

Molecular Architecture and Symmetry Properties of 1,3-Alternate Calix[4]arenes with Orientable Groups at the *para*-Position of the Phenolic Rings

Lucio Toma,^{†*} Laura Legnani,[†] Federica Compostella,[‡] Marta Giuliani,[§] Federica Faroldi,[§]
Alessandro Casnati,[§] Francesco Sansone^{§*}

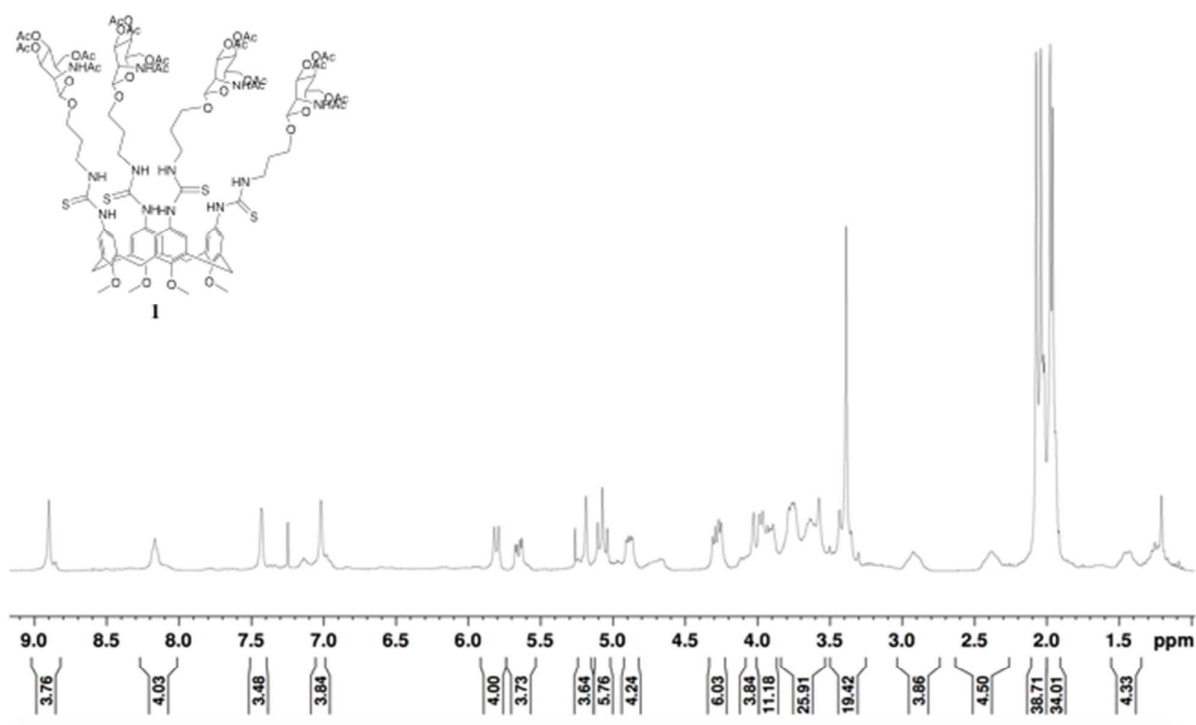
* Tel: (+39) 0382987843. Fax: (+39) 0382987323. E-mail: lucio.toma@unipv.it

* Tel: (+39)0521905458. Fax: (+39) 0521905472. E-mail: francesco.sansone@unipr.it

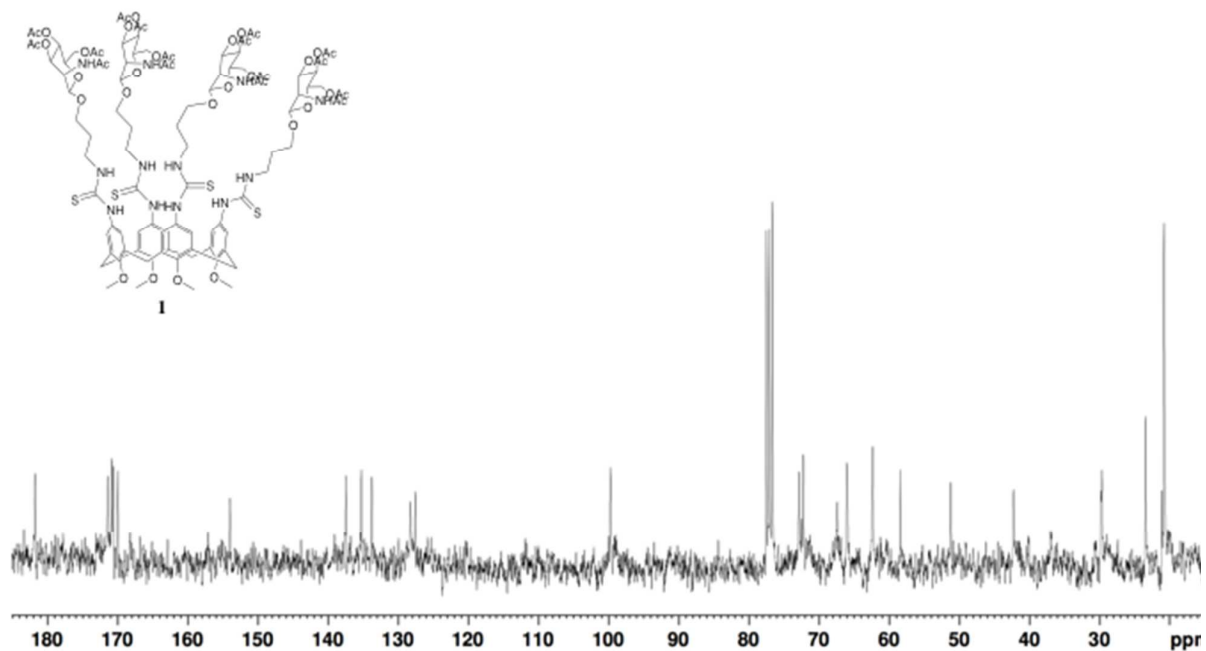
List of contents:

¹ H and ¹³ C NMR spectra of compound 1	pag. 2
¹ H- ¹ H COSY spectrum of compound 1	pag. 3
¹ H- ¹ H HSQC spectrum of compound 1	pag. 4
¹ H and ¹³ C NMR spectra of compound 2	pag. 5
¹ H- ¹ H COSY spectrum of compound 2	pag. 6
¹ H- ¹ H HSQC spectrum of compound 2	pag. 7
¹ H- ¹ H NOESY spectrum of compound 2	pag. 8
Figure 1S	pag. 9
Cartesian coordinates	pag. 10

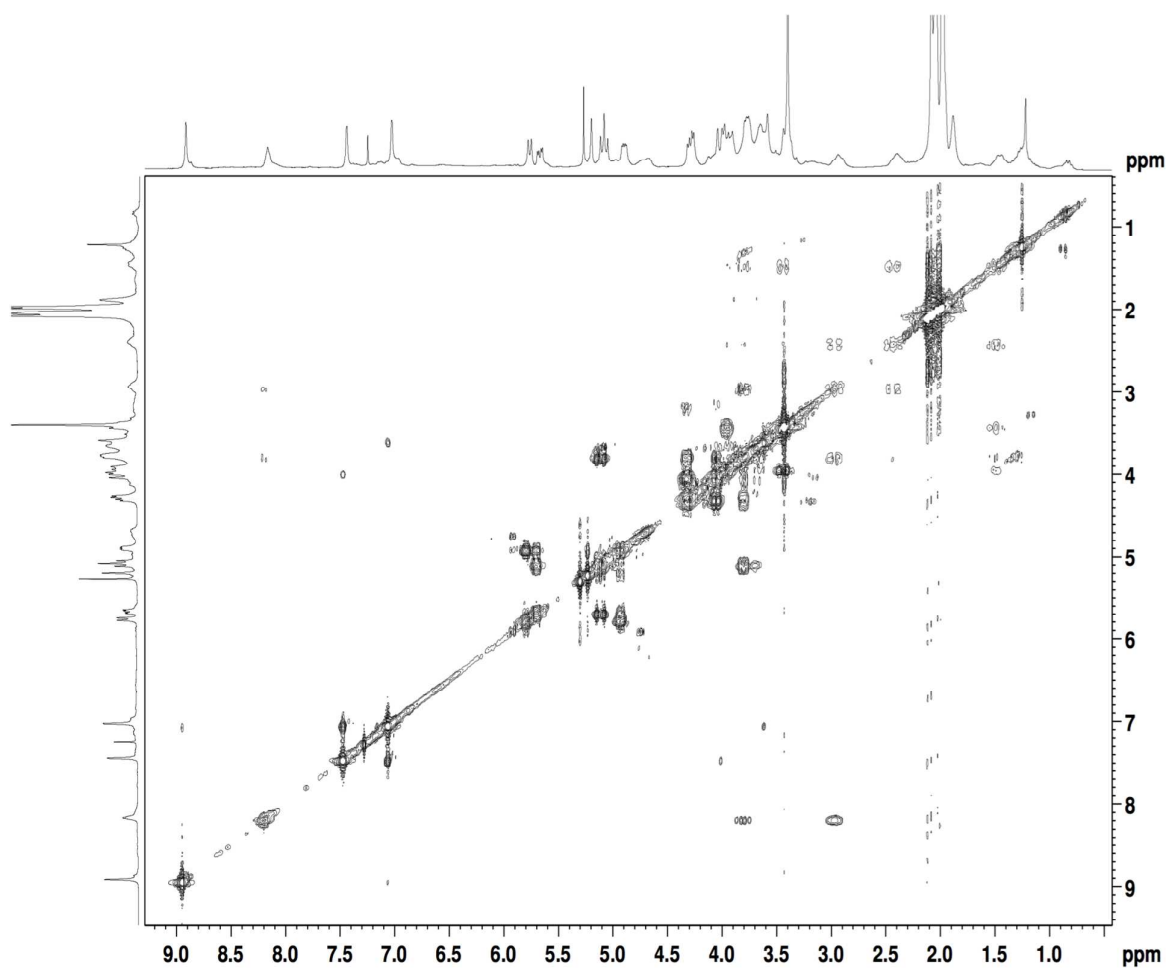
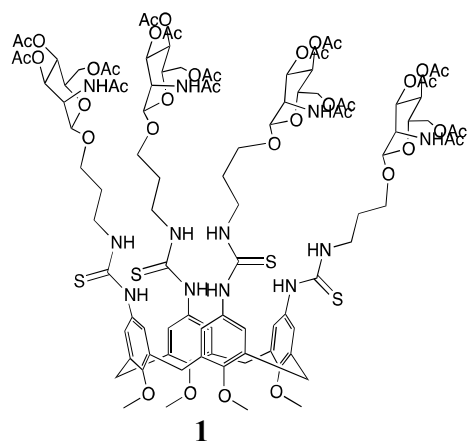
^1H NMR of **1** (CDCl_3 , 300 MHz)



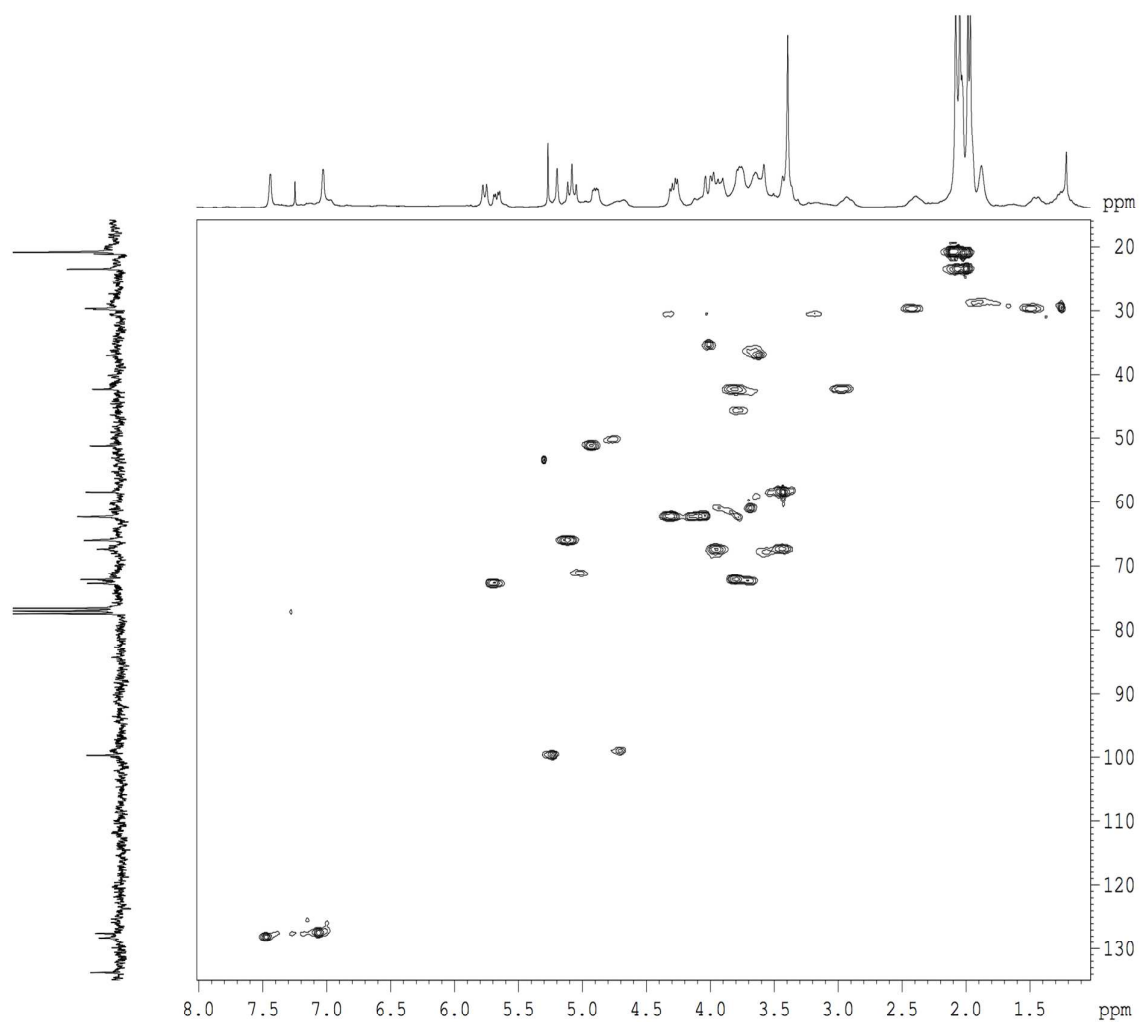
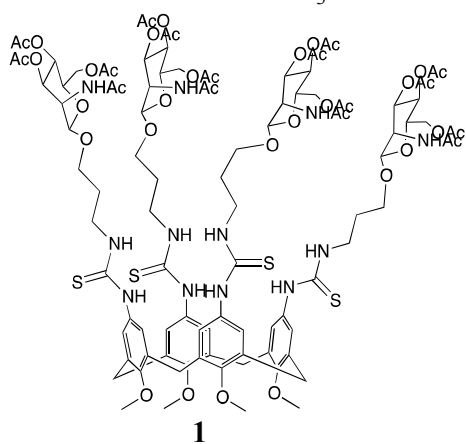
^{13}C NMR of **1** (CDCl_3 , 75 MHz)



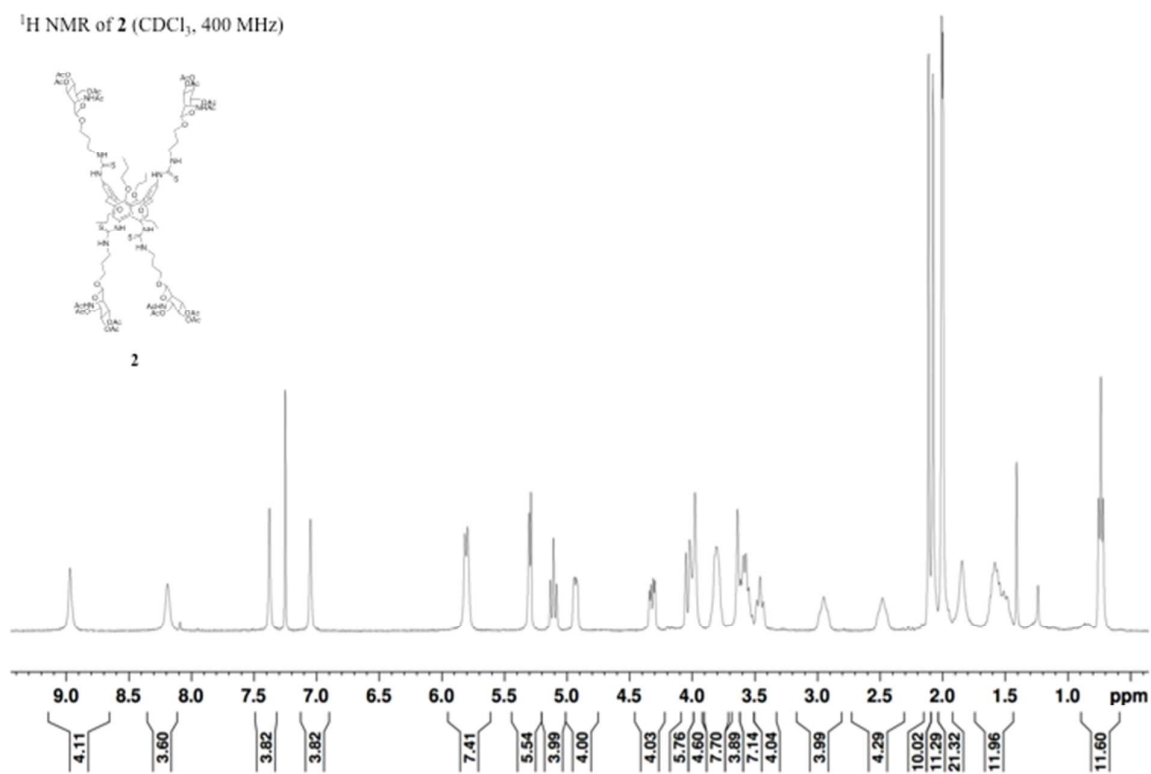
^1H - ^1H COSY of **1** (CDCl_3 , 300 MHz)



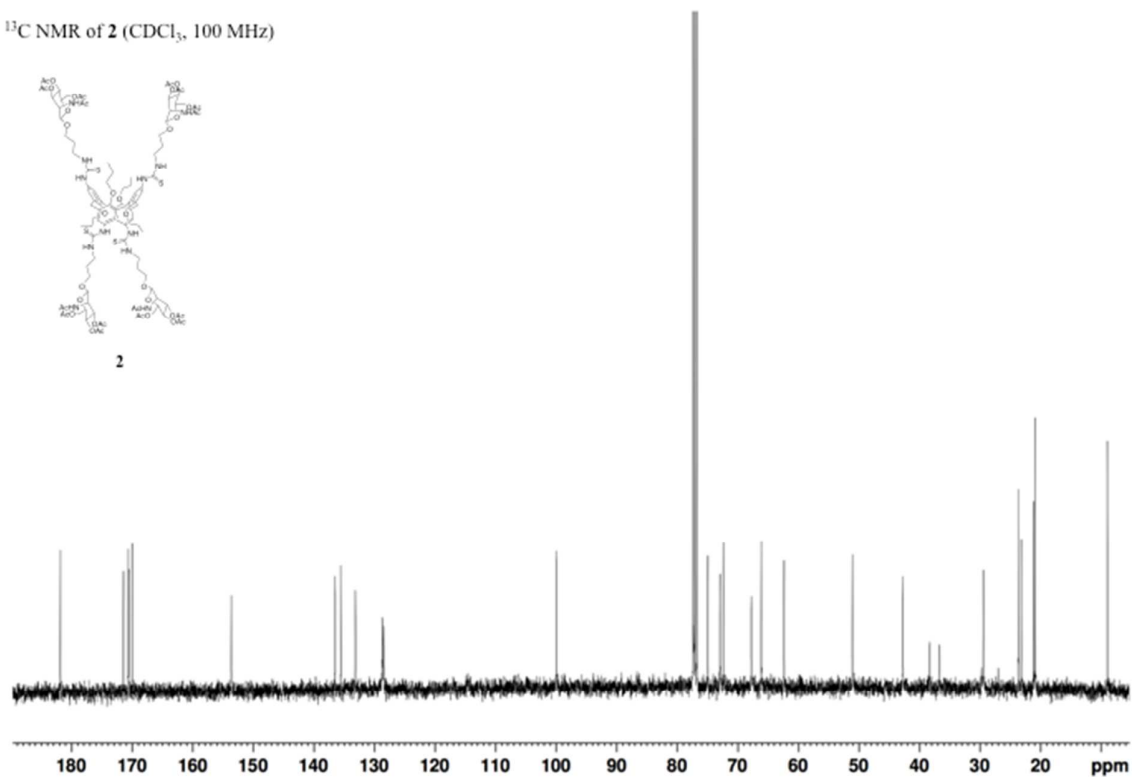
^1H - ^{13}C HSQC of **1** (CDCl_3 , 300 MHz)



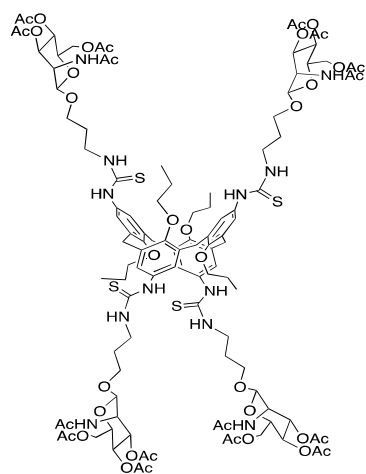
^1H NMR of **2** (CDCl_3 , 400 MHz)



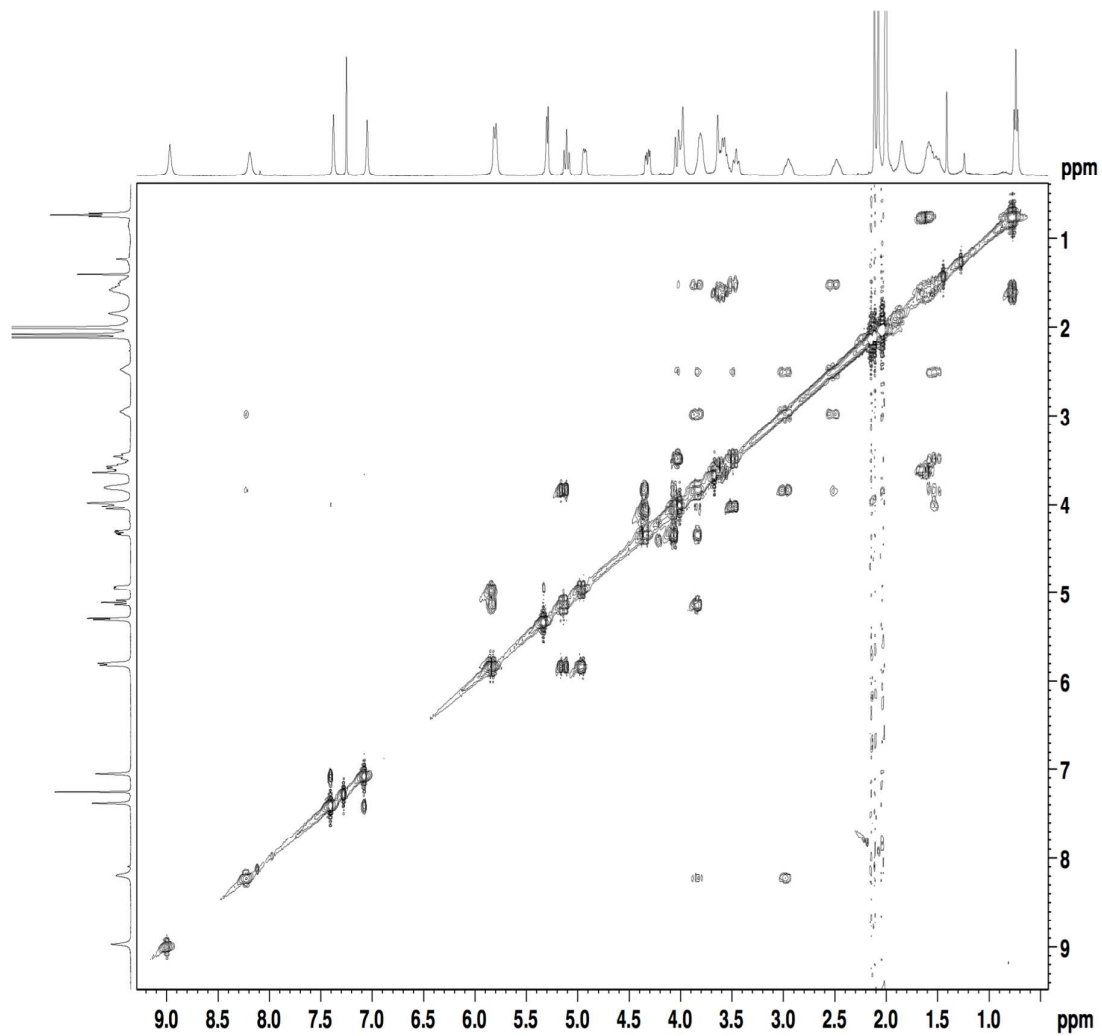
^{13}C NMR of **2** (CDCl_3 , 100 MHz)



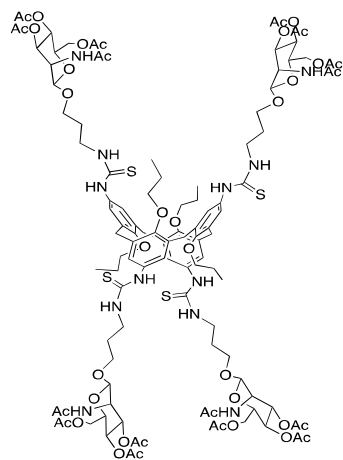
^1H - ^1H COSY of **2** (CDCl_3 , 400 MHz)



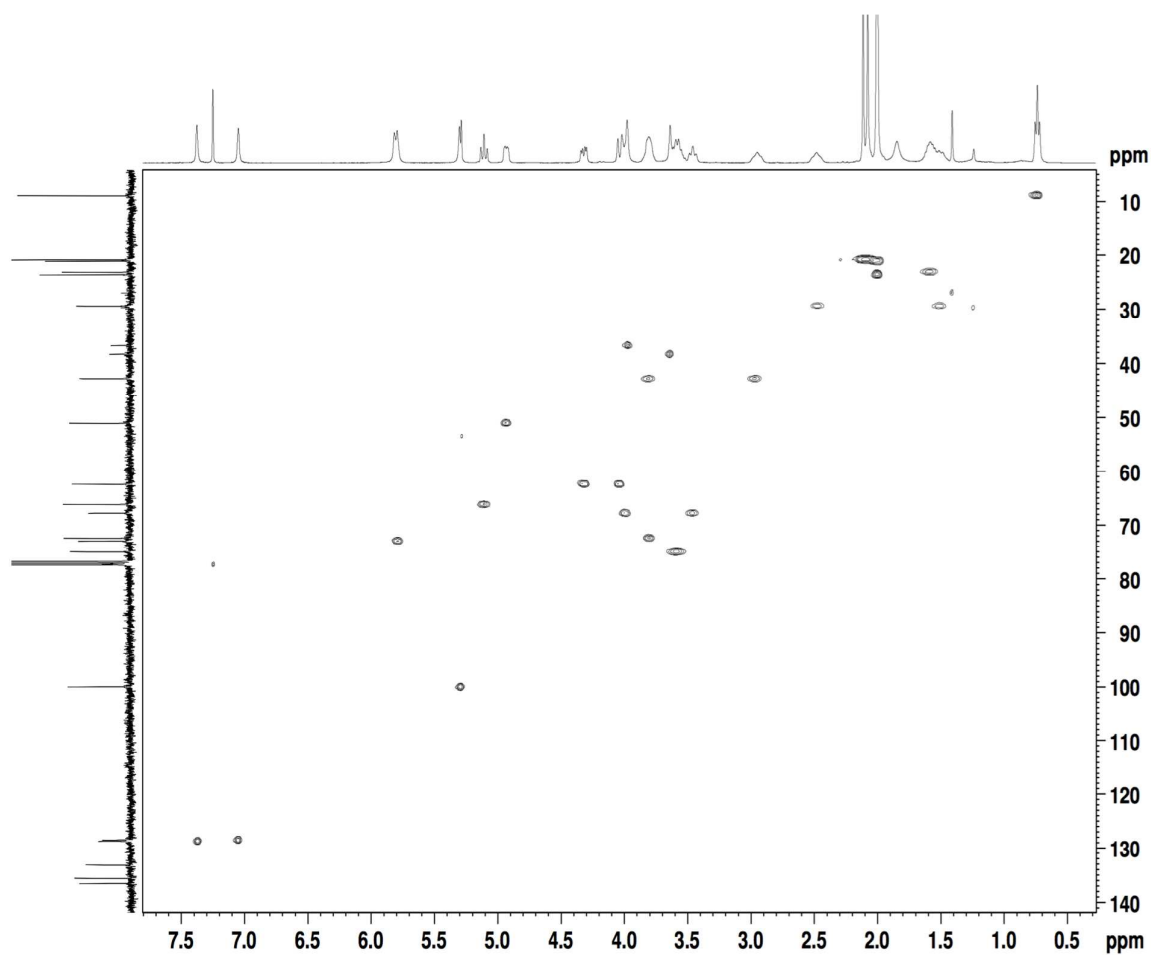
2



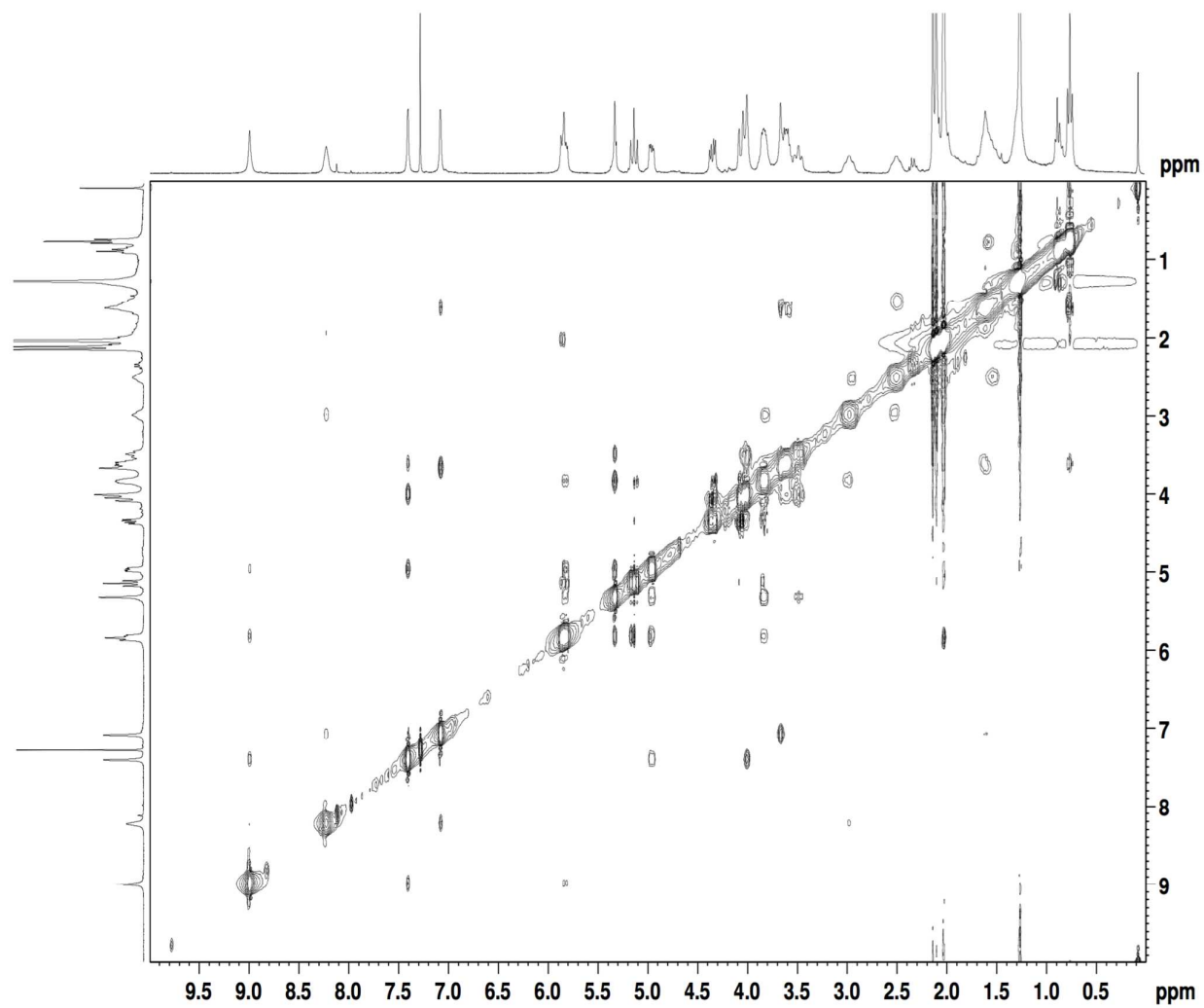
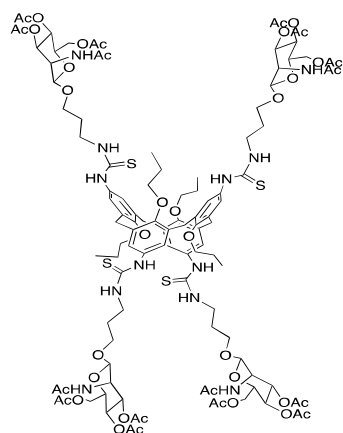
^1H - ^{13}C HSQC of **2** (CDCl_3 , 400 MHz)

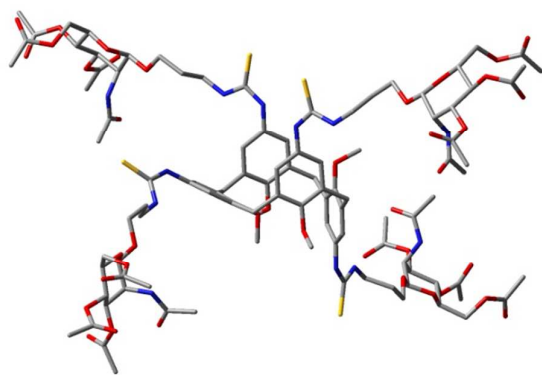


2

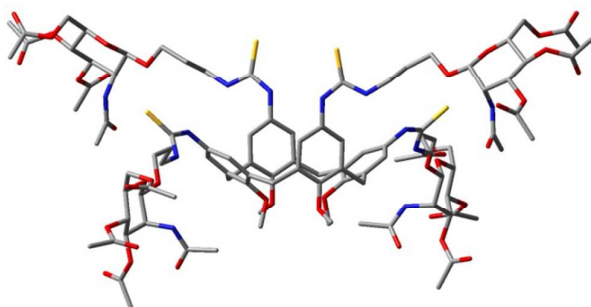


^1H - ^1H NOESY (D8 = 0.2) of **2** (CDCl_3 , 400 MHz)

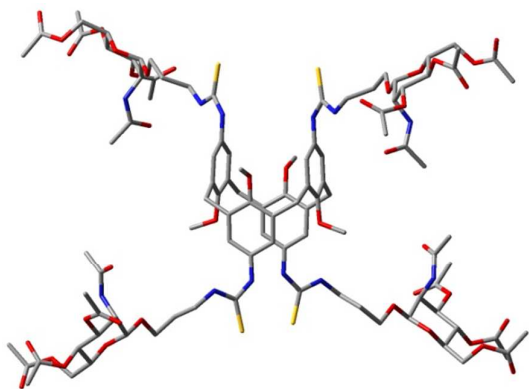




1-pcone-unfolded (0.00)



1-cone-unfolded (1.21)



1-alternate-unfolded (1.96)

Figure 1S. Three-dimensional plots of the partial *cone*, *cone*, and 1,3-alternate unfolded conformers of compound **1** (in parentheses the relative energy, kcal/mol, in methanol).

