

Computational Investigations on the Catalytic Mechanism of Maleate Isomerase: the Role of the Active Site Cysteine Residues

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Supporting Information

(Tables S1 and S2; total pages 240 pages)

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Table S1. Selected optimized geometrical parameters (distances in Angstroms, angles in degrees) obtained in the gas-phase at the B3LYP/6-31G(d,p) level of theory for di- and monoanionic maleate, and maleic acid.

Substrate	r(C1—C2) (Å)	r(C2—C3) (Å)	R(C3—C4) (Å)	∠ C1-C2-C3-C4 (°)
Dianionic maleate	1.537	1.348	1.543	0.0
Monoanionic maleate	1.511	1.345	1.518	0.0
Maleic acid	1.490	1.343	1.491	0.0

Table S2. Cartesian coordinates and partial charges of all species presently obtained using the QM-cluster and ONIOM(QM/MM) approaches for both the Cys76- and Cys194-pathways.

QM-cluster Cys76-pathway

RC_{QM}

C	-1	-6.16565500	-2.51196800	1.19215800
C	0	-6.19468200	-2.44764700	-0.33062500
O	0	-7.10484500	-2.96283200	-0.98865700
N	0	-5.15628000	-1.76779100	-0.86480200
C	-1	1.31809500	-4.02277500	0.51717600
C	0	2.66483400	-4.13006700	-0.14746500
O	0	3.26281800	-5.20977800	-0.20743400
C	0	1.47418000	-4.26179900	2.04420900
S	0	2.60660100	-3.10612100	2.94963700
N	0	3.11671300	-2.93968700	-0.64136000
C	0	4.44329600	-2.65847000	-1.14908700
C	0	5.35844300	-1.81915300	-0.18499200
O	0	6.52099300	-1.58445300	-0.54008100
N	0	4.77335900	-1.28683100	0.92520600
C	0	5.52651300	-0.47777400	1.89432700
C	-1	5.05013900	0.99248200	2.11411400
C	-1	4.06149100	5.62795500	1.30514800
C	0	3.06137000	4.81123200	1.83556100
C	0	4.71757200	5.24082300	0.13507200
C	0	2.71494400	3.61730400	1.21857500
C	0	4.38436500	4.04766100	-0.49829500
C	0	3.38074100	3.21386900	0.03708800
O	0	3.10886300	2.06852400	-0.58287800
C	-1	-4.90977600	2.61233600	5.10528200
C	0	-5.08935300	1.30793000	4.31022100
O	0	-6.14091400	0.67565300	4.40153200
N	0	-4.03970100	0.95533200	3.53699000
C	-1	0.87918800	1.88489700	-2.86515900
C	0	-0.32957200	1.25093200	-3.55890500
O	0	-0.75773900	1.69972400	-4.62894700
C	0	0.63400000	3.34044000	-2.46364800
S	0	-0.60987800	3.56384600	-1.11644200
N	0	-0.85868200	0.15860900	-2.94262500
C	0	-1.99974800	-0.54872700	-3.50518900
C	0	-3.40317100	0.00168300	-3.11610800
O	0	-4.38097400	-0.34038000	-3.80479900
N	0	-3.47550000	0.83206500	-2.06185100
C	0	-4.72654200	1.45980000	-1.64807500
C	-1	-4.64648200	1.94855400	-0.19426900
C	0	0.80082300	-0.09995100	0.50326800
O	0	1.17144500	1.11029900	0.70151200
O	0	1.03565300	-0.75851900	-0.54080400
C	0	0.16966700	-0.78455400	1.68854400
C	0	-1.14303300	-0.92576800	1.92565400
C	0	-2.20426200	-0.42429500	1.00174200
O	0	-1.82823000	0.24293400	0.00112600
O	0	-3.42519100	-0.70943000	1.29030300

H	0	2.31935400	1.58692600	-0.10425700
H	0	-0.14070700	2.58819100	-0.29882700
H	0	2.48300000	-2.14404900	-0.54674500
H	0	3.93697800	-1.76251600	1.30488300
H	0	-5.14617900	-1.58456800	-1.86150100
H	0	-4.46527000	-1.31648300	-0.25478300
H	0	-4.05629300	0.18317800	2.85460700
H	0	-3.23249000	1.55514400	3.46717800
H	0	5.19334900	1.58954000	1.21229000
H	0	5.62955500	1.43659900	2.93305500
H	0	3.98897800	1.02480900	2.37432700
H	0	6.56759400	-0.47907500	1.55686900
H	0	5.48040400	-1.00645000	2.85530600
H	0	-2.72813600	0.78578900	-1.34492600
H	0	-0.48332400	-0.13290200	-2.03894200
H	0	0.84481200	-3.05841000	0.32291000
H	0	0.47047800	-4.21548600	2.48788200
H	0	1.83800400	-5.28972500	2.17018000
H	0	-5.16092600	-2.36440400	1.59426100
H	0	-6.80248200	-1.71840500	1.60058600
H	0	-6.57967100	-3.47154100	1.51436500
H	0	-5.48012000	3.40768100	4.61299700
H	0	-5.33029100	2.47015900	6.10392000
H	0	-3.86804500	2.93669100	5.19147900
H	0	4.88841400	3.72242600	-1.40398000
H	0	5.49831400	5.87338500	-0.28607200
H	0	4.32672400	6.56242900	1.79695100
H	0	2.54354700	5.10884500	2.74573900
H	0	1.94538400	2.96914900	1.62200300
H	0	1.57535200	3.79911000	-2.15335800
H	0	0.23270400	3.89365000	-3.31829600
H	0	-1.96527800	-0.37153700	-4.58457800
H	0	-4.94390000	2.30283200	-2.32228900
H	0	-3.83036200	2.66899700	-0.07583600
H	0	-5.58733300	2.44283400	0.07954100
H	0	-4.46451500	1.11173100	0.48210900
H	0	-5.55229000	0.74914600	-1.76639900
H	0	4.31391800	-1.95694200	-1.98780400
H	0	0.90230300	-1.24576100	2.36351200
H	0	-1.48183900	-1.47435000	2.80287800
H	0	1.20286700	1.28885400	-2.01175500
H	0	1.69665200	1.87622500	-3.59872000
C	-1	5.12843200	-3.91804900	-1.73131600
H	0	4.47546000	-4.37589200	-2.47768200
H	0	5.32753700	-4.65940400	-0.96255500
H	0	6.06503200	-3.60142900	-2.20332000
C	-1	-1.89912800	-2.06477800	-3.23931400
H	0	-2.77878200	-2.56401700	-3.65409200
H	0	-1.85372000	-2.26680500	-2.16453600
H	0	-0.99456100	-2.47204600	-3.70084600
H	0	0.67772000	-4.81428200	0.09912100

TS1_{QM}

C	-1	6.57979700	-1.89509400	-0.82751600
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C	0	5.64549300	-3.04125300	-0.44750300
O	0	6.09001400	-4.15991600	-0.14870600
N	0	4.35113400	-2.69365600	-0.44756000
C	-1	-0.76900900	-4.04387400	-0.47759600
C	0	-2.27212000	-4.09845600	-0.26718600
O	0	-2.97957500	-4.97437500	-0.77724200
C	0	-0.35303700	-3.51192200	-1.87214300
S	0	-1.12754300	-1.93864300	-2.45669400
N	0	-2.74725200	-3.12519600	0.56038000
C	0	-4.15367200	-2.98244800	0.91192400
C	0	-5.06388300	-2.52065900	-0.27265100
O	0	-6.14181500	-3.07234200	-0.52194400
N	0	-4.60410100	-1.42418300	-0.91654300
C	0	-5.21336200	-0.86715600	-2.11538000
C	-1	-4.84140900	0.61662100	-2.30146800
C	-1	-4.29498700	5.32638000	-1.50205900
C	0	-3.24306100	4.41751200	-1.64837700
C	0	-5.24092900	5.10755600	-0.49632300
C	0	-3.13922400	3.30015200	-0.82685800
C	0	-5.15139500	3.99278200	0.33583000
C	0	-4.10571200	3.06186600	0.17430300
O	0	-4.07546300	1.98857500	0.97518500
C	-1	5.06996900	3.07108200	-4.85315500
C	0	5.04247300	1.80666300	-3.95915000
O	0	6.01082000	1.04611100	-3.98474400
N	0	3.93261500	1.63121300	-3.21250000
C	-1	-0.99911200	1.90518800	2.85243700
C	0	0.20978400	1.37737300	3.62933200
O	0	0.56367500	1.89432200	4.69712200
C	0	-0.63886700	3.10161300	1.94079200
S	0	0.78085900	2.96724100	0.74368600
N	0	0.87030600	0.33400200	3.05220400
C	0	2.04328300	-0.26763500	3.67196700
C	0	3.40839700	0.36916100	3.29747600
O	0	4.42209200	0.00385400	3.90765400
N	0	3.42909600	1.30346600	2.32104300
C	0	4.67812500	1.91660800	1.88403200
C	-1	4.61870200	2.42734500	0.43618400
C	0	-1.34192800	-0.23697200	-0.02842200
O	0	-2.50111700	0.32414100	-0.15368300
O	0	-0.98599400	-0.85275600	1.00440400
C	0	-0.45609100	-0.02856800	-1.24000300
C	0	0.90978800	0.36697300	-1.19467000
C	0	2.04383600	-0.45758900	-0.67012100
O	0	1.84374500	-1.37619000	0.16017200
O	0	3.22208100	-0.18331900	-1.15881800
H	0	-3.40569400	1.29653900	0.63755500
H	0	0.67080000	1.68618200	-0.09044900
H	0	-2.10707800	-2.37791900	0.84426100
H	0	-3.70021800	-1.02187800	-0.65572900
H	0	3.66263100	-3.33414500	-0.08241400
H	0	4.00730700	-1.73599100	-0.65435500
H	0	3.77503800	0.85509500	-2.52595600
H	0	3.20755700	2.33118500	-3.22590200

H	0	-5.24877900	1.22550000	-1.49167800
H	0	-5.24204000	0.98530600	-3.25402200
H	0	-3.75793400	0.73938700	-2.29615700
H	0	-6.29886400	-1.00116100	-2.03792300
H	0	-4.88119100	-1.43787200	-2.99575500
H	0	2.55682800	1.60784900	1.89040900
H	0	0.49114900	-0.10068300	2.20568100
H	0	-0.29423800	-3.39980900	0.26838000
H	0	0.73455100	-3.39457600	-1.87002400
H	0	-0.61573300	-4.25886600	-2.63169100
H	0	6.11299300	-1.17072900	-1.50051100
H	0	6.87754700	-1.36277600	0.08380700
H	0	7.48215700	-2.30673500	-1.28865600
H	0	4.16441800	3.68402300	-4.79625600
H	0	5.93114700	3.68088200	-4.56279700
H	0	5.22360300	2.75625900	-5.88979200
H	0	-5.88871200	3.80597100	1.11202400
H	0	-6.06363400	5.80918300	-0.36113300
H	0	-4.37008300	6.19675100	-2.15054500
H	0	-2.48739500	4.57680800	-2.41432000
H	0	-2.33595300	2.58317100	-0.94964400
H	0	-1.53268000	3.39806400	1.38797000
H	0	-0.34719900	3.94547100	2.57575000
H	0	1.95816000	-0.08266900	4.74845600
H	0	4.95262400	2.73961500	2.56646400
H	0	3.89242800	3.24128800	0.33754600
H	0	5.60466100	2.80232100	0.13469900
H	0	4.31541700	1.61414100	-0.23056100
H	0	5.45958700	1.15761000	1.99312400
H	0	-4.17982700	-2.15527600	1.63337500
H	0	-1.02290300	0.54858700	-1.96740300
H	0	1.20898600	0.90280500	-2.09984100
H	0	-1.44796300	1.10193800	2.26373000
H	0	-1.73116200	2.25524800	3.58849300
C	-1	-4.67462200	-4.25278300	1.59312600
H	0	-4.06573600	-4.46368700	2.47880400
H	0	-4.60765300	-5.09025500	0.89949500
H	0	-5.71954300	-4.12526700	1.89364400
C	-1	2.08911400	-1.78576800	3.39894700
H	0	2.98190600	-2.20438200	3.87059100
H	0	2.12729200	-1.95949300	2.31861200
H	0	1.19538000	-2.26751200	3.80972700
H	0	-0.38335700	-5.06559900	-0.35996200

IC1_{QM}

C	-1	6.21165200	-2.39161200	-0.82422000
C	0	6.02588500	-2.34968700	0.68551900
O	0	6.89198300	-2.77766200	1.45840400
N	0	4.86078100	-1.78930700	1.06579200
C	-1	-1.27154900	-4.03096900	-0.58155900
C	0	-2.78326500	-3.89716100	-0.43870800
O	0	-3.56292900	-4.61603300	-1.07082900
C	0	-0.69163900	-3.66515300	-1.95944100
S	0	-0.94827400	-1.96939500	-2.63592700

N	0	-3.16941600	-2.98498700	0.49486000
C	0	-4.56714900	-2.76505400	0.84985900
C	0	-5.41400000	-2.17142000	-0.31752500
O	0	-6.57233500	-2.54700200	-0.52379200
N	0	-4.80573200	-1.17215700	-1.00137900
C	0	-5.40684100	-0.51898500	-2.15882200
C	-1	-4.99522100	0.95810800	-2.27700900
C	-1	-4.12756800	5.59059400	-1.32479700
C	0	-2.92411300	4.87443100	-1.35932400
C	0	-5.18424800	5.08877900	-0.56003100
C	0	-2.77467400	3.66559500	-0.68082800
C	0	-5.05325200	3.88051700	0.12332000
C	0	-3.85667200	3.14073000	0.05200500
O	0	-3.81599100	1.95444100	0.68624500
C	-1	5.08197100	2.79228800	-4.69710900
C	0	5.74162000	1.55977400	-4.07204200
O	0	6.97249500	1.43313600	-4.12301900
N	0	4.90579600	0.69136700	-3.48042100
C	-1	-1.11091800	1.81182700	2.93545200
C	0	-0.06811200	1.07673600	3.75251400
O	0	0.20097700	1.38116600	4.92059000
C	0	-0.62867400	3.24360900	2.60031700
S	0	0.80967000	3.32341900	1.45045300
N	0	0.57708600	0.07286700	3.08833100
C	0	1.73604200	-0.58576000	3.64182600
C	0	3.09883700	0.01080700	3.20760600
O	0	4.12911900	-0.55097200	3.63489000
N	0	3.10423100	1.09432300	2.41169600
C	0	4.34833400	1.78681000	2.07358500
C	-1	4.54748500	2.01550200	0.56654800
C	0	-1.23224000	-0.49135500	-0.31904300
O	0	-2.22074000	0.25847900	-0.59984900
O	0	-1.06436700	-1.09602300	0.77978000
C	0	-0.20104900	-0.72966000	-1.44494700
C	0	1.21665400	-1.01937200	-0.95152300
C	0	2.40254700	-0.57005400	-1.84348100
O	0	2.18167700	0.14840400	-2.85138700
O	0	3.54275800	-0.94288900	-1.41982000
H	0	-3.10702700	1.35096100	0.31584100
H	0	1.36378000	-2.07144900	-0.68676300
H	0	-2.46667900	-2.30945500	0.82419400
H	0	-3.84797900	-0.89300700	-0.77808600
H	0	4.72338200	-1.54281100	2.04412400
H	0	4.22568200	-1.42846700	0.34604100
H	0	5.28700100	-0.06433700	-2.92638300
H	0	3.87818800	0.75494300	-3.38221500
H	0	-5.38968300	1.54377500	-1.44591800
H	0	-5.38097200	1.37472100	-3.21555300
H	0	-3.90680300	1.05406200	-2.26987900
H	0	-6.49208100	-0.62819000	-2.06446700
H	0	-5.11048100	-1.05506900	-3.07377100
H	0	2.22844400	1.60765800	2.17093300
H	0	0.23460800	-0.19731100	2.16953400
H	0	-0.76708800	-3.43467800	0.18257300

H	0	0.37977400	-3.89101700	-1.95728400
H	0	-1.15986800	-4.28993400	-2.72831400
H	0	5.27347500	-2.27050800	-1.36789400
H	0	6.87932900	-1.57057700	-1.11400200
H	0	6.71313400	-3.32628800	-1.09745100
H	0	5.28263500	3.65742400	-4.05588500
H	0	5.54269300	2.98593600	-5.67041800
H	0	3.99881700	2.69257900	-4.80955500
H	0	-5.87377400	3.46977900	0.70562500
H	0	-6.12503900	5.63535400	-0.50190000
H	0	-4.22833300	6.53077900	-1.86259600
H	0	-2.07554600	5.26363600	-1.91703300
H	0	-1.82547100	3.13574700	-0.68709100
H	0	-1.47900400	3.78145500	2.16069100
H	0	-0.39287300	3.73703200	3.55338600
H	0	1.69707600	-0.40515100	4.72221200
H	0	4.34230500	2.75936300	2.58613000
H	0	3.74234900	2.63868000	0.16616800
H	0	5.50284000	2.52813200	0.39572700
H	0	4.54937400	1.07264600	0.01305800
H	0	5.16313400	1.18871100	2.48835900
H	0	-4.54584500	-1.98131500	1.61805300
H	0	-0.16528200	0.15667900	-2.08433000
H	0	1.35045900	-0.46651800	-0.01383000
H	0	-1.34897100	1.27068800	2.01848100
H	0	-2.02367500	1.86795700	3.54762700
C	-1	-5.19754600	-4.03122100	1.46096300
H	0	-4.63496100	-4.32105900	2.35419100
H	0	-5.16858600	-4.84174700	0.73206700
H	0	-6.23951300	-3.83797800	1.72920100
C	-1	1.70815400	-2.10150400	3.38000900
H	0	2.62222800	-2.55611900	3.76705400
H	0	1.64388300	-2.30879300	2.30665900
H	0	0.83423000	-2.54969900	3.86372400
H	0	-1.03869900	-5.08953000	-0.40002200

TS2_{qm}

C	-1	6.20762500	-2.31033900	-1.25968600
C	0	6.09100300	-2.48777700	0.25047900
O	0	6.97216000	-3.06830900	0.89697400
N	0	4.97212900	-1.95864700	0.78383500
C	-1	-1.28124700	-3.94084900	-1.20579800
C	0	-2.78362300	-3.87566400	-0.98603100
O	0	-3.56935400	-4.56952900	-1.64020900
C	0	-0.83405700	-3.39281700	-2.57462700
S	0	-1.20636000	-1.61549400	-2.87096500
N	0	-3.17189300	-3.04861500	0.02719400
C	0	-4.56491500	-2.88820400	0.42012100
C	0	-5.43629400	-2.10681200	-0.61571400
O	0	-6.63822800	-2.36231700	-0.75456200
N	0	-4.79864100	-1.08305300	-1.23350000
C	0	-5.41711300	-0.22016200	-2.23449300
C	-1	-4.99367900	1.25923000	-2.10479900
C	-1	-4.09719800	5.69355300	-0.47613000

C	0	-3.07222100	4.82732300	-0.86837000
C	0	-5.01900400	5.25976200	0.48086200
C	0	-2.97251400	3.54433200	-0.33972800
C	0	-4.93451700	3.97715300	1.01992600
C	0	-3.91883600	3.09292100	0.60514400
O	0	-3.90327400	1.85476100	1.11958200
C	-1	5.07401800	3.39945800	-4.30294700
C	0	5.74957600	2.08891000	-3.89058300
O	0	6.93882100	1.89546200	-4.18451500
N	0	4.97504100	1.22646400	-3.21534400
C	-1	-1.06721700	1.30822400	3.14562100
C	0	0.07006900	0.55156400	3.82473800
O	0	0.47641700	0.83740200	4.95631800
C	0	-0.56333100	2.59897100	2.45598600
S	0	0.84775300	2.52042500	1.24145100
N	0	0.63013400	-0.43188800	3.06021000
C	0	1.78483500	-1.19083500	3.50390000
C	0	3.17728900	-0.57662200	3.19091200
O	0	4.17825000	-1.19064300	3.60543700
N	0	3.23466000	0.56990000	2.49209600
C	0	4.49266600	1.26514300	2.21157400
C	-1	4.57453700	1.84446000	0.78897600
C	0	-1.32514200	-0.22489800	-0.21539400
O	0	-2.36527700	0.48896000	-0.41705100
O	0	-1.19678800	-1.04272500	0.74764200
C	0	-0.16628000	0.01677000	-1.14291700
C	0	1.12692400	-0.05103800	-0.60786800
C	0	2.38213100	0.23412100	-1.41822400
O	0	2.34985700	1.15197900	-2.28676100
O	0	3.40568100	-0.47408800	-1.13478600
H	0	-3.27303400	1.24714000	0.59584700
H	0	1.27978800	-0.80347900	0.16360600
H	0	-2.48342600	-2.38931500	0.40966500
H	0	-3.79756400	-0.95537400	-1.09884600
H	0	4.87725800	-1.93928200	1.79530300
H	0	4.29159400	-1.44991500	0.20265200
H	0	5.40739700	0.37709500	-2.87945100
H	0	3.97169100	1.33535100	-2.92933600
H	0	-5.35296000	1.68570300	-1.16664300
H	0	-5.41323800	1.83567500	-2.93877900
H	0	-3.90606000	1.34647400	-2.12079500
H	0	-6.49994900	-0.33804900	-2.12722000
H	0	-5.14546600	-0.58402000	-3.23657500
H	0	2.37105100	1.05523500	2.21941900
H	0	0.17232500	-0.67490800	2.17750500
H	0	-0.75647000	-3.39592000	-0.41597900
H	0	0.24336200	-3.57364200	-2.67738500
H	0	-1.33909600	-3.97009600	-3.35972200
H	0	5.32243600	-1.83704300	-1.69236500
H	0	7.08933500	-1.69480400	-1.47128700
H	0	6.37954900	-3.28762100	-1.72372400
H	0	5.60762000	4.23033600	-3.82934100
H	0	5.17297800	3.52333000	-5.38656100
H	0	4.01829100	3.44508300	-4.02341700

H	0	-5.65484800	3.62313400	1.75256000
H	0	-5.81917000	5.92389800	0.80647200
H	0	-4.16807300	6.69432900	-0.89705200
H	0	-2.33390400	5.15125600	-1.59834300
H	0	-2.18731300	2.86514900	-0.65265400
H	0	-1.41470700	3.07005300	1.96011900
H	0	-0.21067400	3.28533800	3.23399000
H	0	1.75125400	-1.20442400	4.59952800
H	0	4.61846100	2.07409200	2.94940500
H	0	3.76825500	2.56183600	0.61167700
H	0	5.53188800	2.36886800	0.67278400
H	0	4.50015100	1.05761000	0.03626000
H	0	5.29473300	0.54433500	2.38573700
H	0	-4.53879700	-2.23151200	1.30033500
H	0	-0.34046500	0.72302400	-1.94520100
H	0	0.85633600	1.15822300	0.26583000
H	0	-1.56816600	0.66565600	2.41779300
H	0	-1.78777500	1.59443000	3.91993300
C	-1	-5.19209900	-4.23322300	0.84483900
H	0	-4.61891100	-4.64842200	1.68047600
H	0	-5.16769400	-4.92939400	0.00701600
H	0	-6.22976800	-4.07711400	1.15222800
C	-1	1.73654000	-2.63756300	2.97629200
H	0	2.62565000	-3.17260400	3.31468800
H	0	1.71656500	-2.65481100	1.88184200
H	0	0.83697100	-3.14337800	3.34097400
H	0	-1.00339300	-5.00372600	-1.13309800

PC_{QM}

C	-1	-6.15287600	-2.47707100	0.72843500
C	0	-6.02836500	-2.50943900	-0.78711400
O	0	-6.85850100	-3.06875800	-1.51281900
N	0	-4.91172600	-1.89565900	-1.23657800
C	-1	1.35597900	-3.97930600	1.05254700
C	0	2.77088000	-4.14649500	0.57194400
O	0	3.39050000	-5.19805100	0.76189200
C	0	1.34218000	-3.83234100	2.59970200
S	0	2.25117600	-2.37497200	3.27777300
N	0	3.26399400	-3.04156700	-0.06724200
C	0	4.64541700	-2.80530200	-0.44132000
C	0	5.45161900	-1.84594400	0.50855900
O	0	6.65645200	-1.67862400	0.27152900
N	0	4.74574900	-1.16080000	1.44690900
C	0	5.39493000	-0.24128500	2.39288800
C	-1	4.91017400	1.24084100	2.37502600
C	-1	4.02626000	5.72230500	0.87348700
C	0	3.02550900	4.88315700	1.36311500
C	0	4.83045800	5.28779300	-0.18263300
C	0	2.82706300	3.62039100	0.82146100
C	0	4.64544800	4.02485500	-0.73919400
C	0	3.64493200	3.16866000	-0.23895400
O	0	3.52189400	1.95123400	-0.78071100
C	-1	-5.30750200	3.12208200	4.05756000
C	0	-6.02869400	1.82640100	4.42727300

O	0	-7.10530400	1.85153500	5.04029200
N	0	-5.39874800	0.70613700	4.03262000
C	-1	1.29671100	1.43837100	-3.09217200
C	0	0.17135500	0.71076200	-3.81967500
O	0	-0.19113700	1.05006300	-4.95184200
C	0	0.95717200	2.91174500	-2.85428000
S	0	-0.41154500	3.18088200	-1.64316900
N	0	-0.40114200	-0.31160000	-3.12606300
C	0	-1.48657200	-1.08712300	-3.69993700
C	0	-2.90012100	-0.50269400	-3.46525700
O	0	-3.86946600	-1.06920400	-3.99185100
N	0	-3.00620800	0.59953000	-2.69262000
C	0	-4.26978700	1.30871800	-2.49460900
C	-1	-4.48216700	1.78430200	-1.05363600
C	0	0.66660000	0.06943100	0.30543700
O	0	1.46672200	1.06487300	0.40243300
O	0	0.76008700	-0.84540400	-0.55921100
C	0	-0.50091900	0.15331800	1.24116600
C	0	-1.70911200	-0.31780100	0.91802700
C	0	-2.98164200	-0.05520500	1.67905900
O	0	-2.94341300	0.60997100	2.75348000
O	0	-4.03124600	-0.51863500	1.13314700
H	0	2.74792600	1.44812100	-0.33509100
H	0	-1.82211100	-0.90159600	0.00779400
H	0	2.63653900	-2.24305900	-0.10841200
H	0	3.84453000	-1.56165800	1.78878800
H	0	-4.75092000	-1.81806300	-2.23459700
H	0	-4.34081000	-1.37912600	-0.55945800
H	0	-5.87613500	-0.16563500	4.21081200
H	0	-4.49661400	0.68152500	3.49574600
H	0	5.17138200	1.72653000	1.43352400
H	0	5.38619700	1.78426400	3.20068800
H	0	3.82546400	1.29182500	2.49689500
H	0	6.46881300	-0.28285600	2.18597700
H	0	5.22406700	-0.64975800	3.39750600
H	0	-2.15625800	1.02640200	-2.33767700
H	0	-0.02415400	-0.56230000	-2.19900100
H	0	0.86778800	-3.11186400	0.59903500
H	0	0.29060100	-3.78218100	2.91219200
H	0	1.75912600	-4.76151900	3.01225600
H	0	-5.85181700	-1.51687700	1.14822600
H	0	-7.17978700	-2.73918600	0.99932200
H	0	-5.47958600	-3.22567900	1.16334500
H	0	-5.96713000	3.72005000	3.41996000
H	0	-5.12282600	3.70030400	4.96909300
H	0	-4.36400200	2.94095600	3.53691000
H	0	5.26953000	3.66484300	-1.55240800
H	0	5.61279100	5.93696700	-0.57404000
H	0	4.17752500	6.70999500	1.30515400
H	0	2.39083600	5.21276500	2.18309200
H	0	2.06065500	2.95545100	1.20131800
H	0	1.83859500	3.44936300	-2.50049600
H	0	0.61111000	3.36648300	-3.78684900
H	0	-1.36905500	-1.03859700	-4.78835100

H	0	-4.30571800	2.16693200	-3.18435700
H	0	-3.67923100	2.46278100	-0.74365200
H	0	-5.42635900	2.34034300	-0.99588900
H	0	-4.51606500	0.95413500	-0.34560900
H	0	-5.05984100	0.61842000	-2.79692400
H	0	4.61736300	-2.21973600	-1.37342600
H	0	-0.37016700	0.74720700	2.14005800
H	0	0.18497400	2.52624200	-0.61470300
H	0	1.55484500	0.94124400	-2.15738500
H	0	2.17919500	1.39976600	-3.74425200
C	-1	5.38472100	-4.12285000	-0.77337100
H	0	4.81644700	-4.68246100	-1.52049300
H	0	5.49526900	-4.75326500	0.10408600
H	0	6.36852000	-3.86107200	-1.17701400
C	-1	-1.43671500	-2.55710300	-3.24555700
H	0	-2.30302700	-3.08704700	-3.64598800
H	0	-1.45167200	-2.63013400	-2.15369600
H	0	-0.51703500	-3.03051100	-3.60190800
H	0	0.80237100	-4.88661500	0.76848600

ONIOM(QM/MM) Cys76-pathway

RC

C-CT--0.366200	-1	8.216083	4.637984	-8.143840	L
C-C-0.597200	-1	9.046369	3.891732	-7.104837	L
O-O--0.567900	-1	9.644902	2.853141	-7.386898	L
H-HC-0.112300	-1	7.774823	5.524558	-7.688618	L
H-HC-0.112300	-1	7.423315	3.986106	-8.512481	L
H-HC-0.112300	-1	8.856030	4.937012	-8.974849	L
N-N--0.415700	-1	9.043494	4.450089	-5.887878	L
C-CT--0.087500	-1	9.515087	3.773785	-4.672347	L
C-C-0.597300	-1	8.376711	2.878298	-4.179376	L
O-O--0.567900	-1	7.467220	3.339670	-3.474825	L
C-CT-0.298500	-1	10.000257	4.775206	-3.597073	L
C-CT--0.319200	-1	10.420173	4.075270	-2.298987	L
C-CT--0.319200	-1	11.215473	5.581253	-4.078221	L
H-H-0.271900	-1	8.459786	5.273151	-5.759998	L
H-H1-0.096900	-1	10.351398	3.131285	-4.927465	L
H-HC--0.029700	-1	9.204456	5.482106	-3.379801	L
H-HC-0.079100	-1	11.124598	3.275341	-2.528875	L
H-HC-0.079100	-1	9.549705	3.653469	-1.800295	L
H-HC-0.079100	-1	10.898607	4.782702	-1.623553	L
H-HC-0.079100	-1	12.074674	4.923186	-4.207838	L
H-HC-0.079100	-1	11.463604	6.351854	-3.346240	L
H-HC-0.079100	-1	10.996888	6.061089	-5.031208	L
N-N--0.415700	-1	8.390860	1.605639	-4.611124	L
C-CT--0.087500	-1	7.276585	0.655264	-4.434981	L
C-C-0.597300	-1	7.691421	-0.621002	-3.674285	L
O-O--0.567900	-1	8.836569	-1.074311	-3.799985	L
C-CT-0.298500	-1	6.621152	0.249254	-5.779449	L
C-CT--0.319200	-1	5.764553	1.377075	-6.366583	L
C-CT--0.319200	-1	7.612105	-0.203118	-6.857167	L
H-H-0.271900	-1	9.165046	1.298586	-5.205901	L

H-H1-0.096900	-1	6.506993	1.163347	-3.860887	L
H-HC--0.029700	-1	5.950944	-0.590577	-5.592500	L
H-HC-0.079100	-1	6.283271	2.332653	-6.291185	L
H-HC-0.079100	-1	4.830115	1.426141	-5.812066	L
H-HC-0.079100	-1	5.514859	1.162326	-7.406933	L
H-HC-0.079100	-1	8.213418	0.640562	-7.191785	L
H-HC-0.079100	-1	7.061104	-0.605401	-7.706249	L
H-HC-0.079100	-1	8.265673	-0.977123	-6.462992	L
N-N--0.254800	-1	6.755243	-1.226205	-2.905593	L
C-CT--0.026600	-1	6.885847	-2.579450	-2.358916	L
C-C-0.589600	-1	7.131450	-3.603242	-3.469048	L
O-O--0.574800	-1	6.383616	-3.649818	-4.448814	L
C-CT--0.007000	0	5.547911	-2.876697	-1.657742	L
C-CT-0.018900	0	4.935610	-1.504958	-1.391199	L
C-CT-0.019200	0	5.440849	-0.680872	-2.564219	L
H-H1-0.064100	-1	7.704958	-2.595862	-1.640822	L
H-HC-0.025300	0	4.877722	-3.429984	-2.317534	L
H-HC-0.025300	0	5.697045	-3.437166	-0.739325	L
H-HC-0.021300	0	5.322870	-1.083429	-0.468218	L
H-HC-0.021300	0	3.849645	-1.533115	-1.354225	L
H-H1-0.039100	0	5.494943	0.364218	-2.258019	L
H-H1-0.039100	0	4.760505	-0.794731	-3.409739	L
N-N--0.415700	-1	8.155242	-4.450603	-3.321430	L
C-CT--0.149000	-1	8.522631	-5.447177	-4.340138	L
H-H-0.271900	-1	8.755182	-4.329136	-2.506611	L
H-H1-0.097600	-1	7.778579	-5.446072	-5.136030	L
H-H1-0.097600	-1	8.563278	-6.435934	-3.882132	L
H-H1-0.097600	-1	9.499367	-5.199466	-4.755756	L
C-CT--0.366200	-1	5.220731	-7.426696	-4.092900	L
C-C-0.597200	-1	4.091992	-6.754527	-4.884687	L
O-O--0.567900	-1	3.193031	-7.471513	-5.333657	L
H-HC-0.112300	-1	5.933792	-6.671228	-3.763586	L
H-HC-0.112300	-1	5.727621	-8.153708	-4.727269	L
H-HC-0.112300	-1	4.801668	-7.933028	-3.223270	L
N-N--0.415700	-1	4.081953	-5.423699	-5.023893	L
C-CT-0.014300	-1	2.980613	-4.674684	-5.653666	L H-HC 69
C-C-0.597300	-1	2.785177	-5.015059	-7.165862	L
O-O--0.567900	-1	3.779237	-5.180746	-7.874308	L
C-CT--0.204100	0	3.296084	-3.178438	-5.432406	H
C-C-0.713000	0	2.186921	-2.245864	-5.918004	H
O-O--0.593100	0	2.052509	-1.949128	-7.103415	H
N-N--0.919100	0	1.414684	-1.736502	-4.926698	H
H-H-0.271900	-1	4.851066	-4.887168	-4.656276	L
H-H1-0.104800	-1	2.072939	-4.937251	-5.119929	L
H-HC-0.079700	0	4.202544	-2.947368	-6.003414	H
H-HC-0.079700	0	3.492675	-3.022233	-4.368431	H
H-H-0.419600	0	0.565190	-1.289478	-5.242522	H
H-H-0.419600	0	1.479367	-2.053921	-3.953930	H
N-N--0.415700	-1	1.531319	-5.112552	-7.658828	L
C-CT--0.149000	-1	1.178669	-5.371846	-9.084468	L
H-H-0.271900	-1	0.776420	-4.886173	-7.012270	L
H-H1-0.097600	-1	2.083962	-5.597962	-9.647289	L
H-H1-0.097600	-1	0.699055	-4.488138	-9.506233	L
H-H1-0.097600	-1	0.494543	-6.218555	-9.139626	L

C-CT--0.366200	-1	11.716128	-5.939016	-0.641614	L
C-C-0.597200	-1	10.700546	-6.063942	0.502303	L
O-O--0.567900	-1	11.018055	-5.909431	1.686805	L
H-HC-0.112300	-1	11.214855	-6.113994	-1.593423	L
H-HC-0.112300	-1	12.507227	-6.676177	-0.506913	L
H-HC-0.112300	-1	12.148224	-4.938108	-0.637258	L
N-N--0.415700	-1	9.463519	-6.366291	0.111180	L
C-CT--0.023700	-1	8.303179	-6.562417	0.975293	L
C-C-0.597300	-1	7.247662	-7.404536	0.271240	L
O-O--0.567900	-1	7.069011	-7.245289	-0.943153	L
C-CT-0.034200	0	7.698580	-5.202826	1.366616	L
C-CT-0.001800	0	6.788317	-5.218955	2.610937	L
S-S--0.273700	0	5.070678	-5.791953	2.412010	L
C-CT--0.053600	0	4.216685	-4.235540	2.008091	L
H-H-0.271900	-1	9.294572	-6.439740	-0.885999	L
H-H1-0.088000	-1	8.627210	-7.094797	1.857901	L
H-HC-0.024100	0	7.152432	-4.785423	0.520925	L
H-HC-0.024100	0	8.531120	-4.538817	1.579784	L
H-H1-0.044000	0	6.740861	-4.203842	3.005718	L
H-H1-0.044000	0	7.266405	-5.833675	3.373544	L
H-H1-0.068400	0	3.160561	-4.427298	1.812978	L
H-H1-0.068400	0	4.655340	-3.779555	1.123733	L
H-H1-0.068400	0	4.295868	-3.535401	2.840270	L
N-N--0.415700	-1	6.538699	-8.249394	1.030279	L
C-CT--0.149000	-1	5.315908	-8.953890	0.616524	L
H-H-0.271900	-1	6.854857	-8.381352	1.991010	L
H-H1-0.097600	-1	5.098717	-8.722982	-0.425857	L
H-H1-0.097600	-1	4.482534	-8.632663	1.241561	L
H-H1-0.097600	-1	5.461000	-10.028027	0.728078	L
C-CT--0.366200	-1	3.881038	-9.352110	4.897864	L
C-C-0.597200	-1	3.714999	-7.946081	5.508753	L
O-O--0.567900	-1	4.677833	-7.231170	5.802056	L
H-HC-0.112300	-1	2.898288	-9.791600	4.724050	L
H-HC-0.112300	-1	4.444532	-9.983414	5.584673	L
H-HC-0.112300	-1	4.416892	-9.276439	3.951553	L
N-N--0.415700	-1	2.454066	-7.530042	5.656286	L
C-CT--0.087500	-1	2.019294	-6.124890	5.603956	L
C-C-0.597300	-1	1.898633	-5.566735	7.028367	L
O-O--0.567900	-1	0.861784	-5.658723	7.700816	L
C-CT-0.298500	0	0.696731	-5.952840	4.826571	L
C-CT--0.319200	0	0.347603	-4.469473	4.659397	L
C-CT--0.319200	0	0.780588	-6.592462	3.433213	L
H-H-0.271900	-1	1.717363	-8.222871	5.500145	L
H-H1-0.096900	-1	2.785686	-5.552818	5.077451	L
H-HC--0.029700	0	-0.109844	-6.445601	5.371095	L
H-HC-0.079100	0	1.093567	-3.964835	4.042028	L
H-HC-0.079100	0	0.282853	-3.967240	5.623683	L
H-HC-0.079100	0	-0.621829	-4.373111	4.172963	L
H-HC-0.079100	0	1.621960	-6.165461	2.885854	L
H-HC-0.079100	0	-0.135098	-6.377855	2.880237	L
H-HC-0.079100	0	0.895921	-7.670652	3.507411	L
N-N--0.415700	-1	3.059509	-5.115963	7.503296	L
C-CT--0.149000	-1	3.437211	-4.982335	8.907626	L
H-H-0.271900	-1	3.818613	-5.033730	6.837228	L

H-H1-0.097600	-1	2.550621	-5.086287	9.533291	L
H-H1-0.097600	-1	3.884699	-4.002786	9.072335	L
H-H1-0.097600	-1	4.156968	-5.759337	9.165394	L
C-CT--0.366200	-1	12.482132	-4.252184	6.335335	L
C-C-0.597200	-1	12.278377	-3.528374	4.985835	L
O-O--0.567900	-1	13.245594	-3.313375	4.248742	L
H-HC-0.112300	-1	11.522838	-4.350726	6.843422	L
H-HC-0.112300	-1	13.164461	-3.672996	6.958697	L
H-HC-0.112300	-1	12.902769	-5.241039	6.157616	L
N-N--0.415700	-1	11.043870	-3.099638	4.683943	L
C-CT--0.023700	-1	10.768241	-2.274175	3.510345	L
C-C-0.597300	-1	11.339587	-0.852594	3.647123	L
O-O--0.567900	-1	12.069113	-0.388458	2.769107	L
C-CT-0.034200	0	9.263100	-2.190673	3.246557	L
C-CT-0.001800	0	9.025411	-1.495907	1.899225	L
S-S--0.273700	0	7.464469	-1.907530	1.103832	L
C-CT--0.053600	0	6.265690	-1.085428	2.181081	L
H-H-0.271900	-1	10.278776	-3.327248	5.312582	L
H-H1-0.088000	-1	11.237246	-2.754379	2.649830	L
H-HC-0.024100	0	8.757477	-1.639227	4.040387	L
H-HC-0.024100	0	8.860847	-3.198773	3.222121	L
H-H1-0.044000	0	9.814890	-1.793000	1.207741	L
H-H1-0.044000	0	9.085639	-0.414456	2.029383	L
H-H1-0.068400	0	5.254145	-1.338794	1.860630	L
H-H1-0.068400	0	6.382867	-0.004151	2.107517	L
H-H1-0.068400	0	6.396200	-1.405391	3.212861	L
N-N--0.415700	-1	11.074395	-0.164286	4.762947	L
C-CT--0.149000	-1	11.631465	1.172655	4.992483	L
H-H-0.271900	-1	10.495454	-0.594083	5.483866	L
H-H1-0.097600	-1	12.219852	1.474183	4.125999	L
H-H1-0.097600	-1	12.269432	1.153445	5.875669	L
H-H1-0.097600	-1	10.819397	1.883270	5.146320	L
C-CT--0.366200	-1	6.205138	8.716091	-5.558235	L
C-C-0.597200	-1	6.517548	7.522599	-4.634013	L
O-O--0.567900	-1	6.665456	6.374004	-5.075264	L
H-HC-0.112300	-1	6.116361	9.624753	-4.961832	L
H-HC-0.112300	-1	5.266860	8.534043	-6.083540	L
H-HC-0.112300	-1	7.010322	8.835164	-6.283922	L
N-N--0.415700	-1	6.662830	7.836647	-3.336472	L
C-CT--0.001400	-1	6.702581	6.844242	-2.247047	L
C-C-0.597300	-1	5.325742	6.168530	-2.105360	L
O-O--0.567900	-1	4.454460	6.651062	-1.364532	L
C-CT--0.001400	-1	7.223123	7.475216	-0.942465	L
C-CA--0.001100	-1	7.906520	6.501458	0.011625	L
C-CA--0.190600	-1	9.314217	6.446886	0.060881	L
C-CA--0.190600	-1	7.158808	5.681988	0.882179	L
C-CA--0.234100	-1	9.963045	5.623811	1.000363	L
C-CA--0.234100	-1	7.811980	4.853812	1.821383	L
C-C-0.322600	-1	9.214467	4.847347	1.899052	L
O-OH--0.557900	-1	9.873442	4.099017	2.830441	L
H-H-0.271900	-1	6.601727	8.828567	-3.094004	L
H-H1-0.087600	-1	7.411148	6.070239	-2.528236	L
H-HC-0.029500	-1	7.950779	8.244555	-1.203657	L
H-HC-0.029500	-1	6.412760	7.984476	-0.419392	L

H-HA-0.169900	-1	9.901515	7.069414	-0.599073	L
H-HA-0.169900	-1	6.077775	5.691070	0.839662	L
H-HA-0.165600	-1	11.040245	5.591164	1.048538	L
H-HA-0.165600	-1	7.236137	4.222381	2.482072	L
H-HO-0.399200	-1	9.377022	3.876509	3.634109	L
N-N--0.415700	-1	5.110043	5.148787	-2.941062	L
C-CT-0.033700	-1	3.791602	4.658042	-3.327166	L
C-C-0.597300	-1	2.953918	4.023064	-2.206327	L
O-O--0.567900	-1	1.730782	4.127844	-2.273689	L
C-CT--0.182500	-1	3.976207	3.659635	-4.464815	L
H-H-0.271900	-1	5.891618	4.853905	-3.521334	L
H-H1-0.082300	-1	3.227779	5.504876	-3.719701	L
H-HC-0.060300	-1	3.003905	3.352317	-4.848944	L
H-HC-0.060300	-1	4.511430	2.789326	-4.084964	L
H-HC-0.060300	-1	4.547311	4.119572	-5.271425	L
N-N--0.415700	-1	3.567099	3.378539	-1.202864	L H-HC 209
C-CT-0.021300	0	2.865092	2.676247	-0.111529	H
C-C-0.597300	0	2.326269	3.700529	0.904131	H
O-O--0.567900	0	3.107478	4.508452	1.409273	H
C-CT--0.123100	0	3.939750	1.803521	0.554059	H
S-S--1.036000	0	3.302458	0.595869	1.775426	H
H-H-0.271900	-1	4.570861	3.350911	-1.196091	L
H-H1-0.112400	0	2.072195	2.055395	-0.537059	H
H-H1-0.111200	0	4.633203	2.438698	1.115352	H
H-H1-0.111200	0	4.524087	1.252925	-0.190011	H
N-N--0.415700	0	1.002435	3.640778	1.224255	H
C-CT--0.051800	0	0.432174	4.495607	2.281795	H
C-C-0.597300	0	0.814269	3.987689	3.704897	H
O-O--0.567900	0	1.354915	4.714676	4.537188	H
C-CT--0.110200	-1	-1.100833	4.643371	2.034994	H
C-CT-0.353100	-1	-1.956396	5.549054	2.947022	L H-HC 222
C-CT--0.412100	-1	-2.147315	5.001508	4.362964	L
C-CT--0.412100	-1	-1.422159	6.981447	3.036132	L
H-H-0.271900	0	0.442911	2.860987	0.856790	H
H-H1-0.092200	0	0.916020	5.472342	2.216503	H
H-HC-0.045700	0	-1.219809	5.021366	1.012733	H
H-HC-0.045700	0	-1.570297	3.654526	2.050344	H
H-HC--0.036100	-1	-2.948529	5.600109	2.499954	L
H-HC-0.100000	-1	-1.247253	5.139924	4.958337	L
H-HC-0.100000	-1	-2.394777	3.941784	4.321063	L
H-HC-0.100000	-1	-2.964712	5.535836	4.844806	L
H-HC-0.100000	-1	-0.459325	6.995236	3.547840	L
H-HC-0.100000	-1	-2.131775	7.601104	3.583017	L
H-HC-0.100000	-1	-1.298976	7.384685	2.030101	L
N-N--0.415700	0	0.555421	2.668727	3.967692	H
C-CT--0.087500	0	0.603994	2.152705	5.342116	H
C-C-0.597300	0	2.001679	2.106995	5.974001	H
O-O--0.567900	0	2.097668	2.034271	7.195260	H
C-CT-0.298500	-1	-0.018058	0.741307	5.375518	H
C-CT--0.319200	0	0.806758	-0.329679	4.635028	L H-HC 241
C-CT--0.319200	0	-0.358190	0.197892	6.763095	L H-HC 241
H-H-0.271900	0	0.072897	2.116162	3.262100	H
H-H1-0.096900	0	0.028877	2.829393	5.987430	H
H-HC--0.029700	0	-0.965485	0.809034	4.840773	H

H-HC-0.079100	0	1.691747	-0.605760	5.204224	L
H-HC-0.079100	0	1.129976	0.050888	3.664208	L
H-HC-0.079100	0	0.192239	-1.210660	4.457567	L
H-HC-0.079100	0	0.551779	-0.015528	7.322025	L
H-HC-0.079100	0	-0.934605	-0.720399	6.654866	L
H-HC-0.079100	0	-0.956173	0.931629	7.301032	L
N-N--0.415700	0	3.022938	1.936987	5.103003	H
C-CT-0.033700	0	4.388843	1.782041	5.558279	H
C-C-0.597300	-1	5.107376	3.109797	5.828591	L H-H1 254
O-O--0.567900	-1	6.282730	3.081910	6.183269	L
C-CT--0.182500	-1	5.160384	0.963962	4.521437	L H-H1 254
H-H-0.271900	0	2.863718	2.147876	4.129256	H
H-H1-0.082300	0	4.370368	1.235292	6.504677	H
H-HC-0.060300	-1	6.127031	0.668058	4.926368	L
H-HC-0.060300	-1	5.317620	1.566056	3.626778	L
H-HC-0.060300	-1	4.599607	0.063564	4.267384	L
N-N--0.415700	-1	4.407266	4.239948	5.666450	L
C-CT--0.087500	-1	4.794695	5.600964	6.064321	L
C-C-0.597300	-1	3.955568	6.049379	7.268024	L
O-O--0.567900	-1	4.510219	6.496842	8.272809	L
C-CT-0.298500	-1	4.581412	6.578492	4.891142	L
C-CT--0.319200	-1	4.980178	8.015486	5.244602	L
C-CT--0.319200	-1	5.396069	6.182058	3.660229	L
H-H-0.271900	-1	3.495171	4.128836	5.241217	L
H-H1-0.096900	-1	5.845044	5.626272	6.344586	L
H-HC--0.029700	-1	3.528632	6.569620	4.616528	L
H-HC-0.079100	-1	6.031128	8.049420	5.523388	L
H-HC-0.079100	-1	4.375992	8.393295	6.068688	L
H-HC-0.079100	-1	4.820478	8.656411	4.377859	L
H-HC-0.079100	-1	6.446271	6.100173	3.934380	L
H-HC-0.079100	-1	5.280725	6.931260	2.877384	L
H-HC-0.079100	-1	5.040361	5.226651	3.274528	L
N-N--0.415700	-1	2.623596	5.862877	7.215643	L
C-CT--0.149000	-1	1.718692	6.203617	8.324140	L
H-H-0.271900	-1	2.214634	5.484773	6.366579	L
H-H1-0.097600	-1	2.298575	6.595559	9.159805	L
H-H1-0.097600	-1	1.180462	5.309947	8.641596	L
H-H1-0.097600	-1	1.005409	6.958039	7.992328	L
C-CT--0.366200	-1	4.079813	10.304542	-0.983793	L
C-C-0.597200	-1	2.603711	9.982948	-1.227256	L
O-O--0.567900	-1	1.797011	10.900488	-1.297648	L
H-HC-0.112300	-1	4.652343	9.378652	-0.949880	L
H-HC-0.112300	-1	4.184317	10.831841	-0.035767	L
H-HC-0.112300	-1	4.452565	10.932925	-1.792322	L
N-N--0.415700	-1	2.220831	8.701295	-1.284336	L
C-CT--0.024900	-1	0.806495	8.323871	-1.124190	L
C-C-0.597300	-1	0.222715	8.821324	0.203866	L
O-O--0.567900	-1	-0.869926	9.392310	0.213822	L
C-CT-0.211700	0	0.632741	6.824464	-1.273765	L
O-OH--0.654600	0	0.919490	6.519415	-2.618535	L
H-H-0.271900	-1	2.920877	7.966509	-1.346766	L
H-H1-0.084300	-1	0.234532	8.776867	-1.929720	L
H-H1-0.035200	0	-0.391308	6.537691	-1.042876	L
H-H1-0.035200	0	1.315428	6.294113	-0.607932	L

