

Supporting information

Cone Calix[4]arenes with Orientable Glycosylthioureido Groups at the Upper Rim: An In-depth Analysis of Their Symmetry Properties

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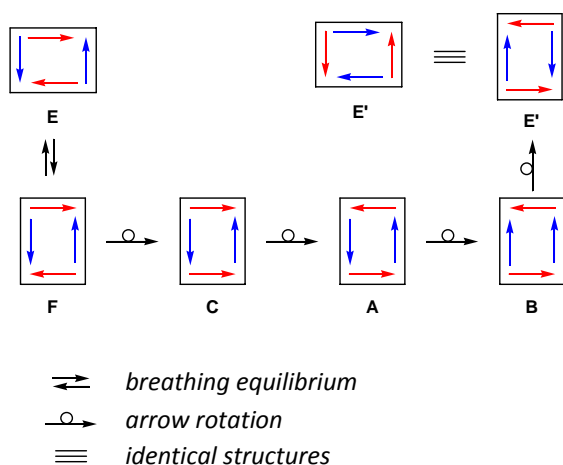
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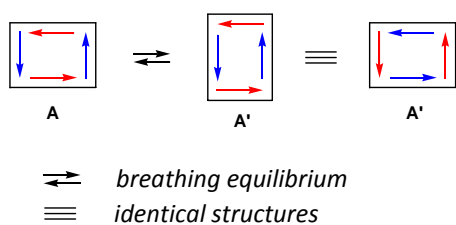
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Scheme 1S. One of the paths that interchange the two couples of mannosyl residues of conformer **E** (in the identical **E** and **E'** structures the blue and red arrows/residues are interchanged).



Scheme 2S. Equilibrium that interchanges the two couples of mannosyl residues of conformer **A** (in the identical **A** and **A'** structures the blue and red arrows/residues are interchanged).

Table 1S. Relative energy (kcal/mol) and population percentage at 298 K (%) of the conformers of compound **1** optimized at the B3LYP/6-31G(d) level in a polarizable continuum model (PCM), choosing water as the solvent.

	E _{rel}	%
1A-ZE	4.43	0.06
1B-ZE	5.29	0.01
1C-ZE	3.09	0.54
1D-ZE	7.59	0.00
1E-ZE	0.00	99.34
1F-ZE	7.65	0.00
1G-ZE	4.87	0.03
1H-ZE	7.80	0.00
1I-ZE	4.79	0.03
1J-ZE	9.67	0.00
1J-EZ	9.19	0.00
1B-ZZ	12.06	0.00
1J-EE	33.00	0.00

Table 2S. Relative energy (kcal/mol) and population percentage at 298 K (%) of the conformers of compound **2** optimized at the B3LYP/6-31G(d) level in a polarizable continuum model (PCM), choosing water as the solvent.

	E _{rel}	%
2A-EZ	0.00	89.39
2B-EZ	1.80	4.28
2C-EZ	3.86	0.13
2D-EZ	8.17	0.00
2E-EZ	2.88	0.69
2F-EZ	7.36	0.00
2G-EZ	1.65	5.49
2H-EZ	5.55	0.01
2I-EZ	7.54	0.00
2J-EZ	8.16	0.00
2I-ZE	5.67	0.01
2I-ZZ	8.84	0.00
2A-EE	25.56	0.00

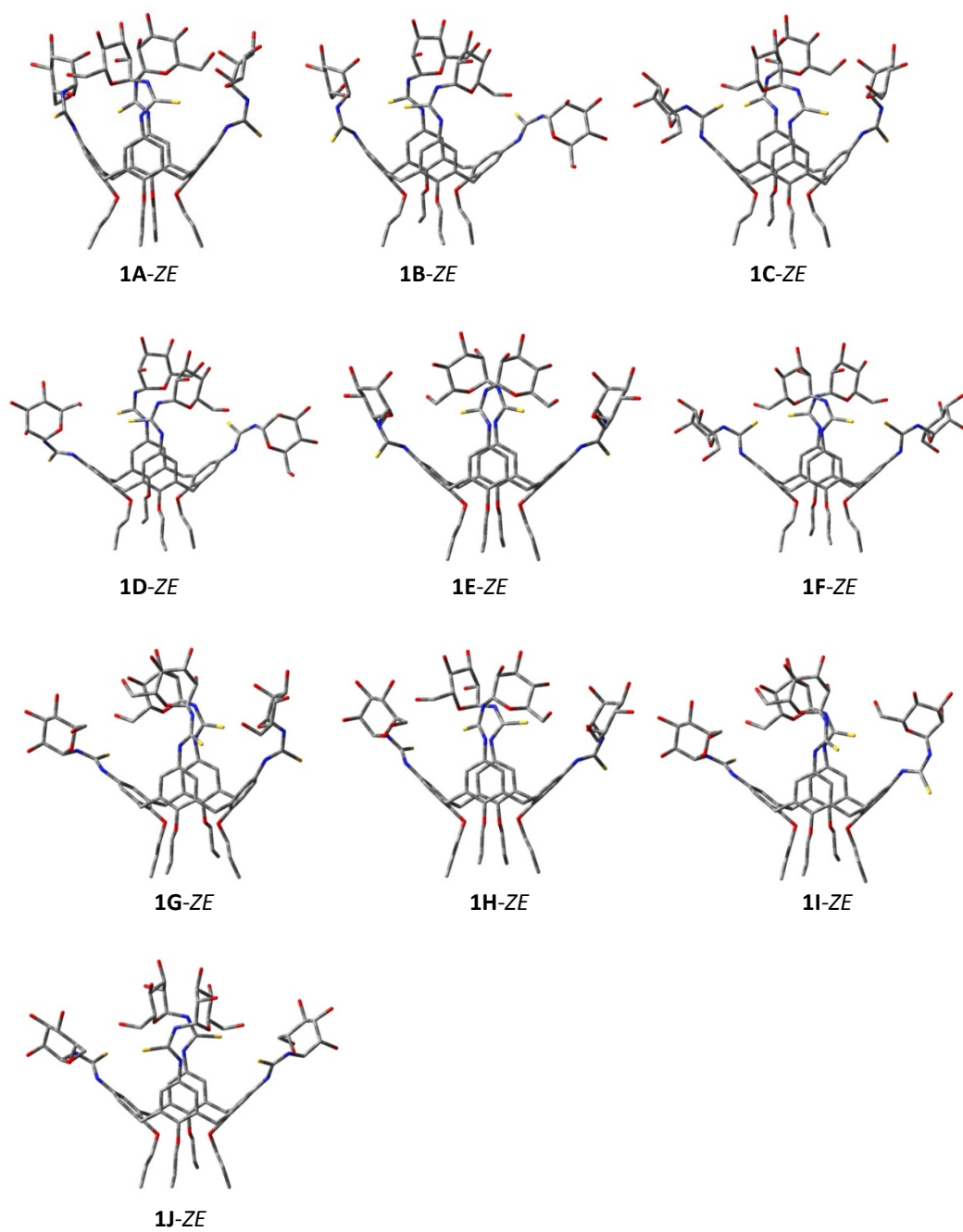


Figure 1S. Three-dimensional plots of the *ZE* conformers of α -D-mannosylthioureidocalix[4]arene **1**. The hydrogen atoms are omitted for clarity.

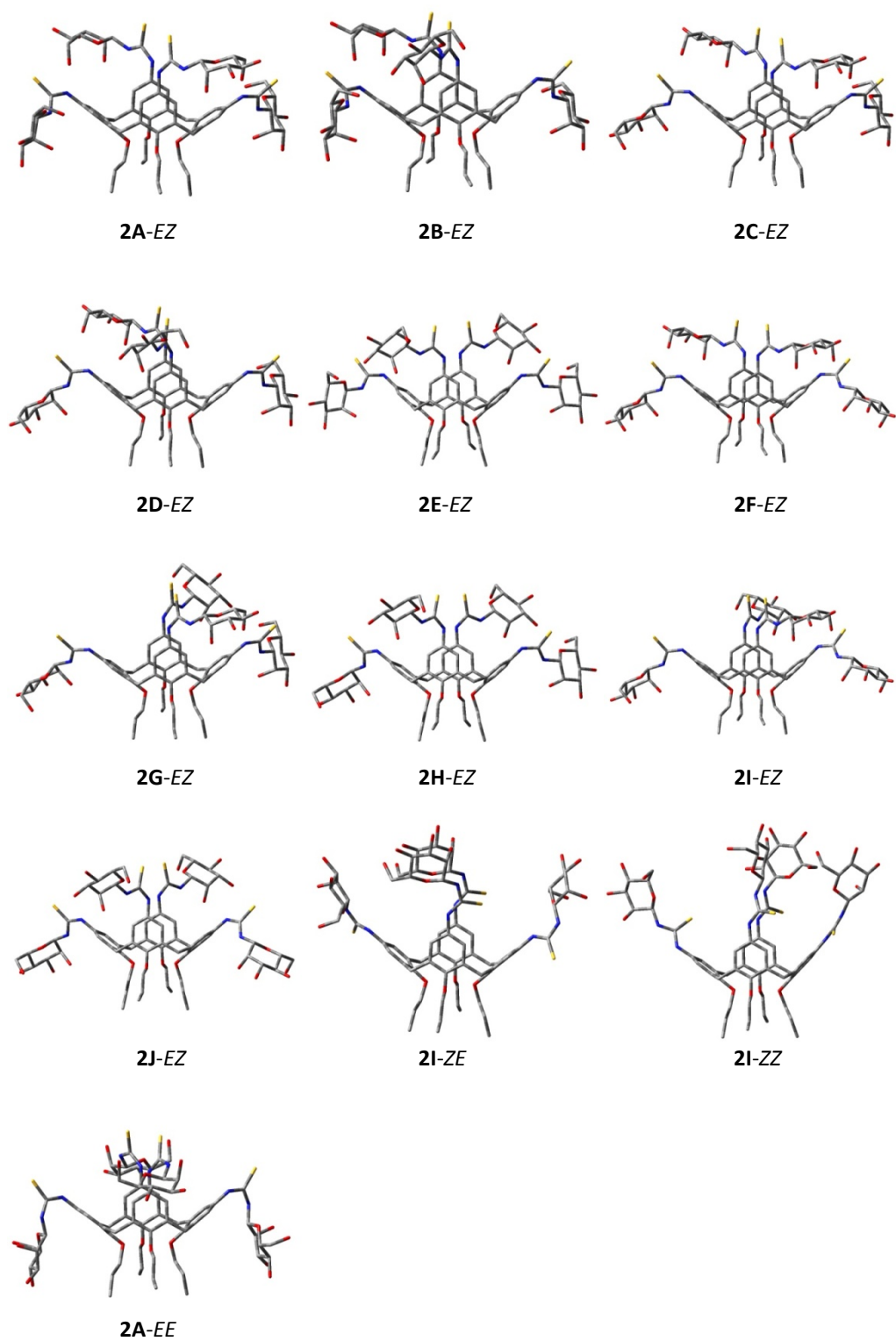


Figure 2S. Three-dimensional plots of the conformers of β -D-mannosylthioureidocalix[4]arene **2**. The hydrogen atoms are omitted for clarity.

E-3 MP2, electron energy = -892.184333 a.u.

N	-2.00890200	0.99498900	-1.12683300
N	-0.74413400	-0.45614000	0.13727000
C	-1.99676100	0.03186600	-0.15839000
H	-1.15347000	1.51550200	-1.31300800
H	-0.75644600	-1.22890500	0.79499800
S	-3.37164100	-0.53957400	0.60965700
C	0.41949900	-0.23981400	-0.70421900
H	0.19136500	-0.46680500	-1.75860100
H	-2.90243000	1.44205800	-1.28727500
C	1.55651900	-1.14543700	-0.21336100
H	1.15684700	-2.17447400	-0.12713800
C	1.22458600	1.61914600	0.57024800
H	1.45383000	2.68297000	0.41675800
H	0.38535600	1.53207500	1.28488400
C	2.44046400	0.83857200	1.06211600
H	2.74232700	1.21596600	2.05335000
H	3.27680200	0.99661900	0.36356600
C	2.09396900	-0.65549400	1.13825700
H	2.97413500	-1.25942200	1.41977800
H	1.32898000	-0.82504900	1.91726000
O	0.80192100	1.14063000	-0.72817200
O	2.55077800	-1.08754100	-1.24256900
H	3.26896800	-1.68703700	-0.99412200

Z-3 MP2, electron energy = -892.174213 a.u.

N	-2.75534900	-1.35756200	-0.87490200
N	-0.71451000	-0.31614600	-0.65815600
C	-2.05495100	-0.28670200	-0.34093300
H	-2.42124400	-1.74592900	-1.75314700
H	-0.36764300	-1.19757100	-1.02621600
S	-2.78584700	0.87940500	0.59411700
C	0.25234800	0.56449000	-0.02449900
H	-0.22188600	1.54842200	0.08336600
H	-3.76245000	-1.25166800	-0.81526600
C	1.49011500	0.66713500	-0.92859300
H	1.13999500	0.88221600	-1.95498900
C	1.29414200	-1.08059700	1.35413500
H	1.46941800	-1.26461600	2.42357200
H	0.64601000	-1.89604200	0.97340300
C	2.60333600	-1.02005900	0.56780900
H	3.11275200	-1.99731100	0.61688700
H	3.25978400	-0.26471700	1.02650100
C	2.30908000	-0.63176200	-0.88836600
H	3.23920800	-0.49775400	-1.46795600
H	1.74825400	-1.44186100	-1.39378900
O	0.59082700	0.17133700	1.30174600
O	2.24267000	1.77492900	-0.41551500
H	2.98796000	1.92715100	-1.01398900

E-3 B3LYP/6-31G(d), electron energy = -894.001542 a.u.

N	2.03404700	1.02626400	1.08765900
N	0.77052500	-0.44528000	-0.15296900
C	2.01521800	0.04925700	0.14634600
H	1.18272900	1.54367300	1.28405200
H	0.79425700	-1.22332100	-0.79815700
S	3.39835300	-0.54083300	-0.60607300
C	-0.40937500	-0.24918600	0.67635400

H	-0.19137900	-0.49330800	1.72166000
H	2.92400300	1.47402400	1.24823900
C	-1.54724200	-1.16005400	0.18014800
H	-1.13083500	-2.16915600	0.02416000
C	-1.29066300	1.64493100	-0.51709300
H	-1.53985900	2.68780600	-0.30476900
H	-0.49413100	1.62474600	-1.27456700
C	-2.50930300	0.85868600	-0.99427200
H	-2.85895300	1.26189000	-1.95221800
H	-3.31815600	0.97658000	-0.26494100
C	-2.14793300	-0.62716400	-1.13042000
H	-3.02825800	-1.22725200	-1.39812900
H	-1.42215700	-0.76356500	-1.94387200
O	-0.79431800	1.12072300	0.72485500
O	-2.49866700	-1.17968500	1.23675900
H	-3.24325300	-1.73280400	0.95359300

Z-3 B3LYP/6-31G(d), electron energy = -893.990015 a.u.

N	-2.79578100	-1.34712100	-0.88633100
N	-0.74828800	-0.37924800	-0.53468500
C	-2.09767200	-0.31769600	-0.30602300
H	-2.41338200	-1.81312200	-1.70158600
H	-0.40304800	-1.24604400	-0.92975500
S	-2.87962900	0.86658400	0.58378100
C	0.23853400	0.45756700	0.13619300
H	-0.27581100	1.37234800	0.42873800
H	-3.79950200	-1.22975700	-0.88639600
C	1.38096500	0.80284100	-0.83956900
H	0.92534700	1.08951400	-1.79937100
C	1.56544700	-1.24164400	1.19344100
H	1.85242100	-1.52197400	2.21053500
H	1.00435200	-2.09206000	0.76681300
C	2.78796500	-0.92881600	0.33015500
H	3.40412300	-1.82871000	0.21252800
H	3.39303400	-0.16906500	0.83582100
C	2.33293100	-0.38999000	-1.03271900
H	3.18980100	-0.08196400	-1.64735900
H	1.82415600	-1.18230600	-1.60402700
O	0.71475200	-0.10709800	1.34355400
O	2.05681300	1.91271900	-0.25618400
H	2.75952000	2.18385500	-0.86715000

E-3 B3LYP/6-31G(d) PCM, electron energy = -894.021136 a.u.

N	-2.02428400	1.02240600	-1.08215500
N	-0.77473000	-0.49212500	0.11348400
C	-1.99292700	0.03943700	-0.16359700
H	-1.16488200	1.50604000	-1.32823100
H	-0.78309200	-1.25191500	0.78117500
S	-3.40240200	-0.53413700	0.61311600
C	0.42717500	-0.27261500	-0.69163400
H	0.22383900	-0.53554800	-1.73517100
H	-2.90442100	1.48853300	-1.24740200
C	1.57038200	-1.15789500	-0.16438900
H	1.17477900	-2.17297300	-0.00805400
C	1.25143200	1.65166800	0.50376000
H	1.48321900	2.69551300	0.28038700
H	0.44014500	1.62730900	1.24406600
C	2.47187000	0.89061200	1.01096500

H	2.78753800	1.30733300	1.97417000
H	3.29898000	1.02306300	0.30476800
C	2.13859100	-0.60128400	1.14956600
H	3.02528700	-1.18176300	1.43262800
H	1.40289900	-0.74812300	1.95159800
O	0.78092100	1.10148100	-0.74548400
O	2.53897900	-1.16641900	-1.20958300
H	3.28889400	-1.70328100	-0.90659100

Z-3 B3LYP/6-31G(d) PCM, electron energy = -894.015693 a.u.

N	-2.79828100	-1.26161600	-0.97893900
N	-0.73912700	-0.34118700	-0.59997300
C	-2.07420100	-0.31082700	-0.35734400
H	-2.39410400	-1.92262600	-1.63096800
H	-0.39523600	-1.08360400	-1.19831600
S	-2.83808800	0.83740800	0.64994800
C	0.25028200	0.52177800	0.03054300
H	-0.22345800	1.48817200	0.20173900
H	-3.80277000	-1.24847100	-0.88479700
C	1.45652800	0.70493400	-0.91228000
H	1.07347500	0.91234300	-1.92206400
C	1.41473500	-1.13593000	1.32033500
H	1.62960100	-1.33527900	2.37347600
H	0.80791500	-1.97074500	0.93767700
C	2.69492200	-0.98289800	0.50268400
H	3.24507400	-1.93092000	0.49711800
H	3.33517400	-0.22961600	0.97478600
C	2.35133600	-0.54464800	-0.92760300
H	3.25736900	-0.33305700	-1.50908700
H	1.83738900	-1.35939100	-1.45791500
O	0.63850400	0.07243400	1.31720400
O	2.15046600	1.84440700	-0.40438000
H	2.92746300	1.98511400	-0.96903800

E-4 MP2, electron energy = -892.184133 a.u.

N	-1.92078500	1.54849300	0.45207400
N	-0.92787900	-0.49074900	0.04667100
C	-2.09647000	0.22418400	0.10499000
H	-1.09288200	1.99895100	0.06387200
H	-0.96951300	-1.39901300	-0.40448300
S	-3.59158900	-0.47582900	-0.15267500
C	0.35651600	0.04356400	0.37539800
H	0.29183300	0.58604000	1.34115100
H	-2.77736700	2.08879200	0.40233100
C	1.36611100	-1.09808400	0.52593400
H	1.04490200	-1.70526800	1.39294700
C	2.02181900	1.57876400	-0.34247800
H	2.19223200	2.32274600	-1.13357200
H	1.96382200	2.10454400	0.63359700
C	3.11554000	0.51476100	-0.30915900
H	4.08713500	0.98796100	-0.08912300
H	3.17974100	0.03851800	-1.29996700
C	2.77144900	-0.53146200	0.75922400
H	3.50211400	-1.35825700	0.76673100
H	2.79702500	-0.06847600	1.76295200
O	0.74291800	0.98481800	-0.64536300
O	1.28190300	-1.87077000	-0.68224800
H	1.77867700	-2.69021500	-0.54741200

Z-4 MP2, electron energy = -892.181692 a.u.

N	-3.14203200	-1.10011500	0.48864000
N	-0.92567100	-0.89112200	-0.07210500
C	-2.15254800	-0.29439200	-0.04114000
H	-3.03675100	-2.10542800	0.38515200
H	-0.76810400	-1.67100900	0.56390100
S	-2.46585200	1.27155200	-0.55383600
C	0.27811500	-0.16118700	-0.39685100
H	0.02925100	0.57359400	-1.18368600
H	-4.08137300	-0.74401800	0.35260900
C	0.83349000	0.57910800	0.82616300
H	0.08436000	1.33772000	1.11353300
C	2.42589300	-0.53077200	-1.29044500
H	3.03489000	-1.35127600	-1.69566600
H	2.21449200	0.19049000	-2.10609000
C	3.11840400	0.17338700	-0.12477000
H	4.05204200	0.63969800	-0.48222500
H	3.37749900	-0.57205200	0.64318900
C	2.17452100	1.22808500	0.46899600
H	2.61011400	1.70311500	1.36432800
H	1.98639900	2.03030800	-0.26849700
O	1.18987200	-1.14504400	-0.87642800
O	0.98007700	-0.41182500	1.86342500
H	0.99788800	0.05226500	2.71139500

E-4 B3LYP/6-31G(d), electron energy = -894.002729 a.u.

N	-1.95673900	1.55854500	0.43037300
N	-0.92742400	-0.46709700	0.06713600
C	-2.09749700	0.23633800	0.10589900
H	-1.12055300	2.02194200	0.08636200
H	-0.95480600	-1.37086200	-0.38659400
S	-3.58405400	-0.49291900	-0.16724700
C	0.36144900	0.05180800	0.40496500
H	0.30474800	0.56077700	1.38176700
H	-2.81378900	2.09102500	0.37046800
C	1.36835200	-1.10337800	0.52365800
H	1.07295300	-1.70159000	1.39925700
C	2.04035300	1.58447100	-0.33511500
H	2.19477700	2.32033700	-1.12890600
H	2.04038300	2.11831000	0.63187800
C	3.11949000	0.50384400	-0.34246600
H	4.10129000	0.95314100	-0.15045100
H	3.14934900	0.03980700	-1.33427700
C	2.79026500	-0.55602200	0.71647600
H	3.50717800	-1.38668100	0.68666500
H	2.86283200	-0.11600300	1.72136600
O	0.74973100	1.02022800	-0.58049900
O	1.24520900	-1.88020100	-0.66779400
H	1.73566200	-2.70620100	-0.53829400

Z-4 B3LYP/6-31G(d), electron energy = -893.999060 a.u.

N	3.09811000	1.13172200	-0.67541900
N	0.90870800	0.70477800	-0.17452200
C	2.19716600	0.26913500	-0.11028800
H	2.79982700	1.75098000	-1.42012500
H	0.69555500	1.58517600	-0.63023000
S	2.70442800	-1.13895300	0.65573300
C	-0.24777200	-0.07023800	0.16245500

H	0.05666800	-0.83246400	0.89099200
H	4.04213000	0.77960800	-0.74570100
C	-1.31800000	0.84131100	0.78482400
H	-0.92977100	1.19899600	1.75038200
C	-1.87190400	-1.50014200	-0.80911200
H	-2.09855000	-1.96178600	-1.77438200
H	-1.63394600	-2.30636600	-0.09363400
C	-3.04240900	-0.66135800	-0.29437300
H	-3.91577700	-1.30004500	-0.11407900
H	-3.31504800	0.07302700	-1.06039200
C	-2.62618000	0.06475300	0.99200900
H	-3.41160200	0.75117300	1.33614600
H	-2.47205900	-0.66404900	1.80055400
O	-0.71935900	-0.69081200	-1.02971600
O	-1.48552400	1.94434300	-0.11520100
H	-2.04235600	2.60446000	0.32457300

E-4 B3LYP/6-31G(d) PCM, electron energy = -894.023257 a.u.

N	-1.96082400	1.56541300	0.39093700
N	-0.92812300	-0.46529800	0.10075500
C	-2.07702700	0.24959800	0.10921700
H	-1.08317600	2.03168800	0.18187600
H	-0.96019100	-1.39942600	-0.28812400
S	-3.58650200	-0.49650200	-0.17124000
C	0.37612800	0.05073500	0.43024100
H	0.33286000	0.55122800	1.41058100
H	-2.80077800	2.12412700	0.34004500
C	1.37586700	-1.11102700	0.51982400
H	1.09829700	-1.72030200	1.39145900
C	2.03809700	1.58796800	-0.32733400
H	2.17575100	2.32785700	-1.11956900
H	2.03996700	2.11380200	0.64079900
C	3.11638300	0.50843700	-0.35500100
H	4.09597400	0.96037800	-0.16179600
H	3.14821500	0.05981600	-1.35427700
C	2.80107300	-0.56787600	0.69205000
H	3.51123000	-1.40105000	0.63410000
H	2.89125500	-0.14430300	1.70157900
O	0.73873800	1.01622100	-0.56099100
O	1.22083700	-1.87341300	-0.68052100
H	1.69752800	-2.71007000	-0.56056400

Z-4 B3LYP/6-31G(d) PCM, electron energy = -894.020747 a.u.

N	3.09949000	1.18200200	-0.56188800
N	0.90615900	0.74076700	-0.10648300
C	2.18937900	0.31190100	-0.08141200
H	2.85699800	2.12350500	-0.84557800
H	0.68471200	1.63452000	-0.53627100
S	2.67810500	-1.21209600	0.51826200
C	-0.25412800	-0.03421200	0.23629000
H	0.01041000	-0.72711500	1.04424900
H	4.07885100	0.94991000	-0.49149800
C	-1.36475500	0.91527400	0.71431300
H	-1.03343100	1.37244600	1.65677400
C	-1.81157700	-1.57808300	-0.67712000
H	-1.98448700	-2.12875600	-1.60588300
H	-1.59386200	-2.30943400	0.11901900
C	-3.01336600	-0.71586700	-0.29624900

H	-3.88083500	-1.35476800	-0.09367600
H	-3.26835400	-0.06653200	-1.14141500
C	-2.67080800	0.13928500	0.93111000
H	-3.47689200	0.84535500	1.16407800
H	-2.54858100	-0.50453400	1.81319800
O	-0.65230400	-0.77019300	-0.91836600
O	-1.49573800	1.92147500	-0.29899400
H	-1.99788100	2.65952000	0.08069500

E-Phenylthiourea B3LYP/6-31G(d), electron energy = -779.267138 a.u.

C	2.88830600	-1.09181400	0.30630600
C	3.40792100	0.17484800	0.02898700
C	2.54196000	1.20350300	-0.34311600
C	1.16804900	0.97905700	-0.44082100
C	0.64442700	-0.28728400	-0.13626200
C	1.51686500	-1.32243200	0.23290300
H	0.50841300	1.76964300	-0.78206400
H	1.11127700	-2.30316000	0.46806700
N	-0.73696300	-0.58132800	-0.24484100
N	-1.59538300	1.37453700	0.68377500
C	-1.83154100	0.16397300	0.10585900
H	-0.98562500	-1.50809700	-0.56569900
H	-0.70567100	1.55778300	1.13201900
S	-3.38584100	-0.40330400	-0.18936000
H	2.93592100	2.18765400	-0.58182800
H	4.47679900	0.35502600	0.09500300
H	3.55151800	-1.90364400	0.59186300
H	-2.40868100	1.82609800	1.07672300

Z-Phenylthiourea B3LYP/6-31G(d), electron energy = -779.260893 a.u.

C	-2.91436800	-0.88991900	-0.36246300
C	-3.26041600	0.42168800	-0.03470400
C	-2.26261000	1.30894800	0.37169900
C	-0.92972400	0.90725800	0.45454600
C	-0.58431600	-0.40580200	0.11050200
C	-1.58560700	-1.30106300	-0.29355000
H	-0.16400500	1.60132500	0.77229800
H	-1.31899700	-2.32159100	-0.56246700
N	0.73181000	-0.92008800	0.21134200
N	2.99183000	-1.19357600	0.25598300
C	1.95082500	-0.31378800	0.05060900
H	0.76440000	-1.93320400	0.21474100
H	2.87475900	-1.93798000	0.93483400
S	2.24263700	1.26873000	-0.40823000
H	-2.51948600	2.33106400	0.63632000
H	-4.29494100	0.74736100	-0.09356100
H	-3.67632400	-1.59659400	-0.67965100
H	3.90422000	-0.75834500	0.25804900

E-Phenylthiourea B3LYP/6-31G(d) PCM, electron energy = -779.282434 a.u.

C	2.86531600	-1.09361300	0.34883600
C	3.40077000	0.16331400	0.05429300
C	2.55572900	1.19188400	-0.36604800
C	1.18287000	0.97302300	-0.49633400
C	0.64663200	-0.28167300	-0.17468700
C	1.49333000	-1.31699400	0.24338200
H	0.53883400	1.76313100	-0.86881300

H	1.07280900	-2.28860400	0.48657800
N	-0.74403500	-0.55811400	-0.31826900
N	-1.57087500	1.30958800	0.78372000
C	-1.80761900	0.16486400	0.11943200
H	-0.99351500	-1.46000300	-0.70424400
H	-0.64585800	1.55648900	1.11324600
S	-3.39870000	-0.37736200	-0.19022800
H	2.96382300	2.16750300	-0.61362200
H	4.46880100	0.33696200	0.14566000
H	3.51477500	-1.90225200	0.67137400
H	-2.35825200	1.79942800	1.18207700

Z-Phenylthiourea B3LYP/6-31G(d) PCM, electron energy = -779.278381 a.u.

C	-2.82358800	-0.86477200	-0.55297400
C	-3.22351000	0.38516700	-0.07599700
C	-2.28779800	1.21925500	0.54194000
C	-0.96064900	0.81436100	0.68640700
C	-0.55931000	-0.43004800	0.18648800
C	-1.49464000	-1.27143800	-0.42789200
H	-0.24069300	1.45130600	1.18514300
H	-1.17793000	-2.23858400	-0.80914500
N	0.76773800	-0.91743300	0.35331600
N	3.04491700	-1.03136200	0.36651800
C	1.94902400	-0.29661700	0.08497400
H	0.82291300	-1.90635100	0.57337900
H	3.00370100	-1.92034600	0.84948700
S	2.10898100	1.26109100	-0.58895600
H	-2.59309100	2.18734700	0.92911900
H	-4.25656000	0.70460300	-0.17872900
H	-3.54201300	-1.52497700	-1.03042900
H	3.95421600	-0.62434700	0.20795300

5-ZZ-a, electron energy = -1661.803223 a.u.

C	3.95697800	-1.44266900	-0.62293300
C	4.45215700	-0.12973700	-0.68693100
C	3.59467000	0.98602000	-0.67965300
C	2.21831800	0.76897200	-0.58227100
C	1.70952100	-0.52748400	-0.47386000
C	2.57383200	-1.62267000	-0.50883900
H	1.53696300	1.61252700	-0.59671300
H	2.16713800	-2.62902900	-0.44830200
C	4.88901500	-2.62911200	-0.68176900
H	5.36789200	-2.81688200	0.28779100
H	4.34596000	-3.53729200	-0.95952200
O	5.81194600	0.07655400	-0.84088500
C	6.56154300	0.17273800	0.38646700
H	6.16065100	0.99096000	1.00039700
H	6.45497900	-0.75835700	0.95943300
C	8.02007500	0.42508600	0.03460200
H	8.08522900	1.34707400	-0.55672100
H	8.37210300	-0.39092100	-0.60908900
C	8.90462300	0.53283200	1.28088600
H	8.58330600	1.35722600	1.92872900
H	8.87336600	-0.38947600	1.87319300
H	9.94781400	0.71504900	1.00229900
N	0.30346900	-0.77149300	-0.42803300
N	-1.88608800	-0.67394600	0.19065500
C	-0.60528100	-0.27992200	0.45646000
H	-0.01990600	-1.49333700	-1.06402100

H	-2.04219600	-1.21134900	-0.65450800
S	-0.20016500	0.69692500	1.78504000
H	5.69070800	-2.46341100	-1.40773400
C	4.15093100	2.38385500	-0.80973700
H	4.67221600	2.69896000	0.10285900
H	4.87647900	2.44647100	-1.62713000
H	3.35008300	3.10484900	-0.99770400
C	-3.04994300	-0.31360700	0.97654600
C	-4.11177300	-1.42604400	0.89784100
H	-2.72765400	-0.20352500	2.01139300
C	-4.89068000	-1.36359300	-0.42197900
H	-3.60743300	-2.40024700	0.98112900
C	-4.23781900	1.04528400	-0.64711700
C	-5.40706300	0.05000900	-0.67180700
H	-4.23709800	-1.64877500	-1.26262500
H	-3.53514800	0.81126800	-1.46105300
H	-6.10608700	0.31833900	0.12688700
O	-3.57926500	0.96083800	0.62905300
O	-4.99960200	-1.23238100	1.98923300
H	-5.80309800	-1.73134500	1.75279000
O	-5.96750200	-2.28882600	-0.31258400
H	-6.60107400	-2.03937100	-1.00884200
O	-6.07111200	0.01923500	-1.93759000
H	-6.78038800	0.68019600	-1.92558700
C	-4.67352800	2.50117000	-0.77965900
H	-3.77735000	3.13829000	-0.79009900
H	-5.20077900	2.64237900	-1.72762500
O	-5.56738800	2.88495800	0.25809000
H	-5.11577700	2.66718800	1.09138600

5-ZE-a, electron energy = -1661.808767 a.u.

C	-3.09195400	1.26272500	-0.21243000
C	-3.96969600	0.21908800	-0.55114700
C	-3.50729600	-1.08905600	-0.78035400
C	-2.14021400	-1.34794200	-0.64237700
C	-1.25814700	-0.33326700	-0.26561600
C	-1.73378300	0.96594900	-0.06732600
H	-1.76001000	-2.34395100	-0.83883800
H	-1.03874500	1.75685600	0.20411200
C	-3.60425200	2.67050200	-0.02514400
H	-4.25312200	2.75369200	0.85508400
H	-2.77482600	3.37146200	0.10550400
O	-5.30882700	0.51365300	-0.74063300
C	-6.15395700	0.30812000	0.40838400
H	-6.11847400	-0.74705500	0.71148000
H	-5.78512500	0.91043800	1.25009100
C	-7.57147300	0.71415500	0.03314500
H	-7.89107200	0.11672300	-0.83003400
H	-7.56224800	1.76217400	-0.29170200
C	-8.55263800	0.52950100	1.19530900
H	-8.59432900	-0.51709300	1.51982500
H	-8.26409300	1.13689100	2.06151900
H	-9.56427000	0.82786100	0.90094100
N	0.14549500	-0.55344900	-0.17071100
N	2.15923000	-1.51996300	0.33816600
C	0.80087200	-1.53371400	0.49806700
H	0.73247000	0.21310300	-0.49709100
H	2.64378500	-2.24463200	0.85116500
S	0.08758400	-2.69934600	1.51130100
H	-4.19789600	2.99269500	-0.88729200

C	-4.45791800	-2.18581200	-1.19754400
H	-4.99297700	-2.60547000	-0.33594000
H	-5.21423900	-1.80875000	-1.89237000
H	-3.91769000	-3.00725400	-1.67754000
C	2.86952900	-0.81773900	-0.72097600
C	4.34462100	-1.24872300	-0.73622200
H	2.42305800	-1.05045300	-1.69302700
C	5.12444600	-0.58167700	0.40436800
H	4.39526700	-2.34273700	-0.62394200
C	3.38019600	1.21737000	0.51557500
C	4.88294400	0.92550300	0.41108400
H	4.79877300	-0.99326600	1.37222000
H	2.98621000	0.81168200	1.45770600
H	5.25394700	1.34795600	-0.52827200
O	2.71525300	0.59740800	-0.60901500
O	4.88058300	-0.85781700	-1.98887400
H	5.84705800	-0.85113600	-1.85933100
O	6.49993100	-0.87405900	0.18287700
H	6.99724400	-0.23343900	0.72197000
O	5.61072600	1.44658400	1.52418300
H	5.88564100	2.35190300	1.31149000
C	3.03725500	2.70011600	0.42694300
H	1.94707600	2.81808100	0.51186600
H	3.49889200	3.22807300	1.26623300
O	3.53246200	3.29961500	-0.76335400
H	3.15304800	2.79539200	-1.50273700

5-EZ-a, electron energy = -1661.807879 a.u.

C	-3.19625000	1.49632200	1.03730500
C	-3.53378300	0.75130500	-0.10812700
C	-2.70086600	0.71478300	-1.23933200
C	-1.49797400	1.43042000	-1.20071500
C	-1.12613600	2.14239700	-0.05603000
C	-1.97861800	2.17989500	1.05168700
H	-0.86527400	1.45792300	-2.08356700
H	-1.68906900	2.74980300	1.93034700
C	-4.13893000	1.55961800	2.21423600
H	-4.29269700	0.57201800	2.66434500
H	-3.74924100	2.22535300	2.98941900
O	-4.75773600	0.11066100	-0.13552400
C	-4.73478200	-1.28593900	0.22462100
H	-4.11166300	-1.84267900	-0.48787000
H	-4.28761700	-1.39989400	1.22171300
C	-6.16555200	-1.80254700	0.20853800
H	-6.58738500	-1.63700800	-0.79084000
H	-6.76291700	-1.20545900	0.90881900
C	-6.24692400	-3.28743800	0.57675000
H	-5.67589900	-3.90507000	-0.12668400
H	-5.84986500	-3.47131700	1.58224900
H	-7.28506700	-3.63511400	0.55931000
N	0.08609100	2.89931500	-0.02008200
N	1.51560100	1.15372600	-0.51842200
C	1.35733700	2.47216900	-0.23900300
H	0.02468300	3.85899000	0.29668600
H	0.68111500	0.57789400	-0.49159800
S	2.64293500	3.58932100	-0.16021200
H	-5.12549900	1.92498300	1.90877400
C	-3.10644400	-0.03841300	-2.48295300
H	-2.83988800	-1.10090200	-2.41544500
H	-4.18774400	0.01497500	-2.63807700

H	-2.60359800	0.36811200	-3.36546200
C	2.79213000	0.50400600	-0.75712400
C	2.59591800	-0.73248200	-1.65349500
H	3.43563300	1.21700800	-1.27212900
C	2.06020800	-1.92663000	-0.85302700
H	1.88518200	-0.47817000	-2.45400100
C	2.93819100	-0.86821000	1.24009100
C	2.90143500	-2.15241800	0.39999900
H	1.01893800	-1.74048500	-0.54293000
H	1.92043100	-0.61533200	1.57352100
H	3.92474500	-2.39936100	0.09930900
O	3.48840800	0.19509700	0.44242000
O	3.86556900	-1.05332800	-2.20245300
H	3.78555800	-1.97842200	-2.49972700
O	2.11312700	-3.05899900	-1.71460900
H	2.05314900	-3.83703700	-1.13191000
O	2.29978500	-3.24479000	1.09866800
H	2.99493600	-3.71714800	1.58214200
C	3.84512700	-0.96384200	2.46290600
H	3.78657400	-0.01760200	3.01993200
H	3.49443500	-1.76606000	3.11861500
O	5.18754600	-1.27123600	2.10688500
H	5.45111000	-0.59763000	1.45692000

5-EE-a, electron energy = -1661.797112 a.u.

C	-2.92761800	1.20344100	1.13679900
C	-3.33627100	0.70207700	-0.11154400
C	-2.55478100	0.87075300	-1.26839500
C	-1.33149500	1.53868800	-1.15577300
C	-0.88858800	2.00596800	0.08577900
C	-1.68977500	1.84887600	1.21883700
H	-0.72856100	1.70783200	-2.04328900
H	-1.34763700	2.23865600	2.17400300
C	-3.80371500	1.05431100	2.35703300
H	-3.72877300	0.04767000	2.78746300
H	-3.51213500	1.76583700	3.13498700
O	-4.57255600	0.09461400	-0.22829500
C	-4.58607800	-1.32694800	0.01606200
H	-3.88674600	-1.82473400	-0.66942900
H	-4.25011700	-1.52989800	1.04182200
C	-6.00514300	-1.83220200	-0.19678800
H	-6.31715000	-1.58436500	-1.21908300
H	-6.67669000	-1.29031600	0.48099500
C	-6.12132100	-3.34155400	0.03980900
H	-5.47334100	-3.90335300	-0.64352100
H	-5.83757500	-3.60816100	1.06486700
H	-7.14974800	-3.68151600	-0.12066600
N	0.33453400	2.73613500	0.21141000
N	1.88226300	1.31493900	-0.85093800
C	1.52691500	2.54735800	-0.41408600
H	0.25641600	3.65097300	0.64002300
H	2.73174800	1.31709100	-1.40071500
S	2.58875200	3.87097100	-0.63220100
H	-4.85596900	1.21829200	2.10648700
C	-3.04794900	0.37789000	-2.60733800
H	-3.06877700	-0.71772500	-2.65234100
H	-4.06871400	0.72278900	-2.80193900
H	-2.40077900	0.73151200	-3.41494800
C	1.43253800	-0.03592200	-0.44322200
C	1.54515200	-0.25613400	1.07824000

H	0.39039800	-0.18608100	-0.72985100
C	2.99146600	-0.52380800	1.50284800
H	1.17879400	0.63947500	1.59705100
C	3.53445200	-1.23016800	-0.82962900
C	3.59716000	-1.63078000	0.64844700
H	3.59144900	0.39042400	1.37669400
H	4.15908600	-0.33805300	-0.98676000
H	3.01764400	-2.54854400	0.78957500
O	2.16167300	-0.97070900	-1.20461200
O	0.72872700	-1.37686700	1.39093200
H	1.03524900	-1.67569400	2.26681700
O	2.95286500	-0.90546600	2.87481000
H	3.80397700	-1.34533400	3.04967400
O	4.94304600	-1.80426300	1.09542000
H	5.19250200	-2.73171500	0.96199800
C	4.00049500	-2.32397600	-1.78551500
H	3.94619400	-1.94061900	-2.81450400
H	5.04386900	-2.57154400	-1.57074400
O	3.24729600	-3.52008800	-1.63747700
H	2.31668700	-3.27094500	-1.76835900

5-ZZ-b, electron energy = -1661.803225 a.u.

