	1.95745000
H	10.40518400	-12.28366100	1.45609300
H	10.83687900	-11.54414800	2.98623900
H	8.59804600	-10.71811200	3.00479200
H	8.39605300	-11.05167400	1.28254000
H	3.12243200	12.78544600	-0.22840800
H	4.04752800	11.39686800	-2.74485400
H	4.51994200	14.58981200	-1.15164500
H	5.21586800	13.47685800	-2.33575400
H	3.38092700	14.10021000	-3.69425900
H	2.45160300	14.70945700	-2.33832400
H	1.91664600	12.21751700	-3.60924400
H	1.37166700	12.63930600	-1.98359800

A1: ground state

N	-0.02622100	-0.03627800	-0.16999500
C	-0.65206600	1.23661200	-0.21677100
C	-1.78999300	1.45135200	-1.01269000
C	-0.14423500	2.31556800	0.52516600
C	-2.40042000	2.69897800	-1.05058500
H	-2.18626800	0.63884700	-1.61214100
C	-0.75132300	3.56500300	0.46940500
H	0.72726800	2.16915500	1.15423400
C	-1.90163500	3.78896700	-0.31105900
H	-3.26014400	2.83873400	-1.69841400
H	-0.33856800	4.37674300	1.05640800
C	1.39169000	-0.12996400	-0.15727000
C	2.04483900	-1.03908200	0.68992000
C	2.17374600	0.68827800	-0.98864100
C	3.43209800	-1.13511800	0.69551000
H	1.45890900	-1.67555600	1.34453300
C	3.56036800	0.59803300	-0.96595900
H	1.69068800	1.40251500	-1.64675400
C	4.22795700	-0.32104000	-0.13337700
H	3.90768500	-1.84496100	1.36137300
H	4.13484600	1.26286000	-1.60305200
C	-0.81403300	-1.21702900	-0.13601800
C	-0.43935100	-2.35286500	-0.87278300

C	-1.98271300	-1.28231700	0.63991200
C	-1.20808600	-3.50960900	-0.82820600
H	0.46320900	-2.32907100	-1.47381800
C	-2.75576500	-2.43781500	0.66599600
H	-2.28702000	-0.41992600	1.22325000
C	-2.39196400	-3.58277700	-0.06880100
H	-0.87400200	-4.37634400	-1.38938400
H	-3.65125000	-2.45713500	1.27518400
C	5.70208700	-0.43056300	-0.15515500
C	6.48475200	-0.80792400	0.97804500
C	6.44977500	-0.16519500	-1.29662200
C	7.91067900	-0.89404600	0.92676800
C	7.86164400	-0.24919400	-1.34726000
H	5.93274100	0.11008500	-2.21027600
C	8.65218800	-0.61875700	-0.26349800
H	8.34456900	0.00425200	-2.28535900
C	-2.57996700	5.10068200	-0.34470400
C	-1.89732700	6.34539100	-0.19232100
C	-3.95273400	5.22468100	-0.52707800
C	-2.58043600	7.60003800	-0.23009500
C	-4.62989300	6.46726700	-0.56098800
H	-4.55351800	4.32462900	-0.61108100
C	-3.99350800	7.69674700	-0.42045100
H	-5.70962700	6.44641500	-0.66743600
C	-3.21763000	-4.80882400	-0.06953500
C	-4.02105900	-5.22298200	1.03607800
C	-3.27460900	-5.66604000	-1.16257900
C	-4.79939600	-6.42167200	1.00829000
C	-4.04301900	-6.85413500	-1.18930700
H	-2.71229900	-5.41558500	-2.05641600
C	-4.83550400	-7.28525600	-0.12993300
H	-3.99203900	-7.46217600	-2.08661700
C	-4.72617600	8.97719800	-0.46441900
C	-5.89610100	9.10856800	-1.23580300
C	-4.29549500	10.10800100	0.26869900
C	-6.64074700	10.28745500	-1.27800800
H	-6.22195900	8.27574400	-1.85136700
C	-5.02360600	11.28273000	0.23758600
H	-3.38581800	10.05239700	0.85589700
C	-6.20988400	11.38492400	-0.51894400
H	-7.51389800	10.34723800	-1.91540500
C	-4.75623100	12.59333200	0.93433300
N	-6.74955400	12.66466900	-0.41681300
C	-5.84462800	13.55373600	0.35034100

C	-4.97156000	12.62192500	2.46943300
H	-3.75448200	12.97196100	0.70582300
C	-7.94398200	13.13446600	-0.98951300
C	-6.51047000	14.25090700	1.56514700
H	-5.39240900	14.28890100	-0.32569500
C	-5.52453800	14.03144700	2.72825000
H	-5.71680800	11.86921900	2.75356600
H	-4.05334700	12.40264700	3.02214000
C	-9.08489300	12.31758400	-1.09598900
C	-8.04357200	14.46576400	-1.43327300
H	-6.72767600	15.30643900	1.38146100
H	-7.46101000	13.75232000	1.78437300
H	-5.99968900	14.13547700	3.70857400
H	-4.71151700	14.76667800	2.67831000
C	-10.25978900	12.80951300	-1.66031100
H	-9.06332600	11.30627100	-0.70762700
C	-9.23130300	14.94540000	-1.98109900
H	-7.19044900	15.13023000	-1.35297300
C	-10.36148000	14.12907300	-2.12062500
H	-11.12423500	12.15311400	-1.72500600
H	-9.27480300	15.97979000	-2.31333700
C	-11.63137400	14.64507200	-2.75442800
H	-11.62748000	14.49069300	-3.84100700
H	-12.51272200	14.13117700	-2.35894400
H	-11.75753400	15.71812200	-2.58178500
C	10.12182600	-0.72100600	-0.35543400
C	10.73965700	-1.07012500	-1.57114200
C	10.96029900	-0.46731200	0.75581300
C	12.12463300	-1.14912000	-1.71572000
H	10.12119700	-1.32300800	-2.42680100
C	12.33501200	-0.54051200	0.62751200
H	10.52004400	-0.21844700	1.71471200
C	12.93488600	-0.86685000	-0.60688600
H	12.54837900	-1.45717700	-2.66332600
C	13.40862300	-0.31131100	1.66197400
N	14.32097800	-0.91174000	-0.48326200
C	14.72508700	-0.73895300	0.93251600
C	13.64962900	1.15592300	2.10054000
H	13.24966600	-0.92999400	2.55133900
C	15.25729100	-1.16647800	-1.50024500
C	15.74936800	0.40124600	1.17011400
H	15.09704900	-1.69193500	1.32723500
C	15.16551200	1.21300800	2.34217100
H	13.37452800	1.83626800	1.28554100

H	13.05532700	1.43169100	2.97655700
C	15.07881700	-0.67623400	-2.80723200
C	16.43253300	-1.88708300	-1.22129900
H	16.75803400	0.02907900	1.36823500
H	15.79982300	1.02661700	0.27223400
H	15.55767700	2.23382600	2.38417800
H	15.40977900	0.72887600	3.29609200
C	16.02462900	-0.93372900	-3.79681200
H	14.21410400	-0.06656100	-3.04154100
C	17.37529000	-2.12268400	-2.21994800
H	16.61171000	-2.26809600	-0.22192200
C	17.19046200	-1.66478700	-3.53096200
H	15.85860000	-0.53753700	-4.79572500
H	18.27356400	-2.68242600	-1.97099100
C	18.19778400	-1.95774900	-4.61733400
H	17.95132300	-2.88355900	-5.15268800
H	18.22845200	-1.15489400	-5.36026400
H	19.20450300	-2.08004600	-4.20691000
C	-5.64175600	-8.51991900	-0.19774500
C	-6.15216600	-8.97424600	-1.42844700
C	-5.92295400	-9.29399200	0.95294100
C	-6.88893400	-10.15241800	-1.54865300
H	-6.00047600	-8.37354600	-2.31986200
C	-6.65137100	-10.46467500	0.84933200
H	-5.56761300	-8.96320200	1.92220100
C	-7.13019800	-10.91659500	-0.39830300
H	-7.28926600	-10.43809500	-2.51323200
C	-7.06428000	-11.43620400	1.92687900
N	-7.85912700	-12.09361300	-0.24818200
C	-8.02408400	-12.42556200	1.18696900
C	-5.94780800	-12.32960200	2.52569700
H	-7.59422800	-10.93151600	2.74146700
C	-8.46564800	-12.85339800	-1.26326300
C	-7.56137700	-13.85526000	1.57012500
H	-9.06502200	-12.25470800	1.48627700
C	-6.66675700	-13.65737300	2.80861900
H	-5.15642000	-12.48261300	1.78196000
H	-5.48724600	-11.88269300	3.41157200
C	-7.85592800	-13.02606100	-2.52005800
C	-9.68883600	-13.50679900	-1.02938000
H	-8.39759500	-14.53577800	1.75112900
H	-6.97111900	-14.27154600	0.74658800
H	-5.98054300	-14.49424700	2.97096500
H	-7.28530700	-13.56099500	3.70978900

C	-8.47171100	-13.78972200	-3.50852600
H	-6.88359400	-12.58823400	-2.71290800
C	-10.28372100	-14.27918200	-2.02523200
H	-10.18083600	-13.41120400	-0.06774900
C	-9.69971800	-14.42929300	-3.28947100
H	-7.97222900	-13.90561600	-4.46743500
H	-11.22939800	-14.77125400	-1.81149600
C	-10.36946200	-15.23483300	-4.37721300
H	-10.97031500	-14.59532500	-5.03630200
H	-9.63439200	-15.74471900	-5.00776900
H	-11.04053400	-15.99070500	-3.95905500
N	8.34941600	-1.28057200	2.14949600
N	6.09096900	-1.13395500	2.23287300
N	7.23229000	-1.40327500	2.85244000
N	-4.19619500	-4.63873300	2.24603800
N	-5.03073300	-5.46199100	2.86662000
N	-5.43806200	-6.53190400	2.19854000
N	-0.57363300	6.59349700	-0.04247000
N	-1.65554400	8.58259600	-0.10294200
N	-0.51305900	7.91786500	-0.00115700
C	7.26226400	-1.73657900	4.27862900
H	8.14059600	-2.36601100	4.42804100
H	6.36621500	-2.32655900	4.47804100
C	0.75410300	8.61410500	0.23359200
H	0.67659800	9.57466200	-0.27790500
H	1.52866100	8.01708400	-0.25027600
C	-5.54960400	-5.15370600	4.20136800
H	-5.76882500	-6.11231900	4.67364300
H	-4.73756900	-4.66867900	4.74555600
C	7.31339000	-0.48726500	5.15698800
H	6.43453000	0.14068700	4.98939700
H	7.33235200	-0.78332200	6.20950100
H	8.21150200	0.09930600	4.94592700
C	1.03996300	8.79645500	1.72351200
H	1.99150800	9.32030600	1.84962500
H	0.25331900	9.38736700	2.20013900
H	1.10803400	7.82860400	2.22712700
C	-6.78992800	-4.26329500	4.14179300
H	-7.14002400	-4.05944200	5.15749900
H	-6.56075000	-3.31088600	3.65674200
H	-7.59531500	-4.75522000	3.58996700

A1: the first excited state

N	-0.00268700	0.02312200	-0.15728400
C	0.91989300	-1.03690400	-0.19155600
C	2.11919800	-0.92821400	-0.91947200
C	0.66766300	-2.23859200	0.49438900
C	3.02210600	-1.96703800	-0.94816200
H	2.32560800	-0.02261500	-1.47853100
C	1.56923600	-3.28072400	0.45492400
H	-0.24412100	-2.34213100	1.07194900
C	2.79258500	-3.18797900	-0.25902600
H	3.91122200	-1.84699700	-1.55420200
H	1.34545700	-4.18700000	0.99905400
C	-1.39036000	-0.24431600	-0.15696400
C	-2.25057100	0.46103200	0.69162000
C	-1.92626400	-1.22179700	-1.00344500
C	-3.61025500	0.20254700	0.68446100
H	-1.84799800	1.21619200	1.35718800
C	-3.28490400	-1.48222500	-0.99402500
H	-1.27166700	-1.77907900	-1.66357000
C	-4.16075900	-0.77263900	-0.15967900
H	-4.25581500	0.75884000	1.35225500
H	-3.67079300	-2.25986700	-1.64392300
C	0.44815800	1.36029200	-0.12322900
C	-0.20133800	2.34923500	-0.87170400
C	1.54892500	1.72258600	0.66157700
C	0.24283700	3.65828300	-0.83085000
H	-1.05930000	2.08825700	-1.48038600
C	1.99332700	3.03327800	0.68573000
H	2.05571000	0.97008500	1.25442800
C	1.35632700	4.03315800	-0.06338700
H	-0.29749000	4.40659300	-1.39944700
H	2.84428500	3.28756700	1.30401600
C	-5.61155900	-1.03762400	-0.19410000
C	-6.45755900	-0.91135200	0.94656600
C	-6.26350200	-1.43447100	-1.34692700
C	-7.84907800	-1.18163400	0.88776500
C	-7.64971200	-1.70317800	-1.40589700
H	-5.69417200	-1.53528200	-2.26475800
C	-8.49675300	-1.58745200	-0.31710200
H	-8.05814800	-2.02995000	-2.35599000
C	3.76268300	-4.26505900	-0.28667900
C	3.49454400	-5.60791700	0.13242700
C	5.08738700	-4.07645000	-0.73231700
C	4.47773900	-6.64695200	0.06804900
C	6.04177800	-5.08654800	-0.79383900

H	5.40654700	-3.07931300	-1.01050900
C	5.80580600	-6.42546400	-0.41966600
H	7.03648100	-4.80251200	-1.11432100
C	1.83729200	5.42841700	-0.06850500
C	2.53999200	6.02111400	1.02231500
C	1.64193800	6.27319300	-1.14512700
C	2.98091000	7.37002900	0.99315100
C	2.08100800	7.61632500	-1.17476600
H	1.14122100	5.89503100	-2.02950700
C	2.76275300	8.21991800	-0.13251900
H	1.84999200	8.19830900	-2.05993200
C	6.82960300	-7.45566400	-0.52010300
C	8.02860300	-7.23263000	-1.24487700
C	6.68723200	-8.73129100	0.08916800
C	9.03986000	-8.17204000	-1.34354800
H	8.15884200	-6.30255100	-1.78328200
C	7.68813000	-9.67035400	-0.00261300
H	5.77671100	-8.96081000	0.62536600
C	8.88136600	-9.40476100	-0.69944900
H	9.91754600	-7.95759300	-1.93910700
C	7.74843500	-11.05966500	0.57033300
N	9.72021900	-10.50480200	-0.67310900
C	9.05389700	-11.65552700	-0.03177000
C	7.93147700	-11.16330000	2.09866300
H	6.88258000	-11.65467100	0.26655900
C	11.01872500	-10.59714500	-1.18554500
C	9.84387000	-12.26472600	1.14460200
H	8.82644600	-12.40966900	-0.79211100
C	8.80964000	-12.40424200	2.26890800
H	8.46058600	-10.27802100	2.46765400
H	6.97780600	-11.22432400	2.62797000
C	11.90559700	-9.51236900	-1.13523700
C	11.47605300	-11.80560100	-1.72882800
H	10.32767000	-13.20866000	0.88567500
H	10.62825400	-11.56387700	1.44630500
H	9.27027600	-12.47514600	3.25739100
H	8.20994600	-13.30918900	2.11953100
C	13.18999700	-9.63261400	-1.64368100
H	11.59847500	-8.58476600	-0.66869100
C	12.76790600	-11.90969300	-2.22129100
H	10.81837200	-12.66577000	-1.77174200
C	13.64950400	-10.82710300	-2.20157700
H	13.85845600	-8.77821800	-1.58740400
H	13.09638500	-12.85793300	-2.63710100

C	15.03692000	-10.93880200	-2.77373000
H	15.04809800	-10.67889600	-3.83807600
H	15.73133100	-10.26370100	-2.26774900
H	15.42394000	-11.95670300	-2.68437500
C	-9.94268000	-1.85255100	-0.40810600
C	-10.64157300	-1.59014000	-1.59491900
C	-10.66752900	-2.38234200	0.67844400
C	-11.99853300	-1.84943100	-1.73555100
H	-10.11613600	-1.13679900	-2.42901100
C	-12.01138500	-2.64613100	0.55325400
H	-10.16272000	-2.57698300	1.61759800
C	-12.69035000	-2.39712500	-0.65244700
H	-12.50109800	-1.59763900	-2.66003900
C	-12.97479300	-3.21009900	1.56049000
N	-14.03521400	-2.71059500	-0.52713500
C	-14.36081900	-3.06638800	0.86621000
C	-12.83995200	-4.71381600	1.87359700
H	-12.95727800	-2.64336800	2.49563300
C	-15.01907600	-2.63013900	-1.52133600
C	-15.07035800	-4.42854200	1.02053400
H	-14.94528700	-2.26194600	1.32615000
C	-14.28398600	-5.15389600	2.12029600
H	-12.43354200	-5.23763700	1.00136500
H	-12.17223100	-4.90609500	2.71682200
C	-14.74408600	-2.96256000	-2.85388400
C	-16.32740600	-2.25683500	-1.19136100
H	-16.13354300	-4.32889300	1.24915800
H	-14.98657100	-4.97969500	0.07890500
H	-14.41692200	-6.23824400	2.08807400
H	-14.61312500	-4.81190300	3.10809500
C	-15.73734500	-2.88423200	-3.81939200
H	-13.75676800	-3.31161000	-3.13015600
C	-17.31262500	-2.19882900	-2.16702500
H	-16.57836200	-2.00845400	-0.16671600
C	-17.04002000	-2.49750200	-3.50215900
H	-15.49463100	-3.15064400	-4.84436300
H	-18.31913100	-1.90758200	-1.87999400
C	-18.10439100	-2.39416300	-4.56200900
H	-18.10978100	-1.40103200	-5.02451700
H	-17.94235100	-3.12219700	-5.36079500
H	-19.09986600	-2.56322300	-4.14452200
C	3.22637300	9.61706200	-0.19597200
C	3.54847800	10.20336400	-1.42858100
C	3.35629000	10.40968300	0.96244400

C	3.96030200	11.52466300	-1.54319900
H	3.51175000	9.59845200	-2.32819900
C	3.76360100	11.71987700	0.86429400
H	3.13961100	9.98212200	1.93395400
C	4.05511600	12.29738100	-0.38368000
H	4.22939300	11.92090900	-2.51317900
C	3.96503500	12.74331000	1.94700800
N	4.46943700	13.61209900	-0.22636300
C	4.61389700	13.94622000	1.20165800
C	2.68983500	13.31672400	2.59702400
H	4.63444000	12.37482300	2.72932600
C	4.80452100	14.52091200	-1.23844800
C	3.83256600	15.20380900	1.63901400
H	5.67629800	14.03302800	1.45471500
C	3.06857000	14.76839800	2.89617000
H	1.86309500	13.28651800	1.87878700
H	2.38219700	12.75202500	3.48033500
C	4.11586800	14.54760800	-2.45826300
C	5.81856800	15.46395700	-1.03369100
H	4.48044700	16.06633300	1.80917000
H	3.12588800	15.47415600	0.84843000
H	2.20612200	15.40568800	3.10721400
H	3.72771400	14.80773700	3.77086700
C	4.46032000	15.46232400	-3.44259200
H	3.28822900	13.86975000	-2.62589600
C	6.14053200	16.38146600	-2.02420100
H	6.36203400	15.48159200	-0.09620500
C	5.48070800	16.39529600	-3.25284500
H	3.90565300	15.46058700	-4.37684200
H	6.93124800	17.10208900	-1.83511000
C	5.86106800	17.36775400	-4.33738800
H	6.57738600	16.92276500	-5.03671500
H	4.98931100	17.67556600	-4.92051100
H	6.32610300	18.26485200	-3.92192100
N	-8.36517100	-0.96793500	2.11450300
N	-6.15816900	-0.54442900	2.20847300
N	-7.32154900	-0.59471600	2.82669800
N	2.89614600	5.49482800	2.21137700
N	3.50332600	6.49285000	2.82091200
N	3.59985100	7.62909500	2.16230000
N	2.35582200	-6.14911700	0.59485200
N	3.89978200	-7.78300500	0.49456700
N	2.65595300	-7.42629800	0.77924100
C	-7.43181700	-0.33570500	4.25869600

H	-8.43859100	0.04740400	4.42377900
H	-6.71153300	0.44953400	4.48828400
C	1.72141000	-8.34748600	1.39843800
H	1.94644600	-9.33683100	0.99802100
H	0.72530000	-8.05590900	1.06271000
C	4.12018100	6.31826100	4.13212900
H	4.09340600	7.29439300	4.61582200
H	3.48162300	5.63024500	4.68620700
C	-7.16952000	-1.59063200	5.07765400
H	-6.16284100	-1.97018900	4.89067600
H	-7.26050600	-1.35904900	6.14104000
H	-7.89226000	-2.37100800	4.82994200
C	1.81782400	-8.33187200	2.91828000
H	1.09970800	-9.03783000	3.34203000
H	2.82012700	-8.61941500	3.24359000
H	1.59617700	-7.33587400	3.30801300
C	5.54219900	5.79013400	4.01874200
H	5.96947900	5.67259600	5.01698000
H	5.55491300	4.81849100	3.52051300
H	6.16817800	6.48423600	3.45393900

B1: ground state

N	0.09521200	0.02444900	0.06549300
C	-1.06722600	0.84013800	0.04496500
C	-1.15127500	1.98926700	0.84733200
C	-2.15801000	0.51666800	-0.77811100
C	-2.28614300	2.79146700	0.81938600
H	-0.32157600	2.25368300	1.49398300
C	-3.29382900	1.31701600	-0.79563600
H	-2.11364200	-0.36667500	-1.40580300
C	-3.38520800	2.47609800	-0.00145300
H	-2.32614100	3.66895100	1.45342000
H	-4.11897300	1.03993300	-1.44026600
C	-0.03050000	-1.38917100	0.04529100
C	0.82576000	-2.17681000	-0.74147000
C	-1.01870700	-2.03262700	0.80771600
C	0.70191900	-3.56056000	-0.75601500
H	1.58482500	-1.69928400	-1.35147700
C	-1.15025700	-3.41577600	0.77516300
H	-1.68194500	-1.44393500	1.43219900
C	-0.29131000	-4.21550000	-0.00230300
H	1.37017600	-4.13825000	-1.38268500
H	-1.92191400	-3.88464000	1.37373700
C	1.38171500	0.62442400	0.07667400

C	2.41409600	0.09549300	0.86852200
C	1.65303800	1.75853600	-0.70541400
C	3.67505800	0.67928200	0.87176200
H	2.22590100	-0.77909700	1.48174700
C	2.91305600	2.34495200	-0.69054400
H	0.87151400	2.18050800	-1.32790800
C	3.95653700	1.82022500	0.09538400
H	4.45045600	0.24407900	1.49010000
H	3.09520800	3.21424100	-1.31050900
C	-0.43896200	-5.68511700	-0.02619200
C	-1.69664000	-6.35863300	0.06800600
C	0.62348800	-6.56332700	-0.14208300
C	-1.82112000	-7.78052700	0.03911400
C	0.49993500	-7.97696200	-0.16778100
C	-0.70017300	-8.66171700	-0.08425700
C	-4.58901700	3.33351700	-0.02128500
C	-5.10348100	4.01025500	1.12789300
C	-5.33717100	3.57802500	-1.15833900
C	-6.26718600	4.83650100	1.08730400
C	-6.49232500	4.40160800	-1.19945500
C	-7.01646700	5.07334100	-0.10859200
C	5.29649200	2.44425900	0.09105900
C	5.88327500	3.05969400	-1.05849000
C	6.12071100	2.50495900	1.20011100
C	7.18013500	3.65689700	-1.04429400
C	7.41035400	3.09780100	1.21411800
C	8.00830400	3.70307800	0.12219800
C	-8.21903000	5.92586500	-0.17075500
C	-8.50238300	6.71160000	-1.30380900
C	-9.12010400	5.98782700	0.91846000
C	-9.63201800	7.52497600	-1.38375600
H	-7.81351500	6.70540900	-2.13992700
C	-10.24697100	6.78442500	0.84867000
H	-8.92193600	5.41063900	1.81450200
C	-10.52461000	7.55192500	-0.30265600
H	-9.78751400	8.13775000	-2.26258400
C	-11.33647100	6.99801000	1.87001100
N	-11.68973600	8.29122700	-0.13095600
C	-12.20688600	8.14120500	1.25031000
C	-12.31823000	5.81951800	2.09566900
H	-10.92630000	7.31395700	2.83481600
C	-12.30727700	9.13793200	-1.06934300
C	-13.68010400	7.66473800	1.33273900
H	-12.06492800	9.07933500	1.79934600

C	-13.66128100	6.51740500	2.36012100
H	-12.38445600	5.21326900	1.18419600
H	-11.99869200	5.16111500	2.90867800
C	-12.34240400	8.82042100	-2.43961400
C	-12.95453000	10.31283300	-0.64741600
H	-14.37034700	8.46884500	1.60116100
H	-13.98541200	7.28219200	0.35275400
H	-14.52188700	5.84872100	2.26111600
H	-13.67664800	6.92259900	3.37972900
C	-12.96870600	9.67031700	-3.34828500
H	-11.90690200	7.89222300	-2.79037500
C	-13.58967800	11.14370000	-1.56817900
H	-12.96138200	10.58186200	0.40310000
C	-13.60174900	10.85154800	-2.93824200
H	-12.98118700	9.39496000	-4.40009000
H	-14.08219900	12.04411000	-1.20927700
C	-14.25721600	11.77721500	-3.93527400
H	-13.53961600	12.50275900	-4.33908900
H	-14.66712100	11.22314100	-4.78529000
H	-15.07043500	12.34747100	-3.47674500
C	-0.81248000	-10.13222700	-0.11573900
C	0.05249800	-10.91898100	-0.89963000
C	-1.81175300	-10.79624300	0.63454400
C	-0.04282600	-12.30931800	-0.94866200
C	-1.91257000	-12.17359200	0.59915600
H	-2.50661400	-10.21948800	1.23429500
C	-1.02756100	-12.94774800	-0.18132400
C	-2.88091300	-13.08438700	1.31100900
N	-1.34232700	-14.29902800	-0.08463000
C	-2.59303300	-14.49044000	0.68888100
C	-2.66917000	-13.26845900	2.83517900
H	-3.91998500	-12.79295600	1.12587800
C	-0.66939500	-15.37442900	-0.69238700
C	-2.46501800	-15.47891700	1.87709700
H	-3.40106900	-14.78930400	0.01070800
C	-3.07580700	-14.72991800	3.07732100
H	-1.60977600	-13.12870300	3.08196100
H	-3.24453300	-12.54930200	3.42539300
C	0.73320800	-15.39632700	-0.80486700
C	-1.38698200	-16.48788200	-1.16300100
H	-2.94920900	-16.43933900	1.68135400
H	-1.40400100	-15.67767700	2.06265600
H	-2.72895100	-15.12112900	4.03867200
H	-4.16927300	-14.81975300	3.06203100

C	1.37947200	-16.47570900	-1.40193900
H	1.31988400	-14.58179800	-0.39648100
C	-0.72275100	-17.56643900	-1.74440500
H	-2.46769900	-16.51320800	-1.07773400
C	0.67014500	-17.58210900	-1.88993000
H	2.46456700	-16.46383500	-1.47076600
H	-1.30636600	-18.41282700	-2.09797600
C	1.38032600	-18.73638100	-2.55614700
H	1.57437400	-18.52831500	-3.61600900
H	2.34849800	-18.93577100	-2.08605700
H	0.78458400	-19.65250800	-2.50890100
C	9.35131900	4.31313000	0.15168700
C	9.83448000	4.97255100	1.29795600
C	10.19192400	4.26513200	-0.98582100
C	11.09818400	5.56036400	1.34351300
H	9.20111500	5.04953000	2.17339700
C	11.44809400	4.83891400	-0.95121900
H	9.84450800	3.78197900	-1.89179600
C	11.92206500	5.48290800	0.21150700
H	11.41132800	6.08631600	2.23652000
C	12.50309100	4.90445900	-2.02676400
N	13.19166100	6.00904900	-0.00220800
C	13.59141500	5.85107400	-1.42140600
C	13.25089200	3.58512300	-2.34804200
H	12.10616400	5.32714900	-2.95559400
C	13.99641800	6.69206600	0.92774200
C	14.95483700	5.14082900	-1.62624500
H	13.57672500	6.82869000	-1.91738200
C	14.67488500	4.05419300	-2.68214300
H	13.26718700	2.94222400	-1.45971400
H	12.77366100	3.02212700	-3.15541700
C	14.05197500	6.30294300	2.27896500
C	14.81048600	7.76111500	0.51455400
H	15.74995200	5.82987700	-1.92300600
H	15.25872600	4.67473400	-0.68273800
H	15.41206200	3.24574800	-2.66005500
H	14.69700400	4.49077600	-3.68856300
C	14.86223200	6.98766900	3.18112300
H	13.48366400	5.44424100	2.61676900
C	15.62678800	8.42576800	1.42799900
H	14.80657000	8.07824300	-0.52246500
C	15.66375800	8.06604200	2.78108600
H	14.88488000	6.66033700	4.21777400
H	16.24467100	9.24845000	1.07674700