H-HO-0.427500	0	1.026923	5.543700	-2.632900	L
N-N--0.415700	-1	0.985986	8.682893	1.298633	L
C-CT-0.033700	-1	0.635142	9.163442	2.636310	L
C-C-0.597300	-1	0.174981	10.626089	2.630245	L
O-O--0.567900	-1	-0.919928	10.947315	3.094670	L
C-CT--0.182500	-1	1.822016	8.921516	3.566444	L
H-H-0.271900	-1	1.872822	8.183935	1.191696	L
H-H1-0.082300	-1	-0.181061	8.573310	3.026143	L
H-HC-0.060300	-1	1.594360	9.291454	4.565494	L
H-HC-0.060300	-1	2.708654	9.420856	3.177935	L
H-HC-0.060300	-1	2.013926	7.851661	3.619187	L
N-N--0.415700	-1	0.975225	11.503438	2.014838	L
C-CT--0.149000	-1	0.638939	12.902335	1.824294	L
H-H-0.271900	-1	1.876402	11.193104	1.659692	L
H-H1-0.097600	-1	-0.346026	13.099882	2.248760	L
H-H1-0.097600	-1	0.628037	13.132216	0.759726	L
H-H1-0.097600	-1	1.380845	13.525881	2.324182	L
C-CT--0.366200	-1	-11.904626	4.615005	4.983839	L
C-C-0.597200	-1	-12.341959	3.197561	4.611082	L
O-O--0.567900	-1	-12.908403	2.490316	5.446692	L
H-HC-0.112300	-1	-11.424689	5.084404	4.125000	L
H-HC-0.112300	-1	-11.199714	4.571424	5.814207	L
H-HC-0.112300	-1	-12.776402	5.199150	5.276952	L
N-N--0.415700	-1	-12.010625	2.757155	3.397013	L
C-CT--0.087500	-1	-12.011241	1.335168	3.036074	L
C-C-0.597300	-1	-10.566717	0.936563	2.720243	L
O-O--0.567900	-1	-9.850380	1.579263	1.945014	L
C-CT-0.298500	-1	-13.009837	0.949370	1.912224	L
C-CT--0.319200	-1	-13.760600	-0.339119	2.296916	L
C-CT--0.319200	-1	-14.085267	2.000925	1.605484	L
H-H-0.271900	-1	-11.599149	3.407914	2.725454	L
H-H1-0.096900	-1	-12.304524	0.775557	3.921898	L
H-HC--0.029700	-1	-12.452631	0.759071	0.998618	L
H-HC-0.079100	-1	-14.391458	-0.156493	3.167538	L
H-HC-0.079100	-1	-13.046802	-1.133870	2.517303	L
H-HC-0.079100	-1	-14.399218	-0.651281	1.470788	L
H-HC-0.079100	-1	-14.717436	2.146075	2.478014	L
H-HC-0.079100	-1	-14.694776	1.667794	0.766879	L
H-HC-0.079100	-1	-13.625783	2.952156	1.345773	L
N-N--0.415700	-1	-10.105339	-0.085737	3.443302	L
C-CT--0.038900	-1	-8.698271	-0.487078	3.523295	L
C-C-0.597300	-1	-8.574436	-2.013042	3.634537	L
O-O--0.567900	-1	-9.506609	-2.671377	4.117575	L
C-CT-0.365400	-1	-7.978321	0.156704	4.732088	L
O-OH--0.676100	-1	-8.146815	-0.558853	5.934261	L
C-CT--0.243800	-1	-8.392387	1.593960	5.041824	L
H-H-0.271900	-1	-10.735378	-0.557572	4.075904	L
H-H1-0.100700	-1	-8.198152	-0.153936	2.613969	L
H-H1-0.004300	-1	-6.919552	0.153935	4.494457	L
H-HC-0.064200	-1	-8.435337	2.159846	4.118708	L
H-HC-0.064200	-1	-7.662165	2.048078	5.712955	L
H-HC-0.064200	-1	-9.375044	1.622632	5.511770	L
H-HO-0.410200	-1	-8.395703	0.080379	6.634105	L
N-N--0.254800	-1	-7.450537	-2.610451	3.199420	L

C-CT--0.026600	-1	-7.203360	-4.037379	3.367318	L
C-C-0.589600	-1	-6.594260	-4.394940	4.724312	L
O-O--0.574800	-1	-6.608136	-5.566190	5.085882	L
C-CT--0.007000	0	-6.229723	-4.397087	2.249656	L
C-CT-0.018900	0	-5.392849	-3.133579	2.102712	L
C-CT-0.019200	0	-6.381515	-2.007252	2.414925	L
H-H1-0.064100	-1	-8.114999	-4.605205	3.223214	L
H-HC-0.025300	0	-5.614702	-5.256126	2.510602	L
H-HC-0.025300	0	-6.781602	-4.583888	1.327547	L
H-HC-0.021300	0	-4.997349	-3.056451	1.093783	L
H-HC-0.021300	0	-4.583273	-3.135570	2.832810	L
H-H1-0.039100	0	-6.787483	-1.616230	1.481645	L
H-H1-0.039100	0	-5.879928	-1.215418	2.972653	L
N-N--0.415700	-1	-5.972417	-3.435606	5.417912	L
C-CT--0.001400	-1	-4.980318	-3.680129	6.476271	L
C-C-0.597300	-1	-5.528898	-4.463375	7.683413	L
O-O--0.567900	-1	-6.714708	-4.344374	7.995824	L
C-CT--0.001400	0	-4.462427	-2.336987	7.006171	L H-HA 373
C-CA--0.001100	0	-4.082772	-1.331604	5.939535	H
C-CA--0.190600	0	-3.219249	-1.697786	4.904989	H
C-CA--0.190600	0	-4.590377	-0.030361	5.979031	H
C-CA--0.234100	0	-2.862318	-0.781326	3.926404	H
C-CA--0.234100	0	-4.230708	0.903315	5.010718	H
C-C-0.322600	0	-3.349921	0.536468	3.984875	H
O-OH--0.557900	0	-2.987354	1.472950	3.083241	H
H-H-0.271900	-1	-6.037863	-2.496224	5.057392	L
H-H1-0.087600	-1	-4.157456	-4.250321	6.043723	L
H-HC-0.029500	0	-5.235840	-1.895240	7.637145	L
H-HC-0.029500	0	-3.588065	-2.516671	7.632949	L
H-HA-0.169900	0	-2.817194	-2.706582	4.842065	H
H-HA-0.169900	0	-5.268044	0.271945	6.778515	H
H-HA-0.165600	0	-2.161442	-1.053741	3.148903	H
H-HA-0.165600	0	-4.584133	1.930116	5.064289	H
H-HO-0.399200	0	-2.157391	1.182429	2.603952	H
N-N--0.415700	-1	-4.651047	-5.156010	8.435610	L
C-CT--0.149000	-1	-5.035044	-5.622738	9.784287	L
H-H-0.271900	-1	-3.656586	-5.151254	8.194778	L
H-H1-0.097600	-1	-6.118529	-5.570035	9.891959	L
H-H1-0.097600	-1	-4.563649	-4.990528	10.535993	L
H-H1-0.097600	-1	-4.706172	-6.653486	9.918808	L
C-CT--0.366200	-1	-0.493618	-10.774029	2.462352	L
C-C-0.597200	-1	-0.673495	-9.831849	1.258784	L
O-O--0.567900	-1	-1.783189	-9.654446	0.751416	L
H-HC-0.112300	-1	0.554673	-10.790846	2.757011	L
H-HC-0.112300	-1	-0.809891	-11.780211	2.186026	L
H-HC-0.112300	-1	-1.100424	-10.419724	3.295635	L
N-N--0.415700	-1	0.441410	-9.287361	0.754442	L
C-CT-0.014300	-1	0.398734	-8.268683	-0.293999	L H-HC 405
C-C-0.597300	-1	0.022390	-8.774158	-1.705508	L
O-O--0.567900	-1	-0.187936	-7.950010	-2.586119	L
C-CT--0.204100	0	1.727435	-7.477013	-0.318342	H
C-C-0.713000	0	1.491231	-5.970616	-0.506342	H
O-O--0.593100	0	0.964676	-5.340880	0.416888	H
N-N--0.919100	0	1.934481	-5.389932	-1.635747	H

H-H-0.271900	-1	1.324278	-9.477599	1.199430	L
H-H1-0.104800	-1	-0.402012	-7.594942	0.011429	L
H-HC-0.079700	0	2.395125	-7.912974	-1.071482	H
H-HC-0.079700	0	2.208060	-7.564166	0.659451	H
H-H-0.419600	0	1.816072	-4.368116	-1.787771	H
H-H-0.419600	0	2.251184	-5.961215	-2.408449	H
N-N--0.415700	-1	-0.077383	-10.086966	-1.944326	L
C-CT--0.149000	-1	-0.620288	-10.635232	-3.199339	L
H-H-0.271900	-1	0.031772	-10.737354	-1.158140	L
H-H1-0.097600	-1	-0.683694	-9.843420	-3.945033	L
H-H1-0.097600	-1	-1.614504	-11.043617	-3.017859	L
H-H1-0.097600	-1	0.035635	-11.426792	-3.563908	L
C-CT--0.366200	-1	-3.891694	-11.686523	-1.430176	L
C-C-0.597200	-1	-4.655337	-10.357974	-1.500291	L
O-O--0.567900	-1	-5.794680	-10.357006	-1.970583	L
H-HC-0.112300	-1	-2.907512	-11.516241	-0.992783	L
H-HC-0.112300	-1	-3.776958	-12.093203	-2.433951	L
H-HC-0.112300	-1	-4.446369	-12.392074	-0.811999	L
N-N--0.415700	-1	-4.024291	-9.232937	-1.124544	L
C-CT--0.087500	-1	-4.584447	-7.870123	-1.285982	L
C-C-0.597300	-1	-4.849455	-7.485695	-2.752767	L
O-O--0.567900	-1	-5.836456	-6.812831	-3.046947	L
C-CT-0.298500	-1	-3.673572	-6.796742	-0.634391	L
C-CT--0.319200	-1	-4.156649	-5.357180	-0.873274	L
C-CT--0.319200	-1	-3.657495	-6.934751	0.885564	L
H-H-0.271900	-1	-3.142274	-9.346819	-0.623145	L
H-H1-0.096900	-1	-5.544858	-7.845851	-0.772447	L
H-HC--0.029700	-1	-2.658610	-6.897588	-1.019296	L
H-HC-0.079100	-1	-5.191974	-5.257776	-0.546357	L
H-HC-0.079100	-1	-4.088610	-5.104838	-1.928850	L
H-HC-0.079100	-1	-3.527067	-4.652253	-0.328246	L
H-HC-0.079100	-1	-4.663339	-6.797224	1.265046	L
H-HC-0.079100	-1	-2.991138	-6.191390	1.325495	L
H-HC-0.079100	-1	-3.311136	-7.913424	1.186469	L
N-N--0.415700	-1	-4.004660	-7.887218	-3.710776	L
C-CT--0.149000	-1	-4.090176	-7.471526	-5.121555	L
H-H-0.271900	-1	-3.284767	-8.552680	-3.455026	L
H-H1-0.097600	-1	-4.906237	-6.758560	-5.241921	L
H-H1-0.097600	-1	-4.275671	-8.345034	-5.748169	L
H-H1-0.097600	-1	-3.152597	-7.003459	-5.420222	L
C-CT--0.366200	-1	-12.102015	3.720551	-1.312147	L
C-C-0.597200	-1	-11.001112	2.651031	-1.277244	L
O-O--0.567900	-1	-11.297797	1.468898	-1.122781	L
H-HC-0.112300	-1	-11.650626	4.702270	-1.455970	L
H-HC-0.112300	-1	-12.651802	3.707891	-0.370650	L
H-HC-0.112300	-1	-12.786512	3.510994	-2.134374	L
N-N--0.415700	-1	-9.743237	3.087919	-1.345377	L
C-CT--0.024900	-1	-8.562969	2.262030	-1.167041	L
C-C-0.597300	-1	-7.447506	3.123821	-0.570078	L
O-O--0.567900	-1	-6.792675	3.910429	-1.268324	L
C-CT-0.211700	0	-8.128490	1.600294	-2.472867	L
O-OH--0.654600	0	-7.162348	0.633809	-2.155630	L
H-H-0.271900	-1	-9.613734	4.084017	-1.415115	L
H-H1-0.084300	-1	-8.802540	1.469954	-0.458928	L

H-H1-0.035200	0	-7.718777	2.329487	-3.168880	L
H-H1-0.035200	0	-8.985111	1.102255	-2.929215	L
H-HO-0.427500	0	-6.260262	1.012449	-2.258578	L
N-N--0.415700	-1	-7.284718	3.048835	0.759734	L
C-CT-0.021300	-1	-6.107364	3.660213	1.394923	L
C-C-0.597300	-1	-4.821361	3.009743	0.860099	L
O-O--0.567900	-1	-3.844429	3.695052	0.599490	L
C-CT--0.123100	-1	-6.164554	3.523321	2.917972	L
S-SH--0.311900	-1	-7.414263	4.633247	3.626993	L
H-H-0.271900	-1	-7.947014	2.504100	1.308796	L
H-H1-0.112400	-1	-6.075707	4.722248	1.146594	L
H-H1-0.111200	-1	-5.192306	3.793194	3.333816	L
H-H1-0.111200	-1	-6.383767	2.489173	3.182466	L
H-HS-0.193300	-1	-8.458273	4.188866	2.918156	L
N-N--0.415700	-1	-4.863916	1.691161	0.653437	L H-HC 478
C-CT-0.021300	0	-3.736175	0.934835	0.088150	H
C-C-0.597300	0	-3.628180	1.249936	-1.396904	H
O-O--0.567900	0	-4.652898	1.441381	-2.059788	H
C-CT--0.123100	0	-4.074322	-0.538963	0.341961	H
S-SH--0.311900	0	-2.767384	-1.759196	-0.053211	H
H-H-0.271900	-1	-5.716330	1.205484	0.859583	L
H-H1-0.112400	0	-2.822792	1.211811	0.615515	H
H-H1-0.111200	0	-4.934975	-0.838855	-0.264032	H
H-H1-0.111200	0	-4.328711	-0.680144	1.391832	H
H-HS-0.193300	0	-1.972082	-1.503526	0.994436	H
N-N--0.415700	0	-2.379035	1.271550	-1.942025	H
C-CT--0.087500	0	-2.259265	1.393417	-3.390646	H
C-C-0.597300	0	-2.281622	0.041988	-4.158798	H
O-O--0.567900	0	-2.594254	0.065110	-5.347984	H
C-CT-0.298500	-1	-1.110820	2.302912	-3.872440	H
C-CT--0.319200	0	-1.224528	3.699408	-3.258083	L H-HC 492
C-CT--0.319200	0	0.287968	1.754410	-3.567033	L H-HC 492
H-H-0.271900	0	-1.563630	1.058667	-1.367364	H
H-H1-0.096900	0	-3.203834	1.844138	-3.709910	H
H-HC--0.029700	0	-1.206087	2.391369	-4.958494	H
H-HC-0.079100	0	-1.043754	3.653644	-2.181903	L
H-HC-0.079100	0	-2.218910	4.093300	-3.444498	L
H-HC-0.079100	0	-0.494120	4.361867	-3.718536	L
H-HC-0.079100	0	0.447147	1.710568	-2.486991	L
H-HC-0.079100	0	1.039311	2.396980	-4.014783	L
H-HC-0.079100	0	0.402156	0.757747	-3.985555	L
N-N--0.415700	0	-1.976478	-1.075075	-3.448530	H
C-CT--0.003100	0	-2.058612	-2.413724	-4.028910	H
C-C-0.597300	0	-3.522709	-2.867543	-4.191472	H
O-O--0.567900	0	-3.830763	-3.657559	-5.077592	H
C-CT--0.003600	-1	-1.305046	-3.438264	-3.119621	H
C-CT--0.064500	-1	-1.442206	-4.891793	-3.610878	L H-HC 508
C-C-0.695100	-1	-0.570673	-5.231941	-4.805093	L
O-O--0.608600	-1	-0.427364	-4.480659	-5.754754	L
N-N--0.940700	-1	0.039878	-6.397410	-4.801238	L
H-H-0.271900	0	-1.419927	-0.977897	-2.600457	H
H-H1-0.085000	0	-1.647408	-2.409901	-5.043779	H
H-HC-0.017100	0	-0.247099	-3.190168	-3.052858	H
H-HC-0.017100	0	-1.732191	-3.385111	-2.115280	H

H-HC-0.035200	-1	-2.471230	-5.143913	-3.851192	L
H-HC-0.035200	-1	-1.158031	-5.540955	-2.790067	L
H-H-0.425100	-1	0.641723	-6.646764	-5.566424	L
H-H-0.425100	-1	-0.070764	-7.018598	-4.001690	L
N-N--0.415700	0	-4.354313	-2.489862	-3.160085	H
C-CT--0.023700	0	-5.741587	-2.929582	-3.233795	H
C-C-0.597300	-1	-6.418635	-2.306680	-4.471488	L H-H1 522
O-O--0.567900	-1	-6.245072	-1.111678	-4.729456	L
C-CT-0.034200	-1	-6.477348	-2.649014	-1.905202	L H-H1 522
C-CT-0.001800	-1	-7.946947	-3.094437	-1.960920	L
S-S--0.273700	-1	-8.849092	-3.067334	-0.384506	L
C-CT--0.053600	-1	-9.213223	-1.298617	-0.251330	L
H-H-0.271900	0	-4.216150	-1.547427	-2.831197	H
H-H1-0.088000	0	-5.687449	-4.007383	-3.348643	H
H-HC-0.024100	-1	-6.404114	-1.602990	-1.644706	L
H-HC-0.024100	-1	-5.984411	-3.203411	-1.110148	L
H-H1-0.044000	-1	-7.975019	-4.119665	-2.331341	L
H-H1-0.044000	-1	-8.486363	-2.466101	-2.669986	L
H-H1-0.068400	-1	-9.817402	-1.113025	0.636648	L
H-H1-0.068400	-1	-9.763624	-0.967204	-1.132084	L
H-H1-0.068400	-1	-8.281848	-0.740964	-0.180246	L
N-N--0.254800	-1	-7.170299	-3.073435	-5.283066	L
C-CT--0.026600	-1	-7.567855	-2.654512	-6.628050	L
C-C-0.589600	-1	-9.016422	-2.167433	-6.617482	L
O-O--0.574800	-1	-9.903527	-2.866146	-6.120431	L
C-CT--0.007000	-1	-7.365465	-3.897967	-7.508380	L
C-CT-0.018900	-1	-6.850257	-4.962834	-6.536893	L
C-CT-0.019200	-1	-7.379826	-4.502702	-5.205076	L
H-H1-0.064100	-1	-6.919094	-1.858692	-6.993437	L
H-HC-0.025300	-1	-8.301147	-4.216124	-7.959162	L
H-HC-0.025300	-1	-6.630520	-3.714365	-8.289856	L
H-HC-0.021300	-1	-5.762102	-4.957241	-6.512037	L
H-HC-0.021300	-1	-7.226808	-5.944249	-6.753364	L
H-H1-0.039100	-1	-6.855731	-5.012648	-4.408470	L
H-H1-0.039100	-1	-8.445696	-4.720966	-5.129551	L
N-N--0.415700	-1	-9.237836	-0.969780	-7.152776	L
C-CT--0.149000	-1	-10.469472	-0.198064	-6.960473	L
H-H-0.271900	-1	-8.432586	-0.501663	-7.567952	L
H-H1-0.097600	-1	-11.230485	-0.834849	-6.509976	L
H-H1-0.097600	-1	-10.823702	0.165095	-7.925191	L
H-H1-0.097600	-1	-10.267974	0.648637	-6.303877	L
C-CT--0.366200	-1	-10.330471	8.879270	-4.219122	L
C-C-0.597200	-1	-9.783617	7.588653	-3.594787	L
O-O--0.567900	-1	-10.225571	7.168658	-2.523994	L
H-HC-0.112300	-1	-9.812819	9.076853	-5.157691	L
H-HC-0.112300	-1	-10.168992	9.710478	-3.533278	L
H-HC-0.112300	-1	-11.397588	8.767182	-4.409981	L
N-N--0.415700	-1	-8.814889	6.964688	-4.259654	L
C-CT--0.024900	-1	-7.871604	6.043956	-3.621718	L
C-C-0.597300	-1	-6.540262	6.773085	-3.401621	L
O-O--0.567900	-1	-6.284334	7.780491	-4.068558	L
C-CT-0.211700	0	-7.652585	4.786725	-4.476047	L
O-OH--0.654600	0	-7.269560	5.090107	-5.803796	L
H-H-0.271900	-1	-8.544609	7.333780	-5.170363	L

H-H1-0.084300	-1	-8.256911	5.704620	-2.659856	L
H-H1-0.035200	0	-8.576461	4.207454	-4.498350	L
H-H1-0.035200	0	-6.873652	4.177638	-4.014952	L
H-HO-0.427500	0	-6.835224	4.313241	-6.176479	L
N-N--0.415700	-1	-5.662422	6.238830	-2.542069	L
C-CT-0.033700	-1	-4.287502	6.744779	-2.440117	L
C-C-0.597300	-1	-3.541678	6.749142	-3.793545	L
O-O--0.567900	-1	-2.641088	7.561299	-4.011081	L
C-CT--0.182500	-1	-3.534162	5.920899	-1.405940	L
H-H-0.271900	-1	-5.946131	5.433713	-1.978827	L
H-H1-0.082300	-1	-4.332386	7.771938	-2.076620	L
H-HC-0.060300	-1	-2.519677	6.300197	-1.301692	L
H-HC-0.060300	-1	-3.501596	4.875076	-1.709513	L
H-HC-0.060300	-1	-4.048272	6.004469	-0.449713	L
N-N--0.415700	-1	-3.966017	5.884199	-4.728581	L
C-CT--0.149000	-1	-3.453034	5.830941	-6.096381	L
H-H-0.271900	-1	-4.695432	5.236695	-4.461144	L
H-H1-0.097600	-1	-2.678240	6.587436	-6.223201	L
H-H1-0.097600	-1	-4.265049	6.023380	-6.797457	L
H-H1-0.097600	-1	-3.032661	4.843815	-6.288450	L
C-CM--0.139000	0	0.961847	-1.947699	0.034102	H
C-C-0.519000	0	1.005234	-1.732930	-1.456742	H
O-O2--0.567000	0	0.381423	-0.781940	-1.966661	H
C-CM--0.117000	0	0.507421	-1.151781	1.021213	H
O-O2--0.618000	0	1.682475	-2.609543	-2.110755	H
C-C--0.553000	0	-0.092230	0.240328	1.055154	H
O-O2--0.556000	0	0.117764	1.100587	0.169566	H
O-O2--0.607000	0	-0.807495	0.431634	2.105300	H
H-HC-0.049000	0	1.306584	-2.933917	0.336777	H
H-HC-0.162000	0	0.505996	-1.606438	2.007770	H
O-OW--0.834000	-1	6.447396	2.944769	-1.181083	L
H-HW-0.417000	-1	6.817779	3.086288	-2.051511	L
H-HW-0.417000	-1	7.128008	3.243348	-0.578274	L
O-OW--0.834000	0	3.437783	7.107492	1.054031	L
H-HW-0.417000	0	3.269960	6.205097	1.396860	L
H-HW-0.417000	0	3.814710	6.909421	0.179733	L
O-OW--0.834000	0	-1.282520	-4.019473	1.706773	H
H-HW-0.417000	0	-0.567740	-4.450409	1.207368	H
H-HW-0.417000	0	-2.024014	-3.993701	1.085601	H
O-OW--0.834000	0	-5.181442	1.027258	-6.021895	L
H-HW-0.417000	0	-4.239442	0.805116	-5.948140	L
H-HW-0.417000	0	-5.599574	0.320686	-5.499428	L
H-HS-0.193300	0	2.557303	-0.147129	0.935827	H

TS1

C-CT--0.366200	-1	8.234350	4.613130	-8.140860	L
C-C-0.597200	-1	9.062106	3.866128	-7.100380	L
O-O--0.567900	-1	9.658719	2.826016	-7.380902	L
H-HC-0.112300	-1	7.794530	5.501060	-7.686890	L
H-HC-0.112300	-1	7.440558	3.962567	-8.509621	L
H-HC-0.112300	-1	8.875693	4.910026	-8.971558	L
N-N--0.415700	-1	9.059275	4.425643	-5.883954	L
C-CT--0.087500	-1	9.528321	3.749506	-4.667345	L
C-C-0.597300	-1	8.387612	2.856878	-4.174583	L

O-O--0.567900	-1	7.478439	3.320826	-3.471315	L
C-CT-0.298500	-1	10.014597	4.750930	-3.592571	L
C-CT--0.319200	-1	10.431839	4.051347	-2.293434	L
C-CT--0.319200	-1	11.231944	5.553968	-4.073356	L
H-H-0.271900	-1	8.477177	5.250051	-5.757395	L
H-H1-0.096900	-1	10.363518	3.105013	-4.921077	L
H-HC--0.029700	-1	9.220078	5.459704	-3.376709	L
H-HC-0.079100	-1	11.134796	3.249725	-2.521909	L
H-HC-0.079100	-1	9.560025	3.631846	-1.795150	L
H-HC-0.079100	-1	10.911129	4.758416	-1.618227	L
H-HC-0.079100	-1	12.089881	4.893978	-4.201550	L
H-HC-0.079100	-1	11.481014	6.324741	-3.341875	L
H-HC-0.079100	-1	11.015250	6.033356	-5.026999	L
N-N--0.415700	-1	8.399492	1.583782	-4.605111	L
C-CT--0.087500	-1	7.283062	0.635913	-4.429103	L
C-C-0.597300	-1	7.694514	-0.640495	-3.666812	L
O-O--0.567900	-1	8.838825	-1.096326	-3.791019	L
C-CT-0.298500	-1	6.628025	0.230002	-5.773794	L
C-CT--0.319200	-1	5.774339	1.359060	-6.362789	L
C-CT--0.319200	-1	7.619024	-0.225468	-6.850161	L
H-H-0.271900	-1	9.173582	1.274543	-5.198879	L
H-H1-0.096900	-1	6.514006	1.146156	-3.856205	L
H-HC--0.029700	-1	5.955883	-0.608243	-5.586671	L
H-HC-0.079100	-1	6.294990	2.313618	-6.287818	L
H-HC-0.079100	-1	4.839492	1.410613	-5.809189	L
H-HC-0.079100	-1	5.525159	1.143848	-7.403169	L
H-HC-0.079100	-1	8.222415	0.616630	-7.185021	L
H-HC-0.079100	-1	7.067968	-0.627403	-7.699372	L
H-HC-0.079100	-1	8.270601	-1.000470	-6.454646	L
N-N--0.254800	-1	6.756358	-1.243003	-2.898417	L
C-CT--0.026600	-1	6.883614	-2.596001	-2.350336	L
C-C-0.589600	-1	7.128097	-3.621359	-3.459269	L
O-O--0.574800	-1	6.381074	-3.667296	-4.439687	L
C-CT--0.007000	0	5.550797	-2.888581	-1.643730	L
C-CT-0.018900	0	4.968621	-1.508599	-1.362322	L
C-CT-0.019200	0	5.449041	-0.691079	-2.547297	L
H-H1-0.064100	-1	7.702024	-2.613449	-1.631466	L
H-HC-0.025300	0	4.867960	-3.423381	-2.305855	L
H-HC-0.025300	0	5.699224	-3.460314	-0.732144	L
H-HC-0.021300	0	5.381118	-1.086586	-0.452325	L
H-HC-0.021300	0	3.890061	-1.527598	-1.296513	L
H-H1-0.039100	0	5.506734	0.355722	-2.247554	L
H-H1-0.039100	0	4.755561	-0.812076	-3.381104	L
N-N--0.415700	-1	8.149972	-4.470725	-3.309899	L
C-CT--0.149000	-1	8.516212	-5.469034	-4.327319	L
H-H-0.271900	-1	8.749410	-4.349743	-2.494638	L
H-H1-0.097600	-1	7.772902	-5.467123	-5.123902	L
H-H1-0.097600	-1	8.554360	-6.457437	-3.868338	L
H-H1-0.097600	-1	9.493852	-5.223765	-4.742264	L
C-CT--0.366200	-1	5.209940	-7.441388	-4.081271	L
C-C-0.597200	-1	4.083345	-6.767603	-4.874742	L
O-O--0.567900	-1	3.183298	-7.483131	-5.323869	L
H-HC-0.112300	-1	5.924277	-6.687105	-3.752012	L
H-HC-0.112300	-1	5.715890	-8.170064	-4.714481	L

H-HC-0.112300	-1	4.789009	-7.946014	-3.211550	L
N-N--0.415700	-1	4.076229	-5.436892	-5.015218	L
C-CT-0.014300	-1	2.977033	-4.686172	-5.646728	L H-HC 69
C-C-0.597300	-1	2.782299	-5.027568	-7.158778	L
O-O--0.567900	-1	3.776666	-5.196011	-7.866143	L
C-CT--0.204100	0	3.288444	-3.188748	-5.424806	H
C-C-0.713000	0	2.180493	-2.260013	-5.919984	H
O-O--0.593100	0	2.035396	-1.984612	-7.109027	H
N-N--0.919100	0	1.411149	-1.731721	-4.935208	H
H-H-0.271900	-1	4.846126	-4.901626	-4.647395	L
H-H1-0.104800	-1	2.068330	-4.946320	-5.113582	L
H-HC-0.079700	0	4.197709	-2.956500	-5.990464	H
H-HC-0.079700	0	3.478962	-3.029939	-4.360183	H
H-H-0.419600	0	0.575859	-1.267727	-5.264491	H
H-H-0.419600	0	1.494640	-2.013233	-3.952840	H
N-N--0.415700	-1	1.528696	-5.122899	-7.652817	L
C-CT--0.149000	-1	1.176824	-5.382806	-9.078535	L
H-H-0.271900	-1	0.773677	-4.894324	-7.007172	L
H-H1-0.097600	-1	2.082162	-5.611355	-9.640302	L
H-H1-0.097600	-1	0.699457	-4.498495	-9.501583	L
H-H1-0.097600	-1	0.490976	-6.228132	-9.133525	L
C-CT--0.366200	-1	11.705243	-5.964055	-0.625366	L
C-C-0.597200	-1	10.688341	-6.085765	0.517726	L
O-O--0.567900	-1	11.005077	-5.930796	1.702373	L
H-HC-0.112300	-1	11.204486	-6.138886	-1.577475	L
H-HC-0.112300	-1	12.494666	-6.702748	-0.489233	L
H-HC-0.112300	-1	12.139434	-4.964051	-0.621558	L
N-N--0.415700	-1	9.451047	-6.385891	0.125740	L
C-CT--0.023700	-1	8.289498	-6.578761	0.988960	L
C-C-0.597300	-1	7.232869	-7.419334	0.284728	L
O-O--0.567900	-1	7.055678	-7.260867	-0.929983	L
C-CT-0.034200	0	7.687335	-5.216441	1.375639	L
C-CT-0.001800	0	6.745381	-5.229050	2.596563	L
S-S--0.273700	0	5.023274	-5.768733	2.345269	L
C-CT--0.053600	0	4.192251	-4.185223	1.996155	L
H-H-0.271900	-1	9.282868	-6.459933	-0.871524	L
H-H1-0.088000	-1	8.611591	-7.110981	1.872374	L
H-HC-0.024100	0	7.166000	-4.789458	0.519225	L
H-HC-0.024100	0	8.520596	-4.561476	1.612326	L
H-H1-0.044000	0	6.706044	-4.217463	3.001333	L
H-H1-0.044000	0	7.192179	-5.860532	3.364392	L
H-H1-0.068400	0	3.140771	-4.356753	1.759646	L
H-H1-0.068400	0	4.659738	-3.686241	1.150499	L
H-H1-0.068400	0	4.250583	-3.528312	2.864453	L
N-N--0.415700	-1	6.521430	-8.261980	1.043908	L
C-CT--0.149000	-1	5.297548	-8.964304	0.629685	L
H-H-0.271900	-1	6.836420	-8.393690	2.005057	L
H-H1-0.097600	-1	5.081809	-8.733932	-0.413116	L
H-H1-0.097600	-1	4.464271	-8.640737	1.253643	L
H-H1-0.097600	-1	5.440282	-10.038636	0.742392	L
C-CT--0.366200	-1	3.857878	-9.355446	4.910066	L
C-C-0.597200	-1	3.694225	-7.948494	5.519468	L
O-O--0.567900	-1	4.658285	-7.235325	5.812988	L
H-HC-0.112300	-1	2.874370	-9.793040	4.735756	L

H-HC-0.112300	-1	4.419411	-9.987279	5.597997	L
H-HC-0.112300	-1	4.394767	-9.281798	3.964182	L
N-N--0.415700	-1	2.434032	-7.529672	5.665435	L
C-CT--0.087500	-1	2.002258	-6.123660	5.611371	L
C-C-0.597300	-1	1.881449	-5.563903	7.035139	L
O-O--0.567900	-1	0.843785	-5.653078	7.706712	L
C-CT-0.298500	0	0.686181	-5.944269	4.823696	L
C-CT--0.319200	0	0.347385	-4.458705	4.652424	L
C-CT--0.319200	0	0.777979	-6.580078	3.428673	L
H-H-0.271900	-1	1.696022	-8.221101	5.509267	L
H-H1-0.096900	-1	2.770336	-5.553699	5.085036	L
H-HC--0.029700	0	-0.127359	-6.433332	5.361138	L
H-HC-0.079100	0	1.113939	-3.953461	4.061039	L
H-HC-0.079100	0	0.256033	-3.961545	5.617212	L
H-HC-0.079100	0	-0.605337	-4.353452	4.134950	L
H-HC-0.079100	0	1.614367	-6.142552	2.881338	L
H-HC-0.079100	0	-0.139591	-6.373173	2.875962	L
H-HC-0.079100	0	0.903938	-7.657227	3.499739	L
N-N--0.415700	-1	3.042828	-5.115114	7.510718	L
C-CT--0.149000	-1	3.419507	-4.980944	8.915273	L
H-H-0.271900	-1	3.802719	-5.035107	6.845278	L
H-H1-0.097600	-1	2.532120	-5.082445	9.540211	L
H-H1-0.097600	-1	3.868897	-4.002180	9.079466	L
H-H1-0.097600	-1	4.137394	-5.759210	9.174443	L
C-CT--0.366200	-1	12.468319	-4.272209	6.350689	L
C-C-0.597200	-1	12.267334	-3.549255	5.000315	L
O-O--0.567900	-1	13.235683	-3.336987	4.263916	L
H-HC-0.112300	-1	11.508350	-4.368257	6.857977	L
H-HC-0.112300	-1	13.151283	-3.693860	6.974135	L
H-HC-0.112300	-1	12.887046	-5.262112	6.174298	L
N-N--0.415700	-1	11.034010	-3.118220	4.696869	L
C-CT--0.023700	-1	10.761200	-2.293295	3.522236	L
C-C-0.597300	-1	11.335401	-0.872783	3.658195	L
O-O--0.567900	-1	12.066712	-0.411015	2.780417	L
C-CT-0.034200	0	9.254930	-2.206899	3.262615	L
C-CT-0.001800	0	9.014166	-1.521972	1.911644	L
S-S--0.273700	0	7.439907	-1.921405	1.137074	L
C-CT--0.053600	0	6.259498	-1.026873	2.178988	L
H-H-0.271900	-1	10.267858	-3.343625	5.325014	L
H-H1-0.088000	-1	11.229993	-2.775297	2.662611	L
H-HC-0.024100	0	8.753246	-1.648000	4.053745	L
H-HC-0.024100	0	8.848173	-3.213609	3.247064	L
H-H1-0.044000	0	9.792479	-1.838388	1.216123	L
H-H1-0.044000	0	9.091050	-0.440156	2.029131	L
H-H1-0.068400	0	5.240173	-1.234068	1.846208	L
H-H1-0.068400	0	6.429572	0.046180	2.093299	L
H-H1-0.068400	0	6.358579	-1.339163	3.216583	L
N-N--0.415700	-1	11.070620	-0.182862	4.773120	L
C-CT--0.149000	-1	11.630282	1.153124	5.001907	L
H-H-0.271900	-1	10.490112	-0.610762	5.493909	L
H-H1-0.097600	-1	12.220102	1.452595	4.135682	L
H-H1-0.097600	-1	12.267388	1.133414	5.885702	L
H-H1-0.097600	-1	10.819564	1.865587	5.154315	L
C-CT--0.366200	-1	6.229570	8.697902	-5.560992	L

C-C-0.597200	-1	6.538621	7.504634	-4.635349	L
O-O--0.567900	-1	6.684527	6.355313	-5.075374	L
H-HC-0.112300	-1	6.142149	9.607313	-4.965531	L
H-HC-0.112300	-1	5.291400	8.517322	-6.086995	L
H-HC-0.112300	-1	7.035676	8.814595	-6.286045	L
N-N--0.415700	-1	6.683359	7.819608	-3.337972	L
C-CT--0.001400	-1	6.720018	6.828158	-2.247571	L
C-C-0.597300	-1	5.341632	6.155470	-2.106522	L
O-O--0.567900	-1	4.470680	6.640531	-1.366959	L
C-CT--0.001400	-1	7.240672	7.459277	-0.943103	L
C-CA--0.001100	-1	7.921143	6.484995	0.012543	L
C-CA--0.190600	-1	9.328676	6.427516	0.063157	L
C-CA--0.190600	-1	7.170905	5.667923	0.883179	L
C-CA--0.234100	-1	9.974904	5.603976	1.004022	L
C-CA--0.234100	-1	7.821467	4.839270	1.823773	L
C-C-0.322600	-1	9.223866	4.829939	1.902752	L
O-OH--0.557900	-1	9.880405	4.081110	2.835460	L
H-H-0.271900	-1	6.624113	8.811883	-3.096501	L
H-H1-0.087600	-1	7.427220	6.052404	-2.527368	L
H-HC-0.029500	-1	7.970186	8.226841	-1.204350	L
H-HC-0.029500	-1	6.430896	7.970731	-0.421267	L
H-HA-0.169900	-1	9.917889	7.048187	-0.596840	L
H-HA-0.169900	-1	6.089933	5.679231	0.839650	L
H-HA-0.165600	-1	11.051987	5.569116	1.053228	L
H-HA-0.165600	-1	7.243690	4.209677	2.484526	L
H-HO-0.399200	-1	9.382777	3.860409	3.638875	L
N-N--0.415700	-1	5.124569	5.135390	-2.941455	L
C-CT-0.033700	-1	3.805462	4.647043	-3.328319	L
C-C-0.597300	-1	2.965408	4.014886	-2.207657	L
O-O--0.567900	-1	1.742558	4.122169	-2.276254	L
C-CT--0.182500	-1	3.989024	3.647172	-4.464849	L
H-H-0.271900	-1	5.906061	4.838317	-3.520722	L
H-H1-0.082300	-1	3.243780	5.494683	-3.722180	L
H-HC-0.060300	-1	3.016435	3.341529	-4.849588	L
H-HC-0.060300	-1	4.522067	2.776102	-4.083676	L
H-HC-0.060300	-1	4.561839	4.105144	-5.271364	L
N-N--0.415700	-1	3.576289	3.369998	-1.202968	L H-H1 209
C-CT-0.021300	0	2.882429	2.733728	-0.080246	H
C-C-0.597300	0	2.342860	3.806418	0.866948	H
O-O--0.567900	0	3.065189	4.714528	1.266456	H
C-CT--0.123100	0	3.900130	1.827196	0.653033	H
S-S--1.036000	0	3.115757	0.622992	1.794808	H
H-H-0.271900	-1	4.580000	3.340305	-1.195284	L
H-H1-0.112400	0	2.086594	2.131273	-0.519022	H
H-H1-0.111200	0	4.608274	2.472630	1.188789	H
H-H1-0.111200	0	4.480367	1.270622	-0.095029	H
N-N--0.415700	0	1.027128	3.691976	1.250235	H
C-CT--0.051800	0	0.438137	4.527508	2.300714	H
C-C-0.597300	0	0.805519	4.027620	3.731968	H
O-O--0.567900	0	1.351862	4.751759	4.560587	H
C-CT--0.110200	-1	-1.091889	4.647739	2.029297	H
C-CT-0.353100	-1	-1.946483	5.556040	2.939692	L H-HC 222
C-CT--0.412100	-1	-2.139845	5.010267	4.355965	L
C-CT--0.412100	-1	-1.409309	6.987421	3.027931	L

H-H-0.271900	0	0.541575	2.836879	1.008275	H
H-H1-0.092200	0	0.910126	5.509145	2.234313	H
H-HC-0.045700	0	-1.207231	5.019361	1.004623	H
H-HC-0.045700	0	-1.556265	3.655818	2.054384	H
H-HC--0.036100	-1	-2.938075	5.608778	2.491644	L
H-HC-0.100000	-1	-1.240048	5.147360	4.952041	L
H-HC-0.100000	-1	-2.389492	3.951026	4.314837	L
H-HC-0.100000	-1	-2.956566	5.546765	4.836539	L
H-HC-0.100000	-1	-0.446921	6.999677	3.540519	L
H-HC-0.100000	-1	-2.118130	7.609084	3.573568	L
H-HC-0.100000	-1	-1.284346	7.389443	2.021633	L
N-N--0.415700	0	0.494542	2.724580	4.005438	H
C-CT--0.087500	0	0.603032	2.159038	5.352913	H
C-C-0.597300	0	2.020344	2.133046	5.946290	H
O-O--0.567900	0	2.121024	2.153930	7.173442	H
C-CT-0.298500	-1	-0.020477	0.746581	5.374520	H
C-CT--0.319200	0	0.727376	-0.281042	4.502546	L H-HC 241
C-CT--0.319200	0	-0.200598	0.125048	6.759176	L H-HC 241
H-H-0.271900	0	0.106933	2.163452	3.261844	H
H-H1-0.096900	0	0.046720	2.811871	6.037565	H
H-HC--0.029700	0	-1.024042	0.838315	4.951169	H
H-HC-0.079100	0	1.674209	-0.570898	4.952556	L
H-HC-0.079100	0	0.938110	0.143205	3.521497	L
H-HC-0.079100	0	0.106698	-1.161833	4.346444	L
H-HC-0.079100	0	0.768851	-0.104979	7.199716	L
H-HC-0.079100	0	-0.779237	-0.793779	6.665285	L
H-HC-0.079100	0	-0.738094	0.821418	7.400648	L
N-N--0.415700	0	3.029080	1.925804	5.082079	H
C-CT-0.033700	0	4.389316	1.773809	5.559406	H
C-C-0.597300	-1	5.109503	3.104740	5.830116	L H-H1 254
O-O--0.567900	-1	6.284463	3.074723	6.185914	L
C-CT--0.182500	-1	5.159211	0.957559	4.525050	L H-H1 254
H-H-0.271900	0	2.882556	1.852752	4.071674	H
H-H1-0.082300	0	4.374473	1.230597	6.510037	H
H-HC-0.060300	-1	6.124863	0.660011	4.931159	L
H-HC-0.060300	-1	5.318544	1.558470	3.629968	L
H-HC-0.060300	-1	4.596786	0.058094	4.271331	L
N-N--0.415700	-1	4.411912	4.236201	5.666256	L
C-CT--0.087500	-1	4.801827	5.596780	6.063198	L
C-C-0.597300	-1	3.962527	6.048096	7.265696	L
O-O--0.567900	-1	4.517185	6.495349	8.270570	L
C-CT-0.298500	-1	4.591684	6.573638	4.888897	L
C-CT--0.319200	-1	4.993135	8.010126	5.241363	L
C-CT--0.319200	-1	5.406647	6.174326	3.659115	L
H-H-0.271900	-1	3.499979	4.126598	5.240283	L
H-H1-0.096900	-1	5.851968	5.620151	6.344415	L
H-HC--0.029700	-1	3.539141	6.566713	4.613313	L
H-HC-0.079100	-1	6.043896	8.042122	5.521094	L
H-HC-0.079100	-1	4.388980	8.389984	6.064529	L
H-HC-0.079100	-1	4.835584	8.650562	4.373864	L
H-HC-0.079100	-1	6.456421	6.090500	3.934319	L
H-HC-0.079100	-1	5.293599	6.923026	2.875454	L
H-HC-0.079100	-1	5.049292	5.219301	3.273989	L
N-N--0.415700	-1	2.630216	5.864338	7.212255	L

C-CT--0.149000	-1	1.725004	6.208027	8.319588	L
H-H-0.271900	-1	2.221250	5.486287	6.363170	L
H-H1-0.097600	-1	2.304931	6.599545	9.155420	L
H-H1-0.097600	-1	1.184607	5.315791	8.637390	L
H-H1-0.097600	-1	1.013613	6.963627	7.986398	L
C-CT--0.366200	-1	4.103346	10.295149	-0.990032	L
C-C-0.597200	-1	2.626800	9.976420	-1.234561	L
O-O--0.567900	-1	1.822092	10.895583	-1.306572	L
H-HC-0.112300	-1	4.673901	9.368092	-0.954711	L
H-HC-0.112300	-1	4.208077	10.823127	-0.042410	L
H-HC-0.112300	-1	4.478165	10.921980	-1.798810	L
N-N--0.415700	-1	2.241284	8.695518	-1.290780	L
C-CT--0.024900	-1	0.826012	8.321216	-1.131592	L
C-C-0.597300	-1	0.242045	8.821152	0.195450	L
O-O--0.567900	-1	-0.849404	9.394439	0.203850	L
C-CT-0.211700	0	0.652254	6.821562	-1.276865	L
O-OH--0.654600	0	0.928404	6.513084	-2.623034	L
H-H-0.271900	-1	2.939844	7.959209	-1.351865	L
H-H1-0.084300	-1	0.255747	8.774645	-1.938080	L
H-H1-0.035200	0	-0.369651	6.534206	-1.036879	L
H-H1-0.035200	0	1.341705	6.294740	-0.615034	L
H-HO-0.427500	0	1.048324	5.538970	-2.635635	L
N-N--0.415700	-1	1.004012	8.682163	1.291056	L
C-CT-0.033700	-1	0.652936	9.164715	2.627949	L
C-C-0.597300	-1	0.195850	10.628317	2.620071	L
O-O--0.567900	-1	-0.898812	10.952281	3.083175	L
C-CT--0.182500	-1	1.838439	8.921185	3.559416	L
H-H-0.271900	-1	1.889895	8.181242	1.185416	L
H-H1-0.082300	-1	-0.164865	8.576668	3.017584	L
H-HC-0.060300	-1	1.610631	9.292546	4.557901	L
H-HC-0.060300	-1	2.726481	9.418293	3.171257	L
H-HC-0.060300	-1	2.028052	7.850977	3.613349	L
N-N--0.415700	-1	0.998505	11.503403	2.004578	L
C-CT--0.149000	-1	0.665329	12.902819	1.812396	L
H-H-0.271900	-1	1.899357	11.190841	1.650562	L
H-H1-0.097600	-1	-0.319613	13.102835	2.235759	L
H-H1-0.097600	-1	0.655896	13.131711	0.747601	L
H-H1-0.097600	-1	1.408078	13.525282	2.312382	L
C-CT--0.366200	-1	-11.898518	4.644820	4.968145	L
C-C-0.597200	-1	-12.338477	3.227941	4.596327	L
O-O--0.567900	-1	-12.907180	2.522681	5.432080	L
H-HC-0.112300	-1	-11.416801	5.112396	4.109307	L
H-HC-0.112300	-1	-11.194468	4.600548	5.799208	L
H-HC-0.112300	-1	-12.769337	5.231070	5.259895	L
N-N--0.415700	-1	-12.006945	2.785689	3.382982	L
C-CT--0.087500	-1	-12.010210	1.363365	3.023391	L
C-C-0.597300	-1	-10.566233	0.961431	2.709280	L
O-O--0.567900	-1	-9.847832	1.601891	1.934107	L
C-CT-0.298500	-1	-13.008570	0.978594	1.898980	L
C-CT--0.319200	-1	-13.762392	-0.307951	2.284197	L
C-CT--0.319200	-1	-14.081507	2.032112	1.590246	L
H-H-0.271900	-1	-11.593482	3.434946	2.711190	L
H-H1-0.096900	-1	-12.305486	0.805212	3.909473	L
H-HC--0.029700	-1	-12.450919	0.786261	0.986073	L

H-HC-0.079100	-1	-14.393671	-0.123174	3.154060	L
H-HC-0.079100	-1	-13.050468	-1.103989	2.506000	L
H-HC-0.079100	-1	-14.400898	-0.619557	1.457772	L
H-HC-0.079100	-1	-14.714178	2.179415	2.462052	L
H-HC-0.079100	-1	-14.690938	1.699462	0.751391	L
H-HC-0.079100	-1	-13.619789	2.982130	1.330060	L
N-N--0.415700	-1	-10.107670	-0.061147	3.433735	L
C-CT--0.038900	-1	-8.701522	-0.465362	3.515415	L
C-C-0.597300	-1	-8.580991	-1.991475	3.628219	L
O-O--0.567900	-1	-9.514992	-2.647395	4.111015	L
C-CT-0.365400	-1	-7.981344	0.178056	4.724265	L
O-OH--0.676100	-1	-8.152452	-0.536005	5.926958	L
C-CT--0.243800	-1	-8.392679	1.616472	5.032253	L
H-H-0.271900	-1	-10.739285	-0.531060	4.066200	L
H-H1-0.100700	-1	-8.199864	-0.134135	2.606238	L
H-H1-0.004300	-1	-6.922365	0.172841	4.487622	L
H-HC-0.064200	-1	-8.433586	2.181568	4.108562	L
H-HC-0.064200	-1	-7.662128	2.069694	5.703634	L
H-HC-0.064200	-1	-9.375710	1.647650	5.501262	L
H-HO-0.410200	-1	-8.400647	0.104414	6.625967	L
N-N--0.254800	-1	-7.457945	-2.591654	3.194712	L
C-CT--0.026600	-1	-7.213921	-4.018936	3.364191	L
C-C-0.589600	-1	-6.606831	-4.376485	4.722089	L
O-O--0.574800	-1	-6.623497	-5.547361	5.084758	L
C-CT--0.007000	0	-6.241150	-4.383502	2.247832	L
C-CT-0.018900	0	-5.401539	-3.122496	2.099409	L
C-CT-0.019200	0	-6.386791	-1.992471	2.409558	L
H-H1-0.064100	-1	-8.126614	-4.584986	3.219780	L
H-HC-0.025300	0	-5.628324	-5.243515	2.510762	L
H-HC-0.025300	0	-6.793113	-4.570558	1.325842	L
H-HC-0.021300	0	-5.006712	-3.049128	1.090604	L
H-HC-0.021300	0	-4.591430	-3.126461	2.828596	L
H-H1-0.039100	0	-6.791698	-1.602223	1.475601	L
H-H1-0.039100	0	-5.882861	-1.200797	2.965309	L
N-N--0.415700	-1	-5.983617	-3.417800	5.415356	L
C-CT--0.001400	-1	-4.993015	-3.663398	6.474866	L
C-C-0.597300	-1	-5.544356	-4.444345	7.682242	L
O-O--0.567900	-1	-6.730203	-4.322560	7.993438	L
C-CT--0.001400	0	-4.493778	-2.325344	7.037140	L H-HA 373
C-CA--0.001100	0	-4.125885	-1.301328	5.992724	H
C-CA--0.190600	0	-3.317706	-1.675277	4.921250	H
C-CA--0.190600	0	-4.607286	0.007514	6.071434	H
C-CA--0.234100	0	-2.997546	-0.760157	3.933647	H
C-CA--0.234100	0	-4.269868	0.946339	5.098994	H
C-C-0.322600	0	-3.451585	0.563664	4.032112	H
O-OH--0.557900	0	-3.115576	1.501015	3.108443	H
H-H-0.271900	-1	-6.046759	-2.478625	5.053886	L
H-H1-0.087600	-1	-4.170952	-4.235725	6.043625	L
H-HC-0.029500	0	-5.275221	-1.902229	7.671216	L
H-HC-0.029500	0	-3.618943	-2.505853	7.663082	L
H-HA-0.169900	0	-2.934927	-2.689224	4.831570	H
H-HA-0.169900	0	-5.244701	0.311374	6.901973	H
H-HA-0.165600	0	-2.355192	-1.049630	3.116709	H
H-HA-0.165600	0	-4.598149	1.979695	5.177562	H