3A-EZ B3LYP/6-31G(d), electr. en. = -3884.827218 a.u.

C	0.74982000	1.02659800	-2.73796400
C	0.06176900	1.94350700	-1.92475300
C	0.74814600	2.77904600	-1.02800200
C	2.14494300	2.76724400	-1.03927700
C	2.85393100	1.94167100	-1.92147800
C	2.14522200	1.05485300	-2.73903900
H	2.68871500	3.37219100	-0.32117000
H	2.69370100	0.37438600	-3.38462500
C	-0.00010400	-0.00000800	-3.57730400
H	-0.72276400	0.49681500	-4.23356200
C	0.00003900	3.61897900	-0.00001800
H	-0.72418500	4.27555900	-0.49475100
C	-0.74996000	-1.02658800	-2.73787300
C	-0.06184600	-1.94350200	-1.92472100
C	-2.14536200	-1.05483200	-2.73882600
C	-0.74815000	-2.77904600	-1.02791500
C	-2.85400200	-1.94163400	-1.92118800
H	-2.69389300	-0.37436800	-3.38436900
C	-2.14494800	-2.76723400	-1.03907000
H	-2.68867000	-3.37220500	-0.32094300
C	-0.74812700	2.77904000	1.02791800
C	-0.06181000	1.94349300	1.92471200
C	-2.14492500	2.76723400	1.03909800
C	-0.74991400	1.02658100	2.73787500
C	-2.85396700	1.94163700	1.92123000
H	-2.68865800	3.37220700	0.32098000
C	-2.14531500	1.05483100	2.73885200
H	-2.69383800	0.37436800	3.38440500
C	-0.00004700	-0.00000200	3.57729300
H	-0.72269900	-0.49682600	4.23356000
C	0.00003100	-3.61898800	0.00000800
H	-0.72418600	-4.27556800	0.49475100
H	0.72427500	-4.27551700	-0.49476400
C	2.14526400	-1.05486100	2.73898800
C	2.85395900	-1.94168000	1.92141600
C	0.74986300	-1.02660800	2.73794100
C	2.14495400	-2.76725300	1.03922800
C	0.06179600	-1.94351800	1.92474400
C	0.74815600	-2.77905700	1.02798000
H	2.68871200	-3.37219700	0.32110700
H	2.69375500	-0.37439200	3.38456100
O	1.32218700	-1.97874500	-1.96392200
O	-1.32224100	-1.97873200	1.96382500
O	1.32222300	1.97873100	1.96388900
O	-1.32226900	1.97872100	-1.96380700
C	1.85267500	2.91607100	2.90121300
H	1.54277400	2.68103100	3.92812700
H	1.53634000	3.94220000	2.67093400
C	-1.85277700	-2.91610300	2.90106900
H	-1.54292800	-2.68112900	3.92801400
H	-1.53646100	-3.94223000	2.67075300
C	-1.85282300	2.91609400	-2.90104100
H	-1.53650100	3.94222000	-2.67073000
H	-1.54299500	2.68112000	-3.92799200
C	1.85262000	-2.91608600	-2.90125400
H	1.54270300	-2.68104400	-3.92816300
H	1.53628400	-3.94221400	-2.67097000
H	0.72256900	0.49683600	4.23359000
H	0.72429100	4.27550800	0.49474100

H	0.72250300	-0.49684800	-4.23360900
H	-2.94075100	2.84833400	-2.82599400
H	-2.94070600	-2.84834300	2.82604400
H	2.94055700	-2.84836800	-2.82630700
H	2.94061100	2.84834900	2.82624800
N	4.27074100	1.92484500	-1.94795600
H	4.72790300	1.02800000	-2.04870500
C	5.15292500	2.97988400	-2.02933000
S	6.81054600	2.68970700	-2.06337700
N	4.60803300	4.21913800	-2.08199200
C	5.39478000	5.42923100	-2.25876800
H	5.90351500	5.44540200	-3.22968800
H	4.71817600	6.28528800	-2.18592800
H	6.15685000	5.49884700	-1.47907200
H	3.60893400	4.28630200	-2.22829300
N	-4.27077700	1.92484300	1.94761000
H	-4.72798500	1.02802700	2.04841000
S	-6.81054700	2.68991200	2.06269000
C	-5.15289700	2.97994500	2.02877300
N	-4.60788400	4.21915800	2.08112800
C	-5.39450900	5.42938400	2.25753500
H	-4.71781200	6.28534800	2.18447700
H	-6.15654600	5.49886200	1.47779500
H	-5.90327300	5.44587800	3.22843400
H	-3.60878000	4.28625500	2.22743300
N	-4.27081200	-1.92483500	-1.94754300
H	-4.72802000	-1.02801800	-2.04834100
C	-5.15293600	-2.97993600	-2.02867300
S	-6.81058700	-2.68990100	-2.06255500
N	-4.60792500	-4.21915000	-2.08101900
C	-5.39455600	-5.42937900	-2.25738500
H	-4.71785600	-6.28534100	-2.18433600
H	-6.15657000	-5.49884700	-1.47762100
H	-5.90334900	-5.44588500	-3.22826900
H	-3.60882400	-4.28625100	-2.22734100
N	4.27077000	-1.92484800	1.94786500
H	4.72792700	-1.02799800	2.04859500
C	5.15296700	-2.97987700	2.02923000
S	6.81058400	-2.68967800	2.06323700
N	4.60809400	-4.21913700	2.08194100
C	5.39486600	-5.42921400	2.25872400
H	4.71826900	-6.28528100	2.18594700
H	6.15690100	-5.49884800	1.47899600
H	5.90364500	-5.44534200	3.22962100
H	3.60900000	-4.28631300	2.22826900

3B-EZ B3LYP/6-31G(d), electr. en. = -3884.833252 a.u.

C	0.64872700	-1.63893900	2.76134800
C	-0.00870100	-2.55532100	1.92550300
C	0.70975400	-3.38893700	1.04973700
C	2.10341900	-3.35689300	1.09879900
C	2.78190400	-2.51277100	1.98456300
C	2.04489000	-1.64839600	2.80139800
H	2.67793700	-3.97945800	0.41898700
H	2.56302000	-0.98295100	3.48404000
C	-0.13063500	-0.61892500	3.58102300
H	-0.87950100	-1.11545600	4.20709400
C	-0.00004100	-4.23518800	0.00021800
H	-0.74126400	-4.89136900	0.46893100
C	-0.84418900	0.41105300	2.71450000

C	-0.12718700	1.32947400	1.92685500	H	-4.62774700	-3.48885800	-2.04591000
C	-2.23905300	0.43966400	2.66315900	S	-6.75163600	-1.91415400	-2.27442800
C	-0.77946700	2.16390100	1.00366200	C	-5.12049900	-1.55323200	-2.05620800
C	-2.91649000	1.33035600	1.82450700	N	-4.64314900	-0.29975100	-1.87648100
H	-2.81054000	-0.24127200	3.28757700	C	-5.51078900	0.86592200	-1.76451400
C	-2.17605000	2.15487000	0.96780700	H	-4.87421200	1.75385200	-1.71445100
H	-2.69451500	2.76989900	0.23912200	H	-6.16257300	0.93152000	-2.63888600
C	-0.70984400	-3.38902800	-1.04936900	H	-6.14040200	0.82591900	-0.86885600
C	0.00860900	-2.55549500	-1.92521400	H	-3.67808000	-0.19041000	-1.58621100
C	-2.10351100	-3.35698900	-1.09843000	N	-4.33484800	1.32894300	1.80176700
C	-0.64882000	-1.63918000	-2.76113500	H	-4.80559200	0.43712400	1.88486400
C	-2.78199500	-2.51294500	-1.98426600	C	-5.19878200	2.39731700	1.92761000
H	-2.67802800	-3.97950500	-0.41857300	S	-6.86161300	2.13860200	1.92907300
C	-2.04498100	-1.64864100	-2.80117700	N	-4.63071300	3.62098700	2.04078200
H	-2.56311400	-0.98326900	-3.48388800	C	-5.39562100	4.83917200	2.25778100
C	0.13053000	-0.61925000	-3.58092800	H	-4.70091000	5.68312900	2.23101400
H	-0.56764800	-0.12626100	-4.26576000	H	-6.14487600	4.95759000	1.47154300
C	0.00018300	3.00443800	-0.00009600	H	-5.91742000	4.82414900	3.22152200
H	-0.70870500	3.66062500	-0.51696600	H	-3.63143000	3.66273900	2.19551400
H	0.70915200	3.66056100	0.51674200	N	4.33497700	1.32854600	-1.80213000
C	2.23907600	0.43929600	-2.66330200	H	4.80569600	0.43671800	-1.88526500
C	2.91661800	1.33000300	-1.82475200	C	5.19891100	2.39691600	-1.92799700
C	0.84420500	0.41074600	-2.71452500	S	6.86174400	2.13820400	-1.92961400
C	2.17628800	2.15462000	-0.96806000	N	4.63081800	3.62058700	-2.04103100
C	0.12731200	1.32926800	-1.92689400	C	5.39569200	4.83879700	-2.25800800
C	0.77970400	2.16374200	-1.00382400	H	4.70098200	5.68274900	-2.23106600
H	2.69484700	2.76967600	-0.23946300	H	6.14504800	4.95713600	-1.47185500
H	2.81048100	-0.24169800	-3.28773200	H	5.91736600	4.82387300	-3.22181900
O	1.25570700	1.38314800	2.03231600	H	3.63151800	3.66233500	-2.19566200
O	-1.25558800	1.38298500	-2.03225300	3C-EZ B3LYP/6-31G(d), electr. en. = -3884.837007			
O	1.39391000	-2.59745900	-1.92623400	a.u.			
O	-1.39400300	-2.59725100	1.92651300	C	0.74335800	-2.76380200	-1.01943400
C	1.94251700	-3.54819400	-2.84052000	C	0.05740900	-1.94544100	-1.93194200
H	1.66091200	-3.32061400	-3.87716900	C	0.74383500	-1.02702000	-2.74621500
H	1.61278300	-4.56935500	-2.60906000	C	2.13850100	-1.01993100	-2.70583500
C	-1.71308300	2.31232500	-3.01875200	C	2.84833300	-1.89374700	-1.87444800
H	-1.31832600	2.07045700	-4.01354900	C	2.13986000	-2.74786400	-1.02291500
H	-1.42060600	3.34048200	-2.76799400	H	2.68745900	-0.31233300	-3.32068900
C	-1.94264500	-3.54794200	2.84082500	H	2.67858600	-3.42065300	-0.36443300
H	-1.61294700	-4.56912200	2.60939800	C	0.00021400	-3.61688700	0.00009900
H	-1.66103300	-3.32034000	3.87746800	H	-0.72547900	-4.27204000	-0.49301900
C	1.71316600	2.31248800	3.01883300	C	0.00010200	0.00002700	-3.59126400
H	1.31834900	2.07064700	4.01361200	H	-0.72545200	-0.49301700	-4.24695000
H	1.42073000	3.34064900	2.76804200	C	-0.74303800	-2.76386300	1.01960100
H	0.87932900	-1.11584800	-4.20702500	C	-0.05720000	-1.94545400	1.93215500
H	0.74118700	-4.89140200	-0.46844300	C	-2.13953900	-2.74801100	1.02299800
H	0.56751700	-0.12592800	4.26587500	C	-0.74373600	-1.02706900	2.74637600
H	-3.02880800	-3.48684200	2.73797800	C	-2.84812200	-1.89393200	1.87448200
H	-2.80271000	2.23829800	-3.03633300	H	-2.67818300	-3.42083200	0.36448200
H	2.80279000	2.23843100	3.03647800	C	-2.13840000	-1.02007100	2.70591200
H	3.02868300	-3.48713000	-2.73767600	H	-2.68744100	-0.31249300	3.32071700
N	4.19561800	-2.57434100	2.04603900	C	-0.74370100	1.02705900	-2.74626100
H	4.62767300	-3.48865100	2.04625100	C	-0.05732700	1.94553300	-1.93200200
C	5.12038100	-1.55300700	2.05637700	C	-2.13836700	1.01989900	-2.70589100
S	6.75153300	-1.91385400	2.27460500	C	-0.74332400	2.76387400	-1.01950800
N	4.64297200	-0.29957400	1.87647800	C	-2.84824600	1.89370600	-1.87454000
C	5.51054600	0.86613700	1.76434400	H	-2.68728400	0.31224900	-3.32072400
H	6.14016500	0.82604100	0.86869500	C	-2.13982300	2.74787600	-1.02301500
H	4.87391400	1.75402000	1.71413900	H	-2.67859400	3.42063800	-0.36454100
H	6.16231200	0.93190800	2.63871700	C	-0.00022700	3.61696100	0.00005600
H	3.67790000	-0.19033200	1.58618300	H	-0.72601100	4.27202500	0.49316300
N	-4.19571000	-2.57453900	-2.04575900				

C	-0.00009700	0.00005500	3.59141100
H	-0.72573000	0.49303100	4.24706200
H	0.72552500	-0.49290900	4.24707800
C	2.13948700	2.74801000	1.02299100
C	2.84801800	1.89391100	1.87449500
C	0.74298400	2.76393100	1.01958600
C	2.13824200	1.02009100	2.70592800
C	0.05709800	1.94557900	1.93215000
C	0.74357800	1.02716000	2.74637900
H	2.68724200	0.31248900	3.32074200
H	2.67816600	3.42079000	0.36446200
O	1.32800700	-2.02192800	2.00851000
O	-1.32810000	2.02216900	2.00852400
O	1.32787800	2.02215900	-2.00824500
O	-1.32780200	-2.02198200	-2.00818200
C	1.78448100	2.98863500	-2.95970300
H	1.41905000	3.99466600	-2.71823400
H	1.45985200	2.73481800	-3.97696700
C	-1.78463500	2.98864000	2.96002400
H	-1.41917700	3.99466300	2.71856200
H	-1.45998000	2.73479100	3.97727100
C	-1.78446800	-2.98840200	-2.95966700
H	-1.45990300	-2.73452800	-3.97693700
H	-1.41902500	-3.99444700	-2.71827500
C	1.78463600	-2.98837500	2.95998600
H	1.41933100	-3.99443900	2.71846300
H	1.45989600	-2.73461500	3.97722800
H	0.72548400	4.27212100	-0.49302600
H	0.72570100	0.49307200	-4.24689700
H	0.72597700	-4.27195800	0.49322600
H	-2.87608700	-2.98158300	-2.91414400
H	-2.87625800	2.98186500	2.91460800
H	2.87625900	-2.98144100	2.91461900
H	2.87610200	2.98181700	-2.91424700
N	4.26244200	-1.90492900	-1.94706200
H	4.68281300	-1.89021000	-2.86696900
C	5.20125600	-1.99588100	-0.94214600
S	6.82285500	-2.21280000	-1.34478700
N	4.74795000	-1.88503900	0.32756000
C	5.64049700	-1.83377600	1.47961900
H	6.29115300	-0.95307600	1.44647000
H	5.02138600	-1.79573500	2.38047400
H	6.26974900	-2.72662600	1.50669000
H	3.78597800	-1.60026900	0.47233200
N	-4.26235600	1.90480400	-1.94714200
H	-4.68273800	1.89003800	-2.86704400
S	-6.82277700	2.21256300	-1.34483300
C	-5.20115700	1.99574600	-0.94221600
N	-4.74780800	1.88503800	0.32748500
C	-5.64031700	1.83382700	1.47957700
H	-5.02117700	1.79591600	2.38041700
H	-6.26963000	2.72663600	1.50657800
H	-6.29090800	0.95307500	1.44653200
H	-3.78581100	1.60034700	0.47224800
N	-4.26223800	-1.90518100	1.94697600
H	-4.68268600	-1.89051400	2.86684800
C	-5.20096500	-1.99612100	0.94197900
S	-6.82259400	-2.21308200	1.34448200
N	-4.74756900	-1.88517300	-0.32768400
C	-5.64003000	-1.83386000	-1.47980700
H	-5.02085200	-1.79573500	-2.38061200
H	-6.26925200	-2.72672800	-1.50698700

H	-6.29071200	-0.95317900	-1.44664400
H	-3.78559200	-1.60037600	-0.47236500
N	4.26213100	1.90508900	1.94700600
H	4.68257000	1.89038200	2.86688200
C	5.20087100	1.99600600	0.94201700
S	6.82250700	2.21288000	1.34453200
N	4.74747200	1.88509100	-0.32764900
C	5.63993000	1.83373400	-1.47977300
H	5.02074900	1.79564400	-2.38057900
H	6.26919700	2.72657100	-1.50695300
H	6.29056700	0.95302100	-1.44661100
H	3.78548500	1.60032700	-0.47233000

3D-EZ B3LYP/6-31G(d), electr. en. = -3884.826021 a.u.

C	0.56524000	2.48853500	1.14904400
C	-0.25687000	1.64435500	1.91420900
C	0.28974100	0.74327900	2.84513000
C	1.66175600	0.79507900	3.09407200
C	2.49099000	1.68902700	2.40831000
C	1.93817400	2.49909400	1.40840200
H	2.09751600	0.12942400	3.83426000
H	2.59291300	3.10996300	0.79557600
C	-0.00100300	3.32406700	0.00746500
H	-0.79788800	3.98004800	0.37515700
C	-0.57965500	-0.28833800	3.55310400
H	-1.39942400	0.20606500	4.08592500
C	-0.56602200	2.49328600	-1.13821100
C	0.25711500	1.65326700	-1.90686100
C	-1.93885100	2.50392500	-1.39819200
C	-0.28830200	0.75622100	-2.84234800
C	-2.49048700	1.69820400	-2.40226200
H	-2.59440500	3.11133500	-0.78279200
C	-1.66019200	0.80824200	-3.09189200
H	-2.09506800	0.14575600	-3.83543300
C	-1.18279700	-1.32025400	2.60861000
C	-0.37093200	-2.21959900	1.89768000
C	-2.56048600	-1.33573900	2.37577200
C	-0.90304500	-3.03860200	0.88661900
C	-3.12705500	-2.22406500	1.45311000
H	-3.19591100	-0.61633200	2.88165500
C	-2.28492900	-3.04275700	0.69334800
H	-2.71782400	-3.69321900	-0.06172200
C	-0.00156300	-3.87749300	-0.00951900
H	-0.63711300	-4.53196400	-0.61581200
C	0.58224900	-0.27166800	-3.55426300
H	-0.02775800	-0.75910500	-4.32263100
H	1.40296800	0.22545800	-4.08302400
C	2.28317000	-3.04149100	-0.70670800
C	3.12645800	-2.21942100	-1.46152800
C	0.90143500	-3.03521700	-0.90091600
C	2.56125200	-1.32599800	-2.38010100
C	0.37070600	-2.21071500	-1.90824300
C	1.18377400	-1.30850100	-2.61411500
H	3.19752000	-0.60439300	-2.88179900
H	2.71503700	-3.69603000	0.04541700
O	1.62462000	1.66202600	-1.69322700
O	-0.99012800	-2.24559800	-2.16872800
O	0.99003400	-2.25680600	2.15714700
O	-1.62448400	1.65336200	1.70129500
C	1.35901200	-3.19820100	3.16504900
H	1.09013200	-4.22380600	2.87943600

H	0.88102400	-2.96971100	4.12691600	C	0.17306400	-2.84723100	1.35603600
C	-1.35925200	-3.18189200	-3.18132000	C	1.53784900	-3.14060900	1.39001200
H	-1.09124300	-4.20904100	-2.90049300	C	2.39757000	-2.46405100	2.26138000
H	-0.88061000	-2.94915700	-4.14184400	C	1.88106600	-1.46290500	3.09002900
C	-2.34037300	2.57554300	2.52289100	H	1.93613600	-3.91124700	0.73815000
H	-2.21989600	2.34525100	3.58993300	H	2.56137800	-0.89613300	3.71919100
H	-2.01095300	3.60941500	2.35327300	C	0.00013800	0.00096600	3.93787500
C	2.34032500	2.58905800	-2.50950700	H	-0.81054600	-0.33117300	4.59538500
H	2.01036500	3.62181800	-2.33427000	C	-0.72782200	-3.52918200	0.33560000
H	2.22028100	2.36461500	-3.57784500	H	-1.57503200	-4.01182600	0.83439500
H	0.63268200	-4.53673100	0.59300600	C	-0.51887000	1.16116200	3.09751000
H	0.03168600	-0.77979000	4.31782400	C	0.33402800	1.89582500	2.25425900
H	0.79486700	3.98312300	-0.35698000	C	-1.88090000	1.46441200	3.08951900
H	-3.39339500	2.48115500	2.24796500	C	-0.17306300	2.84788600	1.35466200
H	-2.44400800	-3.10926700	-3.29187100	C	-2.39747600	2.46517200	2.26043900
H	3.39330800	2.49364300	-2.23478900	H	-2.56115900	0.89797200	3.71903500
H	2.44387500	-3.12685900	3.27540500	C	-1.53785100	3.14129700	1.38864700
N	3.88015500	1.69405300	2.68859100	H	-1.93621100	3.91159100	0.73642700
H	4.32303000	0.80472400	2.87801600	C	-1.28106700	-2.57123200	-0.71237600
C	4.71800100	2.76051900	2.93099400	C	-0.43653400	-1.88884300	-1.60439400
S	6.34159100	2.48998600	3.28352400	C	-2.65220200	-2.30358000	-0.75157800
N	4.15927400	3.99288200	2.87191000	C	-0.93022000	-0.86854500	-2.43648800
C	4.88469500	5.21322100	3.18687000	C	-3.18326400	-1.37966900	-1.66094700
H	5.77168700	5.29820300	2.55455100	H	-3.30683300	-2.78430600	-0.03248200
H	4.21890700	6.05971900	2.99713300	C	-2.30695900	-0.64469900	-2.46752000
H	5.21288500	5.23153900	4.23254700	H	-2.70923500	0.11100300	-3.13714200
H	3.15032500	4.04915300	2.81814100	C	-0.00005500	-0.00083900	-3.27361000
N	-4.52272500	-2.25785100	1.21051400	H	-0.61572900	0.62266800	-3.93118700
H	-4.82833200	-2.37173100	0.25319000	C	0.72770200	3.52932600	0.33377900
S	-7.14882100	-2.43812300	1.54905600	H	0.15500300	4.33143900	-0.14509200
C	-5.56312900	-2.35829600	2.10826500	H	1.57488200	4.01237900	0.83223900
N	-5.22831500	-2.39165900	3.42011400	C	2.30684100	0.64351600	-2.46793100
C	-6.19912400	-2.58345000	4.48582000	C	3.18317700	1.37887000	-1.66174500
H	-5.67352000	-2.49617800	5.44076800	C	0.93009600	0.86736100	-2.43698400
H	-6.97818200	-1.81972800	4.42682400	C	2.65212400	2.30318800	-0.75276100
H	-6.68338000	-3.56477400	4.42173000	C	0.43643300	1.88804900	-1.60537400
H	-4.25010100	-2.50599200	3.65276000	C	1.28099700	2.57084100	-0.71367700
N	-3.87954600	1.70329200	-2.68315700	H	3.30674000	2.78421000	-0.03385500
H	-4.32157300	0.81442300	-2.87666600	H	2.70907500	-0.11252700	-3.13719600
C	-4.71800100	2.77010600	-2.92184500	O	1.69445700	1.63753800	2.26749800
S	-6.34110900	2.49980400	-3.27677100	O	-0.91724900	2.19786000	-1.63728200
N	-4.16024100	4.00262100	-2.85726200	O	0.91716700	-2.19856000	-1.63626700
C	-4.88635200	5.22365500	-3.16791600	O	-1.69438300	-1.63645400	2.26843400
H	-4.22118700	6.06987500	-2.97479300	C	1.23472900	-3.24576200	-2.55697600
H	-5.21418300	5.24561500	-4.21363300	H	1.01291500	-2.95243200	-3.59139600
H	-5.77363900	5.30571600	-2.53561400	H	0.68036900	-4.16484000	-2.32870600
H	-3.15137900	4.05941500	-2.80242500	C	-1.23485700	3.24435200	-2.55877000
N	4.52186800	-2.25530300	-1.21774500	H	-1.01295700	2.95033300	-3.59297300
H	4.82642500	-2.37445500	-0.26073000	H	-0.68059000	4.16364500	-2.33110900
C	5.56312200	-2.35188400	-2.11492800	C	-2.42867500	-2.41743600	3.21226200
S	7.14817400	-2.43570600	-1.55448900	H	-2.34725300	-3.49151000	2.99834300
N	5.22962000	-2.37820000	-3.42726800	H	-2.08230600	-2.24269500	4.23925400
C	6.20137500	-2.56537700	-4.49293900	C	2.42884700	2.41915400	3.21072400
H	5.67684800	-2.47275200	-5.44797300	H	2.08272800	2.24493100	4.23789100
H	6.98103700	-1.80265700	-4.42921100	H	2.34722400	3.49309700	2.99622500
H	6.68471900	-3.54743800	-4.43337100	H	0.61564400	-0.62476500	-3.93076700
H	4.25156900	-2.49076800	-3.66146700	H	-0.15524200	-4.33166400	-0.14280400
3E-EZ B3LYP/6-31G(d), electr. en. = -3884.830598				H	0.81091700	0.33345100	4.59509300
a.u.				H	-3.47263300	-2.10778600	3.12393800
C	0.51903100	-1.15965400	3.09802600	H	-2.30536100	3.43722300	-2.45700100
C	-0.33395300	-1.89472400	2.25522400	H	3.47282800	2.10959800	3.12234600
				H	2.30521000	-3.43866100	-2.45501400

N	3.77688800	-2.78481400	2.33719400	H	3.63166100	-2.93101400	0.89619100
H	4.19178400	-2.88172200	3.25434400	C	-0.19750800	2.89015600	-1.01480200
C	4.69778400	-2.90666100	1.32194700	C	-0.57494200	1.83814700	-1.86699000
S	6.27030100	-3.39546900	1.67330100	C	1.10066300	3.39032000	-1.11479700
N	4.26233300	-2.61243100	0.07243600	C	0.35472100	1.22701500	-2.72527300
C	5.15466100	-2.57510300	-1.07665300	C	2.02105700	2.85443000	-2.01923900
H	5.67447600	-3.53018800	-1.18287200	H	1.41394800	4.19914000	-0.46011400
H	4.54537500	-2.39791400	-1.96928300	C	1.64215300	1.76334800	-2.80836700
H	5.91520200	-1.78983500	-0.98185600	H	2.34970100	1.33686200	-3.51197300
H	3.35630500	-2.16791400	-0.02504100	C	-0.00035900	0.00036700	-3.55477300
N	-4.56813300	-1.10299200	-1.73419900	H	0.84749400	-0.21607600	-4.21430900
H	-4.83836300	-0.15037800	-1.93864400	C	1.14084100	-3.45347500	0.03640800
S	-7.20451100	-1.33723400	-1.88144700	H	2.05485000	-3.83176800	-0.43512400
C	-5.64637500	-1.96235000	-1.76082700	H	0.65473000	-4.32818700	0.48604400
N	-5.37088600	-3.28586500	-1.69304000	C	-1.64261100	-1.76282100	-2.80830300
C	-6.39107500	-4.31800300	-1.79672100	C	-2.02131300	-2.85406100	-2.01929300
H	-5.91181600	-5.28512100	-1.62207800	C	-0.35519200	-1.22642200	-2.72536800
H	-7.16687700	-4.15389600	-1.04547000	C	-1.10071200	-3.39004200	-1.11510600
H	-6.86991300	-4.31821800	-2.78279400	C	0.57465800	-1.83763200	-1.86734700
H	-4.40672400	-3.57130600	-1.80781700	C	0.19743300	-2.88979600	-1.01525700
N	-3.77680000	2.78596200	2.33624800	H	-1.41381800	-4.19899700	-0.46050500
H	-4.19153500	2.88372300	3.25338000	H	-2.35028300	-1.33626400	-3.51173700
C	-4.69776600	2.90752600	1.32104500	O	-0.74368500	-1.97669500	1.67594100
S	-6.27014300	3.39685900	1.67232200	O	1.88882800	-1.38349900	-1.84814100
N	-4.26257500	2.61254100	0.07161900	O	-1.88910500	1.38400700	-1.84760900
C	-5.15510200	2.57471800	-1.07729100	O	0.74396200	1.97671500	1.67615800
H	-4.54600900	2.39684600	-1.96991500	C	-2.72225000	2.06841100	-2.78560300
H	-5.91582700	1.78969900	-0.98188200	H	-2.34708200	1.96459100	-3.81162100
H	-5.67473700	3.52984800	-1.18401600	H	-2.80152500	3.13776500	-2.55089300
H	-3.35659800	2.16791000	-0.02578700	C	2.72171200	-2.06761500	-2.78658800
N	4.56801200	1.10210900	-1.73497900	H	2.34627800	-1.96343500	-3.81247000
H	4.83808000	0.14954500	-1.93987000	H	2.80099500	-3.13705200	-2.55225300
C	5.64641400	1.96129100	-1.76151300	C	1.31613200	3.00408800	2.48372500
S	7.20440000	1.33585800	-1.88233600	H	0.84202700	3.97739200	2.29967700
N	5.37114000	3.28485000	-1.69341300	H	1.22910300	2.77566500	3.55411000
C	6.39147500	4.31684700	-1.79704800	C	-1.31570800	-3.00441400	2.48316500
H	5.91273600	5.28388100	-1.62050400	H	-1.22859500	-2.77639100	3.55363100
H	7.16811000	4.15143800	-1.04696900	H	-0.84155600	-3.97761400	2.29870700
H	6.86912100	4.31828900	-2.78371400	H	-0.84841100	0.21690900	-4.21401800
H	4.40707800	3.57043500	-1.80872500	H	-2.05467300	3.83234800	-0.43413800
3F-EZ B3LYP/6-31G(d), electr. en. = -3884.822038				H	-0.56326200	-0.66639600	4.30249100
a.u.				H	2.37250500	3.05892100	2.21103900
C	-1.01007200	0.81721100	2.84430400	H	3.71191900	-1.60899800	-2.72267400
C	-0.60669400	1.76736500	1.88948700	H	-2.37210400	-3.05921300	2.21056000
C	-1.55340400	2.47502300	1.13197700	H	-3.71242800	1.60973600	-2.72158300
C	-2.91314100	2.31018400	1.41979200	N	-4.67803000	1.27389900	2.83711900
C	-3.33739800	1.41927400	2.41446000	H	-4.80332000	0.99197400	3.80078400
C	-2.37223400	0.65722900	3.08885100	C	-5.88074000	1.59529900	2.24854200
H	-3.63142500	2.93118400	0.89701700	S	-7.27633400	1.65530300	3.18521000
H	-2.69845600	-0.06869900	3.83031100	N	-5.86062100	1.83635800	0.91284100
C	0.00020700	-0.00019600	3.63764100	C	-7.06514600	2.11958300	0.14625500
H	0.56369000	0.66585300	4.30263300	H	-7.60379300	2.95218500	0.60283500
C	-1.14065200	3.45376100	0.03714200	H	-6.76480300	2.39470000	-0.86875600
H	-0.65430200	4.32827800	0.48689600	H	-7.74191900	1.25784400	0.11018200
C	1.01046000	-0.81744100	2.84410700	H	-5.05077600	1.51338500	0.39902800
C	0.60700100	-1.76741800	1.88914100	N	3.30323700	3.44911800	-2.12529600
C	2.37263300	-0.65754200	3.08862000	H	3.35550700	4.45888200	-2.10259600
C	1.55364200	-2.47492600	1.13140800	S	5.92169500	3.80141400	-2.34769800
C	3.33773700	-1.41947700	2.41401400	C	4.54309400	2.85546900	-2.14744400
H	2.69892300	0.06820500	3.83022600	N	4.56919700	1.50790400	-1.99668000
C	2.91340500	-2.31014200	1.41916100	C	5.81005200	0.75762800	-1.90498600
				H	5.56631100	-0.30835900	-1.94650600