C	16.52094400	8.81554900	3.77303700
H	15.94204500	9.58317700	4.30209300
H	16.93346900	8.14448200	4.53301700
H	17.35483400	9.32164900	3.27816000
N	-3.13811100	-8.08569900	0.09647400
N	-2.93969900	-5.83033200	0.14311400
N	5.37355700	3.19459300	-2.30413500
N	7.42542300	4.15145800	-2.27959300
N	-4.63456600	4.00831700	2.39658800
N	-6.47464400	5.32688600	2.33112600
F	-4.98905400	3.02760400	-2.34268600
F	-7.08277600	4.48917800	-2.41310500
F	8.05319200	3.02569300	2.40194900
F	5.72271300	1.98527900	2.38272300
N	6.32676700	3.84707200	-2.95621100
N	-5.48160100	4.80358800	3.03691400
N	-3.72606500	-6.89871200	0.15283400
C	6.20625000	4.14191800	-4.38638800
H	6.76956800	5.06016400	-4.55860500
H	5.14886400	4.33547700	-4.57304700
C	6.72576000	2.99618700	-5.25344200
H	6.61622400	3.26156100	-6.30857400
H	7.78322500	2.80536100	-5.05239400
H	6.16000800	2.07975100	-5.06637200
C	-5.17798400	-6.77415500	0.30484400
H	-5.46131400	-5.84846300	-0.19825900
H	-5.61632400	-7.61690300	-0.23173500
C	-5.60215400	-6.76485800	1.77263800
H	-5.15179600	-5.92120900	2.30220500
H	-6.68988600	-6.67207500	1.83532300
H	-5.30459800	-7.69239900	2.26875800
C	-5.37469800	5.02350900	4.48160400
H	-5.79693000	6.01112600	4.67206700
H	-4.30867900	5.04380100	4.71360700
C	-6.09875500	3.94114900	5.28076900
H	-5.99371800	4.14808800	6.34934000
H	-7.16375800	3.92315500	5.03459200
H	-5.67233800	2.95584300	5.07534900
F	1.89285400	-6.10337500	-0.20680400
F	1.67212700	-8.64642000	-0.25264500
H	0.80859200	-10.43456800	-1.50582500
H	0.62299200	-12.86796400	-1.59416000

B1: the first excited state

N	-0.08331800	0.07463700	0.07045500
C	0.55888600	-1.18685300	0.03171200
C	0.08030900	-2.25210300	0.79939400
C	1.68258300	-1.38959000	-0.77461300
C	0.70635200	-3.48630100	0.75543300
H	-0.78636300	-2.10863000	1.43433900
C	2.30866600	-2.62359900	-0.80889100
H	2.06339700	-0.57364300	-1.37781100
C	1.83380000	-3.70004600	-0.04775300
H	0.32334900	-4.29413300	1.36581200
H	3.17652600	-2.75422700	-1.44230400
C	0.67252100	1.25446900	0.11205200
C	0.24002600	2.41768400	-0.55139400
C	1.88947100	1.31517900	0.81359300
C	0.97523900	3.57757300	-0.50766500
H	-0.67972600	2.39228800	-1.12469100
C	2.63298800	2.47136600	0.85082200
H	2.24006400	0.43929900	1.34777100
C	2.21167300	3.66488700	0.19766100
H	0.61388300	4.43178900	-1.05970200
H	3.55764900	2.47798500	1.40915200
C	-1.49874400	0.13217700	0.06983000
C	-2.17555100	1.02503000	0.90541800
C	-2.24326000	-0.70302600	-0.76730500
C	-3.55870300	1.07975800	0.90065500
H	-1.61114000	1.67703100	1.56193700
C	-3.62678900	-0.64939900	-0.76216800
H	-1.73196500	-1.39616700	-1.42539200
C	-4.31539800	0.24223600	0.07021000
H	-4.05832000	1.77991100	1.55759700
H	-4.18246600	-1.29961400	-1.42568000
C	2.99894400	4.86071900	0.24130200
C	4.37905500	4.92240300	0.65528400
C	2.51876800	6.15129100	-0.13022600
C	5.16768300	6.11478500	0.60183200
C	3.27352300	7.29429000	-0.18262200
C	4.66608900	7.38070200	0.12260600
C	2.49619500	-5.01902100	-0.08245100
C	2.59065400	-5.88728700	1.04672800
C	3.07887600	-5.54791200	-1.20520200
C	3.22795700	-7.15238200	0.99363800
C	3.71735900	-6.81503300	-1.25779600
C	3.82340200	-7.67508400	-0.19471200
C	-5.79089200	0.29365400	0.06337800

C	-6.58508800	0.07555400	-1.10255300
C	-6.54826300	0.54597200	1.17816800
C	-8.00171200	0.12640900	-1.08948400
C	-7.96707400	0.59721600	1.19066600
C	-8.76061800	0.39034800	0.09124300
C	4.48896600	-8.98934700	-0.26726000
C	4.41538100	-9.77689600	-1.42128100
C	5.20906600	-9.49123800	0.83318500
C	5.03402900	-11.01904300	-1.51250900
H	3.84646100	-9.42061700	-2.27098800
C	5.82870900	-10.71755500	0.75372800
H	5.26743000	-8.91405400	1.74840800
C	5.75997200	-11.48863900	-0.41817800
H	4.92404700	-11.60670000	-2.41418500
C	6.64957700	-11.44652600	1.78163600
N	6.43507900	-12.68899200	-0.25030900
C	6.86740600	-12.85199100	1.14947300
C	8.06907100	-10.90203000	2.03597700
H	6.12025000	-11.53463100	2.73455500
C	6.60396100	-13.70379900	-1.20364800
C	8.36796500	-13.17733200	1.31331600
H	6.24193500	-13.60333800	1.64449900
C	8.87823200	-12.16255800	2.34555300
H	8.45082000	-10.42731300	1.12526000
H	8.09411600	-10.15630000	2.83427200
C	6.84363200	-13.40872300	-2.55113100
C	6.58683300	-15.04799400	-0.81614400
H	8.54629600	-14.21338900	1.60917000
H	8.87107200	-13.01856400	0.35469800
H	9.95868600	-12.00842000	2.28686100
H	8.65084800	-12.50938800	3.36001800
C	7.01761900	-14.42822900	-3.47641300
H	6.92321000	-12.37708500	-2.87117000
C	6.77886800	-16.05556300	-1.75203500
H	6.42186500	-15.31124100	0.22217100
C	6.98476100	-15.77176200	-3.10164800
H	7.20372400	-14.16844500	-4.51485200
H	6.76227000	-17.09012900	-1.42079000
C	7.15248900	-16.87070600	-4.11747200
H	6.19161900	-17.14872000	-4.56428100
H	7.81112400	-16.56185400	-4.93309800
H	7.57251100	-17.77164200	-3.66388000
C	5.45363800	8.56228400	-0.03893600
C	5.01045900	9.67635300	-0.82069500

C	6.75275800	8.67809600	0.55094900
C	5.75778400	10.81812000	-0.98766100
C	7.49461800	9.81424500	0.39237600
H	7.14714100	7.85178300	1.12528800
C	7.01233600	10.91065600	-0.35838700
C	8.85736800	10.15016300	0.93080800
N	7.93783200	11.91974600	-0.39818200
C	9.20039100	11.50679100	0.25115600
C	8.94626000	10.42919300	2.44526100
H	9.59329500	9.38942400	0.65669200
C	7.77980300	13.19558700	-0.96135600
C	9.67182000	12.45512700	1.37263300
H	9.97065900	11.37984800	-0.51583200
C	10.01081400	11.52329000	2.54322300
H	7.98517700	10.80990600	2.80744300
H	9.18480400	9.53115600	3.01953600
C	6.55624100	13.87416500	-0.89788800
C	8.86935100	13.83568000	-1.56252800
H	10.50893000	13.08623800	1.06794300
H	8.84535700	13.11610600	1.65114200
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H	9.83103500	13.33890100	-1.61482300
C	7.50279700	15.77801300	-2.07360400
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H	9.58426700	15.57952300	-2.56754500
C	7.34357400	17.13932500	-2.69507400
H	6.95052200	17.06400200	-3.71483300
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H	8.29915900	17.66544000	-2.75160400
C	-10.23420300	0.44655400	0.12140700
C	-10.95555000	-0.00719600	1.23101700
C	-10.95543400	0.94959900	-0.97771400
C	-12.34476400	0.03471000	1.28044500
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H	-10.42635800	1.28954100	-1.86016600
C	-13.03925900	0.55641700	0.18930200
H	-12.86132500	-0.35613800	2.14695700
C	-13.30172300	1.49561900	-1.97451800
N	-14.40581300	0.68123600	-0.01573900

C	-14.68931500	1.07872900	-1.40652000
C	-13.39012700	3.02399000	-2.15505600
H	-13.13116600	1.02623500	-2.94745900
C	-15.42877700	0.36010400	0.88847200
C	-15.60431700	2.31584600	-1.53582400
H	-15.09607900	0.22458300	-1.95950900
C	-14.86279800	3.25188800	-2.49989300
H	-13.14613500	3.52182200	-1.20999300
H	-12.69798600	3.39607400	-2.91433300
C	-15.30426100	0.62593000	2.25774900
C	-16.62976100	-0.19198200	0.43090300
H	-16.61128400	2.06377000	-1.87531500
H	-15.69795600	2.79061200	-0.55439400
H	-15.17457200	4.29454700	-2.39877900
H	-15.05139200	2.95190400	-3.53699700
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H	-14.41081000	1.10889700	2.63397700
C	-17.65520400	-0.48807600	1.31947900
H	-16.76675500	-0.39360000	-0.62509400
C	-17.52697400	-0.25785500	2.68844100
H	-16.20751100	0.52904500	4.19078600
H	-18.57706100	-0.91471800	0.93422900
C	-18.62722000	-0.61696700	3.65187400
H	-18.45901700	-1.60365700	4.09712800
H	-18.68792600	0.10154200	4.47339300
H	-19.59890200	-0.64588000	3.15332100
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N	5.16617000	3.93077700	1.08720800
N	-6.19140600	-0.20040400	-2.35937900
N	-8.43620800	-0.12841700	-2.33790100
N	2.13423300	-5.70480700	2.29936800
N	3.13683000	-7.71294300	2.21419400
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F	4.23591400	-7.13091200	-2.45804800
F	-8.50607800	0.87722400	2.39077100
F	-5.96930600	0.76350100	2.37152600
N	-7.32546500	-0.31207100	-3.01859000
N	2.48413000	-6.81304100	2.91783100
N	6.35026900	4.50501700	1.26851900
C	-7.34614800	-0.54213800	-4.46003300
H	-8.26381100	-1.09111600	-4.67007600
H	-6.49221000	-1.18169100	-4.68275600
C	-7.28429500	0.76383200	-5.23751800
H	-7.30180000	0.55226500	-6.30873300

H	-8.13965100	1.39851300	-4.99613600
H	-6.36587300	1.30785100	-5.00715900
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C	7.43692300	3.87470700	3.39603000
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H	8.28860300	3.33026600	3.81058700
H	7.49449900	4.91330400	3.72961700
C	2.23622900	-6.99637900	4.34475100
H	2.12432500	-8.06901900	4.50103500
H	1.28646700	-6.50644600	4.55884700
C	3.36417300	-6.42173800	5.18817600
H	3.14400300	-6.57608300	6.24660400
H	4.31056000	-6.91490600	4.95607500
H	3.47256700	-5.34984000	5.00990400
F	1.20164700	6.32641600	-0.38333100
F	2.58407400	8.41951900	-0.47673200
H	4.06352100	9.61304500	-1.33440300
H	5.38905100	11.61230800	-1.62353100

C1: ground state

N	0.05527100	-0.00241300	-0.21228200
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C	2.12633800	-0.98411700	0.66898500
C	2.25462800	0.88019000	-0.85757400
C	3.51412400	-1.01606700	0.74564400
H	1.54063700	-1.69943300	1.23611700
C	3.64115000	0.85105700	-0.76484500
H	1.77158100	1.62276800	-1.48337500
C	4.30829500	-0.09870100	0.03215300
H	3.98893500	-1.75798500	1.37571600
H	4.21645500	1.58949000	-1.31444700
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C	-2.42790300	2.66148100	-0.99690500
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C	-0.86544300	3.51374600	0.62050900
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H	-3.27732900	2.79976100	-1.65869200
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H	0.64423600	-2.16003900	-1.68453100
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H	-4.67398700	4.09911600	-0.36582300
C	-4.33969600	7.49386200	-0.11781100
H	-5.97289900	6.14131000	-0.32446300
C	5.78650900	-0.12943100	0.07852200
C	6.52837300	-0.45156100	1.26911200
C	6.55794600	0.16941200	-1.02931400
C	7.98842500	-0.44731300	1.27573200
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H	6.06068900	0.40235600	-1.96556200
C	8.74295400	-0.12065200	0.09126600
H	8.48053900	0.45920900	-1.94220300
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C	10.89250100	-0.51576100	-1.12193200
C	11.00402100	0.29928700	1.14845100
C	12.28251300	-0.49283800	-1.23350100
H	10.31685200	-0.89010600	-1.96295400
C	12.38224600	0.33025400	1.05161300
H	10.52138200	0.59707100	2.07194700
C	13.03839600	-0.05023100	-0.13851600
H	12.75388600	-0.84502800	-2.14232500
C	13.40654400	0.73896600	2.08018500
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C	15.39946500	-0.22923200	-0.95916500
C	15.69889900	1.58855200	1.57913400
H	15.20254400	-0.52907900	1.89914300
C	15.01838500	2.45096200	2.65952300
H	13.21947100	2.83427700	1.50568600
H	12.87842200	2.55965500	3.21856800
C	15.21386000	0.12553000	-2.30807800
C	16.62399200	-0.81665800	-0.59392000
H	16.72536100	1.31393700	1.83619700
H	15.73294000	2.13655900	0.63133700
H	15.33086600	3.49900400	2.62076500
H	15.26758000	2.07087800	3.65814400
C	16.20315800	-0.13690500	-3.25288800
H	14.30760700	0.63596000	-2.61218800
C	17.60870000	-1.05804400	-1.54969600
H	16.80938300	-1.08926400	0.43913800
C	17.41920900	-0.73774900	-2.90035100
H	16.03015600	0.15251400	-4.28661100
H	18.54464800	-1.51266800	-1.23434500
C	18.47506600	-1.03996800	-3.93690900
H	18.33091800	-2.03535300	-4.37610500
H	18.44607000	-0.31803700	-4.75868200
H	19.47909500	-1.02099500	-3.50273300
C	-5.16830400	8.71507800	-0.10006600
C	-6.33382300	8.79162100	-0.88536600
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H	-3.94958600	9.81377800	1.31651000
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H	-8.03947900	9.92955700	-1.52675500
C	-5.53681700	12.21952100	1.51565300
N	-7.49527500	12.20822100	0.11778600
C	-6.67305200	13.12747500	0.94123600
C	-5.81688000	12.13973300	3.03808700
H	-4.55966300	12.68666500	1.35482900
C	-8.70626800	12.61532700	-0.46957700
C	-7.41568100	13.72944400	2.16262300
H	-6.25659400	13.91662600	0.30403300
C	-6.46526400	13.49614300	3.35310400

H	-6.52551200	11.32822300	3.24333000
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C	-11.16187400	13.47748800	-1.62458800
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H	-12.62732300	14.99305000	-2.11472000
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C	-4.99802100	-9.53050200	1.05948200
C	-5.92141200	-9.25292700	-1.15457200
C	-5.69550300	-10.72496800	1.23696900
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C	-6.62173000	-10.43331500	-0.99179100
H	-6.00754700	-8.69819100	-2.08158600
C	-6.53013500	-11.17647000	0.20454200
H	-5.55770300	-11.29692200	2.14589100
C	-7.55372100	-11.13447400	-1.94831900
N	-7.29296300	-12.33673700	0.12175000
C	-7.85654500	-12.49678200	-1.24008900
C	-8.94085000	-10.48062900	-2.17512800
H	-7.07664600	-11.30917700	-2.91825400
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H	-10.93729400	-11.42582300	-2.23929500

H	-9.75035500	-12.11524000	-3.35064500
C	-7.79410900	-13.92600000	3.45473900
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C	-7.79798000	-15.62779400	1.77303600
H	-7.51727600	-14.97622800	-0.24987400
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H	-7.88955000	-13.61749900	4.49301800
H	-7.88198700	-16.67090600	1.47806700
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H	-8.59790800	-17.21562100	3.80606500
N	-2.14654000	8.61624500	0.09996000
N	-0.80123800	6.49633200	0.07033500
N	-2.57189200	-5.47670500	-2.74079000
N	-3.82843000	-7.64826800	-2.63907600
N	5.99770100	-0.76868500	2.45708700
N	8.50820500	-0.78116900	2.46364100
S	-3.02329400	-6.71357800	-3.72345800
S	7.24923200	-1.05491600	3.48211200
S	-0.58202300	8.12153200	0.17079000

C1: the first excited state

N	-0.03066600	-0.16355700	0.02444400
C	-1.39637200	-0.54859800	0.07352400
C	-2.28841200	0.12227600	0.91273500
C	-1.87221300	-1.59312600	-0.72151300
C	-3.62513400	-0.23982400	0.95177100
H	-1.92926900	0.93401300	1.53513100
C	-3.20772100	-1.95790900	-0.66768000
H	-1.19127300	-2.12258200	-1.37802900
C	-4.11391400	-1.28706000	0.16167400
H	-4.29864700	0.29344100	1.61049100
H	-3.55166900	-2.78549400	-1.27866900
C	0.98485200	-1.12563200	0.03567000
C	2.19960900	-0.90182400	-0.63684900
C	0.82425900	-2.34601900	0.71148700
C	3.19938600	-1.84630300	-0.61806200
H	2.34146900	0.01662400	-1.19384500
C	1.82383600	-3.29506900	0.71583200
H	-0.09509800	-2.53948700	1.25161500
C	3.06112600	-3.08423600	0.05989500
H	4.09630700	-1.63980500	-1.18852000
H	1.67021500	-4.22057800	1.25112600

C	0.28522500	1.21952200	-0.03617400
C	1.29031500	1.75691800	0.77024900
C	-0.41312000	2.06567100	-0.90014300
C	1.59129800	3.10765700	0.70239600
H	1.83934700	1.11159600	1.44642600
C	-0.11526600	3.41771800	-0.95325200
H	-1.19482900	1.65814600	-1.53114000
C	0.89306600	3.96783600	-0.15286300
H	2.39004500	3.50034500	1.32226700
H	-0.66783100	4.05523800	-1.63158100
C	4.13879400	-4.04814100	0.07361500
C	3.97455700	-5.43227700	0.42097600
C	5.46391900	-3.65537900	-0.26746000
C	5.10333000	-6.35764500	0.38237500
C	6.52283900	-4.52118400	-0.30648300
H	5.66575500	-2.60945000	-0.45896600
C	6.41518200	-5.91293700	-0.00653400
H	7.49814700	-4.10599600	-0.52310900
C	-5.54385700	-1.66393800	0.15994800
C	-6.34309300	-1.67712800	1.35379700
C	-6.19423900	-2.03425300	-0.98719900
C	-7.73787500	-2.06291000	1.31566000
C	-7.56374800	-2.41972400	-1.02382700
H	-5.64961600	-2.02808100	-1.92537200
C	-8.37278600	-2.44542900	0.08254000
H	-7.97631900	-2.71759800	-1.98155100
C	1.20295300	5.41374200	-0.16862000
C	1.20253700	6.19261300	-1.37592500
C	1.52170900	6.09935000	0.97346900
C	1.52526300	7.60367900	-1.35549800
C	1.84539500	7.48514800	0.99281600
H	1.52223600	5.57088900	1.92087100
C	1.85696000	8.27545800	-0.12719800
H	2.10692100	7.92670700	1.94822000
C	-9.79827600	-2.82189100	0.00174200
C	-10.56040800	-2.44196800	-1.10709600
C	-10.42582100	-3.58415700	1.00452700
C	-11.89547500	-2.80481800	-1.25603200
H	-10.10831600	-1.81542700	-1.86911600
C	-11.74543600	-3.95258400	0.86937300
H	-9.86905800	-3.87973700	1.88587300
C	-12.48980700	-3.58168200	-0.26263300
H	-12.45381900	-2.45782900	-2.11528700
C	-12.61414900	-4.76332800	1.79112700

N	-13.79451600	-4.04612700	-0.15922700
C	-14.03602500	-4.62271600	1.17557600
C	-12.34664300	-6.28097400	1.82552300
H	-12.59951900	-4.37098100	2.81181700
C	-14.82569800	-3.87995400	-1.09452800
C	-14.64427500	-6.04185500	1.14924700
H	-14.65169000	-3.93694200	1.76871400
C	-13.73550400	-6.87598900	2.06300500
H	-11.95966800	-6.60969300	0.85452000
H	-11.61321100	-6.55915600	2.58624400
C	-14.58430800	-3.96283300	-2.47166400
C	-16.14240800	-3.67613300	-0.66819800
H	-15.69115700	-6.05887800	1.45998500
H	-14.59987000	-6.42682500	0.12604600
H	-13.79023700	-7.94634400	1.84866100
H	-14.02391800	-6.73612900	3.11101500
C	-15.62080400	-3.80576800	-3.38052300
H	-13.58631700	-4.18044700	-2.83172300
C	-17.17079300	-3.53663300	-1.59108900
H	-16.36829200	-3.62510000	0.39049100
C	-16.93419800	-3.58438800	-2.96404600
H	-15.40280300	-3.87716500	-4.44257700
H	-18.18332100	-3.38136800	-1.22918500
C	-18.04738000	-3.39352400	-3.96012100
H	-18.10892900	-2.35151300	-4.29263200
H	-17.89464100	-4.00807600	-4.85104400
H	-19.01642900	-3.65538000	-3.52883300
C	7.56642000	-6.77044500	-0.09234800
C	8.73908200	-6.34218300	-0.78253000
C	7.61042800	-8.07274300	0.48964900
C	9.87786300	-7.10615500	-0.87977400
H	8.73319500	-5.39227800	-1.30083400
C	8.74019000	-8.83725500	0.40624900
H	6.73307700	-8.44549400	0.99854800
C	9.89538100	-8.36939600	-0.26164500
H	10.72585500	-6.74692000	-1.44784600
C	9.01497800	-10.20874000	0.95899100
N	10.88547700	-9.30772000	-0.23901900
C	10.42069800	-10.56122800	0.39216800
C	9.16304900	-10.31258000	2.49163000
H	8.27191000	-10.93258200	0.61399500
C	12.20071900	-9.16379400	-0.72205300
C	11.27754500	-11.01672900	1.58995700
H	10.35498100	-11.34218700	-0.37107800

C	10.25323700	-11.37074400	2.67479700
H	9.50319100	-9.35297900	2.89563600
H	8.22046700	-10.56354100	2.98298700
C	12.90961200	-7.97145100	-0.54897400
C	12.83626900	-10.24023900	-1.34729300
H	11.94668800	-11.84256100	1.34054000
H	11.89734600	-10.17860600	1.92352200
H	10.68679400	-11.37376700	3.67775800
H	9.83952200	-12.36878400	2.49189900
C	14.20776000	-7.85589800	-1.02494300
H	12.45576000	-7.14476400	-0.01572500
C	14.13883700	-10.11149600	-1.80621100
H	12.31048100	-11.17837300	-1.48207300
C	14.84763600	-8.91724900	-1.66604500
H	14.74161600	-6.92195600	-0.87604900
H	14.61323200	-10.96036900	-2.28968700
C	16.24759900	-8.77543300	-2.19995500
H	16.23850000	-8.44089200	-3.24294000
H	16.81904200	-8.04104200	-1.62760500
H	16.78396900	-9.72667600	-2.16845200
C	2.17143900	9.71681900	-0.06521700
C	1.73702900	10.48190200	1.02131700
C	2.92837500	10.35761100	-1.06362800
C	2.04109700	11.83341400	1.15262900
H	1.11396900	10.01749400	1.77878900
C	3.23916800	11.69359900	-0.94563100
H	3.26504500	9.79801600	-1.92833500
C	2.81371800	12.44189300	0.16441500
H	1.65316900	12.39207400	1.99399000
C	4.03269100	12.57862800	-1.86694800
N	3.22531200	13.76284200	0.04599700
C	3.82261300	14.00394300	-1.27966900
C	5.56031200	12.37218800	-1.86758800
H	3.66154300	12.53050400	-2.89450900
C	2.99995500	14.80244500	0.95938300
C	5.21610500	14.66775900	-1.23234400
H	3.12758300	14.58230800	-1.89896000
C	6.10412500	13.78006200	-2.11534400
H	5.88459900	12.01322900	-0.88440900
H	5.88273700	11.63915500	-2.61104700
C	3.06436100	14.58857300	2.34188200
C	2.75353700	16.10258800	0.50516400
H	5.19908400	15.71030400	-1.55727700
H	5.58075800	14.65166800	-0.20084800

H	7.16690500	13.88106600	-1.88105700
H	5.97392700	14.04699400	-3.17027600
C	2.84924100	15.63407200	3.22849300
H	3.31312200	13.60632700	2.72436100
C	2.55608300	17.14070000	1.40609400
H	2.71492400	16.30760500	-0.55828100
C	2.58576400	16.93021900	2.78395000
H	2.90768300	15.43769500	4.29553300
H	2.36897700	18.13991200	1.02283800
C	2.33174100	18.05268300	3.75517900
H	1.27599300	18.09674600	4.04436900
H	2.91281000	17.92518700	4.67206300
H	2.59050000	19.02119700	3.32070100
N	4.77266800	-7.60655400	0.69883000
N	2.82726300	-6.01214000	0.76434400
N	0.92767000	5.74008500	-2.59730400
N	1.46644500	8.16533500	-2.56104900
N	-5.92482100	-1.36073900	2.57733700
N	-8.32257900	-2.00837600	2.51037500
S	1.05461000	7.00029200	-3.61841700
S	-7.19572800	-1.52640800	3.57940600
S	3.14081300	-7.62495400	1.03647600

D1: ground state

N	0.03151300	-0.00961800	-0.13189100
C	1.45141800	0.00005500	-0.08826600
C	2.14776800	-0.88979800	0.74487600
C	2.18806300	0.89870400	-0.87638400
C	3.53706100	-0.88043700	0.78668000
H	1.59560900	-1.59004200	1.36221600
C	3.57676800	0.90971800	-0.82415000
H	1.66847000	1.59140700	-1.52941600
C	4.28405600	0.02128500	0.00711900
H	4.04853800	-1.57446700	1.44241000
H	4.11873900	1.61662500	-1.44134700
C	-0.68865000	1.21193600	-0.14274900
C	-1.84833700	1.35545500	-0.92269700
C	-0.25859200	2.30692600	0.62511800
C	-2.55680400	2.55075400	-0.92360700
H	-2.18950800	0.52868400	-1.53587200
C	-0.95933700	3.50657500	0.60309200
H	0.62529100	2.21302700	1.24626500
C	-2.12742400	3.65638900	-0.16634100
H	-3.44278300	2.63385200	-1.54227300

H	-0.60580600	4.33302900	1.20781900
C	-0.66274000	-1.24867500	-0.14717800
C	-1.81516000	-1.43759100	0.63239200
C	-0.20718000	-2.31282200	-0.94177200
C	-2.48953500	-2.65262700	0.61300600
H	-2.18167400	-0.62861000	1.25480100
C	-0.88081400	-3.52853000	-0.95100400
H	0.67932500	-2.18408500	-1.55322200
C	-2.03818800	-3.72661600	-0.17636600
H	-3.37685900	-2.76957900	1.22401100
H	-0.51007000	-4.33155900	-1.57629400
C	-2.88135500	4.92785300	-0.16899700
C	-2.24833500	6.22122400	-0.18900900
C	-4.25559400	4.98659100	-0.15391600
C	-3.02227100	7.45793100	-0.17726200
C	-5.01194600	6.19390900	-0.13821100
C	-4.46504700	7.45783200	-0.14098600
C	5.76253500	0.03229300	0.05537500
C	6.51576400	-0.12545300	1.27277200
C	6.54861500	0.18980200	-1.06222100
C	7.97501300	-0.11255900	1.28333600
C	7.97318300	0.20754900	-1.05205500
C	8.74809500	0.05811600	0.07647600
C	-2.75223600	-5.02214500	-0.18477700
C	-2.96269700	-5.80227800	-1.37690600
C	-3.27241200	-5.59859300	0.95054800
C	-3.66857300	-7.07900300	-1.34732400
C	-3.96461600	-6.84362000	0.97971800
C	-4.19538800	-7.63417900	-0.12386100
C	10.22340300	0.07440100	0.05183500
C	10.93589600	-0.53545800	-0.99781700
C	10.96574900	0.69904300	1.08171400
C	12.32872700	-0.53491000	-1.05242900
H	10.39092800	-1.04474800	-1.78404700
C	12.34619900	0.71185200	1.03627800
H	10.44886200	1.16653300	1.91164900
C	13.04444400	0.10717800	-0.03138500
H	12.83288300	-1.04776500	-1.86165700
C	13.33363000	1.31315000	2.00493200
N	14.41661700	0.21883200	0.15420000
C	14.72040100	0.81711200	1.47652300
C	13.43831300	2.85980300	2.02140300
H	13.16587200	0.95361000	3.02540500
C	15.43081200	-0.22565100	-0.71441800