H-HO-0.399200	0	-2.330018	1.189651	2.610389	H
N-N--0.415700	-1	-4.668657	-5.138104	8.435911	L
C-CT--0.149000	-1	-5.054882	-5.602745	9.784672	L
H-H-0.271900	-1	-3.673966	-5.135663	8.195997	L
H-H1-0.097600	-1	-6.138353	-5.547668	9.891288	L
H-H1-0.097600	-1	-4.582858	-4.970812	10.536214	L
H-H1-0.097600	-1	-4.728299	-6.634053	9.920473	L
C-CT--0.366200	-1	-0.517492	-10.770500	2.471841	L
C-C-0.597200	-1	-0.694277	-9.829089	1.267216	L
O-O--0.567900	-1	-1.803124	-9.649842	0.758650	L
H-HC-0.112300	-1	0.530489	-10.789235	2.767491	L
H-HC-0.112300	-1	-0.835619	-11.776278	2.196177	L
H-HC-0.112300	-1	-1.124325	-10.414133	3.304225	L
N-N--0.415700	-1	0.422236	-9.287421	0.763392	L
C-CT-0.014300	-1	0.382672	-8.269628	-0.286066	L H-HC 405
C-C-0.597300	-1	0.006573	-8.775677	-1.697430	L
O-O--0.567900	-1	-0.201207	-7.951928	-2.579017	L
C-CT--0.204100	0	1.703428	-7.468139	-0.310664	H
C-C-0.713000	0	1.423562	-5.973993	-0.519377	H
O-O--0.593100	0	0.809551	-5.369557	0.368854	H
N-N--0.919100	0	1.904776	-5.376322	-1.621720	H
H-H-0.271900	-1	1.304291	-9.479086	1.209379	L
H-H1-0.104800	-1	-0.416944	-7.593942	0.017993	L
H-HC-0.079700	0	2.381675	-7.901922	-1.055010	H
H-HC-0.079700	0	2.177823	-7.535776	0.671731	H
H-H-0.419600	0	1.759249	-4.358409	-1.792387	H
H-H-0.419600	0	2.321247	-5.933365	-2.356150	H
N-N--0.415700	-1	-0.095733	-10.088497	-1.935097	L
C-CT--0.149000	-1	-0.638623	-10.636816	-3.190093	L
H-H-0.271900	-1	0.011330	-10.738367	-1.148193	L
H-H1-0.097600	-1	-0.699678	-9.845581	-3.936595	L
H-H1-0.097600	-1	-1.633862	-11.042942	-3.009150	L
H-H1-0.097600	-1	0.015974	-11.430096	-3.553303	L
C-CT--0.366200	-1	-3.913867	-11.679563	-1.422973	L
C-C-0.597200	-1	-4.674656	-10.349483	-1.495057	L
O-O--0.567900	-1	-5.813558	-10.346571	-1.966406	L
H-HC-0.112300	-1	-2.929737	-11.510931	-0.984827	L
H-HC-0.112300	-1	-3.799056	-12.087436	-2.426254	L
H-HC-0.112300	-1	-4.470594	-12.383362	-0.804641	L
N-N--0.415700	-1	-4.041597	-9.225415	-1.119792	L
C-CT--0.087500	-1	-4.598744	-7.861583	-1.283040	L
C-C-0.597300	-1	-4.861585	-7.477993	-2.750432	L
O-O--0.567900	-1	-5.846900	-6.803341	-3.046169	L
C-CT-0.298500	-1	-3.686223	-6.789497	-0.631621	L
C-CT--0.319200	-1	-4.166059	-5.349152	-0.872316	L
C-CT--0.319200	-1	-3.671844	-6.926096	0.888479	L
H-H-0.271900	-1	-3.160288	-9.340670	-0.617465	L
H-H1-0.096900	-1	-5.559577	-7.834810	-0.770421	L
H-HC--0.029700	-1	-2.671118	-6.892836	-1.015487	L
H-HC-0.079100	-1	-5.201474	-5.247266	-0.546455	L
H-HC-0.079100	-1	-4.096512	-5.097956	-1.928067	L
H-HC-0.079100	-1	-3.535502	-4.645030	-0.327373	L
H-HC-0.079100	-1	-4.677748	-6.786098	1.266895	L
H-HC-0.079100	-1	-3.004336	-6.183717	1.328323	L

H-HC-0.079100	-1	-3.327819	-7.905206	1.190633	L
N-N--0.415700	-1	-4.016747	-7.882197	-3.707277	L
C-CT--0.149000	-1	-4.100086	-7.467666	-5.118528	L
H-H-0.271900	-1	-3.298489	-8.548924	-3.450228	L
H-H1-0.097600	-1	-4.914535	-6.753106	-5.240329	L
H-H1-0.097600	-1	-4.286833	-8.341379	-5.744487	L
H-H1-0.097600	-1	-3.161250	-7.001851	-5.416767	L
C-CT--0.366200	-1	-12.091948	3.744801	-1.327170	L
C-C-0.597200	-1	-10.993325	2.673008	-1.290233	L
O-O--0.567900	-1	-11.292633	1.491647	-1.134924	L
H-HC-0.112300	-1	-11.638367	4.725435	-1.471505	L
H-HC-0.112300	-1	-12.642634	3.734189	-0.386173	L
H-HC-0.112300	-1	-12.776123	3.535900	-2.149834	L
N-N--0.415700	-1	-9.734474	3.107192	-1.357611	L
C-CT--0.024900	-1	-8.556107	2.279001	-1.177398	L
C-C-0.597300	-1	-7.439391	3.139016	-0.580216	L
O-O--0.567900	-1	-6.782265	3.923586	-1.278598	L
C-CT-0.211700	0	-8.131217	1.616084	-2.485383	L
O-OH--0.654600	0	-7.173622	0.639763	-2.176155	L
H-H-0.271900	-1	-9.602818	4.102950	-1.428174	L
H-H1-0.084300	-1	-8.797997	1.488102	-0.468756	L
H-H1-0.035200	0	-7.717421	2.343678	-3.180683	L
H-H1-0.035200	0	-8.993921	1.127378	-2.940626	L
H-HO-0.427500	0	-6.270908	1.018277	-2.270757	L
N-N--0.415700	-1	-7.277993	3.064951	0.749818	L
C-CT-0.021300	-1	-6.099950	3.674463	1.385521	L
C-C-0.597300	-1	-4.814817	3.020788	0.852507	L
O-O--0.567900	-1	-3.836209	3.703800	0.592155	L
C-CT--0.123100	-1	-6.158838	3.539138	2.908644	L
S-SH--0.311900	-1	-7.406871	4.652356	3.615453	L
H-H-0.271900	-1	-7.941940	2.522129	1.298781	L
H-H1-0.112400	-1	-6.065833	4.736192	1.136214	L
H-H1-0.111200	-1	-5.186410	3.807366	3.325135	L
H-H1-0.111200	-1	-6.380464	2.505704	3.173915	L
H-HS-0.193300	-1	-8.451155	4.209492	2.906068	L
N-N--0.415700	-1	-4.859956	1.702157	0.647039	L H-H1 478
C-CT-0.021300	0	-3.753963	0.939139	0.058865	H
C-C-0.597300	0	-3.663478	1.265584	-1.424233	H
O-O--0.567900	0	-4.682672	1.467751	-2.085374	H
C-CT--0.123100	0	-4.111011	-0.532321	0.303034	H
S-SH--0.311900	0	-2.876321	-1.788851	-0.205888	H
H-H-0.271900	-1	-5.713572	1.218411	0.852871	L
H-H1-0.112400	0	-2.828739	1.195090	0.575561	H
H-H1-0.111200	0	-5.020032	-0.793842	-0.245636	H
H-H1-0.111200	0	-4.293865	-0.692666	1.364868	H
H-HS-0.193300	0	-2.064922	-1.677832	0.853678	H
N-N--0.415700	0	-2.414464	1.268712	-1.980688	H
C-CT--0.087500	0	-2.267768	1.396304	-3.427238	H
C-C-0.597300	0	-2.205820	0.045083	-4.186042	H
O-O--0.567900	0	-2.324360	0.065978	-5.407832	H
C-CT-0.298500	-1	-1.101510	2.301797	-3.875934	H
C-CT--0.319200	0	-1.227673	3.713982	-3.304025	L H-HC 492
C-CT--0.319200	0	0.265635	1.730415	-3.465119	L H-HC 492
H-H-0.271900	0	-1.604276	1.083185	-1.400182	H

H-H1-0.096900	0	-3.211529	1.832595	-3.769042	H
H-HC--0.029700	0	-1.133405	2.354652	-4.966285	H
H-HC-0.079100	0	-1.091765	3.697442	-2.220917	L
H-HC-0.079100	0	-2.210160	4.110830	-3.540513	L
H-HC-0.079100	0	-0.471599	4.356797	-3.751334	L
H-HC-0.079100	0	0.375681	1.758510	-2.378561	L
H-HC-0.079100	0	1.060626	2.313016	-3.920969	L
H-HC-0.079100	0	0.373909	0.698975	-3.793515	L
N-N--0.415700	0	-1.965681	-1.073322	-3.449760	H
C-CT--0.003100	0	-2.059186	-2.416000	-4.022855	H
C-C-0.597300	0	-3.524744	-2.863650	-4.193952	H
O-O--0.567900	0	-3.831884	-3.663420	-5.068227	H
C-CT--0.003600	-1	-1.308192	-3.438540	-3.117753	H
C-CT--0.064500	-1	-1.448161	-4.892047	-3.607858	L H-HC 508
C-C-0.695100	-1	-0.576185	-5.235170	-4.800921	L
O-O--0.608600	-1	-0.430419	-4.485091	-5.751161	L
N-N--0.940700	-1	0.031916	-6.401910	-4.795396	L
H-H-0.271900	0	-1.955568	-1.014494	-2.438811	H
H-H1-0.085000	0	-1.636686	-2.387960	-5.029491	H
H-HC-0.017100	0	-0.252585	-3.180838	-3.028423	H
H-HC-0.017100	0	-1.746671	-3.396559	-2.117275	H
H-HC-0.035200	-1	-2.477436	-5.142250	-3.848870	L
H-HC-0.035200	-1	-1.166056	-5.541037	-2.786149	L
H-H-0.425100	-1	0.633944	-6.653253	-5.559785	L
H-H-0.425100	-1	-0.080771	-7.022106	-3.995361	L
N-N--0.415700	0	-4.363409	-2.463872	-3.167940	H
C-CT--0.023700	0	-5.746249	-2.919943	-3.238238	H
C-C-0.597300	-1	-6.418323	-2.297313	-4.475528	L H-H1 522
O-O--0.567900	-1	-6.241994	-1.102945	-4.734459	L
C-CT-0.034200	-1	-6.480089	-2.637105	-1.908992	L H-H1 522
C-CT-0.001800	-1	-7.950591	-3.079499	-1.965627	L
S-S--0.273700	-1	-8.854135	-3.049005	-0.390076	L
C-CT--0.053600	-1	-9.214678	-1.279404	-0.258914	L
H-H-0.271900	0	-4.281568	-1.489843	-2.921134	H
H-H1-0.088000	0	-5.684745	-3.997054	-3.352066	H
H-HC-0.024100	-1	-6.404924	-1.590991	-1.649393	L
H-HC-0.024100	-1	-5.989077	-3.191780	-1.112929	L
H-H1-0.044000	-1	-7.980468	-4.105018	-2.335101	L
H-H1-0.044000	-1	-8.488028	-2.450707	-2.675786	L
H-H1-0.068400	-1	-9.819290	-1.091702	0.628325	L
H-H1-0.068400	-1	-9.763566	-0.947673	-1.140494	L
H-H1-0.068400	-1	-8.282200	-0.723638	-0.187496	L
N-N--0.254800	-1	-7.170822	-3.063280	-5.287068	L
C-CT--0.026600	-1	-7.566251	-2.644802	-6.632818	L
C-C-0.589600	-1	-9.013803	-2.154678	-6.624056	L
O-O--0.574800	-1	-9.902831	-2.851056	-6.127167	L
C-CT--0.007000	-1	-7.365653	-3.889515	-7.511778	L
C-CT-0.018900	-1	-6.853583	-4.954537	-6.538807	L
C-CT-0.019200	-1	-7.383418	-4.492033	-5.207918	L
H-H1-0.064100	-1	-6.915482	-1.850693	-6.998356	L
H-HC-0.025300	-1	-8.301585	-4.206137	-7.963128	L
H-HC-0.025300	-1	-6.629603	-3.708198	-8.292744	L
H-HC-0.021300	-1	-5.765442	-4.951203	-6.512945	L
H-HC-0.021300	-1	-7.231992	-5.935364	-6.754696	L

H-H1-0.039100	-1	-6.861133	-5.002317	-4.410343	L
H-H1-0.039100	-1	-8.449815	-4.707987	-5.133175	L
N-N--0.415700	-1	-9.232206	-0.957070	-7.160692	L
C-CT--0.149000	-1	-10.462398	-0.182591	-6.970262	L
H-H-0.271900	-1	-8.425592	-0.491040	-7.575561	L
H-H1-0.097600	-1	-11.225162	-0.817350	-6.519869	L
H-H1-0.097600	-1	-10.814972	0.180393	-7.935653	L
H-H1-0.097600	-1	-10.259731	0.664309	-6.314283	L
C-CT--0.366200	-1	-10.306893	8.897031	-4.237389	L
C-C-0.597200	-1	-9.763325	7.605864	-3.611322	L
O-O--0.567900	-1	-10.207152	7.187813	-2.540546	L
H-HC-0.112300	-1	-9.787959	9.092635	-5.175663	L
H-HC-0.112300	-1	-10.144305	9.728549	-3.552183	L
H-HC-0.112300	-1	-11.374064	8.786998	-4.429131	L
N-N--0.415700	-1	-8.795294	6.979238	-4.274698	L
C-CT--0.024900	-1	-7.854535	6.057136	-3.635014	L
C-C-0.597300	-1	-6.521871	6.783679	-3.414372	L
O-O--0.567900	-1	-6.263212	7.789912	-4.082027	L
C-CT-0.211700	0	-7.637886	4.801379	-4.491676	L
O-OH--0.654600	0	-7.258948	5.110716	-5.819499	L
H-H-0.271900	-1	-8.523397	7.346895	-5.185507	L
H-H1-0.084300	-1	-8.241442	5.719523	-2.673188	L
H-H1-0.035200	0	-8.562326	4.222952	-4.513471	L
H-H1-0.035200	0	-6.858015	4.190865	-4.034064	L
H-HO-0.427500	0	-6.837640	4.333387	-6.204412	L
N-N--0.415700	-1	-5.645950	6.248400	-2.553499	L
C-CT-0.033700	-1	-4.270065	6.751561	-2.450750	L
C-C-0.597300	-1	-3.522981	6.753074	-3.803488	L
O-O--0.567900	-1	-2.620487	7.563135	-4.020958	L
C-CT--0.182500	-1	-3.519415	5.927086	-1.415094	L
H-H-0.271900	-1	-5.931869	5.444415	-1.989760	L
H-H1-0.082300	-1	-4.313132	7.779156	-2.088271	L
H-HC-0.060300	-1	-2.504233	6.304355	-1.310263	L
H-HC-0.060300	-1	-3.488763	4.880909	-1.717645	L
H-HC-0.060300	-1	-4.034233	6.012642	-0.459424	L
N-N--0.415700	-1	-3.948268	5.888137	-4.738099	L
C-CT--0.149000	-1	-3.434129	5.832503	-6.105370	L
H-H-0.271900	-1	-4.679287	5.242417	-4.470724	L
H-H1-0.097600	-1	-2.657633	6.587251	-6.232187	L
H-H1-0.097600	-1	-4.245090	6.025980	-6.807382	L
H-H1-0.097600	-1	-3.015653	4.844315	-6.296113	L
C-CM--0.139000	0	1.046184	-2.132069	0.091483	H
C-C-0.519000	0	1.383311	-1.652960	-1.308053	H
O-O2--0.567000	0	1.424280	-0.439732	-1.572504	H
C-CM--0.117000	0	0.421440	-1.512904	1.111400	H
O-O2--0.618000	0	1.608577	-2.615487	-2.135055	H
C-C--0.553000	0	-0.135077	-0.149629	1.190956	H
O-O2--0.556000	0	0.378316	0.830699	0.484075	H
O-O2--0.607000	0	-1.118893	0.080297	1.913486	H
H-HC-0.049000	0	1.262978	-3.182739	0.258535	H
H-HC-0.162000	0	0.155258	-2.120177	1.969904	H
O-OW--0.834000	-1	6.455665	2.930243	-1.178149	L
H-HW-0.417000	-1	6.827149	3.070158	-2.048366	L
H-HW-0.417000	-1	7.136344	3.227965	-0.574990	L

O-OW--0.834000	0	3.560346	7.282775	1.040234	L
H-HW-0.417000	0	3.337946	6.389130	1.374254	L
H-HW-0.417000	0	3.925618	7.062425	0.166100	L
O-OW--0.834000	0	-1.428071	-4.084107	1.676768	H
H-HW-0.417000	0	-0.699626	-4.529701	1.207973	H
H-HW-0.417000	0	-2.176868	-4.163725	1.069605	H
O-OW--0.834000	0	-4.994310	0.875156	-6.159604	L
H-HW-0.417000	0	-4.056376	0.645067	-6.072319	L
H-HW-0.417000	0	-5.433271	0.214281	-5.597500	L
H-HS-0.193300	0	1.343628	0.590971	0.317304	H

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C-CT--0.366200	-1	8.202201	4.639328	-8.138635	L
C-C-0.597200	-1	9.032858	3.893785	-7.099422	L
O-O--0.567900	-1	9.631690	2.855266	-7.381118	L
H-HC-0.112300	-1	7.760713	5.525953	-7.683735	L
H-HC-0.112300	-1	7.409595	3.987038	-8.506900	L
H-HC-0.112300	-1	8.841945	4.938209	-8.969852	L
N-N--0.415700	-1	9.029958	4.452657	-5.882699	L
C-CT--0.087500	-1	9.501923	3.777020	-4.666941	L
C-C-0.597300	-1	8.363897	2.881377	-4.173446	L
O-O--0.567900	-1	7.454347	3.342755	-3.468975	L
C-CT-0.298500	-1	9.986908	4.779054	-3.592154	L
C-CT--0.319200	-1	10.407213	4.079804	-2.293825	L
C-CT--0.319200	-1	11.201802	5.585288	-4.073799	L
H-H-0.271900	-1	8.446000	5.275586	-5.755094	L
H-H1-0.096900	-1	10.338408	3.134682	-4.921893	L
H-HC--0.029700	-1	9.190906	5.485790	-3.375082	L
H-HC-0.079100	-1	11.111867	3.280005	-2.523462	L
H-HC-0.079100	-1	9.536944	3.657935	-1.794843	L
H-HC-0.079100	-1	10.885505	4.787677	-1.618752	L
H-HC-0.079100	-1	12.061198	4.927442	-4.203245	L
H-HC-0.079100	-1	11.449779	6.356279	-3.342177	L
H-HC-0.079100	-1	10.982942	6.064649	-5.026962	L
N-N--0.415700	-1	8.378402	1.608539	-4.604655	L
C-CT--0.087500	-1	7.264454	0.657880	-4.427968	L
C-C-0.597300	-1	7.679798	-0.617929	-3.666782	L
O-O--0.567900	-1	8.825076	-1.070923	-3.792436	L
C-CT-0.298500	-1	6.608982	0.251088	-5.772180	L
C-CT--0.319200	-1	5.751945	1.378385	-6.359682	L
C-CT--0.319200	-1	7.599944	-0.201422	-6.849831	L
H-H-0.271900	-1	9.152611	1.301484	-5.199400	L
H-H1-0.096900	-1	6.494772	1.165959	-3.853991	L
H-HC--0.029700	-1	5.939067	-0.588878	-5.584789	L
H-HC-0.079100	-1	6.270365	2.334161	-6.284757	L
H-HC-0.079100	-1	4.817562	1.427385	-5.805069	L
H-HC-0.079100	-1	5.502188	1.163114	-7.399911	L
H-HC-0.079100	-1	8.200942	0.642310	-7.184884	L
H-HC-0.079100	-1	7.048965	-0.604243	-7.698672	L
H-HC-0.079100	-1	8.253811	-0.975050	-6.455411	L
N-N--0.254800	-1	6.743913	-1.223107	-2.897715	L
C-CT--0.026600	-1	6.875021	-2.576078	-2.350481	L
C-C-0.589600	-1	7.120814	-3.600262	-3.460208	L
O-O--0.574800	-1	6.372869	-3.647493	-4.439861	L

C-CT--0.007000	0	5.540422	-2.871580	-1.646325	L
C-CT-0.018900	0	4.953994	-1.492832	-1.366355	L
C-CT-0.019200	0	5.434625	-0.675036	-2.550333	L
H-H1-0.064100	-1	7.694229	-2.591922	-1.632483	L
H-HC-0.025300	0	4.859902	-3.408027	-2.309728	L
H-HC-0.025300	0	5.688131	-3.442311	-0.733965	L
H-HC-0.021300	0	5.366827	-1.071802	-0.456188	L
H-HC-0.021300	0	3.874383	-1.507763	-1.302509	L
H-H1-0.039100	0	5.488780	0.372115	-2.251275	L
H-H1-0.039100	0	4.743677	-0.798963	-3.385911	L
N-N--0.415700	-1	8.144897	-4.447231	-3.312362	L
C-CT--0.149000	-1	8.512477	-5.444118	-4.330693	L
H-H-0.271900	-1	8.744901	-4.325225	-2.497670	L
H-H1-0.097600	-1	7.768323	-5.443590	-5.126490	L
H-H1-0.097600	-1	8.553500	-6.432667	-3.872273	L
H-H1-0.097600	-1	9.489081	-5.196268	-4.746540	L
C-CT--0.366200	-1	5.211246	-7.424596	-4.082195	L
C-C-0.597200	-1	4.082189	-6.753124	-4.874123	L
O-O--0.567900	-1	3.183402	-7.470592	-5.322676	L
H-HC-0.112300	-1	5.924105	-6.668758	-3.753293	L
H-HC-0.112300	-1	5.718289	-8.151713	-4.716321	L
H-HC-0.112300	-1	4.792456	-7.930693	-3.212297	L
N-N--0.415700	-1	4.071704	-5.422360	-5.013893	L
C-CT-0.014300	-1	2.970043	-4.673968	-5.643843	L H-HC 69
C-C-0.597300	-1	2.774525	-5.015046	-7.155871	L
O-O--0.567900	-1	3.768549	-5.180714	-7.864373	L
C-CT--0.204100	0	3.279528	-3.172863	-5.440892	H
C-C-0.713000	0	2.203249	-2.249213	-6.013971	H
O-O--0.593100	0	2.144364	-1.964415	-7.206915	H
N-N--0.919100	0	1.358185	-1.730978	-5.085216	H
H-H-0.271900	-1	4.840692	-4.885425	-4.646601	L
H-H1-0.104800	-1	2.062523	-4.936598	-5.109881	L
H-HC-0.079700	0	4.213359	-2.957132	-5.971708	H
H-HC-0.079700	0	3.421482	-2.993162	-4.372483	H
H-H-0.419600	0	0.524518	-1.297241	-5.458942	H
H-H-0.419600	0	1.379138	-2.044990	-4.116958	H
N-N--0.415700	-1	1.520636	-5.113152	-7.648637	L
C-CT--0.149000	-1	1.167889	-5.373164	-9.074121	L
H-H-0.271900	-1	0.765747	-4.886743	-7.002078	L
H-H1-0.097600	-1	2.073183	-5.599228	-9.636962	L
H-H1-0.097600	-1	0.687937	-4.489790	-9.496200	L
H-H1-0.097600	-1	0.484029	-6.220118	-9.128832	L
C-CT--0.366200	-1	11.706602	-5.933359	-0.632365	L
C-C-0.597200	-1	10.691204	-6.058127	0.511733	L
O-O--0.567900	-1	11.008815	-5.903011	1.696128	L
H-HC-0.112300	-1	11.205264	-6.108903	-1.584038	L
H-HC-0.112300	-1	12.497954	-6.670209	-0.497453	L
H-HC-0.112300	-1	12.138376	-4.932310	-0.628490	L
N-N--0.415700	-1	9.454226	-6.361040	0.120896	L
C-CT--0.023700	-1	8.294059	-6.557172	0.985239	L
C-C-0.597300	-1	7.238724	-7.399931	0.281678	L
O-O--0.567900	-1	7.059867	-7.241257	-0.932761	L
C-CT-0.034200	0	7.690867	-5.196997	1.377212	L
C-CT-0.001800	0	6.778923	-5.215064	2.620078	L

S-S--0.273700	0	5.057814	-5.773023	2.412387	L
C-CT--0.053600	0	4.217826	-4.203464	2.027526	L
H-H-0.271900	-1	9.285175	-6.434967	-0.876230	L
H-H1-0.088000	-1	8.618373	-7.089074	1.868031	L
H-HC-0.024100	0	7.146382	-4.777776	0.531363	L
H-HC-0.024100	0	8.523448	-4.533630	1.593043	L
H-H1-0.044000	0	6.737964	-4.202452	3.021928	L
H-H1-0.044000	0	7.250663	-5.838686	3.379374	L
H-H1-0.068400	0	3.159305	-4.382981	1.834085	L
H-H1-0.068400	0	4.657283	-3.741502	1.146525	L
H-H1-0.068400	0	4.305922	-3.512034	2.866059	L
N-N--0.415700	-1	6.530128	-8.244693	1.041166	L
C-CT--0.149000	-1	5.307512	-8.949759	0.627865	L
H-H-0.271900	-1	6.846450	-8.376142	2.001913	L
H-H1-0.097600	-1	5.090115	-8.719364	-0.414587	L
H-H1-0.097600	-1	4.474113	-8.628536	1.252871	L
H-H1-0.097600	-1	5.452963	-10.023802	0.739857	L
C-CT--0.366200	-1	3.873313	-9.346623	4.909555	L
C-C-0.597200	-1	3.706900	-7.940388	5.519869	L
O-O--0.567900	-1	4.669541	-7.225043	5.812746	L
H-HC-0.112300	-1	2.890683	-9.786504	4.736052	L
H-HC-0.112300	-1	4.437097	-9.977454	5.596561	L
H-HC-0.112300	-1	4.409022	-9.271181	3.963144	L
N-N--0.415700	-1	2.445852	-7.524693	5.667385	L
C-CT--0.087500	-1	2.010621	-6.119703	5.614515	L
C-C-0.597300	-1	1.889961	-5.560982	7.038704	L
O-O--0.567900	-1	0.853226	-5.653020	7.711324	L
C-CT-0.298500	0	0.689221	-5.950377	4.833788	L
C-CT--0.319200	0	0.312877	-4.471406	4.690437	L
C-CT--0.319200	0	0.790117	-6.559704	3.427528	L
H-H-0.271900	-1	1.709351	-8.217825	5.511632	L
H-H1-0.096900	-1	2.776762	-5.547609	5.087670	L
H-HC--0.029700	0	-0.111749	-6.466585	5.364856	L
H-HC-0.079100	0	1.057968	-3.939757	4.094558	L
H-HC-0.079100	0	0.223438	-3.988850	5.662617	L
H-HC-0.079100	0	-0.649827	-4.384381	4.188839	L
H-HC-0.079100	0	1.623112	-6.103309	2.890657	L
H-HC-0.079100	0	-0.127386	-6.352510	2.874537	L
H-HC-0.079100	0	0.929792	-7.636282	3.480011	L
N-N--0.415700	-1	3.050752	-5.109636	7.513293	L
C-CT--0.149000	-1	3.428589	-4.975289	8.917520	L
H-H-0.271900	-1	3.809745	-5.027441	6.847094	L
H-H1-0.097600	-1	2.542111	-5.079263	9.543341	L
H-H1-0.097600	-1	3.875783	-3.995526	9.081755	L
H-H1-0.097600	-1	4.148629	-5.751951	9.175524	L
C-CT--0.366200	-1	12.472948	-4.243320	6.343769	L
C-C-0.597200	-1	12.268789	-3.520148	4.993989	L
O-O--0.567900	-1	13.235843	-3.305152	4.256681	L
H-HC-0.112300	-1	11.513750	-4.341956	6.852020	L
H-HC-0.112300	-1	13.155169	-3.663647	6.966798	L
H-HC-0.112300	-1	12.893881	-5.232115	6.166416	L
N-N--0.415700	-1	11.034106	-3.091939	4.692071	L
C-CT--0.023700	-1	10.758062	-2.267063	3.518158	L
C-C-0.597300	-1	11.328967	-0.845238	3.654259	L

O-O--0.567900	-1	12.058233	-0.381241	2.775954	L
C-CT-0.034200	0	9.250741	-2.186342	3.259595	L
C-CT-0.001800	0	9.002351	-1.505097	1.907950	L
S-S--0.273700	0	7.420441	-1.899877	1.143674	L
C-CT--0.053600	0	6.249974	-0.981407	2.176417	L
H-H-0.271900	-1	10.269164	-3.319527	5.320903	L
H-H1-0.088000	-1	11.227111	-2.747480	2.657787	L
H-HC-0.024100	0	8.747700	-1.629059	4.051002	L
H-HC-0.024100	0	8.848928	-3.195051	3.245490	L
H-H1-0.044000	0	9.775012	-1.827314	1.208805	L
H-H1-0.044000	0	9.085006	-0.423241	2.021005	L
H-H1-0.068400	0	5.227704	-1.170530	1.840661	L
H-H1-0.068400	0	6.440324	0.088117	2.089520	L
H-H1-0.068400	0	6.339889	-1.293196	3.215041	L
N-N--0.415700	-1	11.063695	-0.156542	4.769824	L
C-CT--0.149000	-1	11.620364	1.180674	4.998722	L
H-H-0.271900	-1	10.484985	-0.586221	5.491000	L
H-H1-0.097600	-1	12.208544	1.482024	4.132036	L
H-H1-0.097600	-1	12.258450	1.162044	5.881836	L
H-H1-0.097600	-1	10.808087	1.891093	5.152361	L
C-CT--0.366200	-1	6.190270	8.717885	-5.554507	L
C-C-0.597200	-1	6.503183	7.524886	-4.629818	L
O-O--0.567900	-1	6.651404	6.376151	-5.070600	L
H-HC-0.112300	-1	6.101277	9.626771	-4.958478	L
H-HC-0.112300	-1	5.251985	8.535312	-6.079615	L
H-HC-0.112300	-1	6.995324	8.836909	-6.280347	L
N-N--0.415700	-1	6.648528	7.839531	-3.332428	L
C-CT--0.001400	-1	6.688736	6.847601	-2.242588	L
C-C-0.597300	-1	5.312132	6.171506	-2.100439	L
O-O--0.567900	-1	4.440790	6.654073	-1.359705	L
C-CT--0.001400	-1	7.209240	7.479297	-0.938339	L
C-CA--0.001100	-1	7.893073	6.506164	0.016077	L
C-CA--0.190600	-1	9.300794	6.452065	0.065177	L
C-CA--0.190600	-1	7.145735	5.686823	0.887074	L
C-CA--0.234100	-1	9.950005	5.629598	1.004926	L
C-CA--0.234100	-1	7.799292	4.859255	1.826546	L
C-C-0.322600	-1	9.201792	4.853276	1.904041	L
O-OH--0.557900	-1	9.861124	4.105552	2.835662	L
H-H-0.271900	-1	6.587137	8.831534	-3.090375	L
H-H1-0.087600	-1	7.397517	6.073708	-2.523539	L
H-HC-0.029500	-1	7.936617	8.248759	-1.199951	L
H-HC-0.029500	-1	6.398780	7.988517	-0.415380	L
H-HA-0.169900	-1	9.887806	7.074503	-0.595115	L
H-HA-0.169900	-1	6.064693	5.695539	0.844690	L
H-HA-0.165600	-1	11.027221	5.597319	1.052978	L
H-HA-0.165600	-1	7.223736	4.227920	2.487577	L
H-HO-0.399200	-1	9.364879	3.883226	3.639487	L
N-N--0.415700	-1	5.096656	5.151341	-2.935680	L
C-CT-0.033700	-1	3.778325	4.660007	-3.321408	L
C-C-0.597300	-1	2.940988	4.025234	-2.200194	L
O-O--0.567900	-1	1.717810	4.129592	-2.267445	L
C-CT--0.182500	-1	3.963106	3.661177	-4.458657	L
H-H-0.271900	-1	5.878252	4.856463	-3.515927	L
H-H1-0.082300	-1	3.214180	5.506492	-3.714232	L

H-HC-0.060300	-1	2.990854	3.353383	-4.842531	L
H-HC-0.060300	-1	4.498657	2.791201	-4.078505	L
H-HC-0.060300	-1	4.533960	4.120955	-5.265534	L
N-N--0.415700	-1	3.554503	3.381327	-1.196528	L H-HC 209
C-CT-0.021300	0	2.815316	2.683655	-0.118111	H
C-C-0.597300	0	2.309910	3.721785	0.885325	H
O-O--0.567900	0	3.074612	4.558147	1.358806	H
C-CT--0.123100	0	3.778170	1.690719	0.565171	H
S-S--1.036000	0	3.004687	0.653194	1.870977	H
H-H-0.271900	-1	4.558274	3.354032	-1.189878	L
H-H1-0.112400	0	1.987502	2.129606	-0.566532	H
H-H1-0.111200	0	4.599107	2.253279	1.028137	H
H-H1-0.111200	0	4.225519	1.044167	-0.200395	H
N-N--0.415700	0	0.981322	3.665933	1.224682	H
C-CT--0.051800	0	0.417526	4.505662	2.289872	H
C-C-0.597300	0	0.788919	3.996843	3.714782	H
O-O--0.567900	0	1.276470	4.742718	4.563623	H
C-CT--0.110200	-1	-1.113419	4.646048	2.041390	H
C-CT-0.353100	-1	-1.969170	5.551827	2.953129	L H-HC 222
C-CT--0.412100	-1	-2.159726	5.004825	4.369329	L
C-CT--0.412100	-1	-1.435378	6.984434	3.041565	L
H-H-0.271900	0	0.421112	2.898039	0.869809	H
H-H1-0.092200	0	0.899414	5.483294	2.225741	H
H-HC-0.045700	0	-1.237113	5.020315	1.017855	H
H-HC-0.045700	0	-1.577940	3.654106	2.068439	H
H-HC--0.036100	-1	-2.961369	5.602378	2.506167	L
H-HC-0.100000	-1	-1.259634	5.143783	4.964529	L
H-HC-0.100000	-1	-2.406853	3.945005	4.327909	L
H-HC-0.100000	-1	-2.977235	5.539095	4.851048	L
H-HC-0.100000	-1	-0.472482	6.998751	3.553145	L
H-HC-0.100000	-1	-2.145124	7.604096	3.588278	L
H-HC-0.100000	-1	-1.312450	7.387284	2.035348	L
N-N--0.415700	0	0.535306	2.680319	3.971867	H
C-CT--0.087500	0	0.602477	2.153417	5.336828	H
C-C-0.597300	0	2.003359	2.126766	5.962828	H
O-O--0.567900	0	2.093861	2.119346	7.190264	H
C-CT-0.298500	-1	-0.028976	0.745751	5.383414	H
C-CT--0.319200	0	0.804744	-0.354767	4.706484	L H-HC 241
C-CT--0.319200	0	-0.400806	0.253296	6.782069	L H-HC 241
H-H-0.271900	0	0.248093	2.071959	3.213338	H
H-H1-0.096900	0	0.032769	2.834589	5.981289	H
H-HC--0.029700	0	-0.962285	0.809262	4.826327	H
H-HC-0.079100	0	1.673879	-0.616016	5.306055	L
H-HC-0.079100	0	1.151675	0.001013	3.739466	L
H-HC-0.079100	0	0.192318	-1.237905	4.533920	L
H-HC-0.079100	0	0.497110	0.077931	7.373061	L
H-HC-0.079100	0	-0.961666	-0.676856	6.696514	L
H-HC-0.079100	0	-1.022996	0.999509	7.273320	L
N-N--0.415700	0	3.020272	1.936557	5.102038	H
C-CT-0.033700	0	4.380812	1.783781	5.568293	H
C-C-0.597300	-1	5.095758	3.116071	5.834839	L H-H1 254
O-O--0.567900	-1	6.271167	3.088713	6.189378	L
C-CT--0.182500	-1	5.149296	0.969698	4.528582	L H-H1 254
H-H-0.271900	0	2.868931	1.931210	4.094404	H

H-H1-0.082300	0	4.370797	1.239435	6.518089	H
H-HC-0.060300	-1	6.116084	0.674279	4.933522	L
H-HC-0.060300	-1	5.306219	1.571465	3.633654	L
H-HC-0.060300	-1	4.588772	0.069012	4.274989	L
N-N--0.415700	-1	4.395264	4.245928	5.672305	L
C-CT--0.087500	-1	4.782305	5.607238	6.069550	L
C-C-0.597300	-1	3.943186	6.055894	7.273169	L
O-O--0.567900	-1	4.497821	6.503962	8.277694	L
C-CT-0.298500	-1	4.568559	6.584199	4.895984	L
C-CT--0.319200	-1	4.966907	8.021471	5.248782	L
C-CT--0.319200	-1	5.383188	6.187504	3.665135	L
H-H-0.271900	-1	3.483150	4.134342	5.247235	L
H-H1-0.096900	-1	5.832683	5.633003	6.349672	L
H-HC--0.029700	-1	3.515746	6.574872	4.621507	L
H-HC-0.079100	-1	6.017882	8.055862	5.527422	L
H-HC-0.079100	-1	4.362704	8.399436	6.072785	L
H-HC-0.079100	-1	4.806891	8.661977	4.381787	L
H-HC-0.079100	-1	6.433451	6.106074	3.939188	L
H-HC-0.079100	-1	5.267502	6.936338	2.881987	L
H-HC-0.079100	-1	5.027738	5.231819	3.279884	L
N-N--0.415700	-1	2.611268	5.868941	7.221036	L
C-CT--0.149000	-1	1.706396	6.209860	8.329504	L
H-H-0.271900	-1	2.202321	5.490345	6.372185	L
H-H1-0.097600	-1	2.286258	6.602343	9.164929	L
H-H1-0.097600	-1	1.168495	5.316152	8.647407	L
H-H1-0.097600	-1	0.992828	6.963911	7.997462	L
C-CT--0.366200	-1	4.065014	10.307593	-0.980468	L
C-C-0.597200	-1	2.588986	9.985421	-1.223609	L
O-O--0.567900	-1	1.781982	10.902671	-1.294288	L
H-HC-0.112300	-1	4.637848	9.381902	-0.946237	L
H-HC-0.112300	-1	4.169469	10.835327	-0.032680	L
H-HC-0.112300	-1	4.437462	10.935753	-1.789312	L
N-N--0.415700	-1	2.206511	8.703620	-1.280095	L
C-CT--0.024900	-1	0.792317	8.325809	-1.119610	L
C-C-0.597300	-1	0.208545	8.823638	0.208310	L
O-O--0.567900	-1	-0.884279	9.394277	0.218163	L
C-CT-0.211700	0	0.620412	6.825790	-1.266630	L
O-OH--0.654600	0	0.898707	6.518941	-2.612760	L
H-H-0.271900	-1	2.906785	7.969034	-1.342303	L
H-H1-0.084300	-1	0.220106	8.778280	-1.925258	L
H-H1-0.035200	0	-0.401562	6.537291	-1.028586	L
H-H1-0.035200	0	1.308634	6.297912	-0.604436	L
H-HO-0.427500	0	1.016929	5.544344	-2.625828	L
N-N--0.415700	-1	0.972000	8.685918	1.303038	L
C-CT-0.033700	-1	0.621171	9.166921	2.640555	L
C-C-0.597300	-1	0.160539	10.629418	2.633927	L
O-O--0.567900	-1	-0.934415	10.950489	3.098356	L
C-CT--0.182500	-1	1.808241	8.925773	3.570642	L
H-H-0.271900	-1	1.858982	8.187199	1.196201	L
H-H1-0.082300	-1	-0.194793	8.576693	3.030743	L
H-HC-0.060300	-1	1.580592	9.296060	4.569562	L
H-HC-0.060300	-1	2.694670	9.425232	3.181808	L
H-HC-0.060300	-1	2.000501	7.856001	3.623814	L
N-N--0.415700	-1	0.960422	11.506764	2.018048	L

C-CT--0.149000	-1	0.623661	12.905470	1.826953	L
H-H-0.271900	-1	1.861654	11.196568	1.662918	L
H-H1-0.097600	-1	-0.361314	13.102881	2.251459	L
H-H1-0.097600	-1	0.612550	13.134896	0.762288	L
H-H1-0.097600	-1	1.365429	13.529467	2.326482	L
C-CT--0.366200	-1	-11.916835	4.615447	4.991608	L
C-C-0.597200	-1	-12.353758	3.197703	4.619509	L
O-O--0.567900	-1	-12.919869	2.490631	5.455491	L
H-HC-0.112300	-1	-11.437157	5.084636	4.132508	L
H-HC-0.112300	-1	-11.211803	4.572444	5.821905	L
H-HC-0.112300	-1	-12.788761	5.199435	5.284583	L
N-N--0.415700	-1	-12.022437	2.756889	3.405584	L
C-CT--0.087500	-1	-12.022641	1.334749	3.045249	L
C-C-0.597300	-1	-10.578029	0.936474	2.729404	L
O-O--0.567900	-1	-9.861998	1.579077	1.953810	L
C-CT-0.298500	-1	-13.021255	0.948152	1.921689	L
C-CT--0.319200	-1	-13.771555	-0.340415	2.307024	L
C-CT--0.319200	-1	-14.097062	1.999231	1.614640	L
H-H-0.271900	-1	-11.611256	3.407495	2.733697	L
H-H1-0.096900	-1	-12.315631	0.775419	3.931347	L
H-HC--0.029700	-1	-12.464104	0.757646	1.008094	L
H-HC-0.079100	-1	-14.402361	-0.157622	3.177649	L
H-HC-0.079100	-1	-13.057473	-1.134843	2.527658	L
H-HC-0.079100	-1	-14.410177	-0.653133	1.481110	L
H-HC-0.079100	-1	-14.729168	2.144547	2.487189	L
H-HC-0.079100	-1	-14.706571	1.665547	0.776254	L
H-HC-0.079100	-1	-13.637918	2.950500	1.354467	L
N-N--0.415700	-1	-10.116229	-0.085370	3.452838	L
C-CT--0.038900	-1	-8.709022	-0.486224	3.532822	L
C-C-0.597300	-1	-8.584681	-2.012101	3.644696	L
O-O--0.567900	-1	-9.516582	-2.670531	4.128132	L
C-CT-0.365400	-1	-7.989126	0.158303	4.741250	L
O-OH--0.676100	-1	-8.157238	-0.556799	5.943748	L
C-CT--0.243800	-1	-8.403615	1.595557	5.050428	L
H-H-0.271900	-1	-10.746037	-0.557140	4.085720	L
H-H1-0.100700	-1	-8.209126	-0.153308	2.623291	L
H-H1-0.004300	-1	-6.930388	0.155773	4.503487	L
H-HC-0.064200	-1	-8.446865	2.161036	4.127078	L
H-HC-0.064200	-1	-7.673455	2.050194	5.721275	L
H-HC-0.064200	-1	-9.386223	1.624111	5.520488	L
H-HO-0.410200	-1	-8.406242	0.082651	6.643354	L
N-N--0.254800	-1	-7.460645	-2.609333	3.209690	L
C-CT--0.026600	-1	-7.212989	-4.036110	3.378162	L
C-C-0.589600	-1	-6.603602	-4.392899	4.735231	L
O-O--0.574800	-1	-6.617055	-5.564000	5.097301	L
C-CT--0.007000	0	-6.236197	-4.391892	2.260626	L
C-CT-0.018900	0	-5.397097	-3.128015	2.119084	L
C-CT-0.019200	0	-6.390402	-2.004343	2.425473	L
H-H1-0.064100	-1	-8.124463	-4.604290	3.234415	L
H-HC-0.025300	0	-5.622398	-5.252241	2.520062	L
H-HC-0.025300	0	-6.786000	-4.575589	1.336668	L
H-HC-0.021300	0	-4.989914	-3.047294	1.114199	L
H-HC-0.021300	0	-4.594699	-3.129888	2.856934	L
H-H1-0.039100	0	-6.795299	-1.617792	1.489869	L

H-H1-0.039100	0	-5.891837	-1.208929	2.980801	L
N-N--0.415700	-1	-5.981980	-3.433071	5.428344	L
C-CT--0.001400	-1	-4.989667	-3.676825	6.486680	L
C-C-0.597300	-1	-5.537842	-4.459736	7.694226	L
O-O--0.567900	-1	-6.723651	-4.340983	8.006735	L
C-CT--0.001400	0	-4.452270	-2.329338	6.982574	L H-HA 373
C-CA--0.001100	0	-4.017658	-1.380150	5.881327	H
C-CA--0.190600	0	-3.112732	-1.799574	4.902396	H
C-CA--0.190600	0	-4.517426	-0.076045	5.833994	H
C-CA--0.234100	0	-2.703990	-0.934738	3.894116	H
C-CA--0.234100	0	-4.108518	0.805549	4.837712	H
C-C-0.322600	0	-3.185358	0.385691	3.870923	H
O-OH--0.557900	0	-2.779312	1.286521	2.949989	H
H-H-0.271900	-1	-6.047773	-2.493863	5.067434	L
H-H1-0.087600	-1	-4.166677	-4.246935	6.054270	L
H-HC-0.029500	0	-5.229970	-1.846009	7.576541	L
H-HC-0.029500	0	-3.598045	-2.507120	7.637013	L
H-HA-0.169900	0	-2.713734	-2.811362	4.908032	H
H-HA-0.169900	0	-5.222779	0.270430	6.590297	H
H-HA-0.165600	0	-1.975248	-1.260924	3.161237	H
H-HA-0.165600	0	-4.447851	1.837889	4.829551	H
H-HO-0.399200	0	-1.938285	0.989532	2.501470	H
N-N--0.415700	-1	-4.659673	-5.151768	8.446605	L
C-CT--0.149000	-1	-5.043349	-5.618047	9.795529	L
H-H-0.271900	-1	-3.665244	-5.146794	8.205644	L
H-H1-0.097600	-1	-6.126837	-5.565647	9.903316	L
H-H1-0.097600	-1	-4.572061	-4.985367	10.546905	L
H-H1-0.097600	-1	-4.714128	-6.648632	9.930444	L
C-CT--0.366200	-1	-0.501194	-10.770984	2.475203	L
C-C-0.597200	-1	-0.681527	-9.829372	1.271259	L
O-O--0.567900	-1	-1.791342	-9.652542	0.763956	L
H-HC-0.112300	-1	0.547141	-10.787338	2.769736	L
H-HC-0.112300	-1	-0.817178	-11.777384	2.199345	L
H-HC-0.112300	-1	-1.108008	-10.416521	3.308413	L
N-N--0.415700	-1	0.433139	-9.284741	0.766543	L
C-CT-0.014300	-1	0.389999	-8.266512	-0.282322	L H-HC 405
C-C-0.597300	-1	0.013642	-8.772717	-1.693571	L
O-O--0.567900	-1	-0.197062	-7.949011	-2.574505	L
C-CT--0.204100	0	1.727660	-7.494048	-0.303811	H
C-C-0.713000	0	1.508909	-5.997369	-0.549045	H
O-O--0.593100	0	1.003775	-5.321828	0.350516	H
N-N--0.919100	0	1.934043	-5.478378	-1.716996	H
H-H-0.271900	-1	1.316126	-9.474505	1.211499	L
H-H1-0.104800	-1	-0.410922	-7.592908	0.022919	L
H-HC-0.079700	0	2.404682	-7.962640	-1.028282	H
H-HC-0.079700	0	2.186015	-7.551876	0.686447	H
H-H-0.419600	0	1.830794	-4.468948	-1.905595	H
H-H-0.419600	0	2.237909	-6.085233	-2.466983	H
N-N--0.415700	-1	-0.085739	-10.085657	-1.931819	L
C-CT--0.149000	-1	-0.628627	-10.634631	-3.186530	L
H-H-0.271900	-1	0.023726	-10.735677	-1.145371	L
H-H1-0.097600	-1	-0.692383	-9.843155	-3.932552	L
H-H1-0.097600	-1	-1.622688	-11.043259	-3.004751	L
H-H1-0.097600	-1	0.027504	-11.426134	-3.550846	L