H	6.46106200	1.01118000	-2.74415700	C	-2.28580400	0.67967900	-2.36263100
H	6.35517900	0.97350700	-0.97791500	C	-0.23015100	1.85082400	-1.95275300
H	3.72034700	1.04895100	-1.68529700	C	-0.93026300	0.84385600	-2.63717700
N	4.67839000	-1.27424400	2.83666100	H	-2.83543400	-0.10578500	-2.87373800
H	4.80370100	-0.99263700	3.80041600	H	-2.68395600	2.96305800	0.11709900
C	5.88106200	-1.59577500	2.24806400	O	-1.34172400	-2.32440400	-2.10618100
S	7.27658300	-1.65641700	3.18479000	O	1.11171600	2.05361700	-2.23918300
N	5.86095600	-1.83640900	0.91229100	O	-1.11239500	2.05120500	2.24124300
C	7.06543700	-2.11977300	0.14568600	O	1.34227100	-2.32596700	2.10429400
H	6.76507900	-2.39420600	-0.86950400	C	-1.35387900	3.08333000	3.19615400
H	7.74259000	-1.25831400	0.11015900	H	-0.91983600	4.03962700	2.87669100
H	7.60367500	-2.95286300	0.60186700	H	-0.93775100	2.82493800	4.18021300
H	5.05118500	-1.51316500	0.39853600	C	1.35302000	3.08666800	-3.19313600
N	-3.30344200	-3.44886200	-2.12519100	H	0.91873400	4.04257200	-2.87283100
H	-3.35558800	-4.45863300	-2.10254100	H	0.93700700	2.82906600	-4.17745200
C	-4.54337800	-2.85538000	-2.14749800	C	1.68454500	-3.33917800	3.04784300
S	-5.92183000	-3.80146500	-2.34808900	H	1.37046300	-3.06425500	4.06464900
N	-4.56971900	-1.50784700	-1.99660800	H	1.22304500	-4.30217900	2.79151000
C	-5.81070700	-0.75774200	-1.90525300	C	-1.68358100	-3.33668200	-3.05087600
H	-5.56697300	0.30828800	-1.94558700	H	-1.22171200	-4.29978900	-2.79560200
H	-6.46107100	-1.01053000	-2.74516700	H	-1.36958800	-3.06050700	-4.06736700
H	-6.35653500	-0.97450800	-0.97881000	H	-0.67201400	4.11174500	0.57028700
H	-3.72096800	-1.04873600	-1.68521300	H	-0.46525300	0.40354200	4.23975000
3C-ZE B3LYP/6-31G(d), electr. en. = -3884.820401 a.u.				H	-0.72453900	-4.36784900	-0.50218100
C	-0.73769100	-2.84106500	1.00488600	H	2.77172100	-3.43675300	3.01072100
C	-0.01854900	-2.11400100	1.96588100	H	2.43826700	3.19115500	-3.26716100
C	-0.63309600	-1.10615300	2.72598300	H	-2.77072100	-3.43471400	-3.01389000
C	-2.00688700	-0.92671100	2.58881100	H	-2.43914500	3.18750800	3.27035400
C	-2.75997200	-1.70308500	1.69876600	N	-4.15824100	-1.44728800	1.70770200
C	-2.11988000	-2.64837700	0.89430000	H	-4.42316300	-0.88512900	2.50642200
H	-2.48900500	-0.12674800	3.14471100	C	-5.15883600	-1.67392600	0.81791800
H	-2.68661800	-3.19901700	0.15789900	S	-5.03240200	-2.43671200	-0.69626100
C	0.00044500	-3.71952600	-0.00156800	N	-6.38413200	-1.23602200	1.22920600
H	0.72565700	-4.36814000	0.49833000	C	-6.65647200	-0.34075400	2.34525200
C	0.19764500	-0.13279300	3.55352000	H	-6.13965400	0.62424400	2.24392800
H	0.93125100	-0.66752900	4.16476800	H	-7.73094300	-0.14960600	2.37002600
C	0.73831200	-2.83970400	-1.00705000	H	-6.38872800	-0.80655300	3.30273000
C	0.01900000	-2.11205300	-1.96745800	H	-7.08830500	-1.31878600	0.51104600
C	2.12039600	-2.64649100	-0.89599900	N	4.32987800	1.22172300	1.26460000
C	0.63327500	-1.10330400	-2.72658600	H	4.60235200	0.34195100	1.69381900
C	2.76026300	-1.70022900	-1.69951800	S	5.20565200	3.15566700	-0.47618600
H	2.68723200	-3.19750000	-0.15996100	C	5.33617100	1.88532000	0.63635900
C	2.00697300	-0.92344700	-2.58906000	N	6.59121900	1.41969000	0.95045300
H	2.48884000	-0.12284000	-3.14425700	C	6.93727800	0.69215800	2.16980900
C	0.92989600	0.84155300	2.63810200	H	8.02632100	0.67887600	2.25646400
C	0.22951800	1.84895600	1.95460100	H	6.52292200	1.17378700	3.06609600
C	2.28548600	0.67800900	2.36341200	H	6.59332300	-0.34819600	2.12735000
C	0.83888000	2.58680900	0.92933200	H	7.30962800	2.00230500	0.54290100
C	2.94017200	1.47520600	1.41348400	N	4.15833000	-1.44350500	-1.70782600
H	2.83530700	-0.10775900	2.87385300	H	4.42284100	-0.87920800	-2.50517500
C	2.20374900	2.40738700	0.67711600	C	5.15946300	-1.67258200	-0.81926200
H	2.68305500	2.96381100	-0.11417200	S	5.03398900	-2.43869300	0.69330300
C	-0.00050800	3.46174600	0.00171600	N	6.38459500	-1.23413300	-1.23043100
H	0.67083200	4.11252300	-0.56616300	C	6.65680700	-0.33763400	-2.34550800
C	-0.19770200	-0.12951700	-3.55337600	H	7.73137300	-0.14705900	-2.37065100
H	0.46509000	0.40758700	-4.23911100	H	6.38819300	-0.80205700	-3.30341100
H	-0.93112800	-0.66393600	-4.16511800	H	6.14060300	0.62753300	-2.24263700
C	-2.20451300	2.40755100	-0.67475700	H	7.08953300	-1.31939600	-0.51332500
C	-2.94068200	1.47585200	-1.41198100	N	-4.33025600	1.22172400	-1.26304700
C	-0.83969300	2.58757300	-0.92679800	H	-4.60236400	0.34158900	-1.69183300
				C	-5.33677100	1.88513000	-0.63504000
				S	-5.20668900	3.15555500	0.47735800

N	-6.59176000	1.41882300	-0.94912300
C	-6.93739400	0.69379100	-2.17020300
H	-8.02644300	0.67992500	-2.25677500
H	-6.52337200	1.17764000	-3.06544300
H	-6.59282800	-0.34642200	-2.12997300
H	-7.31011100	2.00185200	-0.54199700

3E-ZZ B3LYP/6-31G(d), electr. en. = -3884.820138 a.u.

C	-0.75383200	-2.75107500	1.04536500
C	-0.08432900	-1.96447600	1.99930000
C	-0.76509800	-1.00601100	2.76624100
C	-2.15475500	-0.95036000	2.66578500
C	-2.85382900	-1.80900400	1.81071700
C	-2.14939800	-2.67966600	0.97496900
H	-2.70004700	-0.21266100	3.24925500
H	-2.68071600	-3.29290400	0.25909100
C	0.02810200	-3.60403200	0.04917300
H	0.73534200	-4.25987400	0.56703700
C	-0.00009600	-0.00017700	3.61924100
H	0.71247400	-0.51577900	4.27179400
C	0.80464000	-2.72077400	-0.92163900
C	0.12982600	-1.98444700	-1.90927600
C	2.17213100	-2.51023600	-0.73436900
C	0.77924700	-0.97313400	-2.63358100
C	2.85005800	-1.55325300	-1.49212500
H	2.70531200	-3.05806800	0.02966100
C	2.14531500	-0.78476800	-2.42183800
H	2.66247100	0.00376400	-2.95933400
C	0.76495100	1.00569800	2.76632600
C	0.08421800	1.96420000	1.99938800
C	2.15460400	0.95004600	2.66593400
C	0.75377200	2.75084700	1.04554000
C	2.85372900	1.80869100	1.81089600
H	2.69986800	0.21230700	3.24937900
C	2.14934500	2.67940100	0.97516600
H	2.68068600	3.29267500	0.25934000
C	-0.02810300	3.60395900	0.04943600
H	0.67720700	4.25166100	-0.47955900
C	0.00010700	0.00010800	-3.50891800
H	0.70296100	0.53011500	-4.15929000
H	-0.70269100	-0.52986900	-4.15937300
C	-2.17212100	2.51038700	-0.73446400
C	-2.85001200	1.55349500	-1.49235700
C	-0.80458700	2.72085000	-0.92156000
C	-2.14518500	0.78499900	-2.42201100
C	-0.12970700	1.98457500	-1.90918100
C	-0.77909300	0.97331200	-2.63359900
H	-2.66231500	-0.00349600	-2.95959000
H	-2.70532800	3.05817200	0.02958100
O	-1.22613400	-2.20573600	-2.10751100
O	1.22627500	2.20584600	-2.10730100
O	-1.28684100	2.08369400	2.15271200
O	1.28671900	-2.08397700	2.15269800
C	-1.68005300	3.10007800	3.07338500
H	-1.28936500	4.08377100	2.78362800
H	-1.33470800	2.87467400	4.09240400
C	1.50944400	3.19957100	-3.09017100
H	1.06420600	4.16812700	-2.82486200
H	1.13296400	2.90640400	-4.07977300
C	1.67989600	-3.10054900	3.07318700
H	1.33480600	-2.87516300	4.09229700

H	1.28893500	-4.08412600	2.78341400
C	-1.50921900	-3.19944700	-3.09041400
H	-1.06401900	-4.16801000	-2.82506400
H	-1.13264000	-2.90628200	-4.07997900
H	-0.73537400	4.25972000	0.56736000
H	-0.71269700	0.51539500	4.27178100
H	-0.67718100	-4.25165500	-0.47995600
H	2.77203600	-3.13001700	3.05450000
H	2.59725100	3.29802600	-3.12668900
H	-2.59702400	-3.29788800	-3.12703600
H	-2.77220400	3.12930800	3.05491700
N	-4.27360500	-1.79062600	1.92398300
H	-4.58451500	-1.46975200	2.83370800
C	-5.27566100	-2.06605500	1.03805100
S	-5.10783500	-2.22560000	-0.63931600
N	-6.49282800	-2.18392300	1.63850100
C	-7.73534200	-2.45901500	0.93379800
H	-7.67629600	-3.39432000	0.36802600
H	-8.53163000	-2.52928500	1.67900800
H	-7.97430800	-1.65357800	0.23339100
H	-6.51455900	-2.28213500	2.64538200
N	4.27350000	1.79016200	1.92416200
H	4.58437100	1.46907300	2.83382300
S	5.10784700	2.22573800	-0.63899500
C	5.27559500	2.06584600	1.03835800
N	6.49273100	2.18360600	1.63885600
C	7.73530700	2.45871100	0.93425700
H	8.53141700	2.52961500	1.67959600
H	7.97469800	1.65300900	0.23428400
H	7.67603800	3.39371700	0.36803400
H	6.51450700	2.28123900	2.64579200
N	4.20349000	-1.19838300	-1.26484400
H	4.36369600	-0.19237500	-1.28811800
C	5.29110800	-1.98209800	-0.99875500
S	5.29727300	-3.66897600	-0.93759900
N	6.42297600	-1.25175400	-0.78847100
C	7.73628900	-1.83625500	-0.59700800
H	8.44749700	-1.01878600	-0.44226900
H	7.74695200	-2.49689700	0.27528100
H	8.04841300	-2.42693100	-1.46589600
H	6.36703300	-0.24388600	-0.89565200
N	-4.20351200	1.19874700	-1.26535200
H	-4.36383700	0.19277000	-1.28889400
C	-5.29109400	1.98248800	-0.99911200
S	-5.29714400	3.66934700	-0.93736400
N	-6.42304700	1.25219900	-0.78928400
C	-7.73623100	1.83672500	-0.59703300
H	-8.44768000	1.01917800	-0.44384500
H	-7.74698900	2.49594100	0.27635800
H	-8.04793700	2.42891300	-1.46501500
H	-6.36703500	0.24427100	-0.89580100

3A-EE B3LYP/6-31G(d), electr. en. = -3884.818057 a.u.

C	0.78821000	-0.98212200	2.63069600
C	0.12023000	-2.01297400	1.94882700
C	0.77501600	-2.78074000	0.97227400
C	2.14034100	-2.58436200	0.77544600
C	2.84909900	-1.62722800	1.50802600
C	2.16183900	-0.81435700	2.41661300
H	2.64071300	-3.13394300	-0.01265000
H	2.69157000	-0.01520400	2.92514700

C	-0.00003700	0.00003700	3.49520100	H	3.65552000	-4.39117500	2.24539900
H	-0.69849300	-0.53569400	4.14503600	H	5.35557900	-4.87178600	2.49481300
C	-0.00007800	-3.66266800	0.00009700	H	4.80210500	-3.24877100	2.97518700
H	-0.70642600	-4.31261500	0.52605500	H	5.61133700	-4.14456500	0.30992200
C	-0.78828700	0.98220900	2.63071400	N	-4.23244200	-1.39885800	-1.25252500
C	-0.12027600	2.01297200	1.94874200	H	-4.51117300	-0.41848800	-1.15078900
C	-2.16194000	0.81452200	2.41671300	S	-5.82624700	-1.76316400	0.89950100
C	-0.77506300	2.78070900	0.97216800	C	-5.00690400	-2.25534800	-0.49229900
C	-2.84918700	1.62736200	1.50808800	N	-5.08412700	-3.53730300	-0.92197800
H	-2.69170400	0.01545000	2.92533500	C	-4.69550900	-4.04143300	-2.23081800
C	-2.14040300	2.58438400	0.77539300	H	-5.35614500	-4.87169800	-2.49476600
H	-2.64076500	3.13392600	-0.01273600	H	-4.80280000	-3.24866800	-2.97527300
C	-0.77514900	-2.78078500	-0.97213300	H	-3.65606600	-4.39102400	-2.24564200
C	-0.12030000	-2.01309100	-1.94870100	H	-5.61170800	-4.14437600	-0.30991900
C	-2.14047400	-2.58436100	-0.77536500	N	-4.23248100	1.39907900	1.25259600
C	-0.78822300	-0.98225900	-2.63065800	H	-4.51129200	0.41872900	1.15088800
C	-2.84917200	-1.62725600	-1.50803300	C	-5.00680400	2.25557500	0.49221700
H	-2.64088400	-3.13387700	0.01275100	S	-5.82595500	1.76337700	-0.89969000
C	-2.16185700	-0.81444800	-2.41663300	N	-5.08401300	3.53754800	0.92182800
H	-2.69155200	-0.01531500	-2.92523600	C	-4.69541600	4.04174900	2.23064500
C	0.00009700	-0.00014500	-3.49514800	H	-5.35594300	4.87214600	2.49445200
H	-0.69832800	0.53559900	-4.14500500	H	-4.80289300	3.24907700	2.97517400
C	0.00006900	3.66256000	-0.00004100	H	-3.65591900	4.39117800	2.24551700
H	-0.70624700	4.31253900	-0.52600300	H	-5.61144600	4.14464100	0.30966100
H	0.70644100	4.31248200	0.52591100	N	4.23254200	1.39893300	-1.25255300
C	2.16199800	0.81432500	-2.41665500	H	4.51140500	0.41860800	-1.15085700
C	2.84926600	1.62720200	-1.50807900	C	5.00692000	2.25549400	-0.49231400
C	0.78834700	0.98202000	-2.63065400	S	5.82634000	1.76335200	0.89944900
C	2.14048800	2.58427600	-0.77543700	N	5.08400600	3.53745500	-0.92199300
C	0.12035000	2.01283500	-1.94874500	C	4.69520900	4.04160000	-2.23076900
C	0.77514900	2.78062100	-0.97221900	H	5.35569700	4.87198500	-2.49471100
H	2.64086300	3.13385600	0.01265600	H	4.80258200	3.24890400	-2.97529000
H	2.69174600	0.01521600	-2.92523800	H	3.65570800	4.39102300	-2.24550300
O	1.23405900	2.21217000	2.17754700	H	5.61149100	4.14459000	-0.30991400
O	-1.23397500	2.21203500	-2.17757900	4A-EZ B3LYP/6-31G(d), electr. en. = -2367.108850 a.u.			
O	1.23401300	-2.21242300	-2.17752000	C	-8.09595100	0.22291200	1.40439200
O	-1.23406800	-2.21226000	2.17774300	C	-7.59351100	1.44396100	0.92267400
C	1.51580400	-3.19630400	-3.17078400	C	-6.64797600	1.49290700	-0.11399000
H	1.10349500	-2.91139600	-4.14848600	C	-6.22535500	0.29130400	-0.69213800
H	1.10572500	-4.17751500	-2.89466900	C	-6.70898900	-0.93959200	-0.22820300
C	-1.51587300	3.19593000	-3.17079700	C	-7.63608100	-0.95952200	0.82072200
H	-1.10357200	2.91108000	-4.14852000	H	-5.53715100	0.31883300	-1.53159000
H	-1.10586100	4.17716400	-2.89466700	H	-7.99154500	-1.91602600	1.19669200
C	-1.51584100	-3.19615700	3.17099600	C	-9.07973900	0.19088700	2.54891000
H	-1.10579100	-4.17737100	2.89485100	H	-10.10109300	0.41100600	2.21171500
H	-1.10349200	-2.91127000	4.14868800	C	-6.10695400	2.81751500	-0.59634000
C	1.51596800	3.19605100	3.17077700	H	-6.84776300	3.36659900	-1.19142800
H	1.10366100	2.91120500	4.14849900	O	-7.98313100	2.62526800	1.53102400
H	1.10597000	4.17729200	2.89465000	C	-9.14991300	3.23251500	0.97620100
H	0.69856300	-0.53591100	-4.14494000	H	-9.00886300	3.48256900	-0.08314700
H	0.70628000	-4.31261600	-0.52584000	H	-5.22333600	2.67423900	-1.22535300
H	0.69843700	0.53576700	4.14501500	H	-9.09826800	-0.79608600	3.02076900
H	-2.60442800	-3.26319000	3.24051200	H	-9.31913300	4.15046300	1.54388800
H	-2.60446900	3.26289900	-3.24023800	N	-6.32502100	-2.17088200	-0.81875200
H	2.60456400	3.26300600	3.24022300	H	-7.04069200	-2.87814500	-0.92183500
H	2.60439200	-3.26335800	-3.24026400	C	-5.07705000	-2.63507700	-1.16250800
N	4.23233800	-1.39889100	1.25240700	S	-4.91734300	-4.15050000	-1.88362600
H	4.51115400	-0.41855400	1.15070600	N	-4.03052200	-1.82008500	-0.88430100
C	5.00678600	-2.25546000	0.49228000	C	-2.63895300	-2.20089000	-1.09207600
S	5.82641800	-1.76332200	-0.89936300	H	-2.53843800	-2.57276600	-2.11639900
N	5.08377200	-3.53743900	0.92194300				
C	4.69495600	-4.04155300	2.23072900				

H	-2.37166500	-3.03648000	-0.42984200	C	6.14720900	-0.62222700	-0.40132400
H	-4.20381400	-1.02358000	-0.28197300	C	6.48637600	0.05557300	-1.57734000
C	-1.72351400	-0.99953800	-0.84842600	H	5.73939100	-0.42771000	1.70446000
H	-1.83941000	-0.63377600	0.18093000	H	6.58254200	-0.50460500	-2.50450200
H	-1.99560200	-0.17467300	-1.51792100	C	7.03463200	2.16878400	-2.85646500
C	-0.25897700	-1.35477000	-1.06645700	H	8.09352400	2.45679000	-2.88490200
H	0.04794700	-2.18514700	-0.41919500	C	5.97589800	2.26179700	2.09400700
H	-0.08171200	-1.65598600	-2.11092900	H	6.93415100	2.47990100	2.58343600
C	1.86372300	-0.30072000	-1.05364000	O	6.66334400	3.51797300	-0.37649100
H	2.02234200	-0.65047300	-2.09152100	C	7.97518600	3.99493400	-0.07934500
C	2.54383200	1.05805500	-0.85142800	H	8.29651300	3.69352400	0.92593600
H	2.14225200	1.79212600	-1.55444400	H	5.36900700	1.69644100	2.80778900
C	4.05506800	0.88080300	-1.13614100	H	6.84315200	1.54073400	-3.73175900
H	4.19361900	0.64489700	-2.19666000	H	7.92629400	5.08530000	-0.12975000
C	4.63741500	-0.23271900	-0.27156500	N	6.02445300	-2.04155700	-0.45830700
H	4.62960900	0.06357900	0.77776500	H	6.80169300	-2.51778500	-0.90045000
C	3.81800300	-1.52256700	-0.46627500	C	5.35309700	-2.87988900	0.40252100
H	3.90242300	-1.83955200	-1.52061900	S	5.96745900	-4.40081900	0.78111100
O	2.44704500	-1.26019900	-0.16217000	N	4.16561000	-2.44241500	0.90628200
N	2.28484800	1.53442800	0.49533400	C	3.24879500	-1.48788800	0.27830300
C	2.10969800	2.85868300	0.78442300	H	3.52420500	-1.38350200	-0.77637900
O	2.24472900	3.74520800	-0.05278800	H	3.35572800	-0.49501200	0.73499400
C	1.75202000	3.16752200	2.22998700	H	3.74843100	-3.11748300	1.53468900
H	1.55790600	2.27807300	2.83735400	C	1.80284400	-1.97648200	0.40739000
H	2.57365800	3.73083300	2.68426600	H	1.54576000	-2.10749700	1.46691800
H	0.86789000	3.81124300	2.24184800	H	1.69002200	-2.95301000	-0.07739300
H	2.07679500	0.83650900	1.19588900	C	0.81703000	-0.99135000	-0.20740300
O	4.76175900	2.08755300	-0.83650600	H	0.90865900	-0.00011500	0.25327000
O	5.99202100	-0.49857700	-0.67431400	H	0.99920900	-0.88030600	-1.28831100
C	4.29395000	-2.69322800	0.38111300	C	-1.50840600	-0.78458400	-0.60431100
H	3.54192900	-3.48678400	0.34368300	H	-1.28899600	-0.62108700	-1.67665800
H	5.24545400	-3.07184600	0.00531700	C	-2.83958200	-1.52872300	-0.45174200
O	4.45068600	-2.30501700	1.75673900	H	-2.80054100	-2.48954100	-0.97101200
O	0.51648700	-0.19001300	-0.76515300	C	-3.94514300	-0.66289100	-1.10463600
C	4.76536900	3.04127700	-1.81476100	H	-3.76610900	-0.60961000	-2.18384100
O	4.32388700	2.85327200	-2.92561900	C	-3.95388000	0.74040800	-0.50617000
C	6.98389700	-0.21659000	0.22088800	H	-4.27518900	0.70229400	0.53500100
O	6.79068700	0.26293800	1.31498800	C	-2.54561900	1.35618300	-0.60798700
C	5.66648600	-2.53560300	2.32945800	H	-2.27904400	1.45322800	-1.67511400
O	6.58421300	-3.08837500	1.76376800	O	-1.60508400	0.49444400	0.03519300
C	8.32351200	-0.63887200	-0.32280400	N	-3.09265600	-1.78590100	0.95453500
H	9.11216400	-0.07167100	0.17407900	C	-3.71525800	-2.92181800	1.39222800
H	8.45961500	-1.70226800	-0.09275100	O	-4.18470300	-3.75822300	0.62770900
H	8.37630300	-0.50921700	-1.40610000	C	-3.80328700	-3.07486000	2.90268300
C	5.35310900	4.32608800	-1.29849500	H	-3.27088700	-2.29642300	3.45790000
H	6.20603300	4.13646400	-0.64158900	H	-4.85733800	-3.05974200	3.19791900
H	5.64313600	4.96051500	-2.13727800	H	-3.39977600	-4.05319300	3.17929700
H	4.57471100	4.82873700	-0.71325500	H	-2.64650800	-1.17093300	1.62071000
C	5.71600500	-1.97217400	3.72495100	O	-5.23012900	-1.24760300	-0.87889700
H	4.73967500	-2.02050200	4.21238200	O	-4.86031400	1.57584400	-1.24654400
H	6.46667900	-2.50874100	4.30757200	C	-2.42981700	2.74602800	0.00098200
H	6.01751000	-0.92120800	3.64709800	H	-1.37140600	3.01180000	0.07787500
H	-8.82315000	0.93788800	3.30572300	H	-2.94673400	3.47888700	-0.61992900
H	-5.83705200	3.46073000	0.24682400	O	-2.98382800	2.77528200	1.32751600
H	-10.02839900	2.58153200	1.07151400	O	-0.49950500	-1.50763000	0.00567600
4A-EE B3LYP/6-31G(d), electr. en. = -2367.102491 a.u.				C	-5.60069000	-2.23835200	-1.74436600
C	6.68829900	1.43741900	-1.58190200	O	-4.96503000	-2.52622700	-2.73286000
C	6.53044200	2.13864500	-0.37435500	C	-5.97168300	2.03314100	-0.59775800
C	6.16733300	1.48410700	0.81358000	O	-6.24793100	1.75593200	0.54718900
C	5.99139700	0.09659900	0.78780700	C	-3.95347600	3.70272200	1.57211400
				O	-4.32228200	4.52212500	0.75958100
				C	-6.75541200	2.96536600	-1.48367100

H	-7.79385600	2.99636600	-1.15010700
H	-6.32444500	3.96816900	-1.37904300
H	-6.69389300	2.66912400	-2.53318700
C	-6.85918800	-2.91069100	-1.26899900
H	-7.56721400	-2.18401000	-0.86191400
H	-7.30833800	-3.47241300	-2.08922400
H	-6.57572200	-3.60008000	-0.46558600
C	-4.51910000	3.53310500	2.95721200
H	-3.76476700	3.16607400	3.65674600
H	-4.93544500	4.48216600	3.29903200
H	-5.32876900	2.79670700	2.89661900
H	6.45157200	3.08989900	-2.95042800
H	5.48881900	3.22166900	1.89908700
H	8.71083700	3.63151900	-0.80842700

4A-ZZ B3LYP/6-31G(d), electr. en. = -2367.101297 a.u.

C	-9.46180000	1.28108100	0.04640800
C	-10.03231200	0.00351400	0.15712300
C	-9.23983600	-1.15548300	0.17445700
C	-7.84962200	-1.02451700	0.11280100
C	-7.25955200	0.23778500	0.00818200
C	-8.07110400	1.37730100	-0.02963700
H	-7.22663100	-1.90934700	0.12896500
H	-7.61305700	2.35920400	-0.13777100
C	-10.33378500	2.51171500	-0.02172200
H	-10.75746900	2.76774100	0.95827300
C	-9.87713200	-2.52267200	0.25164900
H	-10.16807600	-2.78031100	1.27895200
O	-11.41433200	-0.11357300	0.17353700
C	-11.99588900	-0.13533200	1.47460000
H	-11.63849900	-0.98987700	2.06379800
H	-9.18327600	-3.29394100	-0.09507200
H	-9.76171400	3.37810900	-0.36795800
H	-13.07551000	-0.22506800	1.33049300
N	-5.85516600	0.43660900	0.00543700
H	-5.58323900	1.36761500	0.29947100
C	-4.85491400	-0.29255400	-0.60018500
S	-5.07177400	-1.61288100	-1.60948400
N	-3.61504200	0.21064600	-0.30609400
C	-2.37327700	-0.38956900	-0.77787800
H	-2.41909900	-0.45603200	-1.86940000
H	-2.28261600	-1.42030400	-0.40694100
H	-3.53598300	0.78182600	0.52748800
C	-1.17966300	0.45747400	-0.33122700
H	-1.13756200	0.50891700	0.76552500
H	-1.28439000	1.48467400	-0.70068700
C	0.13706300	-0.12075400	-0.83201000
H	0.26823800	-1.15623600	-0.49553300
H	0.17033400	-0.11576000	-1.93285800
C	2.44774400	0.39995800	-0.81432300
H	2.44206500	0.37763400	-1.92080200
C	3.45719900	1.44136800	-0.31841000
H	3.20024700	2.43301800	-0.69873700
C	4.85012500	1.04872400	-0.86848500
H	4.84355500	1.14532400	-1.95941000
C	5.20004800	-0.38182900	-0.47071500
H	5.34935400	-0.44540700	0.60747200
C	4.07194700	-1.33567300	-0.90712700
H	3.99608300	-1.31436600	-2.00844600
O	2.83601300	-0.89646900	-0.34103700
N	3.42744000	1.49190900	1.13210000

C	3.61979900	2.64922100	1.83299000
O	3.90533100	3.71368700	1.29402900
C	3.47568600	2.52659300	3.34217500
H	3.09005000	1.55688300	3.67186300
H	4.45453400	2.69051900	3.80482500
H	2.80951000	3.31857200	3.69553700
H	3.11783800	0.65868500	1.61276600
O	5.85692100	1.91242600	-0.33458000
O	6.40886200	-0.78795000	-1.13531600
C	4.30213400	-2.78654700	-0.51070900
H	3.37702500	-3.34871100	-0.66779800
H	5.10271600	-3.22223100	-1.10967900
O	4.64448700	-2.89132500	0.88220800
O	1.19276800	0.69619900	-0.31608500
C	6.02085700	3.11091700	-0.97000500
O	5.46015900	3.39491400	-2.00397000
C	7.50789400	-1.02140600	-0.35860700
O	7.52893900	-0.87890200	0.84277300
C	5.80653000	-3.53770300	1.18533900
O	6.52178900	-4.06108900	0.35941600
C	8.65018100	-1.53053400	-1.19765900
H	9.59366900	-1.32809900	-0.68830800
H	8.53351400	-2.61603900	-1.29932300
H	8.64501800	-1.08627500	-2.19548900
C	6.94866600	3.99991500	-0.18814000
H	7.78126600	3.43047500	0.23322800
H	7.31361900	4.80435900	-0.82827300
H	6.37080300	4.42563300	0.64004000
C	6.08984800	-3.46653100	2.66255700
H	5.16806400	-3.44414400	3.24799800
H	6.71373000	-4.31300200	2.95455700
H	6.64693600	-2.54096600	2.84865700
H	-11.17708200	2.35595600	-0.70145900
H	-10.78364900	-2.56552800	-0.35926600
H	-11.78106300	0.78834100	2.02849000

4A-ZE B3LYP/6-31G(d), electr. en. = -2367.101001 a.u.

C	8.19263900	1.95407200	-0.16157000
C	9.25886900	1.07983100	-0.42749600
C	9.08801100	-0.31274900	-0.40313600
C	7.81774300	-0.83503500	-0.13624100
C	6.74296100	0.01631800	0.12765300
C	6.94184000	1.40285500	0.11624700
H	7.67092100	-1.90660800	-0.11356200
H	6.11037900	2.06728800	0.34702600
C	8.41075000	3.44774000	-0.14449800
H	8.60538800	3.84399600	-1.14927400
C	10.25348200	-1.24110800	-0.65130600
H	10.38725700	-1.44922100	-1.72151600
O	10.51765300	1.62084500	-0.64169800
C	10.87093700	1.79201100	-2.01216700
H	10.91018300	0.83281000	-2.54429900
H	10.09619900	-2.20138300	-0.15132300
H	7.53231400	3.96717900	0.25095700
H	11.86410600	2.24800100	-2.02136200
N	5.41626300	-0.43746700	0.35340800
H	4.72426800	0.27421300	0.15761700
C	4.94788500	-1.56737600	0.96884700
S	5.87130200	-2.78259900	1.67985300
N	3.58432400	-1.66030100	0.99041300
C	2.61993400	-0.78789900	0.33781100

H	2.88373000	-0.66436300	-0.72371900	C	-6.19481800	0.38048800	-0.71782600
H	2.62999500	0.21493900	0.79683000	C	-6.47011300	-0.93793900	-0.32964600
H	3.24689400	-2.49514300	1.44946700	C	-7.38515700	-1.17120400	0.70314000
C	1.21352000	-1.38042200	0.45554500	H	-5.51641100	0.56909600	-1.54460900
H	0.95713000	-1.51442000	1.51356400	H	-7.57825600	-2.19337000	1.02007100
H	1.18900700	-2.37027000	-0.01514700	C	-9.00841000	-0.37680900	2.47196600
C	0.15821300	-0.49510700	-0.19452300	H	-10.04910200	-0.35526300	2.12269900
H	0.13584600	0.49961300	0.26768200	C	-6.49448500	2.88208800	-0.47619800
H	0.36306000	-0.36608900	-1.26962300	H	-7.32826800	3.34955700	-1.01507100
C	-2.16870700	-0.51231100	-0.64099800	O	-8.32044200	2.26353400	1.60596100
H	-1.94099100	-0.29747700	-1.70246800	C	-9.58536600	2.68021500	1.09200200
C	-3.41410100	-1.39949000	-0.54452000	H	-9.51229800	2.98259300	0.03943300
H	-3.25501100	-2.33636100	-1.08432000	H	-5.61855200	2.91941900	-1.13046200
C	-4.58798400	-0.64049100	-1.21010700	H	-8.83583100	-1.36151800	2.91686300
H	-4.38499200	-0.53548400	-2.28126000	H	-9.89481700	3.53831300	1.69321700
C	-4.76497900	0.73290500	-0.57160000	N	-5.88169100	-2.05188700	-0.98373200
H	-5.10723600	0.62474000	0.45798900	H	-6.47551500	-2.84877200	-1.17134400
C	-3.43177200	1.50433800	-0.61159200	C	-4.57105700	-2.27746900	-1.33180900
H	-3.15181400	1.67106900	-1.66660500	S	-4.17152100	-3.67658500	-2.19018700
O	-2.41465600	0.73051200	0.02835300	N	-3.67649400	-1.33684800	-0.94727700
N	-3.67585200	-1.71991100	0.84678600	C	-2.24060100	-1.40908700	-1.18892800
C	-4.18892800	-2.92584700	1.23777700	H	-1.85680900	-0.38470600	-1.19089400
O	-4.53959300	-3.78753600	0.43849700	H	-2.09496400	-1.83288600	-2.18651000
C	-4.31438500	-3.12322700	2.74020400	H	-4.00313100	-0.61023200	-0.32194200
H	-3.86440200	-2.31924500	3.33077900	C	-1.48974600	-2.25259300	-0.14825200
H	-5.37560200	-3.19780500	2.99902700	H	-1.88680700	-3.27315100	-0.16783400
H	-3.84425100	-4.07344700	3.00886700	H	-1.65973200	-1.84732200	0.85742600
H	-3.32536900	-1.07488800	1.54117100	C	0.00610900	-2.30749900	-0.41627600
O	-5.80801200	-1.36552000	-1.04062000	H	0.50860300	-2.97627500	0.29123600
O	-5.73677800	1.49084000	-1.31236200	H	0.20601100	-2.67680800	-1.43464300
C	-3.49320800	2.87473700	0.04692500	C	1.83520700	-0.82238200	-0.71956800
H	-2.47608700	3.26235600	0.15751700	H	1.96018000	-1.21594000	-1.74634700
H	-4.08219100	3.56138500	-0.56254700	C	2.21935700	0.66118400	-0.67721100
O	-4.07395400	2.79129300	1.35923100	H	1.58712800	1.23909200	-1.35572700
O	-1.10332000	-1.14241500	-0.02154400	C	3.68839400	0.78330500	-1.14824400
C	-6.04185600	-2.36831300	-1.93971200	H	3.75092500	0.49443400	-2.20279900
O	-5.34669200	-2.56151900	-2.91101100	C	4.59656300	-0.10624400	-0.30524500
C	-6.91067200	1.79658300	-0.68389000	H	4.65094500	0.27482700	0.71473000
O	-7.18437600	1.44881200	0.44208900	C	4.06134100	-1.55086200	-0.30529000
C	-5.14711100	3.59535600	1.61207700	H	4.09980900	-1.94176200	-1.33712700
O	-5.58763900	4.39860300	0.81966100	O	2.70807300	-1.55689100	0.15082100
C	-7.77156700	2.66567700	-1.56236600	N	2.02405100	1.17092100	0.66830000
H	-8.81702100	2.55426100	-1.27025900	C	1.60766500	2.44717400	0.92153000
H	-7.47317600	3.70804200	-1.39857800	O	1.43813300	3.28024900	0.03664200
H	-7.63689400	2.42776400	-2.61978000	C	1.39098200	2.77951700	2.38994800
C	-7.23607500	-3.18217400	-1.52388100	H	1.40476600	1.90427100	3.04686200
H	-8.03079300	-2.54528400	-1.12652300	H	2.17435100	3.47268700	2.71467000
H	-7.59531600	-3.76739600	-2.37148800	H	0.43244100	3.29485200	2.49468200
H	-6.90755300	-3.85790400	-0.72603500	H	2.06715800	0.49841400	1.42151000
C	-5.71809300	3.31171900	2.97595800	O	4.14490800	2.13224300	-1.01128500
H	-4.93937300	3.01952000	3.68407900	O	5.91900900	-0.12350000	-0.87048400
H	-6.25737800	4.19004600	3.33436400	C	4.87334500	-2.50695600	0.55619100
H	-6.42728700	2.48216800	2.87362300	H	4.31632000	-3.44126700	0.67153500
H	9.27679100	3.71043000	0.47129500	H	5.83893700	-2.71044100	0.09137900
H	11.18580300	-0.80247800	-0.28470000	O	5.08697000	-1.96109100	1.86977000
H	10.16436100	2.45393400	-2.53076600	O	0.53566100	-0.97794600	-0.28124700
4B-EZ B3LYP/6-31G(d), electr. en. = -2367.111765				C	3.81283500	2.98581400	-2.02463900
a.u.				O	3.28626300	2.62258600	-3.05185000
C	-8.03751800	-0.11610500	1.34571200	C	6.92513400	0.44284800	-0.14134800
C	-7.74130100	1.19652000	0.94031700	O	6.76368000	0.98069000	0.93052700
C	-6.81210600	1.46041800	-0.07883800	C	6.37752400	-1.87327100	2.30078300
				O	7.32905600	-2.27481300	1.66741400

C	8.25139400	0.24898500	-0.82847600
H	8.94783200	1.02131500	-0.49802900
H	8.64559900	-0.72860100	-0.52641700
H	8.14683600	0.26036900	-1.91561400
C	4.16248600	4.40221300	-1.65805400
H	5.11561200	4.44994200	-1.12485200
H	4.19002700	5.01871600	-2.55767100
H	3.37637300	4.76870300	-0.98817800
C	6.45025800	-1.17581000	3.63347600
H	5.56230500	-1.37224100	4.23846700
H	7.35403500	-1.48861300	4.15910400
H	6.51211800	-0.09850000	3.44074200
H	-8.91355200	0.38331600	3.25268800
H	-6.30029100	3.50110600	0.40531100
H	-10.33869400	1.88696600	1.17995400

4C-EZ B3LYP/6-31G(d), electr. en. = -2367.110553 a.u.