C	3.83494300	-1.28712200	-0.25311100
C	4.46623400	-0.10946200	-0.69306000
C	3.73240600	0.98660100	-1.17745500
C	2.33668200	0.89929300	-1.18161800
C	1.69100000	-0.25280900	-0.72822000
C	2.43882200	-1.34590800	-0.28676200
H	1.74677800	1.73764900	-1.54310500
H	1.93002200	-2.25178400	0.02455500
C	4.64497100	-2.47375000	0.21176100
H	4.99124400	-2.34682800	1.24552300
H	4.04753800	-3.38964400	0.17790500
O	5.84843900	-0.05198600	-0.72811500
C	6.47734700	0.41093000	0.48327800
H	6.10352000	1.41353800	0.73250900
H	6.21875400	-0.25863300	1.31473000
C	7.98167500	0.43464100	0.25700800
H	8.19838000	1.09024300	-0.59573700
H	8.30971600	-0.57360200	-0.02584600
C	8.74602500	0.90964900	1.49686100
H	8.44907500	1.92537400	1.78435400
H	8.56219300	0.25206100	2.35487800
H	9.82467700	0.91842300	1.30846900
N	0.26774800	-0.31885200	-0.82286300
N	-1.91384200	-0.68223500	-0.28172200
C	-0.62537900	-0.59624700	0.16425300
H	-0.11330800	-0.01925400	-1.71457600
H	-2.06625700	-0.61333500	-1.28149900
S	-0.19798700	-0.81210700	1.79351000
H	5.53481000	-2.61097300	-0.40985000
C	4.43592700	2.22030500	-1.69021700
H	4.92220400	2.77740500	-0.87992100
H	5.21939900	1.95797900	-2.40877000
H	3.72835100	2.89627800	-2.17891800
C	-3.08009500	-0.84014700	0.56568700
C	-4.19676400	-1.57443500	-0.19724200
H	-2.78566100	-1.43825800	1.42762600
C	-4.92595700	-0.63212600	-1.16316100
H	-3.75037700	-2.40650000	-0.76200600

C	-4.13864700	1.31438300	0.20433000
C	-5.35809200	0.64222000	-0.44335400
H	-4.26005500	-0.35198400	-1.99588400
H	-3.42422500	1.61231200	-0.57785100
H	-6.06940600	0.37843400	0.34606400
O	-3.52785500	0.39061100	1.12187200
O	-5.10901800	-2.06758500	0.77298700
H	-5.92968400	-2.24870600	0.27886600
O	-6.05332100	-1.34302500	-1.66414800
H	-6.64899000	-0.66654900	-2.03286800
O	-5.97844700	1.47116200	-1.42925600
H	-6.65004800	2.01619000	-0.99094300
C	-4.48994600	2.53966400	1.04204800
H	-3.56043700	2.97832400	1.43297100
H	-4.97943300	3.28809500	0.41213400
O	-5.39295000	2.22201600	2.09430900
H	-4.98004200	1.49143000	2.58576800

5-ZE-b, electron energy = -1661.807493 a.u.

C	3.21467500	0.80432600	-0.90033000
C	3.94695500	0.52274000	0.26763400
C	3.34899900	-0.06001300	1.39814500
C	1.99043700	-0.38959900	1.33101700
C	1.25413500	-0.13878300	0.17399600
C	1.85826700	0.46832500	-0.92761500
H	1.49903400	-0.84019700	2.18887300
H	1.26426500	0.68492300	-1.81034500
C	3.87190000	1.47972200	-2.08000800
H	4.55008200	0.79994200	-2.61070600
H	3.12155400	1.82345300	-2.79783200
O	5.27514800	0.90448000	0.33236000
C	6.22617500	-0.09244600	-0.09170100
H	6.12636400	-0.98925400	0.53468500
H	6.01754200	-0.38468600	-1.12982800
C	7.62115800	0.50178200	0.03267700
H	7.78072000	0.80844800	1.07407600
H	7.67011600	1.41220700	-0.57781800
C	8.71069600	-0.48414500	-0.40090300
H	8.69383400	-1.39295800	0.21247800
H	8.58303900	-0.78479400	-1.44770300
H	9.70377700	-0.03350200	-0.30212900
N	-0.15255100	-0.42200600	0.16519500
N	-2.11776800	-1.49238900	-0.36140500
C	-0.75825100	-1.42279100	-0.50721600
H	-0.76382300	0.25810800	0.61443200
H	-2.53687000	-2.27661800	-0.84395100
S	0.04388500	-2.55385800	-1.49581000
H	4.46961500	2.33921100	-1.75995000
C	4.14651800	-0.30367700	2.65675500
H	4.83870200	-1.14730400	2.54262700
H	4.75144900	0.57122000	2.91541800
H	3.48493600	-0.53196500	3.49740200
C	-2.86839300	-0.88625200	0.73180800
C	-4.32428300	-1.37829800	0.69680200
H	-2.42692900	-1.15737700	1.69693700
C	-5.11301600	-0.67956400	-0.41813000
H	-4.32859900	-2.46546200	0.52154900
C	-3.44335200	1.19164700	-0.39677700
C	-4.93412700	0.83446000	-0.33704200
H	-4.75489500	-1.02308700	-1.40062000

H	-3.01761000	0.85445100	-1.35169200
H	-5.33847100	1.18858500	0.61679900
O	-2.77343500	0.53596100	0.70456000
O	-4.89498800	-1.08189900	1.95999500
H	-5.85876600	-1.10359600	1.81313600
O	-6.47881600	-1.03909200	-0.23742300
H	-6.99383100	-0.38971700	-0.74866300
O	-5.66430600	1.38667500	-1.43358700
H	-5.97733600	2.26823900	-1.17796900
C	-3.16183200	2.67941300	-0.21862300
H	-2.07648700	2.84542200	-0.27952600
H	-3.63346000	3.23581800	-1.03364100
O	-3.69715400	3.18845700	0.99621400
H	-3.30942600	2.65524400	1.71051500

5-EZ-b, electron energy = -1661.807708 a.u.

C	2.34432500	0.22942100	-1.32134800
C	3.45552600	0.60391800	-0.54651100
C	3.42951300	1.73491200	0.29056100
C	2.24542400	2.47127600	0.37631500
C	1.12199300	2.10497600	-0.37060200
C	1.18137300	1.00318300	-1.22962400
H	2.19505200	3.33913900	1.02821700
H	0.32766300	0.76208400	-1.85728600
C	2.41226500	-0.95136400	-2.25913400
H	2.23337900	-1.89621800	-1.73041300
H	1.65575200	-0.86872200	-3.04500700
O	4.63707800	-0.10261800	-0.66328100
C	4.75965800	-1.25272200	0.19903300
H	4.65453000	-0.93923300	1.24666900
H	3.95490100	-1.96722200	-0.01962700
C	6.12275600	-1.88246700	-0.04432000
H	6.89704600	-1.13022800	0.15171000
H	6.20128000	-2.15100600	-1.10529800
C	6.35271700	-3.11861300	0.83128100
H	6.30322500	-2.86750200	1.89755200
H	5.60114700	-3.89247100	0.63449300
H	7.33843200	-3.55388900	0.63671400
N	-0.06094400	2.90706700	-0.29107600
N	-1.45514500	1.22005100	0.44245000
C	-1.30422200	2.52461900	0.10229400
H	0.04243100	3.90691000	-0.41350100
H	-0.61880700	0.64668300	0.42717800
S	-2.56078200	3.67560800	0.16145200
H	3.39882300	-1.02467300	-2.72563500
C	4.65779500	2.14164300	1.06748100
H	4.92344600	1.39484800	1.82499600
H	5.52497800	2.24464100	0.40652500
H	4.49639400	3.09464100	1.57902000
C	-2.70021900	0.60992200	0.87526900
C	-2.40473400	-0.55938600	1.83158600
H	-3.28030600	1.36655500	1.40328600
C	-1.94769000	-1.80532500	1.06255600
H	-1.61540300	-0.25045900	2.53320600
C	-3.06702400	-0.89923300	-0.98874600
C	-2.92124000	-2.12065900	-0.06897300
H	-0.94907800	-1.63914600	0.62622900
H	-2.09695500	-0.67153000	-1.45552400
H	-3.90176700	-2.34945400	0.36093000
O	-3.52759600	0.22100000	-0.21263500

O	-3.60697100	-0.84099000	2.53188700
H	-3.48895700	-1.74308100	2.88240100
O	-1.89345400	-2.87388600	2.00216200
H	-1.88904800	-3.69126000	1.47272100
O	-2.39060000	-3.25737900	-0.75461200
H	-3.13103700	-3.76633700	-1.11924700
C	-4.10803700	-1.08513300	-2.08761400
H	-4.12449800	-0.18219200	-2.71494000
H	-3.82640700	-1.93220100	-2.71967800
O	-5.39704600	-1.36905800	-1.55740500
H	-5.59345900	-0.64859700	-0.93450900

5-EE-b, electron energy = -1661.801160 a.u.

C	2.67620300	0.86738400	-1.18047700
C	3.41763800	0.72719700	0.00666100
C	2.93849000	1.20618600	1.23853500
C	1.67429700	1.80165400	1.27295600
C	0.91493900	1.93222400	0.10782400
C	1.42455000	1.48711100	-1.11568400
H	1.27808900	2.17172200	2.21485100
H	0.84893600	1.62925900	-2.02519300
C	3.23425400	0.39339000	-2.50070800
H	3.13109700	-0.69329600	-2.61430100
H	2.70803700	0.86190300	-3.33743800
O	4.68487800	0.17792900	-0.04942700
C	4.74725700	-1.25412300	0.10922700
H	4.31602600	-1.53735400	1.07901100
H	4.15264200	-1.73985000	-0.67620500
C	6.20629200	-1.67570700	0.02173400
H	6.77195800	-1.14614900	0.79861900
H	6.60915900	-1.34718400	-0.94457000
C	6.38199100	-3.18956200	0.17973800
H	6.00736400	-3.53612300	1.15029400
H	5.84292500	-3.73792700	-0.60203700
H	7.43927400	-3.46650000	0.11248500
N	-0.33688100	2.61868000	0.18857800
N	-1.75410100	1.17909100	-1.02168700
C	-1.49128100	2.41389300	-0.48964700
H	-0.31273400	3.51176500	0.66679400
H	-2.61374700	1.19083700	-1.55771600
S	-2.60594800	3.68667600	-0.68628700
H	4.30066700	0.62384400	-2.58150800
C	3.77424200	1.08785000	2.49000400
H	3.82306200	0.05197900	2.84796000
H	4.80424700	1.40965000	2.30668100
H	3.35583800	1.69684900	3.29642200
C	-1.41589300	-0.10046700	-0.39532300
C	-1.81808500	-1.24941200	-1.33751200
H	-0.34118700	-0.15524100	-0.23720100
C	-3.32613300	-1.52438000	-1.27383200
H	-1.53702600	-0.97442100	-2.36493800
C	-3.40123100	-0.40970400	0.97031500
C	-3.78506500	-1.66549500	0.17475900
H	-3.88417000	-0.69504900	-1.73768800
H	-3.91619900	0.46750500	0.55144000
H	-3.28046500	-2.52708600	0.62400000
O	-1.97238500	-0.23485500	0.90551100
O	-1.10170900	-2.40035200	-0.91722300
H	-1.58639400	-3.15389900	-1.30193500
O	-3.55667900	-2.72626000	-2.00139200

H	-4.43469400	-3.04034000	-1.72047800
O	-5.19855700	-1.87106400	0.13193400
H	-5.45089300	-2.41092600	0.89683100
C	-3.72819400	-0.50531600	2.45710100
H	-3.44425900	0.43983200	2.94194800
H	-4.80555300	-0.64253300	2.58714500
O	-3.08753600	-1.61538200	3.07381300
H	-2.13967100	-1.51895800	2.87931500

6-ZZ-a, electron energy = -1661.807337 a.u.

C	3.90433300	0.50332900	1.44178000
C	4.58825700	-0.33657400	0.54678800
C	3.91153300	-1.28463600	-0.24169200
C	2.51978600	-1.36682000	-0.13798500
C	1.81856900	-0.51226900	0.71486200
C	2.51114500	0.40563100	1.50819900
H	1.97999500	-2.10697600	-0.71789300
H	1.95961300	1.05224700	2.18611300
C	4.65820100	1.47679200	2.31569700
H	5.11101600	2.28439800	1.72765000
H	3.99141600	1.93552900	3.05149400
O	5.97053900	-0.28018400	0.50457600
C	6.52119000	0.59336200	-0.50089100
H	6.17451400	0.28041800	-1.49502400
H	6.16753500	1.61982100	-0.33159900
C	8.03845400	0.52264000	-0.41206500
H	8.35053700	-0.51939500	-0.55645700
H	8.34528400	0.80864700	0.60186800
C	8.72029000	1.42588500	-1.44488400
H	8.44323000	1.14265300	-2.46740900
H	8.44139100	2.47669000	-1.30177600
H	9.81000400	1.35594400	-1.36313000
N	0.40485800	-0.61320000	0.87822400
N	-1.81679800	-0.76854600	0.42625200
C	-0.56378800	-0.57109400	-0.07513700
H	0.09165000	-0.60394100	1.84336700
H	-1.93816300	-0.87611300	1.42901600
S	-0.26309600	-0.31209000	-1.72703600
H	5.47411600	0.97842500	2.84973100
C	4.67219800	-2.21691700	-1.15398300
H	4.95522700	-1.72272500	-2.09218200
H	5.59708900	-2.56178600	-0.68201600
H	4.06424700	-3.08837000	-1.41459900
C	-3.04241300	-0.58229600	-0.29243000
C	-4.13468700	-1.45120100	0.34593000
H	-2.89019800	-0.88438900	-1.33431000
C	-5.50381500	-1.10318800	-0.24342700
H	-3.90434300	-2.50585500	0.13312500
C	-4.61026100	1.13988600	-0.90109000
C	-5.75451800	0.40069200	-0.19092700
H	-5.53690100	-1.42487400	-1.29650500
H	-4.57795300	0.83530500	-1.95968900
H	-5.77640000	0.72182100	0.85574500
O	-3.37616800	0.81022600	-0.24714800
O	-4.12434000	-1.21603500	1.74941300
H	-4.97238000	-1.56443900	2.07894900
O	-6.47495700	-1.81163200	0.52097100
H	-7.32658800	-1.37979600	0.33030100
O	-7.02197000	0.61902500	-0.81517900
H	-7.42372500	1.40831800	-0.42041800

C	-4.72213400	2.65897000	-0.82508600
H	-3.88487900	3.10270700	-1.38303300
H	-5.65410800	2.98378000	-1.29670600
O	-4.74962500	3.12307300	0.51967300
H	-3.95999300	2.74867400	0.94623200

6-EZ-a, electron energy = -1661.811856 a.u.

C	3.76854300	1.49222600	-0.37755200
C	3.71842400	0.39350400	0.49948300
C	2.56830700	0.09929800	1.25193900
C	1.44464500	0.91866500	1.09765500
C	1.45983100	1.98803500	0.19567100
C	2.62093900	2.27537000	-0.52708500
H	0.56335400	0.73584200	1.70605000
H	2.63024400	3.12014600	-1.21057000
C	5.03451100	1.81891800	-1.13191500
H	5.23585300	1.08534500	-1.92216700
H	4.96319100	2.80291700	-1.60374700
O	4.85778500	-0.36624900	0.68655900
C	4.98746100	-1.51185100	-0.18027500
H	4.12708700	-2.18028100	-0.04110300
H	4.98998200	-1.18317300	-1.22836400
C	6.28695300	-2.22227300	0.16696800
H	6.25791200	-2.51054600	1.22524900
H	7.11593000	-1.51248100	0.05322600
C	6.52369700	-3.45585400	-0.71031500
H	5.71565400	-4.18826800	-0.59582800
H	6.58230400	-3.18567400	-1.77144200
H	7.46255400	-3.95010900	-0.43972300
N	0.32643300	2.84635500	0.04898800
N	-1.19737600	1.20057700	-0.49180300
C	-0.95459900	2.51156500	-0.25561500
H	0.49675200	3.84432900	0.06615800
H	-0.43213800	0.53796600	-0.41093000
S	-2.14137000	3.73390400	-0.35654000
H	5.90207600	1.81315600	-0.46430400
C	2.55915600	-1.04832200	2.23225400
H	2.46122600	-2.01411600	1.72077100
H	3.49084400	-1.08338700	2.80492900
H	1.72109200	-0.95927000	2.92953200
C	-2.49105500	0.60950600	-0.67548600
C	-2.35215300	-0.63416400	-1.56382100
H	-3.14935000	1.33948300	-1.15889200
C	-3.66344400	-1.42247500	-1.58454800
H	-2.11050000	-0.30281500	-2.58481300
C	-4.29474000	-0.35707500	0.58912900
C	-4.15960900	-1.68736900	-0.16684300
H	-4.42906900	-0.83795700	-2.11890300
H	-5.03317600	0.28187900	0.07831700
H	-3.42600400	-2.30927500	0.35668700
O	-3.01164900	0.28717900	0.61889500
O	-1.29891100	-1.43537600	-1.04107600
H	-1.40750100	-2.31138700	-1.45332000
O	-3.40144800	-2.64166400	-2.27312700
H	-4.13393400	-3.23933000	-2.04012400
O	-5.40625000	-2.37459300	-0.29626200
H	-5.52277400	-2.94047800	0.48252800
C	-4.70752400	-0.52275200	2.04781600
H	-4.80436000	0.47339200	2.50316000
H	-5.68266800	-1.01564300	2.09934400

O -3.79029200 -1.33459100 2.77172700
H -2.91600800 -0.92861400 2.64413500

6-EE-a, electron energy = -1661.804905 a.u.

C -2.60378400 1.14957600 1.41966700
C -3.15491000 0.89460200 0.15136900
C -2.48102100 1.24474900 -1.03264500
C -1.22400300 1.84906900 -0.92878600
C -0.64584100 2.07657100 0.32301700
C -1.33737400 1.73704100 1.48808900
H -0.69808100 2.15196900 -1.82915600
H -0.88496300 1.93541700 2.45594400
C -3.37269200 0.80969000 2.67336200
H -3.51596300 -0.27202900 2.78108300
H -2.84505900 1.16726300 3.56204800
O -4.42759200 0.35984400 0.07987100
C -4.49159600 -1.07276900 -0.07125500
H -3.97801600 -1.37205800 -0.99460400
H -3.97550700 -1.55452700 0.77055000
C -5.95719500 -1.47843500 -0.11368200
H -6.44292900 -0.95183300 -0.94484500
H -6.44390600 -1.13527500 0.80780900
C -6.13373300 -2.99204100 -0.27291800
H -5.67089700 -3.35227700 -1.19944700
H -5.67852100 -3.53734500 0.56247800
H -7.19552400 -3.25770600 -0.30531100
N 0.61063500 2.75000000 0.44746300
N 1.97309300 1.46687500 -0.98402200
C 1.74493800 2.61807100 -0.27977300
H 0.60647100 3.58084200 1.02765600
H 2.85590600 1.49228200 -1.48436700
S 2.87711600 3.89061800 -0.33376000
H -4.37055900 1.26099000 2.65754800
C -3.11256600 1.01346800 -2.38431300
H -2.96792300 -0.01946000 -2.72575300
H -4.19087100 1.19351700 -2.34913500
H -2.66989400 1.67131900 -3.13799000
C 1.63725500 0.13044600 -0.54553200
C 2.04696000 -0.85850000 -1.64618300
H 0.56124200 0.03711900 -0.37424400
C 1.93815100 -2.29452300 -1.12684500
H 1.36489000 -0.72710100 -2.49935800
C 2.13241600 -1.43273100 1.21676700
C 2.67191000 -2.45206700 0.20211000
H 0.87667700 -2.54418600 -0.97102100
H 1.06104800 -1.62052600 1.39322000
H 3.73721600 -2.25237400 0.04617000
O 2.32817900 -0.11302200 0.68420000
O 3.38481400 -0.57057600 -2.03128400
H 3.69541200 -1.36178200 -2.50745400
O 2.50401700 -3.13745600 -2.12554300
H 2.68791100 -3.98463900 -1.68201500
O 2.46416200 -3.80372700 0.61796000
H 3.23279800 -4.08374100 1.13855400
C 2.86699800 -1.44959900 2.55321600
H 2.39845800 -0.71389500 3.22280300
H 2.76974700 -2.43726100 3.01330900
O 4.25807300 -1.19517000 2.39911200
H 4.32416900 -0.35555900 1.91307400

6-ZZ-b, electron energy = -1661.807329 a.u.

C -3.72099400 0.95087800 -0.70798300
C -4.58614200 -0.15458900 -0.61772400
C -4.09950700 -1.47082100 -0.54515300
C -2.71501400 -1.66583000 -0.52673600
C -1.83972600 -0.57947500 -0.59188900
C -2.34251700 0.71776400 -0.70397600
H -2.31473400 -2.67430900 -0.46082400
H -1.65503600 1.55162200 -0.79705100
C -4.26315000 2.35404100 -0.84062800
H -4.53112100 2.77787900 0.13581800
H -3.51845400 3.01789000 -1.29001400
O -5.95500200 0.03990300 -0.67998400
C -6.59388800 0.32956600 0.57907900
H -6.38947800 -0.48239200 1.29058500
H -6.18113200 1.25577300 1.00102100
C -8.08862300 0.47027100 0.33243000
H -8.46214000 -0.46213700 -0.10909600
H -8.24862500 1.26090300 -0.41154800
C -8.85780600 0.79224800 1.61784900
H -8.73051000 0.00230800 2.36768900
H -8.51427000 1.73390900 2.06241200
H -9.92943900 0.89025200 1.41531900
N -0.43586400 -0.83598500 -0.64146700
N 1.78355500 -0.78029300 -0.15943700
C 0.53494200 -0.35015300 0.17785900
H -0.15907500 -1.56392900 -1.29245000
H 1.91371200 -1.29383700 -1.02574200
S 0.23364600 0.65358200 1.51532300
H -5.16645000 2.37056800 -1.45748700
C -5.05209900 -2.64137100 -0.50067900
H -5.64658900 -2.64675600 0.42084900
H -5.76178300 -2.60544100 -1.33426300
H -4.50715200 -3.58837200 -0.55148100
C 3.00601900 -0.40546100 0.48639000
C 4.02422500 -1.54285600 0.32722600
H 2.80626200 -0.23276800 1.54938800
C 5.40357600 -1.09146400 0.80925500
H 3.68660800 -2.39449700 0.93657700
C 4.71703200 1.28571300 0.42128800
C 5.80213600 0.22970800 0.15899600
H 5.37472000 -0.94794600 1.90105300
H 4.63036900 1.46050000 1.50593000
H 5.88663300 0.08232400 -0.92283500
O 3.47114200 0.81107000 -0.11051800
O 4.07045100 -1.90596000 -1.04814400
H 4.88542700 -2.42893800 -1.15403700
O 6.32141500 -2.12662700 0.47017400
H 7.20542800 -1.72183000 0.52203000
O 7.06590000 0.59044400 0.72187400
H 7.55824100 1.10234600 0.06194700
C 4.97959900 2.61588800 -0.27789200
H 4.18220400 3.32230200 -0.00530700
H 5.93224000 3.03031900 0.06462600
O 5.07281300 2.46285600 -1.68938800
H 4.25981900 2.00306000 -1.96033300

6-ZE-b, electron energy = -1661.810349 a.u.

C 3.48391100 -0.91353000 -0.97374700
C 3.97102200 0.34211400 -0.56787200

C	3.13371400	1.30165600	0.02527100
C	1.79325200	0.96749100	0.24327800
C	1.29679400	-0.28424300	-0.12869200
C	2.13608500	-1.20952500	-0.75399300
H	1.12990200	1.69235000	0.70904100
H	1.73523600	-2.16265600	-1.08072700
C	4.38808400	-1.90571500	-1.66544000
H	5.07217800	-2.39238800	-0.95875300
H	3.80270600	-2.69247100	-2.15017700
O	5.28903200	0.67286900	-0.83211400
C	6.22852900	0.33315400	0.20649400
H	5.94722800	0.84031900	1.13949200
H	6.19965600	-0.74909200	0.39282000
C	7.61491200	0.76634300	-0.24680400
H	7.59513000	1.84310500	-0.45701700
H	7.84903100	0.26210400	-1.19280900
C	8.68956300	0.45230600	0.79912000
H	8.48682500	0.96665400	1.74613200
H	8.74184100	-0.62304800	1.00720900
H	9.67679500	0.77276600	0.45020900
N	-0.09038400	-0.54411700	0.05500500
N	-2.02636100	-1.67691600	0.50674000
C	-0.66912600	-1.63423700	0.62289000
H	-0.70638900	0.25904600	-0.05336200
H	-2.51345800	-2.32846100	1.10904200
S	0.14699600	-2.87616100	1.44949900
H	5.00815900	-1.41394500	-2.42146100
C	3.66570000	2.66197800	0.40767600
H	4.31860900	2.60984000	1.28790000
H	4.26021000	3.09495200	-0.40315400
H	2.84671900	3.34730600	0.64446600
C	-2.83154700	-0.79691900	-0.29304200
C	-4.25670400	-1.35289100	-0.38192400
H	-2.41148100	-0.73221500	-1.30737400
C	-5.18650000	-0.32258600	-1.02884600
H	-4.23048700	-2.25900300	-1.00557000
C	-3.59119200	1.49966500	-0.38227000
C	-5.05502100	1.03515800	-0.34463400
H	-4.91813800	-0.20729300	-2.09071900
H	-3.26235600	1.60566400	-1.42791600
H	-5.35988000	0.93631100	0.70221500
O	-2.78578400	0.51505200	0.29575200
O	-4.69444100	-1.66709800	0.93264100
H	-5.66008700	-1.77879800	0.86458000
O	-6.50958300	-0.83200200	-0.90532900
H	-7.10055200	-0.07270000	-1.05489600
O	-5.92452400	1.92554500	-1.04564800
H	-6.24054100	2.59701700	-0.42144600
C	-3.34741100	2.81326200	0.35246200
H	-2.28239600	3.07422500	0.26863000
H	-3.92828700	3.60816200	-0.12393500
O	-3.76120500	2.75327600	1.71150900
H	-3.28323800	2.00603800	2.10934900

6-EZ-b, electron energy = -1661.811824 a.u.

C	2.88473300	0.31331300	-1.27472200
C	3.79219100	0.47642600	-0.21430900
C	3.57476000	1.41957200	0.80706400
C	2.39995200	2.17421400	0.77600500
C	1.47257800	2.01262300	-0.25807800

C	1.72923200	1.10319900	-1.28911200
H	2.20269700	2.89655700	1.56348500
H	1.04186400	1.02465800	-2.12635000
C	3.16343800	-0.66266500	-2.39204800
H	2.87834400	-1.68503100	-2.11283700
H	2.59703800	-0.39955500	-3.29023500
O	4.97105800	-0.24516800	-0.20890300
C	4.90124500	-1.54008700	0.42263700
H	4.55863400	-1.42575500	1.46015400
H	4.17161400	-2.17025800	-0.10349700
C	6.28763900	-2.16435600	0.37643600
H	6.99215700	-1.49244200	0.88238500
H	6.60838400	-2.23164900	-0.67076000
C	6.31897000	-3.55088500	1.02791600
H	6.02655100	-3.50264200	2.08365000
H	5.63613700	-4.24455000	0.52296200
H	7.32540600	-3.97961000	0.98005000
N	0.30897100	2.84168400	-0.27150500
N	-1.24138800	1.15030800	-0.51598000
C	-0.99479300	2.47536200	-0.38650000
H	0.44064400	3.82406500	-0.06514800
H	-0.47101300	0.49764200	-0.40444300
S	-2.20794400	3.67501000	-0.37824700
H	4.22854000	-0.68150300	-2.64015800
C	4.59373300	1.61171600	1.90379800
H	4.66283400	0.72957700	2.55155700
H	5.59282300	1.77823100	1.48762500
H	4.33226400	2.46745400	2.53264600
C	-2.53892400	0.54180400	-0.58044600
C	-2.43256800	-0.76665600	-1.37568100
H	-3.22625700	1.22895500	-1.08579600
C	-3.73026300	-1.56951800	-1.26075600
H	-2.25341200	-0.51394600	-2.43145700
C	-4.26355100	-0.33616000	0.85025900
C	-4.14927000	-1.72251400	0.19803800
H	-4.53254700	-1.04066800	-1.79922500
H	-5.03620000	0.52535800	0.32933200
H	-3.38181200	-2.29271600	0.73188900
O	-2.98915100	0.31889700	0.75950000
O	-1.33950200	-1.51358100	-0.85356100
H	-1.46568300	-2.42333500	-1.17876100
O	-3.48550100	-2.83858000	-1.85966200
H	-4.19596800	-3.42234400	-1.53936000
O	-5.39127300	-2.43030600	0.18740400
H	-5.45721800	-2.94169300	1.00856000
C	-4.59616300	-0.38500400	2.33776400
H	-4.68815500	0.64428300	2.71351000
H	-5.55748500	-0.88644000	2.48247000
O	-3.62632700	-1.11922700	3.07590800
H	-2.76823400	-0.71232800	2.86702800

6-EE-b, electron energy = -1661.803917 a.u.

C	-1.96151100	1.04932500	1.17144900
C	-2.84962400	1.16929800	0.08736200
C	-2.50111000	1.86958700	-1.08045900
C	-1.22060100	2.42590800	-1.15916400
C	-0.31767900	2.29806800	-0.10109500
C	-0.69276300	1.62601900	1.06548400
H	-0.92456200	2.97174200	-2.05116800
H	-0.00047100	1.55680200	1.89755200

C	-2.39517900	0.35722300	2.44133400	C	3.63165100	1.96901200	-3.03092700
H	-2.59226400	-0.70878800	2.27718300	H	4.68611300	1.76826900	-3.21482300
H	-1.62449000	0.44072800	3.21281400	H	3.26358600	2.56920500	-3.87009400
O	-4.12568500	0.65216400	0.21757200	C	3.56942000	1.36185800	2.52862500
C	-4.30871000	-0.68126600	-0.29904500	C	4.17595800	0.09824300	2.66084800
H	-4.08582200	-0.69685700	-1.37436100	C	2.20838000	1.50461300	2.82117300
H	-3.60904200	-1.36762500	0.19748000	C	3.39863600	-1.03424000	2.97587400
C	-5.74958100	-1.09496200	-0.04023900	C	1.44869500	0.40646900	3.22609100
H	-6.41531700	-0.36913200	-0.52395500	H	1.73716900	2.47121800	2.71390500
H	-5.94378800	-1.03497800	1.03800300	C	2.05210700	-0.85412800	3.28250700
C	-6.04732500	-2.50780500	-0.55285600	H	1.44322400	-1.72026000	3.52620600
H	-5.88234200	-2.58333100	-1.63431200	C	2.87504300	0.64487200	-2.98485300
H	-5.40794500	-3.25267100	-0.06409100	C	3.55186900	-0.57934000	-2.82287700
H	-7.08898900	-2.78120500	-0.35478400	C	1.47679600	0.63970900	-3.05212500
N	0.93979200	2.97542800	-0.20465800	C	2.83772000	-1.77039200	-2.58993100
N	2.49807900	1.31960300	0.43107700	C	0.76068800	-0.55346000	-2.93345000
C	2.17705100	2.62334700	0.22445200	H	0.94377500	1.57534200	-3.20143600
H	0.88177300	3.95566800	-0.45424500	C	1.44453600	-1.73609000	-2.65601200
H	3.44823300	1.18648400	0.76032900	H	0.87557500	-2.63692700	-2.47900100
S	3.35083300	3.83612400	0.49818800	C	3.53691900	-3.06677400	-2.17538800
H	-3.32243700	0.79209100	2.83015900	H	3.25603600	-3.87303900	-2.86291800
C	-3.48423900	2.02967800	-2.21473700	H	4.61452000	-2.93025000	-2.23754100
H	-3.52504200	1.13194700	-2.84471500	C	3.94565700	-2.45600100	2.86798100
H	-4.49583300	2.20198100	-1.83546300	H	5.03040600	-2.41965200	2.79009300
H	-3.20256400	2.86824800	-2.85835700	H	3.69644100	-3.01790600	3.77478500
C	1.94334400	0.14051700	-0.19931800	C	1.91940400	-4.11541200	-0.55421500
C	3.03516600	-0.54499600	-1.04031100	C	1.37224200	-4.27486200	0.72474000
H	1.11675600	0.42547500	-0.85707500	C	3.12704700	-3.44857400	-0.75916500
C	2.55825700	-1.91879400	-1.51518400	C	2.09232500	-3.81562600	1.83206300
H	3.24439300	0.09096000	-1.91378100	C	3.84517300	-3.00007600	0.36626600
C	0.93617500	-1.96460700	0.39345800	C	3.31790000	-3.15735500	1.66331300
C	2.03644600	-2.74322200	-0.34304500	H	1.67823400	-3.92902000	2.82437600
H	1.74119500	-1.78823100	-2.24258800	H	1.36494400	-4.48019500	-1.41500500
H	0.08568800	-1.79602200	-0.28617400	O	5.53783500	-0.04192100	2.46222400
H	2.85784400	-2.92643300	0.35738600	O	5.01960700	-2.30489000	0.17410700
O	1.47031500	-0.70816200	0.84276800	O	4.93339200	-0.60834700	-2.87528800
O	4.19628000	-0.67530300	-0.23055900	O	5.08333200	1.47769500	-0.54509200
H	4.75589400	-1.33443200	-0.67925500	C	5.44563900	-0.89840700	-4.19289000
O	3.67397200	-2.55420300	-2.13186100	H	5.08051100	-0.13971200	-4.89993200
H	3.44903300	-3.50061100	-2.17487800	H	5.06587300	-1.87462600	-4.52665500
O	1.55710500	-3.97173200	-0.89441700	C	6.96579000	-0.90024000	-4.14047700
H	1.66331900	-4.66724100	-0.22720600	H	7.29401700	-1.63974700	-3.39914500
C	0.43731200	-2.66988300	1.65112800	H	7.31035000	0.07913700	-3.78660100
H	-0.36672400	-2.07012500	2.10037500	C	7.58651300	-1.21377700	-5.50607000
H	0.02238000	-3.64577700	1.38286400	H	8.67979700	-1.20868600	-5.44556800
O	1.48708400	-2.90342000	2.58215300	H	7.27644500	-2.20117400	-5.86848300
H	1.89755900	-2.03721500	2.74578300	H	7.29020000	-0.47297100	-6.25827600
1A-ZE, electron energy = -6485.157202 a.u.				C	6.24311300	-2.99692400	0.50375700
C	3.75074400	3.05262900	0.67243800	H	6.09286000	-3.61298900	1.39892400
C	4.11407800	2.45601000	-0.54989100	H	6.95615100	-2.20559300	0.75274700
C	3.42982100	2.76862300	-1.74577600	C	6.77324400	-3.86315600	-0.63608300
C	2.43085300	3.74301700	-1.70968600	H	6.92185600	-3.23539500	-1.52327300
C	2.09625800	4.38511400	-0.51458700	H	6.02184700	-4.61895800	-0.89769700
C	2.75303600	4.03519300	0.66592700	C	8.08945100	-4.55084800	-0.25467600
H	1.88095500	3.98064400	-2.61362900	H	7.95876300	-5.20688900	0.61437300
H	2.47247000	4.52288800	1.59589000	H	8.46378900	-5.16321700	-1.08171800
C	4.33680500	2.57057100	1.99380400	H	8.86468400	-3.81637900	-0.00514400
H	5.38335300	2.29856700	1.87051900	C	6.36607200	1.83176300	-1.10653100
H	4.28495200	3.38828000	2.72207100	H	6.80028600	0.88201800	-1.42798800
				H	6.22359000	2.45763700	-1.99593200

C	7.28605100	2.54308700	-0.11785000	H	-1.77210800	7.67188700	3.53517200
H	7.42056800	1.90556700	0.76390200	O	-2.46750500	5.76753300	3.64857400
H	6.80836900	3.47041600	0.22287600	H	-2.15055200	4.87595300	3.40262100
C	8.64616200	2.86348300	-0.74892500	C	-2.69752300	-4.50528700	0.16709700
H	9.15551200	1.95115300	-1.08225400	C	-4.22861000	-4.63428700	0.20015000
H	8.53572200	3.52123800	-1.61955000	H	-2.43637300	-3.44329000	0.18601900
H	9.30121700	3.36793800	-0.03079900	C	-2.49227000	-6.33650900	-1.43098300
C	6.30474800	0.08632500	3.67695000	C	-4.66798200	-6.04375600	-0.21093000
H	5.93927800	-0.63885100	4.41810100	H	-4.57998100	-4.41329000	1.21815000
H	6.15888600	1.09246300	4.09599800	C	-4.01960400	-6.43318300	-1.53617700
C	7.77260600	-0.16122800	3.36366600	H	-4.36804000	-6.77191000	0.55803800
H	8.10262600	0.56008700	2.60572700	H	-4.35550600	-5.73924300	-2.31278400
H	7.87679500	-1.15911000	2.91978400	H	-2.12868600	-7.04431000	-0.67252700
C	8.65189200	-0.04718400	4.61374700	C	-1.77954100	-6.61707300	-2.75228200
H	9.70350400	-0.22607600	4.36658300	H	-0.69981700	-6.46315300	-2.61273300
H	8.57920900	0.95050100	5.06293200	H	-1.93327200	-7.67041300	-3.00732000
H	8.35835500	-0.77925900	5.37550300	O	-2.13384800	-4.98696900	-1.05034300
N	-0.66133600	-0.51737500	-2.99713000	O	-4.75938100	-3.68413700	-0.71280500
N	0.05526300	0.42348600	3.47619000	H	-5.66744600	-3.99136300	-0.89307700
N	-2.82836900	-1.21327600	-3.30314700	O	-6.08684500	-6.01217000	-0.33220200
N	-2.14022100	0.98274800	3.27733800	H	-6.32355700	-6.79100600	-0.86686400
N	-2.12509200	-5.18533500	1.33346600	O	-4.45369200	-7.76351200	-1.82486000
N	0.04719600	-4.78289000	0.74714200	H	-4.47525000	-7.87211900	-2.78837700
N	0.98643500	5.27060200	-0.43595700	O	-2.28227700	-5.85463600	-3.83742500
N	-0.70417800	6.61363600	-1.17981300	H	-2.01884300	-4.92126900	-3.71172000
C	0.60436200	6.23595300	-1.30968700	C	-2.44780500	-0.30343100	2.66277700
C	-0.82183000	-5.06385300	1.74335800	C	-3.87069800	-0.33601400	2.08776100
C	-1.50315700	-1.42875100	-3.54207700	H	-1.75056600	-0.47755600	1.83977600
C	-0.86562100	1.42008800	3.49219000	C	-3.12210400	-1.46304200	4.67406400
H	-0.37568900	-4.83134000	-0.18101700	C	-4.90078200	-0.46033300	3.21901200
H	-2.75939200	-5.44054900	2.07971300	H	-4.05026400	0.58891400	1.52413800
H	-0.34582500	-0.50635400	3.59283400	C	-4.54515900	-1.63692300	4.12308400
H	-2.86058900	1.68813900	3.36002100	H	-3.06551800	-0.52904100	5.25283300
H	-1.10246000	0.34373400	-2.67613300	H	-4.58383800	-2.55946000	3.53628100
H	-3.43552600	-1.89207600	-3.74380800	C	-3.37701000	-0.37122400	-2.24476000
H	0.37695100	5.14335300	0.37007900	C	-4.88919300	-0.64358200	-1.12236900
H	-0.98694400	7.37228700	-1.78661600	H	-2.90428500	-0.61559600	-1.28808900
S	-0.43140500	-5.32963100	3.38096100	C	-3.74683100	1.60213200	-3.57717200
S	-0.55934700	3.06502800	3.79991900	C	-5.70068700	0.09897100	-3.19532500
S	-1.04869200	-2.75240700	-4.52187600	H	-5.05556300	-1.72509300	-2.19899300
S	1.60772700	6.98630400	-2.45572900	C	-5.25027100	1.55046900	-3.28388000
C	-1.71899900	5.76418400	-0.57109900	H	-3.52097000	1.01144100	-4.47471600
C	-3.12476600	6.19271300	-1.02164000	H	-5.41942600	2.02341300	-2.30773700
H	-1.55730300	4.73008000	-0.88918300	H	-4.87222700	0.45634900	3.83418400
C	-1.93279400	6.92459600	1.54139500	H	-5.55415300	-0.37978600	-4.17497500
C	-3.63446100	7.40351000	-0.23171100	C	-2.68152700	-2.60678900	5.58541000
H	-3.10538300	6.42335400	-2.09528100	H	-1.61690700	-2.47844900	5.82503300
C	-3.41517800	7.20816800	1.26602800	H	-3.24409600	-2.51773700	6.52090900
H	-3.09348300	8.30769300	-0.54894400	C	-3.22917500	3.04174200	-3.78238500
H	-3.99463500	6.34344700	1.60641900	H	-2.26551500	3.14527600	-3.26783500
O	-1.58490400	5.70735000	0.84652400	H	-3.05462700	3.20130300	-4.84956100
O	-3.99441800	5.08009700	-0.79415000	O	-3.06317300	1.00479800	-2.44929400
H	-4.88465000	5.47488400	-0.69670600	O	-4.14766800	4.05703300	-3.38564300
O	-5.02092700	7.52723100	-0.53312000	H	-4.09529000	4.20298900	-2.41546400
H	-5.39799200	8.08242000	0.17282600	O	-6.02632700	2.18680200	-4.28898500
O	-3.87653400	8.40410200	1.89412500	H	-5.81737500	3.13598700	-4.18685500
H	-4.16510400	8.17933100	2.79253900	O	-7.06820900	0.00501600	-2.80334900
H	-1.31534000	7.75441200	1.16786900	H	-7.53039100	0.72904500	-3.26190300
C	-1.62075100	6.71754500	3.02016000	O	-5.29530900	-0.19296600	-0.83167900
H	-0.56085000	6.44745800	3.12432000	H	-6.26221500	-0.06718200	-0.89635200

O	-2.95156000	-3.89917100	5.06569300	H	-0.19793500	4.45742900	5.03156600
H	-2.23302800	-4.14719600	4.44851100	H	-1.85105900	4.83184900	4.50381900
O	-5.52114900	-1.65995800	5.16830800	C	-0.48746500	6.51846800	4.41367200
H	-5.60950100	-2.57689300	5.47210200	H	-1.07688400	7.05619800	3.66007900
O	-6.18944600	-0.61602800	2.64624200	H	0.56889100	6.68397900	4.16839700
H	-6.75980500	-0.90730600	3.37942300	C	-0.79647500	7.06635000	5.81110400
O	-3.91244100	-1.45381600	1.21747300	H	-0.57467500	8.13723400	5.86610300
H	-4.59659100	-1.26433300	0.54203400	H	-1.85377600	6.93059800	6.06830400
O	-2.20403500	-1.38995900	3.55952300	H	-0.19795100	6.56134900	6.57867600

1B-ZE, electron energy = -6485.155831 a.u.