C-CT--0.366200	-1	-3.899469	-11.686224	-1.416506	L
C-C-0.597200	-1	-4.663549	-10.357950	-1.487087	L
O-O--0.567900	-1	-5.802953	-10.357548	-1.957235	L
H-HC-0.112300	-1	-2.915288	-11.515440	-0.979309	L
H-HC-0.112300	-1	-3.784731	-12.093293	-2.420121	L
H-HC-0.112300	-1	-4.453840	-12.391691	-0.797958	L
N-N--0.415700	-1	-4.032817	-9.232551	-1.111899	L
C-CT--0.087500	-1	-4.593433	-7.869986	-1.273843	L
C-C-0.597300	-1	-4.858750	-7.486266	-2.740757	L
O-O--0.567900	-1	-5.846005	-6.813844	-3.035098	L
C-CT-0.298500	-1	-3.682821	-6.796035	-0.622823	L
C-CT--0.319200	-1	-4.166392	-5.356731	-0.862257	L
C-CT--0.319200	-1	-3.666506	-6.933394	0.897188	L
H-H-0.271900	-1	-3.150701	-9.345936	-0.610563	L
H-H1-0.096900	-1	-5.553787	-7.845806	-0.760197	L
H-HC--0.029700	-1	-2.667875	-6.896719	-1.007815	L
H-HC-0.079100	-1	-5.201707	-5.257521	-0.535249	L
H-HC-0.079100	-1	-4.098568	-5.104815	-1.917948	L
H-HC-0.079100	-1	-3.536967	-4.651369	-0.317608	L
H-HC-0.079100	-1	-4.672346	-6.796029	1.276738	L
H-HC-0.079100	-1	-3.000332	-6.189632	1.336718	L
H-HC-0.079100	-1	-3.319795	-7.911827	1.198464	L
N-N--0.415700	-1	-4.013948	-7.887924	-3.698703	L
C-CT--0.149000	-1	-4.099778	-7.472857	-5.109648	L
H-H-0.271900	-1	-3.293809	-8.553045	-3.442762	L
H-H1-0.097600	-1	-4.916082	-6.760206	-5.230213	L
H-H1-0.097600	-1	-4.285071	-8.346692	-5.735868	L
H-H1-0.097600	-1	-3.162387	-7.004616	-5.408632	L
C-CT--0.366200	-1	-12.114734	3.718256	-1.303972	L
C-C-0.597200	-1	-11.013482	2.649105	-1.268756	L
O-O--0.567900	-1	-11.309767	1.466942	-1.113753	L
H-HC-0.112300	-1	-11.663679	4.700060	-1.448270	L
H-HC-0.112300	-1	-12.664398	3.705819	-0.362401	L
H-HC-0.112300	-1	-12.799269	3.508130	-2.126023	L
N-N--0.415700	-1	-9.755758	3.086369	-1.337234	L
C-CT--0.024900	-1	-8.575202	2.260937	-1.158698	L
C-C-0.597300	-1	-7.459939	3.123339	-0.562242	L
O-O--0.567900	-1	-6.805451	3.909862	-1.260905	L
C-CT-0.211700	0	-8.147070	1.600880	-2.467185	L
O-OH--0.654600	0	-7.195658	0.619641	-2.154132	L
H-H-0.271900	-1	-9.626584	4.082479	-1.407412	L
H-H1-0.084300	-1	-8.814428	1.469084	-0.450217	L
H-H1-0.035200	0	-7.726510	2.328617	-3.158366	L
H-H1-0.035200	0	-9.009300	1.116699	-2.927957	L
H-HO-0.427500	0	-6.288805	0.984730	-2.260656	L
N-N--0.415700	-1	-7.296959	3.048970	0.767581	L
C-CT-0.021300	-1	-6.119721	3.660996	1.402361	L
C-C-0.597300	-1	-4.833576	3.010713	0.867649	L
O-O--0.567900	-1	-3.856898	3.696226	0.606625	L
C-CT--0.123100	-1	-6.176674	3.524733	2.925475	L
S-SH--0.311900	-1	-7.426650	4.634558	3.634184	L
H-H-0.271900	-1	-7.959010	2.504255	1.316959	L
H-H1-0.112400	-1	-6.088437	4.722936	1.153577	L
H-H1-0.111200	-1	-5.204459	3.795095	3.341081	L

H-H1-0.111200	-1	-6.395520	2.490627	3.190436	L
H-HS-0.193300	-1	-8.470607	4.189540	2.925668	L
N-N--0.415700	-1	-4.875714	1.692014	0.661545	L H-HC 478
C-CT-0.021300	0	-3.745420	0.945458	0.089235	H
C-C-0.597300	0	-3.656040	1.238393	-1.398973	H
O-O--0.567900	0	-4.679714	1.385365	-2.072236	H
C-CT--0.123100	0	-4.033983	-0.536002	0.359646	H
S-SH--0.311900	0	-2.694587	-1.720557	-0.053190	H
H-H-0.271900	-1	-5.727966	1.206166	0.868013	L
H-H1-0.112400	0	-2.833278	1.248698	0.601907	H
H-H1-0.111200	0	-4.892027	-0.874207	-0.230298	H
H-H1-0.111200	0	-4.261509	-0.682965	1.414876	H
H-HS-0.193300	0	-1.832755	-1.363303	0.911978	H
N-N--0.415700	0	-2.402344	1.264954	-1.936518	H
C-CT--0.087500	0	-2.260306	1.384409	-3.381961	H
C-C-0.597300	0	-2.191651	0.039301	-4.142501	H
O-O--0.567900	0	-2.281108	0.062161	-5.368598	H
C-CT-0.298500	-1	-1.123417	2.303073	-3.865057	H
C-CT--0.319200	0	-1.241685	3.698815	-3.250287	L H-HC 492
C-CT--0.319200	0	0.290666	1.782577	-3.595786	L H-HC 492
H-H-0.271900	0	-1.593516	1.154121	-1.321006	H
H-H1-0.096900	0	-3.210355	1.809384	-3.723459	H
H-HC--0.029700	0	-1.235048	2.391680	-4.948449	H
H-HC-0.079100	0	-1.052071	3.655040	-2.175744	L
H-HC-0.079100	0	-2.239957	4.085707	-3.430089	L
H-HC-0.079100	0	-0.519237	4.366289	-3.716561	L
H-HC-0.079100	0	0.480803	1.768101	-2.522318	L
H-HC-0.079100	0	1.016505	2.430449	-4.076807	L
H-HC-0.079100	0	0.411851	0.779510	-3.998239	L
N-N--0.415700	0	-1.990008	-1.082096	-3.406211	H
C-CT--0.003100	0	-2.075556	-2.413372	-3.996925	H
C-C-0.597300	0	-3.537022	-2.866691	-4.171109	H
O-O--0.567900	0	-3.840534	-3.662659	-5.050786	H
C-CT--0.003600	-1	-1.315696	-3.437862	-3.109779	H
C-CT--0.064500	-1	-1.452440	-4.891629	-3.600412	L H-HC 508
C-C-0.695100	-1	-0.580955	-5.232007	-4.794584	L
O-O--0.608600	-1	-0.438008	-4.481081	-5.744582	L
N-N--0.940700	-1	0.029972	-6.397277	-4.790313	L
H-H-0.271900	0	-1.962145	-1.022406	-2.394594	H
H-H1-0.085000	0	-1.656343	-2.370095	-5.004524	H
H-HC-0.017100	0	-0.259060	-3.181776	-3.047526	H
H-HC-0.017100	0	-1.730569	-3.396479	-2.099049	H
H-HC-0.035200	-1	-2.481419	-5.144186	-3.840479	L
H-HC-0.035200	-1	-1.167958	-5.540354	-2.779351	L
H-H-0.425100	-1	0.631800	-6.646762	-5.555468	L
H-H-0.425100	-1	-0.080369	-7.018161	-3.990486	L
N-N--0.415700	0	-4.375422	-2.472486	-3.145375	H
C-CT--0.023700	0	-5.756385	-2.930401	-3.223087	H
C-C-0.597300	-1	-6.429814	-2.308488	-4.461488	L H-H1 522
O-O--0.567900	-1	-6.256670	-1.113538	-4.719975	L
C-CT-0.034200	-1	-6.488099	-2.649746	-1.895024	L H-H1 522
C-CT-0.001800	-1	-7.957556	-3.095669	-1.950381	L
S-S--0.273700	-1	-8.859508	-3.068187	-0.373864	L
C-CT--0.053600	-1	-9.224193	-1.299531	-0.241392	L

H-H-0.271900	0	-4.292170	-1.500900	-2.887262	H
H-H1-0.088000	0	-5.693084	-4.007411	-3.337762	H
H-HC-0.024100	-1	-6.415162	-1.603591	-1.634996	L
H-HC-0.024100	-1	-5.994877	-3.203650	-1.099811	L
H-H1-0.044000	-1	-7.985344	-4.121064	-2.320363	L
H-H1-0.044000	-1	-8.497263	-2.467808	-2.659645	L
H-H1-0.068400	-1	-9.828319	-1.113757	0.646584	L
H-H1-0.068400	-1	-9.774811	-0.968668	-1.122217	L
H-H1-0.068400	-1	-8.292987	-0.741548	-0.170664	L
N-N--0.254800	-1	-7.181337	-3.075827	-5.272635	L
C-CT--0.026600	-1	-7.579197	-2.657603	-6.617746	L
C-C-0.589600	-1	-9.027920	-2.170986	-6.607200	L
O-O--0.574800	-1	-9.914737	-2.869773	-6.109740	L
C-CT--0.007000	-1	-7.376518	-3.901367	-7.497573	L
C-CT-0.018900	-1	-6.860846	-4.965655	-6.525700	L
C-CT-0.019200	-1	-7.390392	-4.505129	-5.194011	L
H-H1-0.064100	-1	-6.930738	-1.861730	-6.983553	L
H-HC-0.025300	-1	-8.312156	-4.220016	-7.948101	L
H-HC-0.025300	-1	-6.641733	-3.717860	-8.279219	L
H-HC-0.021300	-1	-5.772689	-4.959702	-6.500985	L
H-HC-0.021300	-1	-7.237108	-5.947283	-6.741706	L
H-H1-0.039100	-1	-6.866032	-5.014567	-4.397256	L
H-H1-0.039100	-1	-8.456183	-4.723703	-5.118258	L
N-N--0.415700	-1	-9.249786	-0.973631	-7.142975	L
C-CT--0.149000	-1	-10.481647	-0.202230	-6.950842	L
H-H-0.271900	-1	-8.444741	-0.505433	-7.558451	L
H-H1-0.097600	-1	-11.242398	-0.839069	-6.499979	L
H-H1-0.097600	-1	-10.836116	0.160405	-7.915669	L
H-H1-0.097600	-1	-10.280337	0.644814	-6.294632	L
C-CT--0.366200	-1	-10.345220	8.876311	-4.213363	L
C-C-0.597200	-1	-9.797871	7.586136	-3.588549	L
O-O--0.567900	-1	-10.239554	7.166452	-2.517523	L
H-HC-0.112300	-1	-9.827752	9.073662	-5.152080	L
H-HC-0.112300	-1	-10.183921	9.707861	-3.527892	L
H-HC-0.112300	-1	-11.412325	8.763797	-4.404037	L
N-N--0.415700	-1	-8.829027	6.962200	-4.253274	L
C-CT--0.024900	-1	-7.885365	6.042043	-3.615067	L
C-C-0.597300	-1	-6.554229	6.771693	-3.395448	L
O-O--0.567900	-1	-6.298711	7.778898	-4.062846	L
C-CT-0.211700	0	-7.666278	4.787810	-4.473373	L
O-OH--0.654600	0	-7.293241	5.100242	-5.802165	L
H-H-0.271900	-1	-8.558981	7.330991	-5.164175	L
H-H1-0.084300	-1	-8.270439	5.702991	-2.653011	L
H-H1-0.035200	0	-8.588325	4.205493	-4.492668	L
H-H1-0.035200	0	-6.882300	4.180204	-4.018938	L
H-HO-0.427500	0	-6.860910	4.328687	-6.186419	L
N-N--0.415700	-1	-5.676109	6.238085	-2.535781	L
C-CT-0.033700	-1	-4.301338	6.744520	-2.434219	L
C-C-0.597300	-1	-3.555688	6.748548	-3.787744	L
O-O--0.567900	-1	-2.655387	7.560904	-4.005739	L
C-CT--0.182500	-1	-3.547602	5.921321	-1.399788	L
H-H-0.271900	-1	-5.959487	5.433116	-1.972162	L
H-H1-0.082300	-1	-4.346507	7.771818	-2.071153	L
H-HC-0.060300	-1	-2.533226	6.300990	-1.295830	L

H-HC-0.060300	-1	-3.514738	4.875380	-1.702921	L
H-HC-0.060300	-1	-4.061618	6.005132	-0.443532	L
N-N--0.415700	-1	-3.979867	5.883072	-4.722359	L
C-CT--0.149000	-1	-3.467040	5.829399	-6.090201	L
H-H-0.271900	-1	-4.709040	5.235447	-4.454553	L
H-H1-0.097600	-1	-2.692506	6.586089	-6.217439	L
H-H1-0.097600	-1	-4.279207	6.021279	-6.791255	L
H-H1-0.097600	-1	-3.046375	4.842327	-6.281904	L
C-CM--0.139000	0	1.393007	-1.956579	-0.019162	H
C-C-0.519000	0	1.360338	-1.772952	-1.452266	H
O-O2--0.567000	0	1.001824	-0.608441	-1.963715	H
C-CM--0.117000	0	1.061448	-1.077325	0.981482	H
O-O2--0.618000	0	1.702683	-2.684127	-2.250509	H
C-C--0.553000	0	0.160895	0.122161	0.933408	H
O-O2--0.556000	0	0.036030	0.808549	-0.144603	H
O-O2--0.607000	0	-0.539410	0.328713	1.968587	H
H-HC-0.049000	0	1.807523	-2.911219	0.281433	H
H-HC-0.162000	0	1.156774	-1.471184	1.982582	H
O-OW--0.834000	-1	6.434942	2.948499	-1.174936	L
H-HW-0.417000	-1	6.805168	3.089768	-2.045472	L
H-HW-0.417000	-1	7.115535	3.247553	-0.572339	L
O-OW--0.834000	0	3.446900	7.150579	1.055709	L
H-HW-0.417000	0	3.264668	6.248268	1.392105	L
H-HW-0.417000	0	3.824270	6.949530	0.182159	L
O-OW--0.834000	0	-1.058101	-3.786587	1.697307	H
H-HW-0.417000	0	-0.338482	-4.205313	1.193671	H
H-HW-0.417000	0	-1.837456	-3.920200	1.140590	H
O-OW--0.834000	0	-4.964712	0.858970	-6.127701	L
H-HW-0.417000	0	-4.026671	0.633167	-6.030966	L
H-HW-0.417000	0	-5.407424	0.197923	-5.569405	L
H-HS-0.193300	0	0.674782	0.032204	-1.229148	H

TS2

C-CT--0.366200	-1	8.218554	4.639898	-8.127399	L
C-C-0.597200	-1	9.048383	3.894801	-7.087204	L
O-O--0.567900	-1	9.648517	2.856876	-7.368322	L
H-HC-0.112300	-1	7.775652	5.526021	-7.672892	L
H-HC-0.112300	-1	7.427040	3.987018	-8.496957	L
H-HC-0.112300	-1	8.859218	4.939551	-8.957631	L
N-N--0.415700	-1	9.043275	4.453351	-5.870338	L
C-CT--0.087500	-1	9.514103	3.777807	-4.654092	L
C-C-0.597300	-1	8.376154	2.881045	-4.162444	L
O-O--0.567900	-1	7.465205	3.341453	-3.459141	L
C-CT-0.298500	-1	9.996691	4.779977	-3.578355	L
C-CT--0.319200	-1	10.415763	4.080749	-2.279613	L
C-CT--0.319200	-1	11.211569	5.587390	-4.058067	L
H-H-0.271900	-1	8.458424	5.275741	-5.743347	L
H-H1-0.096900	-1	10.351503	3.136260	-4.908024	L
H-HC--0.029700	-1	9.199773	5.485966	-3.362226	L
H-HC-0.079100	-1	11.121436	3.281625	-2.508460	L
H-HC-0.079100	-1	9.545152	3.658000	-1.781974	L
H-HC-0.079100	-1	10.892482	4.788859	-1.603678	L
H-HC-0.079100	-1	12.071718	4.930322	-4.186466	L
H-HC-0.079100	-1	11.457840	6.358403	-3.325891	L

H-HC-0.079100	-1	10.993646	6.066811	-5.011414	L
N-N--0.415700	-1	8.392377	1.608333	-4.593964	L
C-CT--0.087500	-1	7.279004	0.656663	-4.419106	L
C-C-0.597300	-1	7.694370	-0.618984	-3.657664	L
O-O--0.567900	-1	8.840217	-1.070949	-3.781811	L
C-CT-0.298500	-1	6.625789	0.249656	-5.764350	L
C-CT--0.319200	-1	5.768608	1.376366	-6.352773	L
C-CT--0.319200	-1	7.618670	-0.201709	-6.840713	L
H-H-0.271900	-1	9.167692	1.302107	-5.187691	L
H-H1-0.096900	-1	6.508068	1.163926	-3.846086	L
H-HC--0.029700	-1	5.956339	-0.590938	-5.578131	L
H-HC-0.079100	-1	6.286092	2.332571	-6.276864	L
H-HC-0.079100	-1	4.833397	1.424412	-5.799473	L
H-HC-0.079100	-1	5.520512	1.161149	-7.393412	L
H-HC-0.079100	-1	8.219410	0.642629	-7.174694	L
H-HC-0.079100	-1	7.069243	-0.604786	-7.690440	L
H-HC-0.079100	-1	8.272647	-0.974876	-6.445570	L
N-N--0.254800	-1	6.757923	-1.225174	-2.890080	L
C-CT--0.026600	-1	6.889426	-2.578175	-2.343017	L
C-C-0.589600	-1	7.137682	-3.601854	-3.452663	L
O-O--0.574800	-1	6.391169	-3.649476	-4.433386	L
C-CT--0.007000	0	5.557092	-2.890492	-1.644751	L
C-CT-0.018900	0	4.943615	-1.523220	-1.381534	L
C-CT-0.019200	0	5.439717	-0.690032	-2.552145	L
H-H1-0.064100	-1	7.707631	-2.593496	-1.623861	L
H-HC-0.025300	0	4.889607	-3.445245	-2.306106	L
H-HC-0.025300	0	5.708787	-3.450853	-0.726570	L
H-HC-0.021300	0	5.324970	-1.099317	-0.458312	L
H-HC-0.021300	0	3.861980	-1.567142	-1.344608	L
H-H1-0.039100	0	5.485113	0.354902	-2.243661	L
H-H1-0.039100	0	4.760327	-0.808022	-3.397837	L
N-N--0.415700	-1	8.162286	-4.447972	-3.303584	L
C-CT--0.149000	-1	8.532174	-5.444276	-4.321655	L
H-H-0.271900	-1	8.761030	-4.325660	-2.488010	L
H-H1-0.097600	-1	7.789152	-5.444184	-5.118506	L
H-H1-0.097600	-1	8.573407	-6.432906	-3.863433	L
H-H1-0.097600	-1	9.509154	-5.195468	-4.736049	L
C-CT--0.366200	-1	5.232313	-7.427676	-4.078355	L
C-C-0.597200	-1	4.103802	-6.756977	-4.871708	L
O-O--0.567900	-1	3.206273	-7.475106	-5.321720	L
H-HC-0.112300	-1	5.944049	-6.671308	-3.748245	L
H-HC-0.112300	-1	5.740887	-8.154189	-4.711952	L
H-HC-0.112300	-1	4.812728	-7.934366	-3.209183	L
N-N--0.415700	-1	4.092360	-5.426184	-5.011145	L
C-CT-0.014300	-1	2.990923	-4.678625	-5.642480	L H-HC 69
C-C-0.597300	-1	2.797865	-5.019431	-7.154854	L
O-O--0.567900	-1	3.793036	-5.184056	-7.861987	L
C-CT--0.204100	0	3.289304	-3.177703	-5.418234	H
C-C-0.713000	0	2.195548	-2.252400	-5.954912	H
O-O--0.593100	0	2.094922	-1.984449	-7.149486	H
N-N--0.919100	0	1.389316	-1.713776	-5.004141	H
H-H-0.271900	-1	4.860357	-4.888684	-4.642621	L
H-H1-0.104800	-1	2.082894	-4.942141	-5.109855	L
H-HC-0.079700	0	4.213183	-2.944896	-5.959464	H

H-HC-0.079700	0	3.450487	-3.013800	-4.349314	H
H-H-0.419600	0	0.551305	-1.274973	-5.363383	H
H-H-0.419600	0	1.436058	-1.986926	-4.021382	H
N-N--0.415700	-1	1.544763	-5.118500	-7.649421	L
C-CT--0.149000	-1	1.194259	-5.378442	-9.075472	L
H-H-0.271900	-1	0.788761	-4.892911	-7.003877	L
H-H1-0.097600	-1	2.100548	-5.603574	-9.637088	L
H-H1-0.097600	-1	0.714142	-4.495375	-9.498002	L
H-H1-0.097600	-1	0.511212	-6.225972	-9.131375	L
C-CT--0.366200	-1	11.721479	-5.931716	-0.618926	L
C-C-0.597200	-1	10.704567	-6.057665	0.523693	L
O-O--0.567900	-1	11.020364	-5.902585	1.708579	L
H-HC-0.112300	-1	11.221641	-6.107448	-1.571358	L
H-HC-0.112300	-1	12.513278	-6.667914	-0.483086	L
H-HC-0.112300	-1	12.152379	-4.930297	-0.614180	L
N-N--0.415700	-1	9.468407	-6.361548	0.131027	L
C-CT--0.023700	-1	8.307186	-6.558912	0.993676	L
C-C-0.597300	-1	7.253581	-7.402401	0.288394	L
O-O--0.567900	-1	7.076311	-7.243563	-0.926255	L
C-CT-0.034200	0	7.702378	-5.196918	1.378402	L
C-CT-0.001800	0	6.738758	-5.213162	2.581993	L
S-S--0.273700	0	5.015091	-5.724612	2.286761	L
C-CT--0.053600	0	4.204738	-4.118322	1.993912	L
H-H-0.271900	-1	9.300836	-6.435359	-0.866356	L
H-H1-0.088000	-1	8.630712	-7.090764	1.876783	L
H-HC-0.024100	0	7.197184	-4.763660	0.515488	L
H-HC-0.024100	0	8.533150	-4.545472	1.632557	L
H-H1-0.044000	0	6.705701	-4.206717	3.000010	L
H-H1-0.044000	0	7.161581	-5.861714	3.349163	L
H-H1-0.068400	0	3.157206	-4.268401	1.727184	L
H-H1-0.068400	0	4.694295	-3.583627	1.183043	L
H-H1-0.068400	0	4.249282	-3.502808	2.892701	L
N-N--0.415700	-1	6.544643	-8.247975	1.046655	L
C-CT--0.149000	-1	5.323228	-8.953993	0.631440	L
H-H-0.271900	-1	6.859716	-8.379403	2.007818	L
H-H1-0.097600	-1	5.107106	-8.723514	-0.411261	L
H-H1-0.097600	-1	4.488663	-8.633655	1.255345	L
H-H1-0.097600	-1	5.469450	-10.027940	0.743354	L
C-CT--0.366200	-1	3.883301	-9.353222	4.910987	L
C-C-0.597200	-1	3.714804	-7.947295	5.521430	L
O-O--0.567900	-1	4.676410	-7.231193	5.815862	L
H-HC-0.112300	-1	2.901301	-9.793909	4.735976	L
H-HC-0.112300	-1	4.446661	-9.983744	5.598628	L
H-HC-0.112300	-1	4.420286	-9.277067	3.965357	L
N-N--0.415700	-1	2.453188	-7.532730	5.667267	L
C-CT--0.087500	-1	2.016815	-6.128104	5.614147	L
C-C-0.597300	-1	1.893651	-5.569862	7.038311	L
O-O--0.567900	-1	0.856045	-5.662975	7.709436	L
C-CT-0.298500	0	0.680465	-5.977992	4.859051	L
C-CT--0.319200	0	0.243312	-4.513166	4.763489	L
C-CT--0.319200	0	0.777298	-6.554309	3.440199	L
H-H-0.271900	-1	1.717509	-8.226458	5.510290	L
H-H1-0.096900	-1	2.783207	-5.555209	5.088539	L
H-HC--0.029700	0	-0.092370	-6.535156	5.390742	L

H-HC-0.079100	0	0.920446	-3.948501	4.118565	L
H-HC-0.079100	0	0.206435	-4.036283	5.741254	L
H-HC-0.079100	0	-0.760284	-4.466556	4.346051	L
H-HC-0.079100	0	1.589112	-6.061494	2.902875	L
H-HC-0.079100	0	-0.155162	-6.364540	2.906501	L
H-HC-0.079100	0	0.951845	-7.626724	3.467330	L
N-N--0.415700	-1	3.053376	-5.117634	7.514664	L
C-CT--0.149000	-1	3.429104	-4.983328	8.919457	L
H-H-0.271900	-1	3.813243	-5.034608	6.849564	L
H-H1-0.097600	-1	2.541831	-5.088235	9.543996	L
H-H1-0.097600	-1	3.875215	-4.003219	9.084582	L
H-H1-0.097600	-1	4.149451	-5.759434	9.178283	L
C-CT--0.366200	-1	12.476466	-4.242844	6.358727	L
C-C-0.597200	-1	12.273595	-3.519496	5.008848	L
O-O--0.567900	-1	13.241507	-3.303467	4.272967	L
H-HC-0.112300	-1	11.516634	-4.342445	6.865591	L
H-HC-0.112300	-1	13.157301	-3.662746	6.982874	L
H-HC-0.112300	-1	12.898506	-5.231229	6.181712	L
N-N--0.415700	-1	11.038969	-3.092278	4.705291	L
C-CT--0.023700	-1	10.763875	-2.267333	3.531203	L
C-C-0.597300	-1	11.333352	-0.845053	3.668485	L
O-O--0.567900	-1	12.063461	-0.380191	2.791336	L
C-CT-0.034200	0	9.256904	-2.185341	3.267098	L
C-CT-0.001800	0	9.018194	-1.515320	1.907472	L
S-S--0.273700	0	7.432045	-1.891408	1.141361	L
C-CT--0.053600	0	6.272817	-0.951754	2.166929	L
H-H-0.271900	-1	10.273334	-3.320696	5.332977	L
H-H1-0.088000	-1	11.234560	-2.747120	2.671372	L
H-HC-0.024100	0	8.753147	-1.618246	4.051018	L
H-HC-0.024100	0	8.850110	-3.192192	3.261636	L
H-H1-0.044000	0	9.787025	-1.855894	1.212850	L
H-H1-0.044000	0	9.117398	-0.433741	2.009188	L
H-H1-0.068400	0	5.249343	-1.121649	1.824448	L
H-H1-0.068400	0	6.486346	0.113467	2.083154	L
H-H1-0.068400	0	6.350587	-1.268405	3.205083	L
N-N--0.415700	-1	11.065905	-0.156878	4.783851	L
C-CT--0.149000	-1	11.621087	1.180760	5.013888	L
H-H-0.271900	-1	10.486546	-0.587246	5.504093	L
H-H1-0.097600	-1	12.210234	1.482847	4.148116	L
H-H1-0.097600	-1	12.257935	1.162452	5.897901	L
H-H1-0.097600	-1	10.807978	1.890436	5.166562	L
C-CT--0.366200	-1	6.199427	8.716030	-5.545059	L
C-C-0.597200	-1	6.512062	7.523062	-4.620242	L
O-O--0.567900	-1	6.661904	6.374574	-5.061110	L
H-HC-0.112300	-1	6.108800	9.624687	-4.948922	L
H-HC-0.112300	-1	5.262043	8.532780	-6.071546	L
H-HC-0.112300	-1	7.005404	8.835944	-6.269728	L
N-N--0.415700	-1	6.655295	7.837491	-3.322564	L
C-CT--0.001400	-1	6.694817	6.845309	-2.232925	L
C-C-0.597300	-1	5.318601	6.167986	-2.092907	L
O-O--0.567900	-1	4.445792	6.649602	-1.353283	L
C-CT--0.001400	-1	7.212928	7.477115	-0.927777	L
C-CA--0.001100	-1	7.896246	6.504325	0.027354	L
C-CA--0.190600	-1	9.303943	6.451434	0.078435	L

C-CA--0.190600	-1	7.148387	5.684107	0.897076	L
C-CA--0.234100	-1	9.952535	5.629285	1.018889	L
C-CA--0.234100	-1	7.801328	4.856863	1.837256	L
C-C-0.322600	-1	9.203721	4.852074	1.916740	L
O-OH--0.557900	-1	9.862382	4.104679	2.849101	L
H-H-0.271900	-1	6.592703	8.829379	-3.080339	L
H-H1-0.087600	-1	7.404669	6.072105	-2.513074	L
H-HC-0.029500	-1	7.940005	8.247278	-1.188156	L
H-HC-0.029500	-1	6.401285	7.985495	-0.405834	L
H-HA-0.169900	-1	9.891353	7.074552	-0.580863	L
H-HA-0.169900	-1	6.067397	5.691898	0.853162	L
H-HA-0.165600	-1	11.029710	5.597925	1.068462	L
H-HA-0.165600	-1	7.225383	4.224856	2.497308	L
H-HO-0.399200	-1	9.365188	3.881714	3.652163	L
N-N--0.415700	-1	5.105192	5.147852	-2.928719	L
C-CT-0.033700	-1	3.787838	4.655480	-3.316443	L
C-C-0.597300	-1	2.949461	4.019687	-2.196585	L
O-O--0.567900	-1	1.726289	4.123002	-2.265544	L
C-CT--0.182500	-1	3.975096	3.657107	-4.453689	L
H-H-0.271900	-1	5.887869	4.853806	-3.507933	L
H-H1-0.082300	-1	3.223518	5.501580	-3.709847	L
H-HC-0.060300	-1	3.003657	3.348571	-4.839025	L
H-HC-0.060300	-1	4.510865	2.787494	-4.073007	L
H-HC-0.060300	-1	4.546696	4.117593	-5.259638	L
N-N--0.415700	-1	3.561785	3.375946	-1.191987	L H-HC 209
C-CT-0.021300	0	2.721483	2.626753	-0.193612	H
C-C-0.597300	0	2.333889	3.575102	0.956029	H
O-O--0.567900	0	3.186604	4.226593	1.555820	H
C-CT--0.123100	0	3.466011	1.341052	0.218497	H
S-S--1.036000	0	2.733229	0.195440	1.494988	H
H-H-0.271900	-1	4.565895	3.349620	-1.184151	L
H-H1-0.112400	0	1.812230	2.309244	-0.703680	H
H-H1-0.111200	0	4.423728	1.585958	0.694534	H
H-H1-0.111200	0	3.666029	0.761724	-0.683064	H
N-N--0.415700	0	0.994727	3.660214	1.234569	H
C-CT--0.051800	0	0.429354	4.506121	2.302080	H
C-C-0.597300	0	0.807497	4.000795	3.731784	H
O-O--0.567900	0	1.330178	4.740899	4.564527	H
C-CT--0.110200	-1	-1.111280	4.635825	2.039254	H
C-CT-0.353100	-1	-1.969268	5.540686	2.950202	L H-HC 222
C-CT--0.412100	-1	-2.161406	4.993130	4.365954	L
C-CT--0.412100	-1	-1.436895	6.973716	3.039737	L
H-H-0.271900	0	0.353423	3.038426	0.745299	H
H-H1-0.092200	0	0.898063	5.492681	2.246906	H
H-HC-0.045700	0	-1.227842	5.013920	1.016548	H
H-HC-0.045700	0	-1.565625	3.641172	2.059120	H
H-HC--0.036100	-1	-2.960927	5.590482	2.501816	L
H-HC-0.100000	-1	-1.262279	5.132714	4.962468	L
H-HC-0.100000	-1	-2.407557	3.933108	4.323908	L
H-HC-0.100000	-1	-2.980061	5.526565	4.846653	L
H-HC-0.100000	-1	-0.474738	6.988733	3.552686	L
H-HC-0.100000	-1	-2.147951	7.592618	3.585607	L
H-HC-0.100000	-1	-1.312889	7.376938	2.033801	L
N-N--0.415700	0	0.552246	2.684048	3.991701	H

C-CT--0.087500	0	0.598210	2.150751	5.359436	H
C-C-0.597300	0	1.995729	2.088290	5.986131	H
O-O--0.567900	0	2.095337	1.983081	7.205150	H
C-CT-0.298500	-1	-0.028638	0.735670	5.382037	H
C-CT--0.319200	0	0.817698	-0.338550	4.685423	L H-HC 241
C-CT--0.319200	0	-0.423134	0.208041	6.760872	L H-HC 241
H-H-0.271900	0	0.107858	2.123931	3.264813	H
H-H1-0.096900	0	0.026328	2.823275	6.011807	H
H-HC--0.029700	0	-0.954850	0.803315	4.812214	H
H-HC-0.079100	0	1.653865	-0.649038	5.307954	L
H-HC-0.079100	0	1.213674	0.076702	3.762016	L
H-HC-0.079100	0	0.198796	-1.198345	4.432754	L
H-HC-0.079100	0	0.463493	0.014483	7.362595	L
H-HC-0.079100	0	-0.982534	-0.719108	6.640922	L
H-HC-0.079100	0	-1.053744	0.941623	7.260239	L
N-N--0.415700	0	3.015073	1.939324	5.108553	H
C-CT-0.033700	0	4.378271	1.781942	5.568485	H
C-C-0.597300	-1	5.093631	3.110323	5.841245	L H-H1 254
O-O--0.567900	-1	6.268555	3.083853	6.197456	L
C-CT--0.182500	-1	5.151039	0.964225	4.534470	L H-H1 254
H-H-0.271900	0	2.862780	2.187502	4.141983	H
H-H1-0.082300	0	4.354421	1.234781	6.514201	H
H-HC-0.060300	-1	6.117347	0.669611	4.940752	L
H-HC-0.060300	-1	5.308545	1.566433	3.639970	L
H-HC-0.060300	-1	4.591495	0.063197	4.279895	L
N-N--0.415700	-1	4.392383	4.239573	5.678027	L
C-CT--0.087500	-1	4.777683	5.601115	6.076174	L
C-C-0.597300	-1	3.936468	6.048729	7.278722	L
O-O--0.567900	-1	4.489290	6.497012	8.284150	L
C-CT-0.298500	-1	4.564754	6.578200	4.902563	L
C-CT--0.319200	-1	4.961354	8.015722	5.256301	L
C-CT--0.319200	-1	5.381470	6.182534	3.672767	L
H-H-0.271900	-1	3.480970	4.127311	5.251634	L
H-H1-0.096900	-1	5.827639	5.627717	6.357791	L
H-HC--0.029700	-1	3.512338	6.568031	4.626591	L
H-HC-0.079100	-1	6.011902	8.050950	5.536438	L
H-HC-0.079100	-1	4.355656	8.392947	6.079546	L
H-HC-0.079100	-1	4.802010	8.656314	4.389248	L
H-HC-0.079100	-1	6.431412	6.101939	3.948286	L
H-HC-0.079100	-1	5.266245	6.931472	2.889649	L
H-HC-0.079100	-1	5.027396	5.226640	3.286764	L
N-N--0.415700	-1	2.604788	5.860632	7.224650	L
C-CT--0.149000	-1	1.698049	6.200478	8.331923	L
H-H-0.271900	-1	2.197373	5.481908	6.375120	L
H-H1-0.097600	-1	2.276387	6.593244	9.168271	L
H-H1-0.097600	-1	1.160472	5.306221	8.648829	L
H-H1-0.097600	-1	0.984299	6.953999	7.999065	L
C-CT--0.366200	-1	4.066312	10.302696	-0.973624	L
C-C-0.597200	-1	2.590911	9.979307	-1.218943	L
O-O--0.567900	-1	1.783210	10.895879	-1.290525	L
H-HC-0.112300	-1	4.639896	9.377494	-0.938824	L
H-HC-0.112300	-1	4.168965	10.830272	-0.025552	L
H-HC-0.112300	-1	4.439361	10.931389	-1.781777	L
N-N--0.415700	-1	2.209626	8.697191	-1.276305	L

C-CT--0.024900	-1	0.795534	8.318113	-1.117925	L
C-C-0.597300	-1	0.209449	8.815087	0.209297	L
O-O--0.567900	-1	-0.883882	9.384776	0.217747	L
C-CT-0.211700	0	0.618885	6.818858	-1.271183	L
O-OH--0.654600	0	0.911502	6.513527	-2.614741	L
H-H-0.271900	-1	2.910624	7.963229	-1.337712	L
H-H1-0.084300	-1	0.224074	8.770301	-1.924267	L
H-H1-0.035200	0	-0.407058	6.534921	-1.046068	L
H-H1-0.035200	0	1.294711	6.283805	-0.602960	L
H-HO-0.427500	0	1.023073	5.537977	-2.627426	L
N-N--0.415700	-1	0.971469	8.677743	1.305070	L
C-CT-0.033700	-1	0.618329	9.158093	2.642215	L
C-C-0.597300	-1	0.156436	10.620189	2.635314	L
O-O--0.567900	-1	-0.939453	10.940187	3.098274	L
C-CT--0.182500	-1	1.804287	8.917727	3.573919	L
H-H-0.271900	-1	1.859034	8.179820	1.199359	L
H-H1-0.082300	-1	-0.197673	8.567053	3.031090	L
H-HC-0.060300	-1	1.574901	9.287553	4.572611	L
H-HC-0.060300	-1	2.690833	9.418056	3.186473	L
H-HC-0.060300	-1	1.997400	7.848111	3.627084	L
N-N--0.415700	-1	0.956432	11.498390	2.020800	L
C-CT--0.149000	-1	0.618732	12.896855	1.829593	L
H-H-0.271900	-1	1.858434	11.189069	1.666867	L
H-H1-0.097600	-1	-0.367013	13.093297	2.252753	L
H-H1-0.097600	-1	0.608929	13.126548	0.764974	L
H-H1-0.097600	-1	1.359247	13.521362	2.330334	L
C-CT--0.366200	-1	-11.919045	4.595134	4.974297	L
C-C-0.597200	-1	-12.354213	3.177109	4.601209	L
O-O--0.567900	-1	-12.920895	2.469328	5.436203	L
H-HC-0.112300	-1	-11.438560	5.064964	4.116002	L
H-HC-0.112300	-1	-11.215155	4.552525	5.805581	L
H-HC-0.112300	-1	-12.791892	5.178287	5.266189	L
N-N--0.415700	-1	-12.020788	2.736901	3.387642	L
C-CT--0.087500	-1	-12.019248	1.314857	3.026933	L
C-C-0.597300	-1	-10.573849	0.917916	2.713034	L
O-O--0.567900	-1	-9.857271	1.561341	1.938625	L
C-CT-0.298500	-1	-13.015935	0.927690	1.901856	L
C-CT--0.319200	-1	-13.765659	-0.361629	2.285792	L
C-CT--0.319200	-1	-14.092216	1.977919	1.593559	L
H-H-0.271900	-1	-11.609219	3.388041	2.716506	L
H-H1-0.096900	-1	-12.313010	0.755039	3.912468	L
H-HC--0.029700	-1	-12.457324	0.737903	0.989004	L
H-HC-0.079100	-1	-14.397860	-0.179613	3.155568	L
H-HC-0.079100	-1	-13.051203	-1.155496	2.507230	L
H-HC-0.079100	-1	-14.402840	-0.674687	1.458891	L
H-HC-0.079100	-1	-14.725682	2.122454	2.465248	L
H-HC-0.079100	-1	-14.700244	1.643924	0.754222	L
H-HC-0.079100	-1	-13.633529	2.929649	1.334286	L
N-N--0.415700	-1	-10.112186	-0.103717	3.436851	L
C-CT--0.038900	-1	-8.704749	-0.503374	3.518730	L
C-C-0.597300	-1	-8.579243	-2.029172	3.630380	L
O-O--0.567900	-1	-9.511257	-2.688533	4.112320	L
C-CT-0.365400	-1	-7.987125	0.141463	4.728343	L
O-OH--0.676100	-1	-8.156319	-0.574102	5.930417	L

C-CT--0.243800	-1	-8.403297	1.578275	5.037312	L
H-H-0.271900	-1	-10.742479	-0.576196	4.068720	L
H-H1-0.100700	-1	-8.203849	-0.169783	2.609994	L
H-H1-0.004300	-1	-6.928046	0.139912	4.492081	L
H-HC-0.064200	-1	-8.445727	2.143959	4.114048	L
H-HC-0.064200	-1	-7.674483	2.033369	5.709311	L
H-HC-0.064200	-1	-9.386593	1.605854	5.505983	L
H-HO-0.410200	-1	-8.406871	0.064950	6.629836	L
N-N--0.254800	-1	-7.454072	-2.625314	3.196813	L
C-CT--0.026600	-1	-7.205418	-4.051920	3.365264	L
C-C-0.589600	-1	-6.597643	-4.408535	4.723101	L
O-O--0.574800	-1	-6.610596	-5.579745	5.084847	L
C-CT--0.007000	0	-6.219176	-4.396432	2.249560	L
C-CT-0.018900	0	-5.378028	-3.129753	2.118825	L
C-CT-0.019200	0	-6.380541	-2.012960	2.416802	L
H-H1-0.064100	-1	-8.116195	-4.620852	3.220074	L
H-HC-0.025300	0	-5.605696	-5.257813	2.506408	L
H-HC-0.025300	0	-6.763119	-4.575471	1.321247	L
H-HC-0.021300	0	-4.952757	-3.039846	1.120939	L
H-HC-0.021300	0	-4.587056	-3.131439	2.868822	L
H-H1-0.039100	0	-6.782255	-1.631710	1.477634	L
H-H1-0.039100	0	-5.889036	-1.211810	2.970356	L
N-N--0.415700	-1	-5.977841	-3.448351	5.417345	L
C-CT--0.001400	-1	-4.986818	-3.691525	6.477022	L
C-C-0.597300	-1	-5.536027	-4.475226	7.683586	L
O-O--0.567900	-1	-6.722381	-4.357583	7.994444	L
C-CT--0.001400	0	-4.442590	-2.351109	6.986435	L H-HA 373
C-CA--0.001100	0	-4.061948	-1.349327	5.911132	H
C-CA--0.190600	0	-3.177836	-1.698319	4.885202	H
C-CA--0.190600	0	-4.586773	-0.054717	5.948994	H
C-CA--0.234100	0	-2.819296	-0.770914	3.911495	H
C-CA--0.234100	0	-4.230660	0.885367	4.987805	H
C-C-0.322600	0	-3.335789	0.535674	3.969043	H
O-OH--0.557900	0	-3.009163	1.488552	3.069208	H
H-H-0.271900	-1	-6.043935	-2.509108	5.056587	L
H-H1-0.087600	-1	-4.162720	-4.260806	6.045634	L
H-HC-0.029500	0	-5.200344	-1.898300	7.628387	L
H-HC-0.029500	0	-3.562426	-2.539634	7.602322	L
H-HA-0.169900	0	-2.761158	-2.700545	4.817594	H
H-HA-0.169900	0	-5.276877	0.236948	6.741882	H
H-HA-0.165600	0	-2.119495	-1.049166	3.130653	H
H-HA-0.165600	0	-4.600922	1.906253	5.037449	H
H-HO-0.399200	0	-2.165027	1.268616	2.592935	H
N-N--0.415700	-1	-4.658324	-5.166695	8.437030	L
C-CT--0.149000	-1	-5.043509	-5.633660	9.785286	L
H-H-0.271900	-1	-3.663559	-5.160798	8.197480	L
H-H1-0.097600	-1	-6.127193	-5.582229	9.891550	L
H-H1-0.097600	-1	-4.573833	-5.000770	10.537495	L
H-H1-0.097600	-1	-4.713584	-6.663995	9.920401	L
C-CT--0.366200	-1	-0.486514	-10.780738	2.470062	L
C-C-0.597200	-1	-0.665953	-9.838963	1.266109	L
O-O--0.567900	-1	-1.775205	-9.662964	0.757281	L
H-HC-0.112300	-1	0.561418	-10.796259	2.766077	L
H-HC-0.112300	-1	-0.801231	-11.787337	2.193495	L

H-HC-0.112300	-1	-1.094817	-10.427015	3.302504	L
N-N--0.415700	-1	0.448951	-9.293235	0.763118	L
C-CT-0.014300	-1	0.406467	-8.274633	-0.285522	L H-HC 405
C-C-0.597300	-1	0.032499	-8.780931	-1.697453	L
O-O--0.567900	-1	-0.177668	-7.957177	-2.578472	L
C-CT--0.204100	0	1.706137	-7.434365	-0.296537	H
C-C-0.713000	0	1.401546	-5.929760	-0.449503	H
O-O--0.593100	0	0.813066	-5.345707	0.460756	H
N-N--0.919100	0	1.857545	-5.304462	-1.555958	H
H-H-0.271900	-1	1.331472	-9.482351	1.209276	L
H-H1-0.104800	-1	-0.395519	-7.601940	0.018740	L
H-HC-0.079700	0	2.386135	-7.825626	-1.062826	H
H-HC-0.079700	0	2.194743	-7.526848	0.676931	H
H-H-0.419600	0	1.686426	-4.297462	-1.697711	H
H-H-0.419600	0	2.216425	-5.842777	-2.333168	H
N-N--0.415700	-1	-0.065404	-10.093892	-1.936186	L
C-CT--0.149000	-1	-0.606037	-10.643007	-3.191808	L
H-H-0.271900	-1	0.043506	-10.744023	-1.149756	L
H-H1-0.097600	-1	-0.669420	-9.851392	-3.937716	L
H-H1-0.097600	-1	-1.600000	-11.052546	-3.011546	L
H-H1-0.097600	-1	0.051297	-11.433845	-3.555401	L
C-CT--0.366200	-1	-3.878473	-11.697902	-1.426701	L
C-C-0.597200	-1	-4.643605	-10.370274	-1.498017	L
O-O--0.567900	-1	-5.782341	-10.370732	-1.969781	L
H-HC-0.112300	-1	-2.895061	-11.526375	-0.988064	L
H-HC-0.112300	-1	-3.761956	-12.104608	-2.430256	L
H-HC-0.112300	-1	-4.433107	-12.404006	-0.809123	L
N-N--0.415700	-1	-4.014380	-9.244424	-1.121641	L
C-CT--0.087500	-1	-4.575945	-7.882303	-1.284025	L
C-C-0.597300	-1	-4.839518	-7.498428	-2.751214	L
O-O--0.567900	-1	-5.826936	-6.826785	-3.046775	L
C-CT-0.298500	-1	-3.667190	-6.807733	-0.631435	L
C-CT--0.319200	-1	-4.151671	-5.368786	-0.871176	L
C-CT--0.319200	-1	-3.652911	-6.945478	0.888565	L
H-H-0.271900	-1	-3.132876	-9.357177	-0.619085	L
H-H1-0.096900	-1	-5.537048	-7.859091	-0.771734	L
H-HC--0.029700	-1	-2.651613	-6.907437	-1.015013	L
H-HC-0.079100	-1	-5.187531	-5.270561	-0.545611	L
H-HC-0.079100	-1	-4.082568	-5.116536	-1.926705	L
H-HC-0.079100	-1	-3.523626	-4.663023	-0.325452	L
H-HC-0.079100	-1	-4.659408	-6.809084	1.266723	L
H-HC-0.079100	-1	-2.988005	-6.201252	1.329231	L
H-HC-0.079100	-1	-3.305780	-7.923688	1.190076	L
N-N--0.415700	-1	-3.993010	-7.899102	-3.708066	L
C-CT--0.149000	-1	-4.077198	-7.483738	-5.119022	L
H-H-0.271900	-1	-3.272656	-8.563665	-3.451277	L
H-H1-0.097600	-1	-4.893951	-6.771765	-5.240558	L
H-H1-0.097600	-1	-4.260845	-8.357567	-5.745732	L
H-H1-0.097600	-1	-3.139790	-7.014608	-5.416555	L
C-CT--0.366200	-1	-12.107245	3.699421	-1.321792	L
C-C-0.597200	-1	-11.005117	2.631220	-1.285294	L
O-O--0.567900	-1	-11.300593	1.448760	-1.131020	L
H-HC-0.112300	-1	-11.656836	4.681654	-1.465195	L
H-HC-0.112300	-1	-12.658233	3.686263	-0.381004	L

H-HC-0.112300	-1	-12.790427	3.488921	-2.144867	L
N-N--0.415700	-1	-9.747673	3.069593	-1.351876	L
C-CT--0.024900	-1	-8.566656	2.245134	-1.171879	L
C-C-0.597300	-1	-7.452989	3.108347	-0.573619	L
O-O--0.567900	-1	-6.798193	3.895617	-1.271147	L
C-CT-0.211700	0	-8.138351	1.587585	-2.481664	L
O-OH--0.654600	0	-7.191375	0.601049	-2.173059	L
H-H-0.271900	-1	-9.619264	4.065831	-1.421607	L
H-H1-0.084300	-1	-8.806198	1.452887	-0.463946	L
H-H1-0.035200	0	-7.714237	2.316323	-3.169628	L
H-H1-0.035200	0	-9.001788	1.108643	-2.945663	L
H-HO-0.427500	0	-6.283345	0.968606	-2.260429	L
N-N--0.415700	-1	-7.291832	3.033771	0.756415	L
C-CT-0.021300	-1	-6.116023	3.646647	1.393026	L
C-C-0.597300	-1	-4.828561	2.997624	0.859967	L
O-O--0.567900	-1	-3.852108	3.684052	0.600510	L
C-CT--0.123100	-1	-6.175019	3.509937	2.916019	L
S-SH--0.311900	-1	-7.426958	4.618494	3.623247	L
H-H-0.271900	-1	-7.954187	2.488338	1.304713	L
H-H1-0.112400	-1	-6.085312	4.708683	1.144562	L
H-H1-0.111200	-1	-5.203628	3.781033	3.333077	L
H-H1-0.111200	-1	-6.393345	2.475575	3.180400	L
H-HS-0.193300	-1	-8.469527	4.172756	2.913136	L
N-N--0.415700	-1	-4.869125	1.678861	0.653456	L H-HC 478
C-CT-0.021300	0	-3.684939	0.973094	0.091920	H
C-C-0.597300	0	-3.646232	1.235598	-1.407607	H
O-O--0.567900	0	-4.682154	1.382149	-2.060765	H
C-CT--0.123100	0	-3.782412	-0.523407	0.431879	H
S-SH--0.311900	0	-2.501990	-1.702123	-0.239943	H
H-H-0.271900	-1	-5.721384	1.192300	0.858592	L
H-H1-0.112400	0	-2.784445	1.384023	0.554838	H
H-H1-0.111200	0	-4.698626	-0.944234	-0.000999	H
H-H1-0.111200	0	-3.824673	-0.655919	1.511890	H
H-HS-0.193300	0	-1.029407	-1.418036	-0.050433	H
N-N--0.415700	0	-2.402631	1.257368	-1.967020	H
C-CT--0.087500	0	-2.256433	1.372001	-3.408346	H
C-C-0.597300	0	-2.159795	0.027289	-4.173267	H
O-O--0.567900	0	-2.199280	0.061281	-5.402754	H
C-CT-0.298500	-1	-1.111176	2.294474	-3.867744	H
C-CT--0.319200	0	-1.244557	3.692691	-3.258926	L H-HC 492
C-CT--0.319200	0	0.295456	1.781506	-3.569268	L H-HC 492
H-H-0.271900	0	-1.589642	1.190549	-1.352426	H
H-H1-0.096900	0	-3.203906	1.793572	-3.762918	H
H-HC--0.029700	0	-1.198862	2.379815	-4.953741	H
H-HC-0.079100	0	-1.074341	3.653076	-2.180574	L
H-HC-0.079100	0	-2.240672	4.076133	-3.456702	L
H-HC-0.079100	0	-0.515142	4.360749	-3.713255	L
H-HC-0.079100	0	0.471335	1.838841	-2.497912	L
H-HC-0.079100	0	1.027830	2.398274	-4.080916	L
H-HC-0.079100	0	0.415463	0.753645	-3.903338	L
N-N--0.415700	0	-1.966210	-1.091434	-3.432140	H
C-CT--0.003100	0	-2.056672	-2.428816	-4.013788	H
C-C-0.597300	0	-3.519445	-2.884440	-4.191371	H
O-O--0.567900	0	-3.820608	-3.661409	-5.093039	H