C	7.25960300	-0.67310100	-0.93342900
C	8.31797300	0.18833100	-0.60250700
C	8.23692800	1.06999000	0.48906700
C	7.06755200	1.07183200	1.25338900
C	6.00454900	0.21129100	0.95687300
C	6.11245600	-0.66240000	-0.13364300
H	6.97182400	1.76603600	2.08489000
H	5.30880700	-1.36144300	-0.34555400
C	7.36542800	-1.59264200	-2.12627000
H	8.07114900	-2.41336500	-1.94632600
C	9.36943500	2.01718800	0.80455400
H	10.15789900	1.52520100	1.38924800
O	9.43413900	0.21531000	-1.42102500
C	10.50940800	-0.62649300	-1.00428300
H	10.90010200	-0.32727800	-0.02345000
H	9.01405900	2.86950100	1.39147100
H	6.39548100	-2.04055400	-2.36193400
H	11.29615900	-0.51500600	-1.75400300
N	4.86231000	0.22081500	1.80008800
H	5.01988400	0.31268600	2.79494900
C	3.52823100	0.27376500	1.47212900
S	2.37765100	0.26404100	2.70975900
N	3.23826900	0.33968600	0.15044800
C	1.89616800	0.48790200	-0.39429000
H	1.63032700	1.55306600	-0.47149000
H	1.20374900	0.03488900	0.31412900
H	4.01161200	0.51086700	-0.48237000
C	1.76919600	-0.19157000	-1.76143300
H	2.04650000	-1.24856900	-1.67169800
H	2.45008200	0.26671600	-2.49282100
C	0.34806300	-0.08988700	-2.30253300
H	0.03760300	0.95782000	-2.39465100
H	0.27252800	-0.56237400	-3.29355800
C	-1.86519400	-0.61031100	-1.58689400
H	-2.14495200	-0.86194900	-2.62769500
C	-2.62869500	-1.50560500	-0.60401800
H	-2.42239900	-2.55817100	-0.81485000
C	-4.14286300	-1.25632800	-0.80550400
H	-4.43607100	-1.60961100	-1.79996800
C	-4.46509900	0.22690800	-0.66230800
H	-4.30580700	0.54935100	0.36688300
C	-3.57605400	1.04378500	-1.61902000
H	-3.81098800	0.75011000	-2.65744500
O	-2.20296700	0.76123200	-1.34757600

N	-2.19325400	-1.22543400	0.75183700
C	-2.05016500	-2.21573200	1.69019700
O	-2.41932200	-3.36792100	1.48741200
C	-1.40124000	-1.76673300	2.98861400
H	-0.35706200	-1.47440500	2.82164500
H	-1.92444400	-0.90206100	3.41297400
H	-1.43330500	-2.59253200	3.70042100
H	-1.77520300	-0.32087100	0.92562500
O	-4.89583800	-1.97104800	0.17791200
O	-5.83796300	0.46198700	-1.02359300
C	-3.79256800	2.54714200	-1.52855900
H	-2.99401700	3.05519900	-2.07740200
H	-4.75942700	2.81848200	-1.95437400
O	-3.73530100	2.99230500	-0.16311400
O	-0.50688800	-0.76969800	-1.37797000
C	-5.15520100	-3.28306700	-0.09782200
O	-4.90728000	-3.79920700	-1.16417900
C	-6.68799600	0.87706100	-0.03936400
O	-6.36177200	1.03527800	1.11488400
C	-4.80336200	3.70023100	0.30278900
O	-5.75193600	4.01691900	-0.38157500
C	-8.05488700	1.16139000	-0.60546900
H	-8.79987400	1.08114300	0.18778400
H	-8.05519800	2.19130200	-0.98175500
H	-8.29529600	0.48949000	-1.43238600
C	-5.74613600	-3.96783900	1.10409800
H	-6.45069700	-3.31483500	1.62580600
H	-6.23079000	-4.89592000	0.79754000
H	-4.92013300	-4.19538700	1.78753000
C	-4.65521000	3.98511900	1.77374700
H	-3.60685100	4.10377200	2.05619700
H	-5.23014700	4.87608500	2.03193400
H	-5.06976300	3.12993800	2.32003800
H	7.72629400	-1.05233500	-3.00707200
H	9.83290100	2.39098800	-0.11297700
H	10.20089700	-1.67872800	-0.95610600

4D-EZ B3LYP/6-31G(d), electr. en. = -2367.110226 a.u.

C	-8.15075700	-0.26819400	-0.61348000
C	-7.72101700	1.02823200	-0.28105200
C	-6.36187000	1.33048300	-0.09762800
C	-5.42151100	0.31143300	-0.28089400
C	-5.82471500	-0.99088400	-0.60460200
C	-7.18654900	-1.26816000	-0.76364900
H	-4.36318300	0.54294100	-0.19917400
H	-7.49837600	-2.28466000	-0.99107600
C	-9.62003900	-0.57978200	-0.76503400
H	-9.99714100	-0.28411700	-1.75291500
C	-5.93058500	2.72610100	0.28423500
H	-6.04037300	3.42882600	-0.55120400
O	-8.66146700	2.01764600	-0.05419100
C	-9.05341400	2.75718300	-1.21114800
H	-8.19943300	3.27502800	-1.66611600
H	-4.88008000	2.74190000	0.58916000
H	-9.80533000	-1.65233600	-0.65394500
H	-9.78360400	3.49531900	-0.87161100
N	-4.87933000	-2.03166800	-0.81655400
H	-5.03475900	-2.65072400	-1.60125200
C	-3.86647400	-2.46837300	0.00416100
S	-2.90697500	-3.76893800	-0.49063600
N	-3.72136100	-1.80592000	1.17657000

C	-2.74391600	-2.11274000	2.21652600
H	-2.37868000	-3.12581300	2.03290600
H	-3.27293000	-2.11414100	3.17666300
H	-4.40669200	-1.09194700	1.39266600
C	-1.58254500	-1.10999400	2.27971100
H	-1.00191800	-1.30668900	3.18986300
H	-1.97293300	-0.08786400	2.37071000
C	-0.65290700	-1.17766500	1.07562300
H	-0.14623700	-2.14699700	1.02286700
H	-1.20637900	-1.03671100	0.13679900
C	1.25137300	-0.06153000	0.21684500
H	0.77760300	-0.12639800	-0.78065400
C	2.04639800	1.24436500	0.33285300
H	1.38871300	2.10433500	0.18440900
C	3.12195100	1.24939100	-0.78013500
H	2.62640300	1.30123500	-1.75543400
C	3.98584500	-0.00475000	-0.69781900
H	4.58964900	0.01546800	0.20978400
C	3.08796100	-1.25659500	-0.71054600
H	2.54397200	-1.29350700	-1.67059300
O	2.14920400	-1.17166400	0.36134200
N	2.62344100	1.34034000	1.66213500
C	2.75822100	2.52869100	2.32182500
O	2.49038400	3.61038200	1.80759700
C	3.28211600	2.42653500	3.74623800
H	3.42221000	1.39821100	4.09327200
H	4.23976300	2.95315500	3.80778400
H	2.58349300	2.93880900	4.41437100
H	2.76751700	0.47219200	2.15907200
O	3.97938300	2.38605200	-0.63765700
O	4.85742100	-0.06797200	-1.84065600
C	3.85177600	-2.56755700	-0.59134600
H	3.14079600	-3.37425300	-0.39186200
H	4.39603000	-2.77587300	-1.51325500
O	4.78171900	-2.52603400	0.50630800
O	0.31030900	-0.12255300	1.22523400
C	3.52256300	3.55661300	-1.17084800
O	2.52185400	3.63301100	-1.84743700
C	6.19810500	0.06072300	-1.62029000
O	6.68977000	0.25397800	-0.53147900
C	6.08763100	-2.79027500	0.22240100
O	6.49020600	-3.10660600	-0.87598100
C	6.96578800	-0.13022100	-2.90217700
H	7.93720800	0.36007700	-2.82061300
H	7.12713200	-1.20612500	-3.03854800
H	6.41100700	0.24913700	-3.76323800
C	4.41187300	4.70188500	-0.76955200
H	5.46535400	4.41040500	-0.78723900
H	4.23413400	5.55352700	-1.42781200
H	4.14887100	4.97379400	0.25896900
C	6.95076100	-2.59125300	1.44061800
H	6.41200000	-2.83665800	2.35855600
H	7.85486500	-3.19551500	1.34877900
H	7.23781300	-1.53389000	1.47450400
H	-10.21232000	-0.04120800	-0.01965700
H	-6.54064300	3.11296100	1.10648100
H	-9.51781300	2.10996700	-1.96594500

4E-EZ B3LYP/6-31G(d), electr. en. = -2367.110125 a.u.

C	-6.17188400	1.41876100	0.45282000
C	-6.88639500	1.71269200	-0.71948000

C	-7.18712000	0.71987100	-1.66792100
C	-6.75938400	-0.58613200	-1.41921400
C	-6.06225900	-0.91129300	-0.24985000
C	-5.78112900	0.09549900	0.68349900
H	-6.95560100	-1.36357100	-2.15379900
H	-5.27879700	-0.15503700	1.61324800
C	-5.83842000	2.50933400	1.44234500
H	-6.71901900	2.81709900	2.02064400
C	-7.92103100	1.06741100	-2.94037300
H	-9.00118300	1.16578700	-2.77066100
O	-7.23713100	3.02615100	-0.98083600
C	-8.52841400	3.41155000	-0.51017400
H	-9.32401200	2.82324100	-0.98528900
H	-7.77956700	0.29093600	-3.69816100
H	-5.07986600	2.17311300	2.15530900
H	-8.65158600	4.46404100	-0.77587100
N	-5.69761700	-2.26539700	-0.02824300
H	-6.36415300	-2.97606700	-0.29965200
C	-4.49784700	-2.79881900	0.37908900
S	-4.36316300	-4.47004700	0.58777400
N	-3.48771000	-1.92123700	0.58568200
C	-2.13486300	-2.29079000	0.98238500
H	-2.21152800	-3.11944700	1.69127100
H	-1.69983000	-1.43303900	1.50409300
H	-3.63921800	-0.96037700	0.30323800
C	-1.24140000	-2.69640500	-0.19908300
H	-1.22636000	-1.89138500	-0.94689100
H	-1.67400800	-3.57948300	-0.68344300
C	0.18195400	-3.02603700	0.24393000
H	0.17482800	-3.81640600	1.00113600
H	0.79486000	-3.37307000	-0.59514500
C	1.51792800	-1.06349300	0.02715600
H	0.95481600	-0.85615300	-0.90117700
C	1.82873400	0.25441900	0.74535000
H	0.90260500	0.78295900	0.98473100
C	2.66101900	1.13647300	-0.21458200
H	2.04113500	1.41049300	-1.07509600
C	3.90599200	0.39095400	-0.68375100
H	4.59002800	0.24077000	0.15194700
C	3.49919400	-0.96565100	-1.29083500
H	2.87274400	-0.77962900	-2.18122000
O	2.74819400	-1.70995000	-0.33102600
N	2.52284700	-0.02403600	1.98970300
C	2.32800600	0.72184800	3.11823000
O	1.63339000	1.73350100	3.13350600
C	3.05031800	0.22480400	4.36044000
H	3.54787500	-0.74039200	4.22553700
H	3.79814400	0.96826500	4.65499800
H	2.32763300	0.14552300	5.17756900
H	3.01820600	-0.90298500	2.04977900
O	3.08344300	2.33290300	0.44649300
O	4.57054700	1.15483800	-1.70483900
C	4.67624100	-1.81327900	-1.75174300
H	4.32119700	-2.82555400	-1.96576600
H	5.12743700	-1.38540600	-2.64786100
O	5.67412200	-1.91102600	-0.72105900
O	0.82131500	-1.90001100	0.87858600
C	2.17153200	3.34801700	0.49069800
O	1.11429600	3.31634100	-0.09807400
C	5.80726500	1.65638000	-1.41558600
O	6.35978200	1.51961800	-0.34790800
C	6.94279000	-1.53522600	-1.04976400

O	7.27494800	-1.17987200	-2.15944200
C	6.39537900	2.34079700	-2.62152900
H	7.15229100	3.05767700	-2.29942500
H	6.87915100	1.57498800	-3.23939000
H	5.62502700	2.83272600	-3.21964000
C	2.65734400	4.45790800	1.38233500
H	3.73186600	4.62023100	1.26415700
H	2.10120300	5.37162700	1.16773300
H	2.46875900	4.15102500	2.41735600
C	7.84363700	-1.58184100	0.15609900
H	7.55148700	-2.37812800	0.84434700
H	8.87804400	-1.70948400	-0.16729400
H	7.75456600	-0.62025000	0.67474100
H	-5.46610200	3.40128700	0.92940100
H	-7.57136100	2.02185700	-3.34468900
H	-8.61011000	3.30120500	0.57872800

4F-EZ B3LYP/6-31G(d), electr. en. = -2367.109957
a.u.

C	3.46256300	1.54720000	0.49721200
C	4.47030600	2.21903700	1.20694300
C	5.80753300	1.78504900	1.17838200
C	6.12475800	0.65736700	0.41847200
C	5.14316700	-0.02117900	-0.31427700
C	3.82036700	0.43724500	-0.27539500
H	7.14729400	0.28784900	0.40698300
H	3.06129600	-0.05985500	-0.87158200
C	2.02643900	2.00970700	0.55770500
H	1.83308300	2.83045600	-0.14515800
C	6.86241200	2.50144300	1.98636700
H	7.11127300	3.47866600	1.55349800
O	4.13562900	3.29207100	2.01587500
C	4.13989000	4.56205600	1.36439200
H	5.12825100	4.79884600	0.94979500
H	7.78569100	1.91627800	2.03020300
H	1.33586100	1.20174900	0.29861800
H	3.88291700	5.30091800	2.12712000
N	5.52265300	-1.13694700	-1.10591700
H	6.39228500	-1.07558200	-1.61866500
C	4.92966400	-2.37382500	-1.21182100
S	5.54168400	-3.50735500	-2.29827800
N	3.86342600	-2.59225900	-0.40228100
C	3.15276200	-3.86189200	-0.29185400
H	3.73481000	-4.57638700	0.30607700
H	3.07440400	-4.28717000	-1.29607200
H	3.71175600	-1.92576800	0.34691200
C	1.77431700	-3.64838300	0.34066100
H	1.87589600	-3.13405000	1.30639700
H	1.32740100	-4.62469700	0.55857600
C	0.82835400	-2.84236300	-0.54179700
H	1.29455500	-1.90825600	-0.87318000
H	0.54898900	-3.41608400	-1.43926800
C	-1.34419200	-1.89734000	-0.46061900
H	-1.57570900	-2.40998200	-1.41314100
C	-2.60315100	-1.82028800	0.41047400
H	-2.98215500	-2.82442800	0.61680800
C	-3.68361300	-1.04167300	-0.37822600
H	-3.97736700	-1.62803600	-1.25537600
C	-3.15420000	0.32077000	-0.81395200
H	-2.99733500	0.95881800	0.05622800
C	-1.83459300	0.14047900	-1.58824100
H	-2.03731300	-0.45171000	-2.49763600

O	-0.89937500	-0.56483500	-0.76911400
N	-2.27942500	-1.19181000	1.67872200
C	-2.86920200	-1.56529000	2.85442900
O	-3.77671400	-2.38855600	2.91016900
C	-2.33207600	-0.87658300	4.09940800
H	-1.48632400	-0.20954900	3.90618700
H	-3.14006100	-0.29789200	4.55811400
H	-2.02828200	-1.64186600	4.81973800
H	-1.47624100	-0.57915300	1.69536300
O	-4.83620700	-0.82575100	0.43963400
O	-4.10433300	0.94835200	-1.69242200
C	-1.20488800	1.44490000	-2.05399000
H	-0.18893700	1.24385300	-2.40584200
H	-1.79270000	1.88050700	-2.86285900
O	-1.11426000	2.39268100	-0.97494600
O	-0.34352600	-2.55176500	0.22966800
C	-5.73373200	-1.85499800	0.49929500
O	-5.65602500	-2.84266600	-0.19512000
C	-4.71208700	2.09007800	-1.25528200
O	-4.51324700	2.58881200	-0.17070900
C	-1.68973400	3.61418200	-1.17492400
O	-2.20299400	3.95277500	-2.21838900
C	-5.60400000	2.65910800	-2.32708300
H	-6.36769000	3.28866300	-1.86766400
H	-4.98469500	3.28290100	-2.98253600
H	-6.06172500	1.87114100	-2.92921200
C	-6.77348900	-1.58748100	1.55243300
H	-7.07363800	-0.53630300	1.55517300
H	-7.63535500	-2.23659800	1.39166500
H	-6.31890200	-1.81670400	2.52292500
C	-1.63638800	4.44556700	0.07927700
H	-0.74587200	4.22567800	0.67233200
H	-1.67521200	5.50390200	-0.18422800
H	-2.52294900	4.20025300	0.67534400
H	1.78012400	2.37792000	1.55827300
H	6.51554200	2.68628100	3.00779400
H	3.39881500	4.60389300	0.55596600

4G-EZ B3LYP/6-31G(d), electr. en. = -2367.109635
a.u.

C	-8.32367300	0.85817700	1.02166900
C	-8.64237300	0.90806400	-0.34628000
C	-7.98352000	0.09901700	-1.28571100
C	-7.00957900	-0.79636400	-0.83213800
C	-6.67196900	-0.86376300	0.52640000
C	-7.32909100	-0.02990800	1.43817400
H	-6.53264400	-1.46765800	-1.54017900
H	-7.04696300	-0.06465100	2.48775800
C	-9.01297200	1.76823000	2.00928500
H	-9.99885000	1.38063500	2.29778700
C	-8.32611300	0.19471500	-2.75308100
H	-9.32101900	-0.21544900	-2.96670200
O	-9.57567200	1.82658200	-0.79549600
C	-10.92730000	1.36705500	-0.78507200
H	-11.05619300	0.48171700	-1.42101500
H	-7.60472800	-0.36049900	-3.36002500
H	-8.42276900	1.86986800	2.92493900
H	-11.53400800	2.18569600	-1.17899900
N	-5.71245300	-1.78766200	1.01773200
H	-5.92200900	-2.25414700	1.89035700
C	-4.45252600	-2.08083600	0.55432600
S	-3.54618600	-3.28141400	1.32054900

N	-4.02380800	-1.36191800	-0.51270900	C	8.13849500	1.00409700	1.19934400
C	-2.69319000	-1.46844100	-1.09652100	C	8.01472400	-0.36993400	1.46761900
H	-2.78443900	-1.21790500	-2.16091900	C	7.28078500	-1.15548200	0.57499800
H	-2.38821300	-2.51484900	-1.01862700	C	6.69287900	-0.59978600	-0.56655300
H	-4.58077800	-0.56039500	-0.78479200	C	6.83450900	0.77262400	-0.81355400
C	-1.66083700	-0.55903000	-0.41540200	H	7.14726900	-2.21534200	0.77806200
H	-1.61313700	-0.81126800	0.64881900	H	6.41351200	1.20254300	-1.71774500
H	-1.96890900	0.49110900	-0.49599400	C	7.67032200	3.07541300	-0.17550100
C	-0.27863600	-0.71867500	-1.03331700	H	8.69651200	3.35675400	-0.44240800
H	0.09249800	-1.74253400	-0.90647000	C	8.62607200	-0.97460300	2.70839500
H	-0.30004300	-0.49586700	-2.11330500	H	9.68784100	-1.21308500	2.56219000
C	1.88030400	0.24984700	-0.89913300	O	8.79961100	1.82098200	2.10057000
H	1.86178500	0.38730200	-1.99756200	C	10.21062900	1.91733800	1.90553500
C	2.65676700	1.39749600	-0.24336500	H	10.70344200	0.94485000	2.03009700
H	2.19162000	2.35666300	-0.48459800	H	8.11892000	-1.90541400	2.97973300
C	4.09325600	1.38803700	-0.81943200	H	7.01841300	3.39294300	-0.99475700
H	4.05110800	1.63372300	-1.88595300	H	10.58037200	2.60807600	2.66686900
C	4.74036400	0.02130400	-0.62204000	N	6.00092200	-1.45289300	-1.46695500
H	4.91220800	-0.16291700	0.43865900	H	6.41086700	-2.35641000	-1.66333500
C	3.83229700	-1.07445300	-1.21211700	C	4.75362400	-1.30697000	-2.02607800
H	3.74139300	-0.90929500	-2.30026100	S	4.18203300	-2.47728000	-3.09889500
O	2.53893300	-0.99120000	-0.61330600	N	4.06109200	-0.19958400	-1.66003500
N	2.63412700	1.23224500	1.19932500	C	2.69323200	0.08911500	-2.06996600
C	2.58214700	2.29463900	2.05765400	H	2.57143400	-0.29886700	-3.08424600
O	2.65758600	3.45940600	1.67907600	H	2.58656500	1.18059500	-2.10705000
C	2.44338400	1.93593800	3.52898400	H	4.43386600	0.34601300	-0.89194300
H	2.29791400	0.86690200	3.71154500	C	1.64229700	-0.52182000	-1.13200600
H	3.34335000	2.26481900	4.05861000	H	1.77180100	-0.12872000	-0.11539900
H	1.59713500	2.48966000	3.94572700	H	1.78634400	-1.60606300	-1.08913700
H	2.46258300	0.29947100	1.54874800	C	0.22641900	-0.21476300	-1.59938800
O	4.90464700	2.36019500	-0.15430500	H	0.06351900	0.86646800	-1.69509900
O	5.99908800	-0.02231900	-1.31728500	H	0.03217500	-0.67592500	-2.58042900
C	4.36790500	-2.48680800	-1.02642400	C	-2.01704000	-0.62759700	-0.95894100
H	3.57694700	-3.20108700	-1.27310300	H	-2.21513600	-0.99406900	-1.98399200
H	5.22961000	-2.65556000	-1.67357500	C	-2.86941700	-1.40892600	0.04795200
O	4.75175500	-2.71648600	0.33993000	H	-2.64711300	-2.47715800	-0.01605000
O	0.60130200	0.20309600	-0.37970500	C	-4.35789400	-1.19417700	-0.31905200
C	4.80363000	3.64293700	-0.61130800	H	-4.55749500	-1.66346700	-1.28830400
O	4.18317100	3.94644600	-1.60519400	C	-4.68859900	0.29333600	-0.38052400
C	7.13310900	-0.13736300	-0.56599000	H	-4.63095500	0.73351900	0.61532000
O	7.14306000	-0.17701500	0.64331100	C	-3.70990000	1.00432500	-1.33389100
C	6.02436500	-3.15227000	0.56070000	H	-3.84542100	0.59404000	-2.35010800
O	6.81608000	-3.39790400	-0.32315000	O	-2.37124800	0.76248300	-0.90159900
C	8.34449400	-0.26644800	-1.45207500	N	-2.55790500	-0.96140100	1.39410700
H	9.23094200	0.05824500	-0.90478800	C	-2.56403500	-1.80638300	2.46846300
H	8.46122800	-1.32624500	-1.70803400	O	-2.92955900	-2.97490900	2.39389600
H	8.22917100	0.30354900	-2.37662800	C	-2.10036400	-1.19337300	3.78109400
C	5.53306900	4.58835400	0.30344300	H	-1.72729600	-0.16921100	3.68364000
H	6.47127100	4.15271400	0.65708200	H	-2.93678300	-1.19789500	4.48739700
H	5.71375700	5.53278600	-0.21188300	H	-1.31229400	-1.82420800	4.20242200
H	4.88781200	4.76298400	1.17178700	H	-2.15566400	-0.03899600	1.48619800
C	6.31109100	-3.23967900	2.03643700	O	-5.20505200	-1.79245100	0.66542900
H	5.41640300	-3.50634200	2.60345800	O	-6.02037200	0.47053700	-0.89472700
H	7.10942500	-3.96328500	2.20957000	C	-3.92729000	2.50694400	-1.43590500
H	6.65441300	-2.25272200	2.36738200	H	-3.07365600	2.95415400	-1.95371100
H	-9.17039400	2.76215400	1.58041100	H	-4.84379700	2.72350200	-1.98621500
H	-8.33569100	1.23735900	-3.08627800	O	-4.00742000	3.10550400	-0.13053400
H	-11.26388700	1.12427800	0.23083700	O	-0.68129700	-0.75365300	-0.63064000
				C	-5.44830900	-3.12890600	0.51948100
				O	-5.09784500	-3.76506300	-0.44824500
				C	-6.95909500	0.99289100	-0.05281000
				O	-6.74409000	1.28912500	1.10066700
4H-EZ B3LYP/6-31G(d), electr. en. = -2367.109157							
a.u.							
C	7.54242700	1.59145700	0.07145800				

C	-5.11618700	3.85094100	0.14100600
O	-5.99261800	4.07460600	-0.66509800
C	-8.26379600	1.19825800	-0.77707700
H	-9.08138400	1.21589100	-0.05468000
H	-8.21939300	2.17217900	-1.27883700
H	-8.43005300	0.42661400	-1.53206900
C	-6.16651600	-3.66935000	1.72559500
H	-6.91950500	-2.96413900	2.08736300
H	-6.62088400	-4.63088900	1.48244100
H	-5.41896700	-3.80718000	2.51496400
C	-5.11493500	4.30868100	1.57566400
H	-4.10035600	4.48634800	1.93936600
H	-5.72380100	5.20928500	1.67080200
H	-5.56851300	3.51309900	2.17802000
H	7.40945500	3.64626000	0.72143500
H	8.56296000	-0.28107300	3.55176200
H	10.45281200	2.31121600	0.91003100

1A B3LYP/6-31G(d), electr. en. = -9306.429044 a.u.

C	-2.06269600	3.03451800	1.27888400
C	-2.75808000	2.27279600	2.22050000
N	-4.14770900	2.52930900	2.42268700
C	-2.07709800	-1.29374100	-2.94913600
C	-2.75814900	-2.27283900	-2.22030700
N	-4.14778700	-2.52933700	-2.42247100
C	0.70543300	1.08480700	-2.76892200
C	0.01358900	1.91499500	-1.87041900
C	0.69204100	2.86241300	-1.07909300
C	2.06269000	3.03455000	-1.27846600
C	2.75806900	2.27286000	-2.22009500
C	2.07701800	1.29379500	-2.94898400
H	2.59003100	3.78222400	-0.69336800
H	2.61167600	0.70455800	-3.68916800
C	-0.00003700	0.00006700	-3.57322300
H	-0.74561000	0.45831100	-4.23428300
C	-0.00003900	3.68403500	0.00018500
H	-0.75229300	4.34676300	-0.44164400
C	-0.70551200	-1.08475000	-2.76903900
C	-0.01366800	-1.91497700	-1.87059100
C	-0.69213400	-2.86243500	-1.07930000
H	-2.61172700	-0.70445600	-3.68930300
C	-2.06277500	-3.03456800	-1.27869500
H	-2.59015000	-3.78224300	-0.69362500
C	-0.69207500	2.86234700	1.07943100
C	-0.01360200	1.91486300	1.87068500
C	-0.70543400	1.08465400	2.76915200
H	-2.59006700	3.78220300	0.69382000
C	-2.07701600	1.29366000	2.94927500
H	-2.61163100	0.70436300	3.68944400
C	0.00003300	-0.00017700	3.57332700
H	-0.74553700	-0.45840600	4.23439900
C	-0.00008200	-3.68414400	-0.00008000
H	-0.75233500	-4.34687700	0.44174200
H	0.75214400	-4.34688100	-0.44195700
C	2.07705300	-1.29394400	2.94906300
C	2.75809000	-2.27300600	2.22014800
C	0.70547100	-1.08493400	2.76901800
C	2.06267200	-3.03469600	1.27854500
C	0.01359600	-1.91510600	1.87052000
C	0.69202400	-2.86253900	1.07919000
H	2.58999800	-3.78238000	0.69344100
H	2.61172800	-0.70470400	3.68923400

O	1.36121300	-1.77241900	-1.75388800
O	-1.36128100	-1.77245100	1.75380100
O	1.36127200	1.77228800	1.75390700
O	-1.36129800	1.77240600	-1.75370300
C	2.10047800	2.70520900	2.54589300
H	1.89130000	2.57191400	3.61645000
H	1.88135700	3.74081400	2.26384500
C	-2.10051500	-2.70538900	2.54574800
H	-1.89124200	-2.57220100	3.61629900
H	-1.88151400	-3.74098800	2.26359100
C	-2.10048000	2.70528800	-2.54576100
H	-1.88140200	3.74090700	-2.26374200
H	-1.89123200	2.57194900	-3.61629900
C	2.10036900	-2.70525500	-2.54601800
H	1.89111200	-2.57184300	-3.61654600
H	1.88127400	-3.74088900	-2.26406600
H	0.74564800	0.45799200	4.23439400
H	0.75220400	4.34676900	0.44203900
H	0.74555800	-0.45810800	-4.23431000
H	-3.15920500	2.51038200	-2.35675400
H	-3.15923000	-2.51038200	2.35677800
H	3.15910200	-2.51037100	-2.35702000
H	3.15919700	2.51031300	2.35683500
N	4.14771400	2.52937700	-2.42219800
H	4.41793600	3.50493100	-2.52765900
C	5.18210600	1.66205500	-2.23507700
S	6.79174900	2.21335000	-2.33870800
N	4.85727500	0.37863000	-1.95665300
C	5.81080800	-0.69070300	-1.69538300
H	5.29856900	-1.42541900	-1.06839900
H	6.64532800	-0.27880200	-1.12175700
H	3.87387300	0.15720800	-1.84734000
N	4.14773700	-2.52952600	2.42222400
H	4.41796500	-3.50508000	2.52763400
C	5.18213200	-1.66220400	2.23505800
S	6.79177100	-2.21352200	2.33861000
N	4.85730800	-0.37877200	1.95665300
C	5.81083200	0.69057000	1.69537900
H	6.64533800	0.27869100	1.12171700
H	5.29856300	1.42529200	1.06842500
H	3.87390400	-0.15732800	1.84740900
C	6.35308300	-1.37283000	-2.95871500
H	6.96889100	-0.66019800	-3.51799500
H	5.52579600	-1.67961000	-3.61138700
C	7.18470700	-2.59869000	-2.60426600
H	7.68797200	-3.01069000	-3.48633200
H	7.95541200	-2.34587400	-1.86350000
C	6.35314100	1.37270700	2.95869300
H	6.96891600	0.66006600	3.51799400
H	5.52586300	1.67954200	3.61135100
C	7.18479700	2.59853500	2.60419500
H	7.95547800	2.34568300	1.86341700
H	7.68810400	3.01051800	3.48624600
C	6.79742400	-4.33750700	-1.00698700
H	7.22107500	-3.68970800	-0.22144800
C	5.65958800	-5.18523000	-0.42537800
H	4.88084100	-4.53338100	-0.02769400
C	6.22722700	-6.04495200	0.72638800
H	6.49526500	-5.39149000	1.56302400
C	7.43963100	-6.84497600	0.25652900
H	7.12329500	-7.62126800	-0.44119500
C	8.46489300	-5.91438600	-0.42049700