C	3.20871200	2.73529000	-0.38162700	H	-2.58776700	6.32487300	-1.73469600
C	2.52393800	3.16168800	0.77302700	H	-0.98850400	6.69060500	-1.06431800
C	2.68564800	2.48797600	1.99862000	C	-2.64357800	7.13937300	0.26813800
C	3.64772400	1.47455600	2.09681800	H	-2.02660300	7.09790100	1.17443700
C	4.40217000	1.09877500	0.98078900	H	-3.61749000	6.70151700	0.52148000
C	4.15451600	1.71724400	-0.25409500	C	-2.82888300	8.59537400	-0.17482000
H	3.80448700	0.97502100	3.04285000	H	-3.46745700	8.66295700	-1.06389400
H	4.70422100	1.39011000	-1.13376200	H	-3.29708700	9.18844800	0.61782600
C	2.84371600	3.28368800	-1.75364100	H	-1.86717700	9.06301500	-0.41827600
H	2.76394900	4.36963800	-1.72785500	C	2.03044000	5.47004700	1.19607800
H	3.64331600	3.02781800	-2.45927900	H	1.09737500	5.98469300	1.43312200
C	1.77371500	2.77187700	3.18964400	H	2.57925800	5.31865800	2.13365700
H	1.76537100	3.83396400	3.43847000	C	2.87398500	6.29181000	0.22510500
H	2.17160200	2.23988600	4.06065000	H	2.31297600	6.42001200	-0.70794000
C	1.51829600	2.70548800	-2.24584900	H	3.79192000	5.74278000	-0.02066500
C	0.42741900	3.52451500	-2.59732700	C	3.23494700	7.65925100	0.81765200
C	1.35060100	1.32218100	-2.28879500	H	2.33558500	8.24044100	1.05480500
C	-0.82600000	2.95868000	-2.89504400	H	3.81632000	7.55250300	1.74155900
C	0.13166800	0.74048300	-2.65513400	H	3.83440500	8.24511000	0.11277000
H	2.18210800	0.68131600	-2.00623400	C	1.00088700	5.40222000	-3.91263000
C	-0.95443500	1.56592500	-2.95007700	H	0.26590200	5.10716500	-4.67521500
H	-1.91180900	1.12813700	-3.19504200	H	1.96492800	4.95058800	-4.18741300
C	0.34111400	2.31794400	2.92348600	C	1.11599500	6.91700200	-3.83378800
C	-0.69972500	3.24997500	2.74780900	H	1.84302200	7.17878000	-3.05486100
C	0.05258500	0.95359300	2.79414600	H	0.14945200	7.32936200	-3.51839100
C	-1.97325500	2.83898100	2.31118700	C	1.53812300	7.53137300	-5.17290300
C	-1.23596200	0.52755900	2.46297200	H	1.61391400	8.62084300	-5.09332000
H	0.84274500	0.22242900	2.94743800	H	2.51460400	7.15164300	-5.49667800
C	-2.21967200	1.47337600	2.17477200	H	0.81216400	7.30379100	-5.96259600
H	-3.18507400	1.13673500	1.82366400	N	-1.50018400	-0.86482800	2.31658200
C	-3.04960000	3.84912400	1.90379100	N	0.11394400	-0.67811700	-2.70969400
H	-3.90550500	3.77488800	2.58538500	N	-2.73787600	-2.78993100	2.11336400
H	-2.63883900	4.85376800	1.99136700	N	-0.48976600	-2.88273400	-2.57451100
C	-2.07711400	3.81963900	-3.06892400	N	-7.14487100	-0.49280300	-1.93539800
H	-1.78659900	4.86859700	-3.11980700	N	-5.80903700	1.15761900	-1.10348000
H	-2.57029000	3.56934300	-4.01479500	N	5.44944700	0.13901300	0.98820600
C	-4.56914800	2.68346100	0.25956100	N	6.81873900	-1.65003600	1.39705000
C	-4.86453200	2.21323300	-1.02269900	C	5.73074800	-0.91153700	1.79452100
C	-3.51529100	3.57380600	0.48290600	C	-6.63080800	0.76617700	-2.10671500
C	-4.10000300	2.64988800	-2.10953100	C	-2.63911200	-1.53297200	2.62654900
C	-2.79975700	4.05509900	-0.62787600	C	-0.87625600	-1.57520300	-2.46481500
C	-3.05287200	3.55785500	-1.92415700	H	-5.85748700	0.57571500	-0.26722800
H	-4.28364000	2.23655500	-3.09397000	H	-7.79019900	-0.77998600	-2.65979800
H	-5.14271000	2.31359400	1.10630800	H	1.04764500	-1.08584200	-2.68574200
O	0.58405400	4.89926300	-2.62721800	H	-1.14699000	-3.56632400	-2.20246800
O	-1.75660500	4.93118400	-0.42018400	H	-0.72666400	-1.43914900	1.98879200
O	-0.45902500	4.59293000	2.97009200	H	-3.55797900	-3.29782100	2.41807700
O	1.61723700	4.19147700	0.66150600	H	6.12626900	0.27772300	0.23800000
C	-0.78891100	5.03142100	4.30350300	H	7.00148500	-2.43962500	2.00328400
				S	-7.08233800	1.70139900	-3.45133600

S	-2.47920700	-1.20579200	-2.02862200	C	-2.43996900	-5.79573700	1.38091500
S	-3.89137100	-0.94581600	3.62835100	H	-3.67415800	-4.35819800	0.30747600
S	4.90689100	-1.37018000	3.21178800	C	-0.97985800	-5.94328800	1.79103900
C	7.32358000	-1.72191800	0.02708200	H	-1.10652500	-4.39445700	3.30312800
C	8.36434200	-2.84635600	-0.08306800	H	-0.38977000	-6.11936900	0.88397700
H	6.50312100	-1.92794900	-0.66891100	H	0.28648200	-5.50576500	-1.39504500
C	9.05601600	-0.02128300	0.25201400	H	-3.05398700	-5.66753500	2.28530200
C	9.69752200	-2.42774200	0.54884000	C	3.38529700	-2.79606700	-0.66249400
H	7.97921800	-3.73939600	0.43356800	H	3.15685600	-1.73016900	-0.52717000
C	10.14693500	-1.07272000	0.00910400	H	3.61577800	-3.21687300	0.31983800
H	9.58525400	-2.34966900	1.64101300	C	0.98871200	-4.76410700	2.91320800
H	10.31528000	-1.15735400	-1.06926300	H	1.49844300	-3.81307900	2.70934300
O	7.84180800	-0.46165900	-0.40028400	H	0.99785500	-4.92125500	3.99473700
O	8.54186900	-3.11656900	-1.46377700	O	-0.57961000	-3.58722200	1.46502600
H	9.39581800	-3.58375500	-1.52115700	O	1.69521900	-5.87014800	2.36046000
O	10.64248700	-3.44141500	0.22107400	H	1.91513700	-5.68422800	1.42350200
H	11.51875900	-3.04380600	0.37057100	O	-0.87934900	-7.06102100	2.66378000
O	11.36278400	-0.75118100	0.68745500	H	0.07918500	-7.23777600	2.72084100
H	11.91130500	-0.21607300	0.09330900	O	-2.88457200	-6.93212900	0.64522600
H	8.88370200	0.09124400	1.33108600	H	-2.48665200	-7.70762900	1.07900800
C	9.37336000	1.34239500	-0.35103000	O	-2.00165600	-4.85757300	-0.80514100
H	8.54860200	2.03298600	-0.12280600	H	-2.22783400	-5.78784500	-0.99720900
H	10.28170700	1.73862500	0.11181400	O	4.54450500	-2.97932500	-1.47053600
O	9.61755300	1.27203100	-1.75013900	H	4.33801700	-2.60853100	-2.34519600
H	8.82442900	0.87390600	-2.14674400	O	2.63788200	-5.73183200	-0.29790900
C	-6.52127900	-1.51793000	-1.10251000	H	3.59764200	-5.76092700	-0.15614800
C	-7.12455600	-2.89863200	-1.40549800	O	1.31229800	-6.95444500	-2.48157000
H	-5.44636100	-1.55840400	-1.30747800	H	1.79531800	-7.36620300	-1.74392500
C	-7.91236700	-1.24018600	0.86866300	O	1.69865400	-5.12759600	-4.41821100
C	-8.49953200	-3.06258900	-0.74605000	H	1.91030600	-6.07362800	-4.31178200
H	-7.22337100	-3.01301700	-2.49593100	O	1.90783800	-2.87058100	-2.51598400
C	-8.43565200	-2.67479600	0.72790700	1C-ZE, electron energy = -6485.159339 a.u.			
H	-9.23551700	-2.41566400	-1.24777100	C	2.66652900	3.74353400	-1.54715800
H	-7.74039500	-3.34484800	1.24347500	C	2.39643100	4.17626700	-0.23573300
H	-8.57978600	-0.54592400	0.33789400	C	3.11338400	3.65934400	0.86530300
C	-7.78924100	-0.78076800	2.31952400	C	4.17145400	2.78055700	0.62337000
H	-7.31952000	0.21280200	2.33765500	C	4.49489500	2.39308000	-0.68007200
H	-8.80028800	-0.67665000	2.72685900	C	3.73896400	2.86841200	-1.75234100
O	-6.59145100	-1.18510800	0.28422900	H	4.72180800	2.35838100	1.45723400
O	-6.22096000	-3.86624600	-0.89215100	H	3.97433600	2.53358700	-2.75947800
H	-6.74982600	-4.67974400	-0.79463100	C	1.73636000	4.08853200	-2.70081400
O	-8.86429100	-4.43126900	-0.89677100	H	1.38891900	5.11772300	-2.62550500
H	-9.56592800	-4.59114200	-0.24057400	H	2.28780000	3.98940800	-3.64329800
O	-9.75924600	-2.82578000	1.24358000	C	2.64748400	3.89067000	2.30019300
H	-9.69091200	-3.01953800	2.19163800	H	2.36065900	4.92849200	2.46408900
O	-7.10206300	-1.70149200	3.15110100	H	3.48177800	3.67218700	2.97583600
H	-6.14176600	-1.61419400	2.98282400	C	0.52410400	3.15717800	-2.71405200
C	0.73716900	-3.32636300	-3.20986300	C	-0.78841100	3.65280000	-2.59857200
C	0.73954700	-4.85020000	-3.40992900	C	0.72786000	1.77488000	-2.75774800
H	0.82677800	-2.85443700	-4.19297400	C	-1.87367600	2.77279400	-2.42572600
C	2.16216600	-3.49681000	-1.24006100	C	-0.34970300	0.89174100	-2.68022200
C	1.11012700	-5.59201900	-2.11679600	H	1.73402100	1.38524200	-2.82545000
H	-0.26257000	-5.16634700	-3.73631600	C	-1.63783500	1.39965200	-2.48810300
C	2.37073500	-4.99369400	-1.50128800	H	-2.46828000	0.71141200	-2.34944700
H	1.31077300	-3.34557400	-0.56133100	C	1.46546100	2.98520600	2.64080400
H	3.20559900	-5.11536000	-2.19666100	C	0.16468500	3.49601900	2.81195900
C	-1.91793100	-3.33313300	1.03871300	C	1.66118500	1.60496800	2.75516400
C	-2.60770600	-4.57939100	0.45552900	C	-0.94249000	2.63129900	2.93029800
H	-1.82046200	-2.58464200	0.24780300	C	0.58809700	0.74557200	2.99496700
C	-0.47522500	-4.64958500	2.44168900				

H	2.66591900	1.19816000	2.67437700	H	-2.74000800	7.22291300	-5.63584900
C	-0.71162900	1.25515900	3.01473800	N	0.84898300	-0.64811100	3.15543300
H	-1.54862500	0.57358600	3.11291000	N	-0.21768400	-0.51922900	-2.64529500
C	-2.37533400	3.16300500	2.93975600	N	0.82656800	-2.74439900	4.10272700
H	-2.88107200	2.82072300	3.85007400	N	0.63755000	-2.63251100	-2.66113600
H	-2.34373100	4.25137900	2.96567400	N	-6.19558800	-2.23569600	1.17640500
C	-3.27199800	3.27115400	-2.06880000	N	-5.53626000	-0.06408300	0.81491200
H	-3.29230200	4.35757200	-2.14399700	N	5.45600800	1.37846100	-0.93979200
H	-4.00099300	2.88153300	-2.78813300	N	7.18168100	-0.06355800	-0.56538800
C	-4.00338300	1.56448900	1.83417800	C	6.68372400	1.20076000	-0.39418200
C	-4.65729900	1.05816600	0.71109800	C	-5.17983900	-1.33121700	1.13254900
C	-3.17594800	2.68836400	1.73408600	C	0.42905500	-1.44062100	4.17623300
C	-4.47590400	1.66152400	-0.53447200	C	0.74588500	-1.34818700	-3.11289200
C	-3.05636200	3.32467100	0.48245400	H	-6.44769000	0.03562200	0.37071400
C	-3.65414900	2.78400600	-0.67499400	H	-5.90591900	-3.18368100	1.37752600
H	-4.95039700	1.22767500	-1.41104700	H	-1.01955700	-1.00023400	-2.23795800
H	-4.14239500	1.07902300	2.79487000	H	1.32448700	-3.27338900	-3.03589700
O	-1.01282000	5.01750300	-2.61311000	H	1.62640400	-1.01905400	2.61184300
O	-2.25777100	4.44004700	0.38256100	H	0.51906600	-3.30902500	4.88343100
O	-0.02426700	4.86576400	2.86923900	H	5.17194900	0.66903300	-1.61443500
O	1.33894700	5.03122300	-0.02312200	H	8.11682000	-0.20185000	-0.20457800
C	0.09227000	5.39132800	4.20830700	S	-3.58203700	-1.85560100	1.42934700
H	1.06226200	5.09570000	4.63262500	S	1.97962300	-0.93696500	-4.21506900
H	-0.69375100	4.95453300	4.84104800	S	-0.49383200	-0.93393900	5.51400300
C	-0.03065200	6.90685400	4.16147500	S	7.59535500	2.39194700	0.40036300
H	-0.99779200	7.17430400	3.71851300	C	6.32274100	-1.22066800	-0.78299500
H	0.74527000	7.30555600	3.49632800	C	7.06876700	-2.52141400	-0.44822000
C	0.09764600	7.53287600	5.55465700	H	5.44874200	-1.14692600	-0.12894300
H	0.00464300	8.62256000	5.50060000	C	6.68966700	-1.50579500	-3.16039900
H	-0.68254100	7.16397900	6.23111200	C	7.97813000	-2.97305000	-1.59649400
H	1.06941900	7.30227700	6.00714700	H	7.66114300	-2.37234000	0.46439100
C	-2.92840300	5.69921000	0.15075200	C	7.24277900	-2.91828100	-2.93273800
H	-3.79089900	5.54669000	-0.50875700	H	8.85439600	-2.30985300	-1.65389600
H	-2.19918900	6.31356200	-0.38387600	H	6.39834600	-3.61536700	-2.91022600
C	-3.37914200	6.37907700	1.44036700	O	5.75888000	-1.22614500	-2.09233200
H	-2.50881500	6.51080700	2.09290300	O	6.07370200	-3.51927900	-0.20609800
H	-4.08272300	5.72309100	1.96896600	H	6.52619000	-4.37077600	-0.37132600
C	-4.04303600	7.73258100	1.16122400	O	8.38446800	-4.30292000	-1.28915100
H	-4.93009200	7.61766100	0.52650600	H	8.70353300	-4.68435900	-2.12663600
H	-4.35991900	8.21211100	2.09337500	O	8.19276100	-3.30748300	-3.92456700
H	-3.35412000	8.41664200	0.65101500	H	7.70681500	-3.69198200	-4.67094300
C	1.66964300	6.39627200	0.31398300	H	7.50958400	-0.77309100	-3.13879000
H	0.82763300	6.75088400	0.91406500	C	5.94122900	-1.34957400	-4.48069400
H	2.56776700	6.41656500	0.94375700	H	5.51118700	-0.33969700	-4.52653100
C	1.87349800	7.28172000	-0.91229600	H	6.67073400	-1.43640100	-5.29279400
H	0.97304800	7.23320700	-1.53643200	O	4.95720700	-2.34901700	-4.69680500
H	2.70373600	6.88719100	-1.51190700	H	4.15257300	-2.09703600	-4.20232100
C	2.16454300	8.73432500	-0.51773000	C	-7.61565600	-1.93345400	1.06778400
H	1.34132800	9.16029000	0.06856400	C	-8.43257500	-3.22117300	1.25843100
H	3.07754000	8.80883600	0.08536600	H	-7.90566500	-1.21002400	1.83638200
H	2.30016800	9.36036400	-1.40599800	C	-7.77111300	-2.07670000	-1.35558500
C	-1.27876700	5.54659300	-3.92801400	C	-8.37132400	-4.09717800	0.00008600
H	-2.14157300	5.02334800	-4.36447700	H	-8.02088100	-3.77814700	2.11412600
H	-0.41237600	5.36094100	-4.57884100	C	-8.71646400	-3.28063200	-1.24248900
C	-1.55682600	7.03726800	-3.80835100	H	-7.35712400	-4.50675400	-0.12504800
H	-0.68794800	7.52463100	-3.34845900	H	-9.74309700	-2.91133900	-1.15230000
H	-2.40298100	7.18591300	-3.12589800	H	-6.73330900	-2.42555000	-1.45143300
C	-1.85802100	7.67664600	-5.16816700	C	-8.10251600	-1.14496400	-2.51520400
H	-2.05307000	8.74850300	-5.05832600	H	-7.38085900	-0.31490600	-2.52281500
H	-1.01526200	7.55981800	-5.85992900	H	-7.99687700	-1.69044000	-3.45737000

O	-7.91934700	-1.27265700	-0.15857300	C	3.90176900	2.08071100	-0.82743000
O	-9.76994600	-2.83268200	1.52022800	H	4.18163000	1.69683100	2.53736500
H	-10.30530900	-3.62460700	1.32762100	H	4.33923500	1.70963100	-1.75134900
O	-9.30835800	-5.15135600	0.19188700	C	2.17416700	3.30773400	-2.22049000
H	-9.47219600	-5.52346000	-0.69306100	H	1.94207300	4.37037400	-2.28239200
O	-8.59329100	-4.16869200	-2.35500300	H	2.87719300	3.07389600	-3.02893500
H	-9.22497900	-3.89239000	-3.03682200	C	1.96659000	3.24941100	2.84821600
O	-9.44051800	-0.66633400	-2.46065000	H	1.80850300	4.32040800	2.97739000
H	-9.54052000	-0.23199500	-1.59681700	H	2.57050400	2.90612100	3.69547800
C	-0.13028900	-3.01606400	-1.48204200	C	0.88289000	2.51266400	-2.41184400
C	0.21189700	-4.44207100	-1.02488400	C	-0.35643800	3.14043500	-2.63901300
H	0.09148100	-2.32587800	-0.66327100	C	0.90695800	1.12426600	-2.28734200
C	-2.14742300	-3.77741400	-2.61812300	C	-1.55059900	2.39552400	-2.63663400
C	-0.38061600	-5.45954000	-2.00838400	C	-0.26184400	0.35874600	-2.35869900
H	1.30369000	-4.55439900	-0.98489600	H	1.85629600	0.62774100	-2.10389000
C	-1.88103300	-5.21871500	-2.15641400	C	-1.49083000	1.00209300	-2.51854100
H	-1.72130800	-3.63421800	-3.62160100	H	-2.40636800	0.42593800	-2.53112300
H	-2.35764000	-5.37749400	-1.18466700	C	0.61078100	2.54652000	2.86430700
C	1.40420300	-3.40376900	2.93926900	C	-0.59505800	3.27049400	2.80636900
C	1.44046100	-4.92507800	3.18943800	C	0.55214900	1.14838100	2.88866700
H	0.78773400	-3.21482400	2.05543300	C	-1.82819000	2.61316100	2.62400700
C	3.71687500	-3.15744300	3.56631700	C	-0.67357700	0.48435300	2.81730100
C	2.61072600	-5.33377400	4.09755600	H	1.47271800	0.57457500	2.96373200
H	0.48924300	-5.23570000	3.64343700	C	-1.84647400	1.21775800	2.62770500
C	3.89591800	-4.67923000	3.61011300	H	-2.78287000	0.69355600	2.47713200
H	3.39249800	-2.78779900	4.54813300	C	-3.12187700	3.38687400	2.37107900
H	4.08803700	-5.02329200	2.58633500	H	-3.82783300	3.19540800	3.18789100
H	0.08578200	-5.31900300	-2.99883200	H	-2.89582100	4.45278900	2.37535100
H	2.41501800	-5.01500900	5.13221200	C	-2.91682800	3.07583200	-2.68746600
C	-3.62762400	-3.40953000	-2.65930600	H	-2.77718500	4.13785700	-2.89241500
H	-3.71886700	-2.35546900	-2.95915300	H	-3.50500400	2.66158000	-3.51408500
H	-4.12034900	-4.01842000	-3.42316700	C	-4.86463900	2.10246400	1.05282000
C	5.01400500	-2.42710300	3.16527000	C	-5.40307200	1.64265900	-0.15238500
H	4.75575300	-1.58571900	2.50937600	C	-3.77825700	2.98522600	1.05696400
H	5.47427300	-2.01541100	4.06719700	C	-4.78212600	1.98685600	-1.36015800
O	2.68127100	-2.86632600	2.59869400	C	-3.24883100	3.41565500	-0.17365300
O	6.00351100	-3.26968500	2.57994300	C	-3.68624000	2.85195700	-1.38959700
H	5.80317700	-3.42377600	1.63088500	H	-5.15835800	1.57027500	-2.29161400
O	4.94761000	-5.08286400	4.47603000	H	-5.29340900	1.77497400	1.99071800
H	5.76169700	-4.80732800	4.01265400	O	-0.40406400	4.50922800	-2.83460400
O	2.69612500	-6.75495400	4.02964600	O	-2.21823100	4.32728200	-0.17500700
H	3.60248500	-6.98381900	4.30218200	O	-0.56518900	4.65040200	2.90479900
O	1.59635000	-5.56060600	1.92122100	O	1.26501900	4.36829700	0.27487600
H	1.91785000	-6.46119500	2.12205300	C	-0.70601800	5.13280100	4.25648400
O	-4.30274800	-3.66293100	-1.43457500	H	0.08565200	4.69730200	4.88279500
H	-3.88504700	-3.11559400	-0.73893700	H	-1.67240100	4.80335400	4.66404700
O	-2.35610500	-6.16648800	-3.11733600	C	-0.61236900	6.65111100	4.24814500
H	-3.26927700	-6.39824200	-2.88839600	H	-1.39771100	7.05184300	3.59504100
O	-0.11306000	-6.76724400	-1.52942100	H	0.34854900	6.94467600	3.80760700
H	-0.68407800	-7.35324800	-2.05696800	C	-0.74940700	7.24082900	5.65616400
O	-0.35106500	-4.59009400	0.26724600	H	-0.68123200	8.33332500	5.62802400
H	0.24115700	-5.17761900	0.78337200	H	-1.71393200	6.97756600	6.10635300
O	-1.53325400	-2.85354900	-1.69098900	H	0.04152000	6.87355400	6.32095900
				C	-2.55172300	5.66562000	-0.60634200
				H	-3.27128000	5.62004700	-1.43303800
				H	-1.61733900	6.07545400	-0.99658800
				C	-3.10550200	6.53858300	0.51659500
				H	-2.38073500	6.55997100	1.33892600
				H	-4.02593500	6.08780500	0.90931100
				C	-3.39550400	7.96331000	0.02986100
1D-ZE, electron energy = -6485.152173 a.u.							
C	2.82922100	2.97317700	-0.88796700				
C	2.29398900	3.45616400	0.32169300				
C	2.72790100	2.94745100	1.56086600				
C	3.81424600	2.06492300	1.58890600				
C	4.41688000	1.64234200	0.40020400				

H	-4.13714800	7.96545000	-0.77819500	H	11.81702200	-1.93808100	-0.60544200
H	-3.78806700	8.58208200	0.84374900	O	11.52192100	0.34117400	-0.26289100
H	-2.48742600	8.44747200	-0.34949500	H	12.00099500	0.91783400	-0.87789000
C	1.59851100	5.72759600	0.63646000	H	9.02368100	1.00501900	0.51094200
H	0.66818800	6.15262300	1.02035600	C	9.34871300	2.30226900	-1.17459700
H	2.33092300	5.72480100	1.45303900	H	8.48865100	2.93164300	-0.90356900
C	2.13022400	6.54704600	-0.53633400	H	10.24619800	2.75540300	-0.74385700
H	1.39481000	6.52053000	-1.34916100	O	9.53892200	2.26354700	-2.58335300
H	3.04979300	6.08476600	-0.91761100	H	8.75832200	1.81777100	-2.95314200
C	2.41340000	7.99693700	-0.12584300	C	-8.66206000	-0.68026000	-1.34500000
H	1.50531000	8.49244600	0.23843500	C	-9.99150900	-1.42262400	-1.55434000
H	3.16321600	8.04559200	0.67314800	H	-8.62835600	0.17794100	-2.02500700
H	2.79228100	8.57673100	-0.97416000	C	-7.42592400	-2.76709800	-1.11708200
C	-0.26840900	4.90524200	-4.21410600	C	-9.92891800	-2.83615500	-0.96244600
H	-1.05823900	4.42667700	-4.81065600	H	-10.79663700	-0.85496100	-1.06241200
H	0.69969000	4.55746600	-4.60200200	C	-8.68776500	-3.56990300	-1.46123300
C	-0.37222300	6.42052900	-4.29872700	H	-9.88625200	-2.78038000	0.13602900
H	0.41052500	6.86507200	-3.67132200	H	-8.74847600	-3.67046200	-2.54962400
H	-1.33493200	6.73354500	-3.87583300	H	-7.33516700	-2.66525500	-0.02705500
C	-0.23982000	6.92596400	-5.73958900	C	-6.14589200	-3.37897700	-1.67367200
H	-0.31424800	8.01779500	-5.77663000	H	-5.29126500	-2.74969200	-1.38783400
H	0.72590100	6.64187000	-6.17441600	H	-5.99857600	-4.36779400	-1.22954400
H	-1.02916900	6.51537600	-6.38051800	O	-7.53250600	-1.46047600	-1.73034600
N	-0.69611100	-0.93903300	2.84525600	O	-10.21915100	-1.48660500	-2.95212400
N	-0.08403300	-1.04847100	-2.28610200	H	-10.86699300	-2.20594300	-3.06967300
N	-1.49522200	-3.05792800	3.21183700	O	-11.11481400	-3.50578100	-1.37794100
N	-0.31822300	-3.28038400	-1.83725400	H	-10.93935900	-4.45555000	-1.25308600
N	-8.55886800	-0.23787000	0.04176800	O	-8.69666600	-4.85276600	-0.83246600
N	-6.50686200	0.74789500	-0.23329600	H	-8.26680000	-5.48654600	-1.42742100
N	5.56749100	0.80720300	0.33652400	O	-6.20339100	-3.56325800	-3.08340800
N	7.09810000	-0.86645700	0.66127600	H	-6.37394500	-2.68671100	-3.46709900
C	5.98538500	-0.21090600	1.12494400	C	0.77932500	-3.64089100	-2.71813000
C	-7.64145900	0.67656100	0.50097100	C	0.96445400	-5.16525500	-2.77875300
C	-1.54910700	-1.73500300	3.54058900	H	0.56590900	-3.28223400	-3.72965700
C	-0.85551100	-2.02492600	-1.74398000	C	2.62518300	-3.39370800	-1.14983700
H	-6.44824200	0.07405000	-0.99601800	C	1.73007400	-5.69287700	-1.55626800
H	-9.40430300	-0.25897000	0.59783200	H	-0.02644900	-5.64199100	-2.81981200
H	0.87949700	-1.33560200	-2.45354600	C	2.99385900	-4.87154100	-1.32444600
H	-0.78606600	-3.99983800	-1.29044300	H	1.93308400	-3.27404500	-0.30435800
H	0.08456200	-1.41244900	2.39623600	H	3.65403600	-4.96843700	-2.19056800
H	-2.09391300	-3.64972700	3.77223800	C	-0.85708400	-3.59709200	2.02121600
H	6.17550300	1.00316500	-0.45790400	C	-1.37877500	-5.01866900	1.75015200
H	7.38589400	-1.63078600	1.25879100	H	-1.10831900	-2.96637900	1.16391900
S	-8.00844400	1.57826800	1.89529200	C	1.12266400	-4.41657600	3.11291400
S	-2.35678700	-1.80557800	-0.97442700	C	-0.72957900	-6.04938200	2.68767600
S	-2.60823200	-1.22288400	4.77098900	H	-2.46905500	-5.02707600	1.88760900
S	5.28622700	-0.71813300	2.59154200	C	0.78115900	-5.85945000	2.71913500
C	7.53193900	-0.89591400	-0.73362800	H	0.65773700	-4.17542700	4.07787300
C	8.63802800	-1.94792800	-0.90711500	H	1.16839400	-6.03740400	1.70865600
H	6.69315000	-1.15584700	-1.38810700	H	1.09066500	-5.62127700	-0.66628800
C	9.15164000	0.91418900	-0.57642000	H	-1.12175500	-5.92416800	3.70863000
C	9.96908500	-1.44496100	-0.33577200	C	3.82474400	-2.48033300	-0.93693100
H	8.33887900	-2.86821200	-0.38149200	H	3.47496900	-1.44158500	-0.86470500
C	10.29855600	-0.05854900	-0.88335300	H	4.30981700	-2.73536300	0.00882300
H	9.90537900	-1.38165400	0.76135000	C	2.64418900	-4.18086900	3.21838500
H	10.41785400	-0.12419400	-1.96967200	H	2.88193600	-3.20307800	2.77964500
O	7.94061800	0.39816300	-1.17610500	H	2.92330600	-4.14792600	4.27443800
O	8.76533200	-2.19536700	-2.29729400	O	0.56912700	-3.53825400	2.10575600
H	9.64463900	-2.60375200	-2.40127200	O	3.43750700	-5.21899800	2.64824500
O	10.96233700	-2.39084000	-0.71843000	H	3.39189300	-5.16673600	1.67049800

O	1.32289500	-6.81017900	3.62622300	H	5.02402700	1.73300700	-0.88006700
H	2.28626800	-6.76706700	3.46853700	O	-0.63892000	4.71371900	2.71308000
O	-1.07910000	-7.33536900	2.18340900	O	1.70031200	4.47531300	0.55170800
H	-0.43428200	-7.95903800	2.56152100	O	0.63906900	4.71406800	-2.71292000
O	-1.06817600	-5.33490200	0.39565800	O	-1.70017400	4.47533000	-0.55141700
H	-1.12335100	-6.30804700	0.34003700	C	0.99307700	5.22076800	-4.01613100
O	4.81173300	-2.62470400	-1.95419300	H	0.32015600	4.78900800	-4.77060100
H	4.38854500	-2.38336900	-2.79532300	H	2.01693100	4.90624500	-4.26461100
O	3.64346000	-5.41744300	-0.16441700	C	0.88070400	6.73774700	-4.00244100
H	4.60306700	-5.31776100	-0.27173700	H	1.55148900	7.13795300	-3.23202500
O	2.04336200	-7.05385600	-1.83921900	H	-0.14009200	7.01387800	-3.71025300
H	2.73822100	-7.31196000	-1.20879300	C	1.22271300	7.35040200	-5.36492500
O	1.69546000	-5.44057100	-3.96329800	H	1.13891600	8.44166700	-5.33186200
H	2.06810100	-6.33169700	-3.82807000	H	2.24710900	7.10316000	-5.66832700
O	1.99609200	-2.96277700	-2.37647000	H	0.54528000	6.98669700	-6.14673000
1E-ZE, electron energy = -6485.164266 a.u.				C	1.99801100	5.81792400	0.99420800
C	-3.40425800	3.02529100	0.30795600	H	2.55321700	5.78318600	1.93966800
C	-2.67156500	3.52839500	-0.78290200	H	1.02391500	6.27146600	1.19250500
C	-2.84940900	3.00474200	-2.07973300	C	2.77835700	6.62974400	-0.03601700
C	-3.86873500	2.07352100	-2.30010500	H	2.21757400	6.63549500	-0.97788200
C	-4.68498100	1.64786600	-1.24667500	H	3.73936900	6.13846400	-0.23530100
C	-4.42346000	2.10326300	0.05206300	C	3.02109800	8.06512300	0.44494900
H	-4.01332500	1.66314500	-3.29136300	H	3.60222500	8.08146500	1.37501800
H	-5.02375400	1.73270500	0.88004600	H	3.57548900	8.64019100	-0.30429300
C	-3.04537800	3.40594900	1.73860000	H	2.07507800	8.58699400	0.63375400
H	-2.85393200	4.47596800	1.80954900	C	-1.99785400	5.81797000	-0.99385600
H	-3.90003400	3.17799400	2.38672000	H	-1.02374300	6.27154900	-1.19199100
C	-1.86320500	3.32389600	-3.20054700	H	-2.55293100	5.78328600	-1.93939300
H	-1.69211400	4.39674000	-3.28818900	C	-2.77835000	6.62969900	0.03632400
H	-2.29483200	2.98517200	-4.14882100	H	-2.21767400	6.63544100	0.97825500
C	-1.81168600	2.65634800	2.24351700	H	-3.73936200	6.13836800	0.23547800
C	-0.64209700	3.33164200	2.64303400	C	-3.02110200	8.06509400	-0.44460900
C	-1.81255800	1.25955700	2.27989500	H	-2.07508200	8.58700500	-0.63330500
C	0.52984700	2.61901300	2.96428900	H	-3.60214300	8.08145200	-1.37473100
C	-0.68811100	0.53934900	2.69432100	H	-3.57558100	8.64011500	0.30460400
H	-2.70345500	0.72164300	1.96706400	C	-0.99285800	5.22035400	4.01634000
C	0.48450000	1.22262100	3.01592500	H	-0.31993700	4.78850700	4.77075600
H	1.37039300	0.66751800	3.29813500	H	-2.01672300	4.90586700	4.26482800
C	-0.52970100	2.61938900	-2.96422200	C	-0.88041400	6.73732900	4.00274700
C	0.64224100	3.33199100	-2.64292800	H	-1.55118300	7.13761400	3.23235800
C	-0.48438200	1.22299000	-3.01591900	H	0.14039300	7.01343700	3.71057900
C	1.81182500	2.65666200	-2.24340900	C	-1.22239800	7.34990000	5.36527600
C	0.68820600	0.53970500	-2.69431500	H	-1.13856900	8.44116500	5.33229500
H	-1.37029100	0.66792000	-3.29813400	H	-2.24679900	7.10266400	5.66866500
C	1.81266600	1.25988200	-2.27983700	H	-0.54497100	6.98611500	6.14705000
H	2.70351200	0.72191200	-1.96695400	N	0.82532700	-0.87350200	-2.81749700
C	3.04551000	3.40624000	-1.73842500	N	-0.82527600	-0.87384500	2.81757500
H	3.90015300	3.17838100	-2.38659600	N	0.49466400	-3.13276300	-2.52471800
H	2.85403400	4.47626100	-1.80925700	N	-0.49485100	-3.13312600	2.52470000
C	1.86332500	3.32352400	3.20067900	N	7.17425000	-0.84214100	2.26855100
H	1.69221400	4.39635600	3.28842300	N	5.69794300	0.66442000	1.38753300
H	2.29495200	2.98472400	4.14892600	N	-5.69764300	0.66437100	-1.38768200
C	4.42369500	2.10342800	-0.05205000	N	-7.17409100	-0.84198500	-2.26879800
C	4.68520700	1.64787100	1.24663200	C	-6.47908600	0.32680300	-2.44599300
C	3.40443900	3.02542900	-0.30783900	C	6.47929500	0.32666000	2.44585400
C	3.86890000	2.07331100	2.30010200	C	0.00699100	-1.86079500	-2.38174000
C	2.67173100	3.52837000	0.78308800	C	-0.00708500	-1.86119700	2.38165900
C	2.84956000	3.00453800	2.07985300	H	5.93859000	0.18692900	0.52032400
H	4.01345800	1.66275700	3.29128900	H	7.79606900	-1.08325500	3.02922900
				H	-1.75685600	-1.18701700	3.08819500

H	0.15673000	-3.84327400	2.21649600	H	-2.72576800	-2.64852700	1.04464400
H	1.75692600	-1.18671800	-3.08802300	H	-4.49441800	-4.79219000	2.32222400
H	-0.15702300	-3.84288100	-2.21666800	C	1.60270000	-3.57769000	-3.36928500
H	-5.93831400	0.18682800	-0.52050700	C	1.82768000	-5.08196400	-3.14413000
H	-7.79603700	-1.08292000	-3.02943200	H	1.38543100	-3.39684100	-4.42773400
S	6.68786500	1.21857000	3.87603700	C	3.40486300	-2.99720700	-1.83421900
S	1.51222000	-1.64704400	1.64456900	C	2.48449300	-5.33388500	-1.78120300
S	-1.51247100	-1.64649000	-1.64502400	H	0.85491100	-5.59787400	-3.17799100
S	-6.68774700	1.21892900	-3.87604200	C	3.73673000	-4.47758500	-1.59456500
C	-6.83404700	-1.83868300	-1.26737000	H	2.72549400	-2.64837500	-1.04457500
C	-7.52670800	-3.18092800	-1.54053200	H	4.49401700	-4.79216300	-2.32211400
H	-5.75203400	-2.00617300	-1.28089600	H	-1.77721600	-5.08395800	0.97683700
C	-8.48782200	-1.22857200	0.41067500	H	1.77668000	-5.08383500	-0.97698100
C	-9.00081900	-3.15216100	-1.11751100	C	-4.62843800	-2.09828600	1.86550200
H	-7.44668800	-3.41907000	-2.61015800	H	-4.31807400	-1.05644500	2.01897600
C	-9.13137900	-2.61603400	0.30455700	H	-5.15704200	-2.15764400	0.91836500
H	-9.57428900	-2.50529400	-1.79869300	C	4.62830800	-2.09832600	-1.86525700
H	-8.59714600	-3.28761600	0.98404500	H	4.31808700	-1.05644200	-2.01872100
O	-7.09134300	-1.36034400	0.05376400	H	5.15679200	-2.15778400	-0.91806300
O	-6.83706200	-4.16820200	-0.77483300	O	2.78738300	-2.82780200	-3.13193300
H	-7.46591000	-4.90998200	-0.68861900	O	5.56949900	-2.49479800	-2.86512300
O	-9.47027000	-4.49425800	-1.19935100	H	5.12694800	-2.42428300	-3.72784000
H	-10.27579400	-4.52836300	-0.65286500	O	4.17217800	-4.71136000	-0.25908500
O	-10.52441300	-2.59752700	0.61090000	H	5.11581900	-4.48171100	-0.15142000
H	-10.61234000	-2.66989600	1.57484700	O	2.81253700	-6.71981600	-1.73858400
H	-8.97406600	-0.52769900	-0.28203900	H	3.44503300	-6.81918300	-1.00504900
C	-8.55167100	-0.64760400	1.82366700	O	2.66529500	-5.54247300	-4.19036100
H	-7.90203400	0.23965300	1.86421900	H	3.03673700	-6.38316500	-3.86521500
H	-9.57846600	-0.31237000	2.00220700	O	-5.56957800	-2.49470300	2.86544900
O	-8.24524100	-1.57956900	2.84405100	H	-5.12693700	-2.42427000	3.72812400
H	-7.29423800	-1.81918300	2.78648000	O	-4.17273300	-4.71129900	0.25917700
C	6.83409300	-1.83879600	1.26709700	H	-5.11633100	-4.48144700	0.15157300
C	7.52654800	-3.18115000	1.54025200	O	-2.81306300	-6.71994800	1.73845200
H	5.75205500	-2.00611300	1.28059400	H	-3.44554100	-6.81928700	1.00489900
C	8.48800700	-1.22890000	-0.41089700	O	-2.66554000	-5.54279500	4.19027200
C	9.00069500	-3.15255600	1.11733900	H	-3.03706900	-6.38343800	3.86509400
H	7.44639900	-3.41932300	2.60986400	O	-2.78752600	-2.82802500	3.13200600
C	9.13144000	-2.61641300	-0.30471200				
H	9.57420300	-2.50578400	1.79857700	1F-ZE, electron energy = -6485.152068 a.u.			
H	8.59724000	-3.28796300	-0.98425700	C	-2.85484300	2.83067400	1.90424600
H	8.97428800	-0.52805300	0.28181500	C	-2.71921100	3.41364700	0.62896800
C	8.55195400	-0.64798500	-1.82390200	C	-3.50611800	2.98779300	-0.46020200
H	7.90245300	0.23937300	-1.86449000	C	-4.53723300	2.07609800	-0.21462500
H	9.57879900	-0.31291600	-2.00245000	C	-4.74291600	1.55467400	1.06408900
O	7.09149600	-1.36052000	-0.05405100	C	-3.89231200	1.91476600	2.11063900
O	6.83682000	-4.16827100	0.77444500	H	-5.16562900	1.73968900	-1.03537300
H	7.46552500	-4.91017600	0.68827200	H	-4.04390100	1.48354800	3.09484200
O	9.46996600	-4.49471200	1.19917600	C	-1.86233600	3.14423400	3.01610600
H	10.27561200	-4.52886800	0.65287300	H	-1.69583500	4.21965600	3.08021400
O	10.52451100	-2.59796900	-0.61090700	H	-2.29430900	2.81755500	3.96929200
H	10.61255400	-2.67056500	-1.57482500	C	-3.12874200	3.34369400	-1.89391500
O	8.24539500	-1.57994200	-2.84425900	H	-2.94144500	4.40971900	-2.01892700
H	7.29441600	-1.81960700	-2.78655400	H	-3.96542100	3.08291800	-2.55217300
C	-1.60288800	-3.57802400	3.36925300	C	-0.51313700	2.45529100	2.81002200
C	-1.82799700	-5.08225800	3.14399800	C	0.67185600	3.20005200	2.64236700
H	-1.38558700	-3.39730700	4.42772000	C	-0.45221100	1.05829200	2.74092300
C	-3.40511500	-2.99731500	1.83433200	C	1.88050200	2.56390900	2.30408200
C	-2.48495900	-5.33403600	1.78111500	C	0.76591200	0.41083800	2.51905900
H	-0.85526200	-5.59824500	3.17770600	H	-1.35800200	0.47568300	2.85270700
C	-3.73715700	-4.47764100	1.59463200	C	1.91058800	1.17052700	2.26905200