C-CT--0.003600	-1	-1.299383	-3.446734	-3.114225	H
C-CT--0.064500	-1	-1.434263	-4.900635	-3.605288	L H-HC 508
C-C-0.695100	-1	-0.560769	-5.239921	-4.798382	L
O-O--0.608600	-1	-0.417126	-4.488624	-5.747983	L
N-N--0.940700	-1	0.051159	-6.404664	-4.793549	L
H-H-0.271900	0	-2.061267	-1.045097	-2.417089	H
H-H1-0.085000	0	-1.638747	-2.392111	-5.021986	H
H-HC-0.017100	0	-0.246370	-3.182073	-3.033397	H
H-HC-0.017100	0	-1.730719	-3.407129	-2.111587	H
H-HC-0.035200	-1	-2.462661	-5.153998	-3.846951	L
H-HC-0.035200	-1	-1.150364	-5.549308	-2.784068	L
H-H-0.425100	-1	0.654289	-6.653424	-5.557916	L
H-H-0.425100	-1	-0.059778	-7.025852	-3.994042	L
N-N--0.415700	0	-4.355882	-2.519522	-3.167928	H
C-CT--0.023700	0	-5.741804	-2.949581	-3.235337	H
C-C-0.597300	-1	-6.412623	-2.321565	-4.472800	L H-H1 522
O-O--0.567900	-1	-6.240153	-1.126396	-4.730745	L
C-CT-0.034200	-1	-6.474275	-2.663548	-1.906531	L H-H1 522
C-CT-0.001800	-1	-7.943247	-3.110725	-1.964084	L
S-S--0.273700	-1	-8.847456	-3.084438	-0.388840	L
C-CT--0.053600	-1	-9.213863	-1.316134	-0.256425	L
H-H-0.271900	0	-4.200863	-1.618003	-2.751438	H
H-H1-0.088000	0	-5.694813	-4.027890	-3.346534	H
H-HC-0.024100	-1	-6.402593	-1.617394	-1.646123	L
H-HC-0.024100	-1	-5.981681	-3.217229	-1.110763	L
H-H1-0.044000	-1	-7.969618	-4.136048	-2.334371	L
H-H1-0.044000	-1	-8.482492	-2.483147	-2.673950	L
H-H1-0.068400	-1	-9.819406	-1.131117	0.630741	L
H-H1-0.068400	-1	-9.763517	-0.985519	-1.137942	L
H-H1-0.068400	-1	-8.283243	-0.757364	-0.184230	L
N-N--0.254800	-1	-7.162335	-3.089338	-5.285228	L
C-CT--0.026600	-1	-7.558650	-2.671108	-6.630792	L
C-C-0.589600	-1	-9.007805	-2.185750	-6.622178	L
O-O--0.574800	-1	-9.894724	-2.885434	-6.126153	L
C-CT--0.007000	-1	-7.353647	-3.914466	-7.510655	L
C-CT-0.018900	-1	-6.838431	-4.978561	-6.538334	L
C-CT-0.019200	-1	-7.370262	-4.518840	-5.207276	L
H-H1-0.064100	-1	-6.910364	-1.874575	-6.995473	L
H-HC-0.025300	-1	-8.288366	-4.233807	-7.962595	L
H-HC-0.025300	-1	-6.617912	-3.730116	-8.291217	L
H-HC-0.021300	-1	-5.750315	-4.971670	-6.512072	L
H-HC-0.021300	-1	-7.213533	-5.960459	-6.755129	L
H-H1-0.039100	-1	-6.846591	-5.028035	-4.409909	L
H-H1-0.039100	-1	-8.435970	-4.738358	-5.133090	L
N-N--0.415700	-1	-9.229953	-0.988445	-7.157952	L
C-CT--0.149000	-1	-10.462751	-0.218165	-6.967364	L
H-H-0.271900	-1	-8.424727	-0.519440	-7.572161	L
H-H1-0.097600	-1	-11.223593	-0.855778	-6.517744	L
H-H1-0.097600	-1	-10.816168	0.144416	-7.932598	L
H-H1-0.097600	-1	-10.263109	0.628881	-6.310648	L
C-CT--0.366200	-1	-10.338077	8.859773	-4.227322	L
C-C-0.597200	-1	-9.790498	7.569909	-3.602071	L
O-O--0.567900	-1	-10.233334	7.149561	-2.531779	L
H-HC-0.112300	-1	-9.819451	9.057818	-5.165254	L

H-HC-0.112300	-1	-10.178474	9.691284	-3.541406	L
H-HC-0.112300	-1	-11.404814	8.746385	-4.419537	L
N-N--0.415700	-1	-8.820174	6.946987	-4.265585	L
C-CT--0.024900	-1	-7.876617	6.027482	-3.626279	L
C-C-0.597300	-1	-6.546429	6.758228	-3.404584	L
O-O--0.567900	-1	-6.290838	7.765828	-4.071355	L
C-CT-0.211700	0	-7.655375	4.774076	-4.485085	L
O-OH--0.654600	0	-7.284854	5.088133	-5.814333	L
H-H-0.271900	-1	-8.549156	7.316254	-5.176004	L
H-H1-0.084300	-1	-8.262761	5.687844	-2.664860	L
H-H1-0.035200	0	-8.576126	4.189689	-4.503568	L
H-H1-0.035200	0	-6.869522	4.168125	-4.031646	L
H-HO-0.427500	0	-6.852087	4.317683	-6.199943	L
N-N--0.415700	-1	-5.669063	6.225156	-2.543813	L
C-CT-0.033700	-1	-4.294877	6.732755	-2.440168	L
C-C-0.597300	-1	-3.547313	6.737785	-3.792634	L
O-O--0.567900	-1	-2.647409	7.550978	-4.009138	L
C-CT--0.182500	-1	-3.541895	5.909936	-1.404883	L
H-H-0.271900	-1	-5.952543	5.419794	-1.980804	L
H-H1-0.082300	-1	-4.341453	7.759916	-2.076897	L
H-HC-0.060300	-1	-2.527998	6.290459	-1.299389	L
H-HC-0.060300	-1	-3.507696	4.864104	-1.708242	L
H-HC-0.060300	-1	-4.057338	5.993054	-0.449337	L
N-N--0.415700	-1	-3.969417	5.872185	-4.728074	L
C-CT--0.149000	-1	-3.454606	5.819316	-6.095202	L
H-H-0.271900	-1	-4.698407	5.223860	-4.461473	L
H-H1-0.097600	-1	-2.680548	6.576713	-6.221144	L
H-H1-0.097600	-1	-4.265944	6.010679	-6.797358	L
H-H1-0.097600	-1	-3.032816	4.832660	-6.286565	L
C-CM--0.139000	0	0.761377	-1.623245	0.001228	H
C-C-0.519000	0	1.269066	-1.492881	-1.318218	H
O-O2--0.567000	0	1.483088	-0.233400	-1.780551	H
C-CM--0.117000	0	0.985250	-0.584836	1.057697	H
O-O2--0.618000	0	1.552755	-2.436010	-2.104570	H
C-C--0.553000	0	0.009053	0.577577	1.008276	H
O-O2--0.556000	0	-0.092336	1.216470	-0.093965	H
O-O2--0.607000	0	-0.658656	0.839311	2.049670	H
H-HC-0.049000	0	0.800385	-2.642617	0.370358	H
H-HC-0.162000	0	0.830899	-1.101556	2.001876	H
O-OW--0.834000	-1	6.442890	2.945709	-1.166653	L
H-HW-0.417000	-1	6.814230	3.087526	-2.036627	L
H-HW-0.417000	-1	7.122371	3.245196	-0.563016	L
O-OW--0.834000	0	3.303547	6.877867	1.078131	L
H-HW-0.417000	0	3.201605	5.971078	1.431760	L
H-HW-0.417000	0	3.695744	6.705996	0.206030	L
O-OW--0.834000	0	-1.062194	-3.535955	2.033711	H
H-HW-0.417000	0	-0.488131	-4.156463	1.555112	H
H-HW-0.417000	0	-1.701655	-3.254623	1.358376	H
O-OW--0.834000	0	-4.919069	0.792607	-6.191946	L
H-HW-0.417000	0	-3.980563	0.575392	-6.086199	L
H-HW-0.417000	0	-5.361451	0.150809	-5.611331	L
H-HS-0.193300	0	0.948595	0.377864	-1.210510	H

IC2

C-CT--0.366200	-1	8.188862	4.661426	-8.130106	L
C-C-0.597200	-1	9.021190	3.918125	-7.090623	L
O-O--0.567900	-1	9.623273	2.881466	-7.372241	L
H-HC-0.112300	-1	7.744485	5.546621	-7.675234	L
H-HC-0.112300	-1	7.398407	4.006857	-8.498945	L
H-HC-0.112300	-1	8.828154	4.962413	-8.960912	L
N-N--0.415700	-1	9.015971	4.476700	-5.873772	L
C-CT--0.087500	-1	9.489305	3.802192	-4.657919	L
C-C-0.597300	-1	8.353697	2.903036	-4.165241	L
O-O--0.567900	-1	7.442397	3.361529	-3.461148	L
C-CT-0.298500	-1	9.970719	4.805418	-3.582640	L
C-CT--0.319200	-1	10.392420	4.107123	-2.284249	L
C-CT--0.319200	-1	11.183456	5.615392	-4.063448	L
H-H-0.271900	-1	8.429489	5.297851	-5.746287	L
H-H1-0.096900	-1	10.327841	3.162415	-4.912574	L
H-HC--0.029700	-1	9.172494	5.509721	-3.365828	L
H-HC-0.079100	-1	11.099583	3.309487	-2.513698	L
H-HC-0.079100	-1	9.523150	3.682538	-1.785831	L
H-HC-0.079100	-1	10.868234	4.816264	-1.608756	L
H-HC-0.079100	-1	12.044882	4.960148	-4.192589	L
H-HC-0.079100	-1	11.428737	6.386949	-3.331514	L
H-HC-0.079100	-1	10.963672	6.094320	-5.016616	L
N-N--0.415700	-1	8.372236	1.630348	-4.596739	L
C-CT--0.087500	-1	7.261041	0.676324	-4.420868	L
C-C-0.597300	-1	7.679788	-0.598418	-3.659758	L
O-O--0.567900	-1	8.826482	-1.047957	-3.784906	L
C-CT-0.298500	-1	6.607504	0.267890	-5.765524	L
C-CT--0.319200	-1	5.747415	1.392758	-6.353222	L
C-CT--0.319200	-1	7.600388	-0.181404	-6.842752	L
H-H-0.271900	-1	9.147676	1.325747	-5.191142	L
H-H1-0.096900	-1	6.489538	1.181966	-3.847184	L
H-HC--0.029700	-1	5.940002	-0.574118	-5.578687	L
H-HC-0.079100	-1	6.262936	2.350062	-6.277797	L
H-HC-0.079100	-1	4.812594	1.438836	-5.799095	L
H-HC-0.079100	-1	5.498857	1.176986	-7.393633	L
H-HC-0.079100	-1	8.199040	0.664199	-7.177287	L
H-HC-0.079100	-1	7.051067	-0.585670	-7.691981	L
H-HC-0.079100	-1	8.256353	-0.953167	-6.448162	L
N-N--0.254800	-1	6.745306	-1.206570	-2.891331	L
C-CT--0.026600	-1	6.880166	-2.559271	-2.344342	L
C-C-0.589600	-1	7.129609	-3.582456	-3.454178	L
O-O--0.574800	-1	6.382332	-3.631693	-4.434240	L
C-CT--0.007000	0	5.556607	-2.858075	-1.628748	L
C-CT-0.018900	0	5.013855	-1.471333	-1.316643	L
C-CT-0.019200	0	5.442214	-0.661701	-2.524572	L
H-H1-0.064100	-1	7.699034	-2.572835	-1.625911	L
H-HC-0.025300	0	4.856829	-3.365452	-2.295082	L
H-HC-0.025300	0	5.709229	-3.448795	-0.729992	L
H-HC-0.021300	0	5.480858	-1.049700	-0.435300	L
H-HC-0.021300	0	3.945842	-1.472913	-1.183327	L
H-H1-0.039100	0	5.494425	0.389583	-2.240539	L
H-H1-0.039100	0	4.729411	-0.806008	-3.338302	L
N-N--0.415700	-1	8.156140	-4.426395	-3.305981	L

C-CT--0.149000	-1	8.527241	-5.421941	-4.324349	L
H-H-0.271900	-1	8.755342	-4.302788	-2.490941	L
H-H1-0.097600	-1	7.783513	-5.423450	-5.120543	L
H-H1-0.097600	-1	8.570974	-6.410470	-3.866136	L
H-H1-0.097600	-1	9.503321	-5.171077	-4.739617	L
C-CT--0.366200	-1	5.231810	-7.412333	-4.078075	L
C-C-0.597200	-1	4.101175	-6.744053	-4.870449	L
O-O--0.567900	-1	3.204775	-7.464097	-5.319649	L
H-HC-0.112300	-1	5.942233	-6.654445	-3.748616	L
H-HC-0.112300	-1	5.741363	-8.137783	-4.712099	L
H-HC-0.112300	-1	4.814071	-7.919884	-3.208518	L
N-N--0.415700	-1	4.086788	-5.413292	-5.009915	L
C-CT-0.014300	-1	2.983237	-4.668062	-5.640285	L H-HC 69
C-C-0.597300	-1	2.789540	-5.009355	-7.152490	L
O-O--0.567900	-1	3.784431	-5.171885	-7.860499	L
C-CT--0.204100	0	3.275975	-3.162341	-5.433073	H
C-C-0.713000	0	2.215190	-2.238203	-6.042298	H
O-O--0.593100	0	2.196394	-1.967380	-7.238708	H
N-N--0.919100	0	1.346578	-1.697232	-5.146381	H
H-H-0.271900	-1	4.853972	-4.874148	-4.642087	L
H-H1-0.104800	-1	2.076215	-4.933515	-5.106862	L
H-HC-0.079700	0	4.221910	-2.943038	-5.940565	H
H-HC-0.079700	0	3.392477	-2.978625	-4.361990	H
H-H-0.419600	0	0.510795	-1.280886	-5.540757	H
H-H-0.419600	0	1.336511	-2.002615	-4.180414	H
N-N--0.415700	-1	1.536213	-5.111091	-7.645948	L
C-CT--0.149000	-1	1.185004	-5.371823	-9.071681	L
H-H-0.271900	-1	0.780305	-4.887090	-6.999740	L
H-H1-0.097600	-1	2.091269	-5.595047	-9.634091	L
H-H1-0.097600	-1	0.702639	-4.489787	-9.493810	L
H-H1-0.097600	-1	0.503707	-6.220802	-9.126955	L
C-CT--0.366200	-1	11.720841	-5.902503	-0.624430	L
C-C-0.597200	-1	10.705211	-6.030573	0.519096	L
O-O--0.567900	-1	11.021724	-5.874786	1.703698	L
H-HC-0.112300	-1	11.220538	-6.079321	-1.576411	L
H-HC-0.112300	-1	12.514320	-6.637016	-0.489267	L
H-HC-0.112300	-1	12.149619	-4.900168	-0.620090	L
N-N--0.415700	-1	9.469351	-6.337089	0.127529	L
C-CT--0.023700	-1	8.309315	-6.536890	0.991207	L
C-C-0.597300	-1	7.256878	-7.382633	0.286886	L
O-O--0.567900	-1	7.078196	-7.224209	-0.927611	L
C-CT-0.034200	0	7.701777	-5.180440	1.385613	L
C-CT-0.001800	0	6.774603	-5.205772	2.617331	L
S-S--0.273700	0	5.052272	-5.749932	2.381793	L
C-CT--0.053600	0	4.223289	-4.167027	2.026661	L
H-H-0.271900	-1	9.301055	-6.411286	-0.869705	L
H-H1-0.088000	-1	8.634746	-7.068027	1.874048	L
H-HC-0.024100	0	7.167798	-4.756115	0.535843	L
H-HC-0.024100	0	8.532965	-4.520468	1.615900	L
H-H1-0.044000	0	6.735561	-4.197281	3.029655	L
H-H1-0.044000	0	7.232713	-5.840566	3.375672	L
H-H1-0.068400	0	3.167584	-4.336685	1.810473	L
H-H1-0.068400	0	4.678771	-3.680816	1.166830	L
H-H1-0.068400	0	4.298605	-3.499030	2.885187	L

N-N--0.415700	-1	6.550406	-8.229688	1.045798	L
C-CT--0.149000	-1	5.330123	-8.938306	0.631680	L
H-H-0.271900	-1	6.866607	-8.360416	2.006683	L
H-H1-0.097600	-1	5.112594	-8.708317	-0.410834	L
H-H1-0.097600	-1	4.495435	-8.619722	1.256316	L
H-H1-0.097600	-1	5.478723	-10.011936	0.743499	L
C-CT--0.366200	-1	3.894833	-9.340459	4.912512	L
C-C-0.597200	-1	3.723892	-7.934872	5.523064	L
O-O--0.567900	-1	4.684235	-7.216722	5.816622	L
H-HC-0.112300	-1	2.913614	-9.783234	4.738381	L
H-HC-0.112300	-1	4.460133	-9.969765	5.599672	L
H-HC-0.112300	-1	4.430819	-9.263195	3.966404	L
N-N--0.415700	-1	2.461529	-7.522981	5.670003	L
C-CT--0.087500	-1	2.022130	-6.119286	5.617229	L
C-C-0.597300	-1	1.899041	-5.561262	7.041483	L
O-O--0.567900	-1	0.862228	-5.656555	7.713528	L
C-CT-0.298500	0	0.700193	-5.962775	4.834211	L
C-CT--0.319200	0	0.298492	-4.491329	4.691259	L
C-CT--0.319200	0	0.812595	-6.563629	3.424802	L
H-H-0.271900	-1	1.727186	-8.218274	5.513696	L
H-H1-0.096900	-1	2.786839	-5.544780	5.090926	L
H-HC--0.029700	0	-0.094704	-6.492988	5.360623	L
H-HC-0.079100	0	1.045133	-3.941290	4.113714	L
H-HC-0.079100	0	0.184657	-4.016627	5.664948	L
H-HC-0.079100	0	-0.656703	-4.418259	4.172934	L
H-HC-0.079100	0	1.639611	-6.090845	2.892377	L
H-HC-0.079100	0	-0.106989	-6.371382	2.870421	L
H-HC-0.079100	0	0.971984	-7.637774	3.472577	L
N-N--0.415700	-1	3.058225	-5.106560	7.516797	L
C-CT--0.149000	-1	3.434911	-4.971415	8.921256	L
H-H-0.271900	-1	3.817325	-5.021942	6.851023	L
H-H1-0.097600	-1	2.548414	-5.078183	9.546580	L
H-H1-0.097600	-1	3.879087	-3.990358	9.085959	L
H-H1-0.097600	-1	4.157130	-5.745982	9.179465	L
C-CT--0.366200	-1	12.478412	-4.211817	6.352506	L
C-C-0.597200	-1	12.272813	-3.488943	5.002785	L
O-O--0.567900	-1	13.239614	-3.270884	4.266045	L
H-HC-0.112300	-1	11.519243	-4.313438	6.860222	L
H-HC-0.112300	-1	13.158566	-3.630255	6.976034	L
H-HC-0.112300	-1	12.902393	-5.199309	6.175148	L
N-N--0.415700	-1	11.037017	-3.064354	4.700308	L
C-CT--0.023700	-1	10.759135	-2.240030	3.526440	L
C-C-0.597300	-1	11.325717	-0.816539	3.663178	L
O-O--0.567900	-1	12.054060	-0.350158	2.785370	L
C-CT-0.034200	0	9.252977	-2.161850	3.275385	L
C-CT-0.001800	0	9.004284	-1.471811	1.930403	L
S-S--0.273700	0	7.439356	-1.905632	1.163161	L
C-CT--0.053600	0	6.244316	-1.023755	2.199736	L
H-H-0.271900	-1	10.272424	-3.294374	5.328679	L
H-H1-0.088000	-1	11.230077	-2.718843	2.666209	L
H-HC-0.024100	0	8.750881	-1.610355	4.071460	L
H-HC-0.024100	0	8.853275	-3.171354	3.255707	L
H-H1-0.044000	0	9.787797	-1.769145	1.232263	L
H-H1-0.044000	0	9.057584	-0.389276	2.054271	L

H-H1-0.068400	0	5.229300	-1.251031	1.867475	L
H-H1-0.068400	0	6.396029	0.051283	2.105441	L
H-H1-0.068400	0	6.348419	-1.326930	3.239512	L
N-N--0.415700	-1	11.057793	-0.128901	4.778762	L
C-CT--0.149000	-1	11.610341	1.209920	5.008268	L
H-H-0.271900	-1	10.479985	-0.560475	5.499528	L
H-H1-0.097600	-1	12.198080	1.513230	4.141967	L
H-H1-0.097600	-1	12.248008	1.192990	5.891718	L
H-H1-0.097600	-1	10.795863	1.917872	5.161640	L
C-CT--0.366200	-1	6.163375	8.733346	-5.546102	L
C-C-0.597200	-1	6.479358	7.541071	-4.621524	L
O-O--0.567900	-1	6.631246	6.392888	-5.062495	L
H-HC-0.112300	-1	6.071348	9.641823	-4.949909	L
H-HC-0.112300	-1	5.225919	8.548093	-6.071754	L
H-HC-0.112300	-1	6.968456	8.854946	-6.271484	L
N-N--0.415700	-1	6.623070	7.855845	-3.323984	L
C-CT--0.001400	-1	6.665661	6.863784	-2.234353	L
C-C-0.597300	-1	5.291009	6.183545	-2.093097	L
O-O--0.567900	-1	4.417833	6.663331	-1.352716	L
C-CT--0.001400	-1	7.183581	7.496725	-0.929679	L
C-CA--0.001100	-1	7.869809	6.525416	0.024875	L
C-CA--0.190600	-1	9.277658	6.475514	0.074714	L
C-CA--0.190600	-1	7.124458	5.703641	0.895281	L
C-CA--0.234100	-1	9.928824	5.654770	1.014618	L
C-CA--0.234100	-1	7.779985	4.877810	1.834910	L
C-C-0.322600	-1	9.182454	4.876003	1.913152	L
O-OH--0.557900	-1	9.843522	4.130036	2.844951	L
H-H-0.271900	-1	6.558586	8.847603	-3.081731	L
H-H1-0.087600	-1	7.376902	6.092078	-2.515106	L
H-HC-0.029500	-1	7.908793	8.268420	-1.190723	L
H-HC-0.029500	-1	6.371324	8.003399	-0.407035	L
H-HA-0.169900	-1	9.863161	7.099857	-0.585120	L
H-HA-0.169900	-1	6.043418	5.709137	0.852323	L
H-HA-0.165600	-1	11.006106	5.625699	1.063237	L
H-HA-0.165600	-1	7.205965	4.244604	2.495485	L
H-HO-0.399200	-1	9.347514	3.906038	3.648459	L
N-N--0.415700	-1	5.079028	5.162935	-2.928690	L
C-CT-0.033700	-1	3.762376	4.667755	-3.315237	L
C-C-0.597300	-1	2.926342	4.030220	-2.194618	L
O-O--0.567900	-1	1.702894	4.130938	-2.262498	L
C-CT--0.182500	-1	3.950748	3.669748	-4.452620	L
H-H-0.271900	-1	5.861811	4.870531	-3.508589	L
H-H1-0.082300	-1	3.195914	5.512643	-3.708164	L
H-HC-0.060300	-1	2.979625	3.359140	-4.837085	L
H-HC-0.060300	-1	4.488694	2.801288	-4.072385	L
H-HC-0.060300	-1	4.520656	4.131420	-5.259085	L
N-N--0.415700	-1	3.541251	3.387913	-1.190780	L H-HC 209
C-CT-0.021300	0	2.718910	2.623394	-0.194688	H
C-C-0.597300	0	2.308699	3.564547	0.953673	H
O-O--0.567900	0	3.154896	4.222662	1.554810	H
C-CT--0.123100	0	3.531444	1.384553	0.225484	H
S-S--1.036000	0	2.911256	0.252671	1.561047	H
H-H-0.271900	-1	4.545088	3.363617	-1.183595	L
H-H1-0.112400	0	1.824554	2.265601	-0.704348	H

H-H1-0.111200	0	4.490814	1.683961	0.665267	H
H-H1-0.111200	0	3.742004	0.794778	-0.667636	H
N-N--0.415700	0	0.969512	3.635174	1.235234	H
C-CT--0.051800	0	0.407563	4.495539	2.298602	H
C-C-0.597300	0	0.790098	3.996126	3.726698	H
O-O--0.567900	0	1.303074	4.742070	4.559731	H
C-CT--0.110200	-1	-1.132213	4.637824	2.044939	H
C-CT-0.353100	-1	-1.991065	5.540972	2.956426	L H-HC 222
C-CT--0.412100	-1	-2.180779	4.993023	4.372408	L
C-CT--0.412100	-1	-1.461641	6.975099	3.045493	L
H-H-0.271900	0	0.329103	3.010523	0.752843	H
H-H1-0.092200	0	0.885595	5.476373	2.231067	H
H-HC-0.045700	0	-1.251977	5.016230	1.022852	H
H-HC-0.045700	0	-1.594958	3.645787	2.065730	H
H-HC--0.036100	-1	-2.983210	5.588614	2.508958	L
H-HC-0.100000	-1	-1.281423	5.134530	4.968122	L
H-HC-0.100000	-1	-2.424715	3.932478	4.330610	L
H-HC-0.100000	-1	-3.000137	5.524734	4.853815	L
H-HC-0.100000	-1	-0.499066	6.992173	3.557590	L
H-HC-0.100000	-1	-2.173527	7.592508	3.591971	L
H-HC-0.100000	-1	-1.339382	7.378550	2.039435	L
N-N--0.415700	0	0.551213	2.676343	3.988179	H
C-CT--0.087500	0	0.588776	2.153074	5.360882	H
C-C-0.597300	0	1.983602	2.088718	5.991542	H
O-O--0.567900	0	2.082070	1.965327	7.208215	H
C-CT-0.298500	-1	-0.037855	0.740092	5.386648	H
C-CT--0.319200	0	0.826404	-0.345810	4.726890	L H-HC 241
C-CT--0.319200	0	-0.471576	0.230410	6.760053	L H-HC 241
H-H-0.271900	0	0.125940	2.103727	3.261606	H
H-H1-0.096900	0	0.013936	2.832218	6.003161	H
H-HC--0.029700	0	-0.948051	0.800601	4.791148	H
H-HC-0.079100	0	1.627032	-0.669822	5.388000	L
H-HC-0.079100	0	1.274605	0.060701	3.822475	L
H-HC-0.079100	0	0.207193	-1.194961	4.440662	L
H-HC-0.079100	0	0.397147	0.050561	7.391293	L
H-HC-0.079100	0	-1.022200	-0.701388	6.636008	L
H-HC-0.079100	0	-1.120973	0.967688	7.228850	L
N-N--0.415700	0	3.004513	1.951975	5.111870	H
C-CT-0.033700	0	4.367753	1.796097	5.570179	H
C-C-0.597300	-1	5.079537	3.125616	5.841353	L H-H1 254
O-O--0.567900	-1	6.254831	3.101686	6.196512	L
C-CT--0.182500	-1	5.140190	0.979714	4.534622	L H-H1 254
H-H-0.271900	0	2.855517	2.238386	4.155894	H
H-H1-0.082300	0	4.345065	1.248724	6.515575	H
H-HC-0.060300	-1	6.107635	0.687093	4.940011	L
H-HC-0.060300	-1	5.295785	1.582160	3.639919	L
H-HC-0.060300	-1	4.582489	0.077421	4.280521	L
N-N--0.415700	-1	4.375754	4.253411	5.678708	L
C-CT--0.087500	-1	4.758513	5.615778	6.076477	L
C-C-0.597300	-1	3.917417	6.061642	7.279752	L
O-O--0.567900	-1	4.470174	6.511130	8.284677	L
C-CT-0.298500	-1	4.542475	6.592372	4.903024	L
C-CT--0.319200	-1	4.936338	8.030745	5.256370	L
C-CT--0.319200	-1	5.358942	6.198402	3.672518	L

H-H-0.271900	-1	3.464205	4.139200	5.253125	L
H-H1-0.096900	-1	5.808659	5.644617	6.357164	L
H-HC--0.029700	-1	3.489842	6.579963	4.627983	L
H-HC-0.079100	-1	5.987056	8.068211	5.535578	L
H-HC-0.079100	-1	4.330569	8.406709	6.080138	L
H-HC-0.079100	-1	4.774870	8.670973	4.389439	L
H-HC-0.079100	-1	6.409297	6.120046	3.947112	L
H-HC-0.079100	-1	5.241437	6.947070	2.889483	L
H-HC-0.079100	-1	5.006555	5.241749	3.286855	L
N-N--0.415700	-1	2.586090	5.870723	7.226863	L
C-CT--0.149000	-1	1.679612	6.208676	8.334928	L
H-H-0.271900	-1	2.178730	5.491106	6.377707	L
H-H1-0.097600	-1	2.257854	6.602694	9.170754	L
H-H1-0.097600	-1	1.144215	5.313290	8.652335	L
H-H1-0.097600	-1	0.963972	6.960669	8.002680	L
C-CT--0.366200	-1	4.030940	10.315623	-0.972828	L
C-C-0.597200	-1	2.556010	9.989099	-1.216832	L
O-O--0.567900	-1	1.746306	10.903950	-1.287728	L
H-HC-0.112300	-1	4.606518	9.391640	-0.938506	L
H-HC-0.112300	-1	4.133311	10.843445	-0.024861	L
H-HC-0.112300	-1	4.401939	10.945083	-1.781327	L
N-N--0.415700	-1	2.177397	8.706174	-1.273821	L
C-CT--0.024900	-1	0.764254	8.324101	-1.114179	L
C-C-0.597300	-1	0.178288	8.819872	0.213544	L
O-O--0.567900	-1	-0.916241	9.387240	0.222947	L
C-CT-0.211700	0	0.590725	6.824493	-1.268586	L
O-OH--0.654600	0	0.883627	6.520658	-2.612434	L
H-H-0.271900	-1	2.879897	7.973698	-1.335826	L
H-H1-0.084300	-1	0.191122	8.775049	-1.920028	L
H-H1-0.035200	0	-0.434599	6.538390	-1.043561	L
H-H1-0.035200	0	1.267729	6.290244	-0.601004	L
H-HO-0.427500	0	0.997940	5.545430	-2.626640	L
N-N--0.415700	-1	0.941568	8.684176	1.308648	L
C-CT-0.033700	-1	0.588589	9.163816	2.646090	L
C-C-0.597300	-1	0.123593	10.624931	2.639557	L
O-O--0.567900	-1	-0.972564	10.942619	3.103475	L
C-CT--0.182500	-1	1.775878	8.925997	3.576754	L
H-H-0.271900	-1	1.830093	8.188136	1.202168	L
H-H1-0.082300	-1	-0.225815	8.571060	3.035704	L
H-HC-0.060300	-1	1.546592	9.295368	4.575639	L
H-HC-0.060300	-1	2.661018	9.428195	3.188509	L
H-HC-0.060300	-1	1.971307	7.856793	3.629779	L
N-N--0.415700	-1	0.921179	11.504807	2.024309	L
C-CT--0.149000	-1	0.580341	12.902546	1.833360	L
H-H-0.271900	-1	1.823523	11.197390	1.669589	L
H-H1-0.097600	-1	-0.405445	13.096913	2.257386	L
H-H1-0.097600	-1	0.569112	13.132188	0.768743	L
H-H1-0.097600	-1	1.319975	13.528639	2.333431	L
C-CT--0.366200	-1	-11.937011	4.574342	4.989387	L
C-C-0.597200	-1	-12.369496	3.155387	4.616723	L
O-O--0.567900	-1	-12.933937	2.446430	5.452239	L
H-HC-0.112300	-1	-11.458279	5.045164	4.130653	L
H-HC-0.112300	-1	-11.232296	4.533252	5.820050	L
H-HC-0.112300	-1	-12.810834	5.155653	5.282033	L

N-N--0.415700	-1	-12.036212	2.715850	3.402874	L
C-CT--0.087500	-1	-12.031974	1.293799	3.042207	L
C-C-0.597300	-1	-10.586010	0.899918	2.727040	L
O-O--0.567900	-1	-9.871489	1.544839	1.951979	L
C-CT-0.298500	-1	-13.028829	0.904484	1.918024	L
C-CT--0.319200	-1	-13.775480	-0.386410	2.302658	L
C-CT--0.319200	-1	-14.107609	1.952416	1.610645	L
H-H-0.271900	-1	-11.626619	3.367839	2.731358	L
H-H1-0.096900	-1	-12.323764	0.733389	3.928018	L
H-HC--0.029700	-1	-12.470623	0.715857	1.004682	L
H-HC-0.079100	-1	-14.407294	-0.205707	3.172989	L
H-HC-0.079100	-1	-13.059145	-1.178752	2.523487	L
H-HC-0.079100	-1	-14.412724	-0.700841	1.476330	L
H-HC-0.079100	-1	-14.740611	2.095638	2.482891	L
H-HC-0.079100	-1	-14.715670	1.617109	0.771856	L
H-HC-0.079100	-1	-13.651170	2.905113	1.350940	L
N-N--0.415700	-1	-10.121545	-0.120712	3.450482	L
C-CT--0.038900	-1	-8.713189	-0.517377	3.531125	L
C-C-0.597300	-1	-8.584348	-2.042902	3.642710	L
O-O--0.567900	-1	-9.514535	-2.704227	4.125494	L
C-CT-0.365400	-1	-7.995867	0.129015	4.740087	L
O-OH--0.676100	-1	-8.162482	-0.586868	5.942329	L
C-CT--0.243800	-1	-8.414814	1.564951	5.049380	L
H-H-0.271900	-1	-10.750276	-0.594509	4.082918	L
H-H1-0.100700	-1	-8.213806	-0.182755	2.621938	L
H-H1-0.004300	-1	-6.936999	0.129705	4.502889	L
H-HC-0.064200	-1	-8.459261	2.130516	4.126138	L
H-HC-0.064200	-1	-7.686373	2.021610	5.720722	L
H-HC-0.064200	-1	-9.397752	1.590459	5.518921	L
H-HO-0.410200	-1	-8.413769	0.051670	6.641950	L
N-N--0.254800	-1	-7.458301	-2.636670	3.208165	L
C-CT--0.026600	-1	-7.206471	-4.062740	3.376436	L
C-C-0.589600	-1	-6.596745	-4.418025	4.733747	L
O-O--0.574800	-1	-6.606891	-5.589246	5.095537	L
C-CT--0.007000	0	-6.226818	-4.411948	2.258252	L
C-CT-0.018900	0	-5.390109	-3.145087	2.119932	L
C-CT-0.019200	0	-6.388807	-2.026052	2.424851	L
H-H1-0.064100	-1	-8.116167	-4.633608	3.232070	L
H-HC-0.025300	0	-5.611076	-5.271359	2.516089	L
H-HC-0.025300	0	-6.775258	-4.595102	1.333399	L
H-HC-0.021300	0	-4.975878	-3.059234	1.117851	L
H-HC-0.021300	0	-4.591920	-3.146481	2.861723	L
H-H1-0.039100	0	-6.794629	-1.641920	1.488684	L
H-H1-0.039100	0	-5.893799	-1.227469	2.979036	L
N-N--0.415700	-1	-5.978363	-3.456506	5.427416	L
C-CT--0.001400	-1	-4.985891	-3.697542	6.486225	L
C-C-0.597300	-1	-5.532367	-4.482371	7.693295	L
O-O--0.567900	-1	-6.718693	-4.367235	8.005199	L
C-CT--0.001400	0	-4.441046	-2.349148	6.975818	L H-HA 373
C-CA--0.001100	0	-4.031047	-1.377670	5.879843	H
C-CA--0.190600	0	-3.164177	-1.774379	4.855417	H
C-CA--0.190600	0	-4.515063	-0.066479	5.889571	H
C-CA--0.234100	0	-2.780184	-0.883025	3.858505	H
C-CA--0.234100	0	-4.127662	0.842113	4.908928	H

C-C-0.322600	0	-3.245709	0.441302	3.897597	H
O-OH--0.557900	0	-2.859840	1.371926	2.995660	H
H-H-0.271900	-1	-6.046771	-2.517414	5.066690	L
H-H1-0.087600	-1	-4.160971	-4.265089	6.054122	L
H-HC-0.029500	0	-5.207776	-1.875677	7.591515	L
H-HC-0.029500	0	-3.573759	-2.529398	7.612126	L
H-HA-0.169900	0	-2.780984	-2.791153	4.807198	H
H-HA-0.169900	0	-5.194700	0.264063	6.676251	H
H-HA-0.165600	0	-2.105651	-1.203378	3.071688	H
H-HA-0.165600	0	-4.462359	1.875956	4.939518	H
H-HO-0.399200	0	-2.055191	1.080567	2.501434	H
N-N--0.415700	-1	-4.652535	-5.171952	8.445981	L
C-CT--0.149000	-1	-5.035536	-5.639693	9.794591	L
H-H-0.271900	-1	-3.657998	-5.163950	8.205553	L
H-H1-0.097600	-1	-6.119233	-5.590556	9.901813	L
H-H1-0.097600	-1	-4.566542	-5.005783	10.546367	L
H-H1-0.097600	-1	-4.703308	-6.669321	9.929444	L
C-CT--0.366200	-1	-0.474099	-10.777316	2.475492	L
C-C-0.597200	-1	-0.656603	-9.835964	1.271670	L
O-O--0.567900	-1	-1.766671	-9.662332	0.763818	L
H-HC-0.112300	-1	0.574122	-10.790606	2.770581	L
H-HC-0.112300	-1	-0.786927	-11.784590	2.199230	L
H-HC-0.112300	-1	-1.082414	-10.424862	3.308460	L
N-N--0.415700	-1	0.456699	-9.287885	0.767677	L
C-CT-0.014300	-1	0.411085	-8.269529	-0.280984	L H-HC 405
C-C-0.597300	-1	0.036986	-8.776540	-1.692541	L
O-O--0.567900	-1	-0.175709	-7.953260	-2.573395	L
C-CT--0.204100	0	1.729157	-7.462622	-0.290263	H
C-C-0.713000	0	1.485991	-5.960605	-0.513976	H
O-O--0.593100	0	0.970469	-5.288139	0.376531	H
N-N--0.919100	0	1.936508	-5.430360	-1.676892	H
H-H-0.271900	-1	1.340011	-9.475114	1.213062	L
H-H1-0.104800	-1	-0.392018	-7.598408	0.023997	L
H-HC-0.079700	0	2.417470	-7.904368	-1.020641	H
H-HC-0.079700	0	2.189202	-7.526893	0.699063	H
H-H-0.419600	0	1.803548	-4.434105	-1.862792	H
H-H-0.419600	0	2.190287	-6.029825	-2.451260	H
N-N--0.415700	-1	-0.058344	-10.089716	-1.931147	L
C-CT--0.149000	-1	-0.598920	-10.640015	-3.186277	L
H-H-0.271900	-1	0.052643	-10.739590	-1.144794	L
H-H1-0.097600	-1	-0.664643	-9.848558	-3.932148	L
H-H1-0.097600	-1	-1.591852	-11.051654	-3.005123	L
H-H1-0.097600	-1	0.059768	-11.429468	-3.550427	L
C-CT--0.366200	-1	-3.867549	-11.701793	-1.418244	L
C-C-0.597200	-1	-4.635556	-10.375792	-1.488924	L
O-O--0.567900	-1	-5.774705	-10.378684	-1.959680	L
H-HC-0.112300	-1	-2.884115	-11.528171	-0.980483	L
H-HC-0.112300	-1	-3.751058	-12.108282	-2.421893	L
H-HC-0.112300	-1	-4.420138	-12.409058	-0.800157	L
N-N--0.415700	-1	-4.008391	-9.248601	-1.113136	L
C-CT--0.087500	-1	-4.572989	-7.887679	-1.275062	L
C-C-0.597300	-1	-4.838670	-7.504409	-2.742029	L
O-O--0.567900	-1	-5.827774	-6.834872	-3.036740	L
C-CT-0.298500	-1	-3.665938	-6.811165	-0.623307	L

C-CT--0.319200	-1	-4.153680	-5.373256	-0.862662	L
C-CT--0.319200	-1	-3.650023	-6.948831	0.896682	L
H-H-0.271900	-1	-3.126207	-9.359467	-0.611356	L
H-H1-0.096900	-1	-5.533685	-7.866489	-0.761924	L
H-HC--0.029700	-1	-2.650491	-6.908724	-1.007780	L
H-HC-0.079100	-1	-5.189462	-5.277217	-0.536185	L
H-HC-0.079100	-1	-4.086047	-5.120891	-1.918259	L
H-HC-0.079100	-1	-3.526657	-4.666144	-0.317513	L
H-HC-0.079100	-1	-4.656472	-6.814562	1.275727	L
H-HC-0.079100	-1	-2.986310	-6.203185	1.336740	L
H-HC-0.079100	-1	-3.300551	-7.926295	1.197914	L
N-N--0.415700	-1	-3.992160	-7.903316	-3.699617	L
C-CT--0.149000	-1	-4.078478	-7.488177	-5.110510	L
H-H-0.271900	-1	-3.270173	-8.566343	-3.443447	L
H-H1-0.097600	-1	-4.896844	-6.777940	-5.231346	L
H-H1-0.097600	-1	-4.260825	-8.362415	-5.737033	L
H-H1-0.097600	-1	-3.142331	-7.017067	-5.408885	L
C-CT--0.366200	-1	-12.128871	3.678041	-1.306507	L
C-C-0.597200	-1	-11.024448	2.612178	-1.270952	L
O-O--0.567900	-1	-11.317281	1.429099	-1.116383	L
H-HC-0.112300	-1	-11.680675	4.661222	-1.450335	L
H-HC-0.112300	-1	-12.678996	3.663741	-0.365232	L
H-HC-0.112300	-1	-12.812335	3.466064	-2.128973	L
N-N--0.415700	-1	-9.767999	3.053215	-1.338656	L
C-CT--0.024900	-1	-8.585076	2.231272	-1.159683	L
C-C-0.597300	-1	-7.472714	3.096863	-0.562430	L
O-O--0.567900	-1	-6.820207	3.885502	-1.260561	L
C-CT-0.211700	0	-8.136467	1.562413	-2.456632	L
O-OH--0.654600	0	-7.102327	0.667418	-2.132091	L
H-H-0.271900	-1	-9.641765	4.049722	-1.408533	L
H-H1-0.084300	-1	-8.822313	1.438541	-0.451514	L
H-H1-0.035200	0	-7.784680	2.298378	-3.177056	L
H-H1-0.035200	0	-8.969756	1.002471	-2.883469	L
H-HO-0.427500	0	-6.234313	1.114310	-2.248836	L
N-N--0.415700	-1	-7.310222	3.022669	0.767462	L
C-CT-0.021300	-1	-6.135157	3.638062	1.403013	L
C-C-0.597300	-1	-4.846790	2.991751	0.868837	L
O-O--0.567900	-1	-3.872026	3.680241	0.608494	L
C-CT--0.123100	-1	-6.192514	3.501271	2.926065	L
S-SH--0.311900	-1	-7.446180	4.607189	3.634365	L
H-H-0.271900	-1	-7.970935	2.475850	1.316359	L
H-H1-0.112400	-1	-6.106914	4.700149	1.154493	L
H-H1-0.111200	-1	-5.221334	3.774441	3.342253	L
H-H1-0.111200	-1	-6.408411	2.466454	3.190667	L
H-HS-0.193300	-1	-8.488424	4.159221	2.925188	L
N-N--0.415700	-1	-4.884881	1.672991	0.662398	L H-HC 478
C-CT-0.021300	0	-3.779174	0.939704	0.035502	H
C-C-0.597300	0	-3.692455	1.339299	-1.431256	H
O-O--0.567900	0	-4.673361	1.726968	-2.068212	H
C-CT--0.123100	0	-4.054678	-0.559584	0.253838	H
S-SH--0.311900	0	-2.737539	-1.712476	-0.305573	H
H-H-0.271900	-1	-5.735782	1.184539	0.868303	L
H-H1-0.112400	0	-2.848556	1.212165	0.536672	H
H-H1-0.111200	0	-4.991500	-0.824654	-0.250777	H

H-H1-0.111200	0	-4.202766	-0.721626	1.323872	H
H-HS-0.193300	0	0.451098	-2.369778	0.244775	H
N-N--0.415700	0	-2.444157	1.230138	-1.984202	H
C-CT--0.087500	0	-2.261265	1.345865	-3.418556	H
C-C-0.597300	0	-2.098824	0.004629	-4.168309	H
O-O--0.567900	0	-2.027490	0.033813	-5.400057	H
C-CT-0.298500	-1	-1.132018	2.296323	-3.862099	H
C-CT--0.319200	0	-1.291671	3.682565	-3.232980	L H-HC 492
C-CT--0.319200	0	0.285576	1.806080	-3.570048	L H-HC 492
H-H-0.271900	0	-1.697361	0.877070	-1.392764	H
H-H1-0.096900	0	-3.212467	1.748124	-3.785966	H
H-HC--0.029700	0	-1.215302	2.396402	-4.947381	H
H-HC-0.079100	0	-1.123645	3.629201	-2.155084	L
H-HC-0.079100	0	-2.294411	4.049239	-3.429171	L
H-HC-0.079100	0	-0.573282	4.370517	-3.674938	L
H-HC-0.079100	0	0.457921	1.835902	-2.496212	L
H-HC-0.079100	0	1.004408	2.451257	-4.064556	L
H-HC-0.079100	0	0.431985	0.791607	-3.933741	L
N-N--0.415700	0	-1.951876	-1.101761	-3.406428	H
C-CT--0.003100	0	-2.059375	-2.431787	-3.994137	H
C-C-0.597300	0	-3.529561	-2.862512	-4.189863	H
O-O--0.567900	0	-3.838327	-3.517550	-5.187312	H
C-CT--0.003600	-1	-1.307608	-3.445364	-3.107988	H
C-CT--0.064500	-1	-1.439611	-4.899366	-3.599388	L H-HC 508
C-C-0.695100	-1	-0.566536	-5.236895	-4.793045	L
O-O--0.608600	-1	-0.425327	-4.485323	-5.742792	L
N-N--0.940700	-1	0.047869	-6.400336	-4.788719	L
H-H-0.271900	0	-2.179617	-1.060968	-2.402178	H
H-H1-0.085000	0	-1.648285	-2.393771	-5.004567	H
H-HC-0.017100	0	-0.250048	-3.188884	-3.042575	H
H-HC-0.017100	0	-1.721514	-3.404537	-2.096510	H
H-HC-0.035200	-1	-2.467763	-5.154978	-3.839935	L
H-HC-0.035200	-1	-1.153689	-5.547468	-2.778198	L
H-H-0.425100	-1	0.650847	-6.647841	-5.553612	L
H-H-0.425100	-1	-0.061043	-7.021734	-3.989097	L
N-N--0.415700	0	-4.359565	-2.541744	-3.166836	H
C-CT--0.023700	0	-5.747674	-2.967413	-3.222618	H
C-C-0.597300	-1	-6.424291	-2.330925	-4.462376	L H-H1 522
O-O--0.567900	-1	-6.254572	-1.135423	-4.720507	L
C-CT-0.034200	-1	-6.482894	-2.672992	-1.896067	L H-H1 522
C-CT-0.001800	-1	-7.951004	-3.123278	-1.952284	L
S-S--0.273700	-1	-8.853875	-3.098862	-0.376242	L
C-CT--0.053600	-1	-9.223914	-1.331335	-0.243553	L
H-H-0.271900	0	-3.979731	-2.200037	-2.283922	H
H-H1-0.088000	0	-5.733126	-4.050881	-3.324968	H
H-HC-0.024100	-1	-6.413244	-1.626672	-1.635727	L
H-HC-0.024100	-1	-5.988465	-3.225593	-1.100692	L
H-H1-0.044000	-1	-7.975530	-4.148664	-2.322520	L
H-H1-0.044000	-1	-8.492207	-2.496866	-2.661690	L
H-H1-0.068400	-1	-9.829066	-1.147575	0.644143	L
H-H1-0.068400	-1	-9.775049	-1.001912	-1.124595	L
H-H1-0.068400	-1	-8.294418	-0.770588	-0.172197	L
N-N--0.254800	-1	-7.173076	-3.100337	-5.274118	L
C-CT--0.026600	-1	-7.571467	-2.682988	-6.619343	L