H	8.83268100	-5.18884600	0.32436800	C	-7.43946000	6.84506600	0.25653700
O	7.82730300	-5.21452900	-1.49050200	C	-6.22708400	6.04503300	0.72646700
N	5.07635200	-5.99638300	-1.48143000	H	-6.49515800	5.39162300	1.56313200
C	3.74106200	-6.21777500	-1.59730400	H	-4.88071000	4.53342600	-0.02751900
O	2.92035300	-5.81731700	-0.76793500	O	-7.82716200	5.21449400	-1.49038500
C	3.30781100	-6.99502700	-2.82907000	N	-5.07616100	5.99637700	-1.48128300
H	4.14336700	-7.39196100	-3.41313600	C	-3.74085200	6.21774700	-1.59706100
H	2.66634400	-7.82273500	-2.51398700	O	-2.92022900	5.81735200	-0.76757600
H	2.70727700	-6.34123100	-3.47040400	C	-3.30748500	6.99486000	-2.82887600
H	5.69467800	-6.26807600	-2.23415900	H	-4.14300100	7.39198800	-3.41286100
O	5.23986500	-6.99946400	1.16067500	H	-2.66579500	7.82241000	-2.51383400
O	8.07570000	-7.46654200	1.38702900	H	-2.70716200	6.34090800	-3.47024800
C	9.68368900	-6.64196600	-0.96805200	H	-5.69444900	6.26804100	-2.23405500
H	10.24926200	-5.95510000	-1.60407200	O	-5.23969100	6.99952400	1.16073400
H	10.31756200	-6.99415200	-0.15340400	C	-9.68353500	6.64196700	-0.96804000
O	9.29117500	-7.76405100	-1.78021900	H	-10.24910600	5.95502200	-1.60397900
C	6.79750100	4.33736600	1.00692300	H	-10.31739900	6.99423900	-0.15342500
H	7.22111400	3.68956800	0.22136100	O	-9.29104800	7.76395600	-1.78035300
C	5.65965500	5.18510500	0.42536800	H	-7.12308800	7.62132300	-0.44121300
C	8.46495700	5.91424800	0.42037800	O	-8.07553100	7.46671000	1.38699700
H	8.83270700	5.18871800	-0.32451800	O	-6.30075400	3.59873200	-2.06328600
C	7.43967100	6.84485800	-0.25658900	H	-4.41791900	3.50489600	2.52785800
C	6.22724700	6.04484000	-0.72640300	C	-5.18211900	1.66205200	2.23518600
H	6.49523500	5.39138000	-1.56305700	S	-6.79173400	2.21334900	2.33866500
H	4.88088900	4.53328200	0.02768200	N	-4.85724200	0.37869400	1.95658800
O	7.82741700	5.21437700	1.49040000	C	-5.81070900	-0.69070300	1.69538800
N	5.07642900	5.99625300	1.48143100	H	-6.64520300	-0.27891700	1.12163900
C	3.74113200	6.21763500	1.59729800	H	-5.29840600	-1.42546400	1.06851500
O	2.92042700	5.81717100	0.76792800	H	-3.87382000	0.15724700	1.84749200
C	3.30786000	6.99481600	2.82909700	C	-6.35306400	-1.37272900	2.95874600
H	4.14340400	7.39170800	3.41320700	H	-6.96888600	-0.66005700	3.51796200
H	2.66640600	7.82254500	2.51404500	H	-5.52582000	-1.67947800	3.61148600
H	2.70730500	6.34098500	3.47037800	C	-7.18473400	-2.59856000	2.60429900
H	5.69475500	6.26795800	2.23415500	H	-7.95547000	-2.34567100	1.86359400
O	5.23983600	6.99934100	-1.16062300	H	-7.68796100	-3.01059100	3.48637200
C	9.68379500	6.64179200	0.96789900	C	-6.79756100	-4.33731500	1.00692100
H	10.24934900	5.95489300	1.60390000	H	-7.22118100	-3.68948700	0.22138500
H	10.31766200	6.99395800	0.15323900	C	-5.65977700	-5.18508600	0.42530000
O	9.29136200	7.76388100	1.78010400	C	-8.46510100	-5.91413500	0.42045200
H	7.12336200	7.62113000	0.44117100	H	-8.83286500	-5.18859100	-0.32442600
O	8.07569100	7.46645000	-1.38709400	C	-7.43988600	-6.84476500	-0.25659500
O	6.30093300	-3.59877400	-2.06349000	C	-6.22746300	-6.04476800	-0.72645300
O	6.30104300	3.59863500	2.06344100	H	-6.49548500	-5.39128700	-1.56307900
H	-4.41805200	-3.50491000	-2.52765100	H	-4.88101600	-4.53326100	0.02760100
C	-5.18216900	-1.66204200	-2.23494100	O	-7.82749500	-5.21429100	1.49044600
S	-6.79181500	-2.21327800	-2.33839400	N	-5.07650800	-5.99625700	1.48131000
N	-4.85724900	-0.37867800	-1.95637100	C	-3.74120100	-6.21761800	1.59710500
C	-5.81066200	0.69077500	-1.69519700	O	-2.92055400	-5.81710100	0.76770000
H	-6.64517900	0.27905600	-1.12143100	C	-3.30785400	-6.99486300	2.82884100
H	-5.29830400	1.42550500	-1.06833600	H	-4.14337600	-7.39203800	3.41278600
H	-3.87381400	-0.15725400	-1.84736500	H	-2.66617500	-7.82239000	2.51371900
C	-6.35297600	1.37281900	-2.95856600	H	-2.70752200	-6.34098400	3.47028100
H	-6.96885300	0.66016500	-3.51774100	H	-5.69482300	-6.26802600	2.23402100
H	-5.52571800	1.67948800	-3.61132200	O	-5.24011800	-6.99929900	-1.16075900
C	-7.18455700	2.59871600	-2.60414800	C	-9.68395000	-6.64162500	0.96802800
H	-7.95532400	2.34591300	-1.86344600	H	-10.24943200	-5.95468400	1.60404700
H	-7.68773200	3.01077100	-3.48623800	H	-10.31787200	-6.99377000	0.15340300
C	-6.79727400	4.33750400	-1.00682300	O	-9.29155100	-7.76372000	1.78024100
H	-7.22091800	3.68972700	-0.22125700	H	-7.12355900	-7.62109300	0.44109900
C	-5.65944600	5.18526300	-0.42524000	O	-8.07598000	-7.46628200	-1.38710300
C	-8.46472700	5.91444100	-0.42043000	O	-6.30100700	-3.59861800	2.06341700
H	-8.83251500	5.18896600	0.32450000	C	-8.05159200	-8.82892400	-1.45861000

O	-7.48967800	-9.53896800	-0.65517900
C	-9.81562400	-8.97801200	1.45310900
O	-10.61959400	-9.14970400	0.56303100
C	-4.29427900	-6.57753500	-2.02947000
O	-4.28579000	-5.47766900	-2.54340300
C	-9.81502500	8.97832000	-1.45333400
O	-10.61893500	9.15016700	-0.56323200
C	-8.05120600	8.82936300	1.45831200
O	-7.48936800	9.53932200	0.65475200
C	-4.29382500	6.57769000	2.02938100
O	-4.28532400	5.47777700	2.54321400
C	4.29410000	-6.57776600	2.02949400
O	4.28562500	-5.47793600	2.54349200
C	8.05145700	-8.82918500	1.45839100
O	7.48976700	-9.53921700	0.65478600
C	9.81514900	-8.97837400	-1.45306300
O	10.61905400	-9.15011600	-0.56293500
C	4.29399600	6.57762500	-2.02934600
O	4.28543500	5.47776600	-2.54328400
C	8.05132200	8.82909300	-1.45849600
O	7.48952700	9.53909400	-0.65494100
C	9.81532900	8.97820400	1.45292900
O	10.61919100	9.14995900	0.56276400
C	-8.86163400	-9.31199700	-2.63285200
H	-8.81695200	-8.60992600	-3.46830600
H	-8.50979600	-10.29949500	-2.93601000
H	-9.90475400	-9.39866900	-2.30615900
C	-9.22662200	-10.06455300	2.31424300
H	-8.98943200	-9.69850300	3.31572300
H	-8.30013900	-10.40230600	1.83567100
C	-3.24481300	-7.63546400	-2.23986900
H	-3.67967000	-8.63749900	-2.21855900
H	-2.72549100	-7.45535600	-3.18229000
H	-2.52793700	-7.55212300	-1.41455000
C	-9.22590000	10.06473600	-2.31454200
H	-8.98867800	9.69857300	-3.31597300
H	-8.29941800	10.40246700	-1.83595000
C	-8.86127200	9.31255900	2.63248700
H	-8.81653000	8.61062000	3.46805000
H	-8.50950900	10.30013100	2.93549300
H	-9.90440100	9.39909900	2.30578700
C	-3.24423300	7.63551500	2.23966700
H	-3.67901200	8.63758600	2.21847600
H	-2.72478200	7.45531200	3.18200000
H	-2.52748700	7.55215800	1.41423800
C	8.86149800	-9.31230000	2.63261900
H	8.50977100	-10.29987900	2.93564100
H	9.90464600	-9.39880000	2.30596600
H	8.81668700	-8.61033700	3.46815800
C	3.24475000	-7.63578700	2.24002000
H	3.67969900	-8.63778100	2.21870400
H	2.72549200	-7.45569700	3.18248300
H	2.52778500	-7.55255300	1.41476800
C	9.22599600	-10.06487900	-2.31414100
H	8.98938100	-9.69896900	-3.31581100
H	9.91927200	-10.90622400	-2.36333100
H	8.29914900	-10.40207400	-1.83588000
C	3.24448100	7.63554400	-2.23958500
H	3.67932700	8.63758200	-2.21829300
H	2.72504300	7.45545700	-3.18195000
H	2.52769100	7.55218400	-1.41419400
C	8.86129900	9.31224300	-2.63275300

H	8.50945300	10.29976500	-2.93582400
H	9.90444000	9.39888600	-2.30611700
H	8.81656500	8.61023100	-3.46825500
C	9.22626600	10.06470100	2.31407800
H	8.98971800	9.69877200	3.31575800
H	9.91956900	10.90602500	2.36323500
H	8.29939200	10.40193400	1.83589600
H	-9.91947400	10.90580200	-2.36434400
H	-9.92026100	-10.90557200	2.36392400

1B B3LYP/6-31G(d), electr. en. = -9306.418808 a.u.

C	-1.17095200	-2.12141500	-2.84927700
C	-2.10093100	-2.81675800	-2.06844500
N	-2.30207200	-4.21812500	-2.19978800
C	2.89578200	-2.10921000	1.16075800
C	2.10124300	-2.81644000	2.06853300
N	2.30248700	-4.21779100	2.19991600
C	2.80956300	0.72120300	-1.04904600
C	1.91605400	0.03824700	-1.89416900
C	1.05087800	0.73144000	-2.75605100
C	1.17088000	2.12123000	-2.84933200
C	2.10090500	2.81657000	-2.06855500
C	2.89552900	2.10938800	-1.16081600
H	0.54977900	2.65970100	-3.55874900
H	3.60228600	2.65401500	-0.54300900
C	3.64373900	0.00010100	-0.00008500
H	4.30455800	-0.73414900	-0.47089600
C	-0.00007200	-0.00008100	-3.58138700
H	0.48088800	-0.73284400	-4.23982100
C	2.80971500	-0.72102900	1.04898100
C	1.91614900	-0.03813900	1.89411200
C	1.05107200	-0.73138600	2.75603900
H	3.60256200	-2.65377900	0.54292500
C	1.17122200	-2.12116400	2.84936500
H	0.55020200	-2.65967500	3.55882500
C	-1.05095900	-0.73162600	-2.75600000
C	-1.91611500	-0.03843300	-1.89409800
C	-2.80961500	-0.72138700	-1.04896600
H	-0.54986900	-2.65988200	-3.55871400
C	-2.89555100	-2.10957700	-1.16071200
H	-3.60226800	-2.65420700	-0.54286500
C	-3.64372400	-0.00033100	0.00008500
H	-4.30445100	-0.73464500	0.47092100
C	0.00008200	0.00005500	3.58139800
H	-0.48079100	-0.73275600	4.23983800
H	0.48100800	0.73293100	4.23972400
C	-2.89570000	2.10909800	1.16066600
C	-2.10117600	2.81641300	2.06838700
C	-2.80962000	0.72091500	1.04900200
C	-1.17111500	2.12120700	2.84924000
C	-1.91606400	0.03809800	1.89419200
C	-1.05095800	0.73141800	2.75603300
H	-0.55008800	2.65978800	3.55864300
H	-3.60249400	2.65361100	0.54280000
O	1.86201000	1.34929100	1.86955900
O	-1.86203400	-1.34933900	1.86978700
O	-1.86209000	1.34900000	-1.86958600
O	1.86211900	-1.34918900	-1.86963000
C	-2.80499300	1.96612200	-2.74913400
H	-3.83844200	1.78566200	-2.43368600
H	-2.67805400	1.61353000	-3.78180900
C	-2.80477900	-1.96638100	2.74957800

H	-3.83827500	-1.78591100	2.43429800	H	-4.67778400	7.20957000	2.43522400
H	-2.67762600	-1.61372700	3.78220300	H	-5.90639300	7.25548100	-0.49972600
C	2.80489900	-1.96625500	-2.74936900	O	-7.38904700	4.05848700	-0.95674900
H	2.67772600	-1.61369600	-3.78202400	O	-8.69764000	5.07869600	-3.32241200
H	3.83838500	-1.78570300	-2.43410200	C	-7.70399300	7.68243800	-4.33564700
C	2.80478900	1.96651300	2.74918000	H	-7.04113900	8.36296400	-4.87747100
H	3.83827500	1.78624100	2.43375000	H	-8.41969600	7.23641800	-5.02740000
H	2.67787300	1.61383700	3.78182800	O	-8.41508900	8.45844100	-3.35563500
H	-4.30471400	0.73381800	-0.47063800	C	4.78353600	6.26517800	2.55619100
H	-0.48109500	0.73271300	-4.23973700	H	4.49144600	5.60787800	3.39563000
H	4.30463500	0.73434900	0.47062100	C	5.43081300	5.42933100	1.44584200
H	2.60147200	-3.04057200	-2.71263000	C	6.85980800	6.60330200	3.67091800
H	-2.60129800	-3.04069100	2.71293400	H	6.50812600	5.93445400	4.47663000
H	2.60108500	3.04078300	2.71257000	C	7.63228300	5.75929100	2.63620600
H	-2.60145800	3.04042200	-2.71246000	C	6.68961700	4.73727200	2.01149100
N	2.30209500	4.21791400	-2.19996300	H	6.39013200	4.00070300	2.76404600
H	3.26793400	4.53671700	-2.11912500	H	4.73227300	4.66157500	1.10794400
C	1.36997800	5.21625600	-2.17300400	O	5.73644400	7.22144300	3.04517100
S	1.84475100	6.83554000	-2.37360000	N	5.73207000	6.27827900	0.30724500
N	0.07932400	4.85091700	-1.97059700	C	5.47218500	5.89752100	-0.97309300
C	-1.02240900	5.79587400	-1.81236000	O	5.09724800	4.75149100	-1.25191800
H	-0.65753600	6.67069300	-1.26683700	C	5.66584300	6.95473200	-2.03587300
H	-1.77746600	5.31118500	-1.18810600	H	6.15438400	7.85983200	-1.66289600
H	-0.10458600	3.88009900	-1.74289300	H	6.26036400	6.53228100	-2.85081100
N	-2.30246400	4.21775400	2.19967200	H	4.67719000	7.21011500	-2.43493700
H	-3.26832400	4.53648900	2.11864100	H	5.90557900	7.25595900	0.49987000
C	-1.37039900	5.21614600	2.17256100	O	7.38853300	4.05899800	0.95679800
S	-1.84526500	6.83543300	2.37295400	C	7.70336800	7.68278500	4.33584800
N	-0.07971200	4.85088500	1.97028100	H	7.04050100	8.36325100	4.87772800
C	1.02199100	5.79589900	1.81219500	H	8.41909700	7.23673800	5.02755700
H	1.77714900	5.31123900	1.18804200	O	8.41442500	8.45888100	3.35587500
H	0.65714300	6.67068700	1.26660600	H	8.05795700	6.40219800	1.86511700
H	0.10434100	3.88001800	1.74290900	O	8.69711100	5.07917600	3.32246900
C	-1.63654000	6.24054300	-3.14898800	O	-3.70996200	6.94668700	-2.02971600
H	-2.07170500	5.37506300	-3.66906500	O	3.70936700	6.94707600	2.02985900
H	-0.83999600	6.63414700	-3.79072200	H	3.26835000	-4.53654400	2.11922600
C	-2.68274700	7.33683000	-2.96204300	C	1.37042900	-5.21618000	2.17284600
H	-2.22426100	8.22521400	-2.51845000	S	1.84528700	-6.83544200	2.37348200
H	-3.13798500	7.63090700	-3.91565100	N	0.07976500	-4.85096100	1.97031900
C	1.63591000	6.24061400	3.14891000	C	-1.02189700	-5.79600600	1.81210500
H	2.07108100	5.37516100	3.66902900	H	-1.77698700	-5.31137500	1.18784900
H	0.83924400	6.63414300	3.79053900	H	-0.65698400	-6.67081000	1.26657800
C	2.68204100	7.33700000	2.96214900	H	-0.10424800	-3.88013200	1.74275300
H	3.13716600	7.63102000	3.91583000	C	-1.63598300	-6.24069200	3.14875100
H	2.22349600	8.22538400	2.51861600	H	-2.07120100	-5.37522900	3.66881200
C	-4.78413400	6.26481600	-2.55605800	H	-0.83940200	-6.63423500	3.79047400
H	-4.49205400	5.60755100	-3.39552900	C	-2.68211600	-7.33706000	2.96188100
C	-5.43138400	5.42892500	-1.44572500	H	-3.13726100	-7.63114900	3.91553000
H	-4.73281700	4.66119600	-1.10782300	H	-2.22357500	-8.22541400	2.51828600
C	-6.69015100	4.73684100	-2.01141400	C	-4.78361700	-6.26525300	2.55599000
H	-6.39063100	4.00030700	-2.76398500	H	-4.49156900	-5.60805100	3.39551500
C	-7.63286000	5.75884700	-2.63611100	C	-5.43098600	-5.42934800	1.44574200
H	-8.05858600	6.40170100	-1.86501000	C	-6.85988800	-6.60358900	3.67072300
C	-6.86041100	6.60293900	-3.67077500	H	-6.50824300	-5.93481800	4.47651600
H	-6.50869200	5.93415000	-4.47652000	C	-7.63241400	-5.75945700	2.63612800
O	-5.73707100	7.22108300	-3.04498000	C	-6.68977700	-4.73736500	2.01152300
N	-5.73268600	6.27783500	-0.30710800	H	-6.39026100	-4.00087100	2.76413800
C	-5.47267900	5.89712000	0.97321200	H	-4.73251400	-4.66152800	1.10785600
O	-5.09745800	4.75116600	1.25199900	O	-5.73651500	-7.22162400	3.04491500
C	-5.66640300	6.95428600	2.03601500	N	-5.73226100	-6.27822300	0.30710300
H	-6.15482500	7.85944500	1.66302300	C	-5.47233500	-5.89745400	-0.97322300
H	-6.26107200	6.53183300	2.85084500	O	-5.09735200	-4.75144100	-1.25204900

C	-5.66586800	-6.95469600	-2.03599100	O	-10.22722700	-5.84238900	1.82207800
H	-6.15450400	-7.85976400	-1.66305600	C	-6.92086900	-2.83199700	0.61294700
H	-6.26023700	-6.53225000	-2.85104000	O	-6.06235500	-2.24674600	1.24231200
H	-4.67715700	-7.21014400	-2.43487100	C	-6.92115900	2.83159900	-0.61262000
H	-5.90583600	-7.25589700	0.49970800	O	-6.06256600	2.24632200	-1.24185200
O	-7.38872400	-4.05892500	0.95692300	C	-9.96258500	5.21887200	-2.82464800
C	-7.70341000	-7.68318500	4.33553300	O	-10.22779000	5.84239900	-1.82249800
H	-7.04048500	-8.36379200	4.87716400	C	-9.76928700	8.53555700	-3.48983600
H	-8.41905700	-7.23727100	5.02741100	O	-10.38694100	8.02760400	-4.40043300
O	-8.41460500	-8.45909000	3.35549700	C	6.92082600	2.83202400	0.61272300
H	-8.05810900	-6.40226500	1.86497000	O	6.06248100	2.24653900	1.24209200
O	-8.69722900	-5.07947700	3.32255200	C	9.96201500	5.21932300	2.82459800
O	-3.70943000	-6.94704100	2.02960900	O	10.22712300	5.84271200	1.82233700
H	-3.26792100	-4.53693300	-2.11908000	C	9.76861800	8.53605600	3.49007200
C	-1.36995800	-5.21646000	-2.17272400	O	10.38629800	8.02814800	4.40067800
S	-1.84472300	-6.83574500	-2.37341500	C	10.96330400	-4.54337100	-3.72506500
N	-0.07930800	-4.85117700	-1.97021000	H	10.54608400	-3.64769500	-4.19076600
C	1.02238400	-5.79618300	-1.81199100	H	11.86064000	-4.30095900	-3.15353100
H	1.77744200	-5.31153200	-1.18770600	H	11.23314200	-5.25340200	-4.51573800
H	0.65749300	-6.67100900	-1.26648500	C	10.37972100	-9.29011700	-2.33852500
H	0.10465100	-3.88035500	-1.74257300	H	9.70791400	-10.06706200	-1.96703400
C	1.63653400	-6.24082300	-3.14862100	H	10.56599000	-8.57269300	-1.53090700
H	2.07163600	-5.37531100	-3.66870400	C	7.57486000	-2.33910100	0.64870800
H	0.84000900	-6.63448400	-3.79033900	H	8.63296700	-2.61093300	0.67890400
C	2.68281900	-7.33703900	-2.96171000	H	7.44521800	-1.25940400	0.73804400
H	3.13800800	-7.63110400	-3.91534500	H	7.07117700	-2.83034700	1.48951400
H	2.22441400	-8.22544000	-2.51806800	C	-10.37898700	-9.29105600	2.33852300
C	4.78416100	-6.26490800	-2.55591600	H	-9.70678500	-10.06733000	1.96636100
H	4.49198600	-5.60774000	-3.39542600	H	-10.56633900	-8.57348000	1.53129100
C	5.43145300	-5.42888300	-1.44570800	C	-10.96307100	-4.54425800	3.72451600
C	6.86039200	-6.60295600	-3.67076000	H	-10.54594100	-3.64859500	4.19032900
H	6.50858700	-5.93426200	-4.47654600	H	-11.86030900	-4.30182500	3.15284100
C	7.63284500	-5.75869400	-2.63622100	H	-11.23301800	-5.25433400	4.51511200
C	6.69009900	-4.73672400	-2.01157500	C	-7.57462200	-2.33978700	-0.64878400
H	6.39044100	-4.00028100	-2.76418300	H	-8.63265900	-2.61186500	-0.67918500
H	4.73286400	-4.66118100	-1.10780000	H	-7.44520400	-1.26005600	-0.73804300
O	5.73714800	-7.22115700	-3.04487000	H	-7.07067000	-2.83087700	-1.48952100
N	5.73295100	-6.27767900	-0.30706400	C	-10.96347500	4.54358700	-3.72452900
C	5.47310300	-5.89687200	0.97326400	H	-11.86086500	4.30154200	-3.15292600
O	5.09794400	-4.75090400	1.25204600	H	-11.23316400	5.25336900	-4.51547600
C	5.66694100	-6.95400300	2.03609000	H	-10.54639300	3.64766600	-4.18988700
H	6.15583900	-7.85894900	1.66320000	C	-7.57503500	2.33947900	0.64907400
H	6.26119200	-6.53133500	2.85111000	H	-8.63311400	2.61141400	0.67927800
H	4.67831100	-7.20972300	2.43499600	H	-7.44553000	1.25977100	0.73850300
H	5.90661400	-7.25534300	-0.49964200	H	-7.07126800	2.83076700	1.48980100
O	7.38904300	-4.05821000	-0.95702700	C	-10.37932300	9.29061400	-2.33859400
C	7.70408800	-7.68241300	-4.33556900	H	-9.70726200	10.06721900	-1.96686300
H	7.04131100	-8.36309300	-4.87728800	H	-11.33289800	9.72018600	-2.65018800
H	8.41969900	-7.23635700	-5.02739000	H	-10.56603900	8.57312600	-1.53113200
O	8.41534600	-8.45819600	-3.35548700	C	7.57470100	2.34004100	-0.64902600
H	8.05866700	-6.40144200	-1.86508600	H	8.63274700	2.61210200	-0.67926200
O	8.69752800	-5.07856800	-3.32270400	H	7.44530900	1.26032700	-0.73850700
O	3.71008300	-6.94682200	-2.02947200	H	7.07083700	2.83131900	-1.48970200
C	9.96250900	-5.21850600	-2.82495900	C	10.96298300	4.54408700	3.72443300
O	10.22781400	-5.84173100	-1.82265200	H	11.86029200	4.30193300	3.15274800
C	9.76954500	-8.53514100	-3.48974800	H	11.23280600	5.25395000	4.51526300
O	10.38707900	-8.02728100	-4.40047800	H	10.54591600	3.64824200	4.18994800
C	6.92098200	-2.83139900	-0.61291800	C	10.37860300	9.29130200	2.33892600
O	6.06230600	-2.24624800	-1.24215700	H	9.70646900	10.06787100	1.96725100
C	-9.76879900	-8.53602400	3.48970600	H	11.33212400	9.72094600	2.65058700
O	-10.38637300	-8.02804100	4.40034400	H	10.56541800	8.57391200	1.53139900
C	-9.96211800	-5.21934600	2.82455400	H	-11.33228300	-9.72106300	2.65039800

H	11.33351900	-9.71925400	-2.65003200
1C B3LYP/6-31G(d), electr. en. = -9306.417607 a.u.			
C	-2.09108400	2.94919000	1.22204500
C	-2.78728000	2.19166600	2.16819800
N	-4.16906500	2.47595600	2.37205500
C	-2.09821800	-1.23900600	-2.92552300
C	-2.78703900	-2.19178900	-2.16855800
N	-4.16883900	-2.47600400	-2.37244200
C	0.71958300	1.06436900	-2.77788700
C	0.02750200	1.90200300	-1.88778600
C	0.71103600	2.81555200	-1.06473600
C	2.09093500	2.94912900	-1.22263100
C	2.78722500	2.19150800	-2.16866700
C	2.09856800	1.23855200	-2.92554200
H	2.62718900	3.66961400	-0.61195900
H	2.62784400	0.64805100	-3.66731200
C	0.00023900	-0.00036100	-3.59503400
H	-0.73836500	0.47065800	-4.25462300
C	-0.00013700	3.63937500	-0.00041700
H	-0.74408400	4.29902100	-0.46085200
C	-0.71924500	-1.06490600	-2.77776200
C	-0.02730900	-1.90242700	-1.88741000
C	-0.71100500	-2.81582100	-1.06434700
H	-2.62739100	-0.64860300	-3.66744500
C	-2.09091100	-2.94933800	-1.22237900
H	-2.62725400	-3.66969800	-0.61163900
C	-0.71116900	2.81566100	1.06409600
C	-0.02753700	1.90226300	1.88720500
C	-0.71953800	1.06474600	2.77751000
H	-2.62738500	3.66956500	0.61128400
C	-2.09851700	1.23886600	2.92519500
H	-2.62773900	0.64846700	3.66708600
C	-0.00011300	0.00020700	3.59484600
H	-0.73876700	-0.47082700	4.25436800
C	-0.00006000	-3.63952600	0.00022900
H	-0.74404100	-4.29918000	0.46059500
H	0.74382300	-4.29939400	-0.45998500
C	2.09831600	-1.23861700	2.92551300
C	2.78707600	-2.19153400	2.16868600
C	0.71933200	-1.06450200	2.77776000
C	2.09088900	-2.94919300	1.22260400
C	0.02735600	-1.90217300	1.88761500
C	0.71099700	-2.81568700	1.06461300
H	2.62722400	-3.66965000	0.61197000
H	2.62751000	-0.64807900	3.66731300
O	1.35309300	-1.79813700	-1.81380000
O	-1.35307900	-1.79807000	1.81415300
O	1.35287000	1.79796900	1.81369800
O	-1.35292700	1.79782800	-1.81442900
C	2.04264200	2.74387000	2.63455500
H	1.70436700	2.68647500	3.67795200
H	1.92398200	3.77060800	2.27123200
C	-2.04259800	-2.74381600	2.63543400
H	-1.70400200	-2.68620400	3.67871000
H	-1.92402400	-3.77062400	2.27227200
C	-2.04244200	2.74356300	-2.63571900
H	-1.92392600	3.77036600	-2.27252600
H	-1.70379400	2.68599000	-3.67898100
C	2.04293000	-2.74406400	-2.63457100
H	1.70481000	-2.68663900	-3.67801700
H	1.92416600	-3.77080400	-2.27128700

H	0.73851800	0.47139700	4.25428500
H	0.74369600	4.29925000	0.45986600
H	0.73893700	-0.47153900	-4.25440700
H	-3.10224100	2.48003600	-2.58607100
H	-3.10240400	-2.48032900	2.58573200
H	3.10272700	-2.48061400	-2.58443000
H	3.10243200	2.48035900	2.58457300
N	4.16901300	2.47588600	-2.37246400
H	4.39727400	3.46201400	-2.48263900
C	5.20790100	1.61671400	-2.56009100
S	6.73025100	2.21519500	-3.03653000
N	4.96747800	0.30253300	-2.33451100
C	5.89405700	-0.78610900	-2.63132500
H	6.37001500	-0.57608100	-3.59481700
H	5.29075900	-1.69326100	-2.73976200
H	4.05250200	0.04978800	-1.97870400
N	4.16886500	-2.47583800	2.37256200
H	4.39717000	-3.46195800	2.48272600
C	5.20770500	-1.61662300	2.56026600
S	6.73006800	-2.21505800	3.03672500
N	4.96724000	-0.30244500	2.33472800
C	5.89384700	0.78620300	2.63142000
H	5.29057100	1.69337000	2.73984300
H	6.36986300	0.57622100	3.59489400
H	4.05229600	-0.04972400	1.97882000
C	6.97513200	-1.02085700	-1.56810800
H	6.51647700	-1.10218600	-0.57572900
H	7.64822200	-0.15748300	-1.55383600
C	7.77563000	-2.28833300	-1.84926700
H	8.12598200	-2.31406200	-2.88753300
H	8.65742300	-2.35386700	-1.20295000
C	6.97485300	1.02085400	1.56811300
H	6.51611900	1.10218000	0.57577100
H	7.64788300	0.15743100	1.55381400
C	7.77547200	2.28827800	1.84915400
H	8.65716900	2.35374100	1.20269900
H	8.12599100	2.31398200	2.88736500
C	7.17394600	-4.14668800	-0.49034600
H	7.36637800	-3.46840200	0.35745200
C	5.95292400	-5.01973500	-0.17430200
H	5.09776600	-4.37904300	0.04850100
C	6.26676800	-5.88160900	1.07238500
H	6.32675500	-5.23342800	1.95270700
C	7.57519700	-6.64689000	0.89880200
H	7.46540900	-7.41547200	0.13247700
C	8.69999900	-5.66972100	0.51032900
H	8.83613700	-4.93945400	1.32544500
O	8.32227100	-4.98653700	-0.68516300
N	5.60970500	-5.82583000	-1.33298000
C	4.32423600	-6.05828100	-1.71173200
O	3.35228000	-5.67888200	-1.05393300
C	4.15073100	-6.83436100	-3.00654900
H	5.09534200	-7.10079200	-3.48971700
H	3.59021400	-7.75027700	-2.79549800
H	3.55110000	-6.23720900	-3.70047700
H	6.36658900	-6.07305800	-1.95613100
O	5.22771400	-6.85842900	1.26784700
O	7.92947800	-7.27622500	2.14249300
C	10.04720500	-6.33991300	0.28695100
H	10.72541000	-5.62242900	-0.18365900
H	10.46883500	-6.67661900	1.23484200
O	9.92146400	-7.46542500	-0.60206100

C	7.17376800	4.14672300	0.49036300	H	-10.46855200	6.67635300	1.23551000
H	7.36612500	3.46846300	-0.35747300	O	-9.92154900	7.46522700	-0.60147500
C	5.95275200	5.01981500	0.17443200	H	-7.46532100	7.41530600	0.13261200
C	8.69979100	5.66973200	-0.51038500	O	-7.92899900	7.27594200	2.14271600
H	8.83587700	4.93946600	-1.32551000	O	-6.95097200	3.45694300	-1.66946400
C	7.57498100	6.64691900	-0.89880000	H	-4.39739800	3.46206300	2.48229300
C	6.26652900	5.88165600	-1.07229200	C	-5.20788000	1.61671100	2.55979700
H	6.32646500	5.23345100	-1.95260100	S	-6.73020100	2.21511700	3.03646500
H	5.09754700	4.37915800	-0.04829000	N	-4.96744600	0.30256100	2.33408900
O	8.32212600	4.98654500	0.68512400	C	-5.89391800	-0.78614300	2.63109300
N	5.60969400	5.82594400	1.33313600	H	-5.29054200	-1.69324600	2.73945400
C	4.32428500	6.05843700	1.71206100	H	-6.36974200	-0.57612100	3.59465600
O	3.35222500	5.67901900	1.05442600	H	-4.05243200	0.04984700	1.97835200
C	4.15098100	6.83437200	3.00699200	C	-6.97514800	-1.02096800	1.56805700
H	5.09568300	7.10145400	3.48962100	H	-6.51665300	-1.10255200	0.57563300
H	3.58968300	7.74988100	2.79627600	H	-7.64813700	-0.15751200	1.55372400
H	3.55218400	6.23678400	3.70127400	C	-7.77582000	-2.28823500	1.84968500
H	6.36666400	6.07315000	1.95619200	H	-8.65777800	-2.35376200	1.20358600
O	5.22747300	6.85847500	-1.26773500	H	-8.12594600	-2.31355500	2.88803700
C	10.04701800	6.33990800	-0.28708400	C	-7.17413800	-4.14656300	0.49073400
H	10.72523300	5.62243100	0.18352200	H	-7.36631900	-3.46807600	-0.35695600
H	10.46861500	6.67657400	-1.23500400	C	-5.95303300	-5.01957500	0.17482700
O	9.92132700	7.46545600	0.60188900	C	-8.69994000	-5.66943400	-0.51061400
H	7.46525800	7.41551500	-0.13247800	H	-8.83581000	-4.93905700	-1.32567600
O	7.92919300	7.27623800	-2.14251700	C	-7.57507700	-6.64659300	-0.89884300
O	6.95067900	-3.45693500	-1.66918900	C	-6.26656900	-5.88134600	-1.07201000
O	6.95056800	3.45692600	1.66918900	H	-6.32629800	-5.23310400	-1.95230700
H	-4.39722400	-3.46210000	-2.48264100	H	-5.09783800	-4.37884600	-0.04772400
C	-5.20763000	-1.61671300	-2.56007000	O	-8.32253300	-4.98639600	0.68507800
S	-6.73001400	-2.21505700	-3.03661800	N	-5.61005100	-5.82579400	1.33349800
N	-4.96711400	-0.30257300	-2.33437000	C	-4.32465300	-6.05816400	1.71256500
C	-5.89363400	0.78616000	-2.63110900	O	-3.35256000	-5.67867900	1.05502700
H	-5.29028600	1.69328700	-2.73942900	C	-4.15143200	-6.83411000	3.00750400
H	-6.36957700	0.57626000	-3.59464100	H	-5.09615900	-7.10098700	3.49019600
H	-4.05207300	-0.04990800	-1.97867400	H	-3.59034300	-7.74974500	2.79677300
C	-6.97472300	1.02082200	-1.56789700	H	-3.55245900	-6.23663800	3.70173200
H	-6.51608300	1.10234700	-0.57553500	H	-6.36705100	-6.07289600	1.95655900
H	-7.64765100	0.15732200	-1.55354400	O	-5.22753600	-6.85822300	-1.26726700
C	-7.77554400	2.28805500	-1.84925400	C	-10.04724700	-6.33956900	-0.28768000
H	-8.65735400	2.35345600	-1.20293800	H	-10.72550900	-5.62211000	0.18288200
H	-8.12592500	2.31344000	-2.88752000	H	-10.46867300	-6.67610700	-1.23572200
C	-7.17394500	4.14655800	-0.49048000	O	-9.92181000	-7.46523300	0.60118900
H	-7.36617000	3.46817500	0.35728500	H	-7.46552500	-7.41525100	-0.13256100
C	-5.95288000	5.01962500	-0.17460700	O	-7.92904100	-7.27581500	-2.14269200
C	-8.69981300	5.66952100	0.51063600	O	-6.95123000	-3.45709700	1.66982400
H	-8.83577700	4.93921200	1.32574300	C	-7.92897300	-8.63951000	-2.18605700
C	-7.57495600	6.64667700	0.89891000	O	-7.60469100	-9.34637500	-1.25816800
C	-6.26648100	5.88140600	1.07219800	C	-10.39128600	-8.66313100	0.15478300
H	-6.32629600	5.23316900	1.95249100	O	-10.94297000	-8.81817700	-0.91306000
H	-5.09765200	4.37895100	0.04797000	C	-4.12805600	-6.47840600	-1.95374700
O	-8.32233300	4.98637900	-0.68497400	O	-4.00357200	-5.39806200	-2.49512700
N	-5.60993600	5.82583200	-1.33330100	C	-10.39103600	8.66319900	-0.15527400
C	-4.32455300	6.05830300	-1.71234900	O	-10.94275000	8.81841300	0.91252900
O	-3.35244100	5.67898100	-1.05474400	C	-7.92890800	8.63964000	2.18604900
C	-4.15137100	6.83433000	-3.00724500	O	-7.60453700	9.34647800	1.25817100
H	-5.09610700	7.10099000	-3.49004100	C	-4.12798300	6.47832400	1.95402800
H	-3.59053300	7.75009900	-2.79642700	O	-4.00359700	5.39795900	2.49539200
H	-3.55216900	6.23702100	-3.70141400	C	4.12839400	-6.47849300	1.95453000
H	-6.36695600	6.07289400	-1.95635600	O	4.00410100	-5.39811900	2.49588800
O	-5.22742400	6.85824500	1.26754400	C	7.92945600	-8.63992400	2.18573900
C	-10.04708000	6.33968400	0.28753500	O	7.60485100	-9.34671600	1.25790600
H	-10.72533900	5.62219200	-0.18298100	C	10.39108100	-8.66340900	-0.15600800