H	2.84153400	0.66576500	2.02422200	C	1.05054100	6.53885900	4.13072500
C	-1.88048500	2.56424500	-2.30406900	H	0.07310900	6.93422700	3.82805900
C	-0.67181000	3.20036000	-2.64230900	H	1.77639300	6.87511500	3.37970700
C	-1.91062100	1.17085800	-2.26910700	C	1.42984000	7.08433100	5.51184100
C	0.51315900	2.45556100	-2.80998800	H	1.45971600	8.17886500	5.50187800
C	-0.76596400	0.41115000	-2.51910900	H	0.70482200	6.77702900	6.27493600
H	-2.84158500	0.66611900	-2.02429800	H	2.41767100	6.72597900	5.82523500
C	0.45218700	1.05856700	-2.74092700	N	-0.91139100	-0.99843700	-2.41508300
H	1.35796200	0.47592500	-2.85268000	N	0.91134700	-0.99874500	2.41502600
C	1.86238300	3.14445900	-3.01604200	N	-0.72426500	-3.25262700	-2.75998000
H	2.29432200	2.81782000	-3.96925700	N	0.72433500	-3.25293900	2.75987000
H	1.69592900	4.21989100	-3.08008500	N	7.00151000	-1.23671500	-1.81110400
C	3.12879800	3.34333000	1.89400300	N	5.85252900	0.67966000	-1.27745400
H	2.94156000	4.40935300	2.01913300	N	-5.85258200	0.67977000	1.27723100
H	3.96546300	3.08243400	2.55223200	N	-7.00168800	-1.23652800	1.81092900
C	3.89232800	1.91485400	-2.11072000	C	-5.79975700	-0.61754700	1.65792200
C	4.74290900	1.55459900	-1.06421000	C	5.79962200	-0.61764200	-1.65816700
C	2.85488500	2.83076400	-1.90421800	C	-0.34927400	-1.99419700	-3.14431800
C	4.53724100	2.07587400	0.21456600	C	0.34920800	-1.99454200	3.14418700
C	2.71924900	3.41357000	-0.62886500	H	6.74130900	0.98294900	-0.88234200
C	3.50615200	2.98757100	0.46024900	H	6.94078500	-2.21348900	-2.06597400
H	5.16562500	1.73934500	1.03527400	H	1.71702800	-1.28822500	1.86175200
H	4.04390600	1.48374800	-3.09497500	H	0.30245900	-3.99576700	3.30124900
O	0.64927600	4.57630900	2.78615000	H	-1.71707300	-1.28793100	-1.86181900
O	1.72797700	4.34527600	-0.43374500	H	-0.30240300	-3.99540700	-3.30143600
O	-0.64912800	4.57662700	-2.78601000	H	-6.74131400	0.98309300	0.88203500
O	-1.72796400	4.34540700	0.43401000	H	-6.94102600	-2.21333500	2.06569000
C	-0.99632200	5.01910700	-4.11441900	S	4.36367200	-1.50813400	-1.91075400
H	-1.96948000	4.59400200	-4.39820600	S	-0.70204500	-1.80349900	4.46740100
H	-0.24864400	4.64531900	-4.82875200	S	0.70190500	-1.80306400	-4.46758100
C	-1.05000900	6.53931400	-4.13049700	S	-4.36386900	-1.50811300	1.91056200
H	-0.07233300	6.93433000	-3.82816000	C	-8.30716600	-0.59289600	1.76645700
H	-1.77549200	6.87584200	-3.37924300	C	-9.40262300	-1.62390200	2.08112600
C	-1.42956900	7.08490700	-5.51149300	H	-8.35375800	0.21313700	2.50572700
H	-1.45902300	8.17945300	-5.50154100	C	-8.66503100	-0.79825400	-0.63076000
H	-0.70492800	6.77731500	-6.27483000	C	-9.65337700	-2.54051000	0.87591200
H	-2.41764300	6.72692700	-5.82454400	H	-9.08282000	-2.23034100	2.94280700
C	2.15475800	5.70517900	-0.19621000	C	-9.87008200	-1.71814800	-0.39189500
H	3.08457300	5.70908100	0.38471900	H	-8.78599800	-3.19979200	0.71770500
H	1.36848200	6.14606800	0.42272600	H	-10.76337100	-1.09802000	-0.26555700
C	2.34550300	6.49523800	-1.48724800	O	-8.52371300	0.06832200	0.52259100
H	1.41698000	6.44838000	-2.06662700	O	-10.57857700	-0.89902800	2.39728900
H	3.12722200	6.01592200	-2.09074700	H	-11.30714000	-1.53666400	2.28116000
C	2.72813200	7.95296200	-1.20666000	O	-10.80884600	-3.31219600	1.18523400
H	3.66786500	8.01818900	-0.64474400	H	-11.12199800	-3.67168300	0.33605500
H	2.85954400	8.50939400	-2.14075300	O	-10.05038100	-2.65670300	-1.45407100
H	1.95324400	8.46224200	-0.62085200	H	-10.63889600	-2.26038300	-2.11505900
C	-2.15474900	5.70531300	0.19647300	H	-7.75528600	-1.40001400	-0.76577800
H	-1.36857000	6.14615200	-0.42261800	C	-8.83546500	0.13624500	-1.82235400
H	-3.08466800	5.70921300	-0.38428500	H	-7.93328500	0.75796100	-1.91856600
C	-2.34526700	6.49539500	1.48753000	H	-8.93273300	-0.45808000	-2.73528700
H	-1.41666800	6.44848400	2.06678200	O	-10.00652500	0.93690400	-1.72142800
H	-3.12692400	6.01611300	2.09113700	H	-9.93448700	1.42256400	-0.88250600
C	-2.72785600	7.95314100	1.20700000	C	8.30702600	-0.59314400	-1.76673500
H	-1.95301000	8.46238100	0.62110400	C	9.40243400	-1.62430800	-2.08106400
H	-3.66765300	8.01842400	0.64519700	H	8.35372700	0.21269700	-2.50620800
H	-2.85912700	8.50957300	2.14111300	C	8.66466900	-0.79792600	0.63054800
C	0.99630300	5.01867000	4.11464300	C	9.65303400	-2.54062500	-0.87559500
H	1.96923600	4.59321000	4.39866600	H	9.08265500	-2.23094800	-2.94261300
H	0.24831500	4.64516000	4.82879700	C	9.86968500	-1.71795200	0.39202000

H	8.78559900	-3.19980900	-0.71729100
H	10.76302500	-1.09791200	0.26559900
H	7.75487600	-1.39959800	0.76562300
C	8.83504500	0.13685700	1.82192700
H	7.93289300	0.75865100	1.91790000
H	8.93218700	-0.45725100	2.73501500
O	8.52350700	0.06837300	-0.52302900
O	10.57846200	-0.89959600	-2.39732400
H	11.30697400	-1.53724700	-2.28095600
O	10.80848000	-3.31246300	-1.18463000
H	11.12155500	-3.67173500	-0.33533200
O	10.04984000	-2.65625100	1.45444600
H	10.63828200	-2.25978100	2.11541100
O	10.00616400	0.93741600	1.72091800
H	9.93423300	1.42288700	0.88187900
C	1.40422000	-3.58563500	1.51583700
C	1.43138100	-5.10858800	1.31818400
H	0.87855000	-3.13002600	0.67129300
C	3.67958500	-3.55363100	2.36367200
C	2.49025400	-5.75732600	2.21801200
H	0.43549800	-5.51313300	1.54504700
C	3.83295800	-5.04950700	2.05814000
H	3.33671800	-3.41833700	3.39946200
H	4.16759300	-5.15665400	1.02156800
C	-1.40407900	-3.58538100	-1.51592800
C	-1.43103700	-5.10832900	-1.31821800
H	-0.87844700	-3.12968300	-0.67141000
C	-3.67944600	-3.55369900	-2.36373800
C	-2.48985200	-5.75724300	-2.21799200
H	-0.43510600	-5.51275200	-1.54509100
C	-3.83263500	-5.04957700	-2.05810700
H	-3.33658600	-3.41841600	-3.39953200
H	-4.16719700	-5.15668700	-1.02150600
H	2.18003300	-5.68857500	3.27230500
H	-2.17966400	-5.68850800	-3.27229500
C	4.96821500	-2.75886800	2.17316400
H	4.74833000	-1.69074300	2.31069200
H	5.67583300	-3.05639000	2.95274000
C	-4.96817400	-2.75908100	-2.17329400
H	-4.74839600	-1.69092900	-2.31078700
H	-5.67571100	-3.05666600	-2.95292000
O	-2.70461600	-3.00195900	-1.45053200
O	-5.60787300	-3.00616400	-0.92861800
H	-5.04192900	-2.64819500	-0.21460900
O	-4.74164200	-5.69472700	-2.95138900
H	-5.63471900	-5.61154400	-2.58196900
O	-2.58441900	-7.12157300	-1.82101600
H	-3.43304400	-7.44167100	-2.17560400
O	-1.74884100	-5.34090800	0.04744400
H	-2.04607500	-6.26893600	0.08227700
O	5.60786800	-3.00584500	0.92844300
H	5.04184300	-2.64792100	0.21447300
O	4.74200000	-5.69446600	2.95152900
H	5.63506500	-5.61137000	2.58206200
O	2.58499600	-7.12166300	1.82110700
H	3.43361700	-7.44165800	2.17579600
O	1.74924500	-5.34118300	-0.04746300
H	2.04653700	-6.26919200	-0.08226500
O	2.70468200	-3.00204800	1.45044600

1G-ZE, electron energy = -6485.156499 a.u.

C	2.34276500	3.82637100	-0.94150000
C	1.78156600	3.96901300	0.33934100
C	2.32068800	3.27628300	1.44354400
C	3.50988400	2.56889600	1.26216500
C	4.14906600	2.50999200	0.01287200
C	3.54160600	3.11842300	-1.09056700
H	3.94791400	2.04955900	2.11207600
H	3.99476600	3.03710800	-2.06831400
C	1.60037500	4.32639000	-2.17336600
H	1.22006500	5.33519300	-2.01817300
H	2.29950900	4.36233900	-3.01724600
C	1.59067600	3.20806600	2.78243300
H	1.35493900	4.20740100	3.15071600
H	2.26109200	2.74408000	3.51423100
C	0.42690900	3.40783900	-2.51226100
C	-0.89279900	3.88861400	-2.61969600
C	0.64699500	2.03834900	-2.64941300
C	-1.96962500	2.99605000	-2.76893000
C	-0.40586100	1.14104700	-2.86524400
H	1.66109000	1.65744700	-2.55917900
C	-1.71342800	1.62722100	-2.91520400
H	-2.53776000	0.93944300	-3.03964200
C	0.29729900	2.40211000	2.69273700
C	-0.96100500	3.03008900	2.77356300
C	0.34781100	1.01839400	2.48023600
C	-2.14290100	2.31619800	2.49831600
C	-0.82703500	0.28046100	2.31255500
H	1.31280500	0.51842500	2.44250100
C	-2.05241400	0.94447200	2.26796500
H	-2.94538700	0.38276500	2.03289000
C	-3.49825400	3.01494200	2.35960500
H	-4.17115900	2.68356500	3.15975300
H	-3.35335400	4.08859100	2.46816600
C	-3.42107000	3.46699300	-2.68294500
H	-3.44649300	4.55657500	-2.69494200
H	-3.97580100	3.11705700	-3.56061000
C	-4.93372000	1.55689800	0.87552400
C	-5.31156900	1.08323500	-0.38353000
C	-4.11882600	2.68445800	1.01157000
C	-4.87996600	1.75549200	-1.53198300
C	-3.74787600	3.38575500	-0.14892900
C	-4.08384600	2.89991200	-1.43044700
H	-5.11666400	1.35155500	-2.50907200
H	-5.24100600	1.00972500	1.76365300
O	-1.13283600	5.24930400	-2.54529000
O	-2.93664900	4.49153100	-0.02538700
O	-1.03416600	4.37349700	3.09050900
O	0.63787000	4.72133500	0.48638800
C	-1.26135100	4.62792500	4.49181700
H	-0.44291900	4.18673100	5.07861300
H	-2.19640800	4.14366200	4.80664500
C	-1.33228100	6.13189400	4.70875600
H	-2.14239300	6.54110100	4.09180800
H	-0.39979700	6.58559700	4.35098500
C	-1.56119800	6.48919500	6.18129400
H	-1.60769300	7.57505200	6.31440400
H	-2.50207400	6.06645300	6.55336200
H	-0.75032800	6.10938200	6.81425400
C	-3.55834500	5.77326000	-0.26683300

H	-4.32309100	5.67263300	-1.04696900	H	8.96523900	-1.51074000	-0.39466900
H	-2.75916600	6.40856900	-0.65684300	H	8.63279200	-1.66100900	2.63148600
C	-4.17377700	6.38043400	0.99124700	O	7.02718700	0.18935700	1.66109500
H	-3.39808500	6.46082700	1.76304700	O	9.92132800	0.61338500	2.03418600
H	-4.94674800	5.70544000	1.38031700	H	10.65133700	-0.02299300	2.14934400
C	-4.78219200	7.75989800	0.71279100	O	10.60152100	-1.72901700	0.86768000
H	-5.57892500	7.69947000	-0.03846800	H	10.51008200	-2.68198700	1.04619300
H	-5.21447500	8.18751400	1.62358000	O	8.28513000	-3.27177500	1.35375700
H	-4.02535700	8.46111200	0.34094500	H	8.06965300	-3.73015900	2.18094800
C	0.80982300	6.02324100	1.09256200	H	6.53955000	-1.41560700	0.40434400
H	-0.16905600	6.26490200	1.51114800	C	5.86677200	-1.74167300	2.41918200
H	1.52279500	5.95148700	1.92327100	H	4.92458700	-1.19946400	2.24955500
C	1.26330500	7.09881200	0.10916700	H	5.67863100	-2.80398500	2.23554100
H	0.53660300	7.16102100	-0.70964100	O	6.29328800	-1.62207200	3.77053000
H	2.22544700	6.81036400	-0.33272800	H	6.47522900	-0.67943200	3.92170500
C	1.39978300	8.46296100	0.79608700	C	-5.91721200	-2.93924800	-0.61386400
H	0.44786000	8.78507700	1.23537100	C	-6.15314100	-4.40654700	-1.00576100
H	2.14476800	8.43151600	1.60035600	H	-4.92527600	-2.64279300	-0.97002300
H	1.71359400	9.23079100	0.08100900	C	-6.96884000	-3.25036700	1.55272300
C	-1.08176100	5.91890300	-3.82081700	C	-7.29072200	-5.02569800	-0.18410500
H	-1.82814900	5.47533700	-4.49539300	H	-6.40503200	-4.45273500	-2.07642800
H	-0.09166300	5.76932200	-4.27457800	C	-7.07869700	-4.76004900	1.30302200
C	-1.35955100	7.39916900	-3.60667000	H	-8.25360000	-4.58514500	-0.48620000
H	-0.61112200	7.80390100	-2.91367700	H	-6.14069400	-5.22796400	1.61810200
H	-2.33645900	7.50887300	-3.11950100	H	-7.88797900	-2.74963300	1.21528800
C	-1.33554400	8.18521500	-4.92208000	C	-6.73396300	-2.89542900	3.01863100
H	-1.53457000	9.24706500	-4.74358800	H	-6.57319700	-1.81113200	3.09938100
H	-0.35962000	8.10667500	-5.41594200	H	-7.64662900	-3.13699500	3.57346900
H	-2.09507900	7.81579000	-5.62138100	O	-5.83980200	-2.75409500	0.79933300
N	-0.75223100	-1.12240600	2.07957900	O	-4.94029600	-5.10255100	-0.75814700
N	-0.02996300	-0.21822900	-3.02484300	H	-5.19562500	-6.04182000	-0.69755900
N	-1.48601500	-3.28940100	1.86077000	O	-7.28098300	-6.42304900	-0.45850000
N	0.05106700	-2.50552300	-3.01895300	H	-7.78177000	-6.83715900	0.26696400
N	-6.93227900	-2.08015400	-1.21665100	O	-8.19031200	-5.34722300	1.98153200
N	-5.95367500	-0.18171600	-0.41904400	H	-7.89952100	-5.59629900	2.87279600
N	5.38846300	1.81806800	-0.00703400	O	-5.67856000	-3.62838100	3.61915100
N	7.40873900	0.90521200	-0.58125500	H	-4.82900900	-3.23323100	3.33553200
C	6.22979200	1.44822600	-1.00066000	C	1.29530700	-2.52860500	-3.77074000
C	-6.81143200	-0.71962100	-1.31987500	C	1.73028300	-3.97460200	-4.07513600
C	-1.62926500	-2.08132300	2.47139400	H	1.15016400	-2.01370300	-4.72520700
C	-0.68454500	-1.37985300	-2.76753900	C	2.81987300	-2.36770100	-1.91288600
H	-5.70346500	-0.80248400	0.35019700	C	2.44829400	-4.63347300	-2.88083900
H	-7.60168700	-2.48945600	-1.85521600	H	0.83742300	-4.56441900	-4.33178300
H	0.97799700	-0.33650800	-3.12275500	C	3.49416300	-3.67991800	-2.32273700
H	-0.33643800	-3.37217000	-2.65161100	H	1.97530200	-2.56257800	-1.23790800
H	0.08519300	-1.45780400	1.60865800	H	4.22422200	-3.45384500	-3.10433700
H	-2.09680700	-4.01247200	2.21746300	C	-0.67831700	-3.54792400	0.67780900
H	5.65523800	1.45888200	0.90899300	C	-1.06116000	-4.91458800	0.08180100
H	8.00612400	0.58727900	-1.33296100	H	-0.87495100	-2.77382800	-0.06884600
S	-7.72969100	0.14107400	-2.46082600	C	1.20404100	-4.46300300	1.85634200
S	-2.26813000	-1.53352800	-2.15993900	C	-0.45210900	-6.07261100	0.89129000
S	-2.82531900	-1.90117800	3.67709400	H	-2.15702900	-5.00020900	0.06585500
S	5.94729400	1.54298700	-2.68610400	C	1.02735900	-5.81409400	1.15365700
C	7.91726400	0.87552400	0.78315800	H	0.60265300	-4.43596200	2.77482100
C	9.33233300	0.27468100	0.79089300	H	1.54400500	-5.76641300	0.18792600
H	7.96236100	1.89044500	1.19148300	H	1.71748100	-4.87106500	-2.09695900
C	6.90525600	-1.23710600	1.42453200	H	-0.97094500	-6.16547200	1.85764400
C	9.28226600	-1.25148200	0.62719600	C	3.78011400	-1.41090400	-1.20734300
H	9.90797000	0.71377800	-0.03880800	H	3.41488100	-0.38285400	-1.30996800
C	8.29157200	-1.86679100	1.61184900	H	3.77639600	-1.65691800	-0.14095300

C	2.66733400	-4.17121800	2.22671400	C	4.71542600	1.48750100	0.78659100
H	2.83483000	-3.08812200	2.15513800	C	3.36200600	2.88132500	-0.68772500
H	2.82487900	-4.46211800	3.26835700	C	4.03504500	1.99926100	1.89644000
O	0.71789000	-3.43625200	0.95986100	C	2.78092700	3.47415900	0.44829000
O	3.62677700	-4.90969500	1.47854600	C	3.05698600	2.98643800	1.74248700
H	3.63872300	-4.60131800	0.54743300	H	4.25546900	1.61511700	2.88440200
O	1.53079400	-6.89749000	1.92502400	H	4.83577900	1.46949100	-1.36556700
H	2.50085000	-6.81034700	1.87625900	O	-0.13464500	5.06934000	2.67086800
O	-0.64202200	-7.25317100	0.11757500	O	1.85564300	4.47737300	0.27006400
H	0.00081000	-7.90323300	0.45223100	O	0.43189600	4.61255600	-2.87976700
O	-0.56230400	-4.95376700	-1.25298900	O	-1.65911500	4.77915100	-0.50559300
H	-0.54316200	-5.90059000	-1.49083500	C	0.70493900	5.00641800	-4.24016500
O	5.12670300	-1.53680400	-1.65809000	H	-0.06143800	4.58074300	-4.90356400
H	5.31746700	-0.81096700	-2.28344200	H	1.67775800	4.59888800	-4.55068800
O	4.16215800	-4.32979200	-1.23247200	C	0.70356500	6.52534900	-4.32209500
H	5.01688300	-3.87548600	-1.12665900	H	1.46056500	6.91960900	-3.63263800
O	3.04421600	-5.82756700	-3.38476500	H	-0.26815000	6.89784700	-3.97480300
H	3.73815000	-6.07882800	-2.75077800	C	0.97944000	7.02365000	-5.74486700
O	2.61131500	-3.90630100	-5.18507600	H	0.97332800	8.11802700	-5.78075100
H	3.12189800	-4.73711700	-5.14977800	H	1.95771700	6.68322000	-6.10485800
O	2.33004300	-1.76762900	-3.13130600	H	0.21978300	6.66214600	-6.44819100
1H-ZE, electron energy = -6485.151835 a.u.				C	2.28669900	5.81355900	0.61161400
C	-3.32021000	3.53902300	0.69703500	H	2.90023300	5.78493200	1.52036500
C	-2.69109000	3.86877900	-0.51467600	H	1.36558800	6.35218800	0.84519200
C	-3.03495800	3.20542200	-1.71088600	C	3.05480400	6.50575200	-0.51090100
C	-4.08928300	2.29072600	-1.68152200	H	2.42865100	6.52053200	-1.41038800
C	-4.77785800	2.00288300	-0.49215500	H	3.95400900	5.92439400	-0.75190100
C	-4.38875600	2.63635900	0.68989900	C	3.45220300	7.93456200	-0.12170200
H	-4.36147100	1.77050700	-2.59723000	H	4.09763800	7.94147600	0.76502600
H	-4.89238500	2.40505800	1.61681500	H	3.99835200	8.42391600	-0.93514000
C	-2.76245400	4.01953000	2.02792300	H	2.56987200	8.54593200	0.10325500
H	-2.42786300	5.05350300	1.96089600	C	-1.95291600	6.08349500	-1.05305000
H	-3.55318900	3.97068900	2.78582300	H	-0.99987700	6.44761400	-1.44432000
C	-2.18518600	3.35117600	-2.97135100	H	-2.64920300	5.98364300	-1.89500000
H	-1.96897000	4.39770400	-3.18555800	C	-2.52329800	7.04986100	-0.01850700
H	-2.75337800	2.95572600	-3.82065200	H	-1.82219000	7.12332900	0.82176000
C	-1.58003900	3.14729400	2.45282300	H	-3.46222000	6.64461000	0.37973000
C	-0.30295400	3.69538300	2.67735800	C	-2.77233700	8.43781500	-0.62043600
C	-1.73929700	1.76589800	2.56603200	H	-1.84570500	8.87365700	-1.01324800
C	0.80697700	2.85822900	2.88659200	H	-3.49470100	8.39132700	-1.44438300
C	-0.66199700	0.92250200	2.86973200	H	-3.17080000	9.12495900	0.13348400
H	-2.72462800	1.33424300	2.40807600	C	-0.35757500	5.68213900	3.95651300
C	0.61635800	1.47553200	2.99318300	H	0.32245000	5.23525800	4.69594400
H	1.46700100	0.83182900	3.16813000	H	-1.38689300	5.48035000	4.28602200
C	-0.87129800	2.58284500	-2.83707800	C	-0.11330000	7.17877700	3.83505000
C	0.36893800	3.24121300	-2.70901800	H	-0.78887300	7.58804800	3.07331300
C	-0.90346600	1.18576900	-2.78978500	H	0.90953700	7.34278600	3.47395200
C	1.54142700	2.52345400	-2.40278300	C	-0.32455200	7.90492200	5.16804200
C	0.26290200	0.45604200	-2.56151400	H	-0.14541000	8.97951700	5.05757900
H	-1.84389500	0.66439100	-2.92436300	H	-1.34900000	7.77315800	5.53618500
C	1.46503800	1.12992700	-2.34028300	H	0.35895600	7.52993300	5.93917600
H	2.35668200	0.56058100	-2.09469900	N	0.29654800	-0.97126200	-2.58747000
C	2.86502700	3.22155300	-2.08726800	N	-0.98975000	-0.44710600	3.05610600
H	3.62400200	2.91191100	-2.81557900	N	-0.07552200	-3.15035300	-1.93039400
H	2.72605000	4.29688600	-2.19156700	N	-0.96183900	-2.63903700	3.71366800
C	2.22642000	3.41773200	2.94824800	N	7.20359300	-1.05133100	1.68600700
H	2.17482400	4.50401700	3.02600800	N	5.68688700	0.45699200	0.87638200
H	2.72269200	3.05251200	3.85405200	N	-5.81522000	1.03716000	-0.58957600
C	4.34776900	1.90782300	-0.49785300	N	-7.26104300	-0.69266100	-0.16493300
				C	-6.39802600	0.23869600	0.33614100

C	6.57378500	0.15411600	1.85961400	C	-2.57633600	-3.84855600	5.11554600
C	-0.43434100	-1.83466700	-1.84170200	H	-2.41435200	-1.71964000	4.90045500
C	-0.24057400	-1.55450700	3.29124700	C	-3.48210300	-3.53307400	2.36100400
H	5.81066200	-0.08056600	0.02006300	C	-2.88726300	-5.07155600	4.24287000
H	7.89780000	-1.26757000	2.38937000	H	-1.68524900	-4.05024100	5.72930900
H	-1.98682000	-0.63242400	2.97096400	C	-3.94990300	-4.72502900	3.20628500
H	-0.40830300	-3.47801700	3.82766400	H	-2.52884300	-3.77391000	1.86846000
H	1.12744500	-1.37505600	-3.01760500	H	-4.87143500	-4.43672700	3.72191700
H	-0.65889300	-3.76158100	-1.37404500	C	0.83681400	-3.78049900	-2.88366100
H	-5.97533300	0.72932700	-1.54812000	C	1.02995800	-5.25118700	-2.48053300
H	-7.63438800	-1.32111000	0.53389500	H	0.43765500	-3.72793500	-3.90230900
S	6.97758500	1.12491900	3.19331300	C	2.89656000	-3.11357900	-1.77382600
S	1.43913700	-1.72295600	3.08116600	C	1.88738700	-5.34942300	-1.21320000
S	-1.70152000	-1.39904800	-0.79267300	H	0.04322100	-5.70102200	-2.28698600
S	-6.14858100	0.26187000	2.02912700	C	3.19023200	-4.56160800	-1.35173200
C	-7.78949400	-0.77578700	-1.51970800	H	2.37497300	-2.60209400	-0.95334500
C	-8.76754800	-1.95800100	-1.59650200	H	3.81001700	-5.03496900	-2.12131800
H	-8.31767200	0.14715800	-1.78083400	H	-1.97845800	-5.40208300	3.71592800
C	-5.97807900	-2.08572400	-2.49161500	H	1.33008400	-4.94002800	-0.35762700
C	-8.00226600	-3.28750800	-1.60332000	C	-4.48354400	-3.14499900	1.27671500
H	-9.43353600	-1.92218600	-0.72035900	H	-4.14038800	-2.22375000	0.79054500
C	-6.92520200	-3.27784200	-2.68516600	H	-4.48600700	-3.93774900	0.52171500
H	-7.51889400	-3.44883500	-0.62746700	C	4.14029800	-2.31768800	-2.12870000
H	-7.40716000	-3.18481800	-3.66364200	H	3.85217900	-1.30570500	-2.44171100
O	-6.75241600	-0.86208400	-2.49490400	H	4.78624700	-2.23391000	-1.25925300
O	-9.51542000	-1.81226800	-2.79050600	O	2.07868300	-3.09310600	-2.96698400
H	-9.88497500	-2.69712600	-2.96690100	O	4.93058900	-2.94880400	-3.13913500
O	-8.96297800	-4.30777200	-1.85637900	H	4.40435000	-2.97407700	-3.95585500
H	-8.45315200	-5.09113000	-2.12939200	O	3.81842800	-4.61487300	-0.07489900
O	-6.23406400	-4.52389400	-2.57563000	H	4.79087800	-4.55541100	-0.15351000
H	-5.91447600	-4.77570500	-3.45591900	O	2.15822500	-6.73295200	-1.00955100
H	-5.44301500	-2.18958900	-1.53861900	H	2.88898800	-6.76576300	-0.36685400
C	-4.96443100	-1.92795600	-3.62006600	O	1.66597500	-5.90595800	-3.56403100
H	-4.31531000	-1.06869800	-3.39901700	H	2.04901500	-6.71623700	-3.18073800
H	-4.33324000	-2.82013300	-3.66336800	O	-5.81976200	-3.02011700	1.75077000
O	-5.58686200	-1.79586200	-4.89122200	H	-5.90688000	-2.12402200	2.13716100
H	-6.18424700	-1.03179700	-4.82593300	O	-4.15580200	-5.90448200	2.42674100
C	6.71883900	-2.10231100	0.80789800	H	-5.05960400	-5.87394900	2.07537200
C	7.40550900	-3.44296000	1.10412500	O	-3.34194600	-6.09660900	5.12130300
H	5.64162900	-2.23271200	0.95665300	H	-3.81360600	-6.73613500	4.55836300
C	8.17888100	-1.68052800	-1.09561200	O	-3.68815000	-3.55192500	5.94524600
C	8.81783900	-3.50006600	0.50969900	H	-4.03411700	-4.42087100	6.22192800
H	7.44872900	-3.59504400	2.19151100	O	-3.29607300	-2.40305700	3.24281500
C	8.79237000	-3.07829700	-0.95611600				
H	9.48625400	-2.82402200	1.06430600	II-ZE, electron energy = -6485.156627 a.u.			
H	8.16422500	-3.77967100	-1.51423300	C	-2.21626200	3.74158300	1.24046100
H	8.76502400	-0.94779300	-0.52357200	C	-1.71831700	3.95800900	-0.05567400
C	8.09117000	-1.21079400	-2.54873900	C	-2.34065800	3.36869800	-1.17545800
H	7.46079100	-0.30985100	-2.58589100	C	-3.54949800	2.69800300	-0.98067500
H	9.09808200	-0.92173200	-2.86674900	C	-4.12514200	2.57299200	0.29491600
O	6.83218800	-1.73118900	-0.56663900	C	-3.43314800	3.06994200	1.40471500
O	6.60219000	-4.45972600	0.50840300	H	-4.05436700	2.26265400	-1.84064900
H	7.19123600	-5.23116200	0.40524500	H	-3.83656200	2.93216500	2.39769100
O	9.25721400	-4.84810600	0.64284900	C	-1.38975700	4.12611700	2.45937500
H	9.99174100	-4.95215100	0.01175900	H	-1.00896900	5.14277400	2.36816200
O	10.13924600	-3.13223700	-1.42275700	H	-2.03135700	4.09130200	3.34782200
H	10.11000600	-3.27762200	-2.38201600	C	-1.67975100	3.37577600	-2.55194700
O	7.65106500	-2.20732800	-3.45307200	H	-1.42229600	4.39152800	-2.85547000
H	6.69981200	-2.39256800	-3.29384700	H	-2.40422000	2.99643600	-3.28117100
C	-2.31123100	-2.59837300	4.25699100	C	-0.20665000	3.17559100	2.63504700

C	1.12171500	3.63843200	2.68756600	H	-0.13824500	8.75675700	-0.69737900
C	-0.42899200	1.80057800	2.66812900	H	-1.87645200	8.54496300	-0.96401900
C	2.19717500	2.73261700	2.67800400	H	-1.28971900	9.20030700	0.57192500
C	0.62749700	0.88197100	2.72192400	C	1.42164800	5.55494500	4.04268000
H	-1.45143300	1.43436800	2.62274700	H	2.19923000	5.03894200	4.62390800
C	1.94094800	1.35555200	2.71516200	H	0.45981700	5.38479800	4.54720400
H	2.76679300	0.65731800	2.71154400	C	1.72307100	7.04248400	3.94037400
C	-0.41902200	2.51444400	-2.59527000	H	0.94222600	7.52253100	3.33721300
C	0.86194700	3.08601700	-2.72415000	H	2.66907400	7.17546200	3.40075800
C	-0.52227500	1.12414700	-2.47400100	C	1.80413400	7.70738700	5.31889400
C	2.02347100	2.30104600	-2.58330300	H	2.01881100	8.77675400	5.22228300
C	0.62090800	0.32148100	-2.44439500	H	0.86012400	7.60428000	5.86720300
H	-1.50585600	0.66507800	-2.40634500	H	2.59706300	7.26124900	5.93095900
C	1.88174100	0.92024500	-2.44134200	N	0.47384800	-1.08705000	-2.31514700
H	2.76207700	0.30234600	-2.31852500	N	0.23858400	-0.48220600	2.79246900
C	3.41961900	2.92534100	-2.51680900	N	1.00701500	-3.31632900	-2.40703200
H	4.02091900	2.57132800	-3.36257100	N	0.07322300	-2.75448700	2.61568100
H	3.32483600	4.00686100	-2.60533500	N	8.01991700	-1.65974700	-0.04647100
C	3.63871400	3.21829100	2.53794700	N	6.26486600	-0.19937300	0.13334900
H	3.65398500	4.30618200	2.60266800	N	-5.39407400	1.93735800	0.33594300
H	4.24290300	2.83398800	3.36749200	N	-7.43123900	1.09469100	0.95901300
C	4.98483700	1.45162900	-1.16889200	C	-6.20412200	1.54685200	1.34760800
C	5.49286400	1.00267400	0.05073700	C	7.52925500	-0.40375800	-0.28787500
C	4.12430200	2.55340300	-1.21999200	C	1.21092900	-2.06343000	-2.90813800
C	5.10279600	1.61839300	1.23987700	C	0.82858000	-1.63651500	2.39227800
C	3.81550700	3.21986900	-0.01714100	H	5.77039200	-1.02225600	0.47636400
C	4.23860400	2.71691400	1.22993300	H	8.98393100	-1.78598400	-0.32568000
H	5.45142400	1.21231600	2.18545700	H	-0.76071700	-0.58791800	2.96725700
H	5.24481400	0.92264600	-2.08058200	H	0.38806500	-3.60637300	2.15552800
O	1.37131300	4.99912800	2.71305700	H	-0.35302900	-1.40454600	-1.81472000
O	2.99129200	4.31998800	-0.06693400	H	1.49952700	-4.05042200	-2.89850600
O	0.98147200	4.44259600	-2.96444200	H	-5.72797100	1.65752000	-0.58585100
O	-0.55413000	4.67482700	-0.20932900	H	-8.00822400	0.76486800	1.72152100
C	1.07604400	4.77505900	-4.36457300	S	8.49520700	0.75766900	-1.07314800
H	0.17959200	4.41100200	-4.88671500	S	2.35898500	-1.76775100	1.64708500
H	1.94680300	4.26788600	-4.80369400	S	2.29458600	-1.85219300	-4.20321700
C	1.20376900	6.28476700	-4.50032600	S	-5.83386900	1.51237400	3.01876300
H	2.09137400	6.61648300	-3.94692200	C	-8.01114000	1.18212900	-0.37435300
H	0.33636000	6.75804400	-4.02368500	C	-9.44986500	0.64025400	-0.34390500
C	1.30479800	6.72333400	-5.96527800	H	-8.03103400	2.22341300	-0.71215100
H	1.39694500	7.81194700	-6.03905600	C	-7.12435400	-0.92159900	-1.19889400
H	2.18009800	6.28003300	-6.45488100	C	-9.45591100	-0.89337000	-0.27160800
H	0.41610700	6.42403100	-6.53368700	H	-9.96475200	1.05109900	0.53839500
C	3.61175700	5.59737700	0.20384600	C	-8.54339600	-1.48762900	-1.34089600
H	4.39774200	5.47508800	0.95881700	H	-9.09913100	-1.22467600	0.71572300
H	2.81976800	6.21295000	0.63762800	H	-8.92908300	-1.21326200	-2.32799900
C	4.18996900	6.25001300	-1.04887500	O	-7.20021600	0.52010600	-1.34253200
H	3.39401200	6.35043700	-1.79674000	O	-10.08439200	1.07650700	-1.53314500
H	4.95571700	5.59241200	-1.47979200	H	-10.84617400	0.47827200	-1.64656400
C	4.79900300	7.62265900	-0.73997500	O	-10.80451400	-1.30426600	-0.46923900
H	5.61518000	7.54157800	-0.01188900	H	-10.76198800	-2.24793100	-0.70582300
H	5.20559700	8.08261400	-1.64680300	O	-8.57891800	-2.90426500	-1.16034700
H	4.04883300	8.30703800	-0.32567500	H	-8.42953300	-3.32260000	-2.02250400
C	-0.69783000	6.02047500	-0.72024900	H	-6.70776800	-1.17563900	-0.21478000
H	0.25309700	6.23506800	-1.21211600	C	-6.16705000	-1.40186500	-2.28248800
H	-1.48499700	6.04329300	-1.48391600	H	-5.19681200	-0.90315800	-2.13997600
C	-0.99540200	7.05064900	0.36579900	H	-6.00927000	-2.47879400	-2.17190800
H	-0.20756400	6.99929400	1.12623600	O	-6.66790500	-1.18568400	-3.59593400
H	-1.94133300	6.79837600	0.86184200	H	-6.81959100	-0.22956200	-3.68158000
C	-1.07951900	8.46753500	-0.21439900	C	7.46370600	-2.57962800	0.94243800

C	8.37717700	-3.80664300	1.10145500	O	-3.08185600	-5.95248100	3.07799800
H	7.37422100	-2.08319100	1.91494000	H	-3.86217300	-6.11490800	2.52010700
C	5.97450600	-3.76037700	-0.55788200	O	-2.31902500	-4.20585000	4.93695300
C	8.19083000	-4.79353600	-0.05886900	H	-2.88763100	-4.99818400	4.89876700
H	9.42569800	-3.47042000	1.12894000	O	-2.14722900	-1.93250800	3.01305400
C	6.71023400	-5.08105800	-0.29765100				
H	8.61383500	-4.36740500	-0.98152000	1J-ZE, electron energy = -6485.148853 a.u.			
H	6.28305000	-5.54629700	0.59695800	C	2.99660300	3.12560200	-1.72531000
H	6.42747600	-3.25414200	-1.42253500	C	2.74332800	3.58641900	-0.42060400
C	4.48423700	-3.91477400	-0.83467700	C	3.39501200	3.01156000	0.68978400
H	4.04793200	-2.92501400	-1.01691100	C	4.38255200	2.05351300	0.45305600
H	4.37536800	-4.49798100	-1.75555000	C	4.70522800	1.63963600	-0.84698200
O	6.12159800	-2.93989400	0.62118000	C	4.00374400	2.17509800	-1.93027300
O	8.02742600	-4.42605600	2.32792000	H	4.90091400	1.60871000	1.29953900
H	8.35735800	-5.34060500	2.25051000	H	4.23077200	1.84673400	-2.93536100
O	8.88981600	-5.98105600	0.30083100	C	2.11295500	3.55580100	-2.88893900
H	8.53896800	-6.67986900	-0.27965800	H	1.90356300	4.62358900	-2.84416300
O	6.65242600	-5.97243500	-1.41276300	H	2.64094100	3.35525400	-3.82833900
H	5.85769600	-6.52086000	-1.32337400	C	2.96554500	3.32014700	2.12051000
O	3.78804100	-4.60406500	0.19709100	H	2.86408800	4.39340900	2.27955600
H	3.44474200	-3.93946800	0.82438000	H	3.74993000	2.96647500	2.79905300
C	-1.09711700	-2.78935100	3.48324100	C	0.78982600	2.79215700	-2.86272600
C	-1.57929500	-4.23256600	3.72617300	C	-0.44490100	3.44734300	-2.69104900
H	-0.83249200	-2.36079800	4.45457500	C	0.79760700	1.39911400	-2.94110200
C	-2.79906000	-2.41653700	1.81758700	C	-1.62121300	2.70997300	-2.46200000
C	-2.47183600	-4.76023000	2.58518800	C	-0.37979300	0.65267700	-2.81320400
H	-0.70050400	-4.88668100	3.82963400	H	1.74218000	0.88306100	-3.09470900
C	-3.51071600	-3.71075500	2.21870400	C	-1.57659600	1.31325000	-2.52388000
H	-2.04053100	-2.61646100	1.04959200	H	-2.47573600	0.74076100	-2.34324400
H	-4.12735000	-3.49671900	3.09634300	C	1.64460100	2.64154700	2.47873700
C	0.30188300	-3.61716400	-1.17246700	C	0.47576600	3.38661200	2.72133200
C	0.62202300	-5.04987400	-0.71521100	C	1.58580000	1.24441700	2.51662100
H	0.63269900	-2.92261800	-0.39578300	C	-0.76559100	2.74112100	2.88120500
C	-1.76126800	-4.29203400	-2.20004800	C	0.38254900	0.59144700	2.79643500
C	-0.17107300	-6.09461400	-1.51642500	H	2.47898400	0.66568700	2.32615500
H	1.69995000	-5.22201100	-0.81869400	C	-0.78752100	1.34701200	2.93592300
C	-1.63996000	-5.70010000	-1.60500900	H	-1.73688700	0.83737000	3.08147100
H	-1.25005000	-4.25040100	-3.17110600	C	-2.08056700	3.51788100	2.92205000
H	-2.05345000	-5.67810400	-0.58981400	H	-2.61101600	3.30413000	3.85714400
H	-1.85128400	-4.98042200	1.70769100	H	-1.86021600	4.58411300	2.89864700
H	0.23447800	-6.16332200	-2.53800200	C	-2.93558900	3.39451700	-2.09089500
C	-3.76333500	-1.36099000	1.27048100	H	-2.82361000	4.46975100	-2.22797800
H	-3.36522900	-0.36017800	1.46950400	H	-3.72310000	3.06244200	-2.77672900
H	-3.81496700	-1.48429300	0.18441500	C	-3.98199600	2.17307400	1.93497800
C	-3.22145000	-3.85383800	-2.39920200	C	-4.68747700	1.66561100	0.84099900
H	-3.28682900	-2.77306100	-2.21669700	C	-2.96785500	3.11998800	1.74983100
H	-3.50074100	-4.03123500	-3.44070100	C	-4.36335400	2.10515700	-0.45009300
O	-1.10278100	-3.37529600	-1.29574200	C	-2.71101600	3.60573300	0.45495300
O	-4.16965200	-4.58182400	-1.62499700	C	-3.36827400	3.06024400	-0.66694100
H	-4.06185000	-4.36822300	-0.67340400	H	-4.88499400	1.68174100	-1.30545300
O	-2.31089000	-6.68036800	-2.38672200	H	-4.21069400	1.82470100	2.93293700
H	-3.25984800	-6.50968300	-2.23955800	O	-0.49954200	4.82941100	-2.72575300
O	-0.00631100	-7.33736700	-0.83981200	O	-1.73310500	4.55917800	0.28540600
H	-0.72926100	-7.91185100	-1.14782900	O	0.54449000	4.76717000	2.78176300
O	0.27089300	-5.13488000	0.66672800	O	1.77492500	4.54604000	-0.23169600
H	0.21310100	-6.09042300	0.85741800	C	0.76973000	5.26963500	4.11488100
O	-5.09228400	-1.50335800	1.77040500	H	1.68976300	4.82519500	4.52088300
H	-5.25168800	-0.81498100	2.44524300	H	-0.06250000	4.96520600	4.76572200
O	-4.34618000	-4.23483700	1.17793000	C	0.88547000	6.78537300	4.05719000
H	-5.15513600	-3.69067300	1.19411600	H	-0.03761300	7.19697000	3.63022800