C-C-0.589600	-1	-9.021642	-2.200705	-6.609459	L
O-O--0.574800	-1	-9.906633	-2.902256	-6.112635	L
C-CT--0.007000	-1	-7.364603	-3.925934	-7.499353	L
C-CT-0.018900	-1	-6.846270	-4.988905	-6.527452	L
C-CT-0.019200	-1	-7.377901	-4.530275	-5.195939	L
H-H1-0.064100	-1	-6.925195	-1.885095	-6.984619	L
H-HC-0.025300	-1	-8.299044	-4.247272	-7.950455	L
H-HC-0.025300	-1	-6.629952	-3.740049	-8.280564	L
H-HC-0.021300	-1	-5.758149	-4.979706	-6.502155	L
H-HC-0.021300	-1	-7.219482	-5.971602	-6.743889	L
H-H1-0.039100	-1	-6.852446	-5.038332	-4.399023	L
H-H1-0.039100	-1	-8.443075	-4.752052	-5.120806	L
N-N--0.415700	-1	-9.246801	-1.003893	-7.145072	L
C-CT--0.149000	-1	-10.481063	-0.236222	-6.953418	L
H-H-0.271900	-1	-8.442937	-0.533193	-7.560010	L
H-H1-0.097600	-1	-11.240149	-0.875437	-6.503109	L
H-H1-0.097600	-1	-10.836100	0.125579	-7.918350	L
H-H1-0.097600	-1	-10.282637	0.611266	-6.296903	L
C-CT--0.366200	-1	-10.373228	8.842044	-4.213750	L
C-C-0.597200	-1	-9.822359	7.553363	-3.588945	L
O-O--0.567900	-1	-10.263357	7.132110	-2.518252	L
H-HC-0.112300	-1	-9.855851	9.041160	-5.152145	L
H-HC-0.112300	-1	-10.214780	9.673912	-3.528000	L
H-HC-0.112300	-1	-11.439890	8.726387	-4.405021	L
N-N--0.415700	-1	-8.851300	6.932482	-4.253298	L
C-CT--0.024900	-1	-7.905233	6.014998	-3.614802	L
C-C-0.597300	-1	-6.576401	6.748572	-3.394303	L
O-O--0.567900	-1	-6.323538	7.756693	-4.061328	L
C-CT-0.211700	0	-7.681871	4.762609	-4.474340	L
O-OH--0.654600	0	-7.317851	5.079927	-5.804772	L
H-H-0.271900	-1	-8.581872	7.302293	-5.163968	L
H-H1-0.084300	-1	-8.289806	5.674572	-2.653031	L
H-H1-0.035200	0	-8.600745	4.175253	-4.490370	L
H-H1-0.035200	0	-6.892659	4.158761	-4.023544	L
H-HO-0.427500	0	-6.870126	4.317428	-6.188529	L
N-N--0.415700	-1	-5.697148	6.217389	-2.534291	L
C-CT-0.033700	-1	-4.323952	6.727906	-2.431876	L
C-C-0.597300	-1	-3.577595	6.734480	-3.785002	L
O-O--0.567900	-1	-2.679609	7.549573	-4.002327	L
C-CT--0.182500	-1	-3.568310	5.906721	-1.397235	L
H-H-0.271900	-1	-5.978420	5.411444	-1.971011	L
H-H1-0.082300	-1	-4.372384	7.754980	-2.068595	L
H-HC-0.060300	-1	-2.555130	6.289395	-1.292647	L
H-HC-0.060300	-1	-3.532159	4.860953	-1.700594	L
H-HC-0.060300	-1	-4.083085	5.988771	-0.441234	L
N-N--0.415700	-1	-3.998688	5.867960	-4.720045	L
C-CT--0.149000	-1	-3.484973	5.816139	-6.087625	L
H-H-0.271900	-1	-4.726065	5.218096	-4.452780	L
H-H1-0.097600	-1	-2.712636	6.575171	-6.214274	L
H-H1-0.097600	-1	-4.297335	6.005757	-6.789069	L
H-H1-0.097600	-1	-3.061257	4.830375	-6.279334	L
C-CM--0.139000	0	1.377723	-1.803831	0.088040	H
C-C-0.519000	0	1.505981	-1.544222	-1.394191	H
O-O2--0.567000	0	1.354685	-0.318400	-1.824839	H

C-CM--0.117000	0	1.337663	-0.661066	1.118947	H
O-O2--0.618000	0	1.789032	-2.463724	-2.171870	H
C-C--0.553000	0	0.199295	0.365941	1.007202	H
O-O2--0.556000	0	0.054367	0.952604	-0.121733	H
O-O2--0.607000	0	-0.452144	0.634594	2.041250	H
H-HC-0.049000	0	2.175908	-2.500641	0.356972	H
H-HC-0.162000	0	1.168986	-1.195220	2.053166	H
O-OW--0.834000	-1	6.422952	2.963690	-1.167746	L
H-HW-0.417000	-1	6.793218	3.106269	-2.038050	L
H-HW-0.417000	-1	7.102326	3.264635	-0.564716	L
O-OW--0.834000	0	3.269120	6.874301	1.079305	L
H-HW-0.417000	0	3.173116	5.965890	1.430959	L
H-HW-0.417000	0	3.664195	6.706734	0.207690	L
O-OW--0.834000	0	-0.846789	-3.059409	1.910203	H
H-HW-0.417000	0	-0.564441	-3.897992	1.511614	H
H-HW-0.417000	0	-1.541163	-2.726771	1.290933	H
O-OW--0.834000	0	-4.810005	0.624633	-6.281270	L
H-HW-0.417000	0	-3.873330	0.422106	-6.142614	L
H-HW-0.417000	0	-5.263020	0.029692	-5.660726	L
H-HS-0.193300	0	0.831390	0.256107	-1.122166	H

IC3

C-CT--0.366200	-1	8.165444	4.688577	-8.145437	L
C-C-0.597200	-1	9.000951	3.948411	-7.106267	L
O-O--0.567900	-1	9.606409	2.913744	-7.387978	L
H-HC-0.112300	-1	7.718317	5.572367	-7.690528	L
H-HC-0.112300	-1	7.377010	4.031205	-8.513615	L
H-HC-0.112300	-1	8.803192	4.991528	-8.976716	L
N-N--0.415700	-1	8.994566	4.507293	-5.889562	L
C-CT--0.087500	-1	9.470953	3.834737	-4.673820	L
C-C-0.597300	-1	8.338735	2.931830	-4.180204	L
O-O--0.567900	-1	7.426302	3.387389	-3.475673	L
C-CT-0.298500	-1	9.949588	4.839896	-3.599105	L
C-CT--0.319200	-1	10.374475	4.143399	-2.300787	L
C-CT--0.319200	-1	11.159248	5.653889	-4.080875	L
H-H-0.271900	-1	8.405353	5.326464	-5.761936	L
H-H1-0.096900	-1	10.311520	3.197768	-4.928819	L
H-HC--0.029700	-1	9.149089	5.541519	-3.381991	L
H-HC-0.079100	-1	11.084225	3.348128	-2.530457	L
H-HC-0.079100	-1	9.506971	3.715974	-1.801721	L
H-HC-0.079100	-1	10.848272	4.854348	-1.625776	L
H-HC-0.079100	-1	12.022834	5.001565	-4.210370	L
H-HC-0.079100	-1	11.402334	6.426479	-3.349298	L
H-HC-0.079100	-1	10.937240	6.131805	-5.034036	L
N-N--0.415700	-1	8.361368	1.659097	-4.611373	L
C-CT--0.087500	-1	7.253555	0.701320	-4.434564	L
C-C-0.597300	-1	7.677133	-0.571775	-3.673371	L
O-O--0.567900	-1	8.825283	-1.017418	-3.799103	L
C-CT-0.298500	-1	6.600596	0.290288	-5.778709	L
C-CT--0.319200	-1	5.736299	1.412045	-6.366179	L
C-CT--0.319200	-1	7.594352	-0.155893	-6.856427	L
H-H-0.271900	-1	9.137482	1.356993	-5.206171	L
H-H1-0.096900	-1	6.480677	1.204471	-3.860541	L
H-HC--0.029700	-1	5.936097	-0.553951	-5.591236	L

H-HC-0.079100	-1	6.248584	2.371129	-6.291326	L
H-HC-0.079100	-1	4.801665	1.455070	-5.811490	L
H-HC-0.079100	-1	5.487843	1.195142	-7.406379	L
H-HC-0.079100	-1	8.189898	0.691665	-7.191556	L
H-HC-0.079100	-1	7.045898	-0.562267	-7.705210	L
H-HC-0.079100	-1	8.253198	-0.925299	-6.462033	L
N-N--0.254800	-1	6.745211	-1.182917	-2.904207	L
C-CT--0.026600	-1	6.885039	-2.535001	-2.356939	L
C-C-0.589600	-1	7.137304	-3.557625	-3.466655	L
O-O--0.574800	-1	6.389599	-3.609685	-4.446244	L
C-CT--0.007000	0	5.566723	-2.863901	-1.643907	L
C-CT-0.018900	0	4.711444	-1.606171	-1.725856	L
C-CT-0.019200	0	5.467428	-0.589669	-2.549862	L
H-H1-0.064100	-1	7.704390	-2.545567	-1.639008	L
H-HC-0.025300	0	5.040938	-3.687346	-2.130142	L
H-HC-0.025300	0	5.744253	-3.128661	-0.605634	L
H-HC-0.021300	0	4.525505	-1.212774	-0.728021	L
H-HC-0.021300	0	3.783742	-1.824010	-2.244189	L
H-H1-0.039100	0	5.620330	0.314338	-1.958356	L
H-H1-0.039100	0	4.886912	-0.357242	-3.443777	L
N-N--0.415700	-1	8.166811	-4.398003	-3.318863	L
C-CT--0.149000	-1	8.540695	-5.392546	-4.337193	L
H-H-0.271900	-1	8.766086	-4.272125	-2.504225	L
H-H1-0.097600	-1	7.796488	-5.396817	-5.132929	L
H-H1-0.097600	-1	8.588094	-6.380796	-3.878742	L
H-H1-0.097600	-1	9.515655	-5.138453	-4.753128	L
C-CT--0.366200	-1	5.252252	-7.394147	-4.088361	L
C-C-0.597200	-1	4.118849	-6.729957	-4.880219	L
O-O--0.567900	-1	3.224645	-7.453188	-5.328675	L
H-HC-0.112300	-1	5.960277	-6.633742	-3.759542	L
H-HC-0.112300	-1	5.763898	-8.118018	-4.722504	L
H-HC-0.112300	-1	4.836788	-7.902892	-3.218412	L
N-N--0.415700	-1	4.099818	-5.399291	-5.020032	L
C-CT-0.014300	-1	2.993334	-4.658015	-5.649923	L H-HC 69
C-C-0.597300	-1	2.799879	-5.000377	-7.161917	L
O-O--0.567900	-1	3.794887	-5.159689	-7.870494	L
C-CT--0.204100	0	3.317532	-3.158031	-5.396765	H
C-C-0.713000	0	2.300515	-2.006552	-5.494841	H
O-O--0.593100	0	2.639182	-0.915553	-5.046610	H
N-N--0.919100	0	1.102420	-2.184944	-6.120348	H
H-H-0.271900	-1	4.865376	-4.857423	-4.652820	L
H-H1-0.104800	-1	2.087554	-4.926429	-5.115871	L
H-HC-0.079700	0	4.153098	-2.886983	-6.055207	H
H-HC-0.079700	0	3.697900	-3.062696	-4.376917	H
H-H-0.419600	0	0.423373	-1.436160	-6.055689	H
H-H-0.419600	0	0.664306	-3.103121	-6.184202	H
N-N--0.415700	-1	1.546606	-5.106538	-7.654577	L
C-CT--0.149000	-1	1.195417	-5.368855	-9.080025	L
H-H-0.271900	-1	0.790332	-4.884953	-7.007965	L
H-H1-0.097600	-1	2.102096	-5.589125	-9.642932	L
H-H1-0.097600	-1	0.709775	-4.488590	-9.502093	L
H-H1-0.097600	-1	0.516998	-6.220178	-9.134653	L
C-CT--0.366200	-1	11.738192	-5.861170	-0.639109	L
C-C-0.597200	-1	10.723708	-5.992410	0.505075	L

O-O--0.567900	-1	11.040413	-5.835221	1.689441	L
H-HC-0.112300	-1	11.237913	-6.039957	-1.590735	L
H-HC-0.112300	-1	12.534265	-6.592925	-0.504237	L
H-HC-0.112300	-1	12.163537	-4.857371	-0.635300	L
N-N--0.415700	-1	9.488665	-6.303263	0.114350	L
C-CT--0.023700	-1	8.329851	-6.506803	0.978794	L
C-C-0.597300	-1	7.279885	-7.356335	0.275346	L
O-O--0.567900	-1	7.099916	-7.198851	-0.939083	L
C-CT-0.034200	0	7.718740	-5.143533	1.353258	L
C-CT-0.001800	0	6.901745	-5.128262	2.657971	L
S-S--0.273700	0	5.240641	-5.867803	2.654411	L
C-CT--0.053600	0	4.313740	-4.607179	1.729570	L
H-H-0.271900	-1	9.320013	-6.378304	-0.882761	L
H-H1-0.088000	-1	8.657641	-7.036584	1.861577	L
H-HC-0.024100	0	7.104589	-4.773102	0.532082	L
H-HC-0.024100	0	8.540966	-4.444010	1.478555	L
H-H1-0.044000	0	6.778807	-4.087713	2.959624	L
H-H1-0.044000	0	7.490618	-5.618724	3.432974	L
H-H1-0.068400	0	3.246349	-4.825709	1.757228	L
H-H1-0.068400	0	4.631826	-4.590227	0.688751	L
H-H1-0.068400	0	4.468802	-3.619651	2.166815	L
N-N--0.415700	-1	6.576784	-8.205600	1.034919	L
C-CT--0.149000	-1	5.358682	-8.918505	0.621740	L
H-H-0.271900	-1	6.894021	-8.334986	1.995644	L
H-H1-0.097600	-1	5.139726	-8.689544	-0.420701	L
H-H1-0.097600	-1	4.523291	-8.602614	1.246804	L
H-H1-0.097600	-1	5.511027	-9.991590	0.733755	L
C-CT--0.366200	-1	3.927405	-9.324418	4.903561	L
C-C-0.597200	-1	3.752025	-7.919261	5.513842	L
O-O--0.567900	-1	4.710083	-7.197747	5.806618	L
H-HC-0.112300	-1	2.947601	-9.770598	4.730151	L
H-HC-0.112300	-1	4.495279	-9.951599	5.590542	L
H-HC-0.112300	-1	4.462542	-9.245574	3.957103	L
N-N--0.415700	-1	2.488349	-7.511656	5.661447	L
C-CT--0.087500	-1	2.044112	-6.109489	5.608568	L
C-C-0.597300	-1	1.919987	-5.551506	7.032748	L
O-O--0.567900	-1	0.883919	-5.650168	7.705455	L
C-CT-0.298500	0	0.727852	-5.947231	4.813670	L
C-CT--0.319200	0	0.364815	-4.469317	4.630613	L
C-CT--0.319200	0	0.829101	-6.584522	3.418837	L
H-H-0.271900	-1	1.756296	-8.209502	5.505777	L
H-H1-0.096900	-1	2.806526	-5.532509	5.081641	L
H-HC--0.029700	0	-0.081840	-6.445228	5.348799	L
H-HC-0.079100	0	1.148639	-3.946774	4.076631	L
H-HC-0.079100	0	0.224103	-3.978739	5.592988	L
H-HC-0.079100	0	-0.561587	-4.376418	4.063329	L
H-HC-0.079100	0	1.664886	-6.141219	2.875918	L
H-HC-0.079100	0	-0.084354	-6.383596	2.857036	L
H-HC-0.079100	0	0.964068	-7.660419	3.491720	L
N-N--0.415700	-1	3.077898	-5.092708	7.507228	L
C-CT--0.149000	-1	3.454981	-4.955895	8.911419	L
H-H-0.271900	-1	3.836295	-5.005670	6.840965	L
H-H1-0.097600	-1	2.569239	-5.065530	9.537316	L
H-H1-0.097600	-1	3.895895	-3.973278	9.075586	L

H-H1-0.097600	-1	4.180007	-5.727915	9.169391	L
C-CT--0.366200	-1	12.494249	-4.166020	6.336908	L
C-C-0.597200	-1	12.285347	-3.444218	4.987120	L
O-O--0.567900	-1	13.250943	-3.223047	4.249728	L
H-HC-0.112300	-1	11.535745	-4.270788	6.845240	L
H-HC-0.112300	-1	13.172789	-3.581964	6.959862	L
H-HC-0.112300	-1	12.921501	-5.152101	6.159553	L
N-N--0.415700	-1	11.047918	-3.023945	4.685289	L
C-CT--0.023700	-1	10.766494	-2.200894	3.511372	L
C-C-0.597300	-1	11.328281	-0.775434	3.647381	L
O-O--0.567900	-1	12.054483	-0.306798	2.769001	L
C-CT-0.034200	0	9.256242	-2.119382	3.241147	L
C-CT-0.001800	0	8.999754	-1.342488	1.938669	L
S-S--0.273700	0	7.485505	-1.756802	1.045416	L
C-CT--0.053600	0	6.186215	-0.930415	2.002369	L
H-H-0.271900	-1	10.284504	-3.256414	5.314192	L
H-H1-0.088000	-1	11.238546	-2.678323	2.650980	L
H-HC-0.024100	0	8.738210	-1.628316	4.066078	L
H-HC-0.024100	0	8.872812	-3.130061	3.152130	L
H-H1-0.044000	0	9.821549	-1.549420	1.251918	L
H-H1-0.044000	0	9.008038	-0.271471	2.145461	L
H-H1-0.068400	0	5.209354	-1.136596	1.557504	L
H-H1-0.068400	0	6.343280	0.147597	1.988492	L
H-H1-0.068400	0	6.185745	-1.293748	3.028391	L
N-N--0.415700	-1	11.058688	-0.088417	4.762946	L
C-CT--0.149000	-1	11.606788	1.252350	4.991754	L
H-H-0.271900	-1	10.482804	-0.521774	5.484182	L
H-H1-0.097600	-1	12.192953	1.557438	4.125011	L
H-H1-0.097600	-1	12.245051	1.237842	5.874817	L
H-H1-0.097600	-1	10.789984	1.957550	5.145438	L
C-CT--0.366200	-1	6.127608	8.754232	-5.561277	L
C-C-0.597200	-1	6.448241	7.563295	-4.636575	L
O-O--0.567900	-1	6.603790	6.415520	-5.077332	L
H-HC-0.112300	-1	6.032836	9.662549	-4.965270	L
H-HC-0.112300	-1	5.190470	8.565627	-6.086303	L
H-HC-0.112300	-1	6.931823	8.878393	-6.287186	L
N-N--0.415700	-1	6.591670	7.878909	-3.339207	L
C-CT--0.001400	-1	6.638327	6.887293	-2.249338	L
C-C-0.597300	-1	5.266100	6.202388	-2.107055	L
O-O--0.567900	-1	4.391741	6.679380	-1.366266	L
C-CT--0.001400	-1	7.154877	7.522356	-0.945151	L
C-CA--0.001100	-1	7.845013	6.553660	0.009240	L
C-CA--0.190600	-1	9.253055	6.508594	0.058227	L
C-CA--0.190600	-1	7.103016	5.729572	0.880324	L
C-CA--0.234100	-1	9.907606	5.690338	0.997950	L
C-CA--0.234100	-1	7.761944	4.906244	1.819771	L
C-C-0.322600	-1	9.164459	4.909262	1.897151	L
O-OH--0.557900	-1	9.828650	4.165814	2.828743	L
H-H-0.271900	-1	6.523938	8.870506	-3.097180	L
H-H1-0.087600	-1	7.352035	6.117952	-2.530321	L
H-HC-0.029500	-1	7.877281	8.296460	-1.206847	L
H-HC-0.029500	-1	6.341210	8.026386	-0.422144	L
H-HA-0.169900	-1	9.836011	7.134761	-0.602133	L
H-HA-0.169900	-1	6.021937	5.731354	0.838029	L

H-HA-0.165600	-1	10.985010	5.664970	1.045915	L
H-HA-0.165600	-1	7.190502	4.271254	2.480867	L
H-HO-0.399200	-1	9.333905	3.940335	3.632616	L
N-N--0.415700	-1	5.057104	5.180833	-2.942245	L
C-CT-0.033700	-1	3.741918	4.681042	-3.327850	L
C-C-0.597300	-1	2.908761	4.040950	-2.206547	L
O-O--0.567900	-1	1.684934	4.137458	-2.273702	L
C-CT--0.182500	-1	3.933010	3.683380	-4.465082	L
H-H-0.271900	-1	5.840528	4.890956	-3.522546	L
H-H1-0.082300	-1	3.172325	5.523879	-3.720655	L
H-HC-0.060300	-1	2.962720	3.369344	-4.848867	L
H-HC-0.060300	-1	4.474160	2.816870	-4.084945	L
H-HC-0.060300	-1	4.500838	4.146784	-5.272020	L
N-N--0.415700	-1	3.526481	3.401021	-1.202915	L H-HC 209
C-CT-0.021300	0	2.696083	2.679845	-0.186941	H
C-C-0.597300	0	2.302058	3.644838	0.950612	H
O-O--0.567900	0	3.170393	4.271822	1.557480	H
C-CT--0.123100	0	3.490414	1.462739	0.301483	H
S-S--1.036000	0	2.657335	0.347722	1.522709	H
H-H-0.271900	-1	4.530401	3.380167	-1.196341	L
H-H1-0.112400	0	1.793359	2.310927	-0.681720	H
H-H1-0.111200	0	4.384200	1.776374	0.854020	H
H-H1-0.111200	0	3.818919	0.871520	-0.556691	H
N-N--0.415700	0	0.969949	3.733018	1.219805	H
C-CT--0.051800	0	0.391175	4.543218	2.305676	H
C-C-0.597300	0	0.781411	4.016707	3.727181	H
O-O--0.567900	0	1.317146	4.748558	4.559948	H
C-CT--0.110200	-1	-1.149245	4.635790	2.035349	H
C-CT-0.353100	-1	-2.010633	5.536240	2.947110	L H-HC 222
C-CT--0.412100	-1	-2.197597	4.988024	4.363359	L
C-CT--0.412100	-1	-1.486067	6.972194	3.035472	L
H-H-0.271900	0	0.319855	3.133800	0.703142	H
H-H1-0.092200	0	0.836499	5.541859	2.274215	H
H-HC-0.045700	0	-1.270956	5.010779	1.012548	H
H-HC-0.045700	0	-1.588966	3.635396	2.055277	H
H-HC--0.036100	-1	-3.003207	5.580361	2.500243	L
H-HC-0.100000	-1	-1.298365	5.132771	4.958482	L
H-HC-0.100000	-1	-2.437925	3.926639	4.321995	L
H-HC-0.100000	-1	-3.018476	5.517055	4.845127	L
H-HC-0.100000	-1	-0.523242	6.992703	3.546973	L
H-HC-0.100000	-1	-2.199728	7.587308	3.582223	L
H-HC-0.100000	-1	-1.365808	7.375790	2.029232	L
N-N--0.415700	0	0.530188	2.697172	3.980638	H
C-CT--0.087500	0	0.581557	2.159991	5.348125	H
C-C-0.597300	0	1.978182	2.101800	5.973081	H
O-O--0.567900	0	2.084360	1.986786	7.190168	H
C-CT-0.298500	-1	-0.039495	0.742735	5.377418	H
C-CT--0.319200	0	0.769369	-0.341243	4.643012	L H-HC 241
C-CT--0.319200	0	-0.388872	0.203019	6.763984	L H-HC 241
H-H-0.271900	0	0.056121	2.144461	3.263708	H
H-H1-0.096900	0	0.006987	2.827181	6.003873	H
H-HC--0.029700	0	-0.986535	0.815531	4.841925	H
H-HC-0.079100	0	1.659092	-0.618894	5.203217	L
H-HC-0.079100	0	1.081992	0.034043	3.672396	L

H-HC-0.079100	0	0.150271	-1.218898	4.465274	L
H-HC-0.079100	0	0.517718	-0.025531	7.322092	L
H-HC-0.079100	0	-0.977742	-0.706898	6.653274	L
H-HC-0.079100	0	-0.976444	0.944406	7.302567	L
N-N--0.415700	0	2.998042	1.962431	5.091814	H
C-CT-0.033700	0	4.360934	1.814620	5.554827	H
C-C-0.597300	-1	5.069971	3.145890	5.828341	L H-H1 254
O-O--0.567900	-1	6.245560	3.126082	6.182784	L
C-CT--0.182500	-1	5.137174	0.999858	4.522146	L H-H1 254
H-H-0.271900	0	2.847745	2.261726	4.139922	H
H-H1-0.082300	0	4.337164	1.267199	6.500098	H
H-HC-0.060300	-1	6.105864	0.710661	4.927019	L
H-HC-0.060300	-1	5.290155	1.602591	3.627187	L
H-HC-0.060300	-1	4.582411	0.095591	4.268630	L
N-N--0.415700	-1	4.362231	4.271225	5.665827	L
C-CT--0.087500	-1	4.740566	5.635002	6.062996	L
C-C-0.597300	-1	3.898686	6.078307	7.266669	L
O-O--0.567900	-1	4.450517	6.529956	8.271134	L
C-CT-0.298500	-1	4.520464	6.610534	4.889415	L
C-CT--0.319200	-1	4.909615	8.050343	5.242135	L
C-CT--0.319200	-1	5.337520	6.219031	3.658513	L
H-H-0.271900	-1	3.450818	4.153778	5.240835	L
H-H1-0.096900	-1	5.790779	5.667513	6.343030	L
H-HC--0.029700	-1	3.467711	6.594446	4.615025	L
H-HC-0.079100	-1	5.960369	8.091483	5.520687	L
H-HC-0.079100	-1	4.303067	8.424452	6.066174	L
H-HC-0.079100	-1	4.745423	8.689780	4.375132	L
H-HC-0.079100	-1	6.388306	6.144347	3.932482	L
H-HC-0.079100	-1	5.216971	6.967081	2.875350	L
H-HC-0.079100	-1	4.988175	5.261073	3.273322	L
N-N--0.415700	-1	2.567989	5.882815	7.214649	L
C-CT--0.149000	-1	1.661039	6.217960	8.323181	L
H-H-0.271900	-1	2.161410	5.501576	6.365845	L
H-H1-0.097600	-1	2.238440	6.614181	9.158546	L
H-H1-0.097600	-1	1.128906	5.320831	8.641156	L
H-H1-0.097600	-1	0.942623	6.967408	7.991171	L
C-CT--0.366200	-1	3.992573	10.330428	-0.987116	L
C-C-0.597200	-1	2.518621	9.998788	-1.230127	L
O-O--0.567900	-1	1.705745	10.910842	-1.300770	L
H-HC-0.112300	-1	4.571334	9.408431	-0.952901	L
H-HC-0.112300	-1	4.093717	10.858853	-0.039354	L
H-HC-0.112300	-1	4.360918	10.960937	-1.796012	L
N-N--0.415700	-1	2.144369	8.714559	-1.286540	L
C-CT--0.024900	-1	0.732642	8.327691	-1.125927	L
C-C-0.597300	-1	0.145796	8.821810	0.202023	L
O-O--0.567900	-1	-0.950664	9.385428	0.211947	L
C-CT-0.211700	0	0.564125	6.827620	-1.277320	L
O-OH--0.654600	0	0.859756	6.523493	-2.620519	L
H-H-0.271900	-1	2.849336	7.984477	-1.348781	L
H-H1-0.084300	-1	0.157474	8.776456	-1.931544	L
H-H1-0.035200	0	-0.460332	6.537999	-1.052513	L
H-H1-0.035200	0	1.242659	6.297213	-0.608057	L
H-HO-0.427500	0	0.971363	5.548015	-2.630256	L
N-N--0.415700	-1	0.910208	8.689024	1.296694	L

C-CT-0.033700	-1	0.556409	9.167813	2.634224	L
C-C-0.597300	-1	0.086407	10.627325	2.627587	L
O-O--0.567900	-1	-1.010547	10.941381	3.092093	L
C-CT--0.182500	-1	1.745077	8.934312	3.564222	L
H-H-0.271900	-1	1.800361	8.196002	1.189800	L
H-H1-0.082300	-1	-0.255721	8.572376	3.024497	L
H-HC-0.060300	-1	1.515140	9.303165	4.563149	L
H-HC-0.060300	-1	2.628253	9.439434	3.175299	L
H-HC-0.060300	-1	1.944199	7.865798	3.617413	L
N-N--0.415700	-1	0.880597	11.509761	2.011613	L
C-CT--0.149000	-1	0.534856	12.906273	1.820500	L
H-H-0.271900	-1	1.783771	11.205341	1.656421	L
H-H1-0.097600	-1	-0.451329	13.097377	2.245080	L
H-H1-0.097600	-1	0.522188	13.135589	0.755829	L
H-H1-0.097600	-1	1.272648	13.535031	2.319949	L
C-CT--0.366200	-1	-11.951957	4.536097	4.986446	L
C-C-0.597200	-1	-12.379808	3.115568	4.614427	L
O-O--0.567900	-1	-12.941305	2.404907	5.450480	L
H-HC-0.112300	-1	-11.475368	5.008324	4.127292	L
H-HC-0.112300	-1	-11.246596	4.497644	5.816687	L
H-HC-0.112300	-1	-12.827586	5.114490	5.279474	L
N-N--0.415700	-1	-12.045765	2.676848	3.400491	L
C-CT--0.087500	-1	-12.036878	1.254723	3.040202	L
C-C-0.597300	-1	-10.589767	0.865712	2.724252	L
O-O--0.567900	-1	-9.877935	1.512867	1.948579	L
C-CT-0.298500	-1	-13.033083	0.861693	1.916736	L
C-CT--0.319200	-1	-13.775072	-0.431647	2.302174	L
C-CT--0.319200	-1	-14.115635	1.905841	1.609740	L
H-H-0.271900	-1	-11.638820	3.330055	2.728549	L
H-H1-0.096900	-1	-12.326203	0.693556	3.926342	L
H-HC--0.029700	-1	-12.474795	0.674733	1.003101	L
H-HC-0.079100	-1	-14.406967	-0.252875	3.172845	L
H-HC-0.079100	-1	-13.055892	-1.221471	2.522774	L
H-HC-0.079100	-1	-14.411743	-0.748481	1.476322	L
H-HC-0.079100	-1	-14.748588	2.047129	2.482336	L
H-HC-0.079100	-1	-14.723058	1.568228	0.771414	L
H-HC-0.079100	-1	-13.662621	2.860026	1.349500	L
N-N--0.415700	-1	-10.121365	-0.153126	3.447681	L
C-CT--0.038900	-1	-8.711609	-0.544944	3.527564	L
C-C-0.597300	-1	-8.577476	-2.069988	3.639478	L
O-O--0.567900	-1	-9.505095	-2.734365	4.123010	L
C-CT-0.365400	-1	-7.995764	0.104227	4.735912	L
O-OH--0.676100	-1	-8.159188	-0.611898	5.938448	L
C-CT--0.243800	-1	-8.419437	1.538803	5.045079	L
H-H-0.271900	-1	-10.748081	-0.628904	4.080630	L
H-H1-0.100700	-1	-8.213934	-0.208858	2.617981	L
H-H1-0.004300	-1	-6.937050	0.108480	4.498063	L
H-HC-0.064200	-1	-8.466387	2.103964	4.121713	L
H-HC-0.064200	-1	-7.692152	1.998135	5.715851	L
H-HC-0.064200	-1	-9.402168	1.561071	5.515217	L
H-HO-0.410200	-1	-8.412231	0.025964	6.638052	L
N-N--0.254800	-1	-7.449668	-2.660013	3.204400	L
C-CT--0.026600	-1	-7.192852	-4.085167	3.372897	L
C-C-0.589600	-1	-6.581080	-4.437996	4.729928	L

O-O--0.574800	-1	-6.586992	-5.609147	5.092037	L
C-CT--0.007000	0	-6.211022	-4.428979	2.254256	L
C-CT-0.018900	0	-5.378664	-3.158565	2.116138	L
C-CT-0.019200	0	-6.382414	-2.044312	2.420915	L
H-H1-0.064100	-1	-8.100676	-4.659186	3.229243	L
H-HC-0.025300	0	-5.591742	-5.286065	2.511369	L
H-HC-0.025300	0	-6.758483	-4.613833	1.329184	L
H-HC-0.021300	0	-4.963091	-3.069496	1.114572	L
H-HC-0.021300	0	-4.581235	-3.156695	2.858789	L
H-H1-0.039100	0	-6.789557	-1.662040	1.484571	L
H-H1-0.039100	0	-5.890867	-1.243191	2.974561	L
N-N--0.415700	-1	-5.965569	-3.474177	5.422960	L
C-CT--0.001400	-1	-4.971628	-3.711528	6.481223	L
C-C-0.597300	-1	-5.514672	-4.497898	7.688838	L
O-O--0.567900	-1	-6.701193	-4.386742	8.001441	L
C-CT--0.001400	0	-4.432089	-2.363723	6.980652	L H-HA 373
C-CA--0.001100	0	-4.062560	-1.360813	5.899148	H
C-CA--0.190600	0	-3.206304	-1.714420	4.850287	H
C-CA--0.190600	0	-4.573175	-0.060885	5.948717	H
C-CA--0.234100	0	-2.861645	-0.792895	3.865820	H
C-CA--0.234100	0	-4.224890	0.877232	4.982367	H
C-C-0.322600	0	-3.355202	0.522482	3.941747	H
O-OH--0.557900	0	-3.024244	1.476258	3.049781	H
H-H-0.271900	-1	-6.037415	-2.535423	5.062025	L
H-H1-0.087600	-1	-4.145034	-4.276362	6.048765	L
H-HC-0.029500	0	-5.189538	-1.912856	7.624180	L
H-HC-0.029500	0	-3.547821	-2.543916	7.593198	L
H-HA-0.169900	0	-2.805904	-2.723554	4.779616	H
H-HA-0.169900	0	-5.244934	0.237019	6.755250	H
H-HA-0.165600	0	-2.201323	-1.075832	3.052176	H
H-HA-0.165600	0	-4.582448	1.902256	5.042636	H
H-HO-0.399200	0	-2.182388	1.250944	2.564639	H
N-N--0.415700	-1	-4.632021	-5.184259	8.441168	L
C-CT--0.149000	-1	-5.012590	-5.652946	9.790138	L
H-H-0.271900	-1	-3.637665	-5.172915	8.200127	L
H-H1-0.097600	-1	-6.096383	-5.607492	9.898013	L
H-H1-0.097600	-1	-4.545309	-5.017230	10.541456	L
H-H1-0.097600	-1	-4.676755	-6.681393	9.925062	L
C-CT--0.366200	-1	-0.438075	-10.776887	2.469611	L
C-C-0.597200	-1	-0.624541	-9.836490	1.265649	L
O-O--0.567900	-1	-1.735508	-9.666798	0.758433	L
H-HC-0.112300	-1	0.610366	-10.786508	2.764059	L
H-HC-0.112300	-1	-0.747620	-11.785301	2.193810	L
H-HC-0.112300	-1	-1.047082	-10.426295	3.302858	L
N-N--0.415700	-1	0.486568	-9.284737	0.760826	L
C-CT-0.014300	-1	0.436822	-8.266824	-0.288080	L H-HC 405
C-C-0.597300	-1	0.063596	-8.775496	-1.699270	L
O-O--0.567900	-1	-0.152458	-7.953186	-2.580214	L
C-CT--0.204100	0	1.790398	-7.535957	-0.291640	H
C-C-0.713000	0	1.604363	-6.050771	-0.578909	H
O-O--0.593100	0	1.043640	-5.349577	0.258884	H
N-N--0.919100	0	2.153140	-5.579883	-1.723217	H
H-H-0.271900	-1	1.370789	-9.468820	1.205718	L
H-H1-0.104800	-1	-0.368387	-7.598378	0.017216	L

H-HC-0.079700	0	2.474963	-8.038424	-0.986082	H
H-HC-0.079700	0	2.223440	-7.578545	0.711328	H
H-H-0.419600	0	2.009323	-4.586500	-1.930003	H
H-H-0.419600	0	2.376792	-6.220463	-2.473837	H
N-N--0.415700	-1	-0.027382	-10.089055	-1.937467	L
C-CT--0.149000	-1	-0.566840	-10.641540	-3.192117	L
H-H-0.271900	-1	0.086313	-10.738333	-1.151008	L
H-H1-0.097600	-1	-0.635731	-9.850514	-3.938159	L
H-H1-0.097600	-1	-1.558245	-11.056529	-3.010243	L
H-H1-0.097600	-1	0.094325	-11.428831	-3.556461	L
C-CT--0.366200	-1	-3.830727	-11.714031	-1.421792	L
C-C-0.597200	-1	-4.603315	-10.390687	-1.492354	L
O-O--0.567900	-1	-5.742736	-10.397608	-1.962409	L
H-HC-0.112300	-1	-2.847625	-11.536924	-0.984682	L
H-HC-0.112300	-1	-3.713461	-12.120389	-2.425403	L
H-HC-0.112300	-1	-4.380511	-12.423018	-0.803176	L
N-N--0.415700	-1	-3.979784	-9.261253	-1.117253	L
C-CT--0.087500	-1	-4.549139	-7.902317	-1.279196	L
C-C-0.597300	-1	-4.817032	-7.520354	-2.746102	L
O-O--0.567900	-1	-5.808604	-6.854288	-3.040384	L
C-CT-0.298500	-1	-3.645381	-6.822527	-0.628286	L
C-CT--0.319200	-1	-4.138192	-5.386361	-0.867726	L
C-CT--0.319200	-1	-3.628062	-6.959728	0.891729	L
H-H-0.271900	-1	-3.096918	-9.368962	-0.615986	L
H-H1-0.096900	-1	-5.509587	-7.884279	-0.765473	L
H-HC--0.029700	-1	-2.629842	-6.916711	-1.013357	L
H-HC-0.079100	-1	-5.174096	-5.293783	-0.540638	L
H-HC-0.079100	-1	-4.072072	-5.134051	-1.923432	L
H-HC-0.079100	-1	-3.513260	-4.676959	-0.323151	L
H-HC-0.079100	-1	-4.634732	-6.828805	1.271357	L
H-HC-0.079100	-1	-2.966637	-6.211695	1.331180	L
H-HC-0.079100	-1	-3.275059	-7.935908	1.193008	L
N-N--0.415700	-1	-3.969748	-7.916618	-3.704103	L
C-CT--0.149000	-1	-4.058353	-7.502157	-5.115054	L
H-H-0.271900	-1	-3.245337	-8.577099	-3.448200	L
H-H1-0.097600	-1	-4.879221	-6.794760	-5.235577	L
H-H1-0.097600	-1	-4.238089	-8.377183	-5.741231	L
H-H1-0.097600	-1	-3.124009	-7.027924	-5.414130	L
C-CT--0.366200	-1	-12.144610	3.637447	-1.309089	L
C-C-0.597200	-1	-11.036521	2.575383	-1.273928	L
O-O--0.567900	-1	-11.325205	1.391349	-1.118863	L
H-HC-0.112300	-1	-11.699872	4.622119	-1.453455	L
H-HC-0.112300	-1	-12.694105	3.621517	-0.367472	L
H-HC-0.112300	-1	-12.827848	3.422909	-2.131078	L
N-N--0.415700	-1	-9.781632	3.020702	-1.342522	L
C-CT--0.024900	-1	-8.595791	2.202864	-1.164056	L
C-C-0.597300	-1	-7.486034	3.072421	-0.567718	L
O-O--0.567900	-1	-6.836660	3.863102	-1.266461	L
C-CT-0.211700	0	-8.159412	1.539785	-2.467716	L
O-OH--0.654600	0	-7.154482	0.611137	-2.156055	L
H-H-0.271900	-1	-9.658854	4.017617	-1.412743	L
H-H1-0.084300	-1	-8.829876	1.409516	-0.455530	L
H-H1-0.035200	0	-7.785114	2.275487	-3.176882	L
H-H1-0.035200	0	-9.005927	1.008832	-2.905440	L

H-HO-0.427500	0	-6.273920	1.039651	-2.251795	L
N-N--0.415700	-1	-7.322472	2.999142	0.762093	L
C-CT-0.021300	-1	-6.149132	3.618727	1.396757	L
C-C-0.597300	-1	-4.858887	2.976689	0.861962	L
O-O--0.567900	-1	-3.886647	3.668443	0.600836	L
C-CT--0.123100	-1	-6.205086	3.482151	2.919881	L
S-SH--0.311900	-1	-7.462097	4.583959	3.628656	L
H-H-0.271900	-1	-7.980971	2.450211	1.311542	L
H-H1-0.112400	-1	-6.124680	4.680838	1.147936	L
H-H1-0.111200	-1	-5.234592	3.758758	3.335399	L
H-H1-0.111200	-1	-6.417275	2.446672	3.184892	L
H-HS-0.193300	-1	-8.503236	4.132233	2.920239	L
N-N--0.415700	-1	-4.892585	1.657749	0.655895	L H-HC 478
C-CT-0.021300	0	-3.782528	0.939044	0.017474	H
C-C-0.597300	0	-3.731439	1.316116	-1.458708	H
O-O--0.567900	0	-4.735716	1.645148	-2.093208	H
C-CT--0.123100	0	-4.019279	-0.565406	0.254637	H
S-SH--0.311900	0	-2.684861	-1.701943	-0.307355	H
H-H-0.271900	-1	-5.741684	1.166443	0.862458	L
H-H1-0.112400	0	-2.850505	1.243845	0.496355	H
H-H1-0.111200	0	-4.954523	-0.858913	-0.238431	H
H-H1-0.111200	0	-4.153583	-0.721767	1.327498	H
H-HS-0.193300	0	1.532685	-0.178258	-1.321537	H
N-N--0.415700	0	-2.489349	1.235136	-2.025554	H
C-CT--0.087500	0	-2.298372	1.350671	-3.457118	H
C-C-0.597300	0	-2.116223	-0.000648	-4.194458	H
O-O--0.567900	0	-2.021428	0.014470	-5.427480	H
C-CT-0.298500	-1	-1.144663	2.292711	-3.871067	H
C-CT--0.319200	0	-1.280909	3.669846	-3.219686	L H-HC 492
C-CT--0.319200	0	0.242686	1.720342	-3.513676	L H-HC 492
H-H-0.271900	0	-1.701691	1.048732	-1.410080	H
H-H1-0.096900	0	-3.243730	1.749899	-3.843631	H
H-HC--0.029700	0	-1.182397	2.405207	-4.957071	H
H-HC-0.079100	0	-1.121935	3.595241	-2.140925	L
H-HC-0.079100	0	-2.273814	4.061927	-3.416718	L
H-HC-0.079100	0	-0.545581	4.349138	-3.645493	L
H-HC-0.079100	0	0.360018	1.657234	-2.432016	L
H-HC-0.079100	0	1.016267	2.364179	-3.920583	L
H-HC-0.079100	0	0.385336	0.727783	-3.937287	L
N-N--0.415700	0	-1.972326	-1.098517	-3.419875	H
C-CT--0.003100	0	-2.061013	-2.435147	-3.997515	H
C-C-0.597300	0	-3.526078	-2.875877	-4.195183	H
O-O--0.567900	0	-3.829314	-3.532282	-5.195151	H
C-CT--0.003600	-1	-1.300113	-3.449336	-3.115317	H
C-CT--0.064500	-1	-1.427446	-4.903916	-3.606245	L H-HC 508
C-C-0.695100	-1	-0.553949	-5.238774	-4.800349	L
O-O--0.608600	-1	-0.415898	-4.486979	-5.750384	L
N-N--0.940700	-1	0.064440	-6.400103	-4.796090	L
H-H-0.271900	0	-2.199661	-1.049445	-2.413069	H
H-H1-0.085000	0	-1.654416	-2.391288	-5.010101	H
H-HC-0.017100	0	-0.245930	-3.178133	-3.043050	H
H-HC-0.017100	0	-1.713149	-3.412402	-2.103561	H
H-HC-0.035200	-1	-2.454860	-5.163113	-3.846093	L
H-HC-0.035200	-1	-1.138798	-5.550813	-2.785059	L

H-H-0.425100	-1	0.667793	-6.645747	-5.561287	L
H-H-0.425100	-1	-0.041852	-7.021655	-3.996235	L
N-N--0.415700	0	-4.355492	-2.562049	-3.171635	H
C-CT--0.023700	0	-5.742957	-2.987899	-3.227065	H
C-C-0.597300	-1	-6.421420	-2.352795	-4.466857	L H-H1 522
O-O--0.567900	-1	-6.255954	-1.156789	-4.725412	L
C-CT-0.034200	-1	-6.477275	-2.694370	-1.900422	L H-H1 522
C-CT-0.001800	-1	-7.943868	-3.149696	-1.955615	L
S-S--0.273700	-1	-8.845850	-3.127948	-0.379025	L
C-CT--0.053600	-1	-9.221860	-1.361663	-0.246581	L
H-H-0.271900	0	-3.975775	-2.207535	-2.293533	H
H-H1-0.088000	0	-5.726629	-4.071364	-3.328077	H
H-HC-0.024100	-1	-6.411050	-1.647747	-1.640404	L
H-HC-0.024100	-1	-5.980468	-3.245059	-1.105202	L
H-H1-0.044000	-1	-7.965109	-4.175260	-2.325562	L
H-H1-0.044000	-1	-8.487649	-2.525333	-2.664856	L
H-H1-0.068400	-1	-9.827093	-1.179738	0.641437	L
H-H1-0.068400	-1	-9.774661	-1.034367	-1.127372	L
H-H1-0.068400	-1	-8.294246	-0.797717	-0.175947	L
N-N--0.254800	-1	-7.168062	-3.124986	-5.277933	L
C-CT--0.026600	-1	-7.568706	-2.709366	-6.623024	L
C-C-0.589600	-1	-9.020518	-2.232051	-6.612378	L
O-O--0.574800	-1	-9.902796	-2.936495	-6.114822	L
C-CT--0.007000	-1	-7.358126	-3.951834	-7.502829	L
C-CT-0.018900	-1	-6.835559	-5.012761	-6.530962	L
C-CT-0.019200	-1	-7.367940	-4.555596	-5.199246	L
H-H1-0.064100	-1	-6.925395	-1.909363	-6.988911	L
H-HC-0.025300	-1	-8.291737	-4.276492	-7.953270	L
H-HC-0.025300	-1	-6.624595	-3.763644	-8.284541	L
H-HC-0.021300	-1	-5.747460	-4.999829	-6.506337	L
H-HC-0.021300	-1	-7.205535	-5.996789	-6.746907	L
H-H1-0.039100	-1	-6.840259	-5.061636	-4.402517	L
H-H1-0.039100	-1	-8.432302	-4.781000	-5.123399	L
N-N--0.415700	-1	-9.250104	-1.036161	-7.148172	L
C-CT--0.149000	-1	-10.486870	-0.272670	-6.955965	L
H-H-0.271900	-1	-8.448111	-0.562822	-7.563730	L
H-H1-0.097600	-1	-11.243486	-0.914360	-6.505019	L
H-H1-0.097600	-1	-10.843736	0.087652	-7.920775	L
H-H1-0.097600	-1	-10.290945	0.575669	-6.299799	L
C-CT--0.366200	-1	-10.408449	8.806650	-4.218791	L
C-C-0.597200	-1	-9.852786	7.520031	-3.593980	L
O-O--0.567900	-1	-10.291681	7.097559	-2.522904	L
H-HC-0.112300	-1	-9.892333	9.007284	-5.157557	L
H-HC-0.112300	-1	-10.252431	9.639240	-3.533361	L
H-HC-0.112300	-1	-11.474826	8.687288	-4.409375	L
N-N--0.415700	-1	-8.880014	6.902301	-4.258764	L
C-CT--0.024900	-1	-7.930418	5.988235	-3.620604	L
C-C-0.597300	-1	-6.603972	6.726415	-3.401118	L
O-O--0.567900	-1	-6.354973	7.735216	-4.068568	L
C-CT-0.211700	0	-7.704351	4.736551	-4.479967	L
O-OH--0.654600	0	-7.347542	5.054748	-5.812377	L
H-H-0.271900	-1	-8.612413	7.272787	-5.169698	L
H-H1-0.084300	-1	-8.313233	5.646753	-2.658506	L
H-H1-0.035200	0	-8.620552	4.144911	-4.491664	L

H-H1-0.035200	0	-6.910495	4.136891	-4.031767	L
H-HO-0.427500	0	-6.912165	4.288864	-6.202348	L
N-N--0.415700	-1	-5.722377	6.198478	-2.541505	L
C-CT-0.033700	-1	-4.350875	6.713723	-2.440070	L
C-C-0.597300	-1	-3.605375	6.722489	-3.793656	L
O-O--0.567900	-1	-2.710320	7.540594	-4.011751	L
C-CT--0.182500	-1	-3.591790	5.895410	-1.405674	L
H-H-0.271900	-1	-6.000541	5.391726	-1.977836	L
H-H1-0.082300	-1	-4.402602	7.740723	-2.077034	L
H-HC-0.060300	-1	-2.579863	6.281580	-1.301811	L
H-HC-0.060300	-1	-3.552243	4.849690	-1.708776	L
H-HC-0.060300	-1	-4.106256	5.975954	-0.449379	L
N-N--0.415700	-1	-4.024072	5.854280	-4.728209	L
C-CT--0.149000	-1	-3.511022	5.803850	-6.096090	L
H-H-0.271900	-1	-4.749054	5.202000	-4.460323	L
H-H1-0.097600	-1	-2.741367	6.565489	-6.223417	L
H-H1-0.097600	-1	-4.324459	5.990496	-6.797085	L
H-H1-0.097600	-1	-3.084049	4.819491	-6.287796	L
C-CT--0.139000	0	1.079064	-0.848783	-0.584874	H
C-C-0.519000	0	1.745547	-2.194015	-0.730813	H
O-O2--0.567000	0	2.588508	-2.610452	0.220865	H
C-CT--0.117000	0	1.035649	-0.268783	0.823624	H
O-O2--0.618000	0	1.578107	-2.870525	-1.732952	H
C-C--0.553000	0	-0.073099	0.782308	0.968025	H
O-O2--0.556000	0	-0.301348	1.525744	-0.022759	H
O-O2--0.607000	0	-0.645195	0.837171	2.096440	H
H-HC-0.049000	0	0.042741	-0.993598	-0.911014	H
H-HC-0.162000	0	0.785172	-1.087477	1.507309	H
O-OW--0.834000	-1	6.409633	2.986679	-1.181539	L
H-HW-0.417000	-1	6.778874	3.130290	-2.052109	L
H-HW-0.417000	-1	7.088342	3.290111	-0.579007	L
O-OW--0.834000	0	3.262315	6.922608	1.069864	L
H-HW-0.417000	0	3.163789	6.019867	1.434977	L
H-HW-0.417000	0	3.648757	6.740724	0.197406	L
O-OW--0.834000	0	-0.265360	-2.958926	1.571793	H
H-HW-0.417000	0	0.037548	-3.756124	1.105753	H
H-HW-0.417000	0	-1.081146	-2.685049	1.098623	H
O-OW--0.834000	0	-4.782615	0.422709	-6.436969	L
H-HW-0.417000	0	-3.849067	0.277622	-6.226411	L
H-HW-0.417000	0	-5.249563	-0.093896	-5.758862	L
H-HS-0.193300	0	2.710596	-1.908590	0.889449	H

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C-CT--0.366200	-1	8.198198	4.705162	-8.120991	L
C-C-0.597200	-1	9.031059	3.960683	-7.082780	L
O-O--0.567900	-1	9.635512	2.926030	-7.366690	L
H-HC-0.112300	-1	7.751597	5.588193	-7.664097	L
H-HC-0.112300	-1	7.409426	4.050012	-8.492383	L
H-HC-0.112300	-1	8.837659	5.009738	-8.950359	L
N-N--0.415700	-1	9.023563	4.515880	-5.864395	L
C-CT--0.087500	-1	9.497126	3.838977	-4.649965	L
C-C-0.597300	-1	8.362885	2.936162	-4.160844	L
O-O--0.567900	-1	7.449995	3.390853	-3.456349	L
C-CT-0.298500	-1	9.975491	4.840203	-3.571464	L