O	10.94295000	-8.81866600	0.91170700	N	-4.14770600	-2.49197500	-2.37639000
C	4.12812200	6.47851900	-1.95436100	C	0.68880600	1.09512600	-2.76561700
O	4.00382200	5.39814000	-2.49571000	C	-0.01453700	1.95704600	-1.90279800
C	7.92921500	8.63993600	-2.18575600	C	0.67209400	2.89088000	-1.09429500
O	7.60484200	9.34672900	-1.25784200	C	2.04884600	3.03950900	-1.27465600
C	10.39098200	8.66340600	0.15578500	C	2.75169400	2.25727300	-2.19339900
O	10.94294600	8.81858600	-0.91189200	C	2.06755700	1.27845900	-2.91671300
C	-8.43801500	-9.12639200	-3.51728400	H	2.57739200	3.78690800	-0.69023100
H	-8.15581300	-8.44991800	-4.32707100	H	2.60373900	0.67000000	-3.63914400
H	-8.06281800	-10.13393400	-3.70389200	C	-0.00012400	-0.00018600	-3.57008600
H	-9.53240400	-9.16524000	-3.46220500	H	-0.75310800	0.44736900	-4.22640400
C	-10.08945400	-9.75862300	1.14380700	C	0.00008200	3.71551900	-0.00001700
H	-10.09889700	-9.38613900	2.17058700	H	-0.76268500	4.38078800	-0.41621000
H	-9.08749500	-10.14219400	0.91905100	C	-0.68904600	-1.09544300	-2.76553600
C	-3.07561400	-7.55337800	-1.92592000	C	0.01432700	-1.95733700	-1.90271200
H	-3.52381500	-8.54850500	-1.97813000	C	-0.67228100	-2.89114300	-1.09416000
H	-2.37088400	-7.39937400	-2.74425100	H	-2.60400200	-0.67030200	-3.63899500
H	-2.54291100	-7.46565900	-0.97179700	C	-2.04904600	-3.03974400	-1.27445600
C	-10.08909000	9.75854700	-1.14442100	H	-2.57757200	-3.78711300	-0.68997400
H	-10.09848000	9.38592800	-2.17115200	C	-0.67198200	2.89100000	1.09432400
H	-9.08713000	10.14210600	-0.91964900	C	0.01453400	1.95711800	1.90285900
C	-8.43805400	9.12656200	3.51722100	C	-0.68893200	1.09529100	2.76568900
H	-8.15594900	8.45009300	4.32704500	H	-2.57717800	3.78719500	0.69019100
H	-8.06284000	10.13409500	3.70384600	C	-2.06766500	1.27875000	2.91674400
H	-9.53243600	9.16544900	3.46204100	H	-2.60392100	0.67036800	3.63918500
C	-3.07556100	7.55332100	1.92647900	C	-0.00008800	-0.00002700	3.57023100
H	-3.52378400	8.54843500	1.97872700	H	-0.75309800	-0.44752100	4.22656400
H	-2.37094900	7.39924200	2.74489900	C	-0.00027800	-3.71573000	0.00016600
H	-2.54271100	7.46571400	0.97242800	H	-0.76310200	-4.38092700	0.41636700
C	8.43870900	-9.12690300	3.51684700	H	0.76246300	-4.38104600	-0.41599700
H	8.06377500	-10.13456800	3.70330900	C	2.06749100	-1.27880400	2.91677100
H	9.53310400	-9.16545100	3.46170400	C	2.75152400	-2.25767300	2.19343100
H	8.15638200	-8.45063200	4.32676200	C	0.68874300	-1.09539100	2.76574400
C	3.07597800	-7.55350300	1.92720400	C	2.04857900	-3.03987300	1.27473200
H	3.52421700	-8.54861000	1.97948900	C	-0.01470100	-1.95728600	1.90297900
H	2.37146200	-7.39936200	2.74569400	C	0.67182900	-2.89116100	1.09443700
H	2.54301600	-7.46599400	0.97320600	H	2.57705300	-3.78730400	0.69028400
C	10.08874200	-9.75876700	-1.14502300	H	2.60375200	-0.67036400	3.63915700
H	10.09754600	-9.38613100	-2.17175100	O	1.39170000	-1.83861800	-1.82971900
H	10.80870600	-10.56952300	-1.02124400	O	-1.39207800	-1.83856600	1.83005800
H	9.08695100	-10.14245600	-0.91971600	O	1.39188200	1.83823700	1.82985700
C	3.07574500	7.55356700	-1.92710600	O	-1.39192000	1.83840200	-1.82974100
H	3.52402100	8.54865600	-1.97942400	C	2.14991300	2.91960500	2.40864300
H	2.37124000	7.39941600	-2.74560400	H	1.66323000	3.87834600	2.20247100
H	2.54276200	7.46611600	-0.97311500	C	-2.14990400	-2.91997300	2.40903600
C	8.43857800	9.12690500	-3.51682600	H	-1.66309000	-3.87866700	2.20294100
H	8.06381900	10.13464400	-3.70323600	C	-2.14973500	2.91983400	-2.40868800
H	9.53298000	9.16526200	-3.46167100	H	-1.66301500	3.87853100	-2.20237000
H	8.15614500	8.45072700	-4.32678300	C	2.14958200	-2.92006300	-2.40854500
C	10.08878500	9.75879700	1.14480800	H	1.66287100	-3.87876300	-2.20225500
H	10.09752700	9.38615300	2.17153400	H	0.75293500	0.44752000	4.22651200
H	10.80885900	10.56945700	1.02104200	H	0.76289600	4.38076300	0.41612700
H	9.08704900	10.14262300	0.91949100	H	0.75285100	-0.44779200	-4.22638400
H	-10.80889600	10.56938100	-1.02024800	H	-3.10897400	2.91812100	-1.88122000
H	-10.80928400	-10.56941000	1.01947900	H	-3.10908300	-2.91841700	1.88145700
				H	3.10877300	-2.91832000	-1.88099000
				H	3.10904200	2.91784000	1.88097600
				N	4.14744100	2.49178500	-2.37678200
				H	4.43266800	3.46000000	-2.50794500
				C	5.16817600	1.60692700	-2.19928800
				S	6.78615400	2.13485200	-2.30797100
				N	4.82640600	0.32705300	-1.92480600
2A B3LYP/6-31G(d), electr. en. = -9620.952824 a.u.							
C	-2.04872700	3.03975700	1.27465000				
C	-2.75168600	2.25761600	2.19337700				
N	-4.14742100	2.49227300	2.37665200				
C	-2.06780700	-1.27874700	-2.91656100				
C	-2.75193300	-2.25751300	-2.19316700				

C	5.76549700	-0.75697100	-1.66951700	O	2.94509300	5.99413000	0.57751300
H	5.24286600	-1.48701300	-1.04604600	C	3.36218500	7.37419400	2.50505800
H	6.60617500	-0.36131200	-1.09369600	H	4.09697600	7.43641300	3.31348100
H	3.84031400	0.11524300	-1.82051800	H	3.22972400	8.37516100	2.07899600
N	4.14726500	-2.49231000	2.37673800	H	2.39925800	7.05786800	2.91276600
H	4.43239500	-3.46054600	2.50797200	H	5.70660900	6.41684900	2.08112100
C	5.16807100	-1.60753600	2.19928700	O	5.31220800	6.98113000	-1.33362400
S	6.78600500	-2.13562200	2.30796600	C	9.70989500	6.60954000	0.88256000
N	4.82643300	-0.32761300	1.92484400	H	10.24848400	5.93821000	1.55741100
C	5.76563600	0.75630200	1.66948800	H	10.36554300	6.91165800	0.06500500
H	6.60620600	0.36057100	1.09355700	O	9.32991800	7.77434000	1.63870600
H	5.24301900	1.48642200	1.04609600	H	7.18401700	7.62351100	0.26792000
H	3.84036600	-0.11571800	1.82049900	O	8.16063500	7.36678300	-1.53501300
C	6.29527800	-1.43873700	-2.93817400	O	6.25544700	-3.67056800	-2.03465100
H	6.91271000	-0.72758700	-3.49790300	O	6.25597700	3.66979800	2.03455300
H	5.46196400	-1.73515500	-3.58729600	H	-4.43297500	-3.46016300	-2.50766600
C	7.12610000	-2.66908700	-2.59859000	C	-5.16839200	-1.60703600	-2.19906400
H	7.60756700	-3.08510900	-3.49064400	S	-6.78640000	-2.13486900	-2.30778300
H	7.91421900	-2.41822500	-1.87623500	N	-4.82656300	-0.32715200	-1.92469900
C	6.29563200	1.43798300	2.93809700	C	-5.76557900	0.75694800	-1.66946200
H	6.91304400	0.72676200	3.49775400	H	-6.60642700	0.36129800	-1.09388900
H	5.46241900	1.73449500	3.58730500	H	-5.24300300	1.48683700	-1.04576600
C	7.12656500	2.66823500	2.59842200	H	-3.84046100	-0.11538100	-1.82043500
H	7.91458400	2.41725800	1.87599500	C	-6.29500100	1.43893500	-2.93815100
H	7.60817400	3.08420300	3.49042600	H	-6.91246300	0.72794100	-3.49804700
C	6.77045100	-4.37577100	-0.96324300	H	-5.46151800	1.73525300	-3.58710200
H	7.18987400	-3.69837800	-0.20086900	C	-7.12562600	2.66942700	-2.59860100
C	5.65973600	-5.22734200	-0.33886800	H	-7.91385000	2.41867300	-1.87631900
H	4.86806300	-4.58126900	0.04193400	H	-7.60694800	3.08558500	-3.49066800
C	6.26585200	-6.02098600	0.84306300	C	-6.76992400	4.37602700	-0.96323500
H	6.52794200	-5.32437200	1.64611400	H	-7.18951500	3.69870600	-0.20088400
C	7.49170600	-6.81058200	0.38964100	C	-5.65926700	5.22755500	-0.33871900
H	7.18329400	-7.62430100	-0.26797100	C	-8.48333800	5.88753000	-0.34480300
C	8.48380700	-5.88726300	-0.34455600	H	-8.84733200	5.12305900	0.36197200
H	8.84765900	-5.12283100	0.36233500	C	-7.49134900	6.81077700	0.38964400
O	7.81204000	-5.24733200	-1.43103000	C	-6.26554200	6.02116300	0.84317300
N	5.08593300	-6.10163100	-1.34753900	H	-6.52771600	5.32449800	1.64615400
C	3.76442600	-6.41883100	-1.39453300	H	-4.86764400	4.58147600	0.04216900
O	2.94449500	-5.99467500	-0.57743800	O	-7.81138600	5.24765400	-1.43119500
C	3.36147200	-7.37479500	-2.50499300	N	-5.08532400	6.10188200	-1.34727100
H	4.09571700	-7.43609000	-3.31398600	C	-3.76385500	6.41920700	-1.39394300
H	3.23026200	-8.37604100	-2.07918500	O	-2.94401200	5.99488600	-0.57683600
H	2.39796600	-7.05916100	-2.91185000	C	-3.36050700	7.37520100	-2.50421600
H	5.70591900	-6.41755100	-2.08116300	H	-4.09718900	7.44145900	-3.31058300
O	5.31162000	-6.98172100	1.33367200	H	-3.22291400	8.37495200	-2.07697800
O	8.16001500	-7.36760200	1.53491200	H	-2.39988000	7.05586200	-2.91505300
C	9.70923500	-6.61050800	-0.88275400	H	-5.70530200	6.41819200	-2.08072800
H	10.24787600	-5.93920200	-1.55758900	O	-5.31141100	6.98190600	1.33394300
H	10.36487200	-6.91270200	-0.06521900	C	-9.70865700	6.61082400	-0.88318500
O	9.32915500	-7.77525200	-1.63893400	H	-10.24719300	5.93954800	-1.55813200
C	6.77096600	4.37499100	0.96314000	H	-10.36443300	6.91300800	-0.06575700
H	7.19032400	3.69759200	0.20073400	O	-9.32842900	7.77557900	-1.63927700
C	5.66028100	5.22664100	0.33883000	H	-7.18285500	7.62457400	-0.26783400
C	8.48439500	5.88637800	0.34440500	O	-8.15982700	7.36767100	1.53487600
H	8.84816500	5.12193200	-0.36251500	O	-6.25483300	3.67070800	-2.03452000
C	7.49232900	6.80978400	-0.38972900	H	-4.43255700	3.46049500	2.50790100
C	6.26638900	6.02029600	-0.84310500	C	-5.16824200	1.60750400	2.19924800
H	6.52837600	5.32369500	-1.64620100	S	-6.78616800	2.13560500	2.30788300
H	4.86855300	4.58063300	-0.04196400	N	-4.82659600	0.32758500	1.92482300
O	7.81263500	5.24648800	1.43089800	C	-5.76578000	-0.75635700	1.66953300
N	5.08656100	6.10093200	1.34755000	H	-6.60647700	-0.36058100	1.09382600
C	3.76508300	6.41822300	1.39458600	H	-5.24326400	-1.48638200	1.04594300

H	-3.84051900	0.11564300	1.82066700	H	-9.05123400	-9.78062200	3.08575400
C	-6.29549400	-1.43816900	2.93819200	H	-8.40197900	-10.43409400	1.56513400
H	-6.91281900	-0.72700500	3.49802300	C	-3.34948900	-7.62386400	-2.46750800
H	-5.46214400	-1.73469400	3.58721700	H	-3.81584900	-8.61158100	-2.49251300
C	-7.12641900	-2.66844700	2.59860500	H	-2.83419400	-7.41202100	-3.40554100
H	-7.91455900	-2.41749900	1.87629800	H	-2.62258600	-7.60455300	-1.64704000
H	-7.60787500	-3.08448400	3.49065800	C	-9.31060600	10.09816000	-2.07393100
C	-6.77099500	-4.37508800	0.96320200	H	-9.04898300	9.78182600	-3.08622700
H	-7.19041400	-3.69765000	0.20086300	H	-8.39995100	10.43532400	-1.56552300
C	-5.66043600	-5.22677600	0.33872900	C	-9.00946600	9.13994900	2.84381900
C	-8.48461600	-5.88628600	0.34457100	H	-8.96621400	8.40157800	3.64739300
H	-8.84841000	-5.12173900	-0.36222600	H	-8.68274100	10.11912000	3.19788000
C	-7.49272400	-6.80970300	-0.38978400	H	-10.04792300	9.22197400	2.50140000
C	-6.26673600	-6.02030500	-0.84320200	C	-3.34817500	7.62416300	2.46779200
H	-6.52870100	-5.32361500	-1.64622900	H	-3.81432400	8.61198200	2.49270600
H	-4.86869800	-4.58081000	-0.04211100	H	-2.83301500	7.41225300	3.40588300
O	-7.81265300	-5.24655900	1.43103800	H	-2.62119900	7.60465400	1.64739400
N	-5.08664600	-6.10116800	1.34731600	C	9.00940100	-9.14001700	2.84383300
C	-3.76521700	-6.41865100	1.39405900	H	8.68260500	-10.11922600	3.19772500
O	-2.94528800	-5.99444400	0.57697900	H	10.04792800	-9.22200200	2.50161700
C	-3.36206900	-7.37467800	2.50437900	H	8.96598500	-8.40173000	3.64747700
H	-4.09852300	-7.44028400	3.31100900	C	3.34834800	-7.62398400	2.46745100
H	-3.22529500	-8.37462100	2.07731800	H	3.81448800	-8.61180800	2.49239800
H	-2.40110100	-7.05586400	2.91481700	H	2.83314000	-7.41206500	3.40551400
H	-5.70670000	-6.41740400	2.08074000	H	2.62141500	-7.60448400	1.64701500
O	-5.31270400	-6.98122000	-1.33384500	C	9.31142900	-10.09781400	-2.07364700
C	-9.71010900	-6.60938300	0.88282400	H	9.05033900	-9.78152800	-3.08609600
H	-10.24857300	-5.93804100	1.55776300	H	10.02336400	-10.92450800	-2.09812400
H	-10.36587500	-6.91141300	0.06533000	H	8.40046500	-10.43475000	-1.56564200
O	-9.33014000	-7.77424400	1.63888100	C	3.34890300	7.62360900	-2.46722300
H	-7.18443100	-7.62354900	0.26772800	H	3.81513900	8.61138700	-2.49218700
O	-8.16120400	-7.36649600	-1.53506500	H	2.83359800	7.41176200	-3.40524800
O	-6.25585100	-3.66993600	2.03456300	H	2.62203700	7.60416100	-1.64672700
C	-8.17065900	-8.72497900	-1.66469700	C	9.01007100	9.13916200	-2.84394900
O	-7.61308100	-9.48167500	-0.90172100	H	8.68332300	10.11840900	-3.19777900
C	-9.89004600	-8.96046600	1.27059800	H	10.04864000	9.22104600	-2.50183900
O	-10.71429800	-9.07432500	0.38986900	H	8.96650400	8.40090100	-3.64760700
C	-4.36238500	-6.54566600	-2.19155100	C	9.31229700	10.09692500	2.07330200
O	-4.32428200	-5.42216100	-2.64949800	H	9.05130900	9.78068800	3.08579300
C	-9.88825500	8.96189700	-1.27118100	H	10.02426700	10.92359200	2.09766700
O	-10.71259800	9.07593000	-0.39055800	H	8.40128800	10.43387900	1.56538700
C	-8.16899800	8.72615100	1.66456900	H	-10.02268200	10.92472200	-2.09882100
O	-7.61117400	9.48275700	0.90168500	H	-10.02487500	-10.92333300	2.09807700
C	-4.36128300	6.54617700	2.19179000	C	2.37465600	2.76383500	3.91229100
O	-4.32346500	5.42267300	2.64974900	H	1.40414800	2.71418600	4.42185400
C	4.36148300	-6.54600800	2.19149900	H	2.88573700	1.81113000	4.10168500
O	4.32373000	-5.42255100	2.64959400	C	3.20168300	3.92238500	4.48301000
C	8.16917300	-8.72609300	1.66445400	H	4.15995500	4.02358800	3.95979700
O	7.61146200	-9.48261900	0.90140700	H	2.66525200	4.87424600	4.38675400
C	9.88892100	-8.96157200	-1.27075400	H	3.41092300	3.76859900	5.54714800
O	10.71310600	-9.07561400	-0.38998500	C	2.37418100	-2.76442800	-3.91223000
C	4.36195200	6.54552700	-2.19137800	H	1.40363100	-2.71478500	-4.42171500
O	4.32406100	5.42208500	-2.64949800	H	2.88529600	-1.81177000	-4.10177100
C	8.16993400	8.72527900	-1.66449000	C	3.20110100	-3.92308300	-4.48289800
O	7.61236600	9.48183300	-0.90136600	H	2.66463600	-4.87490800	-4.38646800
C	9.88964900	8.96063000	1.27038300	H	3.41024500	-3.76943700	-5.54707500
O	10.71376700	9.07460500	0.38954200	H	4.15942100	-4.02426100	-3.95976500
C	-9.01100700	-9.13864200	-2.84408000	C	-2.37421900	2.76417600	-3.91238900
H	-8.96746200	-8.40030600	-3.64767100	H	-1.40363800	2.71427300	-4.42178500
H	-8.68442400	-10.11789300	-3.19805300	H	-2.88555200	1.81163400	-4.10192200
H	-10.04954000	-9.22043800	-2.50183800	C	-3.20080500	3.92299200	-4.48321800
C	-9.31269400	-10.09685500	2.07338500	H	-4.15905900	4.02459700	-3.96004800

H	-2.66402000	4.87465700	-4.38701200
H	-3.41006000	3.76922100	-5.54735500
C	-2.37454900	-2.76407800	3.91269000
H	-1.40401300	-2.71419500	4.42217600
H	-2.88579700	-1.81145100	4.10201700
C	-3.20131400	-3.92271800	4.48360400
H	-4.15957300	-4.02422200	3.96042300
H	-2.66466700	-4.87447000	4.38749200
H	-3.41057000	-3.76882000	5.54772300

2B B3LYP/6-31G(d), electr. en. = -9620.937905 a.u.

C	-1.14075100	-2.11219400	-2.80272600
C	-2.06954300	-2.80951000	-2.02528900
N	-2.24977300	-4.21490500	-2.13506900
C	2.88784500	-2.09569600	1.14429100
C	2.06949800	-2.80954600	2.02552200
N	2.24965600	-4.21494600	2.13543100
C	2.83525300	0.70281600	-1.06233500
C	1.96010300	0.01517900	-1.93001700
C	1.05767600	0.71720100	-2.74921300
C	1.14095500	2.11194900	-2.80287600
C	2.06967600	2.80936300	-2.02543600
C	2.88797000	2.09552200	-1.14414800
H	0.49482800	2.65089400	-3.48838200
H	3.58850600	2.64045900	-0.51951800
C	3.67427300	-0.00006700	0.00014200
H	4.33839700	-0.74555200	-0.44530300
C	0.00016200	-0.00019100	-3.57731800
H	0.47311400	-0.73839100	-4.23101800
C	2.83517100	-0.70298200	1.06253200
C	1.95999400	-0.01535700	1.93020300
C	1.05750300	-0.71739500	2.74931700
H	3.58839700	-2.64062800	0.51967300
C	1.14075400	-2.11214100	2.80293500
H	0.49456900	-2.65109300	3.48838500
C	-1.05743700	-0.71744600	-2.74920200
C	-1.95992000	-0.01532000	-1.93014700
C	-2.83512600	-0.70285400	-1.06243700
H	-0.49458000	-2.65122500	-3.48812600
C	-2.88786600	-2.09556700	-1.14411000
H	-3.58845000	-2.64042500	-0.51946200
C	-3.67416300	0.00015300	-0.00006000
H	-4.33832100	-0.74528200	0.44541600
C	-0.00004900	-0.00004500	3.57740300
H	-0.47302800	-0.73819600	4.23114100
H	0.47286500	0.73804500	4.23125200
C	-2.88777900	2.09573000	1.14420300
C	-2.06949800	2.80954500	2.02551400
C	-2.83509300	0.70301500	1.06238500
C	-1.14079600	2.11210900	2.80296400
C	-1.95995000	0.01536200	1.93005500
C	-1.05752600	0.71737000	2.74927600
H	-0.49466900	2.65104600	3.48848000
H	-3.58830700	2.64068100	0.51957700
O	1.93786600	1.37157500	1.96189800
O	-1.93772700	-1.37157400	1.96160700
O	-1.93777900	1.37161800	-1.96191400
O	1.93792200	-1.37175800	-1.96161100
C	-3.05350200	1.99406800	-2.62823900
H	-3.99748500	1.56795600	-2.27621700
C	-3.05336000	-1.99422000	2.62788100
H	-3.99741400	-1.56838300	2.27572000

C	3.05362700	-1.99434600	-2.62782000
H	3.99764000	-1.56850800	-2.27554500
C	3.05358200	1.99405800	2.62818400
H	3.99756100	1.56791200	2.27620200
H	-4.33819300	0.74567800	-0.44558100
H	-0.47271000	0.73789000	-4.23119900
H	4.33832700	0.74544200	0.44565000
H	3.02232900	-3.03977200	-2.30020300
H	-3.02207000	-3.03962700	2.30020500
H	3.02261600	3.03942700	2.30035400
H	-3.02251000	3.03945700	-2.30047700
N	2.24988000	4.21475900	-2.13530900
H	3.21505700	4.54151700	-2.08189700
C	1.30878100	5.20449300	-2.11295200
S	1.77418400	6.82792800	-2.30703400
N	0.01924800	4.83147000	-1.91799600
C	-1.08380500	5.77216000	-1.73755300
H	-0.71758300	6.63721100	-1.17793700
H	-1.83370000	5.27565900	-1.11642100
H	-0.16387600	3.85686600	-1.70671900
N	-2.24969100	4.21493900	2.13546700
H	-3.21484800	4.54173100	2.08195100
C	-1.30855900	5.20464500	2.11300500
S	-1.77392000	6.82810700	2.30689100
N	-0.01904500	4.83151000	1.91809400
C	1.08407600	5.77210300	1.73753600
H	1.83391800	5.27548600	1.11643600
H	0.71791700	6.63714000	1.17785600
H	0.16396700	3.85689600	1.70676700
C	-1.70912600	6.24089400	-3.06068200
H	-2.16629600	5.38878800	-3.58363400
H	-0.91546100	6.62953300	-3.70893500
C	-2.73257400	7.35405900	-2.84620000
H	-2.24970100	8.22983600	-2.40350200
H	-3.19845900	7.66465700	-3.78945900
C	1.70947400	6.24087900	3.06061200
H	2.16661000	5.38877600	3.58360100
H	0.91585700	6.62960300	3.70887000
C	2.73298000	7.35397500	2.84602200
H	3.19891500	7.66460300	3.78924300
H	2.25014700	8.22975400	2.40328400
C	-4.85584100	6.33456500	-2.41258500
H	-4.60341200	5.69382200	-3.27708200
C	-5.49365400	5.48515300	-1.30718800
H	-4.80305100	4.69577800	-1.00449600
C	-6.78000300	4.83221500	-1.85703800
H	-6.51482500	4.10927200	-2.63499500
C	-7.71582900	5.89035000	-2.42934700
H	-8.10689900	6.52012400	-1.62955500
C	-6.95249600	6.74672800	-3.46117700
H	-6.63665300	6.09306700	-4.29376200
O	-5.79962800	7.32470500	-2.85022600
N	-5.75039600	6.31241200	-0.14204400
C	-5.46130600	5.89840600	1.12111500
O	-5.09103400	4.74211200	1.36214200
C	-5.61411800	6.93151400	2.21397300
H	-6.11046800	7.84687500	1.87814300
H	-6.18310700	6.49277100	3.03841900
H	-4.61125900	7.17469000	2.58431900
H	-5.91582300	7.29640400	-0.30806100
O	-7.46531000	4.14223500	-0.80066000
O	-8.81323400	5.25325400	-3.10579400

C	-7.79048000	7.86073500	-4.07392100	H	-5.91613600	-7.29604100	0.30805600
H	-7.12803200	8.54237000	-4.61483100	O	-7.46574700	-4.14183600	0.80023200
H	-8.53346000	7.44838900	-4.75771400	C	-7.79114900	-7.85980400	4.07401000
O	-8.45917000	8.62400100	-3.05453700	H	-7.12888200	-8.54135300	4.61525500
C	4.85614800	6.33426800	2.41238600	H	-8.53422600	-7.44722800	4.75756000
H	4.60366700	5.69348100	3.27683800	O	-8.45975200	-8.62322900	3.05469300
C	5.49391500	5.48486800	1.30695300	H	-8.10728900	-6.51970200	1.62934700
C	6.95276700	6.74621900	3.46104900	O	-8.81386300	-5.25261000	3.10527500
H	6.63685600	6.09246200	4.29353500	O	-3.75154100	-6.97482600	1.89949500
C	7.71609800	5.88991600	2.42911100	H	-3.21494600	-4.54166200	-2.08162200
C	6.78024400	4.83183900	1.85676100	C	-1.30867000	-5.20463400	-2.11262000
H	6.51504400	4.10886800	2.63468600	S	-1.77406200	-6.82807800	-2.30662700
H	4.80326400	4.69554200	1.00424600	N	-0.01914500	-4.83154800	-1.91773100
O	5.79997600	7.32432200	2.85011100	C	1.08397400	-5.77216900	-1.73733500
N	5.75070100	6.31214400	0.14183400	H	1.83387800	-5.27560000	-1.11627000
C	5.46154500	5.89819500	-1.12133000	H	0.71784800	-6.63722700	-1.17766400
O	5.09122900	4.74191700	-1.36238300	H	0.16393700	-3.85692600	-1.70650300
C	5.61436600	6.93132300	-2.21416300	C	1.70923400	-6.24089100	-3.06049600
H	6.11086000	7.84661300	-1.87835300	H	2.16636300	-5.38877800	-3.58347600
H	6.18320800	6.49254000	-3.03868600	H	0.91554400	-6.62954300	-3.70870700
H	4.61149000	7.17461900	-2.58438900	C	2.73270700	-7.35404500	-2.84607400
H	5.91609000	7.29614100	0.30786900	H	3.19856800	-7.66460400	-3.78935800
O	7.46553100	4.14190200	0.80034700	H	2.24985000	-8.22984300	-2.40340100
C	7.79082600	7.86005800	4.07396200	C	4.85593800	-6.33446700	-2.41244500
H	7.12850500	8.54162000	4.61512300	H	4.60344300	-5.69365600	-3.27687100
H	8.53384000	7.44750700	4.75759700	C	5.49371900	-5.48512100	-1.30697600
O	8.45951500	8.62347300	3.05469400	C	6.95255500	-6.74641900	-3.46111700
H	8.10711500	6.51978500	1.62936500	H	6.63667900	-6.09258500	-4.29355600
O	8.81353500	5.25273600	3.10541300	C	7.71591400	-5.89024000	-2.42910800
O	-3.75099700	6.97526100	-1.89940200	C	6.78011300	-4.83214300	-1.85671000
O	3.75134500	6.97504400	1.89921300	H	6.51497800	-4.10909800	-2.63458800
H	3.21480400	-4.54177000	2.08197300	H	4.80310800	-4.69575700	-1.00427700
C	1.30848900	-5.20461800	2.11294700	O	5.79974600	-7.32452200	-2.85022100
S	1.77378600	-6.82809200	2.30692700	N	5.75041100	-6.31244200	-0.14186600
N	0.01899900	-4.83144600	1.91797100	C	5.46126500	-5.89848600	1.12129700
C	-1.08419100	-5.77198300	1.73756100	O	5.09100300	-4.74219300	1.36235600
H	-1.83397900	-5.27542300	1.11635000	C	5.61390300	-6.93166600	2.21411000
H	-0.71807600	-6.63714800	1.17805300	H	6.11018600	-7.84705900	1.87826700
H	-0.16400100	-3.85681200	1.70672600	H	6.18288500	-6.49301800	3.03861000
C	-1.70963700	-6.24047300	3.06071900	H	4.61099600	-7.17476000	2.58438200
H	-2.16676900	-5.38825900	3.58353300	H	5.91570200	-7.29645100	-0.30792200
H	-0.91603900	-6.62908400	3.70906800	O	7.46541700	-4.14233000	-0.80022500
C	-2.73316100	-7.35359300	2.84635000	C	7.79057500	-7.86024400	-4.07411200
H	-3.19908800	-7.66403100	3.78963900	H	7.12823200	-8.54175900	-4.61530400
H	-2.25034400	-8.22946500	2.40377800	H	8.53359900	-7.44766800	-4.75772000
C	-4.85637200	-6.33402600	2.41258100	O	8.45925500	-8.62373200	-3.05489200
H	-4.60394000	-5.69319900	3.27701600	H	8.10687100	-6.52018900	-1.62939600
C	-5.49409600	-5.48469700	1.30706500	O	8.81341300	-5.25309100	-3.10534200
C	-6.95305700	-6.74597900	3.46112200	O	3.75114700	-6.97528500	-1.89928400
H	-6.63723900	-6.09216700	4.29359900	C	10.06113300	-5.40677400	-2.56984900
C	-7.71634900	-5.88976900	2.42907900	O	10.28532400	-6.00510100	-1.54260400
C	-6.78049900	-4.83168600	1.85673100	C	9.81408500	-8.73417500	-3.15171500
H	-6.51539300	-4.10866000	2.63463800	O	10.46631300	-8.26505200	-4.05910800
H	-4.80345000	-4.69536600	1.00436800	C	7.02017200	-2.89496900	-0.50096800
O	-5.80020500	-7.32408200	2.85030500	O	6.19864700	-2.30218100	-1.17106000
N	-5.75074300	-6.31205400	0.14196900	C	-9.81458500	-8.73372100	3.15143700
C	-5.46150000	-5.89817200	-1.12119400	O	-10.46688300	-8.26459600	4.05878000
O	-5.09117500	-4.74190500	-1.36228400	C	-10.06157700	-5.40634400	2.56978300
C	-5.61416700	-6.93137900	-2.21397600	O	-10.28575500	-6.00478500	1.54260000
H	-6.11042500	-7.84677200	-1.87809700	C	-7.02035700	-2.89452900	0.50095100
H	-6.18318400	-6.49275800	-3.03846800	O	-6.19880600	-2.30181500	1.17107700
H	-4.61126900	-7.17446800	-2.58427300	C	-7.02007300	2.89482600	-0.50159900