H	1.69950800	7.05234400	3.37192300	C	9.36627000	-1.65430600	-0.83963000
C	1.13956600	7.39418200	5.44049400	H	8.58562900	0.35561400	-0.84032200
H	1.21673600	8.48456300	5.37643100	C	7.24648600	-1.90824500	1.17195500
H	0.32589400	7.15717800	6.13631800	C	9.00013000	-3.01917200	-0.24182100
H	2.07284500	7.01824800	5.87648800	H	9.59216900	-1.77182800	-1.91090400
C	-2.18276900	5.89920500	-0.01404000	C	8.45219200	-2.85801000	1.17345900
H	-3.05814900	5.85986400	-0.67368100	H	8.23098600	-3.50621100	-0.86078300
H	-1.36039500	6.35242900	-0.57292300	H	9.23214000	-2.42390000	1.80733500
C	-2.51008300	6.71471500	1.23357200	O	7.68018300	-0.63097800	0.63898900
H	-1.63036200	6.72589900	1.88749500	O	10.47963400	-1.10294200	-0.15844400
H	-3.31925900	6.22279800	1.78831000	H	11.07682900	-1.85695100	0.00204600
C	-2.92351200	8.14766300	0.87806800	O	10.19339600	-3.79504400	-0.23846300
H	-3.81984900	8.15959400	0.24614800	H	10.03132700	-4.52712500	0.38301000
H	-3.14530000	8.72581300	1.78136900	O	8.10485000	-4.16861200	1.62362200
H	-2.12580600	8.66916800	0.33528200	H	8.22960200	-4.20330200	2.58466900
C	2.23905300	5.87490000	0.09467100	H	6.43484500	-2.31764500	0.55454800
H	1.41914800	6.32784500	0.65736800	C	6.71084000	-1.60950100	2.56770100
H	3.11011700	5.81271800	0.75822600	H	5.85171300	-0.92844600	2.48442500
C	2.58409500	6.71051200	-1.13496700	H	6.35573900	-2.53975600	3.02041800
H	1.70755300	6.74984100	-1.79198500	O	7.70979800	-1.08256200	3.43198500
H	3.38768700	6.21739700	-1.69668100	H	8.05028900	-0.28023400	3.00179900
C	3.01888500	8.12871100	-0.74716700	C	-8.19847400	-0.61323000	0.65002000
H	2.22657800	8.65192100	-0.19815200	C	-9.36739500	-1.60026700	0.79203100
H	3.91120100	8.11206600	-0.10969100	H	-8.56803900	0.40180100	0.82859400
H	3.25592500	8.72193800	-1.63669100	C	-7.26611500	-1.83144500	-1.24080900
C	-0.72171800	5.35968400	-4.04848100	C	-9.01862700	-2.95591900	0.16361200
H	-1.64720900	4.93311700	-4.46115800	H	-9.58634300	-1.73749500	1.86234500
H	0.10603500	5.05916700	-4.70681000	C	-8.48023700	-2.77050700	-1.25247100
C	-0.82111200	6.87518200	-3.96126300	H	-8.24936000	-3.46281700	0.76624600
H	0.10801700	7.26886800	-3.53054100	H	-9.26121300	-2.31664100	-1.87114200
H	-1.62944500	7.13742100	-3.26747400	H	-6.45449200	-2.26093200	-0.63704300
C	-1.07493800	7.51303700	-5.33150900	C	-6.73710000	-1.50927900	-2.63382100
H	-1.14054700	8.60272800	-5.24626300	H	-5.87204200	-0.83685100	-2.54228100
H	-0.26694100	7.28109800	-6.03561100	H	-6.39273300	-2.43303900	-3.10756300
H	-2.01401600	7.15501300	-5.77006900	O	-7.68438000	-0.56158000	-0.67922500
N	0.22666600	-0.81915100	2.86767200	O	-10.48062800	-1.02494600	0.13073800
N	-0.23581200	-0.75780600	-2.90240600	H	-11.08591900	-1.77003900	-0.04068400
N	0.53900600	-3.07169800	3.17140000	O	-10.21906100	-3.72058300	0.15373000
N	-0.57498200	-3.00953300	-3.18819900	H	-10.06854500	-4.44139200	-0.48363200
N	-7.15798000	-0.94650700	1.61374400	O	-8.14790300	-4.07459900	-1.73190100
N	-5.75573000	0.73477700	0.94010000	H	-8.27949700	-4.08861900	-2.69256000
N	5.77016400	0.70704400	-0.96351300	O	-7.73738600	-0.95663200	-3.48035300
N	7.17073100	-0.96331100	-1.66662500	H	-8.06774600	-0.16016900	-3.03175800
C	6.02909600	-0.24936600	-1.88574300	C	0.81406800	-3.33268000	-3.52266100
C	-6.01160800	-0.24274200	1.84103800	C	0.95154600	-4.85881200	-3.65020800
C	1.09458200	-1.81122700	3.16765700	H	1.10094300	-2.86895200	-4.47308200
C	-1.11613400	-1.74253300	-3.18943300	C	1.72094900	-3.35303100	-1.26059500
H	-6.31654200	0.66931000	0.09123100	C	0.96094100	-5.52359500	-2.26845400
H	-7.32944000	-1.68548200	2.28305900	H	0.10227600	-5.24556700	-4.23517500
H	0.71264400	-1.08732300	-2.71940300	C	1.99741300	-4.85758600	-1.36978400
H	-1.26102900	-3.71247900	-3.43446200	H	0.73679100	-3.19140100	-0.80066900
H	-0.72198100	-1.14010000	2.67125400	H	2.99086000	-4.99557700	-1.80745900
H	1.21622200	-3.78255300	3.41895600	C	-0.85457600	-3.37203000	3.50646900
H	6.32744200	0.62104200	-0.11413100	C	-1.01033600	-4.89210700	3.67899800
H	7.34441900	-1.68653200	-2.35238900	H	-1.14087500	-2.87852100	4.44187400
S	-5.03527400	-0.69616300	3.16904500	C	-1.75485900	-3.45057600	1.24352200
S	-2.77660100	-1.57281300	-3.51898600	C	-1.03164700	-5.59829800	2.31792800
S	2.75434500	-1.65627400	3.50765400	H	-0.16453600	-5.27160500	4.27373300
S	5.06141200	-0.66649600	-3.23205500	C	-2.06112800	-4.94478800	1.40214200
C	8.20525800	-0.65952900	-0.68656800	H	-0.76479000	-3.32587900	0.78478400

H	-3.05486700	-5.04919700	1.84839900	H	-3.94039200	-0.16340900	-2.96488600
H	-0.02768900	-5.43280700	-1.79485300	H	-2.98809000	-1.62113200	-3.25182900
H	-0.04308000	-5.53262100	1.83984900	C	-1.82950500	-3.27521800	1.62751100
C	2.77189500	-2.60615600	-0.44358500	H	-1.58159200	-4.22235800	1.14850000
H	2.55066700	-1.53031200	-0.47418500	H	-2.23488700	-3.51308600	2.61778300
H	2.69339200	-2.92834700	0.59869200	C	-4.55706100	-0.67427500	-0.47571300
C	-2.78545300	-2.70969800	0.39570500	C	-4.82809500	-1.04055100	0.84920400
H	-2.54280400	-1.63810800	0.39466300	C	-3.50225200	-1.26906900	-1.17988600
H	-2.70568000	-3.06525900	-0.63564600	C	-3.96867700	-1.93081900	1.50554300
O	-1.75993200	-2.83086400	2.54989600	C	-2.71618600	-2.23780800	-0.52907800
O	-4.12412500	-2.93950700	0.81281700	C	-2.88210400	-2.50452400	0.84483600
H	-4.26497200	-2.44183200	1.64372600	H	-4.14059800	-2.15689800	2.55445700
O	-1.99605400	-5.64365600	0.15567100	H	-5.13445300	0.11055500	-0.95505900
H	-2.86222700	-5.57637500	-0.27585700	O	0.77108700	-4.25908100	0.86715000
O	-1.37206400	-6.95913300	2.57258200	O	-1.69554200	-2.84015800	-1.22307600
H	-1.66807500	-7.32219700	1.71904000	O	-0.73075700	-1.44044700	-4.08739900
O	-2.22939700	-5.11496300	4.36759500	O	1.74136400	-2.49505500	-1.79368700
H	-2.45534400	-6.04571000	4.18411600	C	-1.01437000	-1.06982700	-5.45390900
O	4.10242000	-2.87512000	-0.86375300	H	-0.26781200	-0.33938200	-5.79586400
H	4.24929800	-2.39784000	-1.70522700	H	-2.00093300	-0.58758400	-5.50200700
O	1.91420700	-5.51266900	-0.10070800	C	-0.97801500	-2.32159900	-6.31695900
H	2.78121000	-5.45346600	0.33019200	H	-1.71944100	-3.03628400	-5.93876000
O	1.28468300	-6.89580200	-2.48143800	H	0.00548000	-2.79619800	-6.21018500
H	1.56939600	-7.23808900	-1.61559700	C	-1.25535100	-2.00864300	-7.79144000
O	2.16916100	-5.11677800	-4.32870900	H	-1.22681100	-2.92262100	-8.39366100
H	2.38299600	-6.04459500	-4.11805200	H	-2.24355700	-1.55222100	-7.92346900
O	1.73065400	-2.77578500	-2.58634900	H	-0.50944000	-1.31612000	-8.19928300
1J-EZ, electron energy = -6485.149628 a.u.				C	-1.88279100	-4.23764800	-1.55009100
C	3.52197600	-1.63260600	-0.44365900	H	-2.42179600	-4.74027700	-0.73831300
C	2.74532500	-1.57473700	-1.61560900	H	-0.87424800	-4.65664300	-1.59554600
C	2.90262900	-0.52226300	-2.54024700	C	-2.61845000	-4.43965500	-2.87109600
C	3.97628100	0.35289400	-2.37285900	H	-2.08081500	-3.89807900	-3.65722700
C	4.82939700	0.24947500	-1.26674300	H	-3.61964800	-3.99535300	-2.79895900
C	4.56303100	-0.70956800	-0.28062100	C	-2.73594700	-5.92552700	-3.23000700
H	4.14375900	1.14399000	-3.09877700	H	-3.28983200	-6.47976400	-2.46258000
H	5.13470600	-0.71694100	0.64260100	H	-3.26289500	-6.05662800	-4.18101600
C	3.14701200	-2.58795500	0.68247800	H	-1.74745900	-6.39035000	-3.32914400
H	3.02757300	-3.60264600	0.30177400	C	1.95995200	-3.47736200	-2.83382700
H	3.95802900	-2.60275900	1.41935200	H	0.96117400	-3.74734900	-3.18530400
C	1.85330400	-0.25200100	-3.60841200	H	2.50016900	-3.01816200	-3.67025900
H	1.61982300	-1.14821800	-4.18301700	C	2.71427200	-4.70600000	-2.33532600
H	2.25320300	0.48597500	-4.31354800	H	2.17394200	-5.12599900	-1.47969600
C	1.84447100	-2.15298100	1.35141800	H	3.70460100	-4.40031500	-1.97369000
C	0.69471300	-2.96714900	1.34943600	C	2.86839600	-5.75895400	-3.43897700
C	1.76046500	-0.88391200	1.92344500	H	1.89162100	-6.09792800	-3.80494900
C	-0.54481500	-2.46149500	1.78264100	H	3.42621900	-5.36154600	-4.29558100
C	0.55361800	-0.38840100	2.42922600	H	3.40827500	-6.63654600	-3.06804200
H	2.64621700	-0.25472200	1.95495600	C	1.05872000	-5.24472400	1.88225800
C	-0.60497800	-1.16301800	2.30365000	H	0.30599500	-5.17628300	2.68011200
H	-1.57688700	-0.74650800	2.54388100	H	2.04005800	-5.03068700	2.32872700
C	0.55734700	0.27774100	-2.99421900	C	1.04107500	-6.62397400	1.24150500
C	-0.67284400	-0.36699500	-3.21945700	H	1.78887000	-6.65332500	0.43937000
C	0.59667700	1.38641500	-2.13961700	H	0.06257300	-6.78245500	0.77107200
C	-1.83275000	0.03441000	-2.52747000	C	1.32144000	-7.73329000	2.26115400
C	-0.57282700	1.87561100	-1.54727900	H	1.30554100	-8.71609700	1.77873900
H	1.56095700	1.81711100	-1.89290500	H	2.30511500	-7.60654800	2.72875200
C	-1.76976300	1.17372300	-1.72543200	H	0.56965300	-7.74046300	3.05930600
H	-2.66382300	1.51009100	-1.20677500	N	-0.60937300	3.00099300	-0.67825600
C	-3.12381500	-0.77966400	-2.57185400	N	0.57348800	0.93440000	2.95149000
				N	0.97075300	4.39304900	-1.67169500

N	-1.02673800	0.79554000	4.63906300	H	-8.99453200	-1.52233800	-4.66973500
N	-7.58266700	-0.51429700	0.07070800	O	-8.26936100	0.67443700	-4.46283400
N	-5.86301500	-0.45183200	1.62604800	H	-8.77939800	1.32859300	-4.96496400
N	5.85319900	1.22884600	-1.14519800	O	-10.24728600	3.01964500	-2.50533000
N	7.58768400	-0.13899900	-0.43949200	H	-10.65104400	2.63467300	-1.70884100
C	7.14769600	1.10296400	-0.76257600	C	-1.84709800	1.30980200	5.72950900
C	-7.15400100	-0.18087000	1.31381900	C	-2.44102900	0.14055300	6.53406000
C	0.03833900	4.19990100	-0.70497900	H	-1.22323000	1.91952400	6.38454500
C	-0.09431000	1.52859500	3.97980600	C	-3.89978900	1.61987500	4.47918300
H	-5.64670800	-0.34414200	2.61965200	C	-3.60871000	-0.51364500	5.78288500
H	-6.94061100	-1.04673800	-0.50588800	H	-1.65615400	-0.61092500	6.71093500
H	1.31686000	1.52238500	2.59389300	C	-4.60995400	0.53241900	5.29872200
H	-1.05682200	-0.19908500	4.44739600	H	-3.48265600	1.18136000	3.56012000
H	-1.35606600	2.98888300	0.00617800	H	-5.08746100	1.00158100	6.16438400
H	1.01467700	3.70646100	-2.41576200	C	1.76311200	5.60893800	-1.81657800
H	5.62836800	2.14049200	-1.55053800	C	2.36850700	5.66937200	-3.22988000
H	6.94947200	-0.90750400	-0.61322000	H	1.11751900	6.47490700	-1.66255000
S	-8.16539900	0.54103700	2.49337600	C	3.82569100	4.77055700	-0.86139200
S	0.28659500	3.14136600	4.37579100	C	3.55783100	4.70881200	-3.36564800
S	-0.36815900	5.37482800	0.45927600	H	1.59601100	5.39658600	-3.96549600
S	8.14932900	2.49225900	-0.72976100	C	4.54490800	4.88410900	-2.21331200
C	8.94674100	-0.45641500	-0.02698700	H	3.42998300	3.75250300	-0.73528100
C	9.29535900	-1.89973000	-0.43417300	H	5.00573200	5.87424500	-2.28352300
H	9.62493000	0.22898700	-0.53538300	H	-3.23061100	-1.05894400	4.90438800
C	8.52273300	-1.11825200	2.26910400	H	3.19945300	3.66732600	-3.35792700
C	8.67600800	-2.91754100	0.53174300	C	-4.80494100	2.79107100	4.10399900
H	8.91838900	-2.08189600	-1.45195200	H	-4.22199300	3.50173400	3.50072600
C	8.99796200	-2.54862000	1.97661900	H	-5.64322200	2.43772100	3.49613900
H	7.58037100	-2.93614100	0.41347600	C	4.71380400	5.10968100	0.33376200
H	10.08268100	-2.58904600	2.11900000	H	4.12606200	4.97537300	1.25317300
O	9.16722500	-0.21444500	1.35438000	H	5.56679700	4.42568500	0.37374200
O	10.71038400	-2.00777300	-0.40573400	O	2.75792800	5.72939000	-0.81444200
H	10.88966500	-2.96511400	-0.36156800	O	5.24160200	6.42719500	0.24529500
O	9.22053100	-4.18961500	0.19621300	H	4.47476900	7.01610800	0.14153800
H	9.05605600	-4.75927800	0.96877300	O	5.53757300	3.86461200	-2.39380100
O	8.34213500	-3.51860400	2.79655800	H	6.36982700	4.10272500	-1.94125900
H	8.86374400	-3.63654500	3.60534100	O	4.17186800	4.99818100	-4.61701300
H	7.42920200	-1.06278200	2.16011100	H	5.04780000	4.57456000	-4.59720000
C	8.90184000	-0.62140400	3.66059600	O	2.79838100	7.00494000	-3.43569800
H	8.49874900	0.39274600	3.79491900	H	3.43156400	6.95743600	-4.17534400
H	8.44961300	-1.26894300	4.41733700	O	-5.36049300	3.42097300	5.25157800
O	10.30815100	-0.65009300	3.87181800	H	-4.60578500	3.66710600	5.81325400
H	10.69791800	-0.13781400	3.14292800	O	-5.58328600	-0.18853900	4.53047500
C	-8.93527800	-0.30355700	-0.42364500	H	-6.42518100	0.30500400	4.48029300
C	-9.27438500	-1.35900600	-1.49191900	O	-4.21619100	-1.42483000	6.69236300
H	-9.62517900	-0.41194800	0.41329600	H	-5.08395500	-1.65146600	6.31448800
C	-8.47865900	1.37885100	-2.11090200	O	-2.89725100	0.67769600	7.76470200
C	-8.63532100	-1.01200700	-2.84272600	H	-3.52144000	0.01604800	8.11518200
H	-8.90641800	-2.33901300	-1.15205200	O	-2.85322300	2.19855000	5.27427500
C	-8.94396500	0.43203400	-3.22613800				
H	-7.54096700	-1.13030000	-2.78669200	1B-ZZ, electron energy = -6485.145041 a.u.			
H	-10.02652800	0.54316400	-3.34556200	C	4.24497000	2.66609000	-1.05625700
H	-7.38718400	1.30310800	-1.99319300	C	3.86362100	3.20514800	0.18674100
C	-8.84414500	2.83896500	-2.35793100	C	4.12605400	2.52094500	1.39217000
H	-8.44791000	3.44665200	-1.53167700	C	4.91592100	1.36843500	1.34934700
H	-8.37667500	3.18163300	-3.28555400	C	5.36988900	0.86160700	0.12896800
O	-9.14341000	1.02189000	-0.88659200	C	5.00848400	1.49372300	-1.06341800
O	-10.68801300	-1.37943200	-1.61891600	H	5.16375900	0.85231000	2.26963600
H	-10.85809200	-1.80382400	-2.48008200	H	5.32927700	1.06786500	-2.01085100
O	-9.17221800	-1.92020000	-3.79876700	C	3.76614800	3.28423600	-2.36318400

H	3.90806800	4.36455100	-2.34727300	H	3.04629100	6.20333800	1.06898300
H	4.37365000	2.88162200	-3.18208300	H	4.49101700	5.28408100	1.51808500
C	3.46212400	2.94051700	2.69993300	C	4.63914000	6.25394800	-0.40653200
H	3.60368400	4.00145700	2.90657200	H	3.96983100	6.48926300	-1.24117000
H	3.93244900	2.38693100	3.52049700	H	5.40630400	5.56880900	-0.78978800
C	2.29121700	2.98835300	-2.62922400	C	5.30336500	7.53130600	0.12061500
C	1.33563600	4.02143400	-2.70786400	H	4.55649700	8.24538500	0.48840300
C	1.86360400	1.66407300	-2.77288300	H	5.99046800	7.31209600	0.94699100
C	-0.03990500	3.73447500	-2.79712300	H	5.87877000	8.02723200	-0.66831300
C	0.51054300	1.37259400	-2.94520900	C	1.97356600	5.88946900	-4.00379000
H	2.58854500	0.85810700	-2.75132700	H	1.06672400	5.75955400	-4.61113800
C	-0.43337800	2.39985300	-2.92415700	H	2.78643100	5.33686900	-4.49646800
H	-1.49011000	2.15385400	-2.99157800	C	2.32245700	7.36404800	-3.87065800
C	1.96625700	2.63568800	2.66358300	H	3.21929600	7.46433500	-3.24708500
C	0.99449200	3.65469700	2.73076400	H	1.50797000	7.87359600	-3.34091700
C	1.53973400	1.32035000	2.46906900	C	2.55790300	8.02239000	-5.23460300
C	-0.36735700	3.38165500	2.49816500	H	2.80937700	9.08144800	-5.11578700
C	0.18541300	1.02316200	2.32352500	H	3.38356600	7.54143900	-5.77254600
H	2.26928200	0.51894100	2.40047200	H	1.66471500	7.96006100	-5.86760900
C	-0.75463300	2.05021000	2.30883300	N	-0.22480500	-0.31877300	2.02390800
H	-1.79636100	1.80956500	2.11989700	N	0.03918300	0.04799100	-3.21348800
C	-1.40165600	4.49961600	2.36601000	N	-0.59936300	-2.54574200	2.31552800
H	-2.16140000	4.39658400	3.14993600	N	-0.40378800	-2.18199400	-3.01867800
H	-0.90295800	5.45725300	2.51149600	N	-6.83917900	1.49860300	-0.86908700
C	-1.10369000	4.82574200	-2.68928300	N	-5.19748400	3.03096900	-0.45591600
H	-0.61442700	5.79922000	-2.69583900	N	6.24744000	-0.26003300	0.05585100
H	-1.76152600	4.78600300	-3.56479600	N	7.20285600	-2.29219200	0.41962400
C	-3.33470600	3.83220400	0.86760800	C	6.11718100	-1.48873400	0.62640200
C	-3.90515200	3.63546600	-0.39263100	C	-5.55472000	1.89492500	-1.11864300
C	-2.08729800	4.44880200	1.00787900	C	-0.33630300	-1.34137100	2.90459000
C	-3.21247400	4.03154700	-1.53839100	C	0.18759000	-1.07527300	-2.47230500
C	-1.42938100	4.89334300	-0.15446000	H	-5.83592200	3.34866800	0.26649800
C	-1.95030700	4.62488700	-1.43675700	H	-7.38703800	2.06487400	-0.23094500
H	-3.64303400	3.84659800	-2.51527600	H	-0.62846900	-0.00051800	-3.97679000
H	-3.86173800	3.48325700	1.75222600	H	-0.86135500	-2.06759700	-3.91629800
O	1.75151300	5.34043300	-2.68786000	H	-0.20805300	-0.55339600	1.02878700
O	-0.20585200	5.50954600	-0.02772400	H	-0.63314500	-2.55846800	1.30026400
O	1.39465300	4.95266700	2.99101300	H	7.01484000	-0.14457100	-0.59819100
O	3.14109800	4.37560900	0.20571800	H	8.00255700	-1.88230700	-0.04919900
C	1.41633900	5.28029700	4.39537700	S	-4.52863100	1.05198000	-2.17539600
H	2.07778900	4.57884900	4.92347500	S	1.05830900	-1.13721800	-1.01091600
H	0.40574300	5.16424400	4.81234300	S	-0.18317200	-1.14615700	4.58809800
C	1.90925400	6.71026600	4.55563600	S	4.75544800	-1.99575100	1.50349400
H	1.24007000	7.38109600	4.00246700	C	7.29661100	-3.68682700	0.80666100
H	2.90023000	6.79626200	4.09258700	C	8.76781200	-4.06750800	1.05282600
C	1.97651300	7.13283800	6.02717100	H	6.73607100	-3.81644500	1.73201100
H	2.33283600	8.16413900	6.11896200	C	7.31309600	-4.71257200	-1.39318100
H	0.99068600	7.07642200	6.50415400	C	9.51342000	-4.29548500	-0.26807900
H	2.66026900	6.49103600	6.59541900	H	9.25334200	-3.25418200	1.61268300
C	-0.16949400	6.92919300	-0.29526200	C	8.73309600	-5.25084500	-1.16604800
H	-0.87629100	7.17503800	-1.09704300	H	9.63841900	-3.33952000	-0.80303100
H	0.84095500	7.12320200	-0.66439100	H	8.65927000	-6.22298900	-0.66788800
C	-0.47027300	7.77399600	0.93959200	O	6.66226900	-4.56073800	-0.11962600
H	0.23041900	7.49677800	1.73570600	O	8.76658600	-5.26333100	1.81811300
H	-1.47957100	7.54053200	1.30209300	H	9.65899700	-5.63846600	1.70259100
C	-0.36272400	9.27301000	0.63634800	O	10.78923100	-4.83393200	0.06341200
H	-1.07561100	9.57493300	-0.14057300	H	11.12739500	-5.23506800	-0.75709700
H	-0.57262600	9.86893500	1.53085400	O	9.47683900	-5.35951000	-2.38210800
H	0.64288200	9.53725500	0.28725900	H	9.32404200	-6.24124000	-2.75554900
C	3.83364400	5.55149200	0.68220700	H	7.36287900	-3.74777200	-1.91991800

C	6.42202800	-5.66034300	-2.18969600	O	0.06049100	-6.08942800	2.79863000
H	5.43969400	-5.18641300	-2.32948300	H	0.06120400	-6.82263000	2.15480700
H	6.85892300	-5.83301300	-3.17754700	O	-5.04381000	-3.80112100	-0.67910900
O	6.29784000	-6.92938100	-1.55909200	H	-4.53691200	-4.42793000	-0.10944100
H	5.99371600	-6.74692200	-0.65359400	O	-4.63249400	-4.43081300	-3.45421500
C	-7.37795200	0.20123800	-1.24071600	H	-5.29291600	-4.47061400	-2.73750500
C	-8.91400700	0.25774000	-1.34143800	O	-2.42077600	-5.91890600	-4.43440800
H	-6.97336800	-0.05204200	-2.21984900	H	-3.37579700	-6.06976900	-4.54981000
C	-7.47596900	-0.83051200	0.94429300	O	-0.72385000	-5.76458900	-2.38472600
C	-9.57888300	0.15634200	0.03793800	H	-1.16518700	-6.47661900	-2.88803600
H	-9.20268800	1.20612800	-1.81883000	O	-1.84715100	-3.17368900	-1.39659900
C	-8.99621500	-1.00643200	0.83639900				
H	-9.40827600	1.08450100	0.60761100				
H	-9.19833700	-1.94416700	0.30795500	1J-EE, electron energy = -6485.111680 a.u.			
H	-7.25394100	0.12914100	1.43800000	C	-3.69088700	1.15384600	-1.22666800
C	-6.77559200	-1.92671500	1.74399100	C	-3.17844400	-0.15113100	-1.36914900
H	-5.70069400	-1.69946100	1.77667900	C	-3.61271400	-1.20434300	-0.53967600
H	-7.15158600	-1.88787500	2.77221300	C	-4.70170900	-0.97376300	0.30732000
O	-6.93081600	-0.84357200	-0.38496500	C	-5.29797100	0.28663900	0.37361000
O	-9.31401900	-0.84268300	-2.14619000	C	-4.76191200	1.35578100	-0.35158000
H	-10.25629900	-0.97841800	-1.93498100	H	-5.08644000	-1.77878200	0.92723800
O	-10.97412200	-0.02185900	-0.18728900	H	-5.17998200	2.35085200	-0.22896400
H	-11.33151200	-0.37543800	0.64684400	C	-2.99705900	2.32842900	-1.89989000
O	-9.65320800	-0.98689100	2.10601200	H	-2.86002400	2.14245900	-2.96528300
H	-9.65385600	-1.88990900	2.45964900	H	-3.62889800	3.21871100	-1.79864900
O	-7.01567500	-3.23383300	1.25105700	C	-2.85168700	-2.52344400	-0.47836100
H	-6.43734400	-3.36207400	0.46676300	H	-2.71521000	-2.95050700	-1.47222900
C	-0.72498700	-3.37277200	-2.25507300	H	-3.44537200	-3.23909500	0.10124400
C	-0.90166600	-4.59026800	-3.18123200	C	-1.63071300	2.58391600	-1.26686400
H	0.11010500	-3.56259900	-1.58178100	C	-0.44935200	2.61638900	-2.03296300
C	-3.11466700	-3.06732400	-2.07770100	C	-1.53225000	2.70681700	0.12098800
C	-2.29258600	-4.63208000	-3.83650500	C	0.81271600	2.68165400	-1.41163400
H	-0.12596200	-4.55866900	-3.95763400	C	-0.28969500	2.81316300	0.74619200
C	-3.37609900	-4.39873800	-2.79081600	H	-2.43243800	2.67305800	0.72848200
H	-3.05591400	-2.25329300	-2.81342200	C	0.87621800	2.78140200	-0.02006100
H	-3.31322000	-5.20157200	-2.04548200	H	1.84409400	2.78099300	0.46997700
C	-0.65451400	-3.82347200	3.00339600	C	-1.48247900	-2.34742900	0.17646900
C	-0.27493900	-4.94651900	2.02452900	C	-0.28583100	-2.56574700	-0.53683200
H	0.05542700	-3.80045300	3.83061800	C	-1.39667600	-1.91384500	1.50203200
C	-3.00627600	-4.27491800	2.72172100	C	0.96705500	-2.23894700	0.01936700
C	-1.42523300	-5.30204100	1.06205500	C	-0.15484700	-1.69531000	2.10351400
H	0.59512700	-4.61913200	1.43443300	H	-2.30360300	-1.75079900	2.07723200
C	-2.72518300	-5.50156000	1.83521400	C	1.01429800	-1.81305800	1.35176400
H	-3.13640300	-3.38634800	2.08460500	H	1.97047800	-1.59636000	1.81863900
H	-2.64009700	-6.38788900	2.47009900	C	2.25246400	-2.33500100	-0.80117900
H	-2.36889600	-3.84966600	-4.60778000	H	2.93426400	-3.05113600	-0.32819700
H	-1.57836900	-4.49417700	0.33954400	H	2.00496300	-2.71841500	-1.79089700
C	-4.20400300	-2.70168500	-1.05423200	C	2.11247700	2.51774400	-2.19777200
H	-3.71808400	-2.25489900	-0.17787100	H	1.87198700	2.38113400	-3.25256200
H	-4.87153600	-1.95109400	-1.47623800	H	2.71368600	3.43095200	-2.12087100
C	-4.24765400	-4.42324500	3.59604200	C	4.10737500	-0.72380800	-0.16326700
H	-4.35069900	-3.51373900	4.20549700	C	4.70320100	0.54070700	-0.20383300
H	-5.13776000	-4.50594900	2.96533400	C	2.96125500	-0.99390700	-0.91627000
O	-1.91066500	-4.07497900	3.62371200	C	4.08383300	1.58378000	-0.89746300
O	-4.19584700	-5.58825500	4.41196900	C	2.43129400	0.03385100	-1.72021200
H	-3.37531500	-5.51909900	4.92884500	C	2.91869000	1.35367900	-1.63549800
O	-3.78279200	-5.69551300	0.88071300	H	4.50942300	2.58294600	-0.85533600
H	-4.48343200	-6.22343100	1.29569700	H	4.54952700	-1.50702900	0.44473600
O	-1.07643100	-6.50342500	0.37728700	O	-0.52313900	2.51216600	-3.40876500
H	-0.86867500	-6.26240000	-0.54845200	O	1.34990500	-0.24734100	-2.51802800
				O	-0.34712500	-3.08801600	-1.81363100

O	-2.15841800	-0.36027400	-2.26379600	H	-8.93394900	1.72405800	-0.24857200
C	-0.31799400	-4.53123300	-1.85338700	S	8.08481900	0.22313100	1.93118600
H	-1.14094100	-4.92964300	-1.24355300	S	0.98297400	2.20836200	4.44841500
H	0.62499500	-4.88854000	-1.41621300	S	-0.87605500	-1.27414500	6.04199900
C	-0.45127600	-4.98117200	-3.30004400	S	-8.49636300	1.70394800	2.35539800
H	0.36991500	-4.54733700	-3.88412200	C	-7.80063400	0.31438500	-1.35575800
H	-1.38379600	-4.57584000	-3.71209400	C	-8.67095800	0.74657600	-2.55054000
C	-0.43774400	-6.50821300	-3.42904900	H	-6.75745600	0.38480300	-1.65818900
H	-0.53783800	-6.80937300	-4.47698800	C	-9.33187100	-1.47783000	-0.77762800
H	0.49816200	-6.93327000	-3.04731900	C	-10.11884100	0.26101100	-2.39634900
H	-1.26446700	-6.96262000	-2.87016900	H	-8.65662700	1.84498700	-2.61897200
C	1.59955400	-0.27095800	-3.94286100	C	-10.15349100	-1.22445800	-2.04920800
H	2.23388600	0.57793800	-4.22413800	H	-10.62318300	-0.81637200	-1.58973900
H	0.61691500	-0.12191500	-4.39766600	H	-9.70593600	-1.79243600	-2.87144800
C	2.23324200	-1.57366500	-4.42358300	O	-7.97559100	-1.05007200	-1.01140800
H	1.59678700	-2.41144600	-4.11598200	O	-8.09127900	0.17145000	-3.71073600
H	3.20886800	-1.70886000	-3.93852700	H	-8.80087600	0.18344500	-4.37947500
C	2.41249500	-1.57949300	-5.94649700	O	-10.76920400	0.51162600	-3.63782200
H	3.05942300	-0.75712900	-6.27514500	H	-11.57069400	-0.04160300	-3.63280200
H	2.86932000	-2.51678000	-6.28116300	O	-11.53084200	-1.56792500	-1.88491500
H	1.45014900	-1.47415300	-6.46184900	H	-11.64383500	-2.49980500	-2.12816900
C	-2.50122700	-1.08208400	-3.47092200	H	-9.77050700	-0.92142200	0.06344700
H	-1.58198300	-1.59458700	-3.76385800	C	-9.22988900	-2.95058200	-0.39631400
H	-3.25615900	-1.84472300	-3.24482600	H	-8.65055900	-3.03465100	0.53445000
C	-2.99845500	-0.16449700	-4.58408300	H	-10.23104400	-3.34964500	-0.21004300
H	-2.24837600	0.61604000	-4.75729300	O	-8.65442500	-3.73242400	-1.43585100
H	-3.91788100	0.33800500	-4.25677100	H	-7.79932200	-3.31726200	-1.64053800
C	-3.26719400	-0.94264600	-5.87748100	C	7.03183500	-0.69870000	-1.79546900
H	-2.35780200	-1.43632800	-6.24098400	C	7.11188900	-2.05429900	-2.51975800
H	-4.02973500	-1.71653000	-5.72729900	H	6.02673500	-0.31113800	-1.93388600
H	-3.62265800	-0.27396900	-6.66856000	C	9.25657600	-0.06878500	-2.55937700
C	-0.59985400	3.77949200	-4.09446000	C	8.56458700	-2.46614900	-2.78673100
H	0.26949600	4.39417600	-3.82155600	H	6.62195700	-2.81401200	-1.89413200
H	-1.50373800	4.31497200	-3.77118100	C	9.33376400	-1.32269700	-3.44222700
C	-0.62853300	3.51909600	-5.59269600	H	9.06546300	-2.72578200	-1.83983400
H	-1.49906200	2.89408400	-5.82794100	H	8.87344600	-1.09518000	-4.40924200
H	0.26260200	2.94047000	-5.86667600	H	9.73837700	-0.26780000	-1.59039900
C	-0.68100200	4.81996600	-6.40106800	C	9.91039200	1.15968700	-3.18411500
H	-0.70208100	4.60839100	-7.47515800	H	9.83467900	1.99769900	-2.47626500
H	-1.57587500	5.40539800	-6.15835400	H	10.97113000	0.95951900	-3.36044500
H	0.19479800	5.44871100	-6.20122000	O	7.87382200	0.28985800	-2.37559700
N	-0.08907800	-1.32436400	3.49024300	O	6.41971100	-1.90381400	-3.75210800
N	-0.25933400	2.77975300	2.17190200	H	6.72747400	-2.64352700	-4.30779000
N	-0.79944700	-3.37296900	4.41700800	O	8.52052200	-3.60625500	-3.63828900
N	1.55246200	4.16921000	2.73074600	H	9.41120400	-3.68108600	-4.02508900
N	7.28354800	-0.88137300	-0.36594400	O	10.67534400	-1.78423800	-3.61312200
N	5.90714000	0.80493500	0.52239700	H	11.04951500	-1.35239200	-4.39654900
N	-6.39185100	0.49463700	1.27339100	O	9.33223800	1.49062000	-4.44060200
N	-8.05905500	1.21471200	-0.22751500	H	8.37804700	1.58549900	-4.27896000
C	-7.58252400	1.09535900	1.04650500	C	1.15604800	5.36888100	1.98750400
C	7.02596600	0.04519000	0.61069100	C	2.36609700	6.31401200	1.87191600
C	-0.55995800	-2.03091100	4.54140600	H	0.85042100	5.08972700	0.98000200
C	0.74507700	3.11157200	3.02540200	C	0.20316000	6.66715800	3.80503800
H	5.86707900	1.54779200	1.21066100	C	2.58438700	7.10586500	3.16852400
H	8.09491600	-1.44186500	-0.13338200	H	3.26224600	5.71480700	1.65082800
H	-0.90750900	2.11718800	2.58103600	C	1.27952500	7.74737600	3.63147100
H	2.30408900	4.27557700	3.40139800	H	0.51748600	5.95015800	4.57759500
H	0.17026000	-0.36250900	3.71190300	H	0.94031800	8.45454000	2.86763700
H	-1.19279400	-3.74992100	5.27054200	C	-0.09271000	-4.32870000	3.56093600
H	-6.19939300	0.34452600	2.25698100	C	-0.60571900	-5.74783500	3.87157900

H	-0.29755800	-4.11799000	2.51345200	C	-0.61360500	-2.72978000	0.91599000
C	1.89416300	-4.65779700	4.91874600	C	0.51610700	-2.28732500	-1.19326600
C	0.02262300	-6.30178500	5.15755600	H	2.61658500	-1.84809600	-1.07514700
H	-1.70002800	-5.71083300	3.98311100	C	-0.65169700	-2.55098100	-0.47008700
C	1.53908900	-6.13550700	5.13218900	H	-1.60619100	-2.58473000	-0.98534800
H	1.50431100	-4.05870100	5.75469700	C	-1.91399200	-2.96156600	1.68653300
H	1.94673300	-6.71485300	4.29737200	H	-2.33486000	-3.93544400	1.41013900
H	2.94502300	6.43805900	3.96732000	H	-1.68365200	-2.99363900	2.75151700
H	-0.36954500	-5.76384100	6.03549500	C	-3.10378600	1.94655300	1.59202700
C	-1.16734300	7.22207800	4.17846800	H	-2.98454200	2.16482500	2.65392900
H	-1.86692500	6.38251200	4.29872800	H	-3.89380500	2.60575500	1.21523300
H	-1.09959900	7.74690500	5.13566300	C	-4.06403700	-2.14736800	0.59722600
C	3.39085400	-4.39881100	4.78235200	C	-4.93201500	-1.12023900	0.20623800
H	3.55170500	-3.31790400	4.66060000	C	-2.94374700	-1.88085800	1.39132500
H	3.90220500	-4.71685200	5.69543200	C	-4.62438000	0.20539700	0.54447700
O	1.31799600	-4.22030000	3.67228500	C	-2.74838500	-0.56556900	1.85173600
O	3.96304900	-5.13094800	3.70528200	C	-3.52948900	0.50046200	1.36304800
H	3.44322600	-4.89641600	2.91770400	H	-5.21842700	1.01885600	0.13809500
O	2.02005100	-6.63681100	6.38113000	H	-4.27251700	-3.16883500	0.29002000
H	2.91173000	-6.99233900	6.24419600	O	-0.69726900	2.83769700	2.93644900
O	-0.33923900	-7.67710900	5.23130100	O	-1.70656700	-0.31232700	2.71054200
H	0.27848000	-8.07851300	5.86827300	O	0.69772100	-2.83798200	2.93630400
O	-0.24846400	-6.56683400	2.76923500	O	1.70712400	0.31206100	2.71053700
H	-0.29050800	-7.47978200	3.10925300	C	0.96724300	-4.20832400	3.30194300
O	-1.64400300	8.15959100	3.22089300	H	1.90750100	-4.53146700	2.83346400
H	-1.63329700	7.69842000	2.36501400	H	0.16339600	-4.85245600	2.91874300
O	1.57455700	8.42369100	4.85498500	C	1.05883500	-4.29703700	4.81748800
H	0.98227300	9.18770300	4.93110600	H	0.11649400	-3.93928800	5.25099400
O	3.56761400	8.09509700	2.88408600	H	1.84721700	-3.61752900	5.16455500
H	3.49203100	8.75469000	3.59668200	C	1.34633300	-5.72528600	5.29274200
O	2.09073200	7.20692300	0.80416000	H	1.40712000	-5.76517000	6.38526600
H	2.68624800	7.96534000	0.94955000	H	0.55689300	-6.41753800	4.97667400
O	0.01265300	5.99725400	2.54277400	H	2.29709800	-6.09603000	4.89151500
2A-EZ, electron energy = -6485.166657 a.u.				C	-2.07063400	-0.02303400	4.08097500
C	2.94407300	1.88060000	1.39110200	H	-2.97572300	0.59610900	4.10088900
C	2.74881000	0.56531800	1.85156800	H	-1.24427400	0.57672200	4.46915000
C	3.52985300	-0.50070700	1.36275900	C	-2.27844500	-1.27970300	4.92081100
C	4.62459400	-0.20564300	0.54399700	H	-1.37103000	-1.89259300	4.86967200
C	4.93211400	1.11998700	0.20561600	H	-3.09456500	-1.87392100	4.49012300
C	4.06419900	2.14711000	0.59676500	C	-2.60396300	-0.93478200	6.37883800
H	5.21861900	-1.01909600	0.13757300	H	-3.52373000	-0.34201700	6.45327300
H	4.27259100	3.16857200	0.28947800	H	-2.74465200	-1.84397500	6.97285100
C	1.91435700	2.96129300	1.68648600	H	-1.79523000	-0.35574000	6.84103600
H	1.68410100	2.99326600	2.75149200	C	2.07140500	0.02271500	4.08089800
H	2.33520900	3.93519300	1.41014400	H	1.24507000	-0.57699100	4.46921000
C	3.10414700	-1.94679800	1.59173600	H	2.97645600	-0.59648800	4.10065200
H	2.98498000	-2.16511600	2.65363600	C	2.27945000	1.27935100	4.92072500
H	3.89411300	-2.60601100	1.21485100	H	1.37206400	1.89230100	4.86978000
C	0.61390300	2.72960100	0.91602200	H	3.09552500	1.87353200	4.48990000
C	-0.62742700	2.62397600	1.57373100	C	2.60521700	0.93437100	6.37868400
C	0.65185900	2.55094500	-0.47007400	H	1.79653700	0.35535900	6.84101200
C	-1.79212300	2.25249900	0.87293000	H	3.52496600	0.34155700	6.45293500
C	-0.51602500	2.28742300	-1.19318000	H	2.74606100	1.84353900	6.97269700
H	1.60630000	2.58472600	-0.98543200	C	-0.96663800	4.20804000	3.30218600
C	-1.72318400	2.11185000	-0.51506200	H	-1.90689700	4.53129800	2.83378800
H	-2.61649400	1.84818800	-1.07491800	H	-0.16275800	4.85212400	2.91897600
C	1.79241000	-2.25265900	0.87272800	C	-1.05812000	4.29665800	4.81774400
C	0.62777600	-2.62419400	1.57359900	H	-0.11579400	3.93875700	5.25115700
C	1.72333500	-2.11184700	-0.51523800	H	-1.84656300	3.61722300	5.16481400
				C	-1.34540300	5.72490600	5.29312700