C	15.63956800	2.06458600	1.41735900
H	15.13826300	0.04973500	2.13866700
C	14.92867800	3.11454900	2.29244100
H	13.16292500	3.26075800	1.03849300
H	12.77382900	3.31382600	2.76223400
C	15.30470100	-0.11459300	-2.11125000
C	16.62758400	-0.75255300	-0.19862200
H	16.66041700	1.85372000	1.74666600
H	15.69403500	2.41802500	0.38196500
H	15.24092500	4.13735600	2.06028900
H	15.15102900	2.93640500	3.35205400
C	16.32572600	-0.55144600	-2.95168800
H	14.41988400	0.34221700	-2.53894000
C	17.64548600	-1.17064800	-1.05375500
H	16.76530600	-0.83967100	0.87351400
C	17.51587800	-1.09274000	-2.44633700
H	16.19928600	-0.44906100	-4.02673400
H	18.55951900	-1.57266900	-0.62375000
C	18.60646900	-1.58430600	-3.36798800
H	18.42500000	-2.61909000	-3.68509200
H	18.66729800	-0.97610500	-4.27583600
H	19.58406100	-1.56217400	-2.87778700
C	-5.27552400	8.69040700	-0.11066100
C	-6.48352400	8.78385700	-0.82685000
C	-4.86214700	9.81555900	0.64086700
C	-7.27264600	9.93312800	-0.81094200
H	-6.80895000	7.94558700	-1.43187400
C	-5.63788400	10.95779600	0.66986400
H	-3.93067700	9.78226800	1.19408400
C	-6.85402600	11.02983100	-0.04341300
H	-8.17606700	9.97043000	-1.40635200
C	-5.40275800	12.25924800	1.39474100
N	-7.43933000	12.28047600	0.11065900
C	-6.54222700	13.19025200	0.86354300
C	-5.58257300	12.24001400	2.93437600
H	-4.42249800	12.68269300	1.15278200
C	-8.67078000	12.71422300	-0.41440800
C	-7.19320400	13.84346800	2.11032400
H	-6.13916200	13.95108200	0.18498200
C	-6.17161400	13.62461800	3.24289700
H	-6.29803200	11.45746000	3.21442800
H	-4.64536200	12.03477200	3.45985000
C	-9.78797700	11.86125700	-0.47261600
C	-8.82809400	14.04031700	-0.85374000

H	-7.44047200	14.89690700	1.95493900
H	-8.12555600	13.31751300	2.34268800
H	-6.62469000	13.68914200	4.23690300
H	-5.38264700	14.38546600	3.19206800
C	-10.99980300	12.31515100	-0.98790100
H	-9.71710600	10.85133000	-0.08591600
C	-10.05208400	14.48212000	-1.35233700
H	-7.99266200	14.73029100	-0.80872400
C	-11.16080200	13.63075700	-1.44365300
H	-11.84545200	11.63229000	-1.01654300
H	-10.14166200	15.51380500	-1.68336000
C	-12.47252900	14.10506600	-2.02234400
H	-12.53732100	13.88765900	-3.09605200
H	-13.32305000	13.61122700	-1.54239600
H	-12.59485900	15.18553500	-1.90282500
C	-4.91582400	-8.92039700	-0.05953100
C	-4.72255000	-9.80526500	1.01760000
C	-5.82111400	-9.30264200	-1.07725600
C	-5.39269600	-11.02406600	1.11072900
H	-4.01353600	-9.54734500	1.79563600
C	-6.49680000	-10.50442900	-0.99336000
H	-5.98391400	-8.65070700	-1.92763200
C	-6.30233900	-11.37371500	0.10183100
H	-5.18396500	-11.68715600	1.94059600
C	-7.50137800	-11.10826000	-1.94258600
N	-7.06300900	-12.52686800	-0.04627400
C	-7.74393400	-12.54139800	-1.36350800
C	-8.90284500	-10.44623800	-1.98364100
H	-7.10390500	-11.17240000	-2.96076900
C	-7.16292900	-13.60241700	0.85586800
C	-9.28100300	-12.72946900	-1.28581500
H	-7.28513500	-13.30314400	-2.00440500
C	-9.85370500	-11.63257200	-2.20339200
H	-9.11542800	-9.96966800	-1.01910400
H	-8.97670700	-9.67611900	-2.75691200
C	-7.18488000	-13.39812100	2.24723100
C	-7.29308800	-14.91886700	0.37877800
H	-9.59937200	-13.73562500	-1.57103000
H	-9.60830000	-12.56062900	-0.25409100
H	-10.89784100	-11.39630100	-1.97658000
H	-9.81083100	-11.95602900	-3.25099900
C	-7.29277500	-14.47849600	3.12032100
H	-7.14937400	-12.39118100	2.64598900
C	-7.41580200	-15.98604800	1.26576000

H	-7.29638200	-15.11181300	-0.68833800
C	-7.40565700	-15.79491800	2.65390100
H	-7.30936400	-14.28776200	4.19056600
H	-7.51564700	-16.99193400	0.86542300
C	-7.49790600	-16.96153600	3.60834900
H	-6.50569700	-17.37303600	3.83324100
H	-7.94748600	-16.66397800	4.56039900
H	-8.09677700	-17.77557300	3.18892100
N	-2.26004200	8.55364100	-0.23929700
N	-0.92941900	6.42503200	-0.25723500
N	-2.55604700	-5.45325000	-2.60097900
N	-3.75422100	-7.65848300	-2.54822100
N	5.98159700	-0.28782900	2.48683000
N	8.49155400	-0.28445800	2.50346200
S	-0.69642300	8.05186800	-0.29910800
S	-3.01707900	-6.65639700	-3.62185700
S	7.23018000	-0.43027900	3.54642500
F	5.99179500	0.33836000	-2.27989600
F	-4.99180500	3.85914000	-0.11001600
F	-3.14723100	-4.99424800	2.14809400
F	-6.34770300	6.01854500	-0.08007400
F	-4.40745000	-7.21147600	2.19899900
F	8.54004200	0.39623700	-2.26084500

D1: the first excited state

N	-0.00169000	-0.10196100	0.10234700
C	-1.35048100	-0.54098900	0.11840500
C	-2.29279300	0.10498800	0.92143300
C	-1.76066600	-1.61369000	-0.67651200
C	-3.61379700	-0.31135100	0.92654000
H	-1.98627500	0.93793100	1.54362800
C	-3.08082500	-2.03169300	-0.66022900
H	-1.04109800	-2.11976600	-1.30960800
C	-4.03360600	-1.38869500	0.13854200
H	-4.32691500	0.20054300	1.56002400
H	-3.37665200	-2.86548600	-1.28487400
C	1.05159100	-1.02418800	0.13310600
C	2.26501000	-0.75459900	-0.52251800
C	0.92850000	-2.24466400	0.81569900
C	3.30493800	-1.65526700	-0.48415300
H	2.37764100	0.16621800	-1.08227400
C	1.96464900	-3.15308900	0.83659700
H	0.01158100	-2.46996700	1.34742600
C	3.19881400	-2.89444900	0.19505100

H	4.20990800	-1.41641000	-1.02402700
H	1.83900900	-4.08108300	1.37505700
C	0.26377500	1.29141800	0.05376800
C	1.23494800	1.85953700	0.88095800
C	-0.45162600	2.11628600	-0.81652400
C	1.48815000	3.22014100	0.82977900
H	1.79189900	1.23047900	1.56572100
C	-0.20089300	3.47800700	-0.85688800
H	-1.20689100	1.68552500	-1.46379800
C	0.77519600	4.05587500	-0.03762300
H	2.24631700	3.63980400	1.47933400
H	-0.76203700	4.09945700	-1.54300100
C	4.28954500	-3.84559100	0.22410600
C	4.11275400	-5.26005900	0.40267800
C	5.64074100	-3.44763100	0.07205500
C	5.24290000	-6.18446900	0.37034200
C	6.70210400	-4.31243000	0.03782600
C	6.58927600	-5.72510600	0.14744200
C	-5.44450800	-1.82869200	0.13930000
C	-6.24941900	-1.89211200	1.32976600
C	-6.10443400	-2.20452400	-0.99207700
C	-7.63133400	-2.32275300	1.29361600
C	-7.46482300	-2.63399900	-1.02693300
C	-8.27680500	-2.71106300	0.06572500
C	1.04146300	5.50912200	-0.07927800
C	1.07269100	6.26862400	-1.30038100
C	1.27585000	6.25268500	1.03819700
C	1.33616700	7.69227300	-1.30573900
C	1.54048700	7.65504700	1.03256800
C	1.58138700	8.42645900	-0.09086300
C	-9.68222600	-3.15438000	-0.00453100
C	-10.50427800	-2.75974200	-1.06470600
C	-10.23060700	-3.98573000	0.98947800
C	-11.82974800	-3.16762700	-1.16661600
H	-10.10647800	-2.10187500	-1.82821300
C	-11.53966400	-4.39977200	0.89776500
H	-9.62272000	-4.29541400	1.83128700
C	-12.34891300	-4.00787500	-0.18184900
H	-12.43817400	-2.81287200	-1.98779500
C	-12.33342500	-5.28396900	1.81980900
N	-13.62719500	-4.52658700	-0.04395900
C	-13.78397900	-5.18760100	1.26401900
C	-11.99446800	-6.78760300	1.78784100
H	-12.29661100	-4.92737900	2.85293200

C	-14.70258300	-4.36997900	-0.93162000
C	-14.31728600	-6.63393900	1.18063000
H	-14.41111100	-4.57059100	1.91717300
C	-13.34666100	-7.45798800	2.03737800
H	-11.61980600	-7.06079700	0.79511800
H	-11.22798000	-7.05882100	2.51781500
C	-14.51525500	-4.40231600	-2.31876300
C	-16.00597200	-4.22673000	-0.44507000
H	-15.35578700	-6.72155700	1.50711300
H	-14.27081800	-6.96820400	0.13970800
H	-13.35619500	-8.52056900	1.78168900
H	-13.61300800	-7.37289800	3.09706500
C	-15.59355100	-4.25513200	-3.17947700
H	-13.52562200	-4.57166900	-2.72515600
C	-17.07624500	-4.09637700	-1.32038000
H	-16.18819800	-4.21561100	0.62324200
C	-16.89510800	-4.09414400	-2.70272200
H	-15.41798200	-4.28608900	-4.25124700
H	-18.07767600	-3.98840900	-0.91334900
C	-18.05474900	-3.91311800	-3.64619700
H	-18.16714400	-2.86388300	-3.94038400
H	-17.91680000	-4.49237800	-4.56276300
H	-18.99507000	-4.22465900	-3.18541700
C	7.72676500	-6.59778600	0.03258200
C	8.90002400	-6.20023700	-0.67711200
C	7.72683600	-7.90853000	0.59587400
C	9.99867200	-7.01303500	-0.81616000
H	8.91824000	-5.23545500	-1.16195400
C	8.81956600	-8.71845200	0.47404800
H	6.84809800	-8.25357900	1.12123000
C	9.97572200	-8.28769200	-0.21961600
H	10.84678700	-6.68292800	-1.40136000
C	9.05269000	-10.10718100	1.00063100
N	10.92277600	-9.26555400	-0.23979400
C	10.42386900	-10.50970000	0.38529100
C	9.24501400	-10.23904100	2.52628300
H	8.26918400	-10.79402400	0.67001000
C	12.23067000	-9.16747500	-0.75528700
C	11.29705800	-11.02136200	1.54786100
H	10.30198500	-11.27193900	-0.38967900
C	10.29233700	-11.34682700	2.65962900
H	9.64049500	-9.30136100	2.93114800
H	8.30834700	-10.45530400	3.04454000
C	12.99551800	-8.01196300	-0.57103500

C	12.79946200	-10.25473900	-1.42375200
H	11.92013300	-11.87185500	1.26467100
H	11.96388100	-10.21708800	1.87376600
H	10.75658800	-11.38395800	3.64798000
H	9.82926300	-12.32277700	2.47619000
C	14.28471800	-7.94169900	-1.07807700
H	12.59242800	-7.18076400	-0.00497500
C	14.09398800	-10.17124700	-1.91469000
H	12.22818500	-11.16443200	-1.56801800
C	14.85890100	-9.01363600	-1.76302600
H	14.86397200	-7.03688000	-0.91977500
H	14.51722400	-11.02665700	-2.43263800
C	16.24954800	-8.91940800	-2.33017200
H	16.23156200	-8.51435200	-3.34769600
H	16.88052200	-8.26042200	-1.72921000
H	16.72692400	-9.90072500	-2.37849300
C	1.85524300	9.87594700	-0.06370600
C	1.30746700	10.68895900	0.93326500
C	2.67430700	10.47632700	-1.03765700
C	1.55101300	12.05694700	0.99103700
H	0.65733900	10.24792000	1.67953000
C	2.92717200	11.82797300	-0.98844600
H	3.10094200	9.87437500	-1.83126100
C	2.37990500	12.63026400	0.02688900
H	1.08032500	12.65309100	1.76140100
C	3.76662900	12.68164600	-1.89851600
N	2.75061200	13.95480200	-0.14885900
C	3.45515700	14.13286400	-1.43142900
C	5.29453100	12.53888000	-1.75354300
H	3.48888900	12.55041800	-2.94806200
C	2.41329000	15.04171600	0.67179400
C	4.81480200	14.85456700	-1.30879400
H	2.79819100	14.64049100	-2.14658600
C	5.80808800	13.94879600	-2.04974000
H	5.54243200	12.25909900	-0.72358400
H	5.70738300	11.77253700	-2.41402400
C	2.38668700	14.92259200	2.06646000
C	2.14308700	16.29448000	0.11139200
H	4.78979200	15.87269100	-1.70313100
H	5.08699800	14.91895800	-0.25098300
H	6.84171000	14.10833500	-1.73242700
H	5.76227800	14.14097400	-3.12769700
C	2.06050600	16.01233100	2.86116200
H	2.65048200	13.98091000	2.53213500

C	1.83408200	17.37891800	0.92189400
H	2.17350000	16.42600400	-0.96397300
C	1.77250000	17.26132800	2.30984200
H	2.04963100	15.89034200	3.94070900
H	1.63087800	18.34020500	0.45832400
C	1.39803300	18.43146500	3.18056700
H	0.32245300	18.44372700	3.38814900
H	1.91267500	18.39186800	4.14396500
H	1.64747300	19.38073800	2.70065400
N	4.88694200	-7.45699100	0.49907600
N	2.93980200	-5.86592900	0.55200800
N	0.87682000	5.77225200	-2.51644700
N	1.31497100	8.21696000	-2.52567600
N	-5.83472600	-1.58043600	2.55228200
N	-8.20911100	-2.30603000	2.48935900
S	3.22995600	-7.50078400	0.66675700
S	1.00297600	7.00777500	-3.56924100
S	-7.09294700	-1.80244400	3.56133500
F	-5.49457600	-2.19102800	-2.18452100
F	5.95493800	-2.13637000	0.03880000
F	1.27101400	5.69213000	2.25461300
F	7.92046000	-3.73784000	-0.01719900
F	1.76042400	8.18253900	2.24517400
F	-7.90726500	-2.97344800	-2.24601600

E1: ground state

N	0.04865700	0.00410900	-0.19412200
C	1.46555400	-0.06434300	-0.13254900
C	2.10404200	-1.02477500	0.66816800
C	2.26138300	0.83120300	-0.86637000
C	3.49110200	-1.09282700	0.72584600
H	1.50841900	-1.72162300	1.24757200
C	3.64674400	0.76762000	-0.79198900
H	1.78979200	1.58479500	-1.48753400
C	4.29984300	-0.19977700	-0.00309500
H	3.95187100	-1.84614900	1.35329100
H	4.23005600	1.49301500	-1.34973800
C	-0.60581200	1.26215900	-0.18244100
C	-1.73470200	1.49080300	-0.98814500
C	-0.13937500	2.31012900	0.62807000
C	-2.37598500	2.72232700	-0.97109500
H	-2.09695400	0.70356500	-1.64029300
C	-0.77672200	3.54496100	0.62794600
H	0.72251100	2.15145600	1.26683400

C	-1.91744100	3.78116400	-0.16297000
H	-3.22491200	2.87681500	-1.62951800
H	-0.39664800	4.32970000	1.27119700
C	-0.71407500	-1.19347300	-0.23233500
C	-1.88347900	-1.32647900	0.53419700
C	-0.31558900	-2.27129400	-1.03890200
C	-2.62297600	-2.50161700	0.49378000
H	-2.21374900	-0.50335100	1.15830000
C	-1.05281700	-3.44939500	-1.06440200
H	0.58003800	-2.18457300	-1.64449300
C	-2.22273000	-3.59774700	-0.29479000
H	-3.53365400	-2.56343200	1.08061400
H	-0.71650900	-4.26414500	-1.69437900
C	-2.62837400	5.07282200	-0.14081800
C	-1.96983100	6.32952900	0.10060200
C	-3.98855900	5.19085800	-0.35463100
C	-2.68830100	7.58385500	0.11407900
C	-4.69871300	6.42646700	-0.33706700
H	-4.57267600	4.28991200	-0.51089300
C	-4.11132900	7.65853500	-0.11001700
H	-5.77306500	6.37829100	-0.47830100
C	5.77336700	-0.27224200	0.03226300
C	6.51437500	-0.74875500	1.17085800
C	6.57378400	0.11942000	-1.02378000
C	7.95976300	-0.79385400	1.18431200
C	7.99813800	0.08207100	-1.00931400
H	6.10192800	0.47329200	-1.93438600
C	8.75465100	-0.37076800	0.05702700
H	8.50787900	0.44716600	-1.89433500
C	-2.99470700	-4.85550000	-0.28145500
C	-3.07537200	-5.74591000	-1.40936400
C	-3.71012000	-5.28815000	0.81846900
C	-3.84451700	-6.96968100	-1.36946000
C	-4.47194900	-6.49193400	0.85779800
H	-3.69049000	-4.68979100	1.72336700
C	-4.57339800	-7.38341600	-0.19527200
H	-5.00851400	-6.70427100	1.77623400
C	10.22463600	-0.42637100	0.03692800
C	10.91515700	-0.57995700	-1.18189600
C	10.99612900	-0.31915900	1.21965700
C	12.30546900	-0.60258000	-1.25872400
H	10.35129400	-0.72421900	-2.09807300
C	12.37579300	-0.34012900	1.15868400
H	10.50299400	-0.21724100	2.17956600

C	13.04862800	-0.46512500	-0.07609800
H	12.78795500	-0.75909700	-2.21525600
C	13.38765500	-0.23802000	2.27250900
N	14.42351400	-0.48987000	0.11382700
C	14.75311800	-0.51295900	1.55963500
C	13.55255900	1.15265600	2.93741500
H	13.20677200	-0.98861000	3.04880300
C	15.41770200	-0.55889900	-0.87991700
C	15.71958300	0.61158900	2.01308400
H	15.14247100	-1.50135000	1.83000900
C	15.05258700	1.21777700	3.26249600
H	13.29027600	1.93994900	2.22043500
H	12.90829200	1.27411700	3.81294400
C	15.28675000	0.12728600	-2.10104700
C	16.59946400	-1.28527000	-0.65250500
H	16.73266100	0.24715900	2.20265800
H	15.78391300	1.36662000	1.22203100
H	15.40394900	2.23161300	3.47721800
H	15.27020600	0.60148300	4.14377800
C	16.28766400	0.05157400	-3.06655700
H	14.41515300	0.74535200	-2.28217800
C	17.59754200	-1.33779400	-1.62352300
H	16.74068900	-1.81348900	0.28398800
C	17.46194800	-0.68405300	-2.85505800
H	16.15860500	0.59568700	-3.99902100
H	18.50031500	-1.90729900	-1.41713800
C	18.52943500	-0.77938400	-3.91883800
H	18.31752200	-1.59226700	-4.62492900
H	18.59629400	0.14401400	-4.50241800
H	19.51242600	-0.97771000	-3.48191000
C	-4.86297100	8.92313700	-0.10503600
C	-6.03328800	9.06128400	-0.87724700
C	-4.45461600	10.03309500	0.67352400
C	-6.79784800	10.22570400	-0.87831500
H	-6.33956000	8.24862700	-1.52847100
C	-5.20357300	11.19335200	0.68344400
H	-3.55000900	9.97327400	1.26805000
C	-6.38869200	11.30220500	-0.07612600
H	-7.66885900	10.29566300	-1.51752800
C	-4.96617000	12.48152000	1.43087500
N	-6.95066700	12.56346400	0.06856200
C	-6.06666500	13.44277400	0.87221000
C	-5.19693200	12.44956600	2.96368300
H	-3.96944700	12.88555100	1.22587900

C	-8.15268800	13.02982600	-0.49560700
C	-6.75345900	14.08736400	2.10379000
H	-5.62394800	14.20693900	0.22302100
C	-5.77522000	13.83976200	3.26800500
H	-5.93212100	11.67486600	3.21262400
H	-4.28037600	12.22521500	3.51692300
C	-9.28237400	12.20008100	-0.61347900
C	-8.26704300	14.36637100	-0.91666200
H	-6.98224600	15.14580800	1.95447600
H	-7.69973600	13.57003600	2.29610800
H	-6.26138600	13.89993700	4.24650400
H	-4.97348900	14.58870200	3.25353600
C	-10.46388300	12.68672800	-1.16831200
H	-9.24661200	11.18246900	-0.24243200
C	-9.46129800	14.84072800	-1.45504700
H	-7.42105500	15.03871000	-0.82654300
C	-10.58141100	14.01273300	-1.60623000
H	-11.32051100	12.02136200	-1.24311900
H	-9.51803300	15.87965200	-1.77032500
C	-11.85861000	14.52338000	-2.22936500
H	-11.86335900	14.36620200	-3.31546400
H	-12.73464000	14.00720100	-1.82514100
H	-11.98644400	15.59625300	-2.05774000
C	-5.33440000	-8.64000100	-0.11672400
C	-5.49658600	-9.29624400	1.11956600
C	-5.93077300	-9.22989200	-1.25764700
C	-6.23048700	-10.47209200	1.25358300
H	-5.00231000	-8.89924000	2.00060300
C	-6.66355400	-10.39484300	-1.13953500
H	-5.81418600	-8.76495100	-2.23004700
C	-6.83486700	-11.02320200	0.11312700
H	-6.29419500	-10.95864100	2.21867000
C	-7.38111000	-11.18982400	-2.20178100
N	-7.57393500	-12.19053100	-0.01934000
C	-7.84955500	-12.47858000	-1.44774600
C	-8.67733700	-10.56675000	-2.78177900
H	-6.70975100	-11.45474200	-3.02502200
C	-7.98569000	-13.05780300	1.00999000
C	-9.35189600	-12.66221000	-1.78317300
H	-7.26498300	-13.34986300	-1.76474800
C	-9.58264900	-11.78375900	-3.02690000
H	-9.13520500	-9.90318600	-2.03831900
H	-8.48726100	-9.97432100	-3.68135600
C	-8.40366500	-12.56994300	2.26110300

C	-8.03338400	-14.44591000	0.79167000
H	-9.62517800	-13.70877300	-1.94136400
H	-9.95154300	-12.28789800	-0.94631500
H	-10.63495300	-11.51728800	-3.16503700
H	-9.25757900	-12.31494900	-3.93024300
C	-8.81476400	-13.44737100	3.26205600
H	-8.43646600	-11.50174600	2.44120600
C	-8.46184100	-15.30797500	1.79871800
H	-7.73274900	-14.85586100	-0.16626500
C	-8.84978600	-14.83332000	3.05881100
H	-9.13498200	-13.03917400	4.21752700
H	-8.48837100	-16.37622500	1.59838600
C	-9.27488000	-15.77760800	4.15790400
H	-8.41574500	-16.10664000	4.75622200
H	-9.98160900	-15.30014800	4.84319500
H	-9.74867600	-16.67648800	3.75227200
N	-1.81972800	8.55854500	0.32139400
N	-0.68729900	6.58000400	0.30190100
N	-2.52437200	-5.63767200	-2.60629300
N	-3.72693200	-7.57312900	-2.53952700
N	6.07218300	-1.19378300	2.33468300
N	8.34978600	-1.27703500	2.35115900
O	-2.92457600	-6.75615000	-3.28836800
O	7.19662700	-1.51585800	3.04737900
O	-0.60459700	7.94036800	0.43874200

E1: the first excited state

N	-0.01010600	0.10503300	-0.04183000
C	1.34570100	0.52157000	-0.00464100
C	2.26003500	-0.12405000	0.83012700
C	1.78900700	1.57779800	-0.80430700
C	3.58678600	0.27315000	0.85954600
H	1.92697500	-0.94220200	1.45835500
C	3.11355700	1.97832600	-0.76003400
H	1.08983600	2.08900100	-1.45595000
C	4.04258100	1.33115300	0.06378900
H	4.27617700	-0.24298900	1.51607000
H	3.42814600	2.81654600	-1.37196000
C	-1.04629300	1.04557900	-0.03027900
C	-2.25550800	0.79670500	-0.70492700
C	-0.91203400	2.26758000	0.64872700
C	-3.27493100	1.71884000	-0.68874500
H	-2.37776700	-0.12571800	-1.26016000
C	-1.93249000	3.19293300	0.65593800

H	0.00311800	2.48080400	1.18854700
C	-3.16430700	2.95808700	-0.00554400
H	-4.16844200	1.48720700	-1.25427500
H	-1.79570300	4.11652000	1.20060700
C	-0.29705000	-1.28392300	-0.08122500
C	-1.29584000	-1.82859500	0.72947700
C	0.42128200	-2.12935600	-0.92927000
C	-1.56864200	-3.18524900	0.68429900
H	-1.86189900	-1.18352700	1.39150400
C	0.15233400	-3.48791300	-0.95956100
H	1.19530900	-1.71695900	-1.56630800
C	-0.84608700	-4.04534500	-0.15148300
H	-2.36453100	-3.58081600	1.30562100
H	0.72302500	-4.12308200	-1.62560000
C	-4.24575300	3.90870600	0.00914400
C	-4.12784500	5.24574100	0.52018900
C	-5.54231400	3.58942100	-0.48634800
C	-5.23227000	6.17463400	0.49484200
C	-6.59311900	4.47153700	-0.51112200
H	-5.73431500	2.58479300	-0.83894400
C	-6.51622500	5.81832200	-0.04231700
H	-7.53880300	4.09848900	-0.88051100
C	5.45837700	1.74814000	0.06606700
C	6.28926000	1.67881800	1.23757600
C	6.09573700	2.24059900	-1.03913700
C	7.65924300	2.10371200	1.22359800
C	7.46089000	2.66888100	-1.05244700
H	5.54893500	2.30895400	-1.97320500
C	8.28987400	2.61879300	0.03562900
H	7.84489000	3.06541400	-1.98556100
C	-1.12319600	-5.49508900	-0.15167200
C	-0.99280000	-6.31360100	-1.32664100
C	-1.53117500	-6.17932700	0.95991200
C	-1.27909000	-7.71914900	-1.30906800
C	-1.82120700	-7.58026900	0.97687900
H	-1.63676000	-5.64338000	1.89679600
C	-1.70677600	-8.39949600	-0.11380300
H	-2.16066000	-8.00273800	1.91584000
C	9.70180100	3.03590500	-0.00189000
C	10.45459600	2.87246600	-1.16963800
C	10.33122300	3.61629000	1.11580200
C	11.78053800	3.27924000	-1.26425500
H	10.00493600	2.38120500	-2.02620700
C	11.64280000	4.02497700	1.03577300

H	9.78303300	3.74235200	2.04238600
C	12.37732000	3.87464300	-0.15257400
H	12.33343900	3.10146600	-2.17710100
C	12.51149000	4.67399000	2.07768200
N	13.67519800	4.33022700	0.01799500
C	13.92624500	4.67282500	1.42982600
C	12.21797000	6.15579000	2.38471100
H	12.51817100	4.10525400	3.01162200
C	14.69330600	4.35908100	-0.94706600
C	14.50580200	6.08850100	1.64115500
H	14.56452500	3.90885100	1.88759700
C	13.60004200	6.72899500	2.70207900
H	11.80719000	6.64263500	1.49319200
H	11.49391500	6.27948000	3.19361600
C	14.42856400	4.70448700	-2.27747200
C	16.01755700	4.08972000	-0.58592900
H	15.55863000	6.07509100	1.93114700
H	14.43101800	6.64508400	0.70212800
H	13.63081300	7.82124200	2.67858200
H	13.91138900	6.41360700	3.70442900
C	15.45182100	4.73719500	-3.21443400
H	13.42302500	4.97714400	-2.57375500
C	17.03206200	4.14253700	-1.53237000
H	16.25942500	3.83661900	0.43974700
C	16.77281700	4.45332700	-2.86681700
H	15.21674100	5.01036200	-4.23939400
H	18.05143100	3.93044600	-1.22226300
C	17.87250100	4.46922300	-3.89539700
H	17.97999600	3.49097800	-4.37668700
H	17.66935200	5.19754900	-4.68445400
H	18.83633200	4.71664800	-3.44410300
C	-7.63407800	6.71402500	-0.10472000
C	-8.82753300	6.35590600	-0.80000500
C	-7.61443300	8.00349800	0.50814400
C	-9.92902100	7.17445200	-0.87258900
H	-8.87534800	5.41356800	-1.32939800
C	-8.70506400	8.82386900	0.44331300
H	-6.72331100	8.32831200	1.02770900
C	-9.88384000	8.42496200	-0.22931900
H	-10.79760800	6.86612800	-1.43939000
C	-8.91055100	10.19724500	1.02017100
N	-10.82687400	9.40953900	-0.18501000
C	-10.29799600	10.62858200	0.46339800
C	-9.05085500	10.28114100	2.55471500