O	-6.19855000	2.30213800	-1.17177900	C	-4.21079900	2.56397000	-4.81050700
C	-10.06095100	5.40633000	-2.57008800	H	-5.14129400	2.09580000	-4.46857400
O	-10.28519500	6.00402500	-1.54249100	H	-4.26953400	3.63443200	-4.57365200
C	-9.81405400	8.73416100	-3.15105900	H	-4.16821600	2.47222400	-5.90101300
O	-10.46640200	8.26496400	-4.05832700	C	2.98792100	1.91369100	4.15375900
C	7.02018900	2.89455900	0.50116000	H	2.07067600	2.40117400	4.50740000
O	6.19850400	2.30194000	1.17120500	H	2.92890200	0.86030900	4.45376400
C	10.06127800	5.40627200	2.56993200	C	4.21081100	2.56409300	4.81045000
O	10.28553100	6.00443800	1.54260600	H	5.14131600	2.09581700	4.46867800
C	9.81433500	8.73402900	3.15157200	H	4.26963200	3.63451600	4.57340700
O	10.46655600	8.26506900	4.05905500	H	4.16812900	2.47254400	5.90097400
C	11.10099000	-4.78216100	-3.46222600	C	2.98834500	-1.91369000	-4.15339600
H	10.71642900	-3.89352200	-3.96776900	H	2.07111800	-2.40096600	-4.50736400
H	11.98731500	-4.54022200	-2.87354400	H	2.92957500	-0.86024800	-4.45323700
H	11.37687500	-5.52311000	-4.22182500	C	4.21129900	-2.56418900	-4.80988000
C	10.37768800	-9.47148000	-1.96568700	H	5.14179500	-2.09614400	-4.46776200
H	9.67679700	-10.21895900	-1.58761200	H	4.26985200	-3.63467000	-4.57303200
H	10.56632800	-8.73636800	-1.17468600	H	4.16893400	-2.47241700	-5.90039800
C	7.64630600	-2.38977000	0.76973600	C	-2.98792800	-1.91365600	4.15345400
H	8.69332600	-2.69391800	0.84446400	H	-2.07065200	-2.40092500	4.50730400
H	7.54882100	-1.30442700	0.82562200	H	-2.92916400	-0.86023300	4.45336400
H	7.09812400	-2.84186400	1.60471900	C	-4.21080200	-2.56424400	4.81000000
C	-10.37811000	-9.47087400	1.96527900	H	-5.14134000	-2.09617300	4.46803500
H	-9.67723400	-10.21837600	1.58722200	H	-4.26937200	-3.63469800	4.57303200
H	-10.56659800	-8.73568200	1.17431600	H	-4.16831500	-2.47259800	5.90052400
C	-11.10146400	-4.78181200	3.46218100	2C B3LYP/6-31G(d), electr. en. = -9620.938639 a.u.			
H	-10.71697800	-3.89311200	3.96767300	C	-2.06786900	-2.99611900	-1.24077500
H	-11.98784000	-4.53999300	2.87352700	C	-2.76846400	-2.21318200	-2.16149400
H	-11.37724100	-5.52275800	4.22182400	N	-4.15493800	-2.47647200	-2.36365600
C	-7.64642700	-2.38923700	-0.76974500	C	-2.07836400	1.24608800	2.89640500
H	-8.69343400	-2.69340200	-0.84458100	C	-2.76870800	2.21267400	2.16199800
H	-7.54895000	-1.30388700	-0.82553600	N	-4.15519900	2.47591400	2.36405900
H	-7.09816700	-2.84124200	-1.60472700	C	0.69640800	-1.08384500	2.76245100
C	-11.10069600	4.78186300	-3.46269500	C	-0.00450800	-1.95270000	1.90606000
H	-11.98708400	4.53980100	-2.87416500	C	0.68656900	-2.86872000	1.08309600
H	-11.37649000	5.52292400	-4.22222000	C	2.06793600	-2.99583700	1.24156600
H	-10.71604000	3.89332900	-3.96835400	C	2.76851800	-2.21274200	2.16217100
C	-7.64619100	2.38944400	0.76904500	C	2.07816400	-1.24610400	2.89649000
H	-8.69317100	2.69369600	0.84390000	H	2.60274700	-3.73215800	0.64831400
H	-7.54881600	1.30407900	0.82472200	H	2.60792500	-0.63571900	3.62055500
H	-7.09790200	2.84131800	1.60407900	C	-0.00011300	-0.00001200	3.57418000
C	-10.37754900	9.47128900	-1.96487500	H	-0.74931000	-0.45500600	4.22976000
H	-9.67670000	10.21883900	-1.58686100	C	0.00003100	-3.69563200	0.00048200
H	-11.32590700	9.93470600	-2.24213400	H	-0.75752700	-4.35754900	0.43218000
H	-10.56596400	8.73609000	-1.17390200	C	-0.69661600	1.08376600	2.76235600
C	7.64620400	2.38927000	-0.76956800	C	0.00430900	1.95251500	1.90586700
H	8.69324900	2.69331500	-0.84436500	C	-0.68675600	2.86847100	1.08283200
H	7.54860700	1.30393500	-0.82542200	H	-2.60812500	0.63579700	3.62055000
H	7.09801800	2.84139200	-1.60453600	C	-2.06812000	2.99564700	1.24129800
C	11.10107100	4.78166100	3.46238300	H	-2.60290800	3.73193100	0.64798100
H	11.98738100	4.53958400	2.87373500	C	-0.68651500	-2.86884300	-1.08223100
H	11.37701500	5.52266400	4.22190800	C	0.00451300	-1.95282100	-1.90522500
H	10.71642900	3.89310800	3.96801600	C	-0.69643700	-1.08411700	-2.76174500
C	10.37793100	9.47129600	1.96551900	H	-2.60262900	-3.73245800	-0.64749800
H	9.67701800	10.21873300	1.58740000	C	-2.07816000	-1.24654200	-2.89586500
H	11.32615500	9.93486800	2.24296800	H	-2.60794200	-0.63629000	-3.62003100
H	10.56660400	8.73615500	1.17455400	C	0.00003700	-0.00031500	-3.57355300
H	-11.32642400	-9.93434800	2.24258600	H	-0.74915400	0.45458900	-4.22920100
H	11.32593400	-9.93500500	-2.24314400	C	-0.00018900	3.69530400	0.00017700
C	-2.98789100	1.91361400	-4.15380800	H	-0.75774400	4.35722000	-0.43153800
H	-2.07066300	2.40107300	-4.50750400	H	0.75734400	4.35725900	0.43186700
H	-2.92886800	0.86022300	-4.45375300				

C	2.07814200	1.24612400	-2.89598400	H	6.35069800	5.14651100	-2.08155500
C	2.76839700	2.21285500	-2.16168500	C	7.63944300	6.56572300	-1.08339600
C	0.69642400	1.08361700	-2.76183700	H	7.54843600	7.37494200	-0.35775200
C	2.06775200	2.99580900	-1.24101100	C	8.71919400	5.56805600	-0.62689900
C	-0.00456800	1.95232000	-1.90535200	H	8.83849300	4.79117200	-1.40033400
C	0.68641400	2.86845600	-1.08244700	O	8.29580500	4.96412500	0.59617900
H	2.60247700	3.73221300	-0.64778400	N	5.61948800	5.95527600	1.15365900
H	2.60794800	0.63585500	-3.62011700	C	4.34474700	6.31958500	1.46209600
O	1.38345900	1.85982800	1.85241000	O	3.36387100	5.92559000	0.82794400
O	-1.38369000	1.85933300	-1.85173400	C	4.20936600	7.29104600	2.62264700
O	1.38364500	-1.85997800	-1.85174700	H	5.07766700	7.29439900	3.28883200
O	-1.38365500	-1.86000600	1.85266700	H	4.07697600	8.30319500	2.22347900
C	2.11989300	-2.96070200	-2.42136000	H	3.31381600	7.03851800	3.19434700
H	1.54953300	-3.89076500	-2.33008600	H	6.38463400	6.24125200	1.74944600
C	-2.12010600	2.95995200	-2.42130500	O	5.31071300	6.85207900	-1.50489000
H	-1.54996500	3.89013500	-2.32986000	O	8.03579600	7.11948700	-2.34997300
C	-2.11975600	-2.96079700	2.42232300	C	10.08741800	6.19783700	-0.41511500
H	-1.54923100	-3.89077000	2.33116200	H	10.73169900	5.48022200	0.10077400
C	2.11954100	2.96066300	2.42202400	H	10.53455300	6.47143800	-1.37165100
H	1.54890200	3.89058000	2.33098600	O	9.99104900	7.36978100	0.41579400
H	0.74930300	-0.45533000	-4.22903800	C	7.11803500	-4.16030500	-0.42331200
H	0.75759200	-4.35759100	-0.43116000	H	7.29476800	-3.44149100	0.39413000
H	0.74907500	0.45503400	4.22973300	C	5.93892200	-5.06674300	-0.05067000
H	-3.01890000	-3.06832300	1.80664900	C	8.72021400	-5.56701700	0.62650300
H	-3.01936700	3.06700300	-1.80571600	H	8.83938700	-4.79008100	1.39990400
H	3.01857900	3.06832600	1.80621900	C	7.64066300	-6.56486000	1.08306100
H	3.01907900	-3.06802600	-1.80571400	C	6.30508100	-5.84338900	1.23866400
N	4.15502800	-2.47586200	2.36419300	H	6.35169900	-5.14585000	2.08123500
H	4.39338900	-3.45286900	2.52498300	H	5.05860000	-4.45269300	0.14629500
C	5.17710400	-1.59319400	2.53659900	O	8.29668000	-4.96323000	-0.59659900
S	6.70242100	-2.14757900	3.05439300	N	5.62044100	-5.95485200	-1.15390500
N	4.91940100	-0.29180300	2.25941600	C	4.34572900	-6.31937600	-1.46221800
C	5.80386300	0.82684800	2.57494300	O	3.36484500	-5.92550900	-0.82800100
H	6.24634800	0.64574200	3.56031700	C	4.21041000	-7.29086200	-2.62275500
H	5.16949700	1.71580100	2.64445000	H	5.07859400	-7.29396000	-3.28909400
H	3.99845100	-0.06419900	1.90217200	H	4.07838500	-8.30305300	-2.22357300
N	4.15484400	2.47623300	-2.36384000	H	3.31468400	-7.03858900	-3.19429300
H	4.39296500	3.45326700	-2.52484000	H	6.38556800	-6.24067500	-1.74978900
C	5.17707400	1.59374600	-2.53629700	O	5.31200600	-6.85162200	1.50464300
S	6.70217200	2.14834400	-3.05448400	C	10.08853800	-6.19657800	0.41472100
N	4.91971000	0.29235000	-2.25879200	H	10.73272100	-5.47885700	-0.10114300
C	5.80412000	-0.82622100	-2.57476900	H	10.53569600	-6.47013500	1.37125900
H	5.16976800	-1.71519600	-2.64411100	O	9.99234100	-7.36851700	-0.41621600
H	6.24622200	-0.64500700	-3.56029600	H	7.54977800	-7.37410900	0.35743800
H	3.99879900	0.06462300	-1.90152600	O	8.03716900	-7.11851200	2.34963800
C	6.92300400	1.08058000	1.55686000	O	6.85554300	3.52575200	1.62485000
H	6.50783200	1.14376800	0.54411900	O	6.85611900	-3.52524800	-1.62538000
H	7.61718600	0.23410700	1.57813300	H	-4.39343300	3.45294400	2.52492400
C	7.68045500	2.36732000	1.87075500	C	-5.17734900	1.59333100	2.53649000
H	7.96033400	2.41200100	2.92933500	S	-6.70257400	2.14781300	3.05441600
H	8.60204900	2.44123000	1.28418900	N	-4.91979800	0.29192600	2.25919900
C	6.92366500	-1.08005600	-1.55715200	C	-5.80425300	-0.82667500	2.57492700
H	6.50888500	-1.14334600	-0.54425800	H	-5.16989500	-1.71563300	2.64441100
H	7.61785200	-0.23359200	-1.57859500	H	-6.24662300	-0.64549900	3.56034000
C	7.68093700	-2.36679200	-1.87151000	H	-3.99883200	0.06423800	1.90205200
H	8.60280900	-2.44080800	-1.28539800	C	-6.92350300	-1.08047900	1.55697800
H	7.96029800	-2.41138100	-2.93022900	H	-6.50843100	-1.14359500	0.54419400
C	7.11729500	4.16099600	0.42285700	H	-7.61775400	-0.23406200	1.57834900
H	7.29411600	3.44231000	-0.39467800	C	-7.68080400	-2.36730300	1.87088100
C	5.93801800	5.06727200	0.05035700	H	-8.60242000	-2.44128400	1.28436100
H	5.05777700	4.45309200	-0.14656400	H	-7.96062200	-2.41205500	2.92947400
C	6.30398300	5.84402100	-1.23896700	C	-7.11754000	-4.16089200	0.42290900

H	-7.29434000	-3.44220800	-0.39463500	H	-7.54923700	7.37429500	0.35740600
C	-5.93826000	-5.06718700	0.05042100	O	-8.03670400	7.11873800	2.34959100
C	-8.71943900	-5.56790000	-0.62689800	O	-6.85573800	3.52521100	-1.62520800
H	-8.83866600	-4.79099500	-1.40031900	C	-8.08822000	8.47769200	2.45832700
C	-7.63971000	-6.56560400	-1.08335100	O	-7.77700700	9.24026800	1.57077800
C	-6.30422600	-5.84393500	-1.23889200	C	-10.51470600	8.52485300	0.07851100
H	-6.35091700	-5.14642600	-2.08148100	O	-11.09035700	8.60665400	1.14177200
H	-5.05801500	-4.45301400	-0.14650900	C	-4.20210800	6.48108100	2.18038800
O	-8.29605600	-4.96401300	0.59621100	O	-4.03284200	5.37683400	2.65741400
N	-5.61972900	-5.95516800	1.15373500	C	-10.51429700	-8.52558900	-0.07933300
C	-4.34500500	-6.31952100	1.46215400	O	-11.08991800	-8.60729900	-1.14261800
O	-3.36411200	-5.92552900	0.82802200	C	-8.08735600	-8.47834100	-2.45861900
C	-4.20958000	-7.29081000	2.62285000	O	-7.77609800	-9.24083700	-1.57101700
H	-5.07806300	-7.29449500	3.28879100	C	-4.20153400	-6.48138100	-2.18040400
H	-4.07656000	-8.30292900	2.22382500	O	-4.03228700	-5.37712500	-2.65742500
H	-3.31431900	-7.03779900	3.19479800	C	4.20126900	6.48139200	-2.18047900
H	-6.38489700	-6.24124700	1.74944200	O	4.03206100	5.37712900	-2.65749500
O	-5.31096900	-6.85201000	-1.50476900	C	8.08702400	8.47845300	-2.45870900
C	-10.08769900	-6.19762500	-0.41518700	O	7.77570700	9.24095900	-1.57113700
H	-10.73195100	-5.48001900	0.10075100	C	10.51391200	8.52578700	-0.07902100
H	-10.53482900	-6.47112100	-1.37175600	O	11.08950400	8.60763500	-1.14231100
O	-9.99140800	-7.36965000	0.41561400	C	4.20254400	-6.48114500	2.18030800
H	-7.54875100	-7.37481700	-0.35769500	O	4.03314600	-5.37689800	2.65728900
O	-8.03603300	-7.11937600	-2.34993300	C	8.08875300	-8.47746200	2.45839700
O	-6.85577700	-3.52564000	1.62489700	O	7.77758400	-9.24007200	1.57086100
H	-4.39310100	-3.45347700	-2.52482400	C	10.51527300	-8.52448800	0.07860700
C	-5.17706400	-1.59386700	-2.53607500	O	11.09081000	-8.60631100	1.14193000
S	-6.70222100	-2.14826300	-3.05432000	C	-8.63491800	8.88042800	3.80261600
N	-4.91957700	-0.29251100	-2.25847500	H	-8.33651200	8.17822200	4.58421500
C	-5.80382900	0.82617200	-2.57453500	H	-8.30378600	9.89225400	4.04189100
H	-5.16937400	1.71508200	-2.64376100	H	-9.72911500	8.87775600	3.73227200
H	-6.24584900	0.64505200	-3.56011800	C	-10.23854300	9.67835000	-0.85035200
H	-3.99854700	-0.06486200	-1.90146600	H	-10.20994200	9.35590900	-1.89356000
C	-6.92343800	1.08004300	-1.55700300	H	-9.25915700	10.09225600	-0.58386200
H	-6.50872400	1.14324800	-0.54407900	C	-3.19918500	7.60149700	2.22969900
H	-7.61767500	0.23361900	-1.57854900	H	-3.69201300	8.57194900	2.32540500
C	-7.68065300	2.36681900	-1.87129700	H	-2.50232900	7.43514900	3.05238800
H	-8.60245300	2.44085500	-1.28507100	H	-2.64695900	7.58653400	1.28275900
H	-7.96014200	2.41143700	-2.92998200	C	-10.23806700	-9.67918200	0.84939000
C	-7.11767700	4.16041700	-0.42323200	H	-10.20955300	-9.35687600	1.89264200
H	-7.29448100	3.44170000	0.39428100	H	-9.25862500	-10.09295900	0.58290100
C	-5.93853000	5.06683400	-0.05063900	C	-8.63391200	-8.88120800	-3.80292700
C	-8.71980300	5.56727500	0.62644000	H	-8.33560500	-8.17896200	-4.58452700
H	-8.83906400	4.79036400	1.39985300	H	-8.30257600	-9.89297700	-4.04216400
C	-7.64019900	6.56505200	1.08302600	H	-9.72811300	-8.87874700	-3.73263100
C	-6.30466600	5.84349700	1.23867600	C	-3.19852600	-7.60172400	-2.22960100
H	-6.35137000	5.14596100	2.08124300	H	-3.69127800	-8.57222300	-2.32522000
H	-5.05821500	4.45276700	0.14630700	H	-2.50167000	-7.43540000	-3.05229400
O	-8.29626100	4.96341700	-0.59662800	H	-2.64631500	-7.58663000	-1.28265400
N	-5.62007400	5.95491200	-1.15390400	C	8.63370200	8.88130100	-3.80297200
C	-4.34537200	6.31934000	-1.46234800	H	8.30244400	9.89309200	-4.04222000
O	-3.36445400	5.92547400	-0.82818000	H	9.72789900	8.87876700	-3.73261000
C	-4.21007300	7.29071700	-2.62298500	H	8.33540000	8.17908100	-4.58459800
H	-5.07830500	7.29384600	-3.28925800	C	3.19827400	7.60174400	-2.22981700
H	-4.07788400	8.30293100	-2.22391600	H	3.69103700	8.57225800	-2.32520400
H	-3.31443400	7.03827000	-3.19458000	H	2.50162400	7.43550200	-3.05270400
H	-6.38523900	6.24078200	-1.74971800	H	2.64581200	7.58653000	-1.28301800
O	-5.31152400	6.85165500	1.50468400	C	10.23759500	9.67928700	0.84979300
C	-10.08807800	6.19691900	0.41458600	H	10.20886600	9.35686300	1.89300100
H	-10.73226100	5.47924200	-0.10134000	H	10.99386400	10.45258200	0.70436300
H	-10.53528700	6.47047200	1.37110100	H	9.25823500	10.09316800	0.58316400
O	-9.99177400	7.36887800	-0.41630800	C	3.19967300	-7.60161400	2.22954000

H	3.69254200	-8.57207900	2.32488100	C	1.13290500	2.75479100	0.13958400
H	2.50298200	-7.43550100	3.05241800	H	-2.51769200	2.08274400	-1.02581700
H	2.64723500	-7.58640000	1.28272700	C	0.77547500	2.89471000	-1.20287100
C	8.63536400	-8.88014400	3.80273700	H	1.54374900	3.10411200	-1.94011500
H	8.30431200	-9.89200300	4.04198200	C	0.00612000	-3.01026400	-0.23365200
H	9.72956800	-8.87735500	3.73250000	C	1.34267500	-2.83224400	0.15340700
H	8.33681000	-8.17796700	4.58430600	C	2.30786200	-2.36917400	-0.75895800
C	10.23923900	-9.67796800	-0.85031600	H	-1.37788600	-2.88873000	-1.87549600
H	10.21053600	-9.35547400	-1.89350300	C	1.94048300	-2.20824200	-2.09418000
H	10.99563300	-10.45114000	-0.70488200	H	2.68053200	-1.87703900	-2.81730000
H	9.25993100	-10.09204000	-0.58379300	C	3.71197300	-2.00273400	-0.29503100
H	-10.99425400	-10.45251200	0.70373000	H	4.33027200	-1.82121200	-1.18041900
H	-10.99481500	10.45162500	-0.70483600	C	2.59192800	2.88172500	0.56169600
C	2.49712000	2.72403000	3.88382500	H	3.16189800	3.27181500	-0.28812400
H	1.58354700	2.63627100	4.48519900	H	2.69428200	3.61580500	1.36854000
H	3.02561000	1.76603600	3.96544600	C	4.00424700	-0.94696800	1.98761300
C	3.37686100	3.85132400	4.43679700	C	3.92974200	0.13934000	2.86926200
H	2.84990100	4.81276800	4.41279900	C	3.72643200	-0.78940400	0.62695200
H	3.65945100	3.65438100	5.47642500	C	3.49283600	1.37784600	2.38713000
H	4.29964100	3.96079000	3.85354900	C	3.36800200	0.48457500	0.15631900
C	2.49710900	-2.72415800	-3.88327000	C	3.18106700	1.56148400	1.03997000
H	1.58338800	-2.63693600	-4.48449700	H	3.37815200	2.20706700	3.07974600
H	3.02513100	-1.76593000	-3.96516400	H	4.22125700	-1.93750600	2.37216200
C	3.37729000	-3.85114100	-4.43617700	O	0.47275400	2.31802200	2.40988100
H	2.85077400	-4.81282200	-4.41192300	O	3.12375600	0.66696400	-1.19459900
H	3.65962500	-3.65425100	-5.47588400	O	1.71691900	-3.05041000	1.46861500
H	4.30020900	-3.96007600	-3.85305000	O	-0.46075400	-0.68610700	1.74313500
C	-2.49717500	2.72351900	-3.88327400	C	2.06910200	-4.40643200	1.75407000
H	-1.58339100	2.63636300	-4.48441500	H	2.90413000	-4.74538700	1.12685600
H	-3.02518200	1.76529500	-3.96530200	H	1.21864900	-5.08322300	1.59933900
C	-3.37730200	3.85054200	-4.43618000	C	4.27514100	1.05487500	-1.94498400
H	-4.30024700	3.95948000	-3.85309500	H	5.06660000	0.29556700	-1.89278800
H	-2.85076900	4.81221000	-4.41187000	H	4.68622700	2.00943100	-1.59012500
H	-3.65959800	3.65370100	-5.47590700	C	-0.22173000	-0.88645400	3.13929600
C	-2.49710400	-2.72419700	3.88419300	H	-0.81499200	-0.19316600	3.74808700
H	-1.58343900	-2.63664000	4.48545500	H	-0.45353600	-1.91513400	3.44018100
H	-3.02541200	-1.76611700	3.96596100	C	0.23253600	3.51692500	3.14873900
C	-3.37697300	-3.85138700	4.43718000	H	-0.83281500	3.78235400	3.14970500
H	-4.29978900	-3.96072800	3.85396500	H	0.80266500	4.36235200	2.74130400
H	-2.85013700	-4.81289700	4.41314200	H	4.17000200	-2.84392900	0.23635100
H	-3.65949500	-3.65443700	5.47682500	H	0.83955200	-0.69355900	3.29336300
1-pcone-unfolded B3LYP/6-31G(d) PCM (methanol),				H	3.94724600	1.16508500	-2.98139200
electr. en. = -9306.358629 a.u.				H	0.55625400	3.32095600	4.17394200
C	-0.33627300	-2.81645400	-1.57582800	H	2.36759800	-4.43449900	2.80467600
C	0.63109800	-2.45835200	-2.52216800	N	-5.66895900	-1.62785100	-0.05500900
N	0.30521500	-2.25820200	-3.88717800	H	-5.75470600	-2.28129400	-0.82258900
C	-1.50284000	2.28444800	-0.69148600	C	-6.89515300	-1.27147900	0.46144400
C	-0.54906400	2.70647800	-1.62200700	S	-8.29760900	-1.75633700	-0.34324700
N	-0.92290300	2.85722600	-2.98222800	N	-6.88474000	-0.55684900	1.60982700
C	-2.65876300	0.15935800	1.27429900	C	-8.08120200	-0.10132300	2.31179000
C	-1.75252700	-0.91317200	1.32589200	H	-7.81188300	0.02533500	3.36374500
C	-2.11374400	-2.19279200	0.86680000	H	-8.83931500	-0.88777300	2.24314300
C	-3.42655300	-2.40480700	0.44146700	H	-5.99366500	-0.41100800	2.06650400
C	-4.36388300	-1.36366600	0.42871100	N	4.18121800	0.00491600	4.25815600
C	-3.95976300	-0.07840500	0.81800500	H	3.58801100	0.52913900	4.88758200
H	-3.73318200	-3.39700800	0.11816300	C	5.18358800	-0.66454900	4.92003700
H	-4.65297300	0.75292000	0.72566100	S	5.16579300	-0.71580300	6.60804800
C	-2.20664100	1.56767100	1.63190700	N	6.13259500	-1.24531200	4.14849300
C	-1.08038200	-3.30667200	0.79265400	C	7.29349500	-1.96356700	4.66150900
C	-1.17193800	2.11129500	0.65470500	H	6.96975300	-2.52624500	5.54129800
C	0.13547400	2.41196300	1.06909700	H	7.60449300	-2.67630300	3.89232100
				H	6.12410900	-1.03124500	3.15866600

C	-8.64049200	1.21220800	1.74799700	O	-9.56272400	1.93229000	3.83956800
H	-8.87762200	1.06988100	0.68819600	O	10.13150100	-2.67929700	4.49892900
H	-7.88259500	2.00262800	1.81767100	H	-1.57326600	2.18372800	-3.36660700
C	-9.90140200	1.66198400	2.46928800	C	-0.72036200	3.92944900	-3.82304400
H	-10.31762500	2.56452300	2.00827000	S	-1.35262100	3.88787200	-5.38662600
H	-10.67149000	0.87528600	2.43316900	N	-0.02011600	4.97061900	-3.31443600
C	8.46591700	-1.04334700	5.03106700	C	0.27672800	6.20129800	-4.03967100
H	8.13728600	-0.34264300	5.80623500	H	-0.59755500	6.46206500	-4.64441400
H	8.77123900	-0.45503100	4.15622000	H	0.42750300	6.98812400	-3.29529900
C	9.66550600	-1.82029400	5.55206500	H	0.23909200	4.93147500	-2.33714600
H	9.38362500	-2.43240700	6.42335600	C	1.51350200	6.08340800	-4.94115800
H	10.47027400	-1.14321100	5.85962600	H	1.34444000	5.28095900	-5.66716000
C	-10.64300500	2.11737800	4.67940200	H	2.39111300	5.81242200	-4.34055800
H	-11.36674700	1.28518400	4.58740600	C	1.80389900	7.36902600	-5.69908200
C	-10.15694600	2.23077200	6.12834900	H	0.92496000	7.68309800	-6.28382500
H	-9.66599500	1.30616000	6.44126600	H	2.64179200	7.23597700	-6.39234700
C	-11.39600100	2.46020300	7.02723300	C	2.19091000	9.67129900	-5.25570500
H	-12.02764600	1.56590400	7.00189800	H	1.27504900	9.91857700	-5.82564900
C	-12.18697700	3.67471500	6.55076300	C	2.38507300	10.67502900	-4.11283200
H	-11.61395500	4.58577700	6.72483900	C	3.37498500	11.01571500	-6.81926100
C	-12.51737100	3.53207200	5.05226800	H	2.41901000	11.20044100	-7.33967800
H	-13.17416300	2.65501000	4.91729300	C	3.59753900	12.13294300	-5.78257500
O	-11.31019500	3.33377000	4.31469200	C	2.49029300	12.08962500	-4.73320000
N	-9.19283800	3.31130800	6.22937000	H	1.52966700	12.35314400	-5.18839000
C	-8.12216000	3.27095500	7.07657600	H	1.52768200	10.65426200	-3.43582700
O	-7.92559600	2.34644700	7.85911300	O	3.31036600	9.75663100	-6.14824600
C	-7.19378300	4.47401200	7.00423900	N	3.56919900	10.31595700	-3.35293400
H	-7.37134300	5.11484500	6.13497900	C	3.66280800	10.49389000	-2.00219200
H	-7.32074500	5.07392400	7.91185100	O	2.77969900	11.02614500	-1.33684100
H	-6.16013400	4.11848000	6.98740000	C	4.96076200	10.00940200	-1.37361400
H	-9.26933000	4.05579300	5.55020900	H	5.56007600	9.37555500	-2.03472200
O	-10.99039700	2.70108300	8.37775400	H	5.56119500	10.87943100	-1.08654900
O	-13.42869100	3.75729600	7.27147400	H	4.72344500	9.45802600	-0.45997300
C	-13.25606700	4.72783400	4.46823000	H	4.28711600	9.80086700	-3.84340600
H	-13.25561900	4.64609600	3.37746400	O	2.80147300	13.05275900	-3.72227200
H	-14.28338600	4.75663600	4.83348600	C	4.45151200	10.94374300	-7.89263800
O	-12.59777400	5.95956900	4.81264800	H	4.33470500	10.00931800	-8.44901600
C	11.06097100	-3.62547600	4.88372900	H	4.36664800	11.79064500	-8.57488400
H	10.71102200	-4.19157500	5.76801700	O	5.76538200	10.93905100	-7.30649800
C	11.32669800	-4.58539500	3.71931100	H	4.57052100	12.01401600	-5.30499900
C	13.25940900	-3.85847600	5.75787100	O	3.56525800	13.39480400	-6.47054600
H	12.82933400	-4.39976100	6.61878000	O	2.12790600	8.39146600	-4.74180600
C	13.64639900	-4.88384700	4.67411000	H	0.76258200	-1.49335000	-4.36631100
C	12.39748400	-5.60553300	4.17703000	C	-0.38087400	-3.08000900	-4.75466800
H	11.97988900	-6.22882400	4.97479900	S	-0.55710300	-2.61467900	-6.36681900
H	10.41652400	-5.13100100	3.45893600	N	-0.86274900	-4.23449600	-4.23908800
O	12.28209300	-2.95941000	5.23171800	C	-1.60287500	-5.23750100	-4.99783800
N	11.74636600	-3.82788400	2.55431000	H	-1.15882500	-5.31052200	-5.99557100
C	11.40862800	-4.18627800	1.28009200	H	-1.46518800	-6.19528000	-4.48857400
O	10.77737400	-5.20604300	1.02053300	H	-0.61536100	-4.46274900	-3.28494600
C	11.89902200	-3.24414600	0.19119900	C	-3.09939400	-4.91642300	-5.11675800
H	12.23570000	-2.27363800	0.56907500	H	-3.21694700	-3.96297600	-5.64263100
H	12.73182500	-3.71874100	-0.33917900	H	-3.53773200	-4.80260700	-4.11722200
H	11.09261100	-3.09245900	-0.53087300	C	-3.86360700	-5.99060700	-5.87460000
H	12.19760900	-2.93960100	2.72382300	H	-3.42156800	-6.15661900	-6.86976700
O	12.77921500	-6.44710400	3.08527300	H	-4.91171300	-5.70380800	-6.01294200
C	14.43274100	-3.05043400	6.29270400	C	-4.23768700	-8.33625200	-5.77320800
H	14.04722500	-2.21757600	6.88793800	H	-3.74369400	-8.44417000	-6.75783700
H	15.07481700	-3.67762700	6.91238600	C	-3.96573000	-9.57481300	-4.91172000
O	15.21121300	-2.49467500	5.21856400	C	-6.17181400	-9.29223800	-6.77508500
H	14.14437900	-4.38349400	3.84303400	H	-5.61840500	-9.34927000	-7.72884100
O	14.55294600	-5.83308900	5.26078200	C	-5.98249600	-10.61879400	-6.01419200

C	-4.50880700	-10.80978000	-5.67028900
H	-3.92361800	-10.95411500	-6.58462400
H	-2.89184400	-9.70553100	-4.75791300
O	-5.65020800	-8.21835000	-5.99106400
N	-4.59038900	-9.40547600	-3.61205800
C	-4.03823100	-9.88603400	-2.45902600
O	-3.00447400	-10.54728500	-2.44038300
C	-4.81216900	-9.56887200	-1.18844300
H	-5.58542000	-8.80591700	-1.32208800
H	-5.28797500	-10.48650400	-0.82584900
H	-4.10651300	-9.23982400	-0.42110200
H	-5.39732800	-8.79847600	-3.56817200
O	-4.39287500	-11.98172200	-4.85790800
C	-7.61981400	-8.98407300	-7.12627800
H	-7.68865200	-7.94835400	-7.47133800
H	-7.97235000	-9.65610600	-7.90978300
O	-8.46796000	-9.11678700	-5.97268600
H	-6.58210900	-10.61834400	-5.10347500
O	-6.42510400	-11.68898500	-6.86631900
O	-3.79268100	-7.20801600	-5.11349200
C	-7.35854200	-12.55070000	-6.36492900
O	-7.80521600	-12.48545300	-5.24229100
C	-9.54051900	-9.95102100	-6.08562900
O	-9.83627100	-10.53475000	-7.10534400
C	-3.17469800	-12.59935500	-4.86199200
O	-2.27163600	-12.28083300	-5.60183900
C	6.63184500	11.90587300	-7.72303800
O	6.37241900	12.71993900	-8.58196400
C	4.62305200	14.23927300	-6.28826600
O	5.56178900	13.99915900	-5.56340300
C	1.74561100	13.52404800	-2.99488800
O	0.59266100	13.26442400	-3.25464100
C	-10.73029300	1.59407400	9.13495300
O	-10.95091400	0.46578200	8.75748100
C	-13.60021800	4.81707500	8.11586300
O	-12.76221900	5.66759300	8.31186600
C	-13.34979700	6.90740800	5.44195700
O	-14.53214100	6.78464600	5.67554600
C	11.96570000	-7.51639100	2.83689700
O	11.04735000	-7.83225100	3.55875600
C	15.74931900	-6.03457200	4.63342900
O	16.07510900	-5.48299500	3.60687900
C	16.54506900	-2.77916600	5.21209500
O	17.10141800	-3.42089200	6.07597000
C	-7.78622200	-13.53907000	-7.41779100
H	-6.96433800	-13.78964200	-8.09212400
H	-8.17952600	-14.43568400	-6.93607100
H	-8.58934700	-13.07663200	-8.00379100
C	-10.26301600	-10.07350100	-4.77013200
H	-10.20668300	-9.14723300	-4.19403500
H	-9.77759600	-10.87244800	-4.19774200
C	-3.12537700	-13.67579600	-3.81225800
H	-4.06746100	-14.22855800	-3.76684200
H	-2.29064100	-14.34830900	-4.01459900
H	-2.97113700	-13.18218200	-2.84596400
C	7.91844700	11.84469900	-6.94263800
H	8.15956900	10.82173500	-6.64521900
H	7.78818400	12.45171400	-6.03921600
C	4.47832600	15.46356900	-7.15305800
H	3.43146800	15.75363500	-7.26713800
H	5.06253600	16.28066100	-6.72683700
H	4.88305000	15.22361600	-8.14342400

C	2.23008800	14.35769200	-1.84017100
H	3.07824000	14.98308900	-2.13098200
H	1.41066100	14.96865900	-1.45893800
H	2.56561800	13.66769400	-1.05757400
C	-14.98441200	4.80264100	8.70908700
H	-14.98313700	5.35845000	9.64811200
H	-15.65587600	5.30828000	8.00498300
H	-15.34585400	3.78338500	8.86222600
C	-10.11471000	1.98697400	10.45000500
H	-10.58666100	2.88569400	10.85577500
H	-10.19112700	1.15727700	11.15415500
H	-9.05833900	2.21009000	10.26174200
C	-12.50245900	8.08815200	5.83638600
H	-11.68859500	8.25312100	5.12684200
H	-13.13159100	8.97618700	5.91714400
H	-12.07166800	7.87386400	6.82129600
C	12.35761800	-8.19194200	1.55125300
H	13.44393700	-8.22073500	1.43329100
H	11.93751200	-9.19832900	1.52239400
H	11.93908200	-7.59941900	0.72967700
C	16.60971700	-6.98301200	5.42598500
H	17.34338500	-7.44655200	4.76459400
H	17.14335500	-6.39845400	6.18478500
H	16.00940100	-7.74233300	5.93204300
C	17.20444400	-2.22733800	3.97585100
H	16.72256200	-1.30597400	3.64131900
H	18.26465300	-2.06018400	4.17322300
H	17.11012500	-2.98010300	3.18468700
H	8.72542900	12.27525700	-7.53792200
H	-11.30186900	-10.35490100	-4.95031300
H	-0.61138700	-3.45456600	1.76752300
H	-1.59354600	-4.24183900	0.53745100
H	-3.08565600	2.22351300	1.64487100
H	-1.78031300	1.58026800	2.63715200

1-cone-unfolded B3LYP/6-31G(d) PCM (methanol),
electr. en. = -9306.356612 a.u.