C-CT--0.319200	-1	10.397390	4.139180	-2.274609	L
C-CT--0.319200	-1	11.187030	5.653961	-4.048891	L
H-H-0.271900	-1	8.435295	5.335484	-5.735196	L
H-H1-0.096900	-1	10.337199	3.201612	-4.905595	L
H-HC--0.029700	-1	9.175633	5.542285	-3.353460	L
H-HC-0.079100	-1	11.106388	3.343618	-2.505593	L
H-HC-0.079100	-1	9.528518	3.711458	-1.778185	L
H-HC-0.079100	-1	10.871131	4.847415	-1.596711	L
H-HC-0.079100	-1	12.049908	5.000824	-4.179027	L
H-HC-0.079100	-1	11.430056	6.423987	-3.314596	L
H-HC-0.079100	-1	10.967168	6.135074	-5.000937	L
N-N--0.415700	-1	8.384416	1.664708	-4.595835	L
C-CT--0.087500	-1	7.274997	0.707947	-4.423649	L
C-C-0.597300	-1	7.695618	-0.568036	-3.665667	L
O-O--0.567900	-1	8.843338	-1.014900	-3.790973	L
C-CT-0.298500	-1	6.623552	0.301910	-5.770045	L
C-CT--0.319200	-1	5.761731	1.426652	-6.355445	L
C-CT--0.319200	-1	7.618358	-0.142393	-6.847569	L
H-H-0.271900	-1	9.161028	1.363330	-5.190344	L
H-H1-0.096900	-1	6.501930	1.210441	-3.849299	L
H-HC--0.029700	-1	5.957589	-0.541963	-5.586165	L
H-HC-0.079100	-1	6.275236	2.384788	-6.276890	L
H-HC-0.079100	-1	4.826298	1.469299	-5.802079	L
H-HC-0.079100	-1	5.514591	1.213252	-7.396681	L
H-HC-0.079100	-1	8.215606	0.705348	-7.179205	L
H-HC-0.079100	-1	7.070656	-0.545422	-7.698431	L
H-HC-0.079100	-1	8.275518	-0.913908	-6.454493	L
N-N--0.254800	-1	6.761652	-1.180202	-2.899807	L
C-CT--0.026600	-1	6.898746	-2.534134	-2.356427	L
C-C-0.589600	-1	7.151311	-3.553738	-3.468846	L
O-O--0.574800	-1	6.405055	-3.601783	-4.449746	L
C-CT--0.007000	0	5.563484	-2.842842	-1.659781	L
C-CT-0.018900	0	4.957549	-1.471795	-1.387318	L
C-CT-0.019200	0	5.450759	-0.638458	-2.554933	L
H-H1-0.064100	-1	7.716967	-2.548025	-1.637263	L
H-HC-0.025300	0	4.892994	-3.390261	-2.324013	L
H-HC-0.025300	0	5.712940	-3.409565	-0.745726	L
H-HC-0.021300	0	5.344095	-1.052718	-0.464362	L
H-HC-0.021300	0	3.876524	-1.496828	-1.352742	L
H-H1-0.039100	0	5.504455	0.404453	-2.241023	L
H-H1-0.039100	0	4.767885	-0.749944	-3.398593	L
N-N--0.415700	-1	8.179415	-4.396001	-3.322012	L
C-CT--0.149000	-1	8.553490	-5.387973	-4.342773	L
H-H-0.271900	-1	8.777598	-4.273429	-2.506070	L
H-H1-0.097600	-1	7.810517	-5.388791	-5.139672	L
H-H1-0.097600	-1	8.598802	-6.377676	-3.887252	L
H-H1-0.097600	-1	9.529449	-5.133984	-4.756425	L
C-CT--0.366200	-1	5.261882	-7.385719	-4.105110	L
C-C-0.597200	-1	4.130636	-6.717552	-4.896702	L
O-O--0.567900	-1	3.236123	-7.438168	-5.348732	L
H-HC-0.112300	-1	5.970455	-6.627310	-3.772887	L
H-HC-0.112300	-1	5.773502	-8.108381	-4.740653	L
H-HC-0.112300	-1	4.844360	-7.896522	-3.237353	L
N-N--0.415700	-1	4.113676	-5.386443	-5.032508	L

C-CT-0.014300	-1	3.009196	-4.641717	-5.661850	L H-HC 69
C-C-0.597300	-1	2.817622	-4.979220	-7.175182	L
O-O--0.567900	-1	3.813501	-5.137771	-7.882698	L
C-CT--0.204100	0	3.298145	-3.141240	-5.421620	H
C-C-0.713000	0	2.183296	-2.219185	-5.914561	H
O-O--0.593100	0	2.049488	-1.932508	-7.100248	H
N-N--0.919100	0	1.393402	-1.694034	-4.936199	H
H-H-0.271900	-1	4.879415	-4.846760	-4.662465	L
H-H1-0.104800	-1	2.102224	-4.910479	-5.130025	L
H-HC-0.079700	0	4.207201	-2.890807	-5.979587	H
H-HC-0.079700	0	3.482098	-2.993130	-4.354014	H
H-H-0.419600	0	0.532899	-1.288528	-5.282606	H
H-H-0.419600	0	1.436094	-2.009154	-3.967788	H
N-N--0.415700	-1	1.564968	-5.082135	-7.670101	L
C-CT--0.149000	-1	1.215626	-5.339637	-9.096881	L
H-H-0.271900	-1	0.807999	-4.861454	-7.023991	L
H-H1-0.097600	-1	2.122873	-5.559468	-9.659045	L
H-H1-0.097600	-1	0.731867	-4.457418	-9.517026	L
H-H1-0.097600	-1	0.536110	-6.189841	-9.155140	L
C-CT--0.366200	-1	11.744589	-5.872274	-0.641181	L
C-C-0.597200	-1	10.728146	-6.005566	0.501023	L
O-O--0.567900	-1	11.043232	-5.852413	1.686352	L
H-HC-0.112300	-1	11.245538	-6.047479	-1.594120	L
H-HC-0.112300	-1	12.539431	-6.605548	-0.507302	L
H-HC-0.112300	-1	12.171324	-4.869092	-0.633672	L
N-N--0.415700	-1	9.493280	-6.313505	0.107446	L
C-CT--0.023700	-1	8.332844	-6.518048	0.969477	L
C-C-0.597300	-1	7.282789	-7.363976	0.261827	L
O-O--0.567900	-1	7.104920	-7.202559	-0.952396	L
C-CT-0.034200	0	7.727020	-5.160690	1.366426	L
C-CT-0.001800	0	6.820121	-5.189623	2.611909	L
S-S--0.273700	0	5.102731	-5.748914	2.393799	L
C-CT--0.053600	0	4.276456	-4.178232	1.985921	L
H-H-0.271900	-1	9.326073	-6.385290	-0.890145	L
H-H1-0.088000	-1	8.658525	-7.050961	1.851152	L
H-HC-0.024100	0	7.177682	-4.741045	0.523882	L
H-HC-0.024100	0	8.557156	-4.494089	1.581653	L
H-H1-0.044000	0	6.775919	-4.180082	3.021050	L
H-H1-0.044000	0	7.293244	-5.819093	3.365442	L
H-H1-0.068400	0	3.242480	-4.362767	1.694809	L
H-H1-0.068400	0	4.778642	-3.682498	1.159416	L
H-H1-0.068400	0	4.281016	-3.510819	2.847876	L
N-N--0.415700	-1	6.577326	-8.214557	1.017729	L
C-CT--0.149000	-1	5.358876	-8.924503	0.600505	L
H-H-0.271900	-1	6.892893	-8.347297	1.978547	L
H-H1-0.097600	-1	5.141857	-8.692075	-0.441574	L
H-H1-0.097600	-1	4.522956	-8.609340	1.225228	L
H-H1-0.097600	-1	5.509552	-9.998132	0.709499	L
C-CT--0.366200	-1	3.721637	-9.139383	4.110675	L
C-C-0.597200	-1	3.613872	-7.975680	5.116585	L
O-O--0.567900	-1	4.599776	-7.490564	5.679463	L
H-HC-0.112300	-1	2.727149	-9.397841	3.745489	L
H-HC-0.112300	-1	4.164267	-10.005688	4.601963	L
H-HC-0.112300	-1	4.348937	-8.837845	3.271668	L

N-N--0.415700	-1	2.382812	-7.491857	5.304249	L
C-CT--0.087500	-1	2.071052	-6.099074	5.663645	L
C-C-0.597300	-1	1.862212	-5.989855	7.180054	L
O-O--0.567900	-1	0.762397	-6.170259	7.721875	L
C-CT-0.298500	0	0.822167	-5.598157	4.900611	L
C-CT--0.319200	0	0.670563	-4.081479	5.045169	L
C-CT--0.319200	0	0.858111	-5.951658	3.407239	L
H-H-0.271900	-1	1.610105	-8.021831	4.892939	L
H-H1-0.096900	-1	2.927904	-5.479501	5.392050	L
H-HC--0.029700	0	-0.066334	-6.077696	5.312856	L
H-HC-0.079100	0	1.521932	-3.569346	4.592083	L
H-HC-0.079100	0	0.589916	-3.795732	6.092995	L
H-HC-0.079100	0	-0.230518	-3.749790	4.528110	L
H-HC-0.079100	0	1.714323	-5.473775	2.931786	L
H-HC-0.079100	0	-0.050074	-5.581982	2.933109	L
H-HC-0.079100	0	0.896051	-7.025649	3.247912	L
N-N--0.415700	-1	3.005882	-5.831100	7.845790	L
C-CT--0.149000	-1	3.258756	-6.170977	9.243357	L
H-H-0.271900	-1	3.828726	-5.632215	7.288996	L
H-H1-0.097600	-1	2.311472	-6.364557	9.746829	L
H-H1-0.097600	-1	3.767100	-5.341237	9.733264	L
H-H1-0.097600	-1	3.885101	-7.061754	9.292636	L
C-CT--0.366200	-1	12.492172	-4.199346	6.341107	L
C-C-0.597200	-1	12.286374	-3.473161	4.993192	L
O-O--0.567900	-1	13.253421	-3.251106	4.257971	L
H-HC-0.112300	-1	11.532740	-4.304314	6.847635	L
H-HC-0.112300	-1	13.170560	-3.618127	6.966881	L
H-HC-0.112300	-1	12.918325	-5.185481	6.161423	L
N-N--0.415700	-1	11.050002	-3.050249	4.690725	L
C-CT--0.023700	-1	10.771547	-2.223248	3.518875	L
C-C-0.597300	-1	11.335107	-0.798995	3.660078	L
O-O--0.567900	-1	12.063325	-0.328713	2.784250	L
C-CT-0.034200	0	9.263300	-2.148319	3.258154	L
C-CT-0.001800	0	9.010416	-1.457014	1.911836	L
S-S--0.273700	0	7.433915	-1.853923	1.134203	L
C-CT--0.053600	0	6.245838	-0.958805	2.168408	L
H-H-0.271900	-1	10.285287	-3.283553	5.317734	L
H-H1-0.088000	-1	11.244266	-2.698724	2.657768	L
H-HC-0.024100	0	8.756212	-1.600601	4.053647	L
H-HC-0.024100	0	8.867271	-3.158932	3.235928	L
H-H1-0.044000	0	9.787960	-1.766367	1.212289	L
H-H1-0.044000	0	9.085451	-0.375759	2.035215	L
H-H1-0.068400	0	5.227662	-1.139237	1.813249	L
H-H1-0.068400	0	6.441026	0.111460	2.108837	L
H-H1-0.068400	0	6.320473	-1.295395	3.200674	L
N-N--0.415700	-1	11.064740	-0.114987	4.777302	L
C-CT--0.149000	-1	11.614353	1.224313	5.011025	L
H-H-0.271900	-1	10.487136	-0.549720	5.496329	L
H-H1-0.097600	-1	12.202286	1.531209	4.146123	L
H-H1-0.097600	-1	12.251224	1.206237	5.895028	L
H-H1-0.097600	-1	10.798293	1.930187	5.165585	L
C-CT--0.366200	-1	6.162020	8.765808	-5.527664	L
C-C-0.597200	-1	6.479554	7.571627	-4.606087	L
O-O--0.567900	-1	6.634189	6.424977	-5.050080	L

H-HC-0.112300	-1	6.067587	9.672445	-4.929054	L
H-HC-0.112300	-1	5.225439	8.580107	-6.054713	L
H-HC-0.112300	-1	6.967534	8.891045	-6.251952	L
N-N--0.415700	-1	6.621410	7.883104	-3.307546	L
C-CT--0.001400	-1	6.664996	6.888123	-2.220619	L
C-C-0.597300	-1	5.291595	6.204707	-2.082540	L
O-O--0.567900	-1	4.416750	6.680676	-1.341661	L
C-CT--0.001400	-1	7.180401	7.518509	-0.913716	L
C-CA--0.001100	-1	7.867706	6.545959	0.038802	L
C-CA--0.190600	-1	9.275608	6.498776	0.089832	L
C-CA--0.190600	-1	7.123208	5.720272	0.906230	L
C-CA--0.234100	-1	9.927556	5.676761	1.028080	L
C-CA--0.234100	-1	7.779530	4.893180	1.844192	L
C-C-0.322600	-1	9.181929	4.894003	1.923756	L
O-OH--0.557900	-1	9.843637	4.146807	2.854117	L
H-H-0.271900	-1	6.554688	8.874056	-3.062618	L
H-H1-0.087600	-1	7.378067	6.118642	-2.502830	L
H-HC-0.029500	-1	7.904289	8.292391	-1.171942	L
H-HC-0.029500	-1	6.366628	8.022089	-0.390440	L
H-HA-0.169900	-1	9.860461	7.126128	-0.567724	L
H-HA-0.169900	-1	6.042201	5.723693	0.862267	L
H-HA-0.165600	-1	11.004848	5.649742	1.077635	L
H-HA-0.165600	-1	7.206179	4.256986	2.502476	L
H-HO-0.399200	-1	9.347327	3.919584	3.656533	L
N-N--0.415700	-1	5.082472	5.185983	-2.921148	L
C-CT-0.033700	-1	3.767194	4.689204	-3.310303	L
C-C-0.597300	-1	2.931404	4.046880	-2.192240	L
O-O--0.567900	-1	1.707814	4.145303	-2.260997	L
C-CT--0.182500	-1	3.958659	3.694729	-4.450259	L
H-H-0.271900	-1	5.866389	4.896772	-3.501111	L
H-H1-0.082300	-1	3.199384	5.534027	-3.701433	L
H-HC-0.060300	-1	2.988531	3.383214	-4.836499	L
H-HC-0.060300	-1	4.498012	2.826315	-4.071918	L
H-HC-0.060300	-1	4.528385	4.159785	-5.254910	L
N-N--0.415700	-1	3.546738	3.403182	-1.189741	L H-HC 209
C-CT-0.021300	0	2.702886	2.688600	-0.185175	H
C-C-0.597300	0	2.330551	3.646471	0.963897	H
O-O--0.567900	0	3.198053	4.276991	1.566338	H
C-CT--0.123100	0	3.448621	1.423857	0.249967	H
S-S--1.036000	0	2.607731	0.354000	1.480011	H
H-H-0.271900	-1	4.550552	3.380770	-1.181533	L
H-H1-0.112400	0	1.786034	2.354334	-0.678790	H
H-H1-0.111200	0	4.395407	1.672579	0.745490	H
H-H1-0.111200	0	3.682723	0.826590	-0.636119	H
N-N--0.415700	0	0.995542	3.742090	1.236325	H
C-CT--0.051800	0	0.410662	4.543948	2.322081	H
C-C-0.597300	0	0.792164	4.013191	3.744555	H
O-O--0.567900	0	1.325796	4.740227	4.582580	H
C-CT--0.110200	-1	-1.132301	4.634536	2.045185	H
C-CT-0.353100	-1	-1.993925	5.533399	2.958296	L H-HC 222
C-CT--0.412100	-1	-2.183822	4.981167	4.372595	L
C-CT--0.412100	-1	-1.467470	6.968358	3.051838	L
H-H-0.271900	0	0.346357	3.136801	0.728569	H
H-H1-0.092200	0	0.851360	5.545079	2.299321	H

H-HC-0.045700	0	-1.249543	5.012767	1.022962	H
H-HC-0.045700	0	-1.569697	3.633681	2.060646	H
H-HC--0.036100	-1	-2.985716	5.580276	2.510040	L
H-HC-0.100000	-1	-1.285317	5.122853	4.969546	L
H-HC-0.100000	-1	-2.425567	3.920250	4.327636	L
H-HC-0.100000	-1	-3.004710	5.509885	4.854696	L
H-HC-0.100000	-1	-0.505413	6.985970	3.564890	L
H-HC-0.100000	-1	-2.181118	7.582808	3.599347	L
H-HC-0.100000	-1	-1.345086	7.374836	2.047016	L
N-N--0.415700	0	0.531763	2.694731	3.994461	H
C-CT--0.087500	0	0.588033	2.147899	5.356813	H
C-C-0.597300	0	1.986693	2.091180	5.979661	H
O-O--0.567900	0	2.090076	1.990701	7.199128	H
C-CT-0.298500	-1	-0.033394	0.729807	5.377328	H
C-CT--0.319200	0	0.773991	-0.338393	4.620998	L H-HC 241
C-CT--0.319200	0	-0.362045	0.173605	6.762780	L H-HC 241
H-H-0.271900	0	0.066583	2.143720	3.273010	H
H-H1-0.096900	0	0.015436	2.810151	6.019472	H
H-HC--0.029700	0	-0.986119	0.807734	4.854022	H
H-HC-0.079100	0	1.664103	-0.628114	5.174601	L
H-HC-0.079100	0	1.084863	0.056941	3.658034	L
H-HC-0.079100	0	0.153016	-1.210484	4.427539	L
H-HC-0.079100	0	0.552512	-0.052428	7.308959	L
H-HC-0.079100	0	-0.945019	-0.739829	6.650652	L
H-HC-0.079100	0	-0.949187	0.905383	7.315010	L
N-N--0.415700	0	3.005436	1.943984	5.101845	H
C-CT-0.033700	0	4.368459	1.793994	5.565026	H
C-C-0.597300	-1	5.078924	3.124473	5.843240	L H-H1 254
O-O--0.567900	-1	6.253899	3.101922	6.199433	L
C-CT--0.182500	-1	5.145170	0.982261	4.530608	L H-H1 254
H-H-0.271900	0	2.851541	2.190571	4.134782	H
H-H1-0.082300	0	4.345393	1.244202	6.509254	H
H-HC-0.060300	-1	6.112784	0.690514	4.936131	L
H-HC-0.060300	-1	5.300339	1.587522	3.637750	L
H-HC-0.060300	-1	4.589501	0.079574	4.273524	L
N-N--0.415700	-1	4.372969	4.251254	5.683038	L
C-CT--0.087500	-1	4.752586	5.613294	6.084924	L
C-C-0.597300	-1	3.909455	6.054122	7.288639	L
O-O--0.567900	-1	4.460356	6.501952	8.295320	L
C-CT-0.298500	-1	4.535667	6.592684	4.913974	L
C-CT--0.319200	-1	4.926273	8.030869	5.271658	L
C-CT--0.319200	-1	5.354088	6.203774	3.683156	L
H-H-0.271900	-1	3.462051	4.136374	5.256277	L
H-H1-0.096900	-1	5.802406	5.643484	6.366684	L
H-HC--0.029700	-1	3.483322	6.578897	4.637905	L
H-HC-0.079100	-1	5.976652	8.069698	5.551963	L
H-HC-0.079100	-1	4.318968	8.403329	6.095892	L
H-HC-0.079100	-1	4.764321	8.673165	4.406349	L
H-HC-0.079100	-1	6.404342	6.126789	3.958522	L
H-HC-0.079100	-1	5.235798	6.954363	2.902079	L
H-HC-0.079100	-1	5.004009	5.247475	3.294521	L
N-N--0.415700	-1	2.578572	5.860646	7.233962	L
C-CT--0.149000	-1	1.670372	6.193697	8.342102	L
H-H-0.271900	-1	2.172782	5.482549	6.383378	L

H-H1-0.097600	-1	2.247025	6.586579	9.179554	L
H-H1-0.097600	-1	1.136496	5.296355	8.656526	L
H-H1-0.097600	-1	0.953515	6.945155	8.011252	L
C-CT--0.366200	-1	4.022082	10.331112	-0.952056	L
C-C-0.597200	-1	2.548049	10.002272	-1.198352	L
O-O--0.567900	-1	1.736557	10.915670	-1.267488	L
H-HC-0.112300	-1	4.599502	9.408209	-0.919742	L
H-HC-0.112300	-1	4.122492	10.856520	-0.002540	L
H-HC-0.112300	-1	4.392560	10.963555	-1.758463	L
N-N--0.415700	-1	2.172097	8.718744	-1.259243	L
C-CT--0.024900	-1	0.759583	8.333363	-1.101986	L
C-C-0.597300	-1	0.171367	8.824274	0.226546	L
O-O--0.567900	-1	-0.924324	9.389392	0.236480	L
C-CT-0.211700	0	0.588950	6.833966	-1.257139	L
O-OH--0.654600	0	0.883233	6.532384	-2.601138	L
H-H-0.271900	-1	2.876139	7.987867	-1.322606	L
H-H1-0.084300	-1	0.186295	8.785372	-1.907130	L
H-H1-0.035200	0	-0.435802	6.545302	-1.032396	L
H-H1-0.035200	0	1.267115	6.301085	-0.589438	L
H-HO-0.427500	0	0.993447	5.557018	-2.613611	L
N-N--0.415700	-1	0.933890	8.687104	1.321990	L
C-CT-0.033700	-1	0.578686	9.162327	2.660417	L
C-C-0.597300	-1	0.110726	10.622509	2.657479	L
O-O--0.567900	-1	-0.986507	10.936685	3.121237	L
C-CT--0.182500	-1	1.765581	8.924347	3.591541	L
H-H-0.271900	-1	1.823521	8.193161	1.214979	L
H-H1-0.082300	-1	-0.234877	8.566844	3.047624	L
H-HC-0.060300	-1	1.534605	9.290490	4.591224	L
H-HC-0.060300	-1	2.650062	9.429411	3.205519	L
H-HC-0.060300	-1	1.963131	7.855400	3.641796	L
N-N--0.415700	-1	0.907101	11.505694	2.045417	L
C-CT--0.149000	-1	0.563602	12.903265	1.858010	L
H-H-0.271900	-1	1.810401	11.201094	1.690700	L
H-H1-0.097600	-1	-0.422971	13.094457	2.281635	L
H-H1-0.097600	-1	0.552904	13.135824	0.794019	L
H-H1-0.097600	-1	1.301495	13.529469	2.360500	L
C-CT--0.366200	-1	-11.939757	4.540988	4.979202	L
C-C-0.597200	-1	-12.369011	3.122195	4.602217	L
O-O--0.567900	-1	-12.932792	2.409786	5.435236	L
H-HC-0.112300	-1	-11.461180	5.015155	4.122225	L
H-HC-0.112300	-1	-11.235744	4.499034	5.810415	L
H-HC-0.112300	-1	-12.815038	5.119715	5.272628	L
N-N--0.415700	-1	-12.033694	2.686689	3.387473	L
C-CT--0.087500	-1	-12.026233	1.265655	3.022884	L
C-C-0.597300	-1	-10.579174	0.875579	2.707995	L
O-O--0.567900	-1	-9.865236	1.524087	1.935392	L
C-CT-0.298500	-1	-13.021238	0.877424	1.896689	L
C-CT--0.319200	-1	-13.765623	-0.416039	2.277053	L
C-CT--0.319200	-1	-14.101854	1.924013	1.591188	L
H-H-0.271900	-1	-11.624799	3.341365	2.718144	L
H-H1-0.096900	-1	-12.317713	0.702208	3.906869	L
H-HC--0.029700	-1	-12.461792	0.692455	0.983358	L
H-HC-0.079100	-1	-14.398619	-0.239025	3.147280	L
H-HC-0.079100	-1	-13.047886	-1.207531	2.496369	L

H-HC-0.079100	-1	-14.401450	-0.729480	1.449258	L
H-HC-0.079100	-1	-14.735965	2.063537	2.463226	L
H-HC-0.079100	-1	-14.708442	1.589790	0.750901	L
H-HC-0.079100	-1	-13.647107	2.878347	1.334546	L
N-N--0.415700	-1	-10.113316	-0.146099	3.429053	L
C-CT--0.038900	-1	-8.704232	-0.540133	3.509930	L
C-C-0.597300	-1	-8.572395	-2.065692	3.617425	L
O-O--0.567900	-1	-9.501694	-2.730236	4.097502	L
C-CT-0.365400	-1	-7.989358	0.104375	4.721353	L
O-OH--0.676100	-1	-8.155649	-0.615166	5.921454	L
C-CT--0.243800	-1	-8.411514	1.538598	5.034213	L
H-H-0.271900	-1	-10.741672	-0.622919	4.059587	L
H-H1-0.100700	-1	-8.204675	-0.201985	2.602147	L
H-H1-0.004300	-1	-6.930273	0.107866	4.485155	L
H-HC-0.064200	-1	-8.456241	2.106620	4.112494	L
H-HC-0.064200	-1	-7.684631	1.994876	5.707501	L
H-HC-0.064200	-1	-9.394940	1.560814	5.502893	L
H-HO-0.410200	-1	-8.408889	0.020924	6.622597	L
N-N--0.254800	-1	-7.444736	-2.655971	3.182308	L
C-CT--0.026600	-1	-7.190171	-4.081988	3.346877	L
C-C-0.589600	-1	-6.580997	-4.439784	4.703777	L
O-O--0.574800	-1	-6.589102	-5.612018	5.062320	L
C-CT--0.007000	0	-6.202313	-4.418387	2.229860	L
C-CT-0.018900	0	-5.367253	-3.147091	2.101839	L
C-CT-0.019200	0	-6.375334	-2.036362	2.402466	L
H-H1-0.064100	-1	-8.098566	-4.654299	3.200075	L
H-HC-0.025300	0	-5.584629	-5.277504	2.484104	L
H-HC-0.025300	0	-6.745674	-4.597716	1.301263	L
H-HC-0.021300	0	-4.942078	-3.051947	1.104204	L
H-HC-0.021300	0	-4.576624	-3.146033	2.852242	L
H-H1-0.039100	0	-6.779736	-1.655682	1.464208	L
H-H1-0.039100	0	-5.887898	-1.233364	2.956953	L
N-N--0.415700	-1	-5.965221	-3.478933	5.400680	L
C-CT--0.001400	-1	-4.973252	-3.720877	6.459757	L
C-C-0.597300	-1	-5.519269	-4.510146	7.664137	L
O-O--0.567900	-1	-6.706119	-4.398279	7.975238	L
C-CT--0.001400	0	-4.441944	-2.378371	6.980091	L H-HA 373
C-CA--0.001100	0	-4.081223	-1.358447	5.915483	H
C-CA--0.190600	0	-3.191151	-1.681957	4.887157	H
C-CA--0.190600	0	-4.626805	-0.072849	5.964495	H
C-CA--0.234100	0	-2.849665	-0.741363	3.921023	H
C-CA--0.234100	0	-4.286921	0.881688	5.011434	H
C-C-0.322600	0	-3.386854	0.557945	3.987216	H
O-OH--0.557900	0	-3.073832	1.516259	3.093975	H
H-H-0.271900	-1	-6.035196	-2.538988	5.042484	L
H-H1-0.087600	-1	-4.146778	-4.285552	6.026870	L
H-HC-0.029500	0	-5.201027	-1.941564	7.631443	L
H-HC-0.029500	0	-3.555964	-2.562517	7.588986	L
H-HA-0.169900	0	-2.758262	-2.677905	4.823317	H
H-HA-0.169900	0	-5.321064	0.200295	6.760382	H
H-HA-0.165600	0	-2.142510	-0.986575	3.136291	H
H-HA-0.165600	0	-4.673970	1.895775	5.071880	H
H-HO-0.399200	0	-2.206415	1.316786	2.630914	H
N-N--0.415700	-1	-4.638747	-5.200019	8.415751	L

C-CT--0.149000	-1	-5.022062	-5.672260	9.762700	L
H-H-0.271900	-1	-3.643999	-5.189336	8.176284	L
H-H1-0.097600	-1	-6.105952	-5.625621	9.869035	L
H-H1-0.097600	-1	-4.555055	-5.039481	10.516664	L
H-H1-0.097600	-1	-4.687866	-6.701579	9.895022	L
C-CT--0.366200	-1	-0.443327	-10.780372	2.433751	L
C-C-0.597200	-1	-0.626611	-9.836070	1.232361	L
O-O--0.567900	-1	-1.736555	-9.663288	0.723940	L
H-HC-0.112300	-1	0.604643	-10.792354	2.729791	L
H-HC-0.112300	-1	-0.753848	-11.787514	2.154415	L
H-HC-0.112300	-1	-1.053138	-10.431458	3.267115	L
N-N--0.415700	-1	0.486046	-9.284341	0.730937	L
C-CT-0.014300	-1	0.439328	-8.263254	-0.314936	L H-HC 405
C-C-0.597300	-1	0.067602	-8.767056	-1.728256	L
O-O--0.567900	-1	-0.145938	-7.941779	-2.607035	L
C-CT--0.204100	0	1.741074	-7.438717	-0.325106	H
C-C-0.713000	0	1.398504	-5.964968	-0.589479	H
O-O--0.593100	0	0.618747	-5.408541	0.186171	H
N-N--0.919100	0	2.002215	-5.360389	-1.628808	H
H-H-0.271900	-1	1.369319	-9.471009	1.176633	L
H-H1-0.104800	-1	-0.365404	-7.594543	-0.008879	L
H-HC-0.079700	0	2.454194	-7.875981	-1.034303	H
H-HC-0.079700	0	2.186199	-7.461203	0.673778	H
H-H-0.419600	0	1.872349	-4.351958	-1.812998	H
H-H-0.419600	0	2.525895	-5.910973	-2.294697	H
N-N--0.415700	-1	-0.024833	-10.079756	-1.970577	L
C-CT--0.149000	-1	-0.563114	-10.627679	-3.227734	L
H-H-0.271900	-1	0.086735	-10.731572	-1.185918	L
H-H1-0.097600	-1	-0.629742	-9.834301	-3.971477	L
H-H1-0.097600	-1	-1.555378	-11.041835	-3.048651	L
H-H1-0.097600	-1	0.097520	-11.414787	-3.593438	L
C-CT--0.366200	-1	-3.831236	-11.700972	-1.465726	L
C-C-0.597200	-1	-4.601868	-10.376342	-1.533467	L
O-O--0.567900	-1	-5.740567	-10.380243	-2.005307	L
H-HC-0.112300	-1	-2.848569	-11.526562	-1.026558	L
H-HC-0.112300	-1	-3.712980	-12.104450	-2.470381	L
H-HC-0.112300	-1	-4.382967	-12.411059	-0.850117	L
N-N--0.415700	-1	-3.977349	-9.248923	-1.153978	L
C-CT--0.087500	-1	-4.544557	-7.888706	-1.312679	L
C-C-0.597300	-1	-4.809641	-7.501924	-2.778832	L
O-O--0.567900	-1	-5.799825	-6.833584	-3.072624	L
C-CT-0.298500	-1	-3.640309	-6.812158	-0.657098	L
C-CT--0.319200	-1	-4.130746	-5.374585	-0.892940	L
C-CT--0.319200	-1	-3.625538	-6.953989	0.862521	L
H-H-0.271900	-1	-3.095413	-9.359383	-0.651670	L
H-H1-0.096900	-1	-5.505776	-7.870885	-0.800391	L
H-HC--0.029700	-1	-2.624302	-6.906596	-1.040881	L
H-HC-0.079100	-1	-5.167023	-5.281550	-0.567177	L
H-HC-0.079100	-1	-4.062635	-5.119170	-1.947771	L
H-HC-0.079100	-1	-3.505668	-4.667711	-0.345251	L
H-HC-0.079100	-1	-4.632614	-6.822811	1.240984	L
H-HC-0.079100	-1	-2.963757	-6.208222	1.305265	L
H-HC-0.079100	-1	-3.274364	-7.931572	1.161383	L
N-N--0.415700	-1	-3.961422	-7.896464	-3.736716	L

C-CT--0.149000	-1	-4.047263	-7.477605	-5.146541	L
H-H-0.271900	-1	-3.238333	-8.558728	-3.481698	L
H-H1-0.097600	-1	-4.866953	-6.768698	-5.266187	L
H-H1-0.097600	-1	-4.227244	-8.350474	-5.775645	L
H-H1-0.097600	-1	-3.111792	-7.003776	-5.442728	L
C-CT--0.366200	-1	-12.123890	3.661700	-1.319319	L
C-C-0.597200	-1	-11.017340	2.597989	-1.285666	L
O-O--0.567900	-1	-11.307911	1.413894	-1.134639	L
H-HC-0.112300	-1	-11.677557	4.646183	-1.460008	L
H-HC-0.112300	-1	-12.674868	3.643687	-0.378607	L
H-HC-0.112300	-1	-12.806150	3.450611	-2.143010	L
N-N--0.415700	-1	-9.761723	3.041759	-1.350962	L
C-CT--0.024900	-1	-8.577302	2.221724	-1.173142	L
C-C-0.597300	-1	-7.467261	3.087916	-0.572454	L
O-O--0.567900	-1	-6.815702	3.879804	-1.267789	L
C-CT-0.211700	0	-8.152530	1.572817	-2.488449	L
O-OH--0.654600	0	-7.223029	0.568120	-2.190012	L
H-H-0.271900	-1	-9.637448	4.038711	-1.417970	L
H-H1-0.084300	-1	-8.813591	1.426561	-0.467394	L
H-H1-0.035200	0	-7.715196	2.302858	-3.166616	L
H-H1-0.035200	0	-9.020860	1.111987	-2.961621	L
H-HO-0.427500	0	-6.309042	0.922670	-2.269847	L
N-N--0.415700	-1	-7.305867	3.010381	0.757380	L
C-CT-0.021300	-1	-6.132651	3.626397	1.395740	L
C-C-0.597300	-1	-4.842473	2.984180	0.860996	L
O-O--0.567900	-1	-3.868865	3.675364	0.603477	L
C-CT--0.123100	-1	-6.191159	3.485281	2.918348	L
S-SH--0.311900	-1	-7.447736	4.586693	3.628519	L
H-H-0.271900	-1	-7.965980	2.460705	1.304143	L
H-H1-0.112400	-1	-6.106335	4.689224	1.150177	L
H-H1-0.111200	-1	-5.220928	3.759271	3.336208	L
H-H1-0.111200	-1	-6.405203	2.449307	3.179893	L
H-HS-0.193300	-1	-8.488402	4.138575	2.917123	L
N-N--0.415700	-1	-4.877742	1.665924	0.650919	L H-HC 478
C-CT-0.021300	0	-3.690928	0.970583	0.081422	H
C-C-0.597300	0	-3.666771	1.219015	-1.420555	H
O-O--0.567900	0	-4.708820	1.312229	-2.073985	H
C-CT--0.123100	0	-3.771065	-0.526063	0.418995	H
S-SH--0.311900	0	-2.404620	-1.684467	-0.135503	H
H-H-0.271900	-1	-5.727790	1.175176	0.854630	L
H-H1-0.112400	0	-2.792885	1.396337	0.533543	H
H-H1-0.111200	0	-4.651172	-0.970552	-0.061577	H
H-H1-0.111200	0	-3.864015	-0.653843	1.496562	H
H-HS-0.193300	0	-1.012869	-1.134422	-0.314521	H
N-N--0.415700	0	-2.426117	1.273368	-1.982816	H
C-CT--0.087500	0	-2.283999	1.394404	-3.424053	H
C-C-0.597300	0	-2.187177	0.045500	-4.185223	H
O-O--0.567900	0	-2.244218	0.071986	-5.413450	H
C-CT-0.298500	-1	-1.121797	2.309329	-3.868282	H
C-CT--0.319200	0	-1.253024	3.710786	-3.268081	L H-HC 492
C-CT--0.319200	0	0.260251	1.753906	-3.485207	L H-HC 492
H-H-0.271900	0	-1.614710	1.306746	-1.359085	H
H-H1-0.096900	0	-3.227734	1.818362	-3.786461	H
H-HC--0.029700	0	-1.163284	2.381442	-4.957238	H

H-HC-0.079100	0	-1.105918	3.674605	-2.185749	L
H-HC-0.079100	0	-2.240897	4.104385	-3.486475	L
H-HC-0.079100	0	-0.507531	4.369006	-3.709989	L
H-HC-0.079100	0	0.388026	1.789604	-2.403281	L
H-HC-0.079100	0	1.035383	2.353275	-3.953914	L
H-HC-0.079100	0	0.376546	0.725423	-3.818171	L
N-N--0.415700	0	-1.965146	-1.071968	-3.443837	H
C-CT--0.003100	0	-2.047731	-2.412400	-4.024852	H
C-C-0.597300	0	-3.508489	-2.874132	-4.201229	H
O-O--0.567900	0	-3.805287	-3.653796	-5.101437	H
C-CT--0.003600	-1	-1.286210	-3.434668	-3.130699	H
C-CT--0.064500	-1	-1.415203	-4.887691	-3.625577	L H-HC 508
C-C-0.695100	-1	-0.540198	-5.220085	-4.819545	L
O-O--0.608600	-1	-0.399627	-4.465608	-5.767079	L
N-N--0.940700	-1	0.076563	-6.382285	-4.817849	L
H-H-0.271900	0	-2.041223	-1.021500	-2.430364	H
H-H1-0.085000	0	-1.633625	-2.371205	-5.034704	H
H-HC-0.017100	0	-0.233039	-3.169800	-3.042283	H
H-HC-0.017100	0	-1.719348	-3.397857	-2.128035	H
H-HC-0.035200	-1	-2.442483	-5.144661	-3.868006	L
H-HC-0.035200	-1	-1.128610	-5.537416	-2.806118	L
H-H-0.425100	-1	0.680761	-6.626452	-5.582853	L
H-H-0.425100	-1	-0.031836	-7.006110	-4.020050	L
N-N--0.415700	0	-4.346870	-2.512092	-3.176620	H
C-CT--0.023700	0	-5.729855	-2.953870	-3.249869	H
C-C-0.597300	-1	-6.404168	-2.326950	-4.486442	L H-H1 522
O-O--0.567900	-1	-6.236620	-1.130380	-4.741049	L
C-CT-0.034200	-1	-6.464528	-2.676200	-1.920992	L H-H1 522
C-CT-0.001800	-1	-7.931609	-3.129317	-1.979931	L
S-S--0.273700	-1	-8.836005	-3.111086	-0.404679	L
C-CT--0.053600	-1	-9.209760	-1.344688	-0.267462	L
H-H-0.271900	0	-4.211425	-1.596366	-2.783118	H
H-H1-0.088000	0	-5.674326	-4.031376	-3.365389	H
H-HC-0.024100	-1	-6.397189	-1.630472	-1.657789	L
H-HC-0.024100	-1	-5.969663	-3.230000	-1.126770	L
H-H1-0.044000	-1	-7.953701	-4.153724	-2.353019	L
H-H1-0.044000	-1	-8.473417	-2.502045	-2.688113	L
H-H1-0.068400	-1	-9.816116	-1.164611	0.620165	L
H-H1-0.068400	-1	-9.760736	-1.013951	-1.148108	L
H-H1-0.068400	-1	-8.281474	-0.782255	-0.193680	L
N-N--0.254800	-1	-7.150613	-3.095620	-5.300951	L
C-CT--0.026600	-1	-7.548587	-2.675361	-6.645395	L
C-C-0.589600	-1	-8.999747	-2.196051	-6.635549	L
O-O--0.574800	-1	-9.883777	-2.900767	-6.141500	L
C-CT--0.007000	-1	-7.338373	-3.915453	-7.528640	L
C-CT-0.018900	-1	-6.818793	-4.980050	-6.559185	L
C-CT-0.019200	-1	-7.352604	-4.526178	-5.226916	L
H-H1-0.064100	-1	-6.903591	-1.875151	-7.007855	L
H-HC-0.025300	-1	-8.271735	-4.237438	-7.981508	L
H-HC-0.025300	-1	-6.603368	-3.725913	-8.308640	L
H-HC-0.021300	-1	-5.730717	-4.968711	-6.532838	L
H-HC-0.021300	-1	-7.189804	-5.962901	-6.778689	L
H-H1-0.039100	-1	-6.826865	-5.035368	-4.430908	L
H-H1-0.039100	-1	-8.417397	-4.750324	-5.153403	L

N-N--0.415700	-1	-9.226837	-0.998222	-7.168068	L
C-CT--0.149000	-1	-10.462835	-0.233592	-6.975460	L
H-H-0.271900	-1	-8.423541	-0.524750	-7.580939	L
H-H1-0.097600	-1	-11.221043	-0.875588	-6.527633	L
H-H1-0.097600	-1	-10.817696	0.130154	-7.939721	L
H-H1-0.097600	-1	-10.266747	0.612479	-6.316418	L
C-CT--0.366200	-1	-10.376013	8.837270	-4.210631	L
C-C-0.597200	-1	-9.823114	7.547987	-3.588869	L
O-O--0.567900	-1	-10.264259	7.122886	-2.519758	L
H-HC-0.112300	-1	-9.858160	9.040027	-5.147983	L
H-HC-0.112300	-1	-10.219898	9.667559	-3.522436	L
H-HC-0.112300	-1	-11.442258	8.719980	-4.403230	L
N-N--0.415700	-1	-8.850173	6.930915	-4.254017	L
C-CT--0.024900	-1	-7.902841	6.013592	-3.617162	L
C-C-0.597300	-1	-6.575714	6.749251	-3.393385	L
O-O--0.567900	-1	-6.324272	7.759719	-4.057385	L
C-CT-0.211700	0	-7.676613	4.763153	-4.478928	L
O-OH--0.654600	0	-7.306756	5.081196	-5.807425	L
H-H-0.271900	-1	-8.580642	7.303787	-5.163407	L
H-H1-0.084300	-1	-8.287623	5.669728	-2.656699	L
H-H1-0.035200	0	-8.595099	4.175248	-4.498860	L
H-H1-0.035200	0	-6.888544	4.159282	-4.026632	L
H-HO-0.427500	0	-6.877854	4.310431	-6.196612	L
N-N--0.415700	-1	-5.696189	6.217477	-2.534014	L
C-CT-0.033700	-1	-4.324131	6.730494	-2.428895	L
C-C-0.597300	-1	-3.576519	6.742320	-3.781291	L
O-O--0.567900	-1	-2.679983	7.559835	-3.995515	L
C-CT--0.182500	-1	-3.567792	5.907988	-1.395808	L
H-H-0.271900	-1	-5.976353	5.409412	-1.973225	L
H-H1-0.082300	-1	-4.374992	7.756462	-2.062823	L
H-HC-0.060300	-1	-2.555491	6.292428	-1.289211	L
H-HC-0.060300	-1	-3.529233	4.863138	-1.702020	L
H-HC-0.060300	-1	-4.083630	5.986350	-0.440075	L
N-N--0.415700	-1	-3.994975	5.877534	-4.719119	L
C-CT--0.149000	-1	-3.479871	5.830537	-6.086353	L
H-H-0.271900	-1	-4.721277	5.225461	-4.454338	L
H-H1-0.097600	-1	-2.708959	6.591482	-6.210172	L
H-H1-0.097600	-1	-4.291959	6.020442	-6.788037	L
H-H1-0.097600	-1	-3.053972	4.846169	-6.280385	L
C-CM--0.139000	0	0.748027	-0.886820	-0.560476	H
C-C-0.519000	0	1.429591	-2.089871	-0.896422	H
O-O2--0.567000	0	1.914567	-2.855495	0.113724	H
C-CM--0.117000	0	0.893871	-0.283896	0.792060	H
O-O2--0.618000	0	1.655218	-2.518822	-2.062324	H
C-C--0.553000	0	-0.153664	0.803248	1.005786	H
O-O2--0.556000	0	-0.738588	0.830451	2.134864	H
O-O2--0.607000	0	-0.397899	1.598576	0.051392	H
H-HC-0.049000	0	0.631504	-0.204483	-1.392186	H
H-HC-0.162000	0	0.737352	-1.026460	1.573580	H
O-OW--0.834000	-1	6.429206	2.984615	-1.165016	L
H-HW-0.417000	-1	6.800001	3.130350	-2.034575	L
H-HW-0.417000	-1	7.107406	3.285267	-0.560518	L
O-OW--0.834000	0	3.288887	6.928029	1.092386	L
H-HW-0.417000	0	3.189859	6.023759	1.453174	L

H-HW-0.417000	0	3.676471	6.750085	0.219571	L
O-OW--0.834000	0	-0.193688	-3.240652	1.808872	H
H-HW-0.417000	0	-0.971677	-2.852208	1.364972	H
H-HW-0.417000	0	-0.074240	-4.095440	1.349032	H
O-OW--0.834000	0	-4.956276	0.812226	-6.195506	L
H-HW-0.417000	0	-4.017842	0.593061	-6.095172	L
H-HW-0.417000	0	-5.396359	0.165585	-5.617991	L
H-HS-0.193300	0	1.300198	-2.803287	0.880369	H

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C-CT--0.366200	-1	8.190705	4.704542	-8.124578	L
C-C-0.597200	-1	9.024020	3.960257	-7.086592	L
O-O--0.567900	-1	9.628197	2.925450	-7.370525	L
H-HC-0.112300	-1	7.744452	5.587759	-7.667700	L
H-HC-0.112300	-1	7.401658	4.049384	-8.495369	L
H-HC-0.112300	-1	8.829769	5.008806	-8.954367	L
N-N--0.415700	-1	9.017231	4.515801	-5.868361	L
C-CT--0.087500	-1	9.491348	3.839185	-4.653987	L
C-C-0.597300	-1	8.357254	2.936649	-4.164015	L
O-O--0.567900	-1	7.444789	3.391651	-3.459170	L
C-CT-0.298500	-1	9.970401	4.840659	-3.576022	L
C-CT--0.319200	-1	10.392894	4.139954	-2.279189	L
C-CT--0.319200	-1	11.181789	5.654133	-4.054315	L
H-H-0.271900	-1	8.429131	5.335514	-5.739087	L
H-H1-0.096900	-1	10.331209	3.201644	-4.909876	L
H-HC--0.029700	-1	9.170743	5.542901	-3.357797	L
H-HC-0.079100	-1	11.101674	3.344239	-2.510319	L
H-HC-0.079100	-1	9.524231	3.712478	-1.782187	L
H-HC-0.079100	-1	10.867077	4.848323	-1.601742	L
H-HC-0.079100	-1	12.044518	5.000854	-4.184718	L
H-HC-0.079100	-1	11.425294	6.424338	-3.320366	L
H-HC-0.079100	-1	10.961486	6.135003	-5.006383	L
N-N--0.415700	-1	8.378400	1.665068	-4.598656	L
C-CT--0.087500	-1	7.268955	0.708492	-4.425617	L
C-C-0.597300	-1	7.689818	-0.567327	-3.667492	L
O-O--0.567900	-1	8.837418	-1.014367	-3.793273	L
C-CT-0.298500	-1	6.616756	0.302152	-5.771554	L
C-CT--0.319200	-1	5.754764	1.426833	-6.356822	L
C-CT--0.319200	-1	7.610941	-0.142579	-6.849474	L
H-H-0.271900	-1	9.154664	1.363426	-5.193486	L
H-H1-0.096900	-1	6.496252	1.211243	-3.851003	L
H-HC--0.029700	-1	5.950785	-0.541588	-5.587085	L
H-HC-0.079100	-1	6.268427	2.384929	-6.278809	L
H-HC-0.079100	-1	4.819627	1.469751	-5.802978	L
H-HC-0.079100	-1	5.507052	1.213167	-7.397869	L
H-HC-0.079100	-1	8.208119	0.704994	-7.181664	L
H-HC-0.079100	-1	7.062744	-0.545783	-7.699934	L
H-HC-0.079100	-1	8.268214	-0.914062	-6.456524	L
N-N--0.254800	-1	6.756179	-1.179162	-2.900968	L
C-CT--0.026600	-1	6.893393	-2.532956	-2.357276	L
C-C-0.589600	-1	7.145250	-3.552907	-3.469537	L
O-O--0.574800	-1	6.398473	-3.601139	-4.450033	L
C-CT--0.007000	0	5.552007	-2.814127	-1.660043	L
C-CT-0.018900	0	4.991343	-1.422580	-1.374876	L

C-CT-0.019200	0	5.473246	-0.602415	-2.541910	L
H-H1-0.064100	-1	7.711989	-2.546743	-1.638537	L
H-HC-0.025300	0	4.865484	-3.335181	-2.328982	L
H-HC-0.025300	0	5.688337	-3.392261	-0.751292	L
H-HC-0.021300	0	5.397491	-1.014052	-0.456163	L
H-HC-0.021300	0	3.917922	-1.388227	-1.352385	L
H-H1-0.039100	0	5.557327	0.436802	-2.223053	L
H-H1-0.039100	0	4.773569	-0.697229	-3.373950	L
N-N--0.415700	-1	8.173327	-4.395254	-3.323003	L
C-CT--0.149000	-1	8.546747	-5.387562	-4.343679	L
H-H-0.271900	-1	8.771954	-4.272524	-2.507410	L
H-H1-0.097600	-1	7.803355	-5.388515	-5.140188	L
H-H1-0.097600	-1	8.592176	-6.377140	-3.887901	L
H-H1-0.097600	-1	9.522519	-5.133810	-4.757915	L
C-CT--0.366200	-1	5.255019	-7.384838	-4.103721	L
C-C-0.597200	-1	4.123440	-6.716756	-4.894909	L
O-O--0.567900	-1	3.228602	-7.437392	-5.346266	L
H-HC-0.112300	-1	5.963858	-6.626421	-3.772086	L
H-HC-0.112300	-1	5.766218	-8.107742	-4.739327	L
H-HC-0.112300	-1	4.837890	-7.895343	-3.235600	L
N-N--0.415700	-1	4.106572	-5.385685	-5.031084	L
C-CT-0.014300	-1	3.001852	-4.641002	-5.660060	L H-HC 69
C-C-0.597300	-1	2.809443	-4.978912	-7.173195	L
O-O--0.567900	-1	3.804932	-5.137785	-7.881188	L
C-CT--0.204100	0	3.300430	-3.141272	-5.433212	H
C-C-0.713000	0	2.185050	-2.221037	-5.923202	H
O-O--0.593100	0	2.072585	-1.888633	-7.097297	H
N-N--0.919100	0	1.361736	-1.747974	-4.941306	H
H-H-0.271900	-1	4.872571	-4.845990	-4.661597	L
H-H1-0.104800	-1	2.095127	-4.909503	-5.127682	L
H-HC-0.079700	0	4.206401	-2.897630	-5.998250	H
H-HC-0.079700	0	3.491363	-2.986536	-4.367969	H
H-H-0.419600	0	0.488203	-1.370647	-5.287239	H
H-H-0.419600	0	1.381990	-2.145540	-4.006881	H
N-N--0.415700	-1	1.556518	-5.081814	-7.667427	L
C-CT--0.149000	-1	1.206396	-5.339680	-9.093950	L
H-H-0.271900	-1	0.799915	-4.860857	-7.020983	L
H-H1-0.097600	-1	2.113321	-5.559781	-9.656528	L
H-H1-0.097600	-1	0.722524	-4.457521	-9.514092	L
H-H1-0.097600	-1	0.526745	-6.189817	-9.151612	L
C-CT--0.366200	-1	11.739728	-5.871201	-0.643624	L
C-C-0.597200	-1	10.723868	-6.004044	0.499152	L
O-O--0.567900	-1	11.039594	-5.850593	1.684272	L
H-HC-0.112300	-1	11.240156	-6.046616	-1.596251	L
H-HC-0.112300	-1	12.534550	-6.604534	-0.509953	L
H-HC-0.112300	-1	12.166588	-4.868069	-0.636623	L
N-N--0.415700	-1	9.488758	-6.311944	0.106310	L
C-CT--0.023700	-1	8.328749	-6.516100	0.969007	L
C-C-0.597300	-1	7.278219	-7.362101	0.262149	L
O-O--0.567900	-1	7.099734	-7.201007	-0.952027	L
C-CT-0.034200	0	7.724309	-5.160982	1.372560	L
C-CT-0.001800	0	6.849298	-5.194847	2.640452	L
S-S--0.273700	0	5.136399	-5.780606	2.468000	L
C-CT--0.053600	0	4.302127	-4.236951	1.988249	L