H	-8.13293200	10.88916200	0.68606200
C	-12.14988500	9.33825600	-0.66166500
C	-11.12769700	11.10863500	1.67078200
H	-10.19493900	11.41612800	-0.28885800
C	-10.08395200	11.39146300	2.75809900
H	-9.44043400	9.33369000	2.94228900
H	-8.09574900	10.47365100	3.04819300
C	-12.91326800	8.17661200	-0.50929800
C	-12.73800100	10.45704900	-1.25827800
H	-11.75355700	11.97184700	1.43619100
H	-11.78934700	10.29861600	1.99300800
H	-10.51465900	11.40079800	3.76221900
H	-9.61915800	12.36937400	2.58987600
C	-14.21828500	8.13285800	-0.97732900
H	-12.49577700	7.31836200	0.00334600
C	-14.04815700	10.39937300	-1.71038300
H	-12.16986700	11.37244500	-1.37653800
C	-14.81149800	9.23716600	-1.59092400
H	-14.79478700	7.22216500	-0.84407000
H	-14.48514300	11.27983800	-2.17201400
C	-16.21986000	9.17165900	-2.11721600
H	-16.23676800	8.80688900	-3.14992200
H	-16.83547900	8.49229900	-1.52289300
H	-16.69315000	10.15616000	-2.11164500
C	-1.97654700	-9.84663800	-0.07123200
C	-1.72230200	-10.57649500	1.09494600
C	-2.50186800	-10.53474100	-1.18160600
C	-1.98905300	-11.93697900	1.19540700
H	-1.26962200	-10.07701800	1.94516500
C	-2.77193700	-11.88143800	-1.09585000
H	-2.69426900	-10.00452900	-2.10722000
C	-2.53295200	-12.59407300	0.09135500
H	-1.74420700	-12.46684900	2.10634600
C	-3.33823200	-12.81513100	-2.12989100
N	-2.85420700	-13.93232900	-0.07234000
C	-3.18528500	-14.22068900	-1.47962900
C	-4.84505700	-12.67712100	-2.42436700
H	-2.78016700	-12.76594600	-3.06898700
C	-2.76428500	-14.94593200	0.89381500
C	-4.53650600	-14.94215900	-1.67383100
H	-2.36550200	-14.77916000	-1.94509400
C	-5.27520000	-14.11219800	-2.73274500
H	-5.36413500	-12.31580500	-1.52962800
H	-5.04983700	-11.97272900	-3.23416800

C	-3.11749900	-14.71546100	2.22868400
C	-2.36330500	-16.23569300	0.53049300
H	-4.41920600	-15.99013900	-1.95785600
H	-5.08902800	-14.91750100	-0.72973600
H	-6.35824000	-14.25530700	-2.70029400
H	-4.93697600	-14.39340700	-3.73654500
C	-3.02959000	-15.73374800	3.16726500
H	-3.48985400	-13.74322400	2.52757400
C	-2.29625700	-17.24763100	1.47899700
H	-2.10062300	-16.45277600	-0.49833700
C	-2.61344700	-17.01875400	2.81733600
H	-3.31175700	-15.52576800	4.19565300
H	-1.98315100	-18.24001800	1.16696400
C	-2.50007700	-18.11060800	3.84811700
H	-1.52130600	-18.09217400	4.33981000
H	-3.25641700	-18.00094000	4.62943000
H	-2.61857400	-19.09835000	3.39647900
N	-4.82984400	7.32013200	1.00606200
N	-3.08171000	5.84992500	1.04538800
N	-0.62848400	-5.98286500	-2.54447000
N	-1.06972900	-8.19524900	-2.51519700
N	6.00000800	1.26162600	2.44899200
N	8.15747700	1.92105900	2.42515600
O	-0.67708000	-7.13379700	-3.25837500
O	7.14251200	1.41159800	3.16231600
O	-3.50554100	7.12988700	1.35263500

F1: ground state

N	0.04295700	-0.05373500	-0.02196100
C	1.42685000	-0.36626100	-0.01230800
C	1.91737800	-1.43214600	0.75919500
C	2.33820900	0.38426000	-0.77372600
C	3.27203400	-1.74015700	0.76173700
H	1.23327800	-2.02116300	1.35987900
C	3.69301600	0.07975900	-0.75958000
H	1.98180500	1.21100700	-1.37800200
C	4.19409800	-0.99226400	0.00482000
H	3.61799000	-2.56714900	1.36969700
H	4.36898000	0.68199000	-1.35338500
C	-0.38075600	1.30083800	-0.02254800
C	-1.45872600	1.71355900	-0.82295100
C	0.26811200	2.25779700	0.77410700
C	-1.87929300	3.03685700	-0.81666400
H	-1.96091300	0.99414400	-1.46029400

C	-0.14406700	3.58452600	0.76325400
H	1.09373900	1.95772600	1.40989400
C	-1.23048100	4.00607000	-0.02683700
H	-2.70434900	3.32527200	-1.45601200
H	0.37360600	4.29808700	1.39302100
C	-0.92138000	-1.09544200	-0.03330100
C	-2.08416700	-1.00378600	0.74918800
C	-0.73578000	-2.23815100	-0.82771500
C	-3.02970400	-2.02077400	0.73393900
H	-2.24619500	-0.13015500	1.37080800
C	-1.67926700	-3.25807700	-0.83203900
H	0.15181900	-2.32612700	-1.44441500
C	-2.84912700	-3.17488400	-0.05304400
H	-3.91797700	-1.91719800	1.34437600
H	-1.50872800	-4.12548900	-1.45813600
C	-1.66625300	5.41537000	-0.02641500
C	-0.76368100	6.52699700	0.12132200
C	-2.97080800	5.82711100	-0.17134100
C	-1.20443900	7.90299400	0.11452800
C	-3.40898100	7.19033100	-0.17494800
C	-2.58724100	8.28728800	-0.03811900
C	5.63265700	-1.32132100	0.02010800
C	6.31587800	-1.85486100	1.16987000
C	6.47894900	-1.16653500	-1.05346800
C	7.72640300	-2.16955800	1.17030600
C	7.87734800	-1.47547600	-1.05321300
C	8.57633200	-1.98620300	0.01814100
C	-3.84974700	-4.25973400	-0.06833700
C	-4.14150900	-5.05727100	-1.23074500
C	-4.60657900	-4.63613200	1.01700700
C	-5.12626500	-6.11461400	-1.23104800
C	-5.58307900	-5.68388500	1.01778000
C	-5.89851500	-6.47324600	-0.06581900
C	10.01280900	-2.30189100	0.00804400
C	10.65712800	-2.74779800	-1.16392700
C	10.79178100	-2.17671000	1.18472200
C	12.01557800	-3.05176600	-1.19628800
H	10.07995300	-2.88498400	-2.06981100
C	12.14000000	-2.47057900	1.16340500
H	10.32934900	-1.84958100	2.10870700
C	12.77258900	-2.89908600	-0.02437000
H	12.45909000	-3.42241500	-2.11175200
C	13.15492500	-2.40515800	2.27711200
N	14.11508000	-3.16042900	0.20126900

C	14.44279700	-3.02714100	1.64175000
C	13.57987500	-0.99060700	2.74875300
H	12.83718100	-2.99341300	3.14402600
C	15.07326500	-3.56567800	-0.74867300
C	15.60152000	-2.04285300	1.94571500
H	14.64631400	-4.01799100	2.06350900
C	15.06857200	-1.15857700	3.08870700
H	13.46251100	-0.27482900	1.92633300
H	12.97612700	-0.63314000	3.58781900
C	15.08737300	-3.03486500	-2.05073500
C	16.07589700	-4.48521600	-0.39648000
H	16.53484900	-2.55340000	2.19733100
H	15.79014100	-1.42946600	1.05781400
H	15.60251300	-0.20683700	3.16902900
H	15.17572200	-1.67734600	4.04953900
C	16.04932500	-3.44460600	-2.97113600
H	14.36327400	-2.27984500	-2.33435800
C	17.03980800	-4.87279700	-1.32498000
H	16.10246300	-4.90280000	0.60400500
C	17.04285600	-4.37393700	-2.63421100
H	16.03643500	-3.01449300	-3.96958600
H	17.80317100	-5.58532100	-1.02255900
C	18.06541500	-4.83016300	-3.64726900
H	17.70075500	-5.69145400	-4.22122700
H	18.29664600	-4.03844500	-4.36636200
H	18.99854100	-5.13483500	-3.16442400
C	-3.04661300	9.68424500	-0.04956300
C	-4.15788100	10.08258400	-0.81990000
C	-2.37449800	10.67609200	0.70644100
C	-4.60868900	11.39950000	-0.84934000
H	-4.67041300	9.35187500	-1.43317000
C	-2.81591200	11.98364900	0.68988700
H	-1.50816200	10.41007700	1.30110400
C	-3.94051200	12.36168400	-0.07664400
H	-5.44512000	11.66492700	-1.48339500
C	-2.27194400	13.19205500	1.41025900
N	-4.17566600	13.72299400	0.03528000
C	-3.10177600	14.38011300	0.81949700
C	-2.51208700	13.25494100	2.94070800
H	-1.20586600	13.33536800	1.20685600
C	-5.22849100	14.45369700	-0.54951800
C	-3.60927900	15.20678400	2.02869900
H	-2.48511400	14.99299100	0.15216300
C	-2.72820100	14.75234100	3.20789300

H	-3.41878600	12.69411600	3.19760100
H	-1.68350900	12.82341200	3.50957300
C	-6.53186700	13.93074900	-0.62422200
C	-5.00657100	15.75352800	-1.03474400
H	-3.56552200	16.28463400	1.85156500
H	-4.65551300	14.94714100	2.22317700
H	-3.18823900	14.95485600	4.17987700
H	-1.76539900	15.27796400	3.18487800
C	-7.56000400	14.67272100	-1.20065200
H	-6.74685700	12.95460700	-0.20496700
C	-6.05007000	16.48806000	-1.59481400
H	-4.01666900	16.19313600	-0.97884000
C	-7.34455200	15.96347400	-1.70290000
H	-8.55778100	14.24275800	-1.24130000
H	-5.84778500	17.49149600	-1.96095100
C	-8.46118500	16.74994300	-2.34695100
H	-8.56087800	16.50212400	-3.41129800
H	-9.42509000	16.53547200	-1.87523300
H	-8.28148700	17.82683500	-2.28017000
C	-6.90037700	-7.54991200	-0.05476300
C	-7.13156100	-8.32235000	1.10133700
C	-7.65551000	-7.85093100	-1.21489200
C	-8.07028600	-9.35032900	1.13369800
H	-6.54585000	-8.13464800	1.99267600
C	-8.59334300	-8.86316400	-1.19278800
H	-7.49774000	-7.28571600	-2.12616600
C	-8.82095400	-9.61878100	-0.02135500
H	-8.18762300	-9.93968400	2.03428400
C	-9.50833700	-9.34972800	-2.28851800
N	-9.77824200	-10.59584100	-0.24645300
C	-10.17158700	-10.62788500	-1.67661700
C	-10.69261400	-8.42319900	-2.66575700
H	-8.94991100	-9.60758300	-3.19413300
C	-10.29232100	-11.51242000	0.69145700
C	-11.69649800	-10.49315000	-1.92212100
H	-9.77417100	-11.53590700	-2.14433900
C	-11.82178600	-9.40669000	-3.00761900
H	-10.97649400	-7.81292000	-1.79993300
H	-10.44238600	-7.74125200	-3.48353300
C	-10.56164500	-11.13168800	2.01799700
C	-10.59357400	-12.82968800	0.30548600
H	-12.16346500	-11.43941500	-2.20766000
H	-12.17759600	-10.15389400	-0.99838400
H	-12.81095700	-8.93907300	-3.02274600

H	-11.64958700	-9.84214000	-3.99983700
C	-11.07556300	-12.05248900	2.92810700
H	-10.39615100	-10.10681200	2.32963000
C	-11.12170900	-13.73383800	1.22479500
H	-10.41291300	-13.15240900	-0.71404000
C	-11.36291100	-13.37311000	2.55699400
H	-11.27565900	-11.72748600	3.94613800
H	-11.34497100	-14.74576300	0.89606700
C	-11.89723300	-14.37009800	3.55731800
H	-11.08217400	-14.88141000	4.08505300
H	-12.51626000	-13.88223900	4.31633100
H	-12.50094100	-15.14127100	3.06999700
N	-0.14309500	8.68018500	0.23026500
N	0.55128900	6.50923000	0.24325800
N	-3.61160500	-4.97892600	-2.43795300
N	-5.15587500	-6.65516700	-2.43545400
N	5.82533400	-2.13275800	2.36419600
N	8.04674300	-2.64117400	2.36136000
O	-4.23355300	-5.95783400	-3.16609200
O	6.88605600	-2.61379400	3.08423000
O	0.92189900	7.82571200	0.31264300
F	6.02110600	-0.69406300	-2.22660400
F	8.49640700	-1.21353700	-2.22002700
F	-4.46626900	-4.01355900	2.20095200
F	-6.20938900	-5.84977600	2.19815800
F	-4.74191300	7.33732800	-0.29721000
F	-3.96490500	4.92922900	-0.29241200

F1: the first excited state

N	0.00460100	-0.00873900	-0.10320400
C	1.41585600	-0.05802600	-0.09898400
C	2.15913100	0.83747400	-0.87912200
C	2.09318800	-0.99792700	0.69010800
C	3.53972600	0.79558200	-0.86509800
H	1.64757500	1.56571700	-1.49776200
C	3.47308100	-1.04175300	0.69268300
H	1.53034900	-1.69318000	1.30218400
C	4.22933600	-0.14463000	-0.08135600
H	4.09201900	1.49477000	-1.47982800
H	3.97298600	-1.77801600	1.30822200
C	-0.74489100	-1.18859700	-0.13689400
C	-1.96572800	-1.28432000	0.54931400
C	-0.29552700	-2.30928300	-0.85042100
C	-2.70631900	-2.44321500	0.51335600

H	-2.31988500	-0.44227600	1.13202600
C	-1.03285400	-3.47197500	-0.87356800
H	0.63548800	-2.25562000	-1.40216900
C	-2.27064600	-3.58563700	-0.19983900
H	-3.62374100	-2.48080400	1.08066700
H	-0.65919200	-4.31119000	-1.44214200
C	-0.64371300	1.24558100	-0.07096000
C	-1.75516200	1.49314600	-0.88862800
C	-0.18080600	2.26210900	0.77527600
C	-2.38640000	2.72031800	-0.85464900
H	-2.11930600	0.71682000	-1.55169900
C	-0.81090900	3.49084300	0.79896100
H	0.67474700	2.08155600	1.41583000
C	-1.92824700	3.74959200	-0.01335200
H	-3.24430700	2.88671600	-1.49281600
H	-0.43895500	4.25891200	1.46496000
C	-3.03587500	-4.82029700	-0.23154800
C	-2.49390200	-6.09888800	-0.59839000
C	-4.38826500	-4.91066700	0.09303400
C	-3.26381800	-7.31879800	-0.56415700
C	-5.13736200	-6.09214400	0.12711000
C	-4.64440900	-7.36854000	-0.15342100
C	5.69928500	-0.18401600	-0.07246200
C	6.50516600	0.12051700	-1.22399600
C	6.45777700	-0.50471400	1.02614900
C	7.94118300	0.07746700	-1.20035900
C	7.88445600	-0.55053600	1.04684300
C	8.69477300	-0.26699200	-0.02334200
C	-2.59533900	5.05895400	0.01934000
C	-2.71007200	5.85628400	1.21013300
C	-3.16980900	5.66287900	-1.07374600
C	-3.36630800	7.13470000	1.22815400
C	-3.82232000	6.93046200	-1.05352600
C	-3.95547800	7.72778600	0.05690300
C	10.16559100	-0.30935000	0.01147500
C	10.87279000	0.04829500	1.16821200
C	10.90173300	-0.70651500	-1.12214500
C	12.25980200	0.01268800	1.22799000
H	10.32810500	0.38066200	2.04287200
C	12.27577600	-0.74857000	-1.07354500
H	10.38716600	-0.97634900	-2.03680900
C	12.96982600	-0.40258900	0.09957600
H	12.76551500	0.32538200	2.13190500
C	13.26159200	-1.14206000	-2.13890900

N	14.33607300	-0.49630800	-0.09867600
C	14.64286600	-0.79427300	-1.50936800
C	13.34305500	-2.64452400	-2.47703400
H	13.10764900	-0.57151600	-3.05902800
C	15.34499100	-0.27410600	0.85067500
C	15.53995500	-2.03358800	-1.71370200
H	15.07702800	0.09035400	-1.98759100
C	14.82487800	-2.85533500	-2.79408600
H	13.06150800	-3.23672900	-1.59933700
H	12.67456900	-2.92508300	-3.29442700
C	15.20289400	-0.69214500	2.17914600
C	16.54708800	0.33334100	0.47201400
H	16.56656300	-1.77413000	-1.98083100
H	15.57668700	-2.60140500	-0.77879400
H	15.12242200	-3.90694200	-2.79054100
H	15.05297600	-2.45259200	-3.78751500
C	16.21795700	-0.47082000	3.09862600
H	14.30639900	-1.21643000	2.48689500
C	17.55921100	0.53200600	1.40049600
H	16.69369700	0.65334100	-0.55310500
C	17.41449000	0.14794200	2.73384000
H	16.08163200	-0.80718100	4.12257200
H	18.48316600	1.00362900	1.07810300
C	18.50102300	0.40295700	3.74444900
H	18.35839900	1.36690600	4.24505700
H	18.51136900	-0.36649500	4.52042300
H	19.48643000	0.42426500	3.27298300
C	-5.42127800	-8.58327700	-0.04048700
C	-6.61919200	-8.63917000	0.71926900
C	-4.99983400	-9.79134800	-0.66264700
C	-7.37108300	-9.78741400	0.84691800
H	-6.94452200	-7.75966600	1.25386700
C	-5.74298800	-10.93451000	-0.54869700
H	-4.08177900	-9.80363500	-1.23325300
C	-6.94486100	-10.95279600	0.19143300
H	-8.25484200	-9.78769600	1.47112800
C	-5.50420700	-12.30024500	-1.13210200
N	-7.49952500	-12.20077200	0.19091000
C	-6.62316500	-13.17473100	-0.49621100
C	-5.70733300	-12.43832600	-2.65593400
H	-4.51749000	-12.68352300	-0.85892700
C	-8.73803800	-12.57972000	0.74714900
C	-7.30781400	-13.92820200	-1.65387700
H	-6.21256000	-13.86585600	0.24582500

C	-6.30409800	-13.83882500	-2.81057000
H	-6.42454600	-11.68657300	-3.00273700
H	-4.77879200	-12.29248100	-3.21237800
C	-9.85930100	-11.75029800	0.65081700
C	-8.87194500	-13.82346300	1.36889300
H	-7.57273700	-14.95407600	-1.39066100
H	-8.23176900	-13.40676400	-1.92217000
H	-6.77035900	-14.00334200	-3.78499200
H	-5.52000300	-14.59447400	-2.68878500
C	-11.07093000	-12.14856400	1.19726100
H	-9.79102200	-10.80790600	0.12076300
C	-10.09418300	-14.21047400	1.90087700
H	-8.01929500	-14.48800400	1.44629200
C	-11.21367700	-13.38056800	1.83716900
H	-11.93076700	-11.49129400	1.10635000
H	-10.17581400	-15.18081800	2.38162100
C	-12.52666800	-13.79188600	2.44750800
H	-12.62320400	-13.40634400	3.46825600
H	-13.37129000	-13.40336700	1.87330300
H	-12.61861500	-14.87907100	2.49911000
C	-4.62401400	9.03906200	0.06523700
C	-4.56210000	9.89122600	-1.04692500
C	-5.33712100	9.47633400	1.19890000
C	-5.18421600	11.13285300	-1.06356500
H	-3.99736600	9.58632800	-1.91881000
C	-5.96003400	10.70279800	1.19261700
H	-5.39272300	8.84890400	2.08055000
C	-5.90202900	11.53875800	0.06326300
H	-5.08509800	11.77072300	-1.93185900
C	-6.77444500	11.37075500	2.26584500
N	-6.57586600	12.72392800	0.30152600
C	-7.01853600	12.80281000	1.70548600
C	-8.18305400	10.79495100	2.51557200
H	-6.22988700	11.41937900	3.21290100
C	-6.76347300	13.78384200	-0.59808100
C	-8.52575900	13.08866500	1.87767300
H	-6.41202300	13.54008400	2.24257600
C	-9.00979600	12.03018700	2.87756700
H	-8.56746900	10.34560800	1.59322700
H	-8.18699000	10.02181800	3.28759000
C	-7.03606100	13.55233300	-1.95161900
C	-6.72981600	15.10733100	-0.14558100
H	-8.72814900	14.11093100	2.20418600
H	-9.02511900	12.94626500	0.91434900

H	-10.08797700	11.85998800	2.82293100
H	-8.77834300	12.34466000	3.90159300
C	-7.22756500	14.61508900	-2.82247000
H	-7.12538800	12.53680400	-2.31777700
C	-6.93998600	16.15855100	-1.02693900
H	-6.53775100	15.31856500	0.89999200
C	-7.18002600	15.93906100	-2.38365100
H	-7.43910300	14.40636500	-3.86739300
H	-6.91049500	17.17615400	-0.64794100
C	-7.36731100	17.08590600	-3.34097100
H	-6.41537400	17.38339200	-3.79426900
H	-8.04425700	16.81782600	-4.15595000
H	-7.77482800	17.96434800	-2.83497900
N	-2.47834400	-8.31015700	-0.90632700
N	-1.26899500	-6.39509200	-0.95939700
N	-2.27955400	5.59365500	2.42536400
N	-3.30494800	7.61232500	2.45358300
N	6.12102200	0.46584500	-2.43347700
N	8.38267600	0.40621500	-2.39565000
O	-2.64364700	6.66857400	3.17989500
O	7.26989700	0.63986200	-3.14322900
O	-1.26305000	-7.74631200	-1.15612300
F	5.88212700	-0.80924900	2.20003200
F	8.40105400	-0.90650200	2.23412800
F	-3.15091100	5.07242400	-2.28019100
F	-4.32120200	7.30742500	-2.24266000
F	-6.44236800	-5.92131800	0.38853500
F	-5.09171800	-3.79682600	0.33359700

A2: ground state

N	-0.04343900	-0.07366900	-0.06382300
C	-1.45535800	-0.20619900	0.01723000
C	-2.21208400	0.64716600	0.83604100
C	-2.12889000	-1.19766000	-0.71504000
C	-3.59497900	0.52117400	0.90951600
H	-1.71128200	1.41544300	1.41552600
C	-3.50922800	-1.32873800	-0.62280500
H	-1.56491400	-1.87285300	-1.34948800
C	-4.28246800	-0.46883300	0.18121800
H	-4.15058100	1.19414200	1.55112700
H	-3.99321000	-2.12326100	-1.18152500
C	0.78020600	-1.22937200	-0.08383600
C	1.90337800	-1.29706600	-0.92553400
C	0.49063500	-2.33603800	0.73099000

C	2.71008000	-2.42805700	-0.93748800
H	2.13383900	-0.46404500	-1.58081600
C	1.29358600	-3.47084100	0.70112900
H	-0.36550500	-2.30189100	1.39617500
C	2.43097100	-3.54459900	-0.12555700
H	3.55233100	-2.45909000	-1.62153600
H	1.04584200	-4.30711000	1.34380000
C	0.54355200	1.21828100	-0.12840700
C	1.71364300	1.51364600	0.59029400
C	-0.02777700	2.22980300	-0.91707200
C	2.28991800	2.77586700	0.51358900
H	2.17608700	0.74648000	1.20192700
C	0.54544300	3.49539100	-0.97575600
H	-0.92796900	2.02105600	-1.48521700
C	1.71914900	3.80399200	-0.26141400
H	3.20860900	2.96139600	1.06074700
H	0.08227900	4.25411600	-1.59486400
C	3.31533100	-4.72798600	-0.13888100
C	2.85573300	-6.06039200	0.08895900
C	4.68023900	-4.63264600	-0.38497400
C	3.73357200	-7.18747900	0.04821000
C	5.54956900	-5.74927700	-0.42581000
H	5.11669500	-3.65189400	-0.54535200
C	5.13255300	-7.05921300	-0.21268200
H	6.59434500	-5.56266900	-0.65238900
C	-5.75411100	-0.59995800	0.23287200
C	-6.54006200	-0.25482700	1.37428000
C	-6.49574700	-1.08213200	-0.83969500
C	-7.96135800	-0.40582400	1.39678200
C	-7.90284300	-1.23349200	-0.81665800
H	-5.98054900	-1.35032100	-1.75648000
C	-8.69681400	-0.90340000	0.27709700
H	-8.37602200	-1.64430700	-1.70265400
C	2.32867600	5.15032600	-0.29847200
C	2.26023100	6.01876200	-1.42989900
C	3.03399700	5.67693000	0.77745400
C	2.87638300	7.30850500	-1.44109300
C	3.64543100	6.95347700	0.76589300
H	3.11893900	5.09098500	1.68705300
C	3.59548000	7.82351100	-0.31865700
H	4.19458900	7.25295900	1.65265700
C	-10.16690600	-1.05235400	0.26502100
C	-10.88183000	-0.89880300	-0.94127100
C	-10.88480100	-1.36656800	1.44469900

C	-12.26899900	-1.05774000	-1.02811400
H	-10.32974300	-0.61994500	-1.83272600
C	-12.25644700	-1.53278100	1.38493300
H	-10.35565300	-1.47456600	2.38420500
C	-12.91997200	-1.38794100	0.15961900
C	-13.27306200	-1.88285400	2.44950500
N	-14.28111000	-1.58070800	0.28336300
C	-14.65172600	-1.85871500	1.68177800
C	-13.16810000	-3.30392100	3.06307700
H	-13.27761800	-1.13930700	3.25365800
C	-15.13654200	-1.28225700	-0.77077900
C	-15.30036000	-3.24432400	1.93299000
H	-15.30043000	-1.05528100	2.05100700
C	-14.62929400	-3.75166800	3.22059300
H	-12.64870300	-3.97032100	2.36445400
H	-12.60796100	-3.30994800	4.00248400
C	-14.59284800	-0.93905900	-2.03724000
C	-16.53020500	-1.31584200	-0.59656100
H	-16.39023200	-3.19759300	2.01002000
H	-15.05451100	-3.90883000	1.09684000
H	-14.73568500	-4.83245200	3.35496000
H	-15.07914300	-3.26622500	4.09591100
C	-15.49387300	-0.66134500	-3.06963800
C	-17.38741900	-1.02387700	-1.65352800
H	-16.94391100	-1.57685000	0.37071700
C	-16.88661700	-0.69143200	-2.91532500
H	-15.09887500	-0.41332400	-4.05116500
H	-18.46146400	-1.06088700	-1.48959500
C	-17.80312700	-0.35528800	-4.06865600
H	-17.88776600	0.72926000	-4.21440200
H	-17.43538200	-0.77618400	-5.01028600
H	-18.81298800	-0.74010700	-3.89922300
C	6.06466300	-8.20554700	-0.24859000
C	7.40431300	-8.03938800	0.15947400
C	5.64855200	-9.47584000	-0.71631700
C	8.34647100	-9.07284100	0.11225300
H	7.70559200	-7.07166700	0.54759800
C	6.55962900	-10.51484100	-0.76969900
H	4.62407000	-9.62199200	-1.03827500
C	7.88066100	-10.30068500	-0.35524000
C	6.41640800	-11.95580100	-1.20846400
N	8.65197100	-11.43821300	-0.48164600
C	7.87133300	-12.54730700	-1.05652200
C	5.51240100	-12.85575400	-0.32571200

H	6.08988000	-12.02491800	-2.25156200
C	10.02742400	-11.38566800	-0.29084200
C	7.72888500	-13.79727000	-0.15020500
H	8.29468600	-12.82108700	-2.03049300
C	6.25100500	-14.20226500	-0.28689600
H	5.44968000	-12.43722100	0.68562900
H	4.49323200	-12.92928500	-0.71583400
C	10.61994700	-10.19293100	0.20349100
C	10.83696700	-12.49471000	-0.58775200
H	8.41791700	-14.60188100	-0.42170100
H	7.94434200	-13.51086300	0.88543600
H	5.91480400	-14.85405500	0.52526000
H	6.09505700	-14.74385500	-1.22841800
C	12.00482200	-10.19413300	0.39332400
C	12.21400500	-12.44482700	-0.38993500
H	10.38526600	-13.39981600	-0.97720600
C	12.82739000	-11.29409400	0.11248000
H	12.47640100	-9.29592000	0.78286200
H	12.81534700	-13.31808100	-0.62997200
C	14.31537200	-11.23537700	0.36831000
H	14.74465700	-10.28569000	0.03161000
H	14.54570700	-11.32871300	1.43724300
H	14.83916600	-12.04393100	-0.14968600
C	4.23135000	9.15725600	-0.29592700
C	4.33845600	9.86781800	0.91787300
C	4.76375600	9.73855200	-1.47252900
C	4.96217700	11.11624600	1.01506000
H	3.89448600	9.43309000	1.80743500
C	5.38893700	10.97015400	-1.40244500
H	4.67929300	9.21484800	-2.41745700
C	5.48739500	11.62903700	-0.17007900
C	6.06353200	11.81594600	-2.46013200
N	6.13475800	12.84269100	-0.28354900
C	6.51439400	13.11215300	-1.68139600
C	7.36178600	11.23553100	-3.07940400
H	5.36579200	12.08242500	-3.26117000
C	6.16034200	13.73359600	0.78298100
C	8.03686800	13.25404200	-1.93911200
H	5.97715300	13.99919200	-2.03794600
C	8.28195400	12.45610500	-3.23170400
H	7.81155400	10.51566800	-2.38550100
H	7.17406300	10.71208700	-4.02127000
C	5.66125200	13.32457500	2.04847100
C	6.67255500	15.03177200	0.62252500