C	-0.58495500	-3.10732800	-0.11917300
C	0.59515400	-2.95861500	-0.85879700
N	0.61363800	-3.03380000	-2.27285700
C	-1.71168000	2.25883600	-0.22677800
C	-0.53974100	2.55774900	-0.92910000
N	-0.57166400	2.59983400	-2.34592900
C	-3.40555300	0.35129200	1.58483100
C	-2.61932200	-0.71248200	2.05614300
C	-2.86314000	-2.03684600	1.65671400
C	-3.98195800	-2.29739600	0.86227700
C	-4.82137900	-1.26190300	0.43040100
C	-4.50215500	0.06261400	0.76575800
H	-4.21684500	-3.32150000	0.58085800
H	-5.09134500	0.87675400	0.35276300
C	-3.00631800	1.78889900	1.88779100
C	-1.89211500	-3.14164700	2.04275600
C	-1.72389400	2.19060400	1.16743200
C	-0.53534700	2.46427900	1.86916200
C	0.66928300	2.69529000	1.18267400
H	-2.62862300	2.07298100	-0.78088900
C	0.65159900	2.73346600	-0.21459200
H	1.58562600	2.85050200	-0.75626900
C	-0.57661000	-3.03542900	1.27707800
C	0.63970700	-2.79078000	1.93742800
C	1.81650300	-2.53995600	1.20794500

H	-1.53144800	-3.22625000	-0.63812800	H	11.06159200	-2.97234500	-0.46842400
C	1.77991600	-2.64726700	-0.18297300	C	-11.76903000	2.80328000	2.37328600
H	2.68822400	-2.47991600	-0.75699500	H	-12.47376200	1.95193600	2.31219600
C	3.11153900	-2.11615200	1.89335800	C	-11.56553200	3.21375300	3.83641800
C	1.99841600	2.81653800	1.92264800	H	-11.16503500	2.37889400	4.41638700
C	4.55924300	-0.43010500	0.65349300	C	-12.94572300	3.60174100	4.41984900
C	4.85811400	0.88117000	0.25410700	H	-13.58200800	2.71120100	4.45766000
C	3.50156500	-0.68956300	1.53152400	C	-13.60408400	4.68156500	3.56679900
C	4.03701400	1.93113400	0.68532000	H	-13.04717100	5.61529800	3.64991300
C	2.73642700	0.39091000	2.00043000	C	-13.65645700	4.22279000	2.09658700
C	2.95715100	1.69959200	1.54053400	H	-14.28894900	3.32025300	2.03015300
H	4.25528500	2.94383500	0.35383700	O	-12.33604400	3.90584600	1.65294700
H	5.13240000	-1.25764600	0.24435300	N	-10.61181600	4.30628400	3.90186500
O	-0.54474300	2.46975700	3.25438000	C	-9.71547000	4.44497900	4.92285200
O	1.70013700	0.14822100	2.87281100	O	-9.68725400	3.69264600	5.89207900
O	0.67261600	-2.75797400	3.32201500	C	-8.76239200	5.62340100	4.79202900
O	-1.54089900	-0.43904600	2.86512600	H	-8.75826300	6.07757000	3.79628600
C	0.93418500	-4.02951100	3.91882700	H	-9.04378100	6.38908400	5.52306700
H	1.90925400	-4.42679900	3.60664500	H	-7.75254200	5.28684400	5.04100500
H	0.15812700	-4.76238300	3.66089100	H	-10.54379700	4.90249500	3.08864500
C	2.07603200	0.18225200	4.24917600	O	-12.79542800	4.11773900	5.74584100
H	2.32970700	1.20133200	4.56951700	O	-14.95271800	4.89867400	4.01517500
H	2.93445500	-0.47216600	4.44744200	C	-14.25911100	5.24943000	1.14887500
C	-1.83982500	-0.42917700	4.26070200	H	-14.06756100	4.93585300	0.11858600
H	-2.69402900	0.22277100	4.48346800	H	-15.33416300	5.33305000	1.31311200
H	-2.06172700	-1.43891500	4.62986300	O	-13.65139400	6.53995000	1.33147500
C	-0.79561400	3.75745000	3.82019900	C	12.13870700	-2.72378800	2.04416400
H	-1.77523300	4.14717300	3.51280100	H	12.74960500	-1.81820100	1.86619800
H	-0.02308500	4.48196100	3.52994700	C	12.08758700	-3.03421200	3.54456400
H	-0.95351800	-0.04064700	4.76048200	C	14.13465200	-3.97042200	1.71276900
H	1.21543700	-0.17699100	4.81261100	H	14.66147400	-3.01823600	1.52635800
H	-0.78119700	3.62812800	4.90521900	C	14.24399300	-4.30871100	3.21216900
H	0.93686300	-3.87052800	5.00001100	C	13.54136300	-3.23420400	4.03667800
N	-5.92825300	-1.57864900	-0.39659400	H	14.08007400	-2.28429300	3.95431200
H	-5.80633100	-2.32629000	-1.06722800	H	11.64626500	-2.19871500	4.09324700
C	-7.24610900	-1.18973500	-0.28919100	O	12.75809500	-3.82178300	1.36065700
S	-8.37685500	-1.80415100	-1.38147900	N	11.26159400	-4.20767700	3.76581600
N	-7.54485700	-0.33589100	0.71567400	C	10.47548300	-4.36135400	4.87201400
C	-8.87922100	0.18590100	0.99473000	O	10.45193900	-3.54897300	5.79163600
H	-8.90026500	0.46713500	2.05117300	C	9.64113800	-5.63310400	4.90153800
H	-9.60380200	-0.61938100	0.83740500	H	9.60874100	-6.16055700	3.94316200
H	-6.81063200	-0.10497000	1.37249500	H	10.05324700	-6.30935700	5.65826200
N	5.92301500	1.16636600	-0.63771100	H	8.62352600	-5.37761900	5.20873500
H	5.76227600	1.87865700	-1.33806800	H	11.18829200	-4.86487500	3.00151800
C	7.25150600	0.80819200	-0.56012900	O	13.54986000	-3.65305900	5.40449400
S	8.33020900	1.39475500	-1.71834200	C	14.76720500	-5.00686100	0.79554700
N	7.60286000	0.00518700	0.46970600	H	14.45922900	-4.80322800	-0.23412500
C	8.96299400	-0.45475400	0.73349500	H	15.85481600	-4.96499900	0.86776300
H	9.65141300	0.36773200	0.51446500	O	14.32227800	-6.33302000	1.12964800
H	9.02668800	-0.68119000	1.80128600	H	13.79936100	-5.28407800	3.41188600
H	6.89723900	-0.20918000	1.16255500	O	15.63874200	-4.34985400	3.55937400
C	-9.24630100	1.39502300	0.12312000	O	-10.54956700	2.48212600	1.81085100
H	-9.24823200	1.08823200	-0.92819500	O	10.85619600	-2.56141800	1.55938100
H	-8.49092800	2.18224200	0.23953200	H	-1.16038400	1.92715200	-2.82027300
C	-10.61306300	1.96369000	0.47174300	C	-0.08914400	3.56777400	-3.20024200
H	-10.89390200	2.76540300	-0.21986500	S	-0.32230900	3.39671100	-4.86180800
H	-11.38778000	1.18241900	0.41882300	N	0.54054100	4.61858700	-2.62479700
C	9.35140600	-1.69015900	-0.09061700	C	1.09829500	5.75335400	-3.35306600
H	9.26260900	-1.44807800	-1.15502100	H	0.42670900	5.99247300	-4.18362000
H	8.66148700	-2.51614400	0.12304600	H	1.11197500	6.60325800	-2.66521800
C	10.77666100	-2.14180700	0.18665100	H	0.53915100	4.67145400	-1.61441500
H	11.48530500	-1.31604900	0.01611000	C	2.51307100	5.48926600	-3.88737300

H	2.47759000	4.64770000	-4.58741400	H	-5.81543600	-8.88986200	-2.23661000
H	3.17805800	5.20824000	-3.06085100	O	-4.91862000	-12.34918000	-2.29427000
C	3.09480500	6.69767700	-4.60431000	C	-6.84297400	-9.93817900	-6.17313400
H	2.43285500	7.02261300	-5.42257500	H	-6.65660400	-9.03613000	-6.76307000
H	4.07598600	6.46608300	-5.03302400	H	-7.02568800	-10.78208900	-6.83969400
C	3.52031800	8.99941200	-4.18451900	O	-8.01630600	-9.70300900	-5.37579800
H	2.82298900	9.25588800	-5.00479600	H	-6.71672600	-11.00093200	-3.58374000
C	3.45122700	10.06516800	-3.08500300	O	-6.17519400	-12.52325600	-4.87387900
C	5.19272700	10.17243000	-5.40408100	O	-3.61131600	-7.87274900	-3.50036100
H	4.44559900	10.36843600	-6.19301400	C	-7.32277700	-13.16798800	-4.50929000
C	5.17816600	11.34699400	-4.40672800	O	-8.07437500	-12.77404000	-3.64678900
C	3.81825800	11.42759300	-3.72040400	C	-9.10521300	-10.48236000	-5.63209800
H	3.04523700	11.70532700	-4.44475600	O	-9.14821300	-11.31173600	-6.51432100
H	2.43890100	10.13066900	-2.67925800	C	-3.85579000	-13.00163500	-1.73797100
O	4.85026300	8.96574600	-4.72033900	O	-2.73355100	-12.94643200	-2.18751700
N	4.34884700	9.70019300	-2.00376200	C	8.62722500	10.83500400	-5.35055700
C	4.07475100	9.96567300	-0.69261200	O	8.68860500	11.59449000	-6.29255000
O	3.07495400	10.57912900	-0.33125600	C	6.44161200	13.36165000	-4.70962800
C	5.11757000	9.47212200	0.29899300	O	7.12034400	13.12818300	-3.73551900
H	5.81466000	8.74173200	-0.12353800	C	2.70817600	13.00686100	-2.33809300
H	5.69282100	10.32985700	0.66456000	O	1.65922300	12.78355000	-2.89867700
H	4.60411400	9.03042800	1.15683500	C	-12.70739300	3.19141800	6.74580700
H	5.14449800	9.12562100	-2.24548700	O	-12.87700100	2.00635500	6.56916200
O	3.89320100	12.44127800	-2.71324100	C	-15.24579000	6.11187500	4.57018400
C	6.52938900	9.97498300	-6.10412100	O	-14.43418300	6.99468700	4.73130100
H	6.51993000	9.01071300	-6.62039000	C	-14.48696500	7.58516800	1.59408900
H	6.70406700	10.77524300	-6.82450000	O	-15.69422000	7.49070300	1.62923200
O	7.60901400	9.94946400	-5.15460300	C	13.43778700	-2.66241100	6.33822400
H	5.96452300	11.21749300	-3.66249900	O	13.46252500	-1.48455800	6.06182500
O	5.42441500	12.55847100	-5.14081800	C	16.10466100	-5.47807800	4.17189600
O	3.22434900	7.76262000	-3.64759700	O	15.40982300	-6.42508200	4.46278900
H	1.25061700	-2.41554400	-2.75893800	C	15.28714500	-7.26033700	1.39200900
C	0.06902200	-3.98033300	-3.11442600	O	16.47528400	-7.03885500	1.30854900
S	0.32963400	-3.85281600	-4.77581100	C	-7.53959100	-14.38784600	-5.36554000
N	-0.64009300	-4.97392800	-2.53015400	H	-6.59331900	-14.85738000	-5.64334500
C	-1.26886700	-6.07753000	-3.24968500	H	-8.18161300	-15.09363600	-4.83613100
H	-0.59479600	-6.39639400	-4.05134600	H	-8.05164200	-14.06819400	-6.28091900
H	-1.37675300	-6.90293900	-2.54045800	C	-10.20889800	-10.19873300	-4.64767400
H	-0.63628600	-5.02267900	-1.51967100	H	-10.20990200	-9.15149900	-4.33719300
C	-2.63868700	-5.71236300	-3.83839200	H	-10.03655400	-10.82551800	-3.76500900
H	-2.50801100	-4.91248500	-4.57465700	C	-4.28093500	-13.74330100	-0.50007000
H	-3.29670600	-5.33280800	-3.04662800	H	-5.26248600	-14.20591700	-0.63240900
C	-3.31057200	-6.89796000	-4.51337600	H	-3.53030400	-14.49249700	-0.24439800
H	-2.64609200	-7.34783500	-5.26800500	H	-4.35460200	-13.00896400	0.31021200
H	-4.23510000	-6.59313600	-5.01525500	C	9.62251100	10.76416000	-4.22266500
C	-3.98600900	-9.11421900	-3.97413500	H	9.69538000	9.75362900	-3.81456800
H	-3.23623200	-9.51435500	-4.68341200	H	9.27621500	11.43850000	-3.43087000
C	-4.16296700	-10.07887800	-2.79548800	C	6.62731100	14.52774200	-5.64441000
C	-5.63216000	-10.21060900	-5.29277000	H	5.67536000	14.86325200	-6.06204800
H	-4.82434800	-10.55611800	-5.96146800	H	7.12677400	15.34120500	-5.11586900
C	-5.87198600	-11.28301500	-4.21284100	H	7.27145500	14.19781800	-6.46808200
C	-4.61585000	-11.44640500	-3.36222400	C	2.90267500	13.89237600	-1.13747400
H	-3.80582000	-11.87098200	-3.96471900	H	3.83702300	14.45545400	-1.20768000
H	-3.21627900	-10.21618800	-2.26758600	H	2.05062700	14.56600900	-1.03578400
O	-5.23483900	-8.98998300	-4.66668000	H	2.96033300	13.24138300	-0.25766500
N	-5.12479700	-9.52446300	-1.85982800	C	-16.71418800	6.20641100	4.89093500
C	-5.02145600	-9.69120100	-0.50834600	H	-16.86833700	6.95433000	5.67033800
O	-4.14220000	-10.37003100	0.01412500	H	-17.23532400	6.53438800	3.98366900
C	-6.09829300	-8.99897100	0.31323500	H	-17.12223900	5.23986400	5.19481100
H	-6.66243200	-8.24600700	-0.24593400	C	-12.34330100	3.85198100	8.04747400
H	-6.80038900	-9.75357400	0.68453700	H	-12.85445100	4.81141500	8.16198100
H	-5.62956700	-8.53017500	1.18228000	H	-12.58069400	3.18463400	8.87718900

H	-11.26354800	4.03904700	8.02783500	C	2.90023900	-2.11237600	-0.10343700
C	-13.70337100	8.84058400	1.87272100	H	3.12813400	-2.90331100	-0.82548800
H	-12.77078900	8.86628900	1.30468300	H	3.73266300	-2.08906100	0.60782900
H	-14.31971500	9.71177300	1.64453300	C	-0.78151500	-2.74747400	2.06913700
H	-13.46331400	8.85229800	2.94224100	C	0.41204400	-2.55629600	2.77231400
C	13.25052300	-3.24957500	7.71050400	C	-0.79734300	-2.80995100	0.67497700
H	13.88048700	-4.13152400	7.85311000	C	1.60014000	-2.35655700	2.05835300
H	13.46574100	-2.49312500	8.46649300	C	0.42599900	-2.72322300	-0.01242400
H	12.20270500	-3.56010500	7.79233400	C	1.62376200	-2.43668100	0.66345500
C	17.59482300	-5.39408400	4.37299300	H	2.50451100	-2.08423500	2.59243500
H	17.88956800	-6.05782500	5.18734500	H	-1.71241700	-2.84364800	2.62057800
H	18.07755800	-5.73712500	3.45018900	O	2.85492100	0.44496000	1.21164400
H	17.91634600	-4.36935600	4.57201400	O	0.44166000	-2.85805600	-1.39072400
C	14.67320900	-8.56165700	1.83593800	O	-2.85549400	-0.44443800	1.21081000
H	13.70310200	-8.73032100	1.36319100	O	-0.44133200	2.85784600	-1.39165700
H	15.35901200	-9.38131400	1.61506000	C	-4.19497500	-0.66139800	1.65656000
H	14.53024000	-8.50754200	2.92138000	H	-4.58333200	-1.62945900	1.31348000
H	10.59569000	11.11066200	-4.57446400	H	-4.87075600	0.12863000	1.30270400
H	-11.16880400	-10.47292700	-5.08837700	C	0.64814400	-4.20059100	-1.83655300
H	-1.67854600	-3.10248100	3.11211700	H	-0.14469500	-4.87068900	-1.47953000
H	-2.36302300	-4.11112200	1.83916200	H	1.61482600	-4.59421600	-1.49580900
H	-3.82355100	2.45154600	1.57875200	C	-0.64770000	4.20024900	-1.83793600
H	-2.86629300	1.92516900	2.96184400	H	-1.61447600	4.59397200	-1.49757500
H	3.92375400	-2.78878700	1.59275500	H	0.14504000	4.87045400	-1.48089200
H	2.98912100	-2.21565300	2.97333200	C	4.19425800	0.66200700	1.65778700
H	2.46797900	3.77982400	1.68883800	H	4.58275200	1.62996900	1.31458300
H	1.80380600	2.79952100	2.99601900	H	4.87013900	-0.12813000	1.30436600
1-alternate-unfolded B3LYP/6-31G(d) PCM				H	-2.90903400	-3.13955100	0.64570300
(methanol), electr. en. = -9306.354647 a.u.				H	-3.73302500	2.08940300	0.60600700
C	-2.74062000	0.77313800	-2.25133200	H	2.90865700	3.13992400	0.64580700
C	-2.55829300	-0.42308200	-2.95280700	H	-0.63215800	4.16998400	-2.92993600
N	-2.48904600	-0.39195300	-4.36959400	H	0.63290600	-4.17064600	-2.92856500
C	2.36663700	1.61140000	-2.23698500	H	4.16365300	0.65093700	2.74998500
C	2.55918500	0.42247200	-2.95206500	H	-4.16473900	-0.65003900	2.74876600
N	2.49045700	0.39095800	-4.36887600	N	-0.37868800	2.48426500	4.18843600
C	0.79695800	2.81031200	0.67447700	H	0.40906600	2.01100600	4.61213000
C	-0.42615100	2.72340100	-0.01331400	C	-1.12595800	3.18376600	5.10990200
C	-1.62414600	2.43705800	0.66224100	S	-0.79774700	2.99764200	6.75475700
C	-1.60099300	2.35731300	2.05716900	N	-2.08701600	3.99823300	4.61460800
C	-0.41313200	2.55722400	2.77147300	C	-2.95608600	4.84046500	5.42978700
C	0.78066400	2.74820800	2.06864600	H	-3.28229200	5.67462500	4.80259300
H	-2.50554300	2.08514000	2.59102200	H	-2.36406600	5.24327100	6.25771300
H	1.71138200	2.84451600	2.62037300	H	-2.14159000	4.10555300	3.60988100
C	2.11868200	2.91035600	-0.07679800	N	0.37714200	-2.48299700	4.18924700
H	2.09583400	3.74213600	-0.78848400	H	-0.41076000	-2.00965800	4.61257800
C	-2.90036600	2.11253900	-0.10498900	C	1.12412000	-3.18229400	5.11111000
H	-3.12803200	2.90327400	-0.82733000	S	0.79542000	-2.99578600	6.75582000
C	2.44201500	1.63274500	-0.84232000	N	2.08533600	-3.99686600	4.61629400
C	2.72080000	0.43238200	-0.16755600	C	2.95416200	-4.83892000	5.43191500
C	2.80255300	-0.79066700	-0.85557200	H	2.36189700	-5.24156600	6.25974400
H	2.10802400	2.51934200	-2.77124000	H	3.28056900	-5.67320300	4.80498800
C	2.74126500	-0.77355700	-2.25020400	H	2.14020700	-4.10442000	3.61160900
H	2.83076000	-1.70468000	-2.80238400	C	-4.17503800	4.08867700	5.98262100
C	-2.80241200	0.79062500	-0.85672800	H	-3.82436100	3.24404000	6.58529100
C	-2.72090500	-0.43223700	-0.16834700	H	-4.77361100	3.68530600	5.15601400
C	-2.44188900	-1.63278200	-0.84268800	C	-5.05362400	4.97246000	6.85362300
H	-2.82991200	1.70411300	-2.80379400	H	-5.87715200	4.39875800	7.29289700
C	-2.36601200	-1.61181500	-2.23733300	H	-4.46777300	5.41140500	7.67653300
H	-2.10719900	-2.51990300	-2.77124300	C	4.17294600	-4.08701500	5.98495700
C	-2.11882100	-2.91018900	-0.07670900	H	3.82209500	-3.24233100	6.58746100
H	-2.09575500	-3.74216800	-0.78815700	H	4.77168300	-3.68369800	5.15844300
				C	5.05138700	-4.97067400	6.85623100

H	4.46538500	-5.40958100	7.67905500	C	6.08655000	2.42540600	-6.08064600
H	5.87479200	-4.39689000	7.29563000	H	5.85526400	1.54442600	-6.68911300
C	-6.19703400	7.05117800	6.72728400	H	6.69079600	2.09300900	-5.22677400
H	-5.53792900	7.44280900	7.52533300	C	6.90217700	3.39572100	-6.92088100
C	-6.57257400	8.17833500	5.75869200	H	6.31119100	3.76232900	-7.77498000
H	-5.67586700	8.60105500	5.29919600	H	7.80421700	2.91389400	-7.31428100
C	-7.28069200	9.28819100	6.57329900	C	7.83089300	5.57642200	-6.76115700
H	-6.56368800	9.73163800	7.27240300	H	7.20496100	5.87721600	-7.62274200
C	-8.47134100	8.71545800	7.33608000	C	8.00125400	6.75817900	-5.80025700
H	-9.25143200	8.41051500	6.63806800	C	9.71688700	6.19554100	-8.07427700
C	-8.01821400	7.51209100	8.18491600	H	9.02997500	6.44909400	-8.90065200
H	-7.29139700	7.86417900	8.93774100	C	9.96197900	7.46120700	-7.22997100
O	-7.39102100	6.54547700	7.34110000	C	8.65597000	7.91837700	-6.58750200
N	-7.41380500	7.64635000	4.70152700	H	7.95909000	8.26715100	-7.35702400
C	-7.36866700	8.11094800	3.41792200	H	7.02936600	7.09330600	-5.43021100
O	-6.65738800	9.04969200	3.07356200	O	9.11979100	5.18749300	-7.25705900
C	-8.28851000	7.39864700	2.43779600	N	8.79968800	6.34161000	-4.66143800
H	-8.70481900	6.46322500	2.82469400	C	8.59804900	6.82539300	-3.40020400
H	-9.11620900	8.06799600	2.17947900	O	7.76537900	7.68946500	-3.14310800
H	-7.73169100	7.19508900	1.51933600	C	9.50488700	6.23802200	-2.32922400
H	-7.95570200	6.82178400	4.91999000	H	10.01431900	5.32053800	-2.64024900
O	-7.76757400	10.31177400	5.70093200	H	10.26244000	6.98188300	-2.05896500
O	-9.00243900	9.71292100	8.22528000	H	8.90757100	6.03670200	-1.43635600
C	-9.14830900	6.83650700	8.94779900	H	9.44341700	5.57691800	-4.81077300
H	-8.78796100	5.88360400	9.34606200	O	8.95697400	9.00739600	-5.70969200
H	-9.48746300	7.47182000	9.76695800	C	10.97621500	5.62399600	-8.70966500
O	-10.25888800	6.55404800	8.07809100	H	10.75446500	4.62605700	-9.09884800
C	6.19491600	-7.04936200	6.73029200	H	11.31998800	6.26570600	-9.52197800
H	5.53568100	-7.44092300	7.52826800	O	12.02743900	5.48890700	-7.73720200
C	6.57061600	-8.17660500	5.76186100	H	10.70764900	7.26122600	-6.46001300
C	8.01585800	-7.51014000	8.18825600	O	10.45684300	8.49057000	-8.10387800
H	7.28891300	-7.86216500	8.94098700	O	7.27249600	4.50777900	-6.08898700
C	8.46913100	-8.71357800	7.33959800	H	-1.98239200	0.37040500	-4.80075600
C	7.27860900	-9.28638800	6.57667600	C	-3.12870600	-1.19368900	-5.28727700
H	6.56149600	-9.72977600	7.27570700	S	-2.83877500	-0.96791900	-6.93348600
H	5.67398200	-8.59936600	5.30225900	N	-3.96734300	-2.13063200	-4.78202300
O	7.38879900	-6.54359900	7.34425600	C	-4.76893000	-3.04526000	-5.58589100
N	7.41200700	-7.64469900	4.70478200	H	-4.15989400	-3.35604700	-6.43926300
C	7.36705800	-8.10938600	3.42120400	H	-4.97526800	-3.92651700	-4.97139700
O	6.65585200	-9.04817400	3.07680800	H	-4.16449300	-2.09481800	-3.78948600
C	8.28697200	-7.39710000	2.44113400	C	-6.08433300	-2.42732300	-6.08217100
H	8.70370600	-6.46195600	2.82824400	H	-5.85293100	-1.54654700	-6.69088900
H	9.11435700	-8.06668100	2.18242600	H	-6.68891800	-2.09466900	-5.22864000
H	7.73005000	-7.19303300	1.52284500	C	-6.89955700	-3.39805600	-6.92230700
H	7.95385200	-6.82010300	4.92326000	H	-6.30823000	-3.76497000	-7.77604000
O	7.76563400	-10.31004700	5.70448000	H	-7.80149700	-2.91647000	-7.31623200
C	9.14581700	-6.83448600	8.95127800	C	-7.82859900	-5.57856300	-6.76198000
H	8.78540400	-5.88153300	9.34936000	H	-7.20274400	-5.87962200	-7.62352600
H	9.48480200	-7.46970900	9.77057600	C	-7.99900000	-6.76008600	-5.80080000
O	10.25657300	-6.55214400	8.08175700	C	-9.71477500	-6.19779700	-8.07480900
H	9.24932900	-8.40869300	6.64167900	H	-9.02799400	-6.45159400	-8.90121600
O	9.00009400	-9.71096000	8.22897000	C	-9.95989200	-7.46325800	-7.23020000
O	-5.58469900	6.02697000	6.03325500	C	-8.65387100	-7.92039700	-6.58773700
O	5.58268800	-6.02522600	6.03606400	H	-7.95708400	-8.26939800	-7.35724100
H	1.98380700	-0.37141200	-4.80002300	H	-7.02711500	-7.09520900	-5.43074300
C	3.13047900	1.19241600	-5.28653900	O	-9.11748900	-5.18961900	-7.25788800
S	2.84113100	0.96621200	-6.93279300	N	-8.79734400	-6.34319600	-4.66202700
N	3.96898200	2.12946100	-4.78123300	C	-8.59562600	-6.82670300	-3.40069700
C	4.77104200	3.04369300	-5.58508500	O	-7.76304600	-7.69082700	-3.14349000
H	4.16238900	3.35428300	-6.43880100	C	-9.50229200	-6.23899600	-2.32975800
H	4.97726000	3.92512500	-4.97080500	H	-10.01164300	-5.32151100	-2.64091800
H	4.16591400	2.09376900	-3.78864600	H	-10.25991500	-6.98270900	-2.05928900

H	-8.90487400	-6.03758000	-1.43698000	H	-6.85289700	13.06185500	4.17445800
H	-9.44086100	-5.57834300	-4.81144900	H	-7.37789400	11.59270600	3.30620000
O	-8.95490000	-9.00920200	-5.70967200	C	-12.50906000	6.77397600	7.38862200
C	-10.97413700	-5.62625900	-8.71014800	H	-12.30442600	5.84314800	6.85496600
H	-10.75236100	-4.62838600	-9.09948300	H	-13.50098300	6.74975100	7.84296900
H	-11.31804300	-6.26805300	-9.52233800	H	-12.47144100	7.60402300	6.67363700
O	-12.02525100	-5.49096100	-7.73759300	C	7.43730900	-12.14337000	4.25447100
H	-10.70548000	-7.26304600	-6.46022500	H	8.48867700	-12.36943500	4.45090800
O	-10.45491300	-8.49276000	-8.10385500	H	6.85117400	-13.06023400	4.17805600
O	-7.27007100	-4.50980800	-6.09008900	H	7.37635200	-11.59114800	3.30979900
C	-11.62667600	-9.10353900	-7.75938000	C	10.69112200	-11.14288200	9.04680500
O	-12.24987000	-8.85155000	-6.75321300	H	11.46029200	-11.80847100	8.65182400
C	-13.21263200	-6.09815200	-8.02255900	H	11.12503900	-10.55282000	9.86283400
O	-13.43772200	-6.68688500	-9.05706600	H	9.84905200	-11.71506100	9.44244400
C	-7.92522300	-9.86422700	-5.43593600	C	12.50686400	-6.77225100	7.39273400
O	-6.85157300	-9.80850200	-5.99129000	H	12.30236300	-5.84149700	6.85889800
C	13.21477000	6.09608200	-8.02241200	H	13.49870700	-6.74799500	7.84725700
O	13.43971300	6.68466200	-9.05703800	H	12.46934300	-7.60240700	6.67787100
C	11.62862800	9.10145400	-7.75966800	H	15.19707400	6.04677300	-7.23384200
O	12.25194100	8.84970000	-6.75351500	H	-15.19484100	-6.04873800	-7.23376100
C	7.92723000	9.86236900	-5.43603300				
O	6.85353800	9.80642400	-5.99128200				
C	-6.86173700	11.26237700	5.32341800				
O	-5.74733900	11.33812100	5.78864200				
C	-10.25584800	10.18830400	7.96494500				
O	-10.92737200	9.84195200	7.01975200				
C	-11.47629300	7.04162700	8.45151600				
O	-11.67505500	7.63950800	9.48620400				
C	6.85986100	-11.26069000	5.32691300				
O	5.74538400	-11.33638200	5.79195600				
C	10.25353100	-10.18639000	7.96885100				
O	10.92518900	-9.84014000	7.02371600				
C	11.47389600	-7.03969800	8.45548300				
O	11.67243300	-7.63748300	9.49027100				
C	-12.05084800	-10.07641200	-8.82791700				
H	-11.18995300	-10.54436300	-9.31046200				
H	-12.70834900	-10.83063400	-8.39255100				
H	-12.61360900	-9.51787500	-9.58530900				
C	-14.16996800	-5.97050100	-6.86716700				
H	-14.02270700	-5.03345900	-6.32547000				
H	-13.97774800	-6.80519000	-6.18321800				
C	-8.31480400	-10.82767500	-4.34837800				
H	-9.34652800	-11.16760400	-4.47146200				
H	-7.62614700	-11.67368700	-4.34246300				
H	-8.24260300	-10.29089300	-3.39563900				
C	14.17224200	5.96867000	-6.86710500				
H	14.02500600	5.03176700	-6.32516100				
H	13.98014300	6.80353600	-6.18333800				
C	12.05262000	10.07417000	-8.82841900				
H	11.19164500	10.54188800	-9.31104500				
H	12.71001700	10.82858300	-8.39322400				
H	12.61545800	9.51556300	-9.58570200				
C	8.31680200	10.82606200	-4.34869100				
H	9.34851600	11.16599000	-4.47185400				
H	7.62812300	11.67205800	-4.34294600				
H	8.24461900	10.28947500	-3.39584100				
C	-10.69360700	11.14489300	9.04274600				
H	-11.46258300	11.81057000	8.64753300				
H	-11.12783700	10.55490700	9.85866400				
H	-9.85157700	11.71697400	9.43860600				
C	-7.43902500	12.14498400	4.25082900				
H	-8.49043200	12.37103600	4.44707300				