H	-1.40611700	5.76471100	6.38565900	H	-9.46686500	3.50800200	-1.71145900
H	-0.55589400	6.41708100	4.97706400	H	-10.39297100	4.53353500	-0.59723800
H	-2.29614600	6.09580600	4.89199100	O	-8.73110200	1.73562400	0.05784900
N	0.48999700	-2.09623700	-2.60820900	O	-7.93788400	1.15119600	2.83137100
N	-0.49005800	2.09666500	-2.60817600	H	-8.20953200	1.49237300	3.70256300
N	-0.62810000	-4.04218800	-3.15275800	O	-10.35039600	1.86978200	3.85870100
N	0.62777500	4.04289000	-3.15229600	H	-10.88631000	2.67640300	3.95972400
N	-7.64029400	-0.24592400	0.54638900	O	-11.23686200	3.71962000	1.91297300
N	-6.04458200	-1.44750400	-0.62096800	H	-10.97782700	4.65202000	1.85167300
N	6.04441600	1.44718400	-0.62195200	O	-8.39575100	4.50055500	-0.21626800
N	7.64045900	0.24571700	0.54502200	H	-7.69015300	3.83173500	-0.19862900
C	7.32719200	1.01780000	-0.52552000	C	1.62672800	4.78351200	-3.86586200
C	-7.32741300	-1.01841500	-0.52396900	C	1.61689900	6.24013800	-3.38815100
C	-0.10699700	-2.85624000	-3.56219200	H	1.41373100	4.73844000	-4.93847100
C	0.10669100	2.85703000	-3.56202700	C	4.05114300	4.79004900	-4.12506700
H	-5.88600900	-2.18305500	-1.31692900	C	2.84864500	6.97883500	-3.91457700
H	-6.91379900	-0.02253000	1.21916400	H	0.70812300	6.72331300	-3.77593000
H	-1.01480100	1.31179700	-2.97466500	C	4.12715900	6.22002300	-3.56764900
H	0.56570700	4.27988800	-2.16659900	H	4.01937900	4.82690500	-5.22435200
H	1.01476600	-1.31131800	-2.97455200	H	4.22315800	6.16948300	-2.47790300
H	-0.56577200	-4.27960100	-2.16717700	C	-1.62713100	-4.78258800	-3.86643700
H	5.88565400	2.18269200	-1.31792000	C	-1.61710100	-6.23941700	-3.38934300
H	6.91433200	0.02308900	1.21844900	H	-1.41432800	-4.73705400	-4.93906500
S	-8.46854700	-1.49851800	-1.70200600	C	-4.05158600	-4.78920400	-4.12519400
S	0.12025400	2.32814000	-5.18115100	C	-2.84888100	-6.97798800	-3.91585600
S	-0.12088100	-2.32677700	-5.18112700	H	-0.70835500	-6.72234800	-3.77749900
S	8.46776000	1.49701500	-1.70446000	C	-4.12738300	-6.21941700	-3.56836200
C	8.86517600	-0.47672500	0.72635600	H	-4.02003500	-4.82560000	-5.22450200
C	9.12843400	-0.65045900	2.22770800	H	-4.22316900	-6.16933800	-2.47857600
H	9.68445600	0.08867100	0.26955600	H	2.77974000	7.06547300	-5.01057500
C	9.87064200	-2.59794300	0.18994200	H	-2.78017200	-7.06415500	-5.01190400
C	10.28978700	-1.62025200	2.45546900	C	5.20267600	3.89248500	-3.67713800
H	9.38780200	0.33286200	2.64777000	H	5.14903400	2.93605000	-4.21259400
C	10.07767100	-2.91606500	1.67873200	H	6.16639400	4.35940100	-3.89434100
H	11.22443500	-1.15388000	2.10598600	C	-5.20311100	-3.89192900	-3.67666900
H	9.17745200	-3.41332500	2.05483100	H	-5.14958400	-2.93523900	-4.21168500
O	8.72952900	-1.73708100	0.05784000	H	-6.16683700	-4.35878500	-3.89396000
O	7.93995900	-1.14860300	2.83156700	O	-2.88250300	-4.13849000	-3.60413500
H	8.21249000	-1.48891000	3.70282400	O	-5.13006000	-3.68201100	-2.26172500
O	10.35326300	-1.86724200	3.85695200	H	-4.18538600	-3.51134200	-2.08978100
H	10.88883700	-2.67403500	3.95838500	O	-5.20627100	-6.96206600	-4.13963000
O	11.23642000	-3.72004700	1.91253400	H	-5.98740600	-6.85492400	-3.57556400
H	10.97685300	-4.65238500	1.85258300	O	-2.84454000	-8.26781900	-3.31383300
H	10.77198500	-2.10440300	-0.20819700	H	-3.74527800	-8.61806100	-3.43343000
C	9.56075100	-3.82526000	-0.66054200	O	-1.61037200	-6.23916500	-1.96621300
H	9.46202400	-3.51217000	-1.70999100	H	-1.85132900	-7.14499400	-1.70126000
H	10.38913600	-4.53670800	-0.59569500	O	5.12980000	3.68190400	-2.26228300
O	8.39244700	-4.50237000	-0.21214200	H	4.18512300	3.51129900	-2.09029200
H	7.68711800	-3.83326700	-0.19453300	O	5.20598000	6.96283800	-4.13882800
C	-8.86522600	0.47605900	0.72814500	H	5.98722500	6.85542000	-3.57496700
C	-9.12680500	0.65159400	2.22958600	O	2.84451100	8.26841000	-3.31200300
H	-9.68473000	-0.09037400	0.27303400	H	3.74524700	8.61864500	-3.43163400
C	-9.87255400	2.59600900	0.19017800	O	1.61043700	6.23928300	-1.96502000
C	-10.28842900	1.62102500	2.45746700	H	1.85150500	7.14498300	-1.69972900
H	-9.38511900	-0.33131600	2.65125400	O	2.88210100	4.13922100	-3.60404800
C	-10.07796600	2.91595200	1.67880800				
H	-11.22322300	1.15366400	2.10969400				
H	-9.17756300	3.41419800	2.05316300				
H	-10.77409700	2.10144800	-0.20624500				
C	-9.56435100	3.82238000	-0.66227700				
				2B-EZ, electron energy = -6485.163789 a.u.			
				C	1.26883400	1.98168000	2.13864500
				C	1.25303700	0.59084000	2.35093400
				C	2.29512100	-0.22732800	1.87374200

C	3.43270000	0.38152100	1.33205800	H	-4.33163600	-3.29196400	3.17191700
C	3.53594100	1.77843800	1.26146400	C	-4.40140800	-2.67279500	5.24638900
C	2.43404600	2.56282200	1.62875300	H	-5.42456100	-2.27905000	5.21511400
H	4.21925300	-0.24449200	0.92073800	H	-4.44876000	-3.69221600	5.64363200
H	2.49117200	3.64340500	1.52841600	H	-3.83084100	-2.06329900	5.95764000
C	0.01562600	2.81179200	2.37464000	C	0.31112000	-0.46148400	4.28494400
H	-0.40637300	2.60095600	3.35732300	H	-0.42602100	-1.26101000	4.39029600
H	0.28535200	3.87416200	2.35093500	H	1.30808200	-0.90325600	4.40175900
C	2.12030300	-1.73893500	1.79779700	C	0.09609900	0.62440300	5.33529000
H	1.82788100	-2.15726200	2.76131400	H	-0.89480300	1.06894400	5.18697400
H	3.08231300	-2.18945400	1.52806700	H	0.83390400	1.42364600	5.18827400
C	-1.05221600	2.53090800	1.31591400	C	0.21829100	0.06370100	6.75714800
C	-2.34523800	2.09424700	1.66632000	H	-0.52281400	-0.72390000	6.93972800
C	-0.72765800	2.63732300	-0.04030800	H	1.21202400	-0.36573000	6.93303200
C	-3.26420500	1.68364500	0.68065400	H	0.05884700	0.85066800	7.50179800
C	-1.66788200	2.33327400	-1.03040600	C	-3.32408700	3.21878200	3.50650100
H	0.28021300	2.92090600	-0.32505700	H	-4.21302200	3.45271100	2.90391400
C	-2.91823500	1.83396400	-0.66363500	H	-2.62290900	4.05959600	3.40949400
H	-3.62297000	1.53939700	-1.43651200	C	-3.70219200	2.99206500	4.96209400
C	1.07448100	-2.11863400	0.75215200	H	-2.79759200	2.73647400	5.52791100
C	-0.11144100	-2.79811500	1.08715300	H	-4.37198800	2.12522800	5.02318100
C	1.27203800	-1.72572400	-0.57296000	C	-4.37631300	4.22326200	5.57731500
C	-1.12773100	-2.99280600	0.13012500	H	-4.63733800	4.03945900	6.62465700
C	0.32843900	-2.02506400	-1.55987700	H	-3.71524700	5.09751100	5.54604400
H	2.16218000	-1.16058700	-0.82895900	H	-5.29849800	4.48150300	5.04330200
C	-0.87974000	-2.62402100	-1.19530700	N	0.54505800	-1.66733500	-2.92300600
H	-1.63938500	-2.79913700	-1.95242600	N	-1.34903600	2.41613400	-2.41912100
C	-2.49342200	-3.55808500	0.51529000	N	2.69632800	-2.48169700	-3.08151800
H	-2.66646600	-4.50102900	-0.01620300	N	-0.51491600	4.56947000	-2.42504700
H	-2.49344200	-3.77665400	1.58317500	N	-8.24438000	-1.91449400	-1.33998600
C	-4.59143200	1.01963900	1.04020100	N	-6.23602600	-2.14747900	-2.44716100
H	-4.70188900	1.01301400	2.12484800	N	4.68033000	2.43614800	0.72888800
H	-5.42275200	1.60766200	0.63544100	N	6.30925000	1.21744700	1.84309500
C	-4.45254400	-2.82594700	-0.92670300	C	5.99672200	2.20558100	0.97090200
C	-5.40496200	-1.87998500	-1.31517300	C	-7.59389200	-2.15846600	-2.50179900
C	-3.61526500	-2.59016600	0.16845400	C	1.67010800	-1.82628300	6.37275900
C	-5.47581700	-0.64914500	-0.65151600	C	-0.72689300	3.41132000	-3.10160400
C	-3.78923500	-1.39989500	0.90039000	H	-5.78517700	-2.47169900	-3.29377900
C	-4.66060200	-0.38545700	0.45325100	H	-7.70065900	-1.71965500	-0.50475900
H	-6.14374600	0.12304800	-1.02321200	H	-1.65063500	1.64539300	-3.00262400
H	-4.36771800	-3.75685700	-1.48082600	H	-0.81459600	4.62483600	-1.45625000
O	-2.70407100	2.01827900	2.99769700	H	-0.24367400	-1.29558200	-3.43730300
O	-3.00694400	-1.18859100	2.00814800	H	2.53982400	-2.92485000	-2.18141700
O	-0.29468700	-3.24301500	2.38185900	H	4.49412900	3.29148300	0.19525800
O	0.14545800	0.02079000	2.93109100	H	5.56295300	0.68645100	2.27911700
C	0.17377200	-4.59015200	2.60641700	S	-8.37499900	-2.49955200	-3.97986100
H	1.23199700	-4.66050700	2.31809500	S	-0.30996800	3.18023800	-4.73724000
H	-0.39306700	-5.28376300	1.96936200	S	1.72346500	-1.21224900	-5.26114400
C	-0.00761900	-4.93089000	4.07749500	S	7.17251800	3.17896700	0.20066600
H	-1.06785800	-4.82586000	4.33894400	C	7.63733100	0.77794400	2.16536300
H	0.54317700	-4.19835500	4.68060800	C	7.62969600	0.17651300	3.57801300
C	0.47394700	-6.34942300	4.40127300	H	8.31371700	1.64009400	2.13780900
H	0.33175100	-6.57395000	5.46347300	C	9.37825700	-0.66417400	1.41624600
H	-0.07924800	-7.09990800	3.82414500	C	8.96807000	-0.50566500	3.87545000
H	1.53968600	-6.47079700	4.17385900	H	7.46923700	0.99147800	4.30003000
C	-3.67667600	-1.24328700	3.29023700	C	9.36603200	-1.44267600	2.74043800
H	-4.68374600	-0.81924900	3.20109200	H	9.74972400	0.26294200	3.98208500
H	-3.09145100	-0.59010300	3.94194600	H	8.62066500	-2.24022000	2.65536400
C	-3.75397900	-2.65759300	3.85660500	O	8.05094100	-0.17418100	1.18048000
H	-2.74101000	-3.07248600	3.90389500	O	6.56547000	-0.76537200	3.65337100

H	6.75775000	-1.31124300	4.43744400	O	4.56196900	-6.60689800	-4.88352100
O	8.80562800	-1.21673300	5.09988800	H	3.77055000	-6.26070500	-4.43705300
H	9.53453900	-1.86152600	5.12883600	O	7.60472600	-4.74937600	-4.20627800
O	10.64355100	-1.98035100	3.08972500	H	7.69284600	-5.71212400	-4.28100600
H	10.73501800	-2.83966200	2.64879400	O	7.20728700	-3.35051500	-1.79822100
H	10.08102600	0.18292800	1.49396100	H	7.96969900	-3.88027200	-2.09436900
C	9.80134600	-1.51284300	0.22064500	O	4.51441600	-3.59628800	-1.47153200
H	9.68181000	-0.91910200	-0.69564500	H	5.26218300	-3.78737900	-0.87812700
H	10.86562900	-1.74605100	0.33190700	O	3.69111400	4.86379900	-0.60317300
O	9.11294500	-2.75214900	0.13488200	H	2.77180200	4.54347500	-0.66515800
H	8.25364700	-2.59883500	-0.29866900	O	3.47772500	8.36254700	-2.04400100
C	-9.66334100	-1.77535700	-1.18491300	H	4.14020500	8.31430900	-1.33801000
C	-10.06194500	-2.25360200	0.21693700	O	0.78519600	9.08919000	-1.59296500
H	-10.16332700	-2.38845100	-1.94231200	H	1.60071700	9.60816000	-1.47557700
C	-11.39144100	-0.10201900	-1.22924300	O	-0.24179400	6.68769900	-0.79379500
C	-11.52607000	-1.91172700	0.49723100	H	-0.24478800	7.56813600	-0.37706600
H	-9.92830900	-3.34485800	0.25952200	O	1.71631300	5.12752400	-2.35143700
C	-11.80305000	-0.43898500	0.21249400				
H	-12.17111000	-2.52068800	-0.15600400	2C-EZ, electron energy = -6485.160498 a.u.			
H	-11.20546900	0.17366400	0.89558700	C	3.60223200	1.16199900	1.78076100
H	-11.99608400	-0.69883700	-1.93118800	C	2.87431300	-0.02886000	1.95962700
C	-11.54089100	1.37569500	-1.57564600	C	3.20217300	-1.19689300	1.24312200
H	-11.25656200	1.52292100	-2.62753400	C	4.37361900	-1.20511400	0.47912400
H	-12.58659500	1.67580100	-1.46141400	C	5.19912000	-0.07339200	0.41750700
O	-9.99571700	-0.39871600	-1.39446200	C	4.78355700	1.11350600	1.03365200
O	-9.21120100	-1.61306000	1.16080000	H	4.62476100	-2.08961900	-0.09911000
H	-9.64248800	-1.73332700	2.02594200	H	5.39589900	2.00663100	0.94033200
O	-11.77010800	-2.22416600	1.86520900	C	3.06718800	2.47963400	2.32113100
H	-12.59070200	-1.75589100	2.10052800	H	2.82337700	2.39179200	3.37999800
O	-13.19977800	-0.23939500	0.44314500	H	3.84778400	3.24349700	2.22475600
H	-13.33271000	0.67720200	0.72988400	C	2.23380600	-2.37255000	1.18415200
O	-10.77126900	2.20403300	-0.71187800	H	1.98685500	-2.73569200	2.18266400
H	-9.86131600	1.86420300	-0.75826300	H	2.72190600	-3.19851500	0.65473900
C	0.43134600	5.57696600	-2.80469800	C	1.81483000	2.92943800	1.56874300
C	0.03407400	6.91483200	-2.17134800	C	0.60156100	3.18662300	2.23664900
H	0.44398700	5.66622100	-3.89526600	C	1.84272700	3.02107000	0.17395700
C	2.80800300	6.04464100	-2.52254500	C	-0.58220800	3.44553900	1.51775100
C	1.16652900	7.93130500	-2.32776000	C	0.69733600	3.37602800	-0.54608200
H	-0.86367800	7.28668800	-2.68673300	H	2.75662300	2.77467300	-0.35643500
C	2.48392100	7.36420700	-1.80421200	C	-0.51062800	3.56189700	0.12762800
H	2.98690800	6.24324100	-3.58993200	H	-1.41023500	3.78011700	-0.44136300
H	2.38188200	7.16646600	-0.73192000	C	0.94272200	-1.99327800	0.46318400
C	4.00729700	-2.68319300	-3.62486500	C	-0.30581000	-2.01559600	1.11641400
C	5.01368300	-2.70291300	-2.46124300	C	0.99556500	-1.57177000	-0.86777200
H	4.24038300	-1.85810300	-4.30692800	C	-1.46236300	-1.50875000	0.49311900
C	5.28317800	-4.27227200	-4.90253700	C	-0.15752700	-1.14169700	-1.52641000
C	6.38759900	-3.15703100	-2.95302600	H	1.94521900	-1.56983000	-1.39585500
H	5.09003400	-1.68402600	-2.05391700	C	-1.36827100	-1.07257100	-0.83184700
C	6.28357100	-4.45261200	-3.74992400	H	-2.23995100	-0.64500500	-1.31805100
H	5.64142100	-3.48322200	-5.58324400	C	-2.78138600	-1.35098300	1.24986500
H	5.91121900	-5.24528100	-3.09275300	H	-3.54041100	-2.00900400	0.81090300
H	1.29100400	8.17609200	-3.39463400	H	-2.63005800	-1.66390600	2.28289800
H	6.82119600	-2.37819000	-3.59771700	C	-1.94244300	3.53381200	2.20789000
C	4.00391400	5.30050000	-1.93157700	H	-1.79905900	3.44617000	3.28502700
H	4.25232800	4.44372300	-2.57073400	H	-2.39136500	4.51555700	2.01985100
H	4.87752800	5.95412300	-1.87042400	C	-4.29417600	0.45440800	0.30151400
C	5.04292100	-5.54814300	-5.70302100	C	-4.65110800	1.79881600	0.14203400
H	4.34187000	-5.32567100	-6.52028300	C	-3.27850400	0.08527300	1.19008500
H	5.98411600	-5.88669000	-6.14587300	C	-3.91926400	2.79266900	0.80089400
O	4.00699500	-3.91563400	-4.34998400	C	-2.63337700	1.09386100	1.92949600

C	-2.87910200	2.45814800	1.67174100	H	-6.69511100	0.56524600	0.80238300
H	-4.15177600	3.83813300	0.61573400	H	-0.07813000	3.02291000	-2.45451900
H	-4.79272800	-0.31056000	-0.28672300	H	2.53009500	4.91189100	-1.19202300
O	0.55699900	3.13436000	3.61613300	H	0.68654300	-0.06752100	-3.11975600
O	-1.66476600	0.73242900	2.83272700	H	-1.78298300	-2.47421400	-2.77000500
O	-0.38456700	-2.50292800	2.40587400	H	6.58634000	0.79456700	-0.88186800
O	1.76113600	-0.00897600	2.76469900	H	6.51939600	-2.03436000	1.15152900
C	-0.68659600	-3.91268800	2.48088600	S	-7.99414000	2.38279400	-2.04629600
H	0.07864400	-4.47755400	1.93010700	S	1.47473200	3.83211000	-4.48188100
H	-1.65572700	-4.10366600	1.99899200	S	-0.53094500	-0.42645300	-5.48381300
C	-0.71627200	-4.32595200	3.94424100	S	8.70211000	-0.78600000	-1.45649400
H	-1.47260200	-3.72690700	4.46665800	C	8.12910400	-3.17920000	0.52168100
H	0.25219300	-4.08397400	4.39946100	C	8.20887900	-3.73216100	1.95052500
C	-1.02068600	-5.81855100	4.11184100	H	9.13178100	-2.92001300	0.16544100
H	-1.04203600	-6.09343800	5.17148600	C	8.22746300	-5.37618000	-0.45663100
H	-1.99452200	-6.07744300	3.67948800	C	8.86615800	-5.11388000	1.94896100
H	-0.26092400	-6.43828900	3.62094000	H	8.81518900	-3.04115700	2.55508800
C	-1.99710800	0.89945500	4.23153700	C	8.19931100	-6.03443200	0.93114000
H	-2.64697000	1.77393900	4.35552300	H	9.92869500	-5.00786800	1.67864300
H	-1.04635000	1.11160300	4.72693500	H	7.15400100	-6.18667200	1.21964700
C	-2.66413300	-0.33673700	4.82731800	O	7.53607400	-4.12035300	-0.38130400
H	-2.01237100	-1.20356800	4.66596400	O	6.88545700	-3.81217200	2.46806800
H	-3.60218600	-0.53552900	4.29309800	H	6.94309600	-4.39771800	3.24452800
C	-2.94757300	-0.15847700	6.32351800	O	8.74050700	-5.63373700	3.26909800
H	-3.61745200	0.69081400	6.50453100	H	8.90197300	-6.59085900	3.19154300
H	-3.42340200	-1.05275500	6.73949100	O	8.92113000	-7.26793900	0.97051600
H	-2.02280200	0.01994700	6.88549400	H	8.31023200	-7.98578600	0.74317000
C	1.88896400	-0.67962700	4.04125100	H	9.27313800	-5.22065500	-0.76812300
H	0.87090700	-0.97370900	4.30563700	C	7.50442900	-6.18051500	-1.53189900
H	2.48394700	-1.59314000	3.92131600	H	7.60037900	-5.65294600	-2.49189000
C	2.50131900	0.20610300	5.12229500	H	7.97509300	-7.16241000	-1.63571600
H	1.91062300	1.12598900	5.19891100	O	6.13896600	-6.40479200	-1.20066100
H	3.51657900	0.49722400	4.82357400	H	5.75877900	-5.52657300	-1.02854000
C	2.54755400	-0.51071800	6.47688100	C	-8.65130100	0.25085100	0.18213000
H	1.54209600	-0.79188400	6.81296300	C	-8.54145400	-1.16958800	0.75276600
H	3.14999700	-1.42574400	6.42467800	H	-9.12099200	0.21858100	-0.80695000
H	2.98761700	0.13419300	7.24483600	C	-10.74273700	0.66067300	1.29987800
C	0.80827500	4.40181900	4.26042800	C	-9.92594200	-1.70035900	1.12977900
H	0.08713400	5.14583700	3.89398200	H	-8.10063500	-1.81736500	-0.01966300
H	1.81552000	4.75229600	3.99455300	C	-10.67196200	-0.70085700	2.00839700
C	0.67668000	4.21762400	5.76443600	H	-10.51313000	-1.86466000	0.21246600
H	1.39081800	3.45212000	6.09260400	H	-10.12281900	-0.57293800	2.94705900
H	-0.32688200	3.83430700	5.98735700	H	-11.30399600	0.55591900	0.35719800
C	0.92301200	5.52511100	6.52532200	C	-11.38808400	1.75526100	2.14349200
H	0.82557700	5.36953100	7.60475600	H	-11.42858900	2.68063000	1.55091600
H	1.92986100	5.91449100	6.33333600	H	-12.41323500	1.46908500	2.39597000
H	0.20314400	6.29882200	6.23293800	O	-9.40549600	1.11354400	1.03889400
N	-0.06626900	-0.70231300	-2.88341900	O	-7.69916400	-1.12158400	1.89882700
N	0.70293300	3.45020300	-1.97165500	H	-7.86573900	-1.95192000	2.38056700
N	-1.68660000	-2.11680200	-3.71550000	O	-9.72311500	-2.93278900	1.81474200
N	2.53966500	4.83012300	-2.20436000	H	-10.55770200	-3.11537000	2.28183600
N	-7.33327800	0.80179400	0.04846000	O	-11.96412800	-1.26299400	2.24862800
N	-5.68042500	2.19308000	-0.76424500	H	-12.27670100	-0.95150000	3.11201100
N	6.40070300	-0.06034300	-0.34787400	O	-10.69584100	1.95761400	3.36990800
N	7.31347400	-2.00039400	0.52023000	H	-9.76863800	2.12270300	3.12778200
C	7.39801300	-0.97923400	-0.36918100	C	3.77497700	5.23129100	-2.81180500
C	-6.96291900	1.74879300	-0.84599200	C	4.31074600	6.47642300	-2.09639100
C	-0.79619700	-1.12336900	-3.94986700	H	3.60256800	5.45042700	-3.87008300
C	1.60185000	4.04668800	-2.79655900	C	6.01873100	4.34218400	-3.14505700
H	-5.48013800	2.97422100	-1.37657700	C	5.75044600	6.75871000	-2.53022100

H	3.67343900	7.33060700	-2.36845600	H	1.19135300	-1.50234400	1.51206800
C	6.62312200	5.51756100	-2.36103700	C	-2.19110000	-1.42624300	1.22329800
H	6.03999700	4.56890200	-4.22161400	H	-3.06731100	-1.07694100	1.76274200
H	6.65637900	5.25231400	-1.29898300	C	0.72997100	2.60718600	-1.81968800
C	-2.67819700	-2.58691500	-4.63869000	C	-0.51978000	2.63493200	-2.46934900
C	-3.00705100	-4.05052700	-4.31586500	C	0.78537100	2.92226800	-0.45905200
H	-2.28117900	-2.51060800	-5.65678200	C	-1.70813400	2.87445400	-1.75041600
C	-4.93115900	-2.11814700	-5.34741000	C	-0.37456200	3.25489600	0.24521200
C	-4.22642700	-4.50984200	-5.11794900	H	1.73545500	2.87326500	0.06463700
H	-2.13789100	-4.66790900	-4.58770700	C	-1.61346800	3.20158000	-0.39515500
C	-5.38596900	-3.53183700	-4.95393000	H	-2.51548700	3.40605800	0.17482700
H	-4.63064100	-2.11114900	-6.40765900	C	-3.08393200	2.73764000	-2.40001000
H	-5.69242400	-3.51644500	-3.90276300	H	-3.59391300	3.70797000	-2.39255900
H	5.75934900	7.05098900	-3.59216300	H	-2.95223300	2.44191300	-3.44076100
H	-3.96024000	-4.55888800	-6.18567500	C	-3.71506900	-1.98856500	-0.70973100
C	6.71926900	3.00929400	-2.88966700	H	-3.64364200	-2.49623800	-1.67185200
H	6.31501600	2.24891000	-3.56992500	H	-4.41002300	-2.56749400	-0.09119100
H	7.79430600	3.09690900	-3.06436500	C	-4.98209700	2.14229000	-0.81930500
C	-5.99663300	-1.04924200	-5.12657800	C	-5.68051800	1.22131500	-0.03286500
H	-5.60056500	-0.08006800	-5.46207500	C	-3.94333300	1.72559100	-1.65743000
H	-6.88073600	-1.28104600	-5.72761400	C	-5.28589800	-0.12249800	-0.02116900
O	-3.82645700	-1.74107800	-4.51182500	C	-3.65492100	0.34974000	-1.73460000
O	-6.41832200	-0.99193800	-3.76842400	C	-4.26301100	-0.57419800	-0.86082500
H	-5.61110000	-0.85722300	-3.24361600	H	-5.75116600	-0.81513800	0.67452400
O	-6.44347300	-4.01957500	-5.78319700	H	-5.25332800	3.19398300	-0.77916500
H	-7.28793000	-3.75292800	-5.38823000	O	-1.32798800	-3.05922100	-1.95173200
O	-4.57565600	-5.80359400	-4.63489500	O	-2.67832200	-0.06999400	-2.60394800
H	-5.48677200	-5.96140700	-4.93990500	O	-0.58419100	2.37750400	-3.82457800
O	-3.26627100	-4.14754600	-2.91986800	O	0.81437500	-0.47077100	-2.74063300
H	-3.71719400	-5.00222500	-2.79635100	C	-0.44852800	3.55278100	-4.65228300
O	6.52974700	2.61757100	-1.52527700	H	0.49907300	4.05710300	-4.41645200
H	5.59132700	2.81283700	-1.34523700	H	-1.26554300	4.25274000	-4.42741900
O	7.92343400	5.86923100	-2.83798500	C	-0.48414400	3.12498500	-6.11128900
H	8.58381400	5.37923900	-2.32454000	H	-1.43377300	2.61179000	-6.30765000
O	6.22382500	7.82655600	-1.71664700	H	0.31485100	2.39307800	-6.28361300
H	7.19348800	7.81682400	-1.80557300	C	-0.32367400	4.31518500	-7.06312000
O	4.25270300	6.24002800	-0.69421000	H	-0.35376900	3.98372900	-8.10624900
H	4.81736500	6.92217000	-0.28841100	H	-1.12549100	5.04990300	-6.92291800
O	4.67224300	4.11709800	-2.69888600	H	0.63214000	4.82813800	-6.90290300

2D-EZ, electron energy = -6485.153642 a.u.

C	2.27287000	-1.39546300	-1.09115500	H	-3.97030400	-1.45286500	-3.49226700
C	1.91334800	-0.32587300	-1.93260500	H	-2.28470600	-1.44924800	-4.03413800
C	2.58456600	0.91292600	-1.87169200	C	-3.52062700	0.09846500	-4.92835500
C	3.73620100	1.00423800	-1.08503000	H	-2.67518300	0.75345600	-5.16757200
C	4.17233200	-0.08512400	-0.32467600	H	-4.35281000	0.74443300	-4.62012300
C	3.41611000	-1.26238700	-0.29576700	C	-3.92749600	-0.71597700	-6.16212700
H	4.29338800	1.93662000	-1.04928600	H	-4.78508700	-1.36486600	-5.94688900
H	3.71012500	-2.07366200	0.36440300	H	-4.20809100	-0.05631300	-6.98996400
C	1.36293100	-2.60750200	-0.95673900	H	-3.10454000	-1.35356000	-6.50717400
H	1.07771700	-2.98435700	-1.93895800	C	1.06384700	-0.57744200	-4.16259900
H	1.90964000	-3.40542400	-0.44087100	H	0.18713500	-0.13084200	-4.63805400
C	2.00163800	2.15487600	-2.53520300	H	1.93959500	0.02507300	-4.43139100
H	1.77156100	1.97948200	-3.58613400	C	1.26065200	-2.02086800	-4.61551900
H	2.74992800	2.95443900	-2.49773600	H	0.39527200	-2.61081900	-4.29243100
C	0.09547900	-2.26564400	-0.17366600	H	2.14259700	-2.44147300	-4.11538600
C	-1.18941600	-2.44594500	-0.72204900	C	1.43329300	-2.11591300	-6.13582800
C	0.20616000	-1.68922500	1.09560600	H	0.55439300	-1.72334500	-6.66152400
C	-2.33599900	-1.97117000	-0.05450200	H	2.30722400	-1.54662500	-6.47495800
C	-0.93172000	-1.31061000	1.81385200	H	1.57177600	-3.15629800	-6.44835600
				C	-1.49238900	-4.49168600	-1.87308500

H	-2.36395600	-4.72332300	-1.24492100	H	-10.24105800	-0.32018400	-1.74045700
H	-0.60737800	-4.93349700	-1.39400000	C	-10.74300800	-3.20039900	0.11085300
C	-1.67857700	-5.03947300	-3.27954200	H	-11.97760500	-1.63129900	-0.67475000
H	-0.80415500	-4.76900700	-3.88442100	H	-9.86055500	-3.77317600	-0.19321000
H	-2.54713300	-4.55045300	-3.73803200	H	-11.31218800	-1.92950400	1.77378100
C	-1.86788700	-6.56035200	-3.28221700	C	-10.00165500	-3.45182400	2.54926900
H	-1.99736900	-6.93239800	-4.30382500	H	-9.82735200	-2.87238600	3.46734300
H	-1.00035400	-7.07145800	-2.84807900	H	-10.80492400	-4.16753800	2.74693400
H	-2.75293800	-6.85382300	-2.70525300	O	-9.31349300	-1.61327900	1.24083600
N	-0.32531800	3.56426000	1.64011000	O	-8.75801600	-1.77463200	-1.63948000
N	-0.82867900	-0.72191400	3.11021300	H	-9.07986500	-2.33720500	-2.36677000
N	1.15698500	5.32236400	1.46403800	O	-11.21677300	-2.77631400	-2.23773300
N	0.42545300	-2.39783400	4.08221900	H	-11.73591200	-3.58440100	-2.07821100
N	-8.34447600	0.18925200	0.16193500	O	-11.89137900	-4.04737100	0.19938500
N	-6.72131600	1.69395100	0.82111000	H	-11.59833200	-4.92926200	0.47580800
N	5.34215900	0.05650000	0.48615400	O	-8.85006000	-4.20534100	2.18804700
N	6.50643300	-1.70069100	-0.44798700	H	-8.17503000	-3.55402200	1.93174100
C	6.48594500	-0.67585300	0.43781000	C	1.31972000	-2.98957000	5.03451000
C	-7.98549600	1.21613100	0.96847900	C	1.25985100	-4.51616300	4.89126100
C	0.38623700	4.54175800	2.25940800	H	1.01040400	-2.69861600	6.04429800
C	-0.17126600	-1.18833400	4.20492300	C	3.65583600	-3.02310200	5.61966500
H	-6.54720600	2.55301100	1.32787300	C	2.37380200	-5.17066000	5.71043600
H	-7.66292200	-0.18430100	-0.49149700	H	0.28320800	-4.85934500	5.26411900
H	-1.39125700	0.10071500	3.28862400	C	3.72551400	-4.54073500	5.39035700
H	0.37266200	-2.88298100	3.19185000	H	3.42751300	-2.82237900	6.67900600
H	-0.96265600	3.06812200	2.25053800	H	3.96121500	-4.71977800	4.33603600
H	1.07386000	5.22189000	0.45658700	C	1.89682900	6.47338000	1.89452700
H	5.39853400	0.86931500	1.08727400	C	3.07496000	6.69683000	0.93628600
H	5.73185500	-1.79697400	-1.09817300	H	2.27070300	6.29333800	2.90838000
S	-9.02959200	1.94525000	2.10327500	C	1.62435300	8.82976800	2.29152500
S	-0.17079000	-0.26729300	5.64011100	C	3.74692600	8.04118800	1.22355100
S	0.28746000	4.70998100	3.95376400	H	3.80320900	5.88643400	1.08947900
S	7.78052600	-0.28585300	1.47658100	C	2.71928800	9.16779500	1.26818100
C	7.64881700	-2.51454200	-0.74963400	H	2.07384300	8.74102800	3.29382100
C	7.17043800	-3.87990500	-1.26127900	H	2.25312400	9.26398900	0.28202500
H	8.23858800	-2.64741100	0.16382700	H	2.16655200	-5.02661200	6.78264200
C	9.60010700	-2.54104000	-2.15861300	H	4.25171700	7.99173000	2.20135900
C	8.35094800	-4.68368500	-1.81101300	C	4.93655700	-2.28789400	5.23851200
H	6.71973000	-4.42564600	-0.41889800	H	4.81365500	-1.21963500	5.46759500
C	9.15398300	-3.85831800	-2.81145300	H	5.77055100	-2.66926800	5.83477100
H	9.01551300	-4.96560100	-0.97888100	C	0.49729900	9.85578400	2.34168800
H	8.51606400	-3.62055000	-3.66927600	H	-0.22050800	9.55453100	3.11826200
O	8.43404900	-1.82377700	-1.72666700	H	0.90256300	10.83432600	2.61520700
O	6.20337900	-3.65635200	-2.28099000	O	1.00475100	7.59236400	1.90965600
H	6.12333000	-4.50320900	-2.75588800	O	-0.14122100	10.00609200	1.07906700
O	7.80692200	-5.84743200	-2.42628900	H	-0.41780400	9.11284500	0.81229500
H	8.51244800	-6.19857800	-2.99806000	O	3.43878000	10.35566100	1.60688200
O	10.25828000	-4.67370000	-3.21071000	H	2.98060600	11.11238100	1.20995900
H	10.50726100	-4.42715600	-4.11470900	O	4.69882500	8.25652400	0.18579000
H	10.25618500	-2.75988700	-1.30047500	H	4.91438100	9.20545900	0.21748300
C	10.32845100	-1.60238300	-3.11500700	O	2.57273300	6.66569500	-0.39501800
H	10.64062600	-0.70540200	-2.56092800	H	3.26821900	7.06757600	-0.94633300
H	11.22694700	-2.09393700	-3.49930300	O	5.27532900	-2.48663600	3.87080300
O	9.52529600	-1.26141600	-4.23872600	H	4.49614900	-2.20911700	3.35972500
H	8.69508800	-0.90881000	-3.87533200	O	4.67939000	-5.18177300	6.24055700
C	-9.54969200	-0.57999200	0.27883600	H	5.53851300	-5.17966800	5.79100400
C	-9.91612300	-1.15118200	-1.09672400	O	2.36565600	-6.55778000	5.38672000
H	-10.35434300	0.07150200	0.63631300	H	3.22813100	-6.90146000	5.68032000
C	-10.42816900	-2.49622600	1.43955000	O	1.40361600	-4.83647000	3.51217600
C	-11.05645400	-2.16249500	-0.96253700	H	1.61991400	-5.78592100	3.48487600

O	2.63144500	-2.47745400	4.77465300	H	4.40600900	5.34480500	4.57265300
				C	-1.94650000	4.40047100	0.90292300
2E-EZ, electron energy = -6485.162070 a.u.				H	-3.02249200	4.38980700	0.69230300
C	2.00058400	1.58175700	-2.86390000	H	-1.43566900	4.81415600	0.02963500
C	2.31186000	2.10571000	-1.59478500	C	-1.66720000	5.23689300	2.14788800
C	3.40614300	1.61631100	-0.85452400	H	-0.59134800	5.21143400	2.35446900
C	4.26662200	0.69315100	-1.45928200	H	-2.17296900	4.78425800	3.01055900
C	4.03644500	0.25112600	-2.76822800	C	-2.14122900	6.68411000	1.97105900
C	2.88974700	0.67533700	-3.44772200	H	-3.22175700	6.73095300	1.78912800
H	5.08656800	0.27685400	-0.88095100	H	-1.92834700	7.27660400	2.86710100
H	2.68681000	0.28973400	-4.44352300	H	-1.63879500	7.16688300	1.12411100
C	0.67552500	1.91188800	-3.53431800	C	1.94262500	4.37982800	-0.92700100
H	0.48253200	2.98385400	-3.49960800	H	1.43258000	4.79690200	-0.05497100
H	0.72685600	1.61459700	-4.58794500	H	3.01908900	4.37313300	-0.71854700
C	3.55050800	1.93496700	0.62802000	C	1.65854100	5.20844600	-2.17606100
H	3.47599700	3.00500300	0.81954500	H	0.58266700	5.17679800	-2.38134800
H	4.54475300	1.61532200	0.96066400	H	2.16566700	4.75370700	-3.03683400
C	-0.47466600	1.18086900	-2.84526600	C	2.12618700	6.65867900	-2.00712200
C	-1.53433400	1.87953900	-2.23322000	H	1.62223100	7.14353600	-1.16226600
C	-0.45836600	-0.21505900	-2.76943300	H	3.20664100	6.71144600	-1.82629900
C	-2.48688700	1.20161800	-1.44935100	H	1.90994400	7.24559800	-2.90603500
C	-1.44086200	-0.90705100	-2.05810900	C	-2.41876000	3.67184800	-3.49945300
H	0.33650400	-0.77050300	-3.25968400	H	-3.41106500	3.20321000	-3.43972000
C	-2.41704600	-0.18994400	-1.36108300	H	-1.94207800	3.32815200	-4.42841100
H	-3.11554800	-0.71439200	-0.71789600	C	-2.53727800	5.18798200	-3.47718800
C	2.48659300	1.20768900	1.44681400	H	-1.53194600	5.62539100	-3.51761600
C	1.53634500	1.89580500	2.22446300	H	-2.97945200	5.49349400	-2.52068200
C	2.41275800	-0.18440400	1.37187700	C	-3.38404500	5.71340500	-4.64161000
C	0.47494700	1.20605500	2.84356800	H	-3.45636000	6.80537800	-4.60626900
C	1.43525500	-0.89212500	2.07665200	H	-2.94668400	5.43872800	-5.60887000
H	3.10928500	-0.71675000	0.73305300	H	-4.40295700	5.30961700	-4.60795900
C	0.45496400	-0.19054200	2.78164700	N	1.36872100	-2.31514700	2.02191500
H	-0.34120500	-0.73900900	3.27761400	N	-1.37754200	-2.32965500	-1.98896200
C	-0.67333200	1.94741900	3.52495000	N	3.60675700	-2.71943900	2.40067800
H	-0.72583000	1.66085600	4.58148300	N	-3.61523900	-2.73219600	-2.37051800
H	-0.47734800	3.01841200	3.47939900	N	-6.92051900	0.29160100	2.95971200
C	-3.54839100	1.94023000	-0.63739600	N	-4.86935700	-0.68216800	3.40715500
H	-3.47024000	3.00815400	-0.83899400	N	4.87554400	-0.71216200	-3.39995900
H	-4.54378700	1.62093500	-0.96690300	N	6.92334700	0.27224400	-2.96014900
C	-2.88676800	0.70990700	3.44664300	C	6.23020900	-0.74097800	-3.52666500
C	-4.03285200	0.27971300	2.76994800	C	-6.22402200	-0.71607900	3.53192600
C	-1.99883300	1.61391400	2.85714800	C	2.38311600	-3.21854900	2.10736900
C	-4.26377500	0.71360000	1.45846200	C	-2.39348700	-3.23165600	-2.06986000
C	-2.31094700	2.13001700	1.58495200	H	-4.40063200	-1.38528900	3.96505300
C	-3.40447700	1.63405200	0.84784400	H	-6.42122400	1.01962400	2.45904900
H	-5.08305200	0.29253900	0.88266100	H	-0.46078300	-2.74860300	-1.89483100
H	-2.68301600	0.33052800	4.44467400	H	-3.69092100	-1.75823800	-2.64750900
O	-1.62308700	3.25107700	-2.37030900	H	0.45084000	-2.73312400	1.93466000
O	-1.45624900	3.04369700	1.01642900	H	3.68585400	-1.74305500	2.66795400
O	1.62855800	3.26839900	2.34805800	H	4.40890900	-1.41964300	-3.95409600
O	1.45555800	3.02107500	-1.03186600	H	6.42178100	1.00004000	-2.46142800
C	2.42324100	3.69843600	3.47433800	S	-6.94314800	-1.99125900	4.40913300
H	3.41518100	3.22838100	3.41997800	S	-2.08257300	-4.88347900	-1.79226000
H	1.94514400	3.36350900	4.40577400	S	2.06794900	-4.87205300	1.84514400
C	2.54294200	5.21421300	3.43859700	S	6.95356800	-2.01700300	-4.39903100
H	1.53774900	5.65251600	3.47265600	C	8.35515500	0.38579800	-2.92851300
H	2.98751100	5.51077100	2.48039600	C	8.72926300	1.87237500	-2.83965400
C	3.38732500	5.74963700	4.60018400	H	8.76469100	-0.04178800	-3.85105100
H	3.46056200	6.84118800	4.55506500	C	10.27144100	-0.30714200	-1.69398600
H	2.94745700	5.48411500	5.56886300	C	10.22954000	2.02947100	-2.57810100