H	8.36139900	14.29568300	-2.01337200
H	8.58249900	12.79451200	-1.10711800
H	9.33372000	12.18704800	-3.36884200
H	7.97874000	13.04965000	-4.10345400
C	5.72268100	14.25071900	3.09370600
C	6.70588800	15.92168100	1.69248000
H	7.05064000	15.34384600	-0.34416800
C	6.23293500	15.54877300	2.95349700
H	5.36089700	13.95198300	4.07396200
H	7.11056100	16.91893700	1.53915600
C	6.24910100	16.50645700	4.12212400
H	5.25072800	16.91530800	4.32331400
H	6.58297900	16.01395100	5.04163900
H	6.91583900	17.35267400	3.93283400
N	2.99850800	-8.29829400	0.29826100
N	1.60575800	-6.51257100	0.35151200
N	1.77041000	-7.82465700	0.45638600
N	1.65899100	5.83202700	-2.62970900
N	1.91038400	6.96154800	-3.27798300
N	2.62610800	7.87993600	-2.64432200
N	-6.15360500	0.24286200	2.57388000
N	-8.40647100	0.01381200	2.60617300
N	-7.29674600	0.37864000	3.23260400
C	-7.32201500	0.83206200	4.62533200
H	-8.27767400	1.33910300	4.76612800
H	-6.51653600	1.56098200	4.72765400
C	0.65580200	-8.70336500	0.81904600
H	-0.23449400	-8.28642800	0.34548700
H	0.87282700	-9.67409300	0.37114500
C	1.49040000	7.14973800	-4.66869800
H	1.31764200	8.21942100	-4.79602400
H	0.54145600	6.62261500	-4.77866200
C	-13.07127100	-0.90662000	-2.32632000
C	-12.71325600	-2.08285300	-3.27461100
H	-11.64088500	-2.08570700	-3.49638800
H	-12.96858900	-3.04351300	-2.81714700
H	-13.25681600	-2.00099700	-4.22118200
C	-12.69202900	0.43016800	-3.01274700
H	-11.62149200	0.46451000	-3.23403300
H	-13.22039500	0.55650000	-3.96130500
H	-12.93496500	1.28086300	-2.36931600
C	9.80271900	-8.92881400	0.57084500
C	10.42855800	-7.68065800	-0.10195100
H	10.43576900	-7.78784800	-1.19063900

H	9.86132800	-6.77959300	0.14794000
H	11.45638500	-7.51757200	0.23247900
C	9.82934500	-8.74204800	2.11187100
H	10.85601200	-8.62428700	2.47303500
H	9.26215600	-7.85175200	2.40328700
H	9.38801800	-9.60689000	2.61643200
C	5.10266400	11.90560400	2.32210700
C	6.08231400	11.14917700	3.25959500
H	5.71113400	10.14098600	3.47178200
H	7.07012500	11.05771600	2.79789600
H	6.19845200	11.67647200	4.21174300
C	3.71840400	12.00777600	3.01178600
H	3.31168600	11.01365700	3.21817900
H	3.78560100	12.53326900	3.96807800
H	3.00573900	12.54242000	2.37692400
C	0.48170800	-8.81293700	2.33311800
H	0.27304500	-7.83360700	2.77165000
H	-0.35771500	-9.47769700	2.55505100
H	1.38137000	-9.22364900	2.79903900
C	-7.15358000	-0.32582000	5.60786500
H	-6.19767000	-0.83232600	5.45087200
H	-7.17756400	0.05951000	6.63096000
H	-7.96122600	-1.05365500	5.49298800
C	2.53423700	6.63093100	-5.65660700
H	2.70548300	5.56072800	-5.51404000
H	2.17942600	6.79201000	-6.67833500
H	3.48303800	7.15949600	-5.53201100

A2: the first excited state

N	-0.02473700	0.08909000	-0.19587000
C	-1.27467800	0.72653500	-0.15231400
C	-1.45434500	1.93479800	0.54282600
C	-2.39126200	0.17609100	-0.80772500
C	-2.68033400	2.55940000	0.58422400
H	-0.61355700	2.37676500	1.06582600
C	-3.61744300	0.79510200	-0.75989000
H	-2.27817200	-0.74349000	-1.37079900
C	-3.82831400	2.01688900	-0.05866700
H	-2.77964900	3.48212800	1.13791700
H	-4.43000000	0.33620400	-1.30856700
C	0.05499300	-1.32496500	-0.17516400
C	0.94295700	-1.99972500	-1.01804200
C	-0.75550300	-2.07292500	0.68300200
C	1.02096600	-3.38157200	-0.99023100

H	1.56282700	-1.43525900	-1.70534800
C	-0.67967600	-3.45600300	0.69649700
H	-1.44194700	-1.56230000	1.34881300
C	0.21654700	-4.14321800	-0.13232500
H	1.69816100	-3.88087900	-1.67479000
H	-1.31597000	-4.01305600	1.37264000
C	1.16795100	0.85052400	-0.25192200
C	2.28511800	0.47885800	0.50172800
C	1.25530000	1.98320300	-1.06629700
C	3.45264300	1.22013200	0.43573800
H	2.23710300	-0.39970900	1.13480000
C	2.42275800	2.72710900	-1.11608300
H	0.40002500	2.27944700	-1.66275500
C	3.54828900	2.36599600	-0.36421500
H	4.31125200	0.89448900	1.01282600
H	2.46704200	3.59722100	-1.75887600
C	0.33477300	-5.61475300	-0.09980800
C	-0.76111200	-6.48108700	0.18194400
C	1.52505900	-6.26490900	-0.34525200
C	-0.62327000	-7.89273000	0.19221400
C	1.66145700	-7.67537800	-0.33732500
H	2.41409500	-5.67653200	-0.54512600
C	0.62010800	-8.53859900	-0.07009700
H	2.63809300	-8.08706400	-0.56762100
C	-5.11495700	2.64627800	-0.00757700
C	-5.37604200	3.93501600	0.57632800
C	-6.28882300	2.02927300	-0.54142400
C	-6.67829800	4.52883300	0.59292000
C	-7.53743300	2.59361900	-0.52420900
H	-6.20795300	1.03926400	-0.97136200
C	-7.83785200	3.88185500	0.02936100
H	-8.34006400	2.00399000	-0.94663100
C	4.79077700	3.16474700	-0.38953900
C	5.24080000	3.87443800	-1.54055700
C	5.61803000	3.27759300	0.70692900
C	6.44576500	4.62270000	-1.54237700
C	6.82293500	4.02356700	0.70390200
H	5.33774600	2.78304500	1.63069400
C	7.28226700	4.72215800	-0.39235200
H	7.41353500	4.02744100	1.61358900
C	-9.15503700	4.43438600	0.01803800
C	-10.24232700	3.74301100	-0.61080100
C	-9.45342800	5.69637300	0.63327000
C	-11.53465800	4.22038400	-0.63816700

H	-10.04545400	2.79815300	-1.09902100
C	-10.73001300	6.18113700	0.61701100
H	-8.65670400	6.25135700	1.10806000
C	-11.75384900	5.44792900	-0.00492100
C	-11.32970500	7.43969100	1.19443700
N	-12.95552200	6.07699500	0.07666800
C	-12.85196800	7.33072600	0.83591800
C	-11.27329300	7.57342600	2.73258100
H	-10.89563600	8.32811900	0.72713900
C	-14.08406900	5.55574700	-0.53845300
C	-13.60072500	7.34325000	2.18296300
H	-13.17804900	8.16020800	0.20128500
C	-12.65648500	8.10517600	3.11669300
H	-11.11752200	6.58729600	3.18162800
H	-10.45495800	8.21739000	3.06166300
C	-13.99514200	4.31852100	-1.21097600
C	-15.29932900	6.25113000	-0.50051000
H	-14.59445100	7.79091100	2.11760500
H	-13.72038500	6.31254100	2.53289600
H	-12.89561000	7.95589600	4.17234900
H	-12.71732000	9.18044200	2.91416600
C	-15.15654000	3.83341500	-1.80910600
C	-16.42490300	5.73157100	-1.11304700
H	-15.35835400	7.20235800	0.01374800
C	-16.37595000	4.50716200	-1.78076600
H	-15.11608300	2.87860800	-2.32445700
H	-17.35763200	6.28614000	-1.06886200
C	-17.59411300	3.94492200	-2.46377800
H	-17.79327300	4.46007600	-3.40983900
H	-17.47000900	2.88317700	-2.68802800
H	-18.48687900	4.05817800	-1.84262100
C	0.78839500	-10.00662100	-0.04880900
C	1.99532200	-10.56572700	0.39205600
C	-0.23884300	-10.86228300	-0.49271200
C	2.22928000	-11.94089200	0.40239200
H	2.76711500	-9.89711700	0.75841500
C	-0.03337800	-12.22466300	-0.48854700
H	-1.17636700	-10.44421200	-0.83950200
C	1.18334600	-12.73639600	-0.03880400
C	-0.92307300	-13.37585500	-0.88809300
N	1.21623400	-14.11196400	-0.10224900
C	-0.01995000	-14.64355200	-0.68179100
C	-2.16543700	-13.61209600	-0.00399100
H	-1.23011900	-13.29771300	-1.93506400

C	2.40278700	-14.79542600	0.11204300
C	-0.82170500	-15.58783700	0.23871700
H	0.20543300	-15.13218700	-1.63667900
C	-2.27644900	-15.13590100	0.07486500
H	-1.98879400	-13.20131100	0.99585400
H	-3.05964100	-13.12958000	-0.40554700
C	3.53565000	-14.09401300	0.58038400
C	2.48936800	-16.16888100	-0.13626800
H	-0.67356700	-16.64381200	0.00104100
H	-0.49696600	-15.43083300	1.27241200
H	-2.92065000	-15.47935800	0.88820900
H	-2.68956900	-15.53020000	-0.86069100
C	4.69971000	-14.82738400	0.79705000
C	3.67330300	-16.85578000	0.08545200
H	1.62209700	-16.70168400	-0.50737800
C	4.80266400	-16.19911000	0.56509000
H	5.57873600	-14.30958100	1.16955900
H	3.71380000	-17.92212100	-0.11812100
C	6.08309000	-16.93998300	0.85078000
H	6.95906300	-16.32557300	0.62643600
H	6.15295900	-17.22907900	1.90537300
H	6.15188900	-17.85545800	0.25809400
C	8.53260000	5.50938200	-0.36736400
C	8.92509800	6.16168200	0.80922400
C	9.35506200	5.60305800	-1.50695500
C	10.10976400	6.89171800	0.90682600
H	8.26501000	6.11002700	1.66856800
C	10.53302000	6.31405400	-1.43399600
H	9.05603900	5.11923200	-2.42912900
C	10.89320100	6.93036000	-0.23612100
C	11.61443200	6.57216700	-2.45362800
N	12.09496800	7.59596100	-0.34236400
C	12.62225800	7.51658000	-1.70746300
C	12.44752700	5.34769600	-2.88585400
H	11.21501100	7.07219300	-3.34075600
C	12.50850100	8.45734600	0.66226600
C	14.00566500	6.84410600	-1.83658500
H	12.63418300	8.51849600	-2.15183800
C	13.86437300	5.90387500	-3.03815200
H	12.42961300	4.59180200	-2.09332200
H	12.06104400	4.88160000	-3.79530900
C	11.79522200	8.49951100	1.88127000
C	13.62306000	9.28085700	0.48041700
H	14.82089400	7.56228600	-1.95147400

H	14.19978500	6.26307900	-0.92925800
H	14.63250400	5.12671600	-3.05971400
H	13.94513900	6.47205700	-3.97200300
C	12.26113200	9.36564400	2.86654900
C	14.04519800	10.13541500	1.48840600
H	14.16695800	9.24637100	-0.45576000
C	13.37323800	10.19323600	2.70485300
H	11.73907700	9.40041500	3.81829100
H	14.91639000	10.76252500	1.32190500
C	13.81161800	11.12189900	3.80740600
H	13.14493100	11.98694100	3.89283600
H	13.81053700	10.61923600	4.77883000
H	14.81979600	11.50194400	3.62674100
N	-1.82737600	-8.42417200	0.48600300
N	-2.04711400	-6.18789300	0.46054000
N	-2.60323100	-7.37037700	0.62057600
N	4.68314500	3.98349500	-2.76309900
N	5.52195000	4.76141700	-3.41433500
N	6.58758200	5.17617900	-2.76396900
N	-4.52666000	4.79160000	1.15771600
N	-6.57461300	5.72516300	1.18436400
N	-5.28338300	5.83520500	1.48358500
C	-4.76954100	6.93951100	2.27094400
H	-5.34734500	7.82103500	1.98932200
H	-3.73455100	7.09105600	1.96095300
C	-4.00084000	-7.50238300	1.01971700
H	-4.53511000	-6.67506700	0.55280000
H	-4.35597300	-8.43981600	0.59215600
C	5.32279500	5.07737100	-4.82520200
H	5.77144500	6.05724900	-4.98713300
H	4.24602100	5.15140600	-4.97692000
C	-12.70073300	3.48866600	-1.29855200
C	-12.91464600	2.13896700	-0.57992700
H	-12.01150700	1.52596300	-0.63893700
H	-13.15347800	2.29375800	0.47518800
H	-13.73305800	1.57728700	-1.03694500
C	-12.35717800	3.22702700	-2.77984000
H	-11.44402200	2.63287800	-2.86440500
H	-13.15650300	2.67539800	-3.27953700
H	-12.20345400	4.16727500	-3.31491800
C	3.52394500	-12.58381300	0.89543000
C	4.72331400	-11.89475000	0.21511900
H	4.68488600	-12.02857600	-0.86877600
H	4.72542200	-10.82295100	0.42648900

H	5.67275800	-12.29539700	0.57580500
C	3.62933000	-12.39000900	2.42313500
H	4.55398300	-12.82899500	2.80815000
H	3.62555600	-11.32610400	2.67775100
H	2.78789900	-12.86503900	2.93421100
C	10.57303800	7.60525600	2.17544900
C	10.96959600	6.54567700	3.22584400
H	10.11963100	5.89719800	3.45793900
H	11.78540700	5.91841000	2.85720400
H	11.29831700	7.02192100	4.15378500
C	9.41706300	8.45902300	2.73254100
H	8.54222000	7.83896400	2.94089200
H	9.69510900	8.94614300	3.66919700
H	9.12470600	9.23219500	2.01778100
C	-4.15547000	-7.48416700	2.53294400
H	-3.78577600	-6.54400400	2.94773000
H	-5.21085300	-7.58649000	2.79445800
H	-3.60434400	-8.31019000	2.98745700
C	-4.86174200	6.67625200	3.76839300
H	-4.28508200	5.78877900	4.03881000
H	-4.46366700	7.52976700	4.32234400
H	-5.90068000	6.52266100	4.06895800
C	5.94255900	4.02192000	-5.72850600
H	5.49131300	3.04434400	-5.54611400
H	5.77575200	4.29082100	-6.77374200
H	7.01875800	3.95031800	-5.55693300

B2: ground state

N	0.02740000	-0.07931600	-0.07465500
C	-1.31181700	-0.54559600	-0.01050900
C	-2.25958100	0.09872800	0.80093000
C	-1.72148400	-1.66217800	-0.75761300
C	-3.57334600	-0.35180500	0.85218500
H	-1.96404200	0.95882900	1.39174200
C	-3.03306200	-2.11625000	-0.69314400
H	-1.00700400	-2.17628300	-1.39113400
C	-3.99498100	-1.46984000	0.10735000
H	-4.28018800	0.16361000	1.49074600
H	-3.31442300	-2.98204000	-1.27949500
C	1.10214400	-1.00660500	-0.11418700
C	2.20283000	-0.79351500	-0.96007200
C	1.08960900	-2.15732800	0.69028900
C	3.26060100	-1.69387700	-0.98725200
H	2.22439700	0.07929600	-1.60350500

C	2.14105800	-3.06524000	0.64448800
H	0.25427600	-2.33546600	1.35872800
C	3.25609300	-2.85335800	-0.18809200
H	4.09048100	-1.50544900	-1.65729300
H	2.10500700	-3.94387900	1.27711200
C	0.29440300	1.31498500	-0.10411600
C	1.36817900	1.85618800	0.62159200
C	-0.50588500	2.18566900	-0.86111700
C	1.63292900	3.21967900	0.58607200
H	1.99941000	1.20304900	1.21412000
C	-0.24468700	3.55063500	-0.88308700
H	-1.33716100	1.78934500	-1.43398300
C	0.83143600	4.10325000	-0.16283500
H	2.47187800	3.60287600	1.15347500
H	-0.87562100	4.19634400	-1.48139400
C	4.37422700	-3.81875500	-0.21982100
C	4.21043300	-5.23148900	-0.07582400
C	5.69873500	-3.45290500	-0.37740000
C	5.30477400	-6.14800900	-0.10928800
C	6.78666600	-4.36392800	-0.40901500
C	6.66489000	-5.73631600	-0.27740000
C	-5.39458300	-1.94061700	0.17072200
C	-6.21181600	-1.85645500	1.34123500
C	-6.06707000	-2.49916800	-0.90143100
C	-7.56599600	-2.30826300	1.37981100
C	-7.41222900	-2.95006800	-0.86264300
C	-8.23360600	-2.87832600	0.24925800
C	1.10668200	5.55494500	-0.20318100
C	0.87386400	6.37854900	-1.34900600
C	1.61078000	6.27224100	0.86682900
C	1.14629900	7.78020500	-1.36830900
C	1.88439900	7.66479700	0.84653100
C	1.66973400	8.49218100	-0.24228400
C	-9.63433600	-3.34556600	0.27116600
C	-10.45806000	-3.21068300	-0.86612000
C	-10.17537600	-3.92980300	1.44271700
C	-11.79065300	-3.63316500	-0.88633900
H	-10.03992600	-2.75029400	-1.75259200
C	-11.48831800	-4.36161700	1.44386100
H	-9.55977900	-4.03179200	2.32857800
C	-12.26739000	-4.21337700	0.28828700
C	-12.32504300	-5.03261900	2.51134700
N	-13.54788900	-4.69063300	0.46529700
C	-13.73644700	-5.21540900	1.82868200

C	-11.88425900	-6.45827200	2.93667500
H	-12.41661000	-4.39901000	3.39994200
C	-14.52064100	-4.49366800	-0.50848600
C	-14.05619400	-6.72942200	1.91848700
H	-14.50687500	-4.62681900	2.34066200
C	-13.20478200	-7.22680200	3.09896100
H	-11.28583100	-6.91344000	2.13886000
H	-11.27198100	-6.44902400	3.84291500
C	-14.15601600	-3.92142800	-1.75578700
C	-15.85736100	-4.85431600	-0.27048300
H	-15.12283300	-6.93415400	2.04512100
H	-13.73123300	-7.21682100	0.99211600
H	-13.07256800	-8.31301700	3.09643300
H	-13.68379900	-6.95653800	4.04848400
C	-15.16644000	-3.76141000	-2.70896200
C	-16.83012400	-4.66770700	-1.24814600
H	-16.13415300	-5.28775200	0.68364800
C	-16.50404500	-4.11867100	-2.49159500
H	-14.90574800	-3.34117200	-3.67671500
H	-17.85573800	-4.95988800	-1.03717500
C	-17.55140700	-3.89400700	-3.55722400
H	-17.90447900	-2.85477900	-3.56352700
H	-17.15851300	-4.10433700	-4.55729200
H	-18.42512700	-4.53245400	-3.39687400
C	7.80649600	-6.67255900	-0.31685900
C	9.05040000	-6.31880100	0.24577800
C	7.66585400	-7.94374000	-0.92543400
C	10.15507700	-7.17598600	0.23084900
H	9.14482100	-5.34762100	0.71603800
C	8.74427200	-8.80769100	-0.95329200
H	6.71851800	-8.22779500	-1.36858000
C	9.95926200	-8.41697400	-0.37388300
C	8.90031300	-10.20370900	-1.51642400
N	10.92443800	-9.39327900	-0.49372800
C	10.40453900	-10.57039800	-1.20993700
C	8.05631900	-11.31672400	-0.84028800
H	8.72310900	-10.21661300	-2.59714600
C	12.24065300	-9.14048300	-0.12427300
C	10.35930200	-11.88221200	-0.38552000
H	10.97646000	-10.71491100	-2.13408800
C	9.01090600	-12.51847600	-0.76220300
H	7.77227800	-11.00167800	0.17045900
H	7.13484200	-11.52929000	-1.38969800
C	12.56467800	-7.91545300	0.51521200

C	13.25272600	-10.07919800	-0.38726500
H	11.21136300	-12.53902600	-0.58114000
H	10.37022600	-11.63207700	0.68158300
H	8.68653900	-13.27814600	-0.04453100
H	9.08553300	-13.00438400	-1.74323000
C	13.90069100	-7.71215500	0.87567100
C	14.57010800	-9.82816400	-0.01701700
H	13.00581200	-11.00836200	-0.88794800
C	14.92156900	-8.63984400	0.63068200
H	14.16837100	-6.78486700	1.37498000
H	15.33234900	-10.57166000	-0.23631000
C	16.34031400	-8.37351300	1.07703100
H	16.57776100	-7.30565700	1.04234600
H	16.50852900	-8.70753000	2.10906400
H	17.06218300	-8.90098500	0.44609800
C	1.96310900	9.93945000	-0.24954100
C	1.77844100	10.72125800	0.91022700
C	2.43347000	10.56616500	-1.42975200
C	2.04506500	12.09336600	0.94453100
H	1.40560900	10.23661900	1.80405500
C	2.71100700	11.91990800	-1.41732100
H	2.56979400	9.98282700	-2.33266400
C	2.52186200	12.65494800	-0.23918000
C	3.23750800	12.84801400	-2.49040500
N	2.84258600	13.98481400	-0.40458600
C	3.28880400	14.25710100	-1.78168500
C	4.68428500	12.57969200	-2.98299800
H	2.56015900	12.88407500	-3.35025800
C	2.57486400	14.91095300	0.59702300
C	4.75313000	14.74646000	-1.92041000
H	2.59830400	14.96655300	-2.25287900
C	5.29386900	13.98154700	-3.14026700
H	5.23608200	12.01866200	-2.21981200
H	4.70590500	11.99102600	-3.90450600
C	2.09347200	14.46085200	1.85520100
C	2.77346000	16.28365500	0.37668500
H	4.83282100	15.83178100	-2.02736500
H	5.31099800	14.45878700	-1.02187100
H	6.38722400	13.97191200	-3.18266200
H	4.93329200	14.44686000	-4.06628500
C	1.85339900	15.42866000	2.83461300
C	2.51274000	17.21116800	1.38161500
H	3.13761200	16.62516100	-0.58538900
C	2.04903900	16.80252300	2.63477800

H	1.49925200	15.10399800	3.80949900
H	2.67818700	18.26711200	1.18342100
C	1.75163600	17.79559400	3.73409200
H	0.67191000	17.91996100	3.88484800
H	2.17189200	17.47296300	4.69288100
H	2.16514000	18.78088400	3.50084400
N	4.80858600	-7.39676500	0.04918200
N	3.07240300	-5.94308400	0.09166400
N	3.50194200	-7.19696000	0.15183300
N	0.38467000	6.03042300	-2.56105400
N	0.36745200	7.17817800	-3.22591100
N	0.80592500	8.25481000	-2.58875800
N	-5.89824500	-1.36871300	2.56317200
N	-8.04858600	-2.07504300	2.62218900
N	-7.02093200	-1.52345100	3.25249100
C	-7.09373400	-1.18051000	4.67517400
H	-8.13393100	-0.91859700	4.87344300
H	-6.47341800	-0.29330100	4.81172100
C	2.57980300	-8.30508100	0.41391700
H	1.63233500	-8.03329800	-0.05369300
H	2.99065600	-9.17571000	-0.09942300
C	-0.03776200	7.23754600	-4.63276300
H	-0.48427000	8.22165200	-4.78278900
H	-0.80826200	6.47621800	-4.76289800
C	-12.70672600	-3.50496600	-2.10938800
C	-12.17167400	-4.43051400	-3.23496500
H	-11.14558300	-4.15784800	-3.50249000
H	-12.17222800	-5.47604200	-2.91233700
H	-12.78947800	-4.35099600	-4.13483900
C	-12.68992200	-2.03714800	-2.60805300
H	-11.67302100	-1.72524400	-2.86303700
H	-13.30208900	-1.91348200	-3.50526900
H	-13.07126500	-1.36031700	-1.83782100
C	11.51387800	-6.82774900	0.85066000
C	11.98556000	-5.45511700	0.30575900
H	12.12289300	-5.49357800	-0.77884300
H	11.25161700	-4.67541300	0.52880000
H	12.93174500	-5.14939700	0.75991300
C	11.35530200	-6.73493400	2.39196300
H	12.30476600	-6.46919600	2.86735700
H	10.61706100	-5.97130100	2.65803200
H	11.02154700	-7.69063600	2.80730700
C	1.86083000	12.96674500	2.19142400
C	2.88611400	12.52307800	3.26924200

H	2.74528100	11.46732600	3.52310100
H	3.91090500	12.65208200	2.90807500
H	2.77078000	13.11077600	4.18534100
C	0.42605400	12.77024500	2.74467600
H	0.24500500	11.71945700	2.98867200
H	0.26816500	13.34829400	3.65908000
H	-0.32074200	13.08318400	2.00904000
C	2.41036400	-8.56668900	1.90965900
H	2.00650500	-7.68535900	2.41481300
H	1.71582900	-9.39848000	2.05609900
H	3.36707400	-8.82920100	2.36873300
C	-6.62607800	-2.33036000	5.56597700
H	-5.58637800	-2.59019600	5.35068000
H	-6.69785800	-2.02895600	6.61465200
H	-7.24935900	-3.21601300	5.41677100
C	1.13965300	7.00799300	-5.57886500
H	1.58475700	6.02326800	-5.41393300
H	0.78892700	7.06058700	-6.61325400
H	1.90869000	7.77148800	-5.43489900
F	2.39704400	8.15599900	1.99822100
F	1.87789800	5.66031100	2.04217000
F	6.04280900	-2.15248100	-0.50851400
F	7.99880600	-3.79200900	-0.59179100
F	-7.86288600	-3.48145100	-2.02246200
F	-5.45564600	-2.64571300	-2.09811800

B2: the first excited state

N	0.15897000	0.00388000	-0.15462200
C	-0.75180300	-1.07924600	-0.10632400
C	-1.88465000	-1.02023300	0.70940200
C	-0.53077300	-2.22733900	-0.87221300
C	-2.77739700	-2.07824300	0.74825600
H	-2.06582700	-0.13928700	1.31476800
C	-1.42067000	-3.28692900	-0.82129800
H	0.34405800	-2.28658300	-1.50951800
C	-2.56372000	-3.23318900	-0.01376000
H	-3.64488000	-2.01331800	1.39278100
H	-1.22840100	-4.16424500	-1.42631000
C	1.54182400	-0.23727600	-0.15721600
C	2.41859700	0.56281200	-0.90995100
C	2.09654600	-1.29465500	0.58223000
C	3.77320300	0.32826200	-0.91416600
H	2.01602500	1.36741300	-1.51510600
C	3.45022700	-1.53931600	0.57179000

H	1.44643300	-1.91960700	1.18475100
C	4.36259300	-0.73517500	-0.16868900
H	4.39520400	0.95256400	-1.53570500
H	3.83429100	-2.35879300	1.16121900
C	-0.33976500	1.32951300	-0.17583400
C	0.27685400	2.33454600	0.57315000
C	-1.46131100	1.65416500	-0.94329900
C	-0.21622400	3.62825700	0.55310700
H	1.14607100	2.09781600	1.17576300
C	-1.95811400	2.94714000	-0.95002500
H	-1.94661700	0.88697000	-1.53568000
C	-1.34686300	3.96095100	-0.20260700
H	0.27945100	4.38799700	1.14392600
H	-2.82542600	3.17659800	-1.55665400
C	5.77002800	-1.00866100	-0.16526900
C	6.35671200	-2.24174400	0.29526500
C	6.77785400	-0.10747800	-0.61490400
C	7.76037100	-2.51557000	0.26540400
C	8.12472800	-0.35477100	-0.62002100
C	8.75262200	-1.56015500	-0.17466700
C	-3.52064100	-4.35750300	0.03512000
C	-4.23653000	-4.73825100	1.21163200
C	-3.82310800	-5.14218900	-1.04679100
C	-5.15568200	-5.81585100	1.23664800
C	-4.74453300	-6.22521900	-1.02023800
C	-5.45319700	-6.61240800	0.08766300
C	-1.88832300	5.33491500	-0.21428900
C	-2.49952000	5.93513100	-1.35464600
C	-1.87340300	6.16373900	0.87758500
C	-3.02795500	7.25067900	-1.34063000
C	-2.39706100	7.48332300	0.88993300
C	-2.99573100	8.08904500	-0.18496600
C	-6.41159200	-7.73613500	0.09902900
C	-7.20865400	-8.00379100	-1.02176200
C	-6.53570100	-8.54662400	1.24418500
C	-8.12582000	-9.05309100	-1.05186400
H	-7.10578600	-7.36800200	-1.89228700
C	-7.43142400	-9.59230500	1.23468800
H	-5.93738100	-8.33850400	2.12325800
C	-8.19728400	-9.83156600	0.09351200
C	-7.77296300	-10.63169600	2.27398000
N	-9.03494500	-10.91153100	0.25668100
C	-8.91473600	-11.47529700	1.60351000
C	-6.66015400	-11.64610300	2.61423100

H	-8.13769800	-10.16818900	3.19508900
C	-10.01775500	-11.18523700	-0.68199600
C	-8.44134700	-12.94266100	1.65834700
H	-9.86554500	-11.35496400	2.13547100
C	-7.40945300	-12.96819100	2.79084300
H	-5.96355700	-11.72483300	1.77275200
H	-6.08284400	-11.35112300	3.49363600
C	-10.04169400	-10.46420800	-1.89714700
C	-10.98024800	-12.16866800	-0.43850200
H	-9.25989900	-13.64965900	1.81138100
H	-7.95963500	-13.19217200	0.70753700
H	-6.75538800	-13.84283900	2.74806700
H	-7.91716500	-12.98437400	3.76195600
C	-11.03611900	-10.78828900	-2.81524100
C	-11.95784800	-12.45256400	-1.38100500
H	-10.95834500	-12.72109300	0.49330400
C	-12.00467300	-11.76853800	-2.59120000
H	-11.06134800	-10.25769500	-3.76248800
H	-12.69160400	-13.22464100	-1.16740600
C	-13.06650100	-12.05382400	-3.62143700
H	-13.83466500	-11.27287300	-3.63367300
H	-12.64417000	-12.10352400	-4.62909700
H	-13.56811500	-13.00313500	-3.41993200
C	10.16134800	-1.79106600	-0.16097200
C	11.11512600	-0.72794000	-0.31715300
C	10.68593800	-3.11686500	0.01933900
C	12.47778500	-0.92751100	-0.32681800
H	10.74154200	0.27888700	-0.41158300
C	12.03381500	-3.32718100	0.01404500
H	10.00009600	-3.94093100	0.14833400
C	12.91445700	-2.24614500	-0.16112600
C	12.85268900	-4.58104700	0.18564400
N	14.21270300	-2.63889500	-0.15862900
C	14.33370900	-4.09008500	0.04948700
C	12.76817800	-5.25367700	1.57323200
H	12.62555200	-5.31052700	-0.59655100
C	15.24056400	-1.73675900	-0.39028400
C	15.04064600	-4.50417900	1.35551300
H	14.82872700	-4.53218300	-0.82041300
C	14.20720900	-5.68238700	1.86843100
H	12.43923800	-4.52112900	2.31746100
H	12.05566700	-6.08121300	1.58858700
C	14.93279400	-0.36883900	-0.55705200
C	16.56774800	-2.17691900	-0.47257600

H	16.09344900	-4.75430200	1.21053100
H	14.99150800	-3.67250600	2.06584400
H	14.38433100	-5.89437100	2.92550000
H	14.45343200	-6.58941700	1.30503300
C	15.99789500	0.49985200	-0.78189000
C	17.59165700	-1.27690000	-0.70481300
H	16.79343500	-3.22996700	-0.35847700
C	17.32664700	0.08446700	-0.85715900
H	15.79012500	1.55844300	-0.90653000
H	18.61359400	-1.63836300	-0.76858300
C	18.43894900	1.07589400	-1.07049900
H	18.08693300	1.96148100	-1.60466300
H	18.85589600	1.41545100	-0.11575900
H	19.25934500	0.63567200	-1.64274000
C	-3.54594600	9.45724100	-0.15026900
C	-4.20276400	9.93112000	0.99370700
C	-3.42352400	10.29906900	-1.27301300
C	-4.74731500	11.21195700	1.06567600
H	-4.28872700	9.27101300	1.84776700
C	-3.95065100	11.57029700	-1.22246000
H	-2.92548900	9.94061900	-2.16608600
C	-4.59346200	12.00316200	-0.06264800
C	-3.97126000	12.69080100	-2.23251600
N	-5.06652000	13.28870600	-0.18789300
C	-4.79869600	13.82276000	-1.52584100
C	-2.60807900	13.33072700	-2.56860900
H	-4.46685700	12.38207300	-3.15737700
C	-5.90770700	13.82561300	0.77600800
C	-3.90780800	15.08242800	-1.56296600
H	-5.74810300	14.00405300	-2.04270500
C	-2.92688400	14.82038900	-2.71004000
H	-1.91250100	13.17739600	-1.73651700
H	-2.15414400	12.89575700	-3.46221500
C	-6.12918200	13.11830100	1.97818000
C	-6.53616400	15.05598900	0.56669200
H	-4.47768900	16.00557300	-1.69162900
H	-3.36353500	15.15700000	-0.61595000
H	-2.03998100	15.45721900	-2.66326100
H	-3.41626200	15.00760300	-3.67272300
C	-6.96456700	13.70720200	2.92369400
C	-7.36862500	15.59976200	1.53418400
H	-6.36695600	15.59374700	-0.35832600
C	-7.59743600	14.93664000	2.73513600
H	-7.13248700	13.19035300	3.86417700

H	-7.84171800	16.55966800	1.34783600
C	-8.50629700	15.50740300	3.79247200
H	-9.47699500	14.99975000	3.80403100
H	-8.07542600	15.39874100	4.79176000
H	-8.69470200	16.56977100	3.62091100
N	7.94512600	-3.75626200	0.72771200
N	5.73742600	-3.32832500	0.76945400
N	6.71893900	-4.19492400	0.99340600
N	-2.69588000	5.42208100	-2.58272300
N	-3.31102900	6.39177400	-3.22496900
N	-3.53886700	7.50330300	-2.55971000
N	-4.19734000	-4.19720200	2.44352000
N	-5.65941500	-5.90190600	2.48267300
N	-5.05668800	-4.92501300	3.12520100
C	-5.26697700	-4.71197000	4.55488600
H	-6.29676800	-5.00282200	4.76105800
H	-5.16095500	-3.64088200	4.72608800
C	6.48291400	-5.46786800	1.64906400
H	5.50879500	-5.81956000	1.30669400
H	7.24780100	-6.15422400	1.28314000
C	-3.64941400	6.27064100	-4.63961700
H	-4.53744400	6.88263700	-4.79647500
H	-3.90690800	5.22490700	-4.80717800
C	-8.99857500	-9.38640400	-2.26023100
C	-8.09597300	-9.92227700	-3.39216100
H	-7.34573000	-9.17596700	-3.66999400
H	-7.57346200	-10.82933500	-3.07708100
H	-8.68688600	-10.16037200	-4.28082500
C	-9.70703100	-8.10669000	-2.74605600
H	-8.97809100	-7.33527700	-3.00512500
H	-10.30569900	-8.29409800	-3.63972300
H	-10.36538600	-7.70716000	-1.97068500
C	13.50164000	0.19300600	-0.48461900
C	13.18999400	0.97811900	-1.77592200
H	13.26921200	0.33048300	-2.65243200
H	12.17698000	1.38529100	-1.74331700
H	13.87789700	1.81621700	-1.90585900
C	13.39492100	1.14166300	0.72833300
H	14.10208200	1.96988200	0.63855500
H	12.38814800	1.56187600	0.79775400
H	13.60834500	0.60969800	1.65877000
C	-5.45370900	11.76923700	2.29985300
C	-4.40832300	11.98535700	3.41517100
H	-3.91736900	11.04156200	3.66945100

H	-3.63951700	12.69380600	3.09596000
H	-4.88045400	12.37882600	4.31951000
C	-6.50601100	10.75361400	2.78554400
H	-6.03826700	9.79498900	3.02185000
H	-7.00532400	11.09909700	3.69277200
H	-7.26611800	10.58303500	2.01919400
C	6.52582400	-5.35273300	3.16691000
H	5.76208000	-4.65686000	3.52152600
H	6.34117600	-6.32936700	3.62057600
H	7.50404700	-4.99692500	3.49821300
C	-4.28006100	-5.51244300	5.39074300
H	-3.25321400	-5.21784200	5.16412500
H	-4.46696100	-5.32887500	6.45090900
H	-4.38983900	-6.58212400	5.19987700
C	-2.50028300	6.71374500	-5.53238100
H	-1.61479500	6.09920400	-5.35705600
H	-2.79117500	6.61077500	-6.57993200
H	-2.24617600	7.75924800	-5.34479200
F	-2.26900400	8.12774100	2.06371700
F	-1.34507100	5.75876200	2.04498400
F	6.42537300	1.11676700	-1.06914100
F	8.88043900	0.64448200	-1.13165300
F	-4.88041000	-6.86680400	-2.19530400
F	-3.24594600	-4.92873600	-2.24178000

C2: ground state

N	-0.11908200	-0.11837100	-0.01691100
C	-1.51902900	-0.32359300	0.09552900
C	-2.30902400	0.53232800	0.88054900
C	-2.14800300	-1.38780400	-0.57145200
C	-3.68090600	0.33469200	0.98851600
H	-1.84292300	1.35810000	1.40718500
C	-3.51774500	-1.58737700	-0.44654800
H	-1.55874400	-2.06440900	-1.18054700
C	-4.32211000	-0.73057900	0.32851100
H	-4.26247400	1.01230400	1.60131000
H	-3.96957400	-2.43360000	-0.95432700
C	0.76935600	-1.22481400	-0.02813800
C	1.87548800	-1.24679600	-0.89399400
C	0.56396200	-2.32460000	0.82136500
C	2.74483300	-2.33064500	-0.90016000
H	2.04247300	-0.41760600	-1.57283800
C	1.42823000	-3.41319300	0.79643800
H	-0.27467700	-2.32118400	1.50923000

C	2.54534300	-3.44234600	-0.05955300
H	3.57299200	-2.33180900	-1.60207900
H	1.24662000	-4.24410900	1.46709300
C	0.39632600	1.20167000	-0.12935000
C	1.53773300	1.58848000	0.59058700
C	-0.22037900	2.14539000	-0.96625900
C	2.04394000	2.87738900	0.46895800
H	2.03125400	0.87337100	1.23990100
C	0.28477800	3.43642600	-1.07414900
H	-1.10145900	1.86307200	-1.53254500
C	1.42928500	3.83570800	-0.35874300
H	2.94068700	3.14173300	1.02057800
H	-0.21126800	4.14306100	-1.72827400
C	3.50264800	-4.56882900	-0.07424700
C	3.10162600	-5.94181500	0.08700900
C	4.85781300	-4.37201500	-0.26631600
C	4.07837700	-7.02558900	0.03762700
C	5.80729900	-5.42641800	-0.32023600
C	5.47999700	-6.76276400	-0.17230100
C	-5.78404000	-0.94345800	0.40435600
C	-6.55408700	-0.69546100	1.59496700
C	-6.50969500	-1.41378300	-0.67471200
C	-7.99337800	-0.93848600	1.63003300
C	-7.90786000	-1.65798800	-0.63872800
C	-8.69852600	-1.43646700	0.47532900
C	1.96618900	5.21243200	-0.43050900
C	1.98760600	5.98498200	-1.64428300
C	2.50223300	5.84319600	0.67667800
C	2.55008600	7.33174000	-1.67366800
C	3.05343500	7.15156400	0.64788600
C	3.10158200	7.93943600	-0.48857500
C	-10.15545500	-1.68273400	0.46359600
C	-10.89524500	-1.43301900	-0.71116000
C	-10.82973900	-2.20023100	1.59650900
C	-12.26780500	-1.68349000	-0.81136300
H	-10.37573700	-1.00317700	-1.56185400
C	-12.18466500	-2.46374300	1.52073900
H	-10.28034600	-2.39151500	2.51049400
C	-12.87489700	-2.21232800	0.32698700
C	-13.15544300	-3.03127700	2.53373000
N	-14.21308800	-2.52703700	0.42975000
C	-14.53639300	-3.04509700	1.76985100
C	-12.91080800	-4.49888500	2.97503300
H	-13.22203800	-2.39007500	3.41911700

C	-15.10032900	-2.20310700	-0.58972300
C	-15.02685800	-4.51458000	1.81315400
H	-15.26481000	-2.38105800	2.24990200
C	-14.31837800	-5.11252300	3.04013300
H	-12.31471500	-5.01829600	2.21570700
H	-12.36583800	-4.56174800	3.92116100
C	-14.60277600	-1.66096400	-1.80403600
C	-16.48171800	-2.40411200	-0.43026600
H	-16.11571400	-4.60093900	1.86436300
H	-14.69444800	-5.02712500	0.90304400
H	-14.31042500	-6.20668400	3.03249300
H	-14.82570600	-4.79392200	3.95944200
C	-15.53333200	-1.36252100	-2.80403500
C	-17.37029800	-2.08513900	-1.45270800
H	-16.86012200	-2.81656700	0.49791500
C	-16.91404600	-1.55824200	-2.66442700
H	-15.17142300	-0.95982100	-3.74640300
H	-18.43348000	-2.25454100	-1.30205900
C	-17.86760400	-1.18993200	-3.77714200
H	-18.08518100	-0.11414000	-3.78313600
H	-17.45309500	-1.43753800	-4.75983900
H	-18.82235500	-1.71351500	-3.67223200
C	6.50121300	-7.82987600	-0.21420000
C	7.78084700	-7.59214000	0.32882500
C	6.24100800	-9.08022300	-0.82618700
C	8.81078400	-8.53797200	0.28646300
H	7.95849000	-6.64221200	0.82278300
C	7.24202100	-10.03210900	-0.88142400
H	5.26656000	-9.27745900	-1.25713800
C	8.49760200	-9.75103000	-0.32536100
C	7.26675400	-11.43140700	-1.45730900
N	9.37317400	-10.80576000	-0.47150300
C	8.73886100	-11.92913000	-1.18167400
C	6.34160900	-12.47323100	-0.77339000
H	7.06956400	-11.41936400	-2.53455100
C	10.71278900	-10.67029800	-0.12655000
C	8.59545200	-13.23588600	-0.36146700
H	9.27832100	-12.11860200	-2.11720200
C	7.19119400	-13.75277100	-0.71687200
H	6.10083200	-12.14181200	0.24333500
H	5.39709300	-12.60286900	-1.30926100
C	11.15202900	-9.48507700	0.51976400
C	11.63374500	-11.69304200	-0.41010400
H	9.38436600	-13.96275500	-0.57354800

H	8.64509400	-12.99292100	0.70619200
H	6.81564100	-14.48580400	0.00354500
H	7.20687700	-14.23818300	-1.70089100
C	12.50597300	-9.40300700	0.86065400
C	12.97333100	-11.56218800	-0.05789100
H	11.29573000	-12.59673200	-0.90404000
C	13.43861500	-10.41232200	0.58750400
H	12.85991300	-8.51178900	1.37187400
H	13.66244700	-12.37132300	-0.28653100
C	14.89454900	-10.24791200	0.95666900
H	15.45462200	-9.72811300	0.16858300
H	15.01191300	-9.66176800	1.87357800
H	15.37851300	-11.21705300	1.11075700
C	3.66525000	9.30520500	-0.47082400
C	3.47431700	10.12263200	0.66231500
C	4.42796700	9.80674100	-1.55348900
C	4.01291700	11.40927800	0.76923900
H	2.85896500	9.74095700	1.47098200
C	4.98026800	11.07116000	-1.46789600
H	4.57915200	9.19603500	-2.43573400
C	4.77288500	11.84295000	-0.31625100
C	5.85267400	11.85297100	-2.42548900
N	5.38648600	13.07453900	-0.40421000
C	6.07599900	13.23458300	-1.69624500
C	7.27461000	11.28590100	-2.67704700
H	5.34866100	12.01104900	-3.38482200
C	5.16525300	14.04927000	0.56188400
C	7.61237900	13.42479400	-1.61015500
H	5.61512800	14.05919600	-2.25305700
C	8.17004200	12.53306000	-2.73282200
H	7.57369800	10.65221400	-1.83390000
H	7.32273800	10.67441800	-3.58258100
C	4.41004900	13.72717400	1.72083200
C	5.67825400	15.34703600	0.40259300
H	7.91890400	14.47025800	-1.70456900
H	7.96221600	13.06238300	-0.63677000
H	9.23243700	12.30539100	-2.60308100
H	8.05743300	13.03407000	-3.70252500
C	4.22821100	14.73696300	2.67014800
C	5.46426100	16.32185800	1.37308700
H	6.25096700	15.59209800	-0.48428600
C	4.73598900	16.03622500	2.53087600
H	3.66557500	14.50786200	3.57148500
H	5.87553400	17.31693800	1.22376000

C	4.48527900	17.08416300	3.59018400
H	3.44642200	17.43695900	3.57151600
H	4.67046000	16.69226800	4.59620700
H	5.12952700	17.95608400	3.44562700
N	3.53094100	-8.23436300	0.21672500
N	1.84815500	-6.37136700	0.28112300
N	1.52767300	5.58022300	-2.83518700
N	2.47753200	7.90464500	-2.88165800
N	-6.06864400	-0.24310100	2.75827200
N	-8.54679000	-0.64156100	2.81251800
S	1.91551900	-8.00800600	0.40932600
S	1.77389800	6.81571700	-3.88998800
S	-7.33772500	-0.12031600	3.79419600
C	10.20209300	-8.32006000	0.89394600
C	10.78145000	-6.97976000	0.37354200
H	10.89715500	-7.00211600	-0.71406200
H	10.12156700	-6.14576300	0.62952600
H	11.75774100	-6.76702100	0.81689900
C	10.07148600	-8.25090700	2.43931900
H	11.04649000	-8.07999700	2.90654000
H	9.40543200	-7.43327100	2.73391000
H	9.66164000	-9.18419500	2.83711000
C	-13.09663800	-1.41998700	-2.07426400
C	-12.87523100	0.04410600	-2.53371700
H	-11.81650700	0.23330800	-2.73358900
H	-13.42324300	0.26055300	-3.45475600
H	-13.20800400	0.74725000	-1.76454900
C	-12.62074800	-2.38186600	-3.19589400
H	-11.55788800	-2.22832700	-3.40939100
H	-12.76080000	-3.42563600	-2.89900800
H	-13.17993400	-2.21281300	-4.12142900
C	3.81537900	12.32156800	1.98579500
C	4.53050900	11.68847800	3.20948200
H	4.39601800	12.30431500	4.10414400
H	4.12578500	10.69297600	3.41967400
H	5.60398500	11.58702100	3.02356100
C	2.30020500	12.44414300	2.29074200
H	1.76896900	12.89331400	1.44649200
H	1.86196800	11.46104900	2.48530700
H	2.12040800	13.06117000	3.17500600
H	3.47173500	7.54003800	1.57078200
H	2.49979400	5.32126500	1.62841700
H	5.22871400	-3.35775300	-0.37511600
H	6.84307300	-5.15924800	-0.50319900

H	-5.99340900	-1.60320600	-1.61049600
H	-8.36996600	-2.05432900	-1.53705400

C2: the first excited state

N	0.23064000	0.10606300	0.06136700
C	1.59339800	0.41347200	-0.04623700
C	2.02582000	1.57638300	-0.70213700
C	2.57227100	-0.43685500	0.49582400
C	3.36739900	1.87664500	-0.81147000
H	1.29394500	2.24615800	-1.13829000
C	3.90984800	-0.13008700	0.38845500
H	2.27153600	-1.34429200	1.00572500
C	4.36994000	1.04039500	-0.26469800
H	3.66682500	2.77071300	-1.33836900
H	4.61941500	-0.83232000	0.80742500
C	-0.20921500	-1.24280500	0.06713100
C	-1.18035800	-1.66418400	0.97776500
C	0.31156700	-2.16832500	-0.84026800
C	-1.62120800	-2.97724400	0.97092100
H	-1.58113600	-0.96037800	1.69835400
C	-0.12286500	-3.48395800	-0.83069200
H	1.05528800	-1.84988200	-1.56197300
C	-1.10514200	-3.91514200	0.06885500
H	-2.35858500	-3.28830700	1.70324500
H	0.29196600	-4.18253700	-1.54617900
C	-0.73702100	1.13958600	0.16380800
C	-1.91623600	1.07801300	-0.58080800
C	-0.53673300	2.22272400	1.02274400
C	-2.87005300	2.07574800	-0.46177100
H	-2.08712800	0.24027900	-1.24724200
C	-1.48908200	3.22383300	1.12647600
H	0.37215200	2.27806600	1.61110700
C	-2.67625800	3.17225000	0.38616800
H	-3.78884500	1.99566800	-1.03269900
H	-1.31359800	4.05257300	1.80050600
C	-1.62255700	-5.29981000	0.06109400
C	-0.78040500	-6.44195900	-0.16450800
C	-2.94529400	-5.57870900	0.28240000
C	-1.32184100	-7.78442500	-0.14835200
C	-3.47646200	-6.89898200	0.30408900
C	-2.72013600	-8.02214300	0.09191000
C	5.78441900	1.34498700	-0.34358500
C	6.35217600	2.29527000	-1.25877800
C	6.71430600	0.68803000	0.50839500

C	7.79445900	2.52445200	-1.30960700
C	8.06242800	0.92703300	0.48780800
C	8.68779200	1.84089800	-0.41182600
C	-3.69453800	4.24229900	0.45855000
C	-4.03594100	4.90646800	1.68612100
C	-4.39001500	4.65570400	-0.64667500
C	-5.05653000	5.93248800	1.72178700
C	-5.39855400	5.65947200	-0.61029600
C	-5.76457200	6.32286300	0.53180700
C	10.11393200	2.03479600	-0.38988300
C	10.88131500	1.60239700	0.73536500
C	10.81979900	2.64335600	-1.47392300
C	12.25025100	1.73413600	0.81955200
H	10.35961200	1.18332100	1.58561300
C	12.17858600	2.77050600	-1.41690500
H	10.26138600	2.99264900	-2.33016400
C	12.87885400	2.31751700	-0.28613300
C	13.17512400	3.32340900	-2.40456700
N	14.21168300	2.52918100	-0.39416600
C	14.55680700	3.13558600	-1.68907200
C	13.29490000	2.56329700	-3.74403000
H	12.98955900	4.38431800	-2.59349000
C	15.07815000	2.23196400	0.65317000
C	15.39646400	2.24391500	-2.62465400
H	15.05385000	4.09342300	-1.51042300
C	14.80105100	2.50820100	-4.01037000
H	12.90188000	1.54817900	-3.62799500
H	12.72978600	3.04569900	-4.54423200
C	14.56565700	1.63906600	1.82558000
C	16.44089500	2.52494100	0.54830900
H	16.46654200	2.45327100	-2.56999700
H	15.24574100	1.19529200	-2.34765500
H	15.07991900	1.74557500	-4.74130200
H	15.15245700	3.47384700	-4.39088900
C	15.47121600	1.35487400	2.84406700
C	17.30395300	2.22949300	1.58985200
H	16.82574900	2.98441400	-0.35345300
C	16.83463200	1.63625100	2.76015300
H	15.10355600	0.88790400	3.75275700
H	18.35951800	2.46209900	1.48752500
C	17.75856800	1.33146200	3.90890200
H	17.77293500	2.15267400	4.63384700
H	17.44536500	0.43205800	4.44477600
H	18.78460600	1.18304300	3.56448300

C	-3.30832200	-9.37805500	0.09144500
C	-4.57691300	-9.57909900	-0.46788400
C	-2.63652000	-10.46862100	0.67722700
C	-5.21105200	-10.82155000	-0.46797400
H	-5.06914100	-8.73383100	-0.93741400
C	-3.24176700	-11.70593800	0.68912400
H	-1.65861800	-10.32596400	1.12118700
C	-4.50320600	-11.86168200	0.11397700
C	-2.78625000	-13.04175500	1.22261200
N	-4.95381400	-13.15899900	0.21007800
C	-4.00102600	-13.99642000	0.94351200
C	-1.58516400	-13.68692100	0.49995800
H	-2.58320400	-12.99354900	2.29634900
C	-6.26408500	-13.47225100	-0.11810300
C	-3.42729700	-15.18719300	0.14681500
H	-4.46128200	-14.34004500	1.87696900
C	-1.93013900	-15.17724000	0.47116600
H	-1.52114700	-13.30151400	-0.52331600
H	-0.63584200	-13.46830500	0.99454800
C	-7.07965300	-12.49702100	-0.73383600
C	-6.78220200	-14.74210900	0.15183400
H	-3.91006300	-16.13648900	0.39015200
H	-3.57865800	-15.00106300	-0.92136900
H	-1.33664500	-15.74264200	-0.25169100
H	-1.75627300	-15.62110000	1.45816200
C	-8.38159100	-12.86517800	-1.06273000
C	-8.08918800	-15.06077500	-0.18603400
H	-6.15366700	-15.48742500	0.62408800
C	-8.91624100	-14.12757200	-0.80302900
H	-9.01968300	-12.13692400	-1.55469100
H	-8.46563900	-16.05619000	0.03186000
C	-10.34272400	-14.45227600	-1.16325800
H	-11.04447500	-14.05245300	-0.42293800
H	-10.61823300	-14.02432700	-2.13105100
H	-10.50240500	-15.53191000	-1.21424800
C	-6.80528900	7.37226500	0.53271400
C	-6.89323200	8.26054200	-0.54715700
C	-7.73769000	7.47615400	1.58327200
C	-7.87765800	9.24536000	-0.63342000
H	-6.14913800	8.18684400	-1.33332600
C	-8.72397900	8.43507100	1.51686700
H	-7.67520600	6.80349400	2.43010200
C	-8.78333000	9.28890300	0.41528400
C	-9.86225800	8.76926900	2.44827000

N	-9.82656700	10.18200700	0.51516500
C	-10.54775900	10.01347900	1.77998800
C	-10.97403600	7.70638100	2.56690600
H	-9.49826000	9.02926400	3.44642100
C	-9.92642500	11.24504500	-0.36951800
C	-12.04104100	9.64785500	1.63928300
H	-10.42440800	10.91402500	2.39234400
C	-12.25968400	8.52906800	2.66353600
H	-10.99445200	7.09247100	1.65998300
H	-10.81949800	7.03604100	3.41569800
C	-9.06206700	11.30596900	-1.48535500
C	-10.87323900	12.25322100	-0.16789800
H	-12.70600200	10.50093000	1.79251100
H	-12.21658900	9.26710000	0.62790700
H	-13.16142800	7.94425200	2.46528200
H	-12.35767800	8.95389300	3.66914400
C	-9.21429000	12.38183700	-2.35560400
C	-10.98243600	13.31144800	-1.05824600
H	-11.53293600	12.20524700	0.69002500
C	-10.15557300	13.39596800	-2.17345800
H	-8.57249100	12.43892200	-3.22998400
H	-11.72900800	14.07987100	-0.87921300
C	-10.25292200	14.54270300	-3.14590000
H	-9.42362300	15.24730000	-3.02013200
H	-10.22228700	14.19315600	-4.18186400
H	-11.18139700	15.10134200	-3.00692200
N	-0.40135800	-8.71685700	-0.38430900
N	0.53004000	-6.41305100	-0.39681500
N	-3.49311200	4.67219400	2.87886500
N	-5.23385200	6.44423300	2.93791000
N	5.67147300	3.02450600	-2.13987000
N	8.15375800	3.42029800	-2.22447500
S	1.01933600	-7.95258500	-0.59085100
S	-4.20735000	5.67794000	3.93975700
S	6.76875200	3.94690900	-2.98551200
C	-6.57874300	-11.08333100	-1.09477700
C	-7.57946300	-10.02467600	-0.59136700
H	-7.70159700	-10.08924800	0.49266000
H	-7.23389400	-9.01764100	-0.83616000
H	-8.56038600	-10.14871100	-1.05433300
C	-6.45448500	-10.97220400	-2.62941200
H	-7.42117100	-11.14288700	-3.11141000
H	-6.10159300	-9.97711000	-2.91577500
H	-5.74576000	-11.70896100	-3.01634600

C	13.07940300	1.28779500	2.02042200
C	12.54858700	1.98931100	3.28794900
H	11.49557900	1.74677200	3.45030800
H	13.10002500	1.67090000	4.17512500
H	12.63939400	3.07449500	3.19894200
C	12.93650200	-0.24044200	2.18419500
H	11.88772400	-0.51288300	2.32865200
H	13.30628000	-0.76343100	1.29882500
H	13.49883000	-0.59520800	3.05118000
C	-8.00551700	10.22627100	-1.79718900
C	-8.43837000	9.44872300	-3.05846300
H	-8.52787100	10.11832700	-3.91831300
H	-7.70405200	8.67594700	-3.30403300
H	-9.40501600	8.96271800	-2.90290200
C	-6.63824300	10.88893500	-2.05680200
H	-6.30727600	11.45374500	-1.18181400
H	-5.87920400	10.13690200	-2.28446000
H	-6.68018000	11.57098500	-2.90832600
H	-5.90819300	5.89352000	-1.53859100
H	-4.16477500	4.20563800	-1.60764300
H	-3.63553000	-4.75707900	0.44120200
H	-4.53518700	-7.01155900	0.51075700
H	6.34625800	-0.01888400	1.24029500
H	8.67828700	0.35358700	1.16747900

D2: ground state

N	0.02465800	-0.16456200	-0.02682800
C	-1.23200600	-0.81609500	0.07102700
C	-2.25893200	-0.27919800	0.86470200
C	-1.47866900	-2.01109200	-0.62478700
C	-3.49351300	-0.91149200	0.94963200
H	-2.08774300	0.63918900	1.41536800
C	-2.71156600	-2.64447100	-0.52746200
H	-0.70058100	-2.44314100	-1.24430000
C	-3.75009800	-2.10929100	0.25740600
H	-4.26586600	-0.47493200	1.57084800
H	-2.87075000	-3.56562900	-1.07529400
C	1.22270500	-0.92594000	-0.05601800
C	2.26680100	-0.58464400	-0.93084200
C	1.39059900	-2.03509200	0.78856900
C	3.44230100	-1.32503600	-0.95154200
H	2.15055200	0.25915600	-1.60208400
C	2.56123700	-2.78328500	0.75059200
H	0.60199200	-2.30613800	1.48207800