H	8.47483500	2.35123500	-3.79726100	H	-5.27974100	-5.86612000	-5.52848100
C	10.67323400	1.14905600	-1.41488400	H	-7.04194000	-5.72982300	-5.69570900
H	10.78685300	1.72474000	-3.47803900	C	6.14877100	-5.14397100	5.47390900
H	10.15934900	1.47326900	-0.50407600	H	5.29640700	-5.83223700	5.56684900
O	8.84216800	-0.35781200	-1.80856900	H	7.06044600	-5.69806700	5.71548900
O	7.97685100	2.45488200	-1.78150000	O	4.99548600	-3.92922200	3.81048200
H	8.42608300	3.29477200	-1.57543100	O	6.05225200	-4.07263200	6.40487000
O	10.45779100	3.40811000	-2.29915500	H	5.28286100	-3.54597900	6.12873700
H	11.32545200	3.44766700	-1.85909700	O	8.66711000	-4.33350700	3.91569600
O	12.08570200	1.32814500	-1.28950300	H	8.94641100	-4.25326100	4.84087600
H	12.32801600	1.14862600	-0.36755100	O	8.34056700	-2.19242700	2.11861300
H	10.73496400	-0.64182100	-2.63769600	H	9.14744700	-2.52681200	2.55061500
C	10.69986500	-1.27455600	-0.59442300	O	5.84658600	-1.31089600	2.77288300
H	10.30291300	-2.27231800	-0.82535600	H	6.69367400	-0.84108200	2.67654700
H	11.79322900	-1.33858900	-0.60735900	O	-6.02379600	-4.11157700	-6.38739600
O	10.32159900	-0.85079700	0.70696700	H	-5.25604300	-3.58433600	-6.10789900
H	9.39702900	-1.12095900	0.85751500	O	-8.66382500	-4.34671200	-3.92324200
C	-8.35277300	0.39883500	2.92553800	H	-8.93361400	-4.27096100	-4.85164500
C	-8.73336400	1.88348000	2.83232100	O	-8.35062300	-2.19763700	-2.13483000
H	-8.76166200	-0.02801900	3.84871300	H	-9.15363400	-2.53358800	-2.57285600
C	-10.26435100	-0.30628500	1.69137100	O	-5.84922100	-1.32356200	-2.77094300
C	-10.23400000	2.03307000	2.56833000	H	-6.69626000	-0.85164700	-2.68510700
H	-8.48247100	2.36592600	3.78908000	O	-4.99252100	-3.95072000	-3.78365000
C	-10.67204700	1.14719700	1.40719800				
H	-10.79108000	1.72854900	3.46847600	2F-EZ, electron energy = -6485.154925 a.u.			
H	-10.15787000	1.47057600	0.49626700	C	-3.52804900	-1.21290700	-0.00986800
H	-10.72655600	-0.63975600	2.63617800	C	-2.57851600	-1.87836700	0.78703800
C	-10.68968200	-1.27901700	0.59510800	C	-2.50273500	-1.65226200	2.17668100
H	-10.28343000	-2.27300900	0.82581100	C	-3.50666900	-0.89132000	2.78151900
H	-11.78248700	-1.35214500	0.61415200	C	-4.52393100	-0.30898400	2.01766900
O	-8.83489600	-0.35000200	1.80694000	C	-4.50248800	-0.43374000	0.62310700
O	-7.98207400	2.46671600	1.77380000	H	-3.48943200	-0.73418900	3.85674600
H	-8.43516600	3.30375400	1.56458300	H	-5.23240600	0.10090400	0.02226100
O	-10.46809100	3.40983700	2.28493600	C	-3.41352300	-1.23382400	-1.52692200
H	-11.33502800	3.44408500	1.84300400	H	-3.28280800	-2.25321100	-1.88989500
O	-12.08497100	1.32001000	1.27857900	H	-4.34424700	-0.84617400	-1.95738900
H	-12.32481100	1.13373300	0.35729500	C	-1.28991900	-2.11220900	2.97607500
O	-10.32133200	-0.85417500	-0.70871400	H	-1.09227900	-3.17430600	2.82788100
H	-9.40104800	-1.13216000	-0.87107200	H	-1.49807700	-1.96914200	4.04241800
C	-4.84204400	-3.46972100	-2.44566100	C	-2.23832300	-0.38185000	-2.00388300
C	-5.99458100	-2.53564400	-2.03852600	C	-1.19286800	-0.91501500	-2.78295900
H	-4.78808700	-4.31918300	-1.75592600	C	-2.15311600	0.95124100	-1.59230100
C	-6.21574100	-4.66537500	-4.01461400	C	-0.03715500	-0.15725700	-3.06068400
C	-7.34297200	-3.19055900	-2.33909200	C	-1.05843100	1.74359400	-1.94599000
H	-5.91545300	-2.34192900	-0.95864400	H	-2.93046300	1.36309400	-0.95560000
C	-7.39414000	-3.70925000	-3.77203400	C	0.00433900	1.17822300	-2.65122900
H	-6.29267200	-5.52682900	-3.33194900	H	0.87904200	1.78335900	-2.87359700
H	-7.29877400	-2.86344100	-4.46065000	C	-0.04487400	-1.31695700	2.58861600
C	4.83354200	-3.45755300	2.47053100	C	1.08642200	-1.94076700	2.02417600
C	5.98338700	-2.52769400	2.04663300	C	-0.03772500	0.07206400	2.74930800
H	4.77272400	-4.31183200	1.78733400	C	2.15628900	-1.17925000	1.51611100
C	6.21949000	-4.64468300	4.03463200	C	1.05237400	0.83263500	2.32425200
C	7.33365200	-3.18277500	2.33828800	H	-0.89180900	0.56743000	3.20280000
H	5.89427900	-2.34058800	0.96636900	C	2.11966800	0.20765600	1.67377800
C	7.39773700	-3.69327600	3.77355500	H	2.91714800	0.81231500	1.25318900
H	6.28765200	-5.51146800	3.35774400	C	3.30514600	-1.80647200	0.72847500
H	7.31201300	-2.84294900	4.45793700	H	4.24675900	-1.65912200	1.27032400
H	-7.49994700	-4.03497500	-1.65155700	H	3.13622300	-2.88025000	0.64978500
H	7.48295000	-4.03118500	1.65402000	C	1.18665500	-0.76655700	-3.74086200
C	-6.13166600	-5.17558700	-5.44928600	H	0.96357600	-1.79493100	-4.02719000

H	1.40426100	-0.21634500	-4.66313100	N	-7.36617600	-0.50689600	1.74429700
C	4.42332900	-0.23862300	-0.92943900	C	-6.86042700	0.42364800	2.58828600
C	4.46226600	0.42301800	-2.16358900	C	6.80671500	1.35422900	-2.32629600
C	3.42577400	-1.18199900	-0.65432500	C	2.00430300	3.05931100	2.96481700
C	3.43371500	0.21394200	-3.09033000	C	-1.86537500	4.10536200	-1.69047800
C	2.46282900	-1.45120400	-1.64357400	H	5.14152100	2.18601100	-3.02637900
C	2.40418900	-0.69188100	-2.82893200	H	6.71798000	-0.53870400	-1.55091700
H	3.42853600	0.77994400	-4.01843100	H	-0.09128100	3.39783600	-1.09836500
H	5.15273500	-0.00436100	-0.16047100	H	-3.06134100	2.86979700	-2.80087600
O	-1.27762100	-2.21731200	-3.23439800	H	0.18804800	2.74092700	2.17934300
O	1.50469900	-2.40374800	-1.39868700	H	3.05647500	1.42429500	3.60044100
O	1.11929600	-3.31687400	1.91705000	H	-5.17591400	1.11413500	3.40475200
O	-1.64763400	-2.67868500	0.17228300	H	-6.73395100	-1.18466200	1.32882700
C	1.72845100	-3.97782500	3.04698800	S	7.73841900	2.67867000	-2.86137800
H	1.19720500	-3.69146500	3.96545900	S	-1.55798000	5.64145000	-1.01748600
H	2.77114800	-3.64428100	3.14533500	S	1.84401600	4.75249200	2.85543900
C	1.65816800	-5.48111600	2.82722000	S	-7.81298300	1.50615400	3.49776600
H	2.17044600	-5.72642700	1.88850400	C	-8.75989400	-0.78624400	1.54797400
H	0.60778600	-5.77234400	2.70262700	C	-8.96244000	-1.34456300	0.13267000
C	2.28705200	-6.25995200	3.98769600	H	-9.32573100	0.14461800	1.66434400
H	2.22504500	-7.33844400	3.80914300	C	-10.54773400	-2.11227900	2.45240400
H	3.34534000	-6.00235900	4.11403500	C	-10.39178200	-1.86513900	-0.03372100
H	1.77554300	-6.04799100	4.93413300	H	-8.78529500	-0.53195600	-0.58771200
C	1.62076800	-3.63258000	-2.15506100	C	-10.76300400	-2.81335400	1.10226100
H	1.98694500	-3.41098500	-3.16483200	H	-11.09034100	-1.01341100	-0.01889800
H	0.59900300	-4.00872100	-2.24189200	H	-10.10960400	-3.69111700	1.06098400
C	2.52870700	-4.65962300	-1.48499100	O	-9.17022000	-1.72055100	2.55060300
H	2.16571900	-4.84093100	-0.46683700	O	-8.02316000	-2.39516000	-0.06478300
H	3.54177200	-4.24645000	-1.39774000	H	-8.34048500	-2.88784100	-0.84296000
C	2.57244500	-5.97273900	-2.27547000	O	-10.44632400	-2.52739800	-1.29354800
H	2.95341900	-5.81484000	-3.29172300	H	-11.24928600	-3.07747800	-1.26830400
H	3.22527400	-6.70220100	-1.78461400	O	-12.12613800	-3.18629500	0.88638700
H	1.57461600	-6.42034200	-2.35875300	H	-12.25867300	-4.07662300	1.24707000
C	-1.81500700	-4.10597700	0.34917900	H	-11.20292800	-1.22816200	2.51625800
H	-0.80466900	-4.51939200	0.29919100	C	-10.80970500	-3.00933400	3.65726200
H	-2.21455700	-4.30952600	1.34993600	H	-10.64914100	-2.42395000	4.57402400
C	-2.71617500	-4.72828600	-0.71345300	H	-11.85069100	-3.34493100	3.64689600
H	-2.32112400	-4.47041000	-1.70299000	O	-9.99542400	-4.17598500	3.63991000
H	-3.71945000	-4.28853800	-0.64212000	H	-9.07700100	-3.86128300	3.58906300
C	-2.80654400	-6.25032200	-0.55520300	C	8.71626200	0.01466200	-1.48503900
H	-1.81951500	-6.71975800	-0.64700400	C	8.85785300	-0.82507000	-0.20814500
H	-3.21752600	-6.52647500	0.42345400	H	9.22071300	0.97735400	-1.35093400
H	-3.45532900	-6.68460100	-1.32315000	C	10.64177500	-0.99991800	-2.50312400
C	-1.87044500	-2.34677300	-4.54436200	C	10.29966000	-1.31100200	-0.04517500
H	-1.30045100	-1.74235100	-5.26384500	H	8.58432000	-0.18921200	0.64670700
H	-2.89761100	-1.95664800	-4.51767400	C	10.79711200	-1.97487900	-1.32579000
C	-1.85587400	-3.81514900	-4.94014100	H	10.95009500	-0.44967800	0.17485400
H	-2.41540900	-4.39015600	-4.19174800	H	10.18705500	-2.86131300	-1.52831800
H	-0.82065500	-4.17759400	-4.91212100	H	11.24733900	-0.09851600	-2.31494100
C	-2.45601500	-4.03987500	-6.33220500	C	11.04381300	-1.59391900	-3.84833200
H	-2.43807400	-5.10264900	-6.59499100	H	10.91772100	-0.82571900	-4.62482700
H	-3.49838300	-3.70227400	-6.37698400	H	12.09900600	-1.88088100	-3.82242000
H	-1.89458900	-3.49585800	-7.10107000	O	9.25457200	-0.65247400	-2.62948700
N	1.02769400	2.25390800	2.46746100	O	7.96968300	-1.93332900	-0.30694100
N	-0.96534700	3.10214200	-1.51505300	H	8.26597000	-2.56689900	0.37117200
N	3.05346200	2.43853200	3.55791500	O	10.30643300	-2.22777500	1.04488300
N	-2.95758000	3.81202400	-2.43675200	H	11.13833700	-2.72725700	0.96451000
N	7.32301700	0.25711100	-1.72813400	O	12.15907700	-2.33898300	-1.08955600
N	5.45513000	1.39293400	-2.48065500	H	12.36147600	-3.12149600	-1.62520300
N	-5.50463200	0.49118300	2.67726500	O	10.30058600	-2.76750800	-4.15657100

H	9.36402000	-2.50981300	-4.11691200	H	2.11116300	-2.37561100	1.69076000
C	-4.12438900	4.63495900	-2.57282000	C	0.00073200	3.51203800	1.11856800
C	-4.80194500	4.31876600	-3.91198500	C	-1.35089800	3.58891800	1.50900100
H	-3.82286200	5.68795600	-2.55051500	C	0.29784800	3.42288200	-0.24518300
C	-6.22405900	5.08943600	-1.48758700	C	-2.38767200	3.48702600	0.56008000
C	-6.16653300	5.00595100	-3.99105800	C	-0.72022200	3.42781000	-1.20465500
H	-4.15784900	4.69327700	-4.72153100	H	1.33104500	3.31497100	-0.55895200
C	-7.00324200	4.69805700	-2.75283100	C	-2.05411900	3.43313000	-0.79480400
H	-6.03155600	6.17456800	-1.49650400	H	-2.84214400	3.37781000	-1.54095900
H	-7.20302200	3.62216100	-2.71683700	C	0.25093500	-1.61734700	0.91437800
C	4.29582300	3.04757100	3.93303400	C	-1.09149600	-1.79224100	1.30046800
C	4.87627300	2.30215200	5.14216500	C	0.53999200	-1.40884700	-0.43532600
H	4.11675300	4.09545600	4.19647700	C	-2.13497400	-1.66778500	0.36118100
C	6.48296400	3.50173700	3.02417900	C	-0.47500300	-1.40428600	-1.39648000
C	6.30943400	2.76529600	5.41402500	H	1.56664200	-1.22184300	-0.73161000
H	4.24747500	2.52506300	6.01707800	C	-1.80717900	-1.50015000	-0.98758800
C	7.15165000	2.68974900	4.14438700	H	-2.59934400	-1.43346000	-1.72861100
H	6.42878200	4.56188300	3.31982500	C	-3.60192400	-1.67292300	0.78753300
H	7.21343000	1.64482500	3.82326900	H	-4.11816000	-2.52269300	0.32609200
H	-6.02053200	6.09616700	-4.05074000	H	-3.65243600	-1.80431500	1.86851800
H	6.29438100	3.80945800	5.76443800	C	-3.85350700	3.37454700	0.97355100
C	-6.94193400	4.72198500	-0.19294100	H	-3.92400400	3.47105500	2.05717100
H	-6.33661400	5.06617900	0.65783600	H	-4.42617600	4.20073500	0.53741600
H	-7.90847800	5.23227200	-0.15081300	C	-5.17823900	-0.37224500	-0.72025100
C	7.20428200	3.39071100	1.68494500	C	-5.73972800	0.82935200	-1.16846500
H	6.68148800	4.01496000	0.94680000	C	-4.30622600	-0.38898500	0.37405300
H	8.22762500	3.76368300	1.78312000	C	-5.34196700	2.03904900	-0.58847700
O	5.16536600	2.97843400	2.79640600	C	-4.01105400	0.82799300	1.01577000
O	7.29172100	2.03815900	1.24364000	C	-4.44667000	2.05896300	0.48355200
H	6.37988600	1.70195800	1.23662200	H	-5.72472700	2.97446900	-0.98835100
O	8.44584900	3.19165200	4.48617000	H	-5.40385700	-1.30075000	-1.23644300
H	9.10111700	2.75150500	3.92310200	O	-1.66837400	3.72584500	2.84602200
O	6.83368900	1.91132300	6.42627600	O	-3.19047000	0.81295400	2.11618500
H	7.80000400	2.02613000	6.39361400	O	-1.38855300	-2.05017500	2.62485500
O	4.85235400	0.90821300	4.85722200	O	0.24589100	0.85885200	2.92134300
H	5.45709000	0.49901700	5.50231700	C	-1.43749900	-3.45696400	2.94630800
O	-7.20285300	3.32529600	-0.11020600	H	-0.48111400	-3.92591200	2.67545100
H	-6.34280200	2.88664400	-0.22408000	H	-2.22637500	-3.93889800	2.35166700
O	-8.22036500	5.43484300	-2.89468000	C	-1.70980000	-3.60929900	4.43492500
H	-8.92678100	4.94444200	-2.44688900	H	-2.65667800	-3.11052800	4.67619400
O	-6.80245300	4.52633000	-5.17175400	H	-0.92313100	-3.08741900	4.99399100
H	-7.74564700	4.74599900	-5.07129300	C	-1.77008700	-5.08083400	4.85907200
O	-4.94982500	2.90674900	-4.01018600	H	-1.97171900	-5.16684300	5.93186000
H	-5.59726000	2.76027000	-4.72321300	H	-2.56385800	-5.61747200	4.32589400
O	-4.98608500	4.36266500	-1.46251900	H	-0.82314900	-5.59465300	4.65504600
2G-EZ, electron energy = -6485.164024 a.u.				C	-3.81802700	1.10013800	3.38856500
C	1.98395500	2.20411100	1.97146600	H	-4.60906300	1.84704600	3.25151300
C	1.46594400	0.93657300	2.29490400	H	-3.03040800	1.55097500	3.99726600
C	2.11916200	-0.24145300	1.88419400	C	-4.38682900	-0.14674000	4.05882600
C	3.38342500	-0.13701800	1.29386100	H	-3.58833700	-0.89187200	4.14921100
C	3.98743000	1.11495100	1.10626900	H	-5.16290000	-0.58133800	3.41560200
C	3.26352400	2.27535200	1.41152900	C	-4.97693600	0.17335400	5.43713500
H	3.87544500	-1.03710600	0.93654200	H	-5.79120400	0.90435900	5.36284200
H	3.71008400	3.24773000	1.22104000	H	-5.38126300	-0.72908900	5.90765500
C	1.13175200	3.45262500	2.14660300	H	-4.21617500	0.58827300	6.10938000
H	0.69482000	3.48332700	3.14481000	C	0.26344800	0.43995000	4.30618000
H	1.77196500	4.33582100	2.03779900	H	-0.70454600	-0.04068600	4.46756700
C	1.39405800	-1.58092400	1.92621600	H	1.04513100	-0.31471700	4.45502600
H	0.99518400	-1.79121700	2.91876900	C	0.46836400	1.60075900	5.27470400
				H	-0.30794700	2.35278300	5.09328100

H	1.43508900	2.07856400	5.06956000	H	6.60294900	-4.77146800	0.05914100
C	0.42278300	1.13168000	6.73365000	C	-9.31486400	-1.52606100	-1.46955200
H	-0.54210600	0.66859900	6.97330200	C	-9.02488700	-2.83897100	-0.72884400
H	1.20768700	0.39420700	6.94084700	H	-9.62129300	-1.74009700	-2.49904000
H	0.56758600	1.97376200	7.41862100	C	-11.58341700	-1.44442100	-0.66791000
C	-1.81121000	5.09770200	3.27320200	C	-10.32541100	-3.59928400	-0.46189300
H	-2.58148000	5.59026200	2.66325200	H	-8.36786000	-3.45319700	-1.36257600
H	-0.86347000	5.62946700	3.10880000	C	-11.35929800	-2.69313100	0.19894300
C	-2.19536500	5.11331800	4.74469900	H	-10.73750100	-3.95864500	-1.41815500
H	-1.41902700	4.59360900	5.31983800	H	-10.97955000	-2.37275900	1.17479800
H	-3.12359900	4.54303200	4.87435900	H	-11.97684600	-1.74600000	-1.65202100
C	-2.37407700	6.54039300	5.27423600	C	-12.53401700	-0.42989800	-0.04095900
H	-2.64612600	6.52922000	6.33474800	H	-12.65704000	0.41457000	-0.73429500
H	-1.45002600	7.12173700	5.17205400	H	-13.51455000	-0.89007900	0.11133800
H	-3.16538200	7.07111800	4.73159100	O	-10.33146000	-0.75752300	-0.81880400
N	-0.18383200	-1.22385000	-2.78029200	O	-8.37374500	-2.52022200	0.49591000
N	-0.43740900	3.32335300	-2.59995600	H	-8.44599400	-3.32029600	1.04709100
N	1.54982900	-2.73860700	-2.90702100	O	-9.99588900	-4.69997000	0.37999100
N	1.10555600	5.03500800	-2.73223100	H	-10.83930400	-5.00204000	0.76146600
N	-8.11841300	-0.73439600	-1.50111800	O	-12.54541800	-3.47684600	0.34918900
N	-6.64204500	0.86554100	-2.27302200	H	-13.02501300	-3.15611600	1.12847300
N	5.27153300	1.26157100	0.50924000	O	-12.07591800	0.00967300	1.23236900
N	6.38924600	-0.34695600	1.74779400	H	-11.16766100	0.32792100	1.09317500
C	6.42172200	0.58848800	0.76874900	C	2.34618400	5.60869600	-3.16473500
C	-7.78935100	0.16009000	-2.46261600	C	2.49139700	7.01118700	-2.56389900
C	0.81137100	-1.78433600	-3.52085600	H	2.35959700	5.66526400	-4.25763700
C	0.47490100	3.99951700	-3.34422600	C	4.73444900	5.16637100	-2.93585300
H	-6.49906600	1.59758100	-2.95772800	C	3.91567500	7.53057600	-2.76783300
H	-7.57557800	-0.75282200	-0.64284200	H	1.78262200	7.67930600	-3.07484500
H	-1.01094400	2.68272200	-3.13497300	C	4.93991600	6.52482700	-2.24737400
H	0.87592600	5.23328000	-1.76290800	H	4.94835800	5.26531100	-4.01065600
H	-0.80227200	-0.62184200	-3.30918800	H	4.79498900	6.40008600	-1.16898400
H	1.25140800	-3.07859100	-1.99795300	C	2.72490000	-3.37458500	-3.42704000
H	5.38597300	2.07202600	-0.10766000	C	3.65138700	-3.71288500	-2.24669600
H	5.52111200	-0.51142800	2.24661800	H	3.22921500	-2.68295500	-4.11118600
S	-8.71035200	0.42672500	-3.87348700	C	3.42154600	-5.30729200	-4.67329100
S	0.72973700	3.56335500	-4.97092300	C	4.80285600	-4.60453600	-2.71117100
S	1.06419900	-1.27379100	-5.12613000	H	4.05797100	-2.77240500	-1.84636100
S	7.83464600	0.97232400	-0.11451900	C	4.28582100	-5.80108800	-3.50220200
C	7.47212600	-1.21696400	2.10952900	H	4.03344100	-4.68391400	-5.34506000
C	7.32185100	-1.60404600	3.58797800	H	3.66043600	-6.41799300	-2.84864500
H	8.41934200	-0.68525000	1.96333200	H	4.09449900	7.68849000	-3.84325700
C	8.48720700	-3.29579400	1.53405500	H	5.47819200	-4.02138500	-3.35483200
C	8.31819800	-2.70716100	3.95579400	C	5.58460100	4.04263200	-2.34643600
H	7.52404900	-0.71275300	4.20105200	H	5.48663800	3.14567600	-2.97100100
C	8.25905700	-3.85004300	2.94835500	H	6.63834000	4.32946900	-2.31188800
H	9.33784200	-2.29078000	3.95016600	C	2.79016100	-6.43514700	-5.48219600
H	7.26230500	-4.30206300	2.97814000	H	2.21697500	-5.99704800	-6.31185500
O	7.43739800	-2.36042000	1.25060400	H	3.57685100	-7.06467300	-5.90780700
O	5.98707100	-2.05249500	3.79472500	O	2.32601100	-4.54613500	-4.14300200
H	6.00378600	-2.53652900	4.64031400	O	1.97277900	-7.27582400	-4.67656600
O	7.97480600	-3.15357100	5.26489100	H	1.32549200	-6.68996600	-4.24851400
H	8.40451100	-4.02104500	5.36899600	O	5.43961100	-6.52546700	-3.93311600
O	9.25477500	-4.79400100	3.34946600	H	5.20215100	-7.46296500	-4.00376500
H	8.98280700	-5.66797600	3.02843800	O	5.49722700	-5.04393800	-1.54230500
H	9.46516500	-2.78627000	1.49258700	H	6.03943800	-5.80506000	-1.81801200
C	8.47422800	-4.37273100	0.45349900	O	2.86974100	-4.37517100	-1.25826100
H	8.56111100	-3.89087800	-0.52963200	H	3.50279700	-4.78869600	-0.64524000
H	9.35631700	-5.00627600	0.59488300	O	5.16254400	3.77040400	-1.00472100
O	7.33601700	-5.21995100	0.51862400	H	4.18835800	3.78930400	-1.04931400

O	6.22751600	7.07786700	-2.52699400	C	0.90150200	-5.21490400	3.22076600
H	6.84227000	6.79718300	-1.83191800	H	-0.12947900	-5.19419300	3.59531100
O	4.00992400	8.76270700	-2.06146000	H	1.50821900	-4.63143400	3.92454200
H	4.96253000	8.94284600	-1.97017300	C	1.40815300	-6.66019700	3.16045700
O	2.18738200	6.93222500	-1.17587900	H	1.36370000	-7.12789600	4.14950400
H	2.52047100	7.76025700	-0.78568200	H	0.80301600	-7.26725500	2.47659900
O	3.38534400	4.72287000	-2.72384900	H	2.44831100	-6.70448300	2.81642700
2H-EZ, electron energy = -6485.157812 a.u.							
C	2.22521000	1.97165300	2.74644300	C	-2.69031600	-1.41504100	3.70974000
C	2.18303700	0.56705200	2.66838500	H	-3.67594200	-0.95249600	3.84022300
C	3.11222000	-0.14529000	1.88537700	H	-2.00366000	-0.95346100	4.42337600
C	4.17870800	0.55259800	1.30753900	C	-2.78480300	-2.92074900	3.93548900
C	4.31055900	1.93538100	1.49073400	H	-1.79550900	-3.36237600	3.77096200
C	3.31463300	2.63754800	2.17839600	H	-3.46236200	-3.35743400	3.19039800
H	4.87312600	0.01905200	0.66454200	C	-3.28682000	-3.24854700	5.34652900
H	3.38839100	3.71854300	2.26641400	H	-4.28534500	-2.83030600	5.52269000
C	1.05555000	2.74798800	3.33108900	H	-3.34803300	-4.33154700	5.49696600
H	0.74320100	2.31880100	4.28283500	H	-2.61504200	-2.84244400	6.11249300
H	1.37133400	3.78090100	3.51794100	C	1.46355900	-0.87817400	4.44188400
C	2.85887500	-1.60104000	1.51694700	H	0.74422500	-1.70139100	4.44296800
H	2.64148500	-2.20797300	2.39578100	H	2.46818000	-1.30554100	4.33813800
H	3.76533200	-2.01057900	1.05674400	C	1.36915100	-0.06521500	5.72928900
C	-0.13298500	2.73646600	2.37043800	H	0.36784500	0.37650500	5.79263100
C	-1.38872100	2.22148400	2.74915000	H	2.08554200	0.76534400	5.68601600
C	0.03136300	3.19956200	1.06247700	C	1.65081800	-0.92743700	6.96513400
C	-2.42180000	2.06156900	1.80545100	H	0.93776000	-1.75713900	7.04337100
C	-1.00834100	3.11703000	0.13446700	H	2.65958300	-1.35645200	6.93099600
H	0.98557700	3.61825500	0.75507000	H	1.57245600	-0.33297900	7.88148400
C	-2.21378500	2.51092700	0.49838600	C	-2.11082800	2.86978100	4.90897800
H	-2.98552500	2.35349000	-0.24900200	H	-3.03830600	3.27088200	4.47676100
C	1.69519600	-1.71484900	0.53384700	H	-1.38142400	3.69061500	4.95710500
C	0.53124000	-2.44813200	0.83064100	C	-2.36579800	2.28726500	6.29051400
C	1.75895900	-1.01363300	-0.67184400	H	-1.42716400	1.87382000	6.68000000
C	-0.58636100	-2.40786200	-0.02689600	H	-3.06824200	1.44971600	6.19665600
C	0.70152400	-1.05555400	-1.58468100	C	-2.92102600	3.33512500	7.26124700
H	2.63102900	-0.40411000	-0.88272000	H	-3.09568200	2.89487800	8.24842900
C	-0.47425100	-1.72766100	-1.24300500	H	-2.22342700	4.17166700	7.38699600
H	-1.31758400	-1.70829800	-1.92820300	H	-3.87369300	3.74416800	6.90432000
C	-1.92054600	-3.04040000	0.36417600	N	0.76197700	-0.35224800	-2.82306200
H	-2.18293900	-3.82525100	-0.35444500	N	-0.78048600	3.57682300	-1.19822400
H	-1.81273500	-3.51059800	1.34166300	N	2.87784200	-1.02870200	-3.44313400
C	-3.72261700	1.33937400	2.14908300	N	-2.66082600	4.90498400	-1.36419500
H	-3.71185000	1.07816800	3.20748500	N	-6.80289100	-2.94346600	-1.41121300
H	-4.56959800	2.01699600	1.99306000	N	-5.89135100	-0.84907100	-1.74128900
C	-3.98017600	-1.94924700	-0.64378600	N	5.37094200	2.68151900	0.90120000
C	-4.92438200	-0.91716500	-0.69241700	N	7.14340100	1.32772900	1.52213300
C	-3.03468900	-2.00397500	0.38585000	C	6.71206600	2.44785000	0.90023400
C	-4.86531700	0.12321600	0.24033200	C	-6.80565100	-1.78379900	-2.11166600
C	-3.06308100	-1.00483000	1.37721100	C	1.79654600	-0.25618900	-3.70204800
C	-3.91535800	0.11302600	1.26527300	C	-1.53231400	4.43009500	-1.94283400
H	-5.55776100	0.95655500	0.15461800	H	-5.99577300	0.03783800	-2.21845600
H	-3.96711900	-2.70414200	-1.42460100	H	-6.22153700	-3.00994000	-0.58074600
O	-1.59863500	1.82435700	4.05482800	H	0.10269200	3.32952500	-1.62698000
O	-2.15797800	-1.07492300	2.40738600	H	-2.82971400	4.70202700	-0.38339200
O	0.47214500	-3.18225600	1.99929500	H	-0.07648900	0.13097200	-3.12034500
O	1.14038400	-0.09731900	3.26740000	H	2.81538500	-1.73007700	-2.71148000
C	0.94540300	-4.53908000	1.85903700	H	5.12767300	3.59661700	0.54242500
H	1.97039300	-4.52754800	1.46268600	H	6.46731200	0.70575400	1.95341400
H	0.31268300	-5.07191700	1.13518300	S	-7.85922300	-1.45758200	-3.41259200
				S	-1.03143600	4.82722300	-3.52421300
				S	1.67746800	0.79688800	-5.03596400

S	7.74759700	3.57801300	0.15030500	C	6.31519100	-2.63761200	-5.12220800
C	8.50584100	0.87400200	1.56948200	H	5.49439200	-1.12129000	-6.44062500
C	8.69585900	0.02257300	2.83306800	H	5.99628200	-3.60567600	-4.72213900
H	9.16875300	1.74618600	1.60842700	H	-6.06800000	6.74479800	-2.87209000
C	10.12070600	-0.36532100	0.33139100	H	6.92519700	-0.72224300	-4.36720900
C	10.06033700	-0.67197800	2.80988600	C	-3.14518400	9.52758900	-1.73695100
H	8.64068500	0.68585500	3.70941500	H	-2.18201000	9.53861600	-2.26721700
C	10.29306200	-1.37451200	1.47669500	H	-3.72478800	10.39426300	-2.06782000
H	10.85150300	0.08164200	2.94815700	C	4.84039400	-3.03451200	-7.17834300
H	9.54347700	-2.16252600	1.35009100	H	4.05134900	-2.56443300	-7.78267400
O	8.77555700	0.13145700	0.37819700	H	5.71571500	-3.18100500	-7.81776500
O	7.64895400	-0.94053400	2.87676300	O	4.00205900	-1.96941100	-5.24434500
H	7.94483000	-1.61736300	3.51232300	O	4.44201000	-4.31983400	-6.71667600
O	10.06888800	-1.59980700	3.89150600	H	3.70882800	-4.16740200	-6.09657600
H	10.79323000	-2.22148200	3.69981000	O	7.56894900	-2.75450700	-5.79702300
O	11.60763200	-1.93244700	1.54029700	H	7.61444200	-3.63319500	-6.20469500
H	11.63650100	-2.69772200	0.94491600	O	7.47863000	-2.22267900	-3.03491200
H	10.83292600	0.46660400	0.46583200	H	8.18653200	-2.62459400	-3.57060000
C	10.35972300	-0.96903000	-1.04930700	O	4.83570300	-2.57791200	-2.49248400
H	10.13871000	-0.20955400	-1.81151000	H	5.63796100	-2.93473500	-2.07200700
H	11.42207100	-1.22329000	-1.12879800	O	-2.96270100	9.65858600	-0.33196000
O	9.62672800	-2.16388300	-1.27493700	H	-2.52457800	8.84010700	-0.04264500
H	8.72298600	-1.91941300	-1.54734600	O	-6.18510300	9.12743700	-1.90614500
C	-7.75366000	-4.00736300	-1.56394100	H	-6.08911200	9.91297100	-1.34578100
C	-7.11046400	-5.32246900	-1.10195100	O	-7.11861500	6.58844500	-1.08200900
H	-8.03460100	-4.08097600	-2.62022200	H	-7.58271100	7.44355500	-1.12019400
C	-9.93806300	-4.68160800	-0.82781800	O	-4.87411100	5.54010500	0.03310000
C	-8.16209900	-6.43234800	-1.02268300	H	-5.78228700	5.66674400	0.36249000
H	-6.33819000	-5.60518200	-1.83286500	O	-3.06284200	7.17278500	-1.61815100
C	-9.37942100	-5.97773800	-0.22247300				
H	-8.49264200	-6.69100600	-2.04110600	2I-EZ, electron energy = -6485.154641 a.u.			
H	-9.07211400	-5.77202000	0.80823200	C	2.50091000	-0.97311600	-1.45212300
H	-10.25255200	-4.86673300	-1.86768100	C	1.60098200	-0.19253300	-2.19962900
C	-11.11379200	-4.09800000	-0.05162400	C	1.74012400	1.20879500	-2.27123400
H	-11.45895900	-3.18916000	-0.56521800	C	2.89319000	1.79002500	-1.73625500
H	-11.93920400	-4.81564000	-0.04026500	C	3.85000900	1.01509500	-1.07114800
O	-8.91001600	-3.68087300	-0.78825000	C	3.62212100	-0.35437700	-0.89078300
O	-6.52520300	-5.10169800	0.17627600	H	3.03510700	2.86520800	-1.80944600
H	-6.37459800	-5.98835800	0.55110500	H	4.30050900	-0.94415200	-0.28339700
O	-7.53255800	-7.55250900	-0.40761500	C	2.17872200	-2.42525600	-1.14008300
H	-8.25588300	-8.13491200	-0.11501100	H	1.84400800	-2.94842800	-2.03504000
O	-10.31649900	-7.05613200	-0.26685000	H	3.08762200	-2.92373900	-0.78322500
H	-10.84955000	-7.02919900	0.54277400	C	0.60372900	2.08994500	-2.77270400
O	-10.77667900	-3.82862500	1.30432200	H	0.22944000	1.75700900	-3.74036800
H	-9.99396300	-3.25241300	1.27624500	H	0.98332200	3.10916100	-2.90624300
C	-3.55444600	5.86825700	-1.94015400	C	1.09110000	-2.52144800	-0.07103800
C	-4.96608400	5.63363100	-1.38401200	C	-0.12977500	-3.18219600	-0.30617100
H	-3.55793900	5.73887400	-3.02784800	C	1.27236600	-1.86604800	1.14966500
C	-3.88785900	8.24540700	-2.09755200	C	-1.18762800	-3.10414500	0.62335900
C	-5.89470700	6.78200400	-1.78493800	C	0.26967000	-1.86855600	2.12301500
H	-5.34939100	4.69213900	-1.80509700	H	2.19374900	-1.32231900	1.33464100
C	-5.27184600	8.13124100	-1.44062400	C	-0.96284900	-2.46082300	1.84403400
H	-3.99474400	8.18772300	-3.19284500	H	-1.75926900	-2.41017000	2.58144400
H	-5.14519400	8.19778100	-0.35489500	C	-0.55279900	2.10538200	-1.77441400
C	4.11345300	-1.03305400	-4.17021700	C	-1.83662700	1.63409900	-2.11256800
C	5.24478400	-1.41130500	-3.19810400	C	-0.31533800	2.53219400	-0.46449400
H	4.28867900	-0.03123400	-4.57788100	C	-2.83976600	1.50329700	-1.13188700
C	5.19743900	-2.09899700	-6.02790500	C	-1.33576400	2.51384900	0.49012600
C	6.54254100	-1.67165300	-3.96422500	H	0.68414300	2.84925200	-0.18337000
H	5.39502600	-0.57449300	-2.50005600	C	-2.57906600	1.97173500	0.15797800

H	-3.35046500	1.90381900	0.92038200	N	0.46281300	-1.19174600	3.36693300
C	-4.17468000	0.82317100	-1.42849500	N	-0.11949400	4.97629300	1.31802600
H	-4.99352900	1.53674100	-1.28122000	N	2.35827100	-2.34442100	4.00256700
H	-4.19025700	0.51798300	-2.47472400	N	-8.20153100	-0.90059700	1.34847800
C	-2.57655200	-3.65739300	0.31223600	N	-6.28899500	-1.26809700	2.58643900
H	-2.54081400	-4.16946400	-0.64950300	N	4.96713800	1.68067600	-0.48749200
H	-2.85298000	-4.40420800	1.06476700	N	6.62882000	0.17245000	-1.05758900
C	-5.28104700	-0.29376200	0.56398600	C	6.28158100	1.33186400	-0.45286100
C	-5.38936100	-1.34650800	1.47970400	C	-7.63175100	-1.05632300	2.56827600
C	-4.39444200	-0.37324000	-0.51438700	C	-0.56362900	4.11934300	2.26699700
C	-4.53942100	-2.45202600	1.37198200	C	1.47731500	-1.34813800	4.25781700
C	-3.62363300	-1.54160200	-0.66485500	H	-5.91860400	-1.48253300	3.50381300
C	-3.62493100	-2.55105600	0.31935300	H	-7.63744900	-1.07669000	0.52214400
H	-4.58329700	-3.23496500	2.12447500	H	-0.25653100	-0.54497800	3.66603300
H	-5.87904500	0.60235600	0.70225700	H	2.21961100	-2.92087000	3.17831700
O	-0.30671600	-3.88657800	-1.47920000	H	-1.53435500	2.40311800	2.56614300
O	-2.76496900	-1.62930300	-1.73333600	H	-0.32613200	4.77859000	0.34352800
O	-2.09806600	1.24972500	-3.41300900	H	4.79061900	2.60458000	-0.11254800
O	0.51159200	-0.81042600	-2.76232700	H	5.93935400	-0.31962300	-1.61709400
C	-2.60912800	2.31287200	-4.24585500	S	-8.49131300	-0.98211800	4.03856000
H	-1.90046100	3.15292800	-4.23886000	S	1.56321300	-0.33116500	5.62430100
H	-3.56091500	2.67441200	-3.83182400	S	-0.44397800	4.40699000	3.94400100
C	-2.79797100	1.77662100	-5.65642400	S	7.38857000	2.35878400	0.34101200
H	-3.48958000	0.92545100	-5.62356400	C	7.95848100	-0.36126100	-1.13539200
H	-1.83690500	1.39208500	-6.01994800	C	7.87905300	-1.89352300	-1.17160000
C	-3.33261000	2.84980100	-6.61095500	H	8.51529300	-0.04288000	-0.24801400
H	-3.46220400	2.44216600	-7.61886800	C	9.90708900	-0.31216000	-2.54328300
H	-4.30478300	3.23170000	-6.27732700	C	9.24812200	-2.49123200	-1.50612200
H	-2.64444600	3.70063600	-6.68044400	H	7.56037800	-2.23805800	-0.17697400
C	-3.15383800	-2.53648500	-2.79245800	C	9.84332300	-1.83350300	-2.74684200
H	-3.57595500	-3.45155200	-2.36154500	H	9.93384400	-2.32136400	-0.66094700
H	-2.21813100	-2.79543400	-3.29031100	H	9.19639700	-2.04082300	-3.60575000
C	-4.13830800	-1.91832400	-3.78120300	O	8.57756400	0.17500000	-2.30790300
H	-3.69456000	-1.00500300	-4.19449700	O	6.92129100	-2.26294100	-2.15835300
H	-5.05339200	-1.62398200	-3.25175200	H	7.08613100	-3.20521700	-2.34281700
C	-4.48792300	-2.89467800	-4.91067500	O	9.05133000	-3.88742800	-1.71038200
H	-4.95614600	-3.80598000	-4.51954700	H	9.84348500	-4.19937300	-2.18288300
H	-5.18795000	-2.43757000	-5.61790700	O	11.13486200	-2.41780400	-2.93191400
H	-3.59376800	-3.19278400	-5.47156000	H	11.34278300	-2.40265300	-3.87879700
C	0.49845700	-0.93711800	-4.20190500	H	10.55744500	-0.08452400	-1.68309700
H	-0.56040500	-0.98266700	-4.46878100	C	10.41424200	0.44889700	-3.76336000
H	0.92387100	-0.03636100	-4.65954900	H	10.45484900	1.52029900	-3.51934400
C	1.24231100	-2.17358900	-4.69627500	H	11.42774100	0.11821600	-4.00850700
H	0.81018600	-3.05822200	-4.21512800	O	9.60890700	0.21142700	-4.91214200
H	2.29306300	-2.11537000	-4.38421700	H	8.69869900	0.43215500	-4.65034500
C	1.16114200	-2.30544600	-6.22177900	C	-9.60896700	-0.77633100	1.09865700
H	0.12057100	-2.38546500	-6.55880500	C	-9.81612500	-0.03053800	-0.22662200
H	1.60853900	-1.43800500	-6.72198400	H	-10.06473000	-0.20897800	1.91768400
H	1.69281300	-3.19912800	-6.56505600	C	-11.57608700	-2.12313000	0.78056900
C	0.04820000	-5.28257200	-1.38028700	C	-11.28826800	-0.08142900	-0.64056800
H	-0.53842100	-5.75091000	-0.57742500	H	-9.51451900	1.01774500	-0.08279900
H	1.11066000	-5.37002900	-1.11269600	C	-11.81303900	-1.51361900	-0.60986200
C	-0.23379400	-5.95420700	-2.71535800	H	-11.88346800	0.52300200	0.06193500
H	0.35321900	-5.45429500	-3.49572400	H	-11.26401200	-2.10956600	-1.34650300
H	-1.29122300	-5.80774400	-2.96825600	H	-12.13207000	-1.54301500	1.53478900
C	0.09966700	-7.44988000	-2.68654600	C	-11.98282400	-3.58976400	0.88278300
H	-0.10635200	-7.91188300	-3.65760700	H	-11.81169000	-3.93274600	1.91338600
H	1.15809100	-7.61775700	-2.45431700	H	-13.04969900	-3.69209600	0.66382100
H	-0.49642500	-7.97723200	-1.93230900	O	-10.16909900	-2.09221300	1.06347500
N	-1.11887600	2.95759600	1.82793800	O	-9.00047200	-0.64849400	-1.21521600