C	3.61648500	-2.44460600	-0.11633100
H	4.22545800	-1.04421100	-1.64574300
H	2.66511100	-3.63177600	1.41559200
C	0.08695100	1.25217400	-0.10660900
C	1.06348500	1.96662100	0.60579100
C	-0.82360600	1.96849500	-0.89990300
C	1.12640400	3.35233700	0.52292800
H	1.77497200	1.43190500	1.22548500
C	-0.76257000	3.35527200	-0.97097600
H	-1.58236000	1.43442700	-1.46135700
C	0.21399800	4.08002400	-0.26357500
H	1.89304600	3.87589000	1.08180800
H	-1.47578400	3.88204700	-1.59309300
C	4.86633000	-3.23394200	-0.14786100
C	4.89824400	-4.67024400	-0.04129200
C	6.11179000	-2.66381400	-0.27716500
C	6.15093600	-5.41826400	-0.07538300
C	7.33419600	-3.39434400	-0.31834600
C	7.42933800	-4.76443600	-0.21950800
C	-5.06791900	-2.77549800	0.34127400
C	-5.83923300	-2.85828800	1.55513200
C	-5.68014800	-3.36606700	-0.74006300
C	-7.14349300	-3.51220600	1.59753300
C	-6.94930300	-4.01179000	-0.69736200
C	-7.73619000	-4.11570800	0.42803000
C	0.27494800	5.55624400	-0.33645900
C	0.05735100	6.29956800	-1.55088600
C	0.53745500	6.35035300	0.75567000
C	0.11982400	7.75720900	-1.58382400
C	0.60420700	7.77317000	0.72282200
C	0.40199000	8.53837100	-0.40369600
C	-9.05528000	-4.78015100	0.43607000
C	-9.93288700	-4.63168100	-0.65806700
C	-9.45715600	-5.57686400	1.53568500
C	-11.19054000	-5.23985100	-0.70345400
H	-9.61862500	-4.01139500	-1.48865100
C	-10.69290700	-6.19461400	1.50995500
H	-8.79757000	-5.69713100	2.38669600
C	-11.53069300	-6.02334900	0.39896700
C	-11.38183700	-7.10592000	2.50190500
N	-12.72141400	-6.70044500	0.54243600
C	-12.78306100	-7.40015500	1.83783800
C	-10.73206400	-8.49672000	2.72587000
H	-11.52070000	-6.60869700	3.46768700

C	-13.75559900	-6.51934100	-0.37030600
C	-12.89586800	-8.94387600	1.75340300
H	-13.60305100	-6.98407500	2.43503100
C	-11.92800800	-9.45486500	2.83446700
H	-10.12065600	-8.76342900	1.85586600
H	-10.08024000	-8.51260200	3.60399600
C	-13.52783600	-5.75138700	-1.54211700
C	-15.02018300	-7.08769500	-0.14341400
H	-13.91861700	-9.30518300	1.89118300
H	-12.55749000	-9.27174800	0.76390900
H	-11.65218500	-10.50417600	2.69253600
H	-12.39094200	-9.36786100	3.82546800
C	-14.59346200	-5.61260100	-2.43708500
C	-16.05274300	-6.91551900	-1.06021000
H	-15.19343100	-7.67141300	0.75327100
C	-15.86012600	-6.17468200	-2.23009900
H	-14.43510100	-5.04293400	-3.34868500
H	-17.01965500	-7.37030100	-0.86013200
C	-16.97738700	-5.96362900	-3.22505300
H	-17.50461000	-5.01784700	-3.04515700
H	-16.59940000	-5.92960300	-4.25177700
H	-17.72044500	-6.76442500	-3.16506100
C	8.71298300	-5.49366600	-0.26441900
C	9.85374400	-4.96998900	0.37843600
C	8.82057400	-6.72034000	-0.96389200
C	11.09281900	-5.61709500	0.35885900
H	9.75751700	-4.03488800	0.91709800
C	10.03520500	-7.37805300	-0.99786400
H	7.95621600	-7.13028800	-1.47266200
C	11.14068700	-6.82549600	-0.33577000
C	10.45512900	-8.68182100	-1.64122900
N	12.26618200	-7.60721600	-0.47284800
C	11.98983000	-8.79941700	-1.29290600
C	9.80166000	-9.96983900	-1.07342200
H	10.31744400	-8.65087200	-2.72722500
C	13.50380300	-7.15548200	-0.02689000
C	12.15428700	-10.15756400	-0.56465400
H	12.60856400	-8.76811400	-2.19745100
C	10.95063100	-10.98960100	-1.03819100
H	9.43968400	-9.78254800	-0.05579900
H	8.94712200	-10.29874900	-1.67147700
C	13.58323900	-5.94273800	0.70534000
C	14.67314400	-7.88742400	-0.29508400
H	13.11403200	-10.63931900	-0.77057800

H	12.09086300	-9.99050100	0.51675500
H	10.74602900	-11.84469900	-0.38684400
H	11.13726900	-11.38177600	-2.04588200
C	14.84880800	-5.53809100	1.14321600
C	15.91091900	-7.44131200	0.15623600
H	14.60964200	-8.81280300	-0.85585300
C	16.02498100	-6.25436700	0.88734300
H	14.93037000	-4.62031000	1.71917600
H	16.79800400	-8.03042100	-0.06258600
C	17.36633100	-5.74739000	1.36342100
H	17.85431100	-5.12337000	0.60357700
H	17.26585100	-5.13682800	2.26592400
H	18.04881100	-6.57293700	1.58785800
C	0.47070500	10.01380100	-0.40367200
C	-0.06314700	10.75083000	0.67361300
C	1.07610800	10.70775000	-1.47914100
C	-0.02126900	12.14717700	0.72457300
H	-0.53328200	10.20793600	1.48481900
C	1.13961400	12.08768300	-1.44567900
H	1.48475300	10.15574200	-2.31720500
C	0.60089100	12.77945700	-0.35169200
C	1.73199700	13.09074700	-2.41136500
N	0.74485800	14.14304100	-0.48323700
C	1.41429100	14.48750000	-1.74970300
C	3.27379500	13.05504700	-2.58150700
H	1.25516900	13.02327800	-3.39496300
C	0.11453300	15.01230000	0.40123100
C	2.77950400	15.20671500	-1.60313100
H	0.73074000	15.07788400	-2.37120000
C	3.67690400	14.53602400	-2.65712100
H	3.73223300	12.58971800	-1.70113100
H	3.58047700	12.47608100	-3.45724000
C	-0.55033800	14.48835300	1.54144800
C	0.12563000	16.39804100	0.17493500
H	2.70711500	16.29021400	-1.73176000
H	3.17569600	15.01664700	-0.59908400
H	4.74256100	14.70098300	-2.47161000
H	3.45089600	14.93652900	-3.65334600
C	-1.16115000	15.40215000	2.40484600
C	-0.50350100	17.26881900	1.06048900
H	0.63198000	16.79543800	-0.69709400
C	-1.15993500	16.78860400	2.19658200
H	-1.66174000	15.02420800	3.29229700
H	-0.47702400	18.33709800	0.86136700

C	-1.85747100	17.71760000	3.16268100
H	-2.94870100	17.65286700	3.06795000
H	-1.61309300	17.47478400	4.20251200
H	-1.57478300	18.75915800	2.98555200
N	5.97767400	-6.73711500	0.05077000
N	3.82201100	-5.45142200	0.08923600
N	-0.20941800	5.75686100	-2.74247100
N	-0.12064100	8.26494300	-2.79605200
N	-5.45751500	-2.36796900	2.73814300
N	-7.70908700	-3.47503200	2.80739500
S	4.36097000	-7.00156400	0.18056700
S	-0.38399000	6.99688900	-3.80737300
S	-6.66351300	-2.69456800	3.80625200
F	-5.09125300	-3.36259900	-1.95191900
F	6.25147200	-1.32711300	-0.37283000
F	0.75128600	5.80461200	1.96865700
F	8.43625100	-2.63363100	-0.47620900
F	0.89559500	8.34825900	1.90735900
F	-7.34792400	-4.54062700	-1.87242600
C	12.34504600	-5.08516900	1.06605100
C	12.58417900	-3.61335500	0.64189200
H	12.76620700	-3.54340900	-0.43452800
H	11.71541800	-2.99330700	0.88108800
H	13.44315800	-3.18220700	1.16283900
C	12.11799300	-5.14142400	2.60058000
H	12.98925300	-4.75598500	3.13939700
H	11.24950600	-4.53781500	2.88419200
H	11.94025900	-6.16944200	2.93051400
C	-12.16127700	-5.10678000	-1.88283300
C	-12.35521800	-3.60634900	-2.21951700
H	-11.39795600	-3.13587200	-2.46149700
H	-13.00857800	-3.47195600	-3.08557000
H	-12.79430600	-3.07069900	-1.37276900
C	-11.55243300	-5.82953100	-3.11458800
H	-10.58246500	-5.39360300	-3.37587000
H	-11.40235300	-6.89319800	-2.90654300
H	-12.21061200	-5.74145300	-3.98465900
C	-0.58508200	12.97822100	1.88338000
C	0.28128600	12.72662800	3.14696900
H	-0.10128100	13.29311500	4.00188900
H	0.27558700	11.66415300	3.41226500
H	1.31871300	13.02867600	2.97445300
C	-2.04147500	12.53327000	2.17109200
H	-2.68065400	12.70457500	1.30001100

H	-2.07961900	11.46865600	2.41844100
H	-2.46570200	13.07675300	3.01923900

D2: the first excited state

N	0.09624700	-0.16635000	-0.04567800
C	-1.09159700	-0.93729400	0.03178600
C	-2.13212400	-0.55185200	0.87979500
C	-1.24255800	-2.08915600	-0.74360900
C	-3.29548900	-1.30069500	0.94826400
H	-2.02595500	0.33943100	1.48750900
C	-2.40429000	-2.83885100	-0.66478100
H	-0.44458600	-2.39599000	-1.40986500
C	-3.45323300	-2.45960100	0.18053800
H	-4.08769300	-0.98764600	1.61649700
H	-2.49986700	-3.72865100	-1.27495200
C	1.35045600	-0.79742200	-0.05208800
C	2.41836300	-0.27517400	-0.79791200
C	1.57122700	-1.97190300	0.68132500
C	3.65010100	-0.89309100	-0.79865300
H	2.26819200	0.61572000	-1.39648100
C	2.79945700	-2.59893300	0.66400900
H	0.76902200	-2.38647300	1.28077600
C	3.89182200	-2.08196600	-0.06906900
H	4.43483100	-0.46962500	-1.40838000
H	2.93619600	-3.50144500	1.24146800
C	-0.00016900	1.24572000	-0.11294100
C	0.86225600	2.05527200	0.63055300
C	-0.96768700	1.85163600	-0.91811200
C	0.76131300	3.43468100	0.56221000
H	1.61349500	1.59918100	1.26476900
C	-1.07041400	3.23168900	-0.97495000
H	-1.64194100	1.23554800	-1.50172300
C	-0.20706300	4.05074300	-0.23897600
H	1.44067700	4.04186000	1.14769600
H	-1.82415100	3.67983800	-1.60973400
C	5.18448300	-2.74363500	-0.07836800
C	5.35937300	-4.15128500	0.14580700
C	6.39109500	-2.04754800	-0.32316500
C	6.67453100	-4.78411700	0.06681200
C	7.63128700	-2.63185700	-0.36400500
C	7.87161700	-4.01820600	-0.17033300
C	-4.69489300	-3.25796600	0.25272900
C	-5.38275100	-3.53281400	1.48560600
C	-5.29397200	-3.79779500	-0.84535000

C	-6.59773800	-4.31909300	1.52091300
C	-6.48911700	-4.57720700	-0.80981000
C	-7.18449100	-4.86876400	0.32586200
C	-0.31938200	5.52324200	-0.29674600
C	-0.58588800	6.24555600	-1.51192600
C	-0.18578300	6.32107600	0.79978800
C	-0.69240800	7.68933500	-1.53266300
C	-0.28485100	7.74463800	0.77816200
C	-0.53694400	8.48221600	-0.34025100
C	-8.42010900	-5.67740800	0.33091800
C	-9.38495900	-5.49497200	-0.66835300
C	-8.63619400	-6.64469600	1.33121000
C	-10.56280800	-6.23896700	-0.71424000
H	-9.20510100	-4.74174800	-1.42611000
C	-9.78773300	-7.39860600	1.29988400
H	-7.90175400	-6.78769600	2.11467300
C	-10.71923000	-7.19093300	0.28197500
C	-10.28782600	-8.50546000	2.19453900
N	-11.80524400	-8.02560700	0.40408800
C	-11.69393900	-8.86842500	1.59793100
C	-9.47997300	-9.81977400	2.16612200
H	-10.39325300	-8.16381200	3.22823200
C	-12.92943700	-7.83679700	-0.38629100
C	-11.65742100	-10.38705700	1.32648400
H	-12.50035200	-8.61840600	2.29651200
C	-10.54917500	-10.91116400	2.24530400
H	-8.93923900	-9.89945800	1.21697200
H	-8.74292800	-9.87197600	2.97087400
C	-12.88859500	-6.89839200	-1.44188300
C	-14.09860500	-8.56311500	-0.14666500
H	-12.61960000	-10.87530500	1.49730700
H	-11.38222600	-10.55089100	0.27949700
H	-10.18179100	-11.89603500	1.94628100
H	-10.92174800	-10.99690800	3.27250300
C	-14.03597200	-6.75455900	-2.21620400
C	-15.22169600	-8.38008400	-0.94085000
H	-14.12790300	-9.27955000	0.66537000
C	-15.21212800	-7.47322000	-1.99495300
H	-14.02073200	-6.04971500	-3.04237100
H	-16.11726800	-8.95891400	-0.73409100
C	-16.42135000	-7.25984200	-2.86800100
H	-16.84196400	-6.25781800	-2.73306100
H	-16.17350100	-7.36274300	-3.92880000
H	-17.20745500	-7.98203800	-2.63648300

C	9.19230300	-4.59243800	-0.20777400
C	10.35018300	-3.80520900	0.08027200
C	9.38712800	-5.97194600	-0.52897000
C	11.63064400	-4.31030700	0.05266300
H	10.20748400	-2.77210200	0.35883700
C	10.64904200	-6.48965100	-0.56785100
H	8.52666700	-6.58808900	-0.74406000
C	11.75173200	-5.66565700	-0.27862500
C	11.15567800	-7.87792600	-0.86465900
N	12.92176300	-6.33551000	-0.36384600
C	12.70818300	-7.75304900	-0.69825500
C	10.71851400	-8.98144600	0.12457600
H	10.90898700	-8.17373900	-1.88794100
C	14.14136400	-5.69018900	-0.18176100
C	13.09346200	-8.74751800	0.41412900
H	13.23633400	-7.97904800	-1.62871400
C	11.98805700	-9.80549500	0.35370400
H	10.39670500	-8.52549400	1.06612400
H	9.88265600	-9.57021200	-0.25850900
C	14.15271300	-4.32463600	0.17007000
C	15.34095700	-6.38755200	-0.35309000
H	14.09436400	-9.16448500	0.28784800
H	13.06501900	-8.23158600	1.37945200
H	11.94332600	-10.41930900	1.25630100
H	12.16013700	-10.47803300	-0.49399600
C	15.39586900	-3.72444500	0.34876100
C	16.55418700	-5.74765300	-0.17045700
H	15.32219400	-7.43443300	-0.62864100
C	16.60467200	-4.40077000	0.18595900
H	15.43328600	-2.67688300	0.63107000
H	17.47541900	-6.30612300	-0.30445700
C	17.91860900	-3.68884600	0.36424800
H	18.24343600	-3.22003400	-0.57106500
H	17.84534700	-2.89847400	1.11505900
H	18.70609100	-4.38060600	0.67206900
C	-0.63656400	9.95553800	-0.33139600
C	-1.29805100	10.61011500	0.71598200
C	-0.06170700	10.71632400	-1.36760200
C	-1.41302600	11.99796600	0.77540500
H	-1.73938800	10.00879400	1.50166000
C	-0.15492300	12.08925200	-1.32484200
H	0.44402300	10.22054200	-2.18731400
C	-0.81622700	12.70182400	-0.25981400
C	0.36749500	13.16073200	-2.24914000

N	-0.81649900	14.07203300	-0.37754600
C	-0.16590500	14.49666300	-1.62070000
C	1.90100700	13.32021200	-2.30440900
H	-0.02352800	13.03804300	-3.26321500
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C	1.07160700	15.40055800	-1.43631400
H	-0.90479100	14.97705100	-2.27209100
C	2.10913200	14.83201200	-2.41000000
H	2.34331800	12.94979200	-1.37334000
H	2.34798600	12.75919700	-3.12847300
C	-2.24753900	14.24556000	1.56516000
C	-1.74648100	16.21931300	0.23619000
H	0.85808300	16.45756700	-1.61095700
H	1.43112800	15.29942000	-0.40721500
H	3.12892400	15.14407200	-2.17118400
H	1.89231400	15.16966000	-3.42994700
C	-3.00523200	15.06939100	2.39266000
C	-2.51914600	16.99972900	1.08393700
H	-1.24829700	16.67848400	-0.60904200
C	-3.16325100	16.44009500	2.18229200
H	-3.49848300	14.62924300	3.25434800
H	-2.61556900	18.06317700	0.88479900
C	-4.01410100	17.26998100	3.10818700
H	-5.08116200	17.07694600	2.95330400
H	-3.79737700	17.04933700	4.15735600
H	-3.84711700	18.33756800	2.94778400
N	6.64128000	-6.09466100	0.27500900
N	4.37769100	-5.00889300	0.40566900
N	-0.75372000	5.69554300	-2.70901600
N	-0.95071100	8.17120800	-2.74305900
N	-4.99638400	-3.11956600	2.68713600
N	-7.08872700	-4.45699900	2.74728500
S	5.05488800	-6.52123700	0.54738300
S	-1.03542400	6.90501900	-3.76190900
S	-6.08822700	-3.67057200	3.76185200
F	-4.77924900	-3.62243200	-2.06937200
F	6.37369200	-0.71241800	-0.51576600
F	0.05479600	5.79857200	2.00948400
F	8.65329300	-1.79822200	-0.64848400
F	-0.10362100	8.33093000	1.97039500
F	-6.89562900	-5.02388200	-2.00688100
C	12.87565700	-3.49175900	0.37762100
C	12.91238200	-2.25274800	-0.54147400
H	12.97716000	-2.54887100	-1.59114100

H	12.00876700	-1.65267600	-0.41155000
H	13.76850800	-1.61556600	-0.31081600
C	12.80292500	-3.03448800	1.85044800
H	13.67039300	-2.42415400	2.11268800
H	11.90491800	-2.43460600	2.01924500
H	12.77177600	-3.89385400	2.52467000
C	-11.63280700	-6.07348300	-1.79121400
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H	-11.11935900	-3.98432000	-2.15992800
H	-12.73147000	-4.41556900	-2.71055000
H	-12.42055600	-4.20505100	-0.98038500
C	-11.06445900	-6.56927300	-3.13793000
H	-10.16911500	-6.00224200	-3.40923600
H	-10.79262500	-7.62641500	-3.07997400
H	-11.79922200	-6.44962400	-3.93895100
C	-2.11447700	12.74719200	1.90630100
C	-1.27729800	12.59869800	3.19469900
H	-1.75817200	13.11094700	4.03264900
H	-1.16360400	11.54341600	3.45976300
H	-0.27968800	13.02512900	3.06145400
C	-3.50912100	12.13279300	2.13633700
H	-4.13178400	12.23580800	1.24426700
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H	-4.02463900	12.61224200	2.97082900

E2: ground state

N	0.06047300	0.21957800	-0.10926600
C	1.40957700	0.64783400	0.00918000
C	2.30473300	-0.03164100	0.85067900
C	1.87773100	1.75989300	-0.70995300
C	3.62759000	0.38050100	0.96015900
H	1.96006300	-0.88848000	1.41927800
C	3.19796700	2.17415700	-0.58628700
H	1.20138400	2.30307800	-1.36087500
C	4.10952800	1.49156000	0.24207200
H	4.29407000	-0.16604600	1.61666200
H	3.52259600	3.05124400	-1.13675300
C	-0.99088700	1.17027400	-0.13407400
C	-2.09474100	0.99755000	-0.98723600
C	-0.95304600	2.30915500	0.68716600
C	-3.12733700	1.92536500	-1.00184700
H	-2.13211200	0.14026900	-1.65036100
C	-1.98293800	3.24184600	0.65549300
H	-0.11596800	2.45731800	1.36055800

C	-3.10323800	3.06922800	-0.17990800
H	-3.94914000	1.77858000	-1.69539300
H	-1.92756000	4.10378600	1.30963900
C	-0.23152300	-1.16781800	-0.19352600
C	-1.31365000	-1.72000000	0.51160500
C	0.55496600	-2.01796100	-0.98722800
C	-1.59545400	-3.07723100	0.42041900
H	-1.93770900	-1.08031200	1.12599100
C	0.27522900	-3.37731000	-1.06389100
H	1.39063900	-1.60902800	-1.54475900
C	-0.80493900	-3.94285400	-0.35978700
H	-2.45294200	-3.46852400	0.95828600
H	0.90196800	-4.00722300	-1.68383100
C	-4.22676300	4.02442300	-0.18985000
C	-4.07039600	5.43063700	0.07470800
C	-5.52966300	3.65223200	-0.46102300
C	-5.18814200	6.34705700	0.04410000
C	-6.63166400	4.55579200	-0.49478800
H	-5.74533100	2.60597500	-0.65126700
C	-6.53286800	5.91230400	-0.24322400
H	-7.60171000	4.14002500	-0.74551400
C	5.51922600	1.92092200	0.32456500
C	6.32098500	1.76792200	1.50982900
C	6.19146100	2.50992900	-0.72863100
C	7.69791800	2.20401200	1.56750400
C	7.54904000	2.94231100	-0.67232400
H	5.66984800	2.64788300	-1.67010900
C	8.36105500	2.81048500	0.43938400
H	7.95365500	3.41217400	-1.56233500
C	-1.09701500	-5.38879800	-0.40884700
C	-0.83871900	-6.20604000	-1.56493700
C	-1.65085600	-6.08263200	0.64945100
C	-1.14971400	-7.61740100	-1.59280800
C	-1.95971800	-7.47436900	0.62248200
H	-1.86087500	-5.54980400	1.57111200
C	-1.72834600	-8.30073600	-0.46210200
H	-2.41697000	-7.89469900	1.51179000
C	9.77351800	3.22734300	0.46567600
C	10.54367000	3.17266600	-0.71589700
C	10.38209300	3.69673300	1.65617000
C	11.88294700	3.56807000	-0.76650200
H	10.08013100	2.77463100	-1.61268500
C	11.70194600	4.10414500	1.62965700
H	9.81141100	3.74043400	2.57655300

C	12.42487200	4.04022500	0.42974400
C	12.60035700	4.66810000	2.70775000
N	13.72361900	4.46833700	0.58812100
C	13.99008400	4.85694900	1.98503700
C	12.22436200	6.07241800	3.24918400
H	12.70332100	3.97037400	3.54542100
C	14.64990800	4.32488800	-0.43983900
C	14.38044700	6.34233000	2.19751600
H	14.75329800	4.19123700	2.40504800
C	13.57811800	6.77339000	3.43745500
H	11.62928200	6.60928000	2.50120800
H	11.63041800	6.01708900	4.16583000
C	14.21916900	3.86122700	-1.71030000
C	16.00454300	4.63293500	-0.23173100
H	15.45775400	6.48731500	2.31574800
H	14.06014900	6.92279000	1.32492500
H	13.49053500	7.86041700	3.52666000
H	14.06759000	6.40712700	4.34855900
C	15.18512900	3.75081100	-2.71532000
C	16.93120500	4.49930700	-1.26119900
H	16.33184600	4.98356600	0.74010200
C	16.53976100	4.05687100	-2.52814700
H	14.87397600	3.41289900	-3.70019800
H	17.97225700	4.74851500	-1.07210800
C	17.53674300	3.88944700	-3.65100900
H	17.87153900	2.84807500	-3.74116900
H	17.10495800	4.17153000	-4.61668100
H	18.42724200	4.50327500	-3.48700500
C	-7.68996400	6.82380200	-0.24729600
C	-8.96505700	6.34052300	0.11727600
C	-7.55877300	8.18172500	-0.63114300
C	-10.10970600	7.14161100	0.11001100
H	-9.04899700	5.30937800	0.44493100
C	-8.67572900	8.99485200	-0.64700800
H	-6.59038400	8.57186100	-0.92222800
C	-9.92184500	8.46940600	-0.27609200
C	-8.84932100	10.45700000	-0.99621400
N	-10.92033800	9.41360500	-0.34851300
C	-10.39375200	10.71348600	-0.79992300
C	-8.13788300	11.47298900	-0.06347700
H	-8.56419700	10.65203700	-2.03545400
C	-12.25025300	9.06253500	-0.14354400
C	-10.50229600	11.86808300	0.22811900
H	-10.87640300	10.99099100	-1.74418000

C	-9.15961000	12.60833400	0.10670200
H	-7.93800000	11.00503200	0.90734100
H	-7.17990500	11.80823400	-0.47067700
C	-12.56876900	7.74216600	0.26963900
C	-13.27814200	9.99903100	-0.34135000
H	-11.36505600	12.51631200	0.05225500
H	-10.60482600	11.44229300	1.23285500
H	-8.95001900	13.24764500	0.96956800
H	-9.16285000	13.24936000	-0.78384500
C	-13.91792000	7.44224700	0.47968100
C	-14.60867300	9.65096500	-0.12715000
H	-13.03337700	11.00591500	-0.65940100
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H	-14.18147300	6.44159100	0.81213300
H	-15.38316000	10.39715300	-0.28510000
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H	-16.51030900	7.35117900	1.41332900
H	-17.04037000	8.84325800	0.62220100
C	-2.02683900	-9.74298800	-0.46054300
C	-1.94669100	-10.47625500	0.74290100
C	-2.41195100	-10.41688900	-1.64626800
C	-2.24018100	-11.84025400	0.81954800
H	-1.61088300	-9.96167100	1.63752400
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H	-2.47260400	-9.87457600	-2.58272500
C	-2.63457000	-12.44757900	-0.37345900
C	-3.17930000	-12.72990400	-2.66262800
N	-2.95960500	-13.77840700	-0.50663800
C	-3.29702500	-14.10768800	-1.90304000
C	-4.58583600	-12.46812400	-3.26279600
H	-2.44569400	-12.80751000	-3.47190800
C	-2.78912600	-14.66267500	0.55342100
C	-4.74944600	-14.59739500	-2.13713400
H	-2.57534800	-14.83878900	-2.28594800
C	-5.19306800	-13.87091400	-3.41826000
H	-5.18456400	-11.88097700	-2.55673900
H	-4.53827600	-11.90796400	-4.20085000
C	-2.39549800	-14.16522300	1.82304200
C	-3.00206700	-16.04018700	0.37868400
H	-4.82544700	-15.68537300	-2.21558900
H	-5.37245400	-14.28005600	-1.29312300
H	-6.28025500	-13.85692500	-3.54100500
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C	-2.83969100	-16.92552400	1.43984000
H	-3.30177700	-16.41764000	-0.59206000
C	-2.46255300	-16.46900700	2.70624200
H	-1.96627200	-14.73021500	3.84416100
H	-3.01448400	-17.98585300	1.27620100
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N	5.99533500	1.25498100	2.68405500
N	8.17113500	1.93075600	2.77105300
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O	-3.39464100	7.41005500	0.52043300
C	-11.50140200	6.64897900	0.52413400
C	-11.85144400	5.37653100	-0.28980800
H	-11.88017700	5.59611500	-1.36110100
H	-11.10756000	4.59219400	-0.12228200
H	-12.82361600	4.97090500	0.00254200
C	-11.48343700	6.29757400	2.03588800
H	-12.45927500	5.92487100	2.36227800
H	-10.73867500	5.52230600	2.24384000
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C	-2.14880600	-12.66357600	2.11016000
C	-0.74234700	-12.47627800	2.73566900
H	-0.65143200	-13.01949900	3.67995200
H	0.03585500	-12.83732300	2.05695200
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C	-3.22220100	-12.15249300	3.10807000
H	-3.17353500	-12.70372300	4.05218200
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H	-4.22775800	-12.27309000	2.69395000
C	12.74651700	3.50590100	-2.03232500
C	12.19295100	4.52088000	-3.06805500
H	11.15093100	4.29109800	-3.31346400
H	12.23293500	5.54083700	-2.67403900
H	12.77386100	4.49030600	-3.99500300
C	12.67265800	2.07733700	-2.63059400
H	11.64009200	1.80834600	-2.87145800

H	13.25114400	2.00242500	-3.55500500
H	13.06141500	1.33930800	-1.92292600

E2: the first excited state

N	0.01136400	-0.16719000	0.06436800
C	-1.31419600	-0.66579500	0.12163100
C	-2.27741500	-0.02843800	0.90697700
C	-1.68239600	-1.79993000	-0.60728600
C	-3.57563700	-0.50935100	0.95733200
H	-2.00531400	0.84964400	1.48123500
C	-2.97716600	-2.28429900	-0.53946300
H	-0.94676600	-2.30719200	-1.22054700
C	-3.95491100	-1.64736300	0.23505300
H	-4.30194300	0.00371100	1.57513900
H	-3.22822100	-3.18200200	-1.09351600
C	1.10614300	-1.04215100	0.09817700
C	2.28277200	-0.75401500	-0.61518500
C	1.06135500	-2.23421200	0.83743500
C	3.35524300	-1.61500400	-0.58472100
H	2.33840200	0.14840700	-1.21258700
C	2.13382400	-3.09965200	0.85762200
H	0.17335300	-2.47420900	1.41055200
C	3.33151700	-2.82738500	0.15121900
H	4.22094000	-1.35693400	-1.18134200
H	2.06373100	-4.00356400	1.44609700
C	0.21604400	1.23349700	-0.02758800
C	1.18273100	1.86440600	0.75906700
C	-0.54875000	2.00430000	-0.90563100
C	1.37807000	3.23173700	0.66222800
H	1.78518100	1.27741900	1.44277600
C	-0.35742100	3.37385800	-0.98784200
H	-1.29814400	1.52504500	-1.52517100
C	0.60781000	4.01726000	-0.20381200
H	2.15034800	3.69501300	1.26640200
H	-0.96340600	3.94973100	-1.67627000
C	4.46346900	-3.72066400	0.17091500
C	4.42673600	-5.04378300	0.72675400
C	5.72556300	-3.35843200	-0.37611600
C	5.57477500	-5.91956500	0.69707600
C	6.82407700	-4.18211900	-0.38834600
H	5.84951800	-2.36831300	-0.79437400
C	6.83366300	-5.51019100	0.13588200
H	7.72233100	-3.79000700	-0.84520300
C	-5.33764400	-2.16263800	0.26367900

C	-6.19252800	-2.04440700	1.41441300
C	-5.91886300	-2.80589900	-0.79429000
C	-7.52536200	-2.57560500	1.42927700
C	-7.24495800	-3.34221100	-0.77713700
H	-5.35449700	-2.92138800	-1.71300000
C	-8.09312000	-3.25584700	0.29374500
H	-7.57869400	-3.85925100	-1.66964800
C	0.80311400	5.47929500	-0.25976200
C	0.62709900	6.24384500	-1.46481200
C	1.17211100	6.22700200	0.82411100
C	0.83477900	7.66264700	-1.50114900
C	1.38388700	7.64180900	0.78718900
H	1.30751900	5.73351300	1.78025200
C	1.22492400	8.41058600	-0.33387700
H	1.69930000	8.11805300	1.70871600
C	-9.46317800	-3.80017700	0.29020700
C	-10.19851900	-3.82818600	-0.90326900
C	-10.04220900	-4.32195100	1.46415800
C	-11.47962800	-4.37048000	-0.98450400
H	-9.75599500	-3.38810900	-1.79047600
C	-11.30574100	-4.86582100	1.40820800
H	-9.49359800	-4.29875500	2.39816000
C	-11.99239600	-4.89328500	0.19393800
C	-12.16535200	-5.51493200	2.46416200
N	-13.23220300	-5.47342400	0.32002800
C	-13.49573500	-5.86520300	1.70778100
C	-11.64926900	-6.85530200	3.02810400
H	-12.36964400	-4.82561300	3.28841300
C	-14.14412500	-5.41856500	-0.72387700
C	-13.72243700	-7.37511800	1.93212600
H	-14.34008600	-5.28438000	2.09553500
C	-12.91546100	-7.69739300	3.19410800
H	-10.98255000	-7.32907200	2.29966000
H	-11.08619600	-6.72652900	3.95540800
C	-13.73737400	-4.91191500	-1.97774400
C	-15.45819000	-5.85983700	-0.54519400
H	-14.77838100	-7.64005400	2.02229000
H	-13.31335400	-7.92376400	1.07746200
H	-12.71066600	-8.76525300	3.30402200
H	-13.46637000	-7.37477700	4.08500500
C	-14.68345400	-4.89316500	-2.99910400
C	-16.36889800	-5.81457000	-1.59031500
H	-15.76730200	-6.24682100	0.41820100
C	-15.99871200	-5.33123500	-2.84128400

H	-14.38652000	-4.52373900	-3.97635100
H	-17.38303800	-6.16706100	-1.42546600
C	-16.97912200	-5.26135600	-3.98311600
H	-17.36047400	-4.24381700	-4.12248300
H	-16.51655200	-5.56310200	-4.92692100
H	-17.83938400	-5.91124600	-3.80656200
C	8.00076000	-6.34428900	0.09582000
C	9.25776100	-5.82361400	-0.34352500
C	7.95630600	-7.72070200	0.48371400
C	10.40833600	-6.57705400	-0.41654700
H	9.32137500	-4.77891600	-0.61605400
C	9.08586000	-8.48501900	0.41738600
H	7.02148900	-8.14543300	0.82163900
C	10.29189500	-7.91645500	-0.02654000
C	9.33924700	-9.93045000	0.76352500
N	11.30457100	-8.81427900	-0.03586700
C	10.86306600	-10.12859700	0.45640700
C	9.16257500	-10.31114400	2.25022900
H	8.73856900	-10.59359100	0.13501600
C	12.56625900	-8.47559400	-0.51315800
C	11.50495200	-10.57713400	1.78396700
H	11.02481200	-10.87307500	-0.32851100
C	10.34870200	-11.23288200	2.54415900
H	9.22892200	-9.41201500	2.87107600
H	8.19345800	-10.77500100	2.44493800
C	12.81554600	-7.15026000	-0.92414100
C	13.57520500	-9.44113000	-0.59037500
H	12.35868800	-11.24291900	1.64308700
H	11.85558600	-9.69353700	2.32726100
H	10.55390700	-11.34049000	3.61181600
H	10.15708600	-12.23428800	2.14273800
C	14.09631500	-6.85717700	-1.38631300
C	14.83176300	-9.10526500	-1.06214300
H	13.37314900	-10.45761800	-0.27688900
C	15.11749500	-7.80254200	-1.46922300
H	14.31858000	-5.84103400	-1.69729600
H	15.60270100	-9.86829300	-1.11082900
C	16.47499800	-7.43328000	-2.00465400
H	16.54982900	-7.64914500	-3.07608300
H	16.67975700	-6.36852100	-1.87153800
H	17.26618800	-7.99777700	-1.50509200
C	1.41612500	9.87228200	-0.35116300
C	1.09423700	10.62902600	0.78418200
C	1.93558500	10.52497400	-1.48665500

C	1.27786600	12.00931300	0.84376000
H	0.66173300	10.11717600	1.63721200
C	2.13269800	11.88707700	-1.44918100
H	2.17936300	9.95676100	-2.37656400
C	1.81261200	12.59904000	-0.29252600
C	2.68760800	12.84915300	-2.46941900
N	2.06484100	13.94347300	-0.43278400
C	2.54850500	14.25322400	-1.78193200
C	4.18893600	12.70166300	-2.79257000
H	2.11014600	12.82384100	-3.39788700
C	1.61257600	14.84513600	0.52001900
C	3.95098600	14.89511200	-1.84241900
H	1.81112900	14.87908300	-2.29721800
C	4.66895000	14.14327500	-2.96817900
H	4.70440500	12.24027700	-1.94334500
H	4.36589700	12.07246000	-3.66797600
C	1.05935000	14.36429400	1.72659400
C	1.70188900	16.22203700	0.29574200
H	3.91907900	15.97486800	-2.00511400
H	4.46112200	14.71761900	-0.89016000
H	5.75597200	14.24441900	-2.91799900
H	4.34743900	14.52869400	-3.94250700
C	0.63897900	15.30824200	2.66039100
C	1.26194400	17.12529200	1.25153100
H	2.12526000	16.58762200	-0.63191800
C	0.72262300	16.68569600	2.45668300
H	0.22801100	14.95983400	3.60327500
H	1.34646400	18.18999400	1.05345500
C	0.22462800	17.65421400	3.49775300
H	-0.85781600	17.80492400	3.41975100
H	0.42726600	17.29262200	4.50938900
H	0.69802700	18.63282000	3.38778500
N	5.24280200	-7.06375600	1.25904600
N	3.42821400	-5.67883200	1.30596100
N	0.28047700	5.84753100	-2.66817900
N	0.59767000	8.08065500	-2.72359300
N	-5.95913300	-1.48731600	2.58082700
N	-8.05793500	-2.31383000	2.60111400
O	0.26397800	6.97164300	-3.42496400
O	-7.09932500	-1.65498400	3.29369500
O	3.92207200	-6.92630700	1.63825900
C	11.76069100	-6.03058900	-0.86574100
C	11.60723600	-5.39259600	-2.26196100
H	11.28897300	-6.13606000	-2.99663100

H	10.86247500	-4.59348400	-2.24019400
H	12.54817700	-4.95539900	-2.60206600
C	12.22280800	-4.95458900	0.14042000
H	13.18351500	-4.52855700	-0.15863500
H	11.49451600	-4.14100100	0.19275300
H	12.33323600	-5.37914400	1.14128400
C	0.94548200	12.86383600	2.06530900
C	-0.48409100	12.53905100	2.54134700
H	-0.74297700	13.10069000	3.44108200
H	-1.21628600	12.77780000	1.76612500
H	-0.58033500	11.47891900	2.78684100
C	1.94322100	12.52651500	3.19386700
H	1.72979100	13.11430000	4.09093900
H	1.88025300	11.46674500	3.45801300
H	2.96926000	12.73958600	2.88298800
C	-12.30291800	-4.42555600	-2.26970700
C	-11.62907200	-5.40821400	-3.25099900
H	-10.60996100	-5.08399800	-3.48112600
H	-11.57826500	-6.41230800	-2.82214100
H	-12.18709800	-5.46612300	-4.18952700
C	-12.34458400	-3.02272600	-2.90744300
H	-11.33554700	-2.66460200	-3.12489800
H	-12.89365500	-3.02964800	-3.85119300
H	-12.82436600	-2.30500600	-2.23751700

F2: ground state

N	-0.05583800	0.18491500	0.10971600
C	-1.39165600	0.65455900	0.01512800
C	-2.32412200	0.00150200	-0.80682100
C	-1.81173800	1.78052700	0.74236000
C	-3.63499000	0.45386300	-0.88904000
H	-2.01918300	-0.86534200	-1.38243400
C	-3.12064700	2.23557600	0.64929600
H	-1.10834700	2.30023600	1.38344900
C	-4.06664100	1.58079300	-0.16356900
H	-4.32936400	-0.07155400	-1.53328500
H	-3.41100700	3.10889300	1.21971900
C	1.02365100	1.10457800	0.14726800
C	2.12375400	0.88255700	0.99241900
C	1.01889200	2.25454000	-0.65879800
C	3.19005500	1.77149800	1.01529300
H	2.13764100	0.01248900	1.63943200
C	2.07906800	3.15159000	-0.61802700
H	0.18512900	2.43968000	-1.32689700

C	3.19443700	2.92816100	0.21152700
H	4.01753800	1.57731000	1.68634300
H	2.04920200	4.02567100	-1.25743700
C	0.20169500	-1.21066800	0.15776300
C	1.27060400	-1.76841500	-0.56262000
C	-0.60546400	-2.06321700	0.92765400
C	1.52419200	-3.13281600	-0.51049800
H	1.90553200	-1.12797400	-1.16470800
C	-0.35459400	-3.42920300	0.96900200
H	-1.43244600	-1.65225500	1.49615600
C	0.71605100	-3.99779100	0.25301200
H	2.35948600	-3.53013900	-1.07340400
H	-0.99335400	-4.06009900	1.57504700
C	4.32605900	3.87440900	0.23263300
C	4.17954400	5.29639700	0.06445700
C	5.64139800	3.50791000	0.39946900
C	5.29995500	6.20851700	0.08209800
C	6.75243900	4.41147600	0.41828100
C	6.66527300	5.77658400	0.25943100
C	-5.46231100	2.05151000	-0.25579400
C	-6.26225400	1.94430100	-1.44808200
C	-6.16053200	2.62596800	0.78099600
C	-7.63228900	2.39844400	-1.51915300
C	-7.51714100	3.07973200	0.71058000
C	-8.32530600	2.99289500	-0.40130000
C	0.98101600	-5.44870300	0.30912300
C	0.73974400	-6.25851500	1.47487800
C	1.47808900	-6.18988200	-0.73771500
C	1.01105900	-7.67725900	1.51544700
C	1.75027900	-7.59543400	-0.69734100
C	1.53927000	-8.41207900	0.39127500
C	-9.72508400	3.44530600	-0.46068400
C	-10.55807200	3.35915100	0.67646500
C	-10.26094000	3.96548600	-1.66596200
C	-11.89395200	3.76545900	0.66304500
H	-10.14565400	2.94486100	1.58762700
C	-11.57661100	4.38247900	-1.69943700
H	-9.64033600	4.03595100	-2.55130300
C	-12.36617100	4.28183300	-0.54443600
C	-12.40966600	4.99103900	-2.80573100
N	-13.64798900	4.73086100	-0.75700000
C	-13.83028900	5.18716600	-2.14691500
C	-11.98207900	6.40091100	-3.29249200
H	-12.48303500	4.31488600	-3.66389900

C	-14.62846400	4.57542900	0.21881100
C	-14.16942100	6.69027600	-2.31297300
H	-14.58723800	4.56275700	-2.63545000
C	-13.31098200	7.14154700	-3.50691900
H	-11.40047200	6.90160600	-2.50974500
H	-11.35817300	6.35686600	-4.18959300
C	-14.27007700	4.07030400	1.49560700
C	-15.96549500	4.91137300	-0.04955500
H	-15.23704400	6.87342000	-2.46155500
H	-13.86209000	7.22668700	-1.40803800
H	-13.19374600	8.22830200	-3.55579400
H	-13.77461800	6.81822500	-4.44731300
C	-15.28764900	3.94822700	2.44697800
C	-16.94543800	4.76548200	0.92758700
H	-16.23757100	5.29244500	-1.02698600
C	-16.62588900	4.28216200	2.19987200
H	-15.03250600	3.57798200	3.43629800
H	-17.97147800	5.03727900	0.69315000
C	-17.68171600	4.10044100	3.26516200
H	-18.05061000	3.06714900	3.29463500
H	-17.29005700	4.32940500	4.26140700
H	-18.54498900	4.74762200	3.08445900
C	7.81315900	6.69862000	0.27043200
C	9.06334600	6.29734100	-0.24873600
C	7.67778400	8.00501400	0.80394900
C	10.17685600	7.13992000	-0.26332000
H	9.15271300	5.30202100	-0.66547300
C	8.76609700	8.85459000	0.80241200
H	6.72964400	8.32738500	1.21802300
C	9.98657600	8.41679500	0.26715400
C	8.93031700	10.27889100	1.28635600
N	10.95970700	9.38456200	0.34730800
C	10.44266300	10.61005100	0.98177500
C	8.10889600	11.35907700	0.53355900
H	8.73764100	10.35544900	2.36163700
C	12.27991500	9.09743500	0.01308100
C	10.42502500	11.86908800	0.07818700
H	11.00336200	10.80336100	1.90357100
C	9.07958600	12.54252600	0.39645300
H	7.83324100	10.98775900	-0.46021300
H	7.18363300	11.61501600	1.05730100
C	12.59909000	7.83344700	-0.54824300
C	13.29537500	10.04320500	0.22813700
H	11.28240500	12.52655900	0.24576600

H	10.44703300	11.55441100	-0.97149900
H	8.77466400	13.26024900	-0.37104200
H	9.14718800	13.08693400	1.34675400
C	13.93714500	7.59582500	-0.87623300
C	14.61543600	9.75815100	-0.10857700
H	13.04955200	11.00784500	0.65688900
C	14.96457100	8.52651800	-0.66958100
H	14.20106300	6.64035600	-1.32150700
H	15.38059600	10.51014200	0.06630400
C	16.39523000	8.19440100	-1.02367700
H	16.86498400	7.56662800	-0.25578300
H	16.45810300	7.64452100	-1.96843300
H	17.00151800	9.09975900	-1.11934900
C	1.82117700	-9.85661700	0.42481700
C	1.65953400	-10.64988000	-0.73228000
C	2.25930300	-10.47294000	1.62427000
C	1.91578200	-12.02254000	-0.74458000
H	1.30817200	-10.17434800	-1.63932500
C	2.52835100	-11.82693900	1.63251100
H	2.38484000	-9.88263600	2.52422500
C	2.36035200	-12.57464700	0.45767100
C	3.02671300	-12.74570800	2.72636600
N	2.66606900	-13.90165800	0.64491200
C	3.08693100	-14.16180800	2.03332800
C	4.46390300	-12.47767500	3.24658500
H	2.33007100	-12.76903100	3.57087400
C	2.42656500	-14.83753800	-0.35689700
C	4.54701400	-14.65357000	2.20322300
H	2.38534300	-14.86446100	2.49759500
C	5.06561200	-13.88005000	3.42725200
H	5.03309000	-11.92443000	2.49060500
H	4.46773200	-11.88182800	4.16358000
C	1.97791200	-14.39876800	-1.63023500
C	2.62139000	-16.20732000	-0.11843100
H	4.62164800	-15.73807600	2.32053200
H	5.12300400	-14.37449600	1.31347500
H	6.15789000	-13.87303600	3.49076500
H	4.68578600	-14.33690400	4.34970300
C	1.76358800	-15.37535700	-2.60694100
C	2.38792700	-17.14405200	-1.12132000
H	2.96085000	-16.53951600	0.85575500
C	1.95559200	-16.74688500	-2.38942400
H	1.43405900	-15.06000100	-3.59335500
H	2.54966900	-18.19786800	-0.90970300

C	1.68574600	-17.75050200	-3.48608700
H	0.60962600	-17.89511700	-3.64432700
H	2.10768700	-17.42435400	-4.44275000
H	2.11494300	-18.72699300	-3.24451500
N	4.84215800	7.43352500	-0.10134500
N	3.07350600	5.99516600	-0.11605800
N	0.26646600	-5.88959200	2.65141500
N	0.68174000	-8.12980300	2.71142000
N	-5.92294300	1.45298700	-2.62607600
N	-8.08784700	2.15676500	-2.73476700
O	0.23188900	-7.03635200	3.39904700
O	-7.04188600	1.58385000	-3.40445400
O	3.48587500	7.29707500	-0.21835400
F	-5.58458500	2.79962800	1.98392600
F	-7.97220700	3.62463400	1.85521200
F	1.75240600	-5.61042300	-1.91995200
F	2.25772200	-8.08853700	-1.84330700
F	7.94261800	3.81332600	0.61626900
F	5.97957400	2.21581400	0.55707100
C	11.53949300	6.74308100	-0.84354900
C	11.40135300	6.57460700	-2.38041600
H	12.35499200	6.27788300	-2.82803900
H	10.66017100	5.80459400	-2.61849600
H	11.08200600	7.51101700	-2.84765300
C	11.98457700	5.39454600	-0.22186700
H	12.10531200	5.48629800	0.86148700
H	11.24445300	4.61321900	-0.41717300
H	12.93355500	5.05389200	-0.64417600
C	-12.82138600	3.68243800	1.88120500
C	-12.79842700	2.23704800	2.44148500
H	-11.78226900	1.94475300	2.72156100
H	-13.42028200	2.14638500	3.33591400
H	-13.16513100	1.52526600	1.69613200
C	-12.30534700	4.65996800	2.97097200
H	-11.27956000	4.40833500	3.25933900
H	-12.31242800	5.69087400	2.60452100
H	-12.93074800	4.61225900	3.86766900
C	1.75102600	-12.90849200	-1.98519700
C	0.32447600	-12.71807000	-2.56161000
H	-0.43314100	-13.02330500	-1.83393600
H	0.14709700	-11.66997100	-2.81965500
H	0.18093500	-13.30632100	-3.47175800
C	2.79321200	-12.47571000	-3.05100100
H	2.69221800	-13.07295800	-3.96240500

H	2.65612000	-11.42292600	-3.31875300
H	3.81209600	-12.60056900	-2.67227000

F2: the first excited state

N	-0.10977400	-0.04507200	-0.15526200
C	-1.51189100	-0.05698400	-0.08444600
C	-2.20858000	0.94517800	0.60629800
C	-2.26024200	-1.07271900	-0.70039300
C	-3.58488400	0.93293900	0.67743600
H	-1.65784000	1.73758800	1.09942600
C	-3.63561400	-1.08317400	-0.63168100
H	-1.75027400	-1.86078800	-1.24185200
C	-4.36011200	-0.07831200	0.05899600
H	-4.08190000	1.71613800	1.23135700
H	-4.16317300	-1.89014100	-1.11606100
C	0.62332900	-1.25660200	-0.15509100
C	1.72490600	-1.41620500	-1.00005700
C	0.26417300	-2.30866400	0.69104700
C	2.45145900	-2.59404400	-0.99124800
H	2.00625200	-0.61443700	-1.67283800
C	0.98344000	-3.49175400	0.68390000
H	-0.57895000	-2.19403900	1.36216200
C	2.09430200	-3.65697200	-0.15202700
H	3.29467600	-2.69643800	-1.66222600
H	0.68595900	-4.29129500	1.35079700
C	0.59141700	1.18561200	-0.21431400
C	1.73652600	1.38607800	0.56011400
C	0.15303400	2.21383700	-1.05161300
C	2.42378700	2.58608800	0.49825800
H	2.08787600	0.59597100	1.21358300
C	0.83821800	3.41598100	-1.10377800
H	-0.72905900	2.06769200	-1.66414400
C	1.98600200	3.62679400	-0.33038200
H	3.30959400	2.71664100	1.10639500
H	0.48145700	4.19633200	-1.76417400
C	2.86240500	-4.91587500	-0.14628300
C	2.26360900	-6.20826300	0.05502000
C	4.21049300	-4.99419800	-0.32093200
C	3.02379100	-7.42457700	0.05530800
C	4.97163400	-6.21259600	-0.32227300
C	4.45120800	-7.45793500	-0.13761300
C	-5.80382300	-0.07575300	0.15161200
C	-6.53804400	0.68663300	1.12399600
C	-6.65984900	-0.82577300	-0.69196100

C	-7.97789700	0.63976800	1.23340600
C	-8.03319000	-0.85036200	-0.60743500
C	-8.80580600	-0.12201300	0.33724400
C	2.71139300	4.91006000	-0.39156900
C	2.83357500	5.69539100	-1.59073600
C	3.33148500	5.49312800	0.67105800
C	3.54171900	6.94205200	-1.63396400
C	4.04322100	6.74031400	0.62702900
C	4.18461900	7.51989700	-0.48117700
C	-10.24214700	-0.13282700	0.39369500
C	-11.03539700	-0.54973500	-0.72104300
C	-10.92615600	0.29701100	1.57475600
C	-12.41191300	-0.56140300	-0.70180800
H	-10.52926800	-0.84523900	-1.62690800
C	-12.28989600	0.28222800	1.61513900
H	-10.35389100	0.62581000	2.43035900
C	-13.01792700	-0.14439600	0.48992100
C	-13.26517700	0.63628800	2.70797900
N	-14.35209800	-0.08461500	0.69612500
C	-14.66634800	0.36892800	2.06125900
C	-13.21562500	-0.24997300	3.97254900
H	-13.17304000	1.68964800	2.98608100
C	-15.25580400	-0.38273300	-0.31831100
C	-15.34946500	-0.68441300	2.95558000
H	-15.26537500	1.28164100	1.99894500
C	-14.68695100	-0.48591000	4.32194700
H	-12.73353400	-1.20366600	3.73539200
H	-12.64665200	0.21545800	4.77984300
C	-14.77001600	-0.81940700	-1.56753800
C	-16.63124900	-0.24096600	-0.10295200
H	-16.43565600	-0.58019500	2.98620400
H	-15.11956700	-1.68319000	2.57051600
H	-14.83780000	-1.33715400	4.98980100
H	-15.10456200	0.39861700	4.81557800
C	-15.71308600	-1.11075000	-2.55035200
C	-17.53056700	-0.53661300	-1.11055800
H	-16.99468100	0.10124300	0.85783100
C	-17.08710900	-0.98024100	-2.35706600
H	-15.36690600	-1.45966600	-3.51820400
H	-18.59413400	-0.42350400	-0.92404700
C	-18.06028700	-1.28524000	-3.46367200
H	-18.39826000	-0.36698200	-3.95603900
H	-17.60786700	-1.92025900	-4.22837800
H	-18.95003100	-1.79234300	-3.08167700

C	5.23723300	-8.70372900	-0.13739000
C	6.53457700	-8.72625100	0.39416600
C	4.69160700	-9.88575500	-0.67755800
C	7.31257400	-9.88134400	0.41400700
H	6.93715800	-7.81229700	0.81249900
C	5.44333000	-11.03801100	-0.66941300
H	3.69367400	-9.88194500	-1.09954600
C	6.72686600	-11.01983800	-0.12102300
C	5.14298900	-12.43524800	-1.15247200
N	7.33048700	-12.25054000	-0.19351900
C	6.46375400	-13.23042200	-0.85433000
C	4.02929500	-13.18858400	-0.39438600
H	4.92932000	-12.44642300	-2.22503400
C	8.66641900	-12.40359800	0.14871900
C	6.04288400	-14.43021300	0.01961500
H	6.94090500	-13.57313100	-1.77906900
C	4.55543900	-14.62151800	-0.29213600
H	3.91477100	-12.76413100	0.60861500
H	3.06180600	-13.11415900	-0.89617400
C	9.36789300	-11.31692600	0.71686700
C	9.32166600	-13.61839400	-0.06620700
H	6.63744700	-15.32679900	-0.16973400
H	6.17175300	-14.16164300	1.07328600
H	4.03766900	-15.21656100	0.46425200
H	4.43596100	-15.13501000	-1.25306800
C	10.70107600	-11.52308100	1.05835400
C	10.65555900	-13.77501900	0.28292500
H	8.78289400	-14.44806700	-0.50761500
C	11.37184700	-12.73070500	0.85722400
H	11.25477200	-10.70457500	1.50926900
H	11.14104200	-14.73033200	0.10593000
C	12.81772200	-12.88346700	1.25216900
H	13.45812400	-12.18008300	0.71042700
H	12.96410100	-12.69247100	2.31995800
H	13.17959000	-13.89234700	1.04180000
C	4.90890300	8.80206500	-0.51528000
C	4.87577200	9.66505500	0.58960100
C	5.64115600	9.17409100	-1.66072700
C	5.54652800	10.88533200	0.60290600
H	4.29850600	9.37138800	1.45721700
C	6.31871800	10.37168400	-1.66581800
H	5.66811000	8.52197600	-2.52553400
C	6.26779500	11.19668500	-0.54092200
C	7.19211100	11.02687800	-2.70700300

N	6.99609500	12.34675800	-0.71726000
C	7.60210800	12.39315600	-2.05091200
C	8.52079300	10.30997700	-3.02796600
H	6.63809900	11.20395500	-3.63322800
C	6.93132400	13.37377300	0.21365700
C	9.14453300	12.42212400	-2.06998600
H	7.19166900	13.24263700	-2.60794400
C	9.52680700	11.45125000	-3.19120700
H	8.81192400	9.67798400	-2.18221900
H	8.44395300	9.66773900	-3.90831900
C	6.23111500	13.17307800	1.42371700
C	7.55051500	14.60088000	-0.03657800
H	9.55184400	13.42504500	-2.21639300
H	9.51607100	12.04860600	-1.11011200
H	10.56642900	11.12027600	-3.12865900
H	9.39274400	11.93257800	-4.16671100
C	6.20646300	14.22718200	2.33237200
C	7.49310200	15.62625800	0.89626300
H	8.08470400	14.75214100	-0.96674600
C	6.82102600	15.45897300	2.10246300
H	5.68627300	14.08815100	3.27563000
H	7.98515200	16.56968400	0.67799500
C	6.74076400	16.56343700	3.12397500
H	5.73567200	16.99645700	3.16808000
H	6.97691400	16.19857000	4.12779900
H	7.43678400	17.37153100	2.88784500
N	2.19914100	-8.42313800	0.26571200
N	1.00293000	-6.51064600	0.25588800
N	2.36509400	5.44652000	-2.79060300
N	3.47069200	7.41142200	-2.85704200
N	-6.07482000	1.49296300	2.05674400
N	-8.34836400	1.41785100	2.22812200
O	2.75624000	6.49609000	-3.55286300
O	-7.18355100	1.94643400	2.74277600
O	0.97415600	-7.85906800	0.38436100
F	-6.14211100	-1.58094900	-1.68223300
F	-8.64068600	-1.66536900	-1.49295700
F	3.31827000	4.91801400	1.87772800
F	4.58158900	7.09753100	1.79952000
F	6.28175200	-6.03232300	-0.52969800
F	4.94617900	-3.89409900	-0.51016500
C	8.72165600	-9.94518500	0.99927600
C	8.64016500	-9.73014800	2.52525500
H	9.63562900	-9.75493300	2.97675200

H	8.18901100	-8.76025900	2.75393600
H	8.03281000	-10.50767500	2.99562000
C	9.57857200	-8.82592600	0.37450300
H	9.66559600	-8.96080100	-0.70640800
H	9.13260000	-7.84590900	0.56059000
H	10.58443900	-8.80972900	0.79921300
C	-13.27455400	-0.99973500	-1.88046700
C	-12.90212500	-0.15789000	-3.11877400
H	-11.84288600	-0.27588700	-3.35851800
H	-13.47462600	-0.47043100	-3.99441900
H	-13.09681800	0.90244300	-2.94145000
C	-12.99452000	-2.49014600	-2.17149300
H	-11.93582100	-2.64230400	-2.39692900
H	-13.25269500	-3.11051100	-1.30979900
H	-13.57607400	-2.83599700	-3.02928800
C	5.53627100	11.84572600	1.79004200
C	4.07775700	12.11670800	2.20994500
H	3.52049200	12.58943200	1.39746400
H	3.57112600	11.18540200	2.47432800
H	4.02901100	12.76999500	3.08359700
C	6.28880600	11.19001100	2.96732200
H	6.28447400	11.84222200	3.84475400
H	5.81662500	10.24330700	3.24549200
H	7.32858200	10.98594000	2.69914200