H	-9.34767900	-0.33843300	-2.07113500	H	-4.79722100	2.02152000	-0.00807700
O	-11.36733400	0.46475600	-1.95395000	C	-2.59703700	2.41642300	-1.59406500
H	-12.22778900	0.17755300	-2.30781200	H	-2.38729800	2.48891200	-2.66111400
O	-13.19997800	-1.44094200	-0.94860900	H	-3.25308800	3.25305500	-1.32704100
H	-13.45142600	-2.27170200	-1.38078200	C	-2.51612700	-2.63868700	-1.50903700
O	-11.28438200	-4.40119600	-0.05418100	H	-2.34740000	-2.79532600	-2.57464600
H	-10.33910600	-4.23090800	0.09840200	H	-3.12193600	-3.47858800	-1.15071500
C	3.60787600	-2.55628900	4.67324000	C	-1.27957100	2.52689700	-0.82754100
C	3.92778900	-4.05728000	4.68106100	C	-0.04961100	2.70667800	-1.49131400
H	3.52368300	-2.18916300	5.70136200	C	-1.27532700	2.39850800	0.56381400
C	5.93871700	-1.95189600	4.48736100	C	1.16899500	2.63632700	-0.78939300
C	5.35937000	-4.29276700	5.16537100	C	-0.07859000	2.40305900	1.28321300
H	3.22440800	-4.55545500	5.36473300	H	-2.21497000	2.27879600	1.09581400
C	6.34492000	-3.43006200	4.38312800	C	1.13778400	2.47787900	0.59890500
H	5.98554200	-1.63328600	5.54103900	H	2.07150600	2.37559800	1.14335800
H	6.31481700	-3.72375800	3.32862300	C	-1.16896100	-2.63639300	-0.78936300
C	0.45223300	6.27051300	1.55700600	C	0.04963700	-2.70675000	-1.49129500
C	1.45162600	6.58846900	0.43570300	C	-1.13773800	-2.47793000	0.59893400
H	0.97048900	6.25333000	2.52164700	C	1.27960300	-2.52696000	-0.82753500
C	-0.19102600	8.57763500	1.79065900	C	0.07864100	-2.40309600	1.28323000
C	1.89579900	8.05058200	0.51537500	H	-2.07145800	-2.37565200	1.14339200
H	2.32728200	5.93429900	0.56106100	C	1.27537200	-2.39855300	0.56381700
C	0.69067500	8.98230300	0.59964400	H	2.21502000	-2.27883000	1.09580600
H	0.38586200	8.67656300	2.72445500	C	2.59706400	-2.41649100	-1.59407000
H	0.09940100	8.88571100	-0.31699700	H	3.25311400	-3.25312300	-1.32704800
H	5.43024700	-4.02595400	6.23177400	H	2.38731900	-2.48898300	-2.66111800
H	2.50988000	8.19357100	1.41849100	C	2.51615300	2.63861100	-1.50908400
C	6.80604200	-1.01944200	3.64659700	H	2.34741200	2.79523000	-2.57469400
H	6.47221200	0.01550400	3.80550500	H	3.12196500	3.47852000	-1.15078600
H	7.84923000	-1.09344900	3.96619400	C	4.39683900	-1.08807100	-0.39307000
C	-1.47224300	9.39646500	1.90937200	C	4.95925800	0.12603700	0.01648700
H	-2.02295000	9.06416200	2.80122500	C	3.30840200	-1.11125500	-1.27124700
H	-1.22222400	10.45340400	2.03931800	C	4.37673000	1.33275000	-0.38288300
O	-0.61711400	7.21894800	1.60753700	C	2.80569900	0.11445800	-1.74755200
O	-2.27660700	9.29799600	0.73984700	C	3.27395400	1.34439900	-1.24147800
H	-2.41397700	8.34705000	0.59010400	H	4.77816700	2.26966000	-0.00601100
O	1.21358500	10.30627500	0.72914400	H	4.79721500	-2.02157900	-0.00803700
H	0.57990200	10.92402800	0.33300100	O	-0.03462800	2.90962100	-2.85721000
O	2.66601400	8.31305200	-0.65398800	O	1.76130700	0.09742200	-2.63851400
H	2.70313400	9.28290700	-0.73294300	O	0.03463600	-2.90970600	-2.85718900
O	0.81591100	6.32987100	-0.81142500	O	-1.76121700	-0.09750400	-2.63842800
H	1.35578200	6.78974200	-1.47958600	C	0.08956700	-4.29934800	-3.24522700
O	6.76519400	-1.36392200	2.26469700	H	-0.74901500	-4.83960900	-2.78395600
H	5.82372500	-1.37804000	2.02407900	H	1.02176300	-4.74573600	-2.87150400
O	7.63485400	-3.68420800	4.94408500	C	0.01707200	-4.38296900	-4.76201200
H	8.29911300	-3.56360900	4.24815800	H	0.85069700	-3.81162400	-5.18894200
O	5.63576800	-5.67795400	4.98173700	H	-0.90745500	-3.89794400	-5.09914500
H	6.60525200	-5.76058900	5.02168900	C	0.06421000	-5.83193600	-5.25944400
O	3.76586800	-4.55217800	3.35608600	H	0.01334300	-5.86837100	-6.35259400
H	4.22300500	-5.41235300	3.34045300	H	0.99140900	-6.32953200	-4.95122000
O	4.60527300	-1.79910600	3.97667000	H	-0.77613400	-6.41629200	-4.86612700
2J-EZ, electron energy = -6485.153649 a.u.				C	2.07097800	0.48528400	-3.99871000
C	-3.30837300	1.11118600	-1.27123900	H	2.83606200	1.27079200	-3.99447000
C	-2.80565200	-0.11453100	-1.74751500	H	1.14560900	0.91732900	-4.38690700
C	-3.27392400	-1.34446800	-1.24144800	C	2.53221000	-0.68930400	-4.85631500
C	-4.37672300	-1.33281200	-0.38288400	H	1.76950800	-1.47550200	-4.81727300
C	-4.95926000	-0.12609600	0.01646300	H	3.45223700	-1.11045400	-4.43089500
C	-4.39683200	1.08800900	-0.39309000	C	2.78181000	-0.26237400	-6.30758700
H	-4.77817300	-2.26971900	-0.00601900	H	3.55579400	0.51229000	-6.36811300
				H	3.11331700	-1.11266100	-6.91283400

H	1.87053900	0.13951100	-6.76678000	H	-12.15349300	1.90270900	-4.24820200
C	-2.07081000	-0.48540400	-3.99863000	H	-11.42092200	1.40068700	-1.09258100
H	-1.14542000	-0.91746500	-4.38675700	C	-11.52194400	-0.34226600	-2.35253400
H	-2.83589900	-1.27090900	-3.99441100	H	-11.65912300	-0.99741000	-1.48020600
C	-2.53198400	0.68916200	-4.85629600	H	-12.51018100	-0.10295400	-2.75583900
H	-1.76928000	1.47535700	-4.81722800	O	-10.79774900	-1.00175500	-3.38448900
H	-3.45203500	1.11032800	-4.43094400	H	-9.89773900	-1.12915200	-3.03905900
C	-2.78149600	0.26219200	-6.30757100	C	8.77029500	-1.58975400	-0.84064100
H	-1.87020000	-0.13971600	-6.76669400	C	8.51213000	-2.70605500	-1.86116300
H	-3.55548500	-0.51246500	-6.36812400	H	9.29280700	-1.99870400	0.03129100
H	-3.11295500	1.11246400	-6.91286500	C	10.82844500	-0.93814500	-1.89838600
C	-0.08956600	4.29925800	-3.24526100	C	9.82873200	-3.15383500	-2.49979400
H	0.74902500	4.83952400	-2.78401300	H	8.05548900	-3.55746400	-1.33473100
H	-1.02175400	4.74565000	-2.87152300	C	10.61686000	-1.95846000	-3.02715800
C	-0.01710300	4.38286500	-4.76204800	H	10.44097600	-3.66602200	-1.74063800
H	-0.85073900	3.81152000	-5.18895500	H	10.04293700	-1.47675000	-3.82588100
H	0.90741500	3.89783200	-5.09919600	H	11.42096300	-1.40066700	-1.09242900
C	-0.06424400	5.83182700	-5.25949200	C	11.52197700	0.34228200	-2.35238800
H	-0.01339700	5.86825200	-6.35264300	H	11.65913700	0.99743100	-1.48006100
H	-0.99143400	6.32943000	-4.95125500	H	12.51022100	0.10298200	-2.75568100
H	0.77611100	6.41618300	-4.86619700	O	9.54545200	-0.52696800	-1.40306800
N	0.12686500	-2.23559000	2.69981100	O	7.62344700	-2.20189100	-2.85149700
N	-0.12679500	2.23557100	2.69980000	H	7.68834100	-2.82070200	-3.60106100
N	-1.27631400	-3.98482600	3.24609400	O	9.49312000	-4.05190800	-3.55319400
N	1.27630400	3.98488800	3.24604200	H	10.28813900	-4.11237300	-4.11202300
N	7.51330500	-1.04452700	-0.41494400	O	11.84787800	-2.48112100	-3.53236900
N	6.06546600	0.15207900	0.92188500	H	12.15359100	-1.90269200	-4.24803300
N	-6.06549300	-0.15213200	0.92183200	O	10.79778300	1.00175700	-3.38435300
N	-7.51328500	1.04449600	-0.41502800	H	9.89776500	1.12913300	-3.03893600
C	-7.29610700	0.39819900	0.75610800	C	1.98409500	4.90006800	4.09426800
C	7.29609300	-0.39823100	0.75618400	C	3.21600800	5.42471300	3.34217600
C	-0.50238900	-2.95618700	3.66610800	H	2.30043500	4.36930300	4.99886700
C	0.50241100	2.95623200	3.66608100	C	1.68405400	6.96852400	5.27850900
H	5.96943500	0.70655100	1.76363900	C	3.86203400	6.57793600	4.11336000
H	6.80821600	-0.98055500	-1.14356100	H	3.93889200	4.60056600	3.24840400
H	-0.77993900	1.55110000	3.06013700	C	2.82509400	7.63045800	4.49197800
H	1.25233200	4.24622200	2.26488500	H	2.08570500	6.52145800	6.20229900
H	0.78003700	-1.55113700	3.06013300	H	2.40708700	8.06530100	3.57789700
H	-1.25231800	-4.24621000	2.26495100	C	-1.98416500	-4.89994400	4.09434000
H	-5.96949000	-0.70661200	1.76358400	C	-3.21610000	-5.42454700	3.34225600
H	-6.80818600	0.98050000	-1.14363400	H	-2.30047900	-4.36913300	4.99892100
S	8.45390800	-0.26421700	2.00127500	C	-1.68422900	-6.96839000	5.27862900
S	0.29753100	2.52378600	5.30296800	C	-3.86218300	-6.57772200	4.11346400
S	-0.29752900	-2.52367500	5.30298300	H	-3.93894300	-4.60036800	3.24846300
S	-8.45395100	0.26420100	2.00117200	C	-2.82529600	-7.63028700	4.49210600
C	-8.77025900	1.58973600	-0.84075300	H	-2.08586600	-6.52129000	6.20240800
C	-8.51205800	2.70602900	-1.86127700	H	-2.40730500	-8.06517100	3.57803800
H	-9.29278200	1.99870000	0.03116600	H	4.31386700	6.18680300	5.03868400
C	-10.82840000	0.93815300	-1.89852800	H	-4.31399500	-6.18654700	5.03878000
C	-9.82864200	3.15382400	-2.49993200	C	0.55398500	7.92568900	5.64197200
H	-8.05541400	3.55743400	-1.33484000	H	-0.20402000	7.37472500	6.21714300
C	-10.61678000	1.95845900	-3.02730100	H	0.94229700	8.72896100	6.27478800
H	-10.44089100	3.66602600	-1.74079100	C	-0.55420300	-7.92559800	5.64211700
H	-10.04285400	1.47673300	-3.82601300	H	0.20382100	-7.37465600	6.21728400
O	-9.54541900	0.52696000	-1.40318900	H	-0.94255100	-8.72884400	6.27494300
O	-7.62336600	2.20184600	-2.85159300	O	-1.08826300	-5.95615500	4.45303700
H	-7.68824500	2.82064900	-3.60116500	O	0.01551000	-8.53952000	4.49185300
O	-9.49299900	4.05188400	-3.55333400	H	0.28500500	-7.81212300	3.90560300
H	-10.28800800	4.11235900	-4.11217500	O	-3.51784700	-8.62121800	5.25452300
O	-11.84778300	2.48113600	-3.53253500	H	-3.06617600	-9.47023600	5.13040800

O	-4.86725300	-7.12794800	3.26688500	O	-2.93669800	4.05901300	0.63154400
H	-5.07083500	-8.00622100	3.63457800	O	-0.65169100	4.36500700	3.11669800
O	-2.79529000	-5.86178600	2.05494900	O	0.48337600	4.68393200	0.02832500
H	-3.51734700	-6.42458100	1.72141100	C	-0.47314900	4.68609500	4.51105200
O	-0.01574700	8.53956900	4.49169400	H	0.52261300	4.35304800	4.83720400
H	-0.28519700	7.81215200	3.90544900	H	-1.21871900	4.14370300	5.10992100
O	3.51759200	8.62144000	5.25437500	C	-0.62299900	6.18920000	4.69193800
H	3.06588500	9.47043400	5.13023300	H	-1.61684100	6.49281800	4.33978600
O	4.86707600	7.12819500	3.26676800	H	0.10987400	6.69744700	4.05288000
H	5.07061700	8.00648400	3.63444300	C	-0.43250900	6.61279500	6.15235600
O	2.79518100	5.86190200	2.05485700	H	-0.54461000	7.69667500	6.26009600
H	3.51721400	6.42472000	1.72130700	H	-1.17101700	6.13393100	6.80634000
O	1.08814000	5.95624500	4.45293200	H	0.56478700	6.34180000	6.51904600
2I-ZE, electron energy = -6485.157616 a.u.				C	-3.58238600	5.34442000	0.49449400
C	1.94516100	3.71234100	-1.60180100	H	-4.45038100	5.25571700	-0.16998400
C	1.64007600	3.99648700	-0.25828500	H	-2.84339700	5.98004400	-0.00020700
C	2.44190400	3.49558000	0.78648800	C	-4.01160600	5.94511700	1.83032400
C	3.64248800	2.86693000	0.45361300	H	-3.13454500	6.01791500	2.48368500
C	4.02368200	2.67903400	-0.88257300	H	-4.72400600	5.26906900	2.32024600
C	3.14519100	3.05800600	-1.90378300	C	-4.65131000	7.32640600	1.64679400
H	4.28570700	2.50030800	1.25119700	H	-5.54780100	7.27062200	1.01746900
H	3.39688200	2.85203100	-2.93577800	H	-4.94764700	7.75117500	2.61174800
C	0.93601600	4.01803000	-2.70110100	H	-3.95435200	8.02839200	1.17297900
H	0.55589800	5.03443800	-2.59925400	C	0.64808300	6.04052100	0.49851100
H	1.44040200	3.94718100	-3.67181800	H	-0.24449400	6.24254100	1.09567700
C	1.96700800	3.51616900	2.23457200	H	1.51830300	6.10032700	1.16331500
H	1.66017300	4.51649200	2.54046200	C	0.78963700	7.05253900	-0.63477800
H	2.80617200	3.22658700	2.87738200	H	-0.08150600	6.96682700	-1.29430500
C	-0.24264300	3.04727400	-2.66108300	H	1.67452700	6.80420300	-1.23476800
C	-1.56532300	3.48498800	-2.45964000	C	0.91183200	8.48431900	-0.10038700
C	-0.00717800	1.67505600	-2.77512500	H	0.03207500	8.76496700	0.49142900
C	-2.60800100	2.56007800	-2.25185800	H	1.79476500	8.59746300	0.54037800
C	-1.04621200	0.74855900	-2.66016100	H	1.00307100	9.20187400	-0.92270400
H	1.00724900	1.32206500	-2.94487800	C	-2.17948100	5.38866100	-3.71998300
C	-2.33338100	1.19404100	-2.35427800	H	-3.02862700	4.83282900	-4.14261300
H	-3.12310500	0.47363300	-2.18095500	H	-1.32727500	5.26471400	-4.40352100
C	0.79908400	2.55709300	2.45720000	C	-2.52944000	6.85938900	-3.55134700
C	-0.47668900	3.02284000	2.82994600	H	-1.67234900	7.37971900	-3.10582600
C	0.97383500	1.18878300	2.23871900	H	-3.35971500	6.94631300	-2.83931400
C	-1.57426000	2.14434800	2.89009900	C	-2.90614100	7.51667500	-4.88345700
C	-0.08946800	0.28951000	2.37897300	H	-3.15323500	8.57353500	-4.73853600
H	1.95430600	0.81853800	1.94783900	H	-2.08026200	7.46247200	-5.60276300
C	-1.36041700	0.77687200	2.69071300	H	-3.77737300	7.02915400	-5.33710700
H	-2.19483800	0.09249600	2.76289700	N	0.20694200	-1.09339500	2.24628300
C	-3.00029800	2.65026200	3.10778400	N	-0.70802900	-0.62703900	-2.75373700
H	-3.41769900	2.20324200	4.01763300	N	-0.02603700	-3.36423800	2.05659200
H	-2.97242000	3.73015000	3.25100500	N	-0.84210200	-2.88223300	-3.10953600
C	-4.01064900	3.01039200	-1.84682100	N	-7.86866600	-1.87570400	1.68707300
H	-4.05538900	4.09875500	-1.88227300	N	-6.34162000	-0.35453400	0.92458500
H	-4.73984600	2.63449600	-2.57361800	N	5.25450600	2.01047600	-1.09306900
C	-4.76549500	1.19830300	2.00682800	N	7.08496600	1.03759500	-2.05147300
C	-5.48192300	0.77675900	0.88330600	C	6.09298500	1.96999200	-2.16278100
C	-3.89394900	2.28786200	1.92876700	C	-7.33050000	-0.62949100	1.81395400
C	-5.26390200	1.39568600	-0.35063200	C	-0.57069100	-2.13223700	1.84046200
C	-3.76820200	2.96503300	0.69960800	C	-1.39475200	-1.65278700	-3.32084000
C	-4.38480100	2.47677900	-0.46882100	H	-6.35904300	-0.92145500	0.07880600
H	-5.77353000	1.02132500	-1.23528500	H	-8.75419200	-2.03812200	2.14949000
H	-4.88139100	0.66635200	2.94457600	H	0.26928200	-0.83446700	-2.55880300
O	-1.84256200	4.84033600	-2.42957600	H	-1.16857300	-3.63221600	-3.70586400
				H	1.19484400	-1.31955600	2.33606200

H	-0.46855000	-4.13798100	1.57659100	C	1.17090000	-3.65582100	2.79330100
H	5.65717500	1.62523500	-0.24149400	C	1.23449300	-5.16665900	3.06770700
H	7.86400600	1.12805200	-2.69176800	H	1.15321400	-3.12516000	3.75694300
S	-7.92620400	0.43504900	2.99840200	C	3.54931700	-3.44308200	2.70125600
S	-2.80905100	-1.52032000	-4.25628500	C	2.61284200	-5.56761000	3.61548400
S	-2.09082900	-2.02891300	1.08526100	H	0.46504800	-5.40578500	3.81678200
S	6.02693700	2.95436700	-3.54605500	C	3.71940200	-4.96634400	2.76041100
C	7.20544300	0.06014200	-1.00736700	H	3.50418100	-3.02897500	3.72060100
C	8.25146300	-0.98880600	-1.39281800	H	3.61659600	-5.35594700	1.74048800
H	6.23992700	-0.44637500	-0.86460100	H	1.65067300	-4.71408100	-0.31274900
C	7.72282000	-0.11251500	1.35273800	H	2.71777400	-5.19679300	4.64646300
C	8.52864900	-1.90769700	-0.20021100	C	3.73626800	-1.99261700	-2.74378500
H	7.84475400	-1.58575300	-2.22304800	H	3.48019100	-0.92396600	-2.70184100
C	8.86421300	-1.09340500	1.04681500	H	4.68612600	-2.13451800	-2.22041400
H	7.63377100	-2.51429800	0.00975400	C	4.69505600	-2.75244400	1.94569600
H	9.77853700	-0.51908600	0.86521000	H	4.29848700	-1.85586900	1.44987700
O	7.53498300	0.74849300	0.21226000	H	5.44345700	-2.42989000	2.67381800
O	9.43371700	-0.31442400	-1.79829900	O	2.29765400	-3.17241100	2.03759800
H	10.13405200	-0.99188500	-1.78885700	O	5.39171400	-3.59788400	1.03614300
O	9.62235300	-2.74040600	-0.57390900	H	4.80721000	-3.82895500	0.28309400
H	9.96493200	-3.11453100	0.25711200	O	4.96707400	-5.35890600	3.31815700
O	9.05707000	-2.03674800	2.10291100	H	5.62669100	-5.15142000	2.63083500
H	9.70094600	-1.66882400	2.72756400	O	2.65761700	-6.99143400	3.59364200
H	6.79992900	-0.67596400	1.55589200	H	3.60040100	-7.23189800	3.62572300
C	8.00830700	0.81595700	2.52818100	O	0.96324100	-5.84925500	1.85240500
H	7.13479500	1.46499500	2.68758000	H	1.32111300	-6.74880200	1.96965300
H	8.15574900	0.22019600	3.43354700	O	3.93231200	-2.42857300	-4.08171200
O	9.19194200	1.57933100	2.33470500	H	3.07012200	-2.34950000	-4.52397800
H	9.07348000	2.05764600	1.49665200	O	4.07162100	-4.63240800	-1.24151500
C	-7.35379800	-2.93342300	0.86270000	H	4.82866600	-4.71190100	-1.84360600
C	-8.07254600	-4.24262400	1.20320200	O	1.87440100	-6.43740500	-1.45149200
H	-6.27770300	-3.05904400	1.05263800	H	2.78877500	-6.63390700	-1.18458400
C	-7.07141300	-3.54804600	-1.45913300	O	0.40706800	-5.26168600	-3.39239300
C	-7.70239200	-5.32677300	0.18660100	H	0.74098900	-6.16994400	-3.27856900
H	-7.74627200	-4.56129600	2.20469400	O	1.44064200	-2.55208800	-2.78851600
C	-7.89397200	-4.82716800	-1.24297100				
H	-6.64398700	-5.60092400	0.31989900	2I-ZZ, electron energy = -6485.152564 a.u.			
H	-8.95133400	-4.59032600	-1.40085100	C	4.86074900	-1.96502300	1.05299900
H	-6.00309200	-3.76334900	-1.30139000	C	4.60475400	-2.61652100	-0.16954400
C	-7.25402000	-2.92493800	-2.83853100	C	4.82953500	-1.97173700	-1.40306900
H	-6.61951800	-2.02945000	-2.90992200	C	5.44392800	-0.71554000	-1.39027200
H	-6.92264000	-3.63402400	-3.60241700	C	5.78831700	-0.09484000	-0.18683200
O	-7.52374900	-2.55662600	-0.51549000	C	5.48053200	-0.71162400	1.02724300
O	-9.47183700	-3.99909700	1.19028000	H	5.63534300	-0.20120400	-2.32872700
H	-9.88763600	-4.87999800	1.16373800	H	5.72795800	-0.21398700	1.95811500
O	-8.54226700	-6.44315700	0.45725300	C	4.40795000	-2.57291600	2.37334800
H	-8.50316900	-7.00381000	-0.33790800	H	4.69944900	-3.62151000	2.43349000
O	-7.47707300	-5.89202800	-2.09871100	H	4.90874200	-2.04193800	3.19137200
H	-7.98112200	-5.83483700	-2.92515400	C	4.27603800	-2.53866500	-2.70604900
O	-8.61504000	-2.62090600	-3.11541300	H	4.57169200	-3.57722900	-2.85503300
H	-8.91484900	-2.03484200	-2.40013200	H	4.69275700	-1.96243500	-3.53997900
C	0.26212500	-3.17186600	-2.23831500	C	2.89441100	-2.47501900	2.54961600
C	0.41806600	-4.68855800	-2.09220100	C	2.09118700	-3.62458100	2.67149400
H	0.07202700	-2.73538300	-1.24770900	C	2.27249400	-1.22018500	2.55315700
C	2.64400300	-2.78737600	-2.03557000	C	0.68487100	-3.53051300	2.66566300
C	1.72466500	-5.02298100	-1.36392300	C	0.88452000	-1.11082300	2.64335000
H	-0.42844400	-5.06393500	-1.49809500	H	2.87880400	-0.32053600	2.48121000
C	2.90200000	-4.30038500	-2.01098900	C	0.09948200	-2.26430600	2.64852000
H	2.52826400	-2.41422300	-1.00601100	H	-0.97953700	-2.17138200	2.62931600
H	3.02647100	-4.65303900	-3.03824100	C	2.75189000	-2.45232900	-2.72637100

C	1.94086400	-3.60159400	-2.78405200	H	2.81370000	-7.36187700	3.58754400
C	2.13648600	-1.20579700	-2.60091500	C	3.72532200	-7.22063200	5.55166700
C	0.54706200	-3.51039200	-2.60282600	H	4.15622800	-8.22692800	5.52539600
C	0.74833300	-1.09230900	-2.49066000	H	4.41594700	-6.57620100	6.10860900
H	2.75112600	-0.30983100	-2.55798600	H	2.78733000	-7.27355500	6.11707100
C	-0.03403600	-2.24736500	-2.45899500	N	0.22395100	0.20822900	-2.26679000
H	-1.09902100	-2.16457800	-2.28932500	N	0.28556800	0.18469100	2.61945800
C	-0.33026600	-4.75561500	-2.45886800	N	-1.17014400	1.96396600	-1.98030600
H	-1.05463100	-4.79497600	-3.28089300	N	-1.12910500	1.92019100	3.07265400
H	0.30100400	-5.64098300	-2.52877600	N	-6.31542500	-2.40618100	0.06329400
C	-0.21066200	-4.76817900	2.59541500	N	-4.34314000	-3.49934100	0.29535600
H	0.40914300	-5.66065700	2.67337000	N	6.49762100	1.14218500	-0.24259200
H	-0.89780200	-4.77386800	3.44927100	N	7.13426800	3.28775200	0.15126100
C	-2.39834300	-4.24939400	-1.09436900	C	6.19046400	2.32521300	0.35331700
C	-3.04419900	-4.04393100	0.12953700	C	-5.31578500	-3.09690600	-0.56917700
C	-1.08310900	-4.72996800	-1.13596100	C	-0.98092800	0.75943800	-2.58308400
C	-2.34005900	-4.29145700	1.31955600	C	-0.70508200	0.66295000	3.41822500
C	-0.42653800	-5.04448500	0.06524900	H	-4.53667300	-3.28970800	1.26924400
C	-1.02608800	-4.75804600	1.30811700	H	-6.16947600	-2.10750100	1.02337700
H	-2.81208800	-4.07430900	2.27581100	H	0.69727000	0.83418500	1.95695300
H	-2.91081700	-4.01705200	-2.01696800	H	-0.82032400	2.29613000	2.18160300
O	2.68730300	-4.86882200	2.77316100	H	0.87171900	0.82005200	-1.78157700
O	0.86305900	-5.52506400	0.01927100	H	-0.45957500	2.34071500	-1.35747700
O	2.52971700	-4.83906500	-2.97323700	H	7.28005200	1.14852500	-0.88858500
O	4.03020400	-3.86569900	-0.14277800	H	7.93954300	3.08098600	-0.43243300
C	2.63842300	-5.22830500	-4.35698700	S	-5.37144100	-3.44444000	-2.22869400
H	3.20806900	-4.46587000	-4.90732700	S	-1.32383800	-0.17108000	4.76216400
H	1.63455900	-5.28071300	-4.80211200	S	-2.12972900	0.05997900	-3.62100100
C	3.33459900	-6.57890600	-4.43026100	S	4.78213000	2.59429800	1.26614000
H	2.75503900	-7.30835500	-3.85055600	C	7.01728900	4.66847000	0.51653600
H	4.31679400	-6.49757200	-3.94787700	C	8.42106700	5.24056600	0.75759500
C	3.49566900	-7.06520800	-5.87466700	H	6.42326600	4.74182000	1.43372800
H	3.99822600	-8.03765400	-5.90286500	C	6.18484700	6.76391300	-0.32285100
H	2.52332800	-7.17721500	-6.36890800	C	8.35715300	6.76090600	0.91954000
H	4.09361400	-6.36294800	-6.46772800	H	8.82180700	4.79330100	1.67954200
C	1.04318000	-6.91335600	0.37453400	C	7.58010000	7.39995000	-0.22719400
H	0.33422700	-7.19069300	1.16439800	H	7.84471000	7.00313800	1.86412000
H	2.05276900	-6.97376000	0.79066000	H	8.11082000	7.21185000	-1.16637700
C	0.88788300	-7.85402200	-0.81736000	O	6.33778200	5.35358700	-0.54219000
H	1.58886800	-7.54818900	-1.60313600	O	9.23743900	4.89359700	-0.35544300
H	-0.12370900	-7.74990400	-1.23027300	H	10.01624600	5.47634000	-0.30036600
C	1.13998900	-9.31379600	-0.42258200	O	9.70200800	7.22988200	0.95244400
H	0.43172800	-9.64721000	0.34560800	H	9.65216400	8.18626500	0.77673200
H	1.03043000	-9.97706000	-1.28709600	O	7.52816300	8.80093500	0.05308800
H	2.15274200	-9.44912400	-0.02390900	H	7.48240000	9.27780200	-0.78997700
C	4.87146400	-4.97274100	-0.53876600	H	5.63186000	6.95002000	0.61221200
H	4.18260900	-5.72285400	-0.93492900	C	5.35835700	7.27618400	-1.49769400
H	5.53671200	-4.66190400	-1.35302200	H	4.37076200	6.79332500	-1.47189300
C	5.69269100	-5.53881200	0.61572500	H	5.21080100	8.35570800	-1.40052500
H	5.01006100	-5.82542000	1.42303700	O	6.00926400	7.05351600	-2.74319700
H	6.35144500	-4.75488100	1.01141700	H	6.21294100	6.10309000	-2.77097700
C	6.53125900	-6.74325000	0.17214100	C	-7.34675400	-1.66375100	-0.60266400
H	5.89653500	-7.55126100	-0.21159800	C	-8.53807100	-1.48720200	0.35152500
H	7.23663500	-6.46801500	-0.62141600	H	-7.66720100	-2.22084300	-1.49006100
H	7.11208400	-7.14475300	1.00933700	C	-7.74138000	0.42500000	-1.68539600
C	2.90078500	-5.29136100	4.13595600	C	-9.55661700	-0.50174800	-0.23725000
H	1.94401600	-5.27620700	4.67701100	H	-9.01833900	-2.46733300	0.48971700
H	3.57685500	-4.58253900	4.63519900	C	-8.85712000	0.77226900	-0.69102200
C	3.49210900	-6.69290400	4.13167200	H	-10.05464600	-0.96580700	-1.10268500
H	4.43852700	-6.67958200	3.57715700	H	-8.39031400	1.23517200	0.18488500

H	-8.15973200	-0.12682100	-2.54360800	C	-2.82597900	0.03241100	1.22428700
C	-7.02025600	1.66890400	-2.21893600	C	-3.36360200	1.24674600	0.74684900
H	-6.02721000	1.36223500	-2.57838300	C	-4.45426700	1.19319300	-0.12568600
H	-7.58060200	2.05474400	-3.07548900	C	-4.98050500	-0.03740900	-0.53123100
O	-6.79133300	-0.40669300	-1.00445300	C	-4.36359000	-1.22642100	-0.13941500
O	-8.04455100	-1.00304100	1.59630600	H	-4.88951000	2.11304600	-0.50573900
H	-8.81585100	-0.61408100	2.04792500	H	-4.74974200	-2.17332600	-0.50659400
O	-10.50579500	-0.22827300	0.79170300	C	-2.50110500	-2.48729700	1.03953800
H	-10.93684800	0.60785400	0.54093100	H	-2.29140200	-2.55781300	2.10660300
O	-9.84650600	1.63898100	-1.23986100	H	-3.12513800	-3.34629600	0.76676700
H	-9.44938600	2.52668900	-1.24605300	C	-2.67911100	2.57574600	1.04416700
O	-6.94194100	2.74095300	-1.28788200	H	-2.52810600	2.71956500	2.11425500
H	-6.43710700	2.43741200	-0.50202700	H	-3.32933900	3.38688800	0.69814600
C	-2.33343100	2.51779300	3.57376500	C	-1.17876300	-2.54738200	0.27662600
C	-2.26492500	4.05388900	3.50865100	C	0.05526800	-2.67448700	0.94631900
H	-2.45482100	2.20763000	4.61684800	C	-1.17207900	-2.39855000	-1.11293200
C	-4.71195800	2.46042700	3.23133300	C	1.27552300	-2.55091800	0.25343700
C	-3.62295000	4.61573600	3.93630700	C	0.03057100	-2.37808300	-1.82193000
H	-1.49306100	4.39152000	4.21203700	H	-2.10971900	-2.28491000	-1.64830500
C	-4.77139600	3.99200600	3.13976400	C	1.24451200	-2.42093500	-1.13804700
H	-4.89170300	2.15624000	4.27518900	H	2.17351100	-2.34322800	-1.69575500
H	-4.68922800	4.29091500	2.09026500	C	-1.32872100	2.66059100	0.33653900
C	-2.28998500	2.84048600	-2.12940400	C	-0.11828100	2.75738400	1.05076000
C	-2.47095100	3.59530400	-0.79890400	C	-1.27799800	2.58198300	-1.05818200
H	-3.18327300	2.25310200	-2.36655100	C	1.12542200	2.65519300	0.39473500
C	-3.01724300	4.74245200	-3.42474500	C	-0.05435300	2.56423500	-1.72552600
C	-3.51034600	4.70539000	-0.97783500	H	-2.19881700	2.52570900	-1.63179700
H	-2.83287200	2.88912100	-0.04107100	C	1.13811700	2.55886000	-0.99947700
C	-3.14988200	5.60056300	-2.15613200	H	2.08295600	2.46473300	-1.52596000
H	-3.98845400	4.27104000	-3.64662600	C	2.43707300	2.56549200	1.17363700
H	-2.18965000	6.08656800	-1.95546600	H	3.06436800	3.43431300	0.94272900
H	-3.77241900	4.36298600	4.99871400	H	2.21259600	2.59459200	2.23962400
H	-4.48653100	4.23608300	-1.17991600	C	2.61522100	-2.49251800	0.98399800
C	-5.73079100	1.76291300	2.33600000	H	2.44759600	-2.67534800	2.04559300
H	-5.74732400	0.68654500	2.53974900	H	3.27086200	-3.29049500	0.61821800
H	-6.72849400	2.16230900	2.53326500	C	4.30814200	1.35063400	-0.03719800
C	-2.55582500	5.52799500	-4.64802300	C	4.92757400	0.17783900	-0.47339400
H	-2.52748000	4.84955600	-5.51301000	C	3.20227900	1.29993000	0.81837600
H	-3.27230000	6.32557300	-4.86494900	C	4.39717700	-1.06721600	-0.11860100
O	-2.01136200	3.74172900	-3.20967900	C	2.76292000	0.04104000	1.26955200
O	-1.29202500	6.14616000	-4.43590800	C	3.30302100	-1.15319400	0.74650500
H	-0.69450700	5.43554400	-4.14652000	H	4.83041800	-1.97295400	-0.53264000
O	-4.19827400	6.56814800	-2.26400400	H	4.69439800	2.31209700	-0.36485300
H	-3.82048800	7.38931100	-2.61466400	O	0.07102100	-2.88110000	2.31147200
O	-3.59478200	5.47059500	0.22657900	O	1.71479100	-0.01586600	2.15545100
H	-4.09008500	6.27701000	-0.00391200	O	-0.15327100	2.91093300	2.42242100
O	-1.19332500	4.09953300	-0.42527600	O	-1.78264400	0.05458400	2.11623900
H	-1.21072900	4.22255000	0.54556900	C	-0.15818200	4.28767300	2.85806900
O	-5.45220000	2.00069100	0.95256700	H	-1.00949400	4.81101500	2.40059800
H	-4.64276000	1.51203500	0.73456000	H	0.76183300	4.78184400	2.51546200
O	-5.97631300	4.51208400	3.71392300	C	-0.25825600	4.31720200	4.37532500
H	-6.62497400	4.63686300	3.00459500	H	0.59156100	3.76699000	4.79802400
O	-3.60210700	6.02496400	3.75920400	H	-1.16697000	3.78324400	4.67997400
H	-4.53038400	6.30547800	3.85000000	C	-0.28030700	5.74933000	4.92067200
O	-1.89913900	4.49432500	2.20248500	H	-0.35208400	5.74660900	6.01323700
H	-2.58821500	5.08413600	1.83174500	H	0.63057500	6.29505000	4.64712100
O	-3.42358600	2.00883100	2.79478000	H	-1.13724800	6.31149700	4.53091800
				C	2.03984700	-0.40828800	3.51033100
2A-EE, electron energy = -6485.125926 a.u.				H	2.84043400	-1.15765000	3.49691600
C	-3.26251100	-1.20906600	0.72375300	H	1.13471300	-0.88802400	3.89009900

C	2.44474300	0.77370800	4.38618000	O	-7.82179300	-0.94554700	1.20360500
H	1.64533100	1.52308700	4.35765100	O	-9.61898800	1.31063100	1.78411100
H	3.34381900	1.24430600	3.96786100	H	-10.11972800	1.61056500	2.56400000
C	2.71366700	0.33756900	5.83119900	O	-9.03165700	1.31834400	4.44115300
H	3.52551900	-0.39808400	5.88143100	H	-9.15366300	0.74538000	5.21885300
H	3.00113100	1.19388400	6.45030400	O	-8.28052000	-1.37908800	4.84367900
H	1.82313400	-0.11680600	6.28208100	H	-8.89571300	-2.11533000	4.98394100
C	-2.11380800	0.39522400	3.48406200	H	-6.54382000	-1.47931700	2.77140400
H	-1.21285200	0.86654500	3.88325300	C	-7.94031200	-3.04288100	2.28108200
H	-2.91910200	1.13946000	3.49548300	H	-7.24735300	-3.46693000	1.54007300
C	-2.51366400	-0.82095300	4.31383100	H	-7.80073200	-3.58045100	3.22337200
H	-1.71248100	-1.56646000	4.25367100	O	-9.29472000	-3.23174100	1.88946400
H	-3.41287800	-1.27743300	3.87991200	H	-9.42420100	-2.68310200	1.09723000
C	-2.78023200	-0.44288500	5.77559000	C	7.48541300	-0.61506000	1.08138200
H	-1.89012100	-0.00329000	6.24170800	C	8.15094000	-1.64780600	2.00173700
H	-3.59483000	0.28687100	5.85744300	H	6.42716000	-0.54375600	1.34701200
H	-3.06258700	-1.32419500	6.36108500	C	8.03522200	1.22201900	2.52959100
C	0.07909500	-4.27404700	2.69229700	C	8.21420800	-1.10809600	3.43297700
H	0.94038000	-4.77332600	2.22663400	H	7.54445300	-2.56565500	1.98550800
H	-0.83265000	-4.75987400	2.31719800	C	8.82351200	0.29082200	3.46367700
C	0.15788100	-4.36343300	4.20841900	H	7.19387500	-1.05278500	3.84443400
H	-0.70224100	-3.83695600	4.64035200	H	9.85657000	0.23677900	3.10462400
H	1.05787700	-3.83538000	4.54730700	H	6.99160900	1.29488800	2.87608900
C	0.18362000	-5.81610400	4.69649700	C	8.62322600	2.62526500	2.42595400
H	0.23867400	-5.85679200	5.78928400	H	7.98855400	3.22574300	1.75835400
H	-0.71835900	-6.35740700	4.38700800	H	8.61997600	3.09758200	3.41260600
H	1.05109800	-6.35543400	4.29785800	O	8.08249300	0.67984700	1.20013300
N	-0.04114800	2.44418200	-3.15293700	O	9.45888200	-1.90856000	1.50969200
N	0.03879500	-2.20741900	-3.24396300	H	9.93187100	-2.34385900	2.24175100
N	1.14037500	4.39694800	-3.75376200	O	9.00142300	-2.02605100	4.18490400
N	-1.16645200	-4.11700700	-3.92911800	H	9.26557200	-1.54871700	4.99145300
N	7.64390700	-1.05657000	-0.28654500	O	8.78130100	0.71770900	4.82699300
N	6.03166300	0.27819500	-1.37615700	H	9.52383000	1.32228600	4.97979400
N	-6.08899900	-0.09445400	-1.43562200	O	9.97285000	2.60606700	1.97696400
N	-7.77284100	0.94996300	-0.14931000	H	9.96987200	2.11472900	1.13794600
C	-7.31304900	0.47256200	-1.34387700	C	-0.62086100	-5.11723600	-3.03891600
C	7.19959900	-0.40578900	-1.40431100	C	-1.54009700	-6.34586500	-3.07062300
C	0.63253500	3.16954900	-4.07413700	H	-0.57820400	-4.74305900	-2.01240500
C	-0.63684500	-2.88627000	-4.19906900	C	1.35433400	-6.44175300	-2.69618200
H	5.86795700	0.81893700	-2.21737800	C	-0.88204100	-7.50581600	-2.31993000
H	8.53767600	-1.51267000	-0.43994200	H	-2.48627600	-6.08248000	-2.57465800
H	0.47945600	-1.36313000	-3.59048200	C	0.54224000	-7.74075000	-2.81524300
H	-1.61403300	-4.52763600	-4.74220900	H	1.40749200	-6.13617400	-1.63867400
H	-0.46105500	1.60479700	-3.53525000	H	0.50914100	-8.03187000	-3.87038400
H	1.58328000	4.84661800	-4.54850500	C	0.58113000	5.35185200	-2.82291200
H	-5.90582200	-0.50333300	-2.34456600	C	1.47542100	6.59921500	-2.81547000
H	-8.72225800	1.30156500	-0.21961200	H	0.55418200	4.93962200	-1.81038400
S	8.11027100	-0.47218200	-2.84461500	C	-1.41727400	6.62270200	-2.41759600
S	-0.84639900	-2.19581000	-5.74608300	C	0.79995800	7.71730000	-2.01811700
S	0.86756800	2.54132600	-5.64441000	H	2.43035100	6.33698700	-2.33591400
S	-8.28980800	0.60998500	-2.73873300	C	-0.63211900	7.94129100	-2.49523800
C	-7.47036600	0.44024500	1.16996100	H	-1.45566600	6.27811700	-1.37149900
C	-8.25991100	1.26222600	2.19769100	H	-0.61248800	8.27067300	-3.53926200
H	-6.40450400	0.54128800	1.39218700	H	-0.84086400	-7.26378900	-1.24602800
C	-7.60271400	-1.56899600	2.47923000	H	0.77169100	7.43506300	-0.95370100
C	-8.14033700	0.61704500	3.58042700	C	2.77005400	-6.55086100	-3.25203500
H	-7.83246100	2.27552900	2.23180700	H	3.28085900	-5.58794500	-3.10713600
C	-8.48545900	-0.86874800	3.52428100	H	3.32325500	-7.31491100	-2.69825200
H	-7.10347100	0.71934500	3.93799400	C	-2.83939300	6.72360700	-2.95823500
H	-9.53226900	-0.98049300	3.22316500	H	-3.33073700	5.74661200	-2.84331200

H	-3.40200600	7.45711800	-2.37348000
O	-0.75504000	5.64783700	-3.23928900
O	-2.86727500	7.15996500	-4.31183700
H	-2.30480600	6.53981100	-4.80616100
O	-1.18215700	8.95661800	-1.65301500
H	-1.84530900	9.44772000	-2.16217600
O	1.58969600	8.88825100	-2.19886200
H	1.02148200	9.63316800	-1.93361000
O	1.69064300	7.00478900	-4.16068900
H	2.03136700	7.91587900	-4.10816600
O	2.77888800	-6.93976300	-4.62029300
H	2.22385300	-6.29255800	-5.08760100
O	1.07662800	-8.79654900	-2.01365100
H	1.72988900	-9.27984500	-2.54269500
O	-1.69627700	-8.65346000	-2.53771800
H	-1.14140000	-9.41870700	-2.30393000
O	-1.77251700	-6.69697300	-4.42830100
H	-2.12954900	-7.60306000	-4.40703500
O	0.70605900	-5.42468800	-3.47665200