H-H-0.271900	-1	9.321019	-6.383992	-0.891173	L
H-H1-0.088000	-1	8.654827	-7.048803	1.850663	L
H-HC-0.024100	0	7.151990	-4.748266	0.541730	L
H-HC-0.024100	0	8.554952	-4.488416	1.566687	L
H-H1-0.044000	0	6.799128	-4.183107	3.043296	L
H-H1-0.044000	0	7.350269	-5.811635	3.386445	L
H-H1-0.068400	0	3.277162	-4.442420	1.679472	L
H-H1-0.068400	0	4.818825	-3.766537	1.156201	L
H-H1-0.068400	0	4.282610	-3.539188	2.825727	L
N-N--0.415700	-1	6.573050	-8.212380	1.018662	L
C-CT--0.149000	-1	5.354294	-8.922296	0.602279	L
H-H-0.271900	-1	6.889104	-8.344886	1.979352	L
H-H1-0.097600	-1	5.136757	-8.690138	-0.439752	L
H-H1-0.097600	-1	4.518740	-8.606853	1.227351	L
H-H1-0.097600	-1	5.504896	-9.995912	0.711500	L
C-CT--0.366200	-1	3.718870	-9.135979	4.113368	L
C-C-0.597200	-1	3.611775	-7.971977	5.119004	L
O-O--0.567900	-1	4.598033	-7.486821	5.681227	L
H-HC-0.112300	-1	2.724159	-9.394419	3.748778	L
H-HC-0.112300	-1	4.161653	-10.002198	4.604670	L
H-HC-0.112300	-1	4.345766	-8.834756	3.273946	L
N-N--0.415700	-1	2.380872	-7.487950	5.307177	L
C-CT--0.087500	-1	2.069472	-6.095026	5.666340	L
C-C-0.597300	-1	1.861440	-5.985352	7.182827	L
O-O--0.567900	-1	0.761887	-6.165467	7.725276	L
C-CT-0.298500	0	0.829799	-5.587676	4.892045	L
C-CT--0.319200	0	0.692937	-4.068236	5.023777	L
C-CT--0.319200	0	0.881815	-5.946715	3.399647	L
H-H-0.271900	-1	1.607885	-8.017947	4.896421	L
H-H1-0.096900	-1	2.926257	-5.475636	5.394119	L
H-HC--0.029700	0	-0.066923	-6.056541	5.298688	L
H-HC-0.079100	0	1.562407	-3.568769	4.591874	L
H-HC-0.079100	0	0.588596	-3.777665	6.068322	L
H-HC-0.079100	0	-0.190175	-3.727992	4.480929	L
H-HC-0.079100	0	1.762096	-5.499845	2.939469	L
H-HC-0.079100	0	-0.002911	-5.549711	2.904271	L
H-HC-0.079100	0	0.887938	-7.022361	3.246268	L
N-N--0.415700	-1	3.005478	-5.826548	7.847918	L
C-CT--0.149000	-1	3.259044	-6.166058	9.245449	L
H-H-0.271900	-1	3.828054	-5.627922	7.290637	L
H-H1-0.097600	-1	2.312001	-6.359379	9.749472	L
H-H1-0.097600	-1	3.767746	-5.336241	9.734853	L
H-H1-0.097600	-1	3.885306	-7.056898	9.294652	L
C-CT--0.366200	-1	12.491178	-4.196381	6.337797	L
C-C-0.597200	-1	12.284761	-3.470554	4.989783	L
O-O--0.567900	-1	13.251448	-3.248826	4.253992	L
H-HC-0.112300	-1	11.531998	-4.301088	6.844857	L
H-HC-0.112300	-1	13.169964	-3.615068	6.963049	L
H-HC-0.112300	-1	12.917115	-5.182619	6.158169	L
N-N--0.415700	-1	11.048281	-3.047576	4.687844	L
C-CT--0.023700	-1	10.769313	-2.220874	3.515905	L
C-C-0.597300	-1	11.333122	-0.796650	3.656408	L
O-O--0.567900	-1	12.060937	-0.326706	2.780064	L
C-CT-0.034200	0	9.262025	-2.145934	3.258388	L

C-CT-0.001800	0	9.007688	-1.444063	1.918656	L
S-S--0.273700	0	7.444052	-1.866228	1.133050	L
C-CT--0.053600	0	6.236709	-1.012791	2.179683	L
H-H-0.271900	-1	10.283867	-3.280609	5.315320	L
H-H1-0.088000	-1	11.241523	-2.696653	2.654686	L
H-HC-0.024100	0	8.754881	-1.605702	4.058960	L
H-HC-0.024100	0	8.868883	-3.157299	3.227922	L
H-H1-0.044000	0	9.794348	-1.731400	1.219870	L
H-H1-0.044000	0	9.060435	-0.362941	2.054265	L
H-H1-0.068400	0	5.224124	-1.234581	1.834782	L
H-H1-0.068400	0	6.387300	0.064336	2.112475	L
H-H1-0.068400	0	6.333957	-1.340211	3.212901	L
N-N--0.415700	-1	11.063425	-0.112292	4.773580	L
C-CT--0.149000	-1	11.613323	1.227008	5.006634	L
H-H-0.271900	-1	10.486144	-0.546750	5.493032	L
H-H1-0.097600	-1	12.200839	1.533586	4.141336	L
H-H1-0.097600	-1	12.250655	1.209104	5.890308	L
H-H1-0.097600	-1	10.797430	1.933024	5.161421	L
C-CT--0.366200	-1	6.156383	8.766174	-5.531337	L
C-C-0.597200	-1	6.474256	7.572217	-4.609588	L
O-O--0.567900	-1	6.628517	6.425421	-5.053336	L
H-HC-0.112300	-1	6.062376	9.672993	-4.932934	L
H-HC-0.112300	-1	5.219503	8.580439	-6.057841	L
H-HC-0.112300	-1	6.961533	8.891107	-6.256083	L
N-N--0.415700	-1	6.616831	7.884046	-3.311209	L
C-CT--0.001400	-1	6.660865	6.889367	-2.224023	L
C-C-0.597300	-1	5.287453	6.206159	-2.085029	L
O-O--0.567900	-1	4.413056	6.682445	-1.343827	L
C-CT--0.001400	-1	7.177032	7.520061	-0.917570	L
C-CA--0.001100	-1	7.864718	6.547699	0.034865	L
C-CA--0.190600	-1	9.272641	6.500358	0.085169	L
C-CA--0.190600	-1	7.120574	5.722350	0.902918	L
C-CA--0.234100	-1	9.924980	5.678531	1.023309	L
C-CA--0.234100	-1	7.777287	4.895443	1.840770	L
C-C-0.322600	-1	9.179727	4.896118	1.919598	L
O-OH--0.557900	-1	9.841832	4.149105	2.849824	L
H-H-0.271900	-1	6.550358	8.875075	-3.066527	L
H-H1-0.087600	-1	7.373694	6.119720	-2.506390	L
H-HC-0.029500	-1	7.900879	8.293782	-1.176395	L
H-HC-0.029500	-1	6.363595	8.023890	-0.394010	L
H-HA-0.169900	-1	9.857225	7.127452	-0.572872	L
H-HA-0.169900	-1	6.039545	5.725890	0.859520	L
H-HA-0.165600	-1	11.002295	5.651393	1.072307	L
H-HA-0.165600	-1	7.204204	4.259507	2.499535	L
H-HO-0.399200	-1	9.345916	3.922171	3.652565	L
N-N--0.415700	-1	5.077766	5.187223	-2.923238	L
C-CT-0.033700	-1	3.762223	4.690494	-3.311562	L
C-C-0.597300	-1	2.926941	4.048589	-2.192878	L
O-O--0.567900	-1	1.703328	4.147143	-2.261021	L
C-CT--0.182500	-1	3.952968	3.695671	-4.451335	L
H-H-0.271900	-1	5.861343	4.897751	-3.503530	L
H-H1-0.082300	-1	3.194311	5.535274	-3.702634	L
H-HC-0.060300	-1	2.982600	3.384165	-4.836978	L
H-HC-0.060300	-1	4.492414	2.827299	-4.073030	L

H-HC-0.060300	-1	4.522329	4.160429	-5.256417	L
N-N--0.415700	-1	3.542725	3.405100	-1.190523	L H-HC 209
C-CT-0.021300	0	2.784181	2.689922	-0.125926	H
C-C-0.597300	0	2.315885	3.704531	0.930352	H
O-O--0.567900	0	3.126908	4.452085	1.474888	H
C-CT--0.123100	0	3.721839	1.628043	0.490524	H
S-S--1.036000	0	2.922114	0.464454	1.681364	H
H-H-0.271900	-1	4.546539	3.382569	-1.182832	L
H-H1-0.112400	0	1.927556	2.191123	-0.587451	H
H-H1-0.111200	0	4.533534	2.137882	1.024072	H
H-H1-0.111200	0	4.183930	1.052699	-0.319882	H
N-N--0.415700	0	0.980982	3.713616	1.228061	H
C-CT--0.051800	0	0.403533	4.531728	2.302553	H
C-C-0.597300	0	0.778798	4.004946	3.723213	H
O-O--0.567900	0	1.301289	4.730739	4.568423	H
C-CT--0.110200	-1	-1.134474	4.637938	2.046513	H
C-CT-0.353100	-1	-1.995502	5.537179	2.959816	L H-HC 222
C-CT--0.412100	-1	-2.184726	4.985367	4.374373	L
C-CT--0.412100	-1	-1.468824	6.972095	3.052677	L
H-H-0.271900	0	0.359499	3.056677	0.753805	H
H-H1-0.092200	0	0.858945	5.525057	2.267546	H
H-HC-0.045700	0	-1.260146	5.013687	1.023810	H
H-HC-0.045700	0	-1.580520	3.639618	2.063994	H
H-HC--0.036100	-1	-2.987524	5.584044	2.512068	L
H-HC-0.100000	-1	-1.285891	5.127113	4.970813	L
H-HC-0.100000	-1	-2.426624	3.924467	4.329843	L
H-HC-0.100000	-1	-3.005297	5.514322	4.856755	L
H-HC-0.100000	-1	-0.506496	6.989735	3.565218	L
H-HC-0.100000	-1	-2.182110	7.586788	3.600385	L
H-HC-0.100000	-1	-1.346918	7.378273	2.047674	L
N-N--0.415700	0	0.508301	2.688447	3.974895	H
C-CT--0.087500	0	0.582353	2.150197	5.337531	H
C-C-0.597300	0	1.986647	2.132196	5.956201	H
O-O--0.567900	0	2.085778	2.128687	7.182061	H
C-CT-0.298500	-1	-0.034292	0.734028	5.379187	H
C-CT--0.319200	0	0.729146	-0.312931	4.544683	L H-HC 241
C-CT--0.319200	0	-0.250618	0.150158	6.775355	L H-HC 241
H-H-0.271900	0	0.092292	2.125012	3.239511	H
H-H1-0.096900	0	0.010993	2.815523	5.998030	H
H-HC--0.029700	0	-1.024564	0.815478	4.929330	H
H-HC-0.079100	0	1.674142	-0.578449	5.013426	L
H-HC-0.079100	0	0.944472	0.080772	3.552703	L
H-HC-0.079100	0	0.119608	-1.203998	4.412038	L
H-HC-0.079100	0	0.706416	-0.078370	7.242714	L
H-HC-0.079100	0	-0.836151	-0.765006	6.692767	L
H-HC-0.079100	0	-0.794635	0.868383	7.386670	L
N-N--0.415700	0	3.005195	1.937418	5.095138	H
C-CT-0.033700	0	4.367122	1.794531	5.565664	H
C-C-0.597300	-1	5.078563	3.128203	5.841737	L H-H1 254
O-O--0.567900	-1	6.253722	3.105610	6.197319	L
C-CT--0.182500	-1	5.143860	0.985609	4.529678	L H-H1 254
H-H-0.271900	0	2.847501	1.970509	4.094097	H
H-H1-0.082300	0	4.353204	1.246964	6.513027	H
H-HC-0.060300	-1	6.111651	0.693860	4.934777	L

H-HC-0.060300	-1	5.298633	1.590598	3.636568	L
H-HC-0.060300	-1	4.587946	0.082918	4.273142	L
N-N--0.415700	-1	4.372663	4.255025	5.681584	L
C-CT--0.087500	-1	4.752657	5.617132	6.082884	L
C-C-0.597300	-1	3.910211	6.058405	7.286916	L
O-O--0.567900	-1	4.461694	6.506454	8.293180	L
C-CT-0.298500	-1	4.535243	6.596216	4.911769	L
C-CT--0.319200	-1	4.926212	8.034455	5.268840	L
C-CT--0.319200	-1	5.352969	6.206856	3.680633	L
H-H-0.271900	-1	3.461506	4.140135	5.255334	L
H-H1-0.096900	-1	5.802627	5.647274	6.364085	L
H-HC--0.029700	-1	3.482750	6.582480	4.636257	L
H-HC-0.079100	-1	5.976742	8.073235	5.548583	L
H-HC-0.079100	-1	4.319384	8.407223	6.093286	L
H-HC-0.079100	-1	4.763884	8.676524	4.403434	L
H-HC-0.079100	-1	6.403358	6.129821	3.955470	L
H-HC-0.079100	-1	5.234362	6.957237	2.899406	L
H-HC-0.079100	-1	5.002570	5.250490	3.292453	L
N-N--0.415700	-1	2.579275	5.865077	7.232992	L
C-CT--0.149000	-1	1.671697	6.198553	8.341513	L
H-H-0.271900	-1	2.172993	5.486788	6.382729	L
H-H1-0.097600	-1	2.248837	6.591602	9.178551	L
H-H1-0.097600	-1	1.137876	5.301366	8.656472	L
H-H1-0.097600	-1	0.954759	6.950004	8.010825	L
C-CT--0.366200	-1	4.019037	10.333040	-0.955053	L
C-C-0.597200	-1	2.544834	10.004311	-1.200482	L
O-O--0.567900	-1	1.733418	10.917788	-1.269451	L
H-HC-0.112300	-1	4.596362	9.410076	-0.922779	L
H-HC-0.112300	-1	4.120010	10.858705	-0.005738	L
H-HC-0.112300	-1	4.389170	10.965209	-1.761833	L
N-N--0.415700	-1	2.168694	8.720811	-1.260811	L
C-CT--0.024900	-1	0.756217	8.335647	-1.102703	L
C-C-0.597300	-1	0.168757	8.827008	0.225997	L
O-O--0.567900	-1	-0.926860	9.392263	0.236346	L
C-CT-0.211700	0	0.588545	6.835782	-1.255099	L
O-OH--0.654600	0	0.878502	6.533989	-2.599867	L
H-H-0.271900	-1	2.872614	7.989830	-1.324335	L
H-H1-0.084300	-1	0.182561	8.787498	-1.907675	L
H-H1-0.035200	0	-0.434634	6.544484	-1.026102	L
H-H1-0.035200	0	1.271756	6.306451	-0.589182	L
H-HO-0.427500	0	0.988356	5.558424	-2.613024	L
N-N--0.415700	-1	0.931838	8.690056	1.321080	L
C-CT-0.033700	-1	0.577393	9.165702	2.659558	L
C-C-0.597300	-1	0.109611	10.625940	2.656452	L
O-O--0.567900	-1	-0.987340	10.940383	3.120696	L
C-CT--0.182500	-1	1.764748	8.927842	3.590127	L
H-H-0.271900	-1	1.821352	8.195974	1.213743	L
H-H1-0.082300	-1	-0.236039	8.570429	3.047362	L
H-HC-0.060300	-1	1.534341	9.294297	4.589828	L
H-HC-0.060300	-1	2.649088	9.432688	3.203498	L
H-HC-0.060300	-1	1.962193	7.858884	3.640583	L
N-N--0.415700	-1	0.905772	11.508855	2.043720	L
C-CT--0.149000	-1	0.562345	12.906414	1.856096	L
H-H-0.271900	-1	1.808849	11.204043	1.688616	L

H-H1-0.097600	-1	-0.423981	13.097847	2.280185	L
H-H1-0.097600	-1	0.551119	13.138672	0.792045	L
H-H1-0.097600	-1	1.300579	13.532671	2.358022	L
C-CT--0.366200	-1	-11.940396	4.546553	4.986222	L
C-C-0.597200	-1	-12.370021	3.127706	4.609866	L
O-O--0.567900	-1	-12.933452	2.415602	5.443383	L
H-HC-0.112300	-1	-11.462210	5.020418	4.128860	L
H-HC-0.112300	-1	-11.235951	4.504748	5.817078	L
H-HC-0.112300	-1	-12.815451	5.125470	5.279943	L
N-N--0.415700	-1	-12.035394	2.691814	3.395069	L
C-CT--0.087500	-1	-12.028297	1.270675	3.030880	L
C-C-0.597300	-1	-10.581451	0.880332	2.715343	L
O-O--0.567900	-1	-9.867840	1.528534	1.942182	L
C-CT-0.298500	-1	-13.023940	0.882246	1.905318	L
C-CT--0.319200	-1	-13.768284	-0.411019	2.286440	L
C-CT--0.319200	-1	-14.104589	1.928880	1.600087	L
H-H-0.271900	-1	-11.626769	3.346249	2.725341	L
H-H1-0.096900	-1	-12.319382	0.707514	3.915179	L
H-HC--0.029700	-1	-12.464996	0.696948	0.991746	L
H-HC-0.079100	-1	-14.400802	-0.233679	3.156949	L
H-HC-0.079100	-1	-13.050528	-1.202536	2.505604	L
H-HC-0.079100	-1	-14.404584	-0.724617	1.459068	L
H-HC-0.079100	-1	-14.738225	2.068729	2.472417	L
H-HC-0.079100	-1	-14.711659	1.594493	0.760213	L
H-HC-0.079100	-1	-13.649861	2.883085	1.342935	L
N-N--0.415700	-1	-10.115340	-0.141197	3.436447	L
C-CT--0.038900	-1	-8.706262	-0.535380	3.516698	L
C-C-0.597300	-1	-8.574555	-2.060926	3.624557	L
O-O--0.567900	-1	-9.503683	-2.725219	4.105310	L
C-CT-0.365400	-1	-7.990674	0.109384	4.727561	L
O-OH--0.676100	-1	-8.156423	-0.609796	5.927954	L
C-CT--0.243800	-1	-8.412491	1.543747	5.040237	L
H-H-0.271900	-1	-10.743423	-0.617761	4.067446	L
H-H1-0.100700	-1	-8.207140	-0.197551	2.608556	L
H-H1-0.004300	-1	-6.931713	0.112679	4.490807	L
H-HC-0.064200	-1	-8.457633	2.111513	4.118379	L
H-HC-0.064200	-1	-7.685200	2.000128	5.713013	L
H-HC-0.064200	-1	-9.395668	1.566217	5.509425	L
H-HO-0.410200	-1	-8.409218	0.026525	6.629050	L
N-N--0.254800	-1	-7.447196	-2.651465	3.189016	L
C-CT--0.026600	-1	-7.192719	-4.077468	3.353856	L
C-C-0.589600	-1	-6.582877	-4.434951	4.710538	L
O-O--0.574800	-1	-6.590937	-5.607083	5.069419	L
C-CT--0.007000	0	-6.213886	-4.425863	2.236186	L
C-CT-0.018900	0	-5.382426	-3.156854	2.096726	L
C-CT-0.019200	0	-6.381299	-2.038996	2.405295	L
H-H1-0.064100	-1	-8.101262	-4.649709	3.207694	L
H-HC-0.025300	0	-5.595212	-5.283123	2.494200	L
H-HC-0.025300	0	-6.762577	-4.611217	1.311876	L
H-HC-0.021300	0	-4.977834	-3.073184	1.091323	L
H-HC-0.021300	0	-4.579183	-3.154730	2.833828	L
H-H1-0.039100	0	-6.789089	-1.653247	1.470630	L
H-H1-0.039100	0	-5.887354	-1.241428	2.961671	L
N-N--0.415700	-1	-5.966619	-3.473979	5.406845	L

C-CT--0.001400	-1	-4.974124	-3.715743	6.465471	L
C-C-0.597300	-1	-5.519605	-4.504602	7.670361	L
O-O--0.567900	-1	-6.706278	-4.392503	7.982053	L
C-CT--0.001400	0	-4.446291	-2.371352	6.983392	L H-HA 373
C-CA--0.001100	0	-4.075749	-1.363345	5.911757	H
C-CA--0.190600	0	-3.180828	-1.702664	4.893581	H
C-CA--0.190600	0	-4.618438	-0.075907	5.940144	H
C-CA--0.234100	0	-2.831603	-0.777416	3.916111	H
C-CA--0.234100	0	-4.270882	0.864246	4.975636	H
C-C-0.322600	0	-3.365152	0.524152	3.961190	H
O-OH--0.557900	0	-3.039254	1.472068	3.061550	H
H-H-0.271900	-1	-6.036667	-2.534127	5.048419	L
H-H1-0.087600	-1	-4.147945	-4.280642	6.032310	L
H-HC-0.029500	0	-5.210812	-1.928580	7.624306	L
H-HC-0.029500	0	-3.565591	-2.552163	7.600870	L
H-HA-0.169900	0	-2.746239	-2.698936	4.848487	H
H-HA-0.169900	0	-5.315020	0.210281	6.729281	H
H-HA-0.165600	0	-2.108204	-1.033201	3.150853	H
H-HA-0.165600	0	-4.652266	1.881046	5.022767	H
H-HO-0.399200	0	-2.195700	1.238218	2.571896	H
N-N--0.415700	-1	-4.638773	-5.194370	8.421709	L
C-CT--0.149000	-1	-5.021439	-5.666180	9.768993	L
H-H-0.271900	-1	-3.644149	-5.183876	8.181717	L
H-H1-0.097600	-1	-6.105268	-5.619379	9.875884	L
H-H1-0.097600	-1	-4.553961	-5.033246	10.522532	L
H-H1-0.097600	-1	-4.687301	-6.695504	9.901433	L
C-CT--0.366200	-1	-0.447173	-10.776935	2.439095	L
C-C-0.597200	-1	-0.630972	-9.832951	1.237534	L
O-O--0.567900	-1	-1.741162	-9.660179	0.729645	L
H-HC-0.112300	-1	0.600951	-10.788960	2.734589	L
H-HC-0.112300	-1	-0.757964	-11.784118	2.160209	L
H-HC-0.112300	-1	-1.056505	-10.427710	3.272680	L
N-N--0.415700	-1	0.481489	-9.281502	0.735370	L
C-CT-0.014300	-1	0.434348	-8.260706	-0.310769	L H-HC 405
C-C-0.597300	-1	0.061819	-8.764864	-1.723751	L
O-O--0.567900	-1	-0.152082	-7.939810	-2.602652	L
C-CT--0.204100	0	1.766714	-7.487060	-0.311223	H
C-C-0.713000	0	1.537357	-6.012128	-0.648652	H
O-O--0.593100	0	0.803688	-5.344929	0.081185	H
N-N--0.919100	0	2.220178	-5.507873	-1.695452	H
H-H-0.271900	-1	1.364973	-9.468151	1.180656	L
H-H1-0.104800	-1	-0.370142	-7.591810	-0.004480	L
H-HC-0.079700	0	2.482396	-7.989169	-0.973182	H
H-HC-0.079700	0	2.177449	-7.486569	0.702817	H
H-H-0.419600	0	2.111017	-4.509679	-1.926726	H
H-H-0.419600	0	2.673705	-6.125333	-2.354061	H
N-N--0.415700	-1	-0.030904	-10.077622	-1.965650	L
C-CT--0.149000	-1	-0.569911	-10.625836	-3.222368	L
H-H-0.271900	-1	0.080996	-10.729228	-1.180865	L
H-H1-0.097600	-1	-0.636833	-9.832661	-3.966303	L
H-H1-0.097600	-1	-1.562131	-11.039819	-3.042648	L
H-H1-0.097600	-1	0.090435	-11.413128	-3.588196	L
C-CT--0.366200	-1	-3.837239	-11.698228	-1.458342	L
C-C-0.597200	-1	-4.607746	-10.373524	-1.526056	L

O-O--0.567900	-1	-5.746693	-10.377419	-1.997297	L
H-HC-0.112300	-1	-2.854320	-11.523814	-1.019739	L
H-HC-0.112300	-1	-3.719559	-12.102006	-2.462945	L
H-HC-0.112300	-1	-4.388734	-12.408074	-0.842243	L
N-N--0.415700	-1	-3.982889	-9.246073	-1.147215	L
C-CT--0.087500	-1	-4.550015	-7.885832	-1.306004	L
C-C-0.597300	-1	-4.815820	-7.499435	-2.772128	L
O-O--0.567900	-1	-5.806077	-6.831057	-3.065591	L
C-CT-0.298500	-1	-3.645292	-6.809209	-0.651203	L
C-CT--0.319200	-1	-4.135677	-5.371643	-0.887198	L
C-CT--0.319200	-1	-3.629741	-6.950609	0.868447	L
H-H-0.271900	-1	-3.100704	-9.356499	-0.645339	L
H-H1-0.096900	-1	-5.510963	-7.867747	-0.793217	L
H-HC--0.029700	-1	-2.629497	-6.903880	-1.035492	L
H-HC-0.079100	-1	-5.171772	-5.278388	-0.560917	L
H-HC-0.079100	-1	-4.068087	-5.116535	-1.942136	L
H-HC-0.079100	-1	-3.510226	-4.664689	-0.340037	L
H-HC-0.079100	-1	-4.636602	-6.819201	1.247402	L
H-HC-0.079100	-1	-2.967636	-6.204797	1.310632	L
H-HC-0.079100	-1	-3.278530	-7.928150	1.167403	L
N-N--0.415700	-1	-3.968153	-7.894350	-3.730345	L
C-CT--0.149000	-1	-4.054681	-7.475881	-5.140244	L
H-H-0.271900	-1	-3.245010	-8.556631	-3.475518	L
H-H1-0.097600	-1	-4.874348	-6.766908	-5.259661	L
H-H1-0.097600	-1	-4.235098	-8.348906	-5.769005	L
H-H1-0.097600	-1	-3.119308	-7.002250	-5.437056	L
C-CT--0.366200	-1	-12.127940	3.665498	-1.311951	L
C-C-0.597200	-1	-11.021503	2.601662	-1.278576	L
O-O--0.567900	-1	-11.312138	1.417645	-1.127061	L
H-HC-0.112300	-1	-11.681561	4.649886	-1.453155	L
H-HC-0.112300	-1	-12.678426	3.647820	-0.370946	L
H-HC-0.112300	-1	-12.810657	3.454259	-2.135225	L
N-N--0.415700	-1	-9.765865	3.045259	-1.344657	L
C-CT--0.024900	-1	-8.581451	2.225130	-1.167226	L
C-C-0.597300	-1	-7.470989	3.091358	-0.567366	L
O-O--0.567900	-1	-6.819699	3.882968	-1.263268	L
C-CT-0.211700	0	-8.162109	1.579954	-2.486355	L
O-OH--0.654600	0	-7.267258	0.544993	-2.190975	L
H-H-0.271900	-1	-9.641504	4.042177	-1.412013	L
H-H1-0.084300	-1	-8.817467	1.430196	-0.461127	L
H-H1-0.035200	0	-7.696879	2.304269	-3.152033	L
H-H1-0.035200	0	-9.038113	1.149378	-2.973619	L
H-HO-0.427500	0	-6.341281	0.862967	-2.286563	L
N-N--0.415700	-1	-7.308908	3.014180	0.762405	L
C-CT-0.021300	-1	-6.135282	3.630234	1.399974	L
C-C-0.597300	-1	-4.845463	2.987707	0.864737	L
O-O--0.567900	-1	-3.871907	3.678699	0.606510	L
C-CT--0.123100	-1	-6.193008	3.489558	2.922654	L
S-SH--0.311900	-1	-7.449078	4.591326	3.633171	L
H-H-0.271900	-1	-7.968801	2.464740	1.309670	L
H-H1-0.112400	-1	-6.108964	4.692987	1.154096	L
H-H1-0.111200	-1	-5.222525	3.763548	3.339926	L
H-H1-0.111200	-1	-6.407041	2.453684	3.184604	L
H-HS-0.193300	-1	-8.490171	4.143132	2.922448	L

N-N--0.415700	-1	-4.881015	1.669404	0.655058	L H-HC 478
C-CT-0.021300	0	-3.756064	0.926198	0.074792	H
C-C-0.597300	0	-3.695286	1.173821	-1.426560	H
O-O--0.567900	0	-4.729193	1.191708	-2.102189	H
C-CT--0.123100	0	-4.036160	-0.549272	0.384853	H
S-SH--0.311900	0	-2.710787	-1.739627	-0.055028	H
H-H-0.271900	-1	-5.731004	1.178810	0.859349	L
H-H1-0.112400	0	-2.836808	1.254903	0.558003	H
H-H1-0.111200	0	-4.910681	-0.896639	-0.175231	H
H-H1-0.111200	0	-4.231843	-0.676621	1.449374	H
H-HS-0.193300	0	-1.794168	-1.341549	0.840753	H
N-N--0.415700	0	-2.451889	1.294782	-1.966217	H
C-CT--0.087500	0	-2.299937	1.409831	-3.409193	H
C-C-0.597300	0	-2.214790	0.054455	-4.157645	H
O-O--0.567900	0	-2.308163	0.063314	-5.382713	H
C-CT-0.298500	-1	-1.127349	2.311060	-3.866301	H
C-CT--0.319200	0	-1.236662	3.709502	-3.256474	L H-HC 492
C-CT--0.319200	0	0.257350	1.741645	-3.512331	L H-HC 492
H-H-0.271900	0	-1.644406	1.359080	-1.331968	H
H-H1-0.096900	0	-3.237160	1.837933	-3.783073	H
H-HC--0.029700	0	-1.188838	2.390607	-4.953764	H
H-HC-0.079100	0	-1.072843	3.664099	-2.176910	L
H-HC-0.079100	0	-2.224054	4.113612	-3.457129	L
H-HC-0.079100	0	-0.492788	4.363472	-3.706965	L
H-HC-0.079100	0	0.400998	1.743299	-2.431821	L
H-HC-0.079100	0	1.029448	2.351952	-3.971628	L
H-HC-0.079100	0	0.365594	0.723360	-3.877882	L
N-N--0.415700	0	-1.958413	-1.060497	-3.415752	H
C-CT--0.003100	0	-2.049847	-2.397079	-4.006719	H
C-C-0.597300	0	-3.511505	-2.853893	-4.183912	H
O-O--0.567900	0	-3.804305	-3.650300	-5.067340	H
C-CT--0.003600	-1	-1.292049	-3.432715	-3.127003	H
C-CT--0.064500	-1	-1.421524	-4.885856	-3.621393	L H-HC 508
C-C-0.695100	-1	-0.547171	-5.218698	-4.815728	L
O-O--0.608600	-1	-0.407003	-4.464506	-5.763550	L
N-N--0.940700	-1	0.069449	-6.380972	-4.814026	L
H-H-0.271900	0	-2.006187	-1.003155	-2.402283	H
H-H1-0.085000	0	-1.637515	-2.350603	-5.017204	H
H-HC-0.017100	0	-0.237958	-3.176325	-3.029489	H
H-HC-0.017100	0	-1.719073	-3.400507	-2.120811	H
H-HC-0.035200	-1	-2.448946	-5.142770	-3.863213	L
H-HC-0.035200	-1	-1.134564	-5.535385	-2.801903	L
H-H-0.425100	-1	0.673217	-6.625430	-5.579277	L
H-H-0.425100	-1	-0.038607	-7.004557	-4.015992	L
N-N--0.415700	0	-4.357301	-2.469490	-3.161854	H
C-CT--0.023700	0	-5.733317	-2.944810	-3.243277	H
C-C-0.597300	-1	-6.410613	-2.324749	-4.480375	L H-H1 522
O-O--0.567900	-1	-6.243051	-1.128273	-4.735407	L
C-CT-0.034200	-1	-6.469669	-2.673266	-1.914789	L H-H1 522
C-CT-0.001800	-1	-7.936835	-3.126219	-1.972832	L
S-S--0.273700	-1	-8.840403	-3.107430	-0.397111	L
C-CT--0.053600	-1	-9.213870	-1.340948	-0.260200	L
H-H-0.271900	0	-4.293400	-1.497592	-2.897052	H
H-H1-0.088000	0	-5.659332	-4.020893	-3.362496	H

H-HC-0.024100	-1	-6.402064	-1.627471	-1.651920	L
H-HC-0.024100	-1	-5.974454	-3.226900	-1.120672	L
H-H1-0.044000	-1	-7.959248	-4.150729	-2.345617	L
H-H1-0.044000	-1	-8.478938	-2.499082	-2.680909	L
H-H1-0.068400	-1	-9.819738	-1.160543	0.627694	L
H-H1-0.068400	-1	-9.765267	-1.010393	-1.140651	L
H-H1-0.068400	-1	-8.285476	-0.778606	-0.187065	L
N-N--0.254800	-1	-7.157577	-3.093561	-5.294271	L
C-CT--0.026600	-1	-7.556205	-2.673635	-6.638625	L
C-C-0.589600	-1	-9.007301	-2.194145	-6.628154	L
O-O--0.574800	-1	-9.891157	-2.898612	-6.133441	L
C-CT--0.007000	-1	-7.346605	-3.914004	-7.521627	L
C-CT-0.018900	-1	-6.826647	-4.978388	-6.552144	L
C-CT-0.019200	-1	-7.359704	-4.524074	-5.219724	L
H-H1-0.064100	-1	-6.911302	-1.873607	-7.001651	L
H-HC-0.025300	-1	-8.280244	-4.236004	-7.973916	L
H-HC-0.025300	-1	-6.611986	-3.724775	-8.302067	L
H-HC-0.021300	-1	-5.738557	-4.967175	-6.526370	L
H-HC-0.021300	-1	-7.197893	-5.961256	-6.771173	L
H-H1-0.039100	-1	-6.833610	-5.033101	-4.423847	L
H-H1-0.039100	-1	-8.424485	-4.748067	-5.145588	L
N-N--0.415700	-1	-9.234524	-0.996439	-7.160895	L
C-CT--0.149000	-1	-10.470327	-0.231603	-6.967856	L
H-H-0.271900	-1	-8.431386	-0.523183	-7.574322	L
H-H1-0.097600	-1	-11.228378	-0.873379	-6.519448	L
H-H1-0.097600	-1	-10.825650	0.131912	-7.932034	L
H-H1-0.097600	-1	-10.273790	0.614631	-6.309156	L
C-CT--0.366200	-1	-10.380948	8.840033	-4.205651	L
C-C-0.597200	-1	-9.827880	7.550859	-3.583811	L
O-O--0.567900	-1	-10.268516	7.126115	-2.514349	L
H-HC-0.112300	-1	-9.863562	9.042460	-5.143332	L
H-HC-0.112300	-1	-10.224370	9.670498	-3.517773	L
H-HC-0.112300	-1	-11.447308	8.722819	-4.397656	L
N-N--0.415700	-1	-8.855363	6.933478	-4.249294	L
C-CT--0.024900	-1	-7.907810	6.016221	-3.612676	L
C-C-0.597300	-1	-6.580475	6.751781	-3.389804	L
O-O--0.567900	-1	-6.329258	7.762031	-4.054224	L
C-CT-0.211700	0	-7.682066	4.765284	-4.473986	L
O-OH--0.654600	0	-7.313054	5.082374	-5.802891	L
H-H-0.271900	-1	-8.586264	7.306060	-5.158931	L
H-H1-0.084300	-1	-8.292130	5.672677	-2.651914	L
H-H1-0.035200	0	-8.600357	4.177030	-4.492839	L
H-H1-0.035200	0	-6.893472	4.161938	-4.021993	L
H-HO-0.427500	0	-6.882587	4.311787	-6.190963	L
N-N--0.415700	-1	-5.700565	6.220144	-2.530744	L
C-CT-0.033700	-1	-4.328389	6.733023	-2.426490	L
C-C-0.597300	-1	-3.581485	6.744374	-3.779281	L
O-O--0.567900	-1	-2.684963	7.561718	-3.994208	L
C-CT--0.182500	-1	-3.571608	5.910718	-1.393567	L
H-H-0.271900	-1	-5.980533	5.412272	-1.969579	L
H-H1-0.082300	-1	-4.378932	7.759101	-2.060683	L
H-HC-0.060300	-1	-2.559205	6.295065	-1.287609	L
H-HC-0.060300	-1	-3.533338	4.865776	-1.699502	L
H-HC-0.060300	-1	-4.086935	5.989415	-0.437584	L

N-N--0.415700	-1	-4.000538	5.879373	-4.716644	L
C-CT--0.149000	-1	-3.486158	5.831924	-6.084135	L
H-H-0.271900	-1	-4.726781	5.227463	-4.451296	L
H-H1-0.097600	-1	-2.715217	6.592740	-6.208574	L
H-H1-0.097600	-1	-4.298590	6.021729	-6.785447	L
H-H1-0.097600	-1	-3.060481	4.847449	-6.278110	L
C-CM--0.139000	0	0.872900	-0.971833	-0.732735	H
C-C-0.519000	0	1.638418	-2.160388	-0.958481	H
O-O2--0.567000	0	2.383607	-2.605075	0.079775	H
C-CM--0.117000	0	0.663783	-0.519107	0.542726	H
O-O2--0.618000	0	1.712509	-2.772409	-2.047736	H
C-C--0.553000	0	-0.228473	0.644510	0.825588	H
O-O2--0.556000	0	-0.835573	0.621228	1.945821	H
O-O2--0.607000	0	-0.384898	1.529795	-0.065565	H
H-HC-0.049000	0	0.513703	-0.431978	-1.596925	H
H-HC-0.162000	0	0.786909	-1.195748	1.374154	H
O-OW--0.834000	-1	6.425152	2.986189	-1.167187	L
H-HW-0.417000	-1	6.795509	3.131631	-2.036981	L
H-HW-0.417000	-1	7.103706	3.286930	-0.563131	L
O-OW--0.834000	0	3.357989	7.068251	1.079484	L
H-HW-0.417000	0	3.216984	6.164316	1.429687	L
H-HW-0.417000	0	3.737762	6.876955	0.205256	L
O-OW--0.834000	0	-0.509439	-3.331297	1.678262	H
H-HW-0.417000	0	-1.362675	-3.662481	1.363436	H
H-HW-0.417000	0	0.122629	-3.837520	1.135468	H
O-OW--0.834000	0	-4.986954	0.842668	-6.164765	L
H-HW-0.417000	0	-4.048306	0.623507	-6.061671	L
H-HW-0.417000	0	-5.427005	0.188371	-5.595869	L
H-HS-0.1933	0	2.584071	-1.840672	0.673106	H

ONIOM(QM/MM) Cys194-pathway

TS1'

C-CT--0.366200	-1	8.23547400	4.62388800	-8.15383800	L
C-C-0.597200	-1	9.06481000	3.87587400	-7.11534400	L
O-O--0.567900	-1	9.66168700	2.83649200	-7.39800400	L
H-HC-0.112300	-1	7.79567000	5.51093000	-7.69811700	L
H-HC-0.112300	-1	7.44163100	3.97340600	-8.52262800	L
H-HC-0.112300	-1	8.87572000	4.92231800	-8.98483200	L
N-N--0.415700	-1	9.06303200	4.43366800	-5.89812400	L
C-CT--0.087500	-1	9.53381600	3.75607200	-4.68300000	L
C-C-0.597300	-1	8.39415700	2.86211100	-4.19022400	L
O-O--0.567900	-1	7.48551400	3.32455600	-3.48528300	L
C-CT-0.298500	-1	10.02073700	4.75624200	-3.60735500	L
C-CT--0.319200	-1	10.43982600	4.05505600	-2.30967700	L
C-CT--0.319200	-1	11.23710300	5.56063900	-4.08836400	L
H-H-0.271900	-1	8.48061800	5.25757000	-5.76974700	L
H-H1-0.096900	-1	10.36908600	3.11240200	-4.93857900	L
H-HC--0.029700	-1	9.22607000	5.46426700	-3.38959900	L
H-HC-0.079100	-1	11.14297200	3.25414900	-2.54007400	L
H-HC-0.079100	-1	9.56880600	3.63436400	-1.81101200	L
H-HC-0.079100	-1	10.91948100	4.76143500	-1.63400600	L
H-HC-0.079100	-1	12.09526200	4.90130900	-4.21845300	L
H-HC-0.079100	-1	11.48656300	6.33051600	-3.35607200	L

H-HC-0.079100	-1	11.01907300	6.04125600	-5.04108500	L
N-N--0.415700	-1	8.40626000	1.58963300	-4.62256800	L
C-CT--0.087500	-1	7.29055500	0.64089500	-4.44665100	L
C-C-0.597300	-1	7.70357000	-0.63636300	-3.68662900	L
O-O--0.567900	-1	8.84799400	-1.09137800	-3.81276300	L
C-CT-0.298500	-1	6.63423700	0.23652200	-5.79118000	L
C-CT--0.319200	-1	5.77926300	1.36593500	-6.37762200	L
C-CT--0.319200	-1	7.62428200	-0.21687500	-6.86930100	L
H-H-0.271900	-1	9.17985600	1.28166400	-5.21763800	L
H-H1-0.096900	-1	6.52185900	1.14989700	-3.87217000	L
H-HC--0.029700	-1	5.96277000	-0.60236100	-5.60449100	L
H-HC-0.079100	-1	6.29946900	2.32067800	-6.30188100	L
H-HC-0.079100	-1	4.84501000	1.41618500	-5.82290200	L
H-HC-0.079100	-1	5.52903700	1.15205600	-7.41802400	L
H-HC-0.079100	-1	8.22683100	0.62603300	-7.20364300	L
H-HC-0.079100	-1	7.07249700	-0.61791200	-7.71846400	L
H-HC-0.079100	-1	8.27673300	-0.99207000	-6.47561300	L
N-N--0.254800	-1	6.76660900	-1.24048000	-2.91803700	L
C-CT--0.026600	-1	6.89523300	-2.59417900	-2.37201600	L
C-C-0.589600	-1	7.13904200	-3.61783200	-3.48267200	L
O-O--0.574800	-1	6.39094800	-3.66279800	-4.46231400	L
C-CT--0.007000	0	5.55798900	-2.89285000	-1.67053500	L
C-CT-0.018900	0	4.93605700	-1.52406200	-1.41217000	L
C-CT-0.019200	0	5.45392800	-0.69211300	-2.57503200	L
H-H1-0.064100	-1	7.71445700	-2.61218900	-1.65408900	L
H-HC-0.025300	0	4.89212000	-3.45467000	-2.32714000	L
H-HC-0.025300	0	5.70841200	-3.44713600	-0.74833500	L
H-HC-0.021300	0	5.30571200	-1.10376100	-0.48096700	L
H-HC-0.021300	0	3.84933800	-1.56052000	-1.39434900	L
H-H1-0.039100	0	5.51409100	0.34967100	-2.25856600	L
H-H1-0.039100	0	4.77703300	-0.79234000	-3.42479800	L
N-N--0.415700	-1	8.16155500	-4.46683800	-3.33564700	L
C-CT--0.149000	-1	8.52720900	-5.46350200	-4.35489000	L
H-H-0.271900	-1	8.76183900	-4.34667600	-2.52088800	L
H-H1-0.097600	-1	7.78300600	-5.46088000	-5.15063700	L
H-H1-0.097600	-1	8.56642100	-6.45253400	-3.89735200	L
H-H1-0.097600	-1	9.50424600	-5.21710500	-4.77058300	L
C-CT--0.366200	-1	5.22231000	-7.43804400	-4.10793200	L
C-C-0.597200	-1	4.09445500	-6.76376700	-4.89918600	L
O-O--0.567900	-1	3.19430200	-7.47915800	-5.34831600	L
H-HC-0.112300	-1	5.93659800	-6.68382900	-3.77840500	L
H-HC-0.112300	-1	5.72795500	-8.16554200	-4.74273800	L
H-HC-0.112300	-1	4.80263400	-7.94413500	-3.23845600	L
N-N--0.415700	-1	4.08644000	-5.43286000	-5.03777100	L
C-CT-0.014300	-1	2.98613200	-4.68185600	-5.66698100	L H-HC 69
C-C-0.597300	-1	2.78988100	-5.02122400	-7.17929800	L
O-O--0.567900	-1	3.78354800	-5.18811400	-7.88801400	L
C-CT--0.204100	0	3.28779300	-3.18384500	-5.42914200	H
C-C-0.713000	0	2.15248200	-2.25838000	-5.86401300	H
O-O--0.593100	0	1.96717200	-1.96768600	-7.03988100	H
N-N--0.919100	0	1.40430200	-1.73387100	-4.85077100	H
H-H-0.271900	-1	4.85645100	-4.89768700	-4.67005400	L
H-H1-0.104800	-1	2.07816100	-4.94327100	-5.13319000	L
H-HC-0.079700	0	4.17186800	-2.93123800	-6.02434100	H

H-HC-0.079700	0	3.52837400	-3.04095800	-4.37171200	H
H-H-0.419600	0	0.52556200	-1.33309700	-5.15331100	H
H-H-0.419600	0	1.47147400	-2.04033200	-3.88510700	H
N-N--0.415700	-1	1.53577900	-5.11655500	-7.67206500	L
C-CT--0.149000	-1	1.18245400	-5.37464100	-9.09775800	L
H-H-0.271900	-1	0.78135600	-4.88931300	-7.02525600	L
H-H1-0.097600	-1	2.08728800	-5.60189000	-9.66085900	L
H-H1-0.097600	-1	0.70412100	-4.48999800	-9.51901800	L
H-H1-0.097600	-1	0.49701300	-6.22026900	-9.15317700	L
C-CT--0.366200	-1	11.72066000	-5.96198700	-0.65721500	L
C-C-0.597200	-1	10.70510800	-6.08588100	0.48684000	L
O-O--0.567900	-1	11.02308400	-5.93241000	1.67135200	L
H-HC-0.112300	-1	11.21893400	-6.13574900	-1.60901000	L
H-HC-0.112300	-1	12.51064800	-6.70043000	-0.52301200	L
H-HC-0.112300	-1	12.15430000	-4.96174900	-0.65247800	L
N-N--0.415700	-1	9.46754100	-6.38614000	0.09581700	L
C-CT--0.023700	-1	8.30706700	-6.58087900	0.96006400	L
C-C-0.597300	-1	7.25011700	-7.42104200	0.25582400	L
O-O--0.567900	-1	7.07147700	-7.26095400	-0.95846000	L
C-CT-0.034200	0	7.70408100	-5.21972900	1.34929900	L
C-CT-0.001800	0	6.77481500	-5.23351400	2.57970000	L
S-S--0.273700	0	5.05533600	-5.79065600	2.35000800	L
C-CT--0.053600	0	4.20883400	-4.21845000	1.99138700	L
H-H-0.271900	-1	9.29828800	-6.45886400	-0.90136300	L
H-H1-0.088000	-1	8.63044800	-7.11416900	1.84236100	L
H-HC-0.024100	0	7.17260400	-4.79618100	0.49738500	L
H-HC-0.024100	0	8.53738700	-4.56149200	1.57615500	L
H-H1-0.044000	0	6.73056700	-4.21988700	2.97883100	L
H-H1-0.044000	0	7.23540500	-5.85628100	3.34654100	L
H-H1-0.068400	0	3.15474000	-4.40038700	1.77597100	L
H-H1-0.068400	0	4.65936100	-3.73065200	1.13006300	L
H-H1-0.068400	0	4.27793100	-3.54856700	2.84901300	L
N-N--0.415700	-1	6.53999900	-8.26515900	1.01460800	L
C-CT--0.149000	-1	5.31604300	-8.96757600	0.60076200	L
H-H-0.271900	-1	6.85613900	-8.39805100	1.97521600	L
H-H1-0.097600	-1	5.09900800	-8.73584800	-0.44146900	L
H-H1-0.097600	-1	4.48328700	-8.64535600	1.22611000	L
H-H1-0.097600	-1	5.45950000	-10.04198700	0.71178800	L
C-CT--0.366200	-1	3.88139000	-9.36557800	4.88219500	L
C-C-0.597200	-1	3.71763800	-7.95957900	5.49377100	L
O-O--0.567900	-1	4.68163000	-7.24629000	5.78722000	L
H-HC-0.112300	-1	2.89793000	-9.80347200	4.70836700	L
H-HC-0.112300	-1	4.44404300	-9.99807000	5.56860100	L
H-HC-0.112300	-1	4.41717700	-9.29029300	3.93581500	L
N-N--0.415700	-1	2.45737600	-7.54166600	5.64174200	L
C-CT--0.087500	-1	2.02476000	-6.13582100	5.59015100	L
C-C-0.597300	-1	1.90523500	-5.57814400	7.01484600	L
O-O--0.567900	-1	0.86837600	-5.66884700	7.68745300	L
C-CT-0.298500	0	0.70211600	-5.95719200	4.81834500	L
C-CT--0.319200	0	0.37655200	-4.47012900	4.64762500	L
C-CT--0.319200	0	0.76940700	-6.60373600	3.42783100	L
H-H-0.271900	-1	1.71957500	-8.23328500	5.48542200	L
H-H1-0.096900	-1	2.79193200	-5.56468600	5.06376300	L
H-HC--0.029700	0	-0.10785000	-6.43627300	5.36990400	L

H-HC-0.079100	0	1.10571700	-3.98446900	3.99576000	L
H-HC-0.079100	0	0.35620200	-3.95409900	5.60662200	L
H-HC-0.079100	0	-0.61056500	-4.36531100	4.20575800	L
H-HC-0.079100	0	1.61795100	-6.19595900	2.87671300	L
H-HC-0.079100	0	-0.14369500	-6.37334800	2.87671600	L
H-HC-0.079100	0	0.86388600	-7.68361200	3.50748500	L
N-N--0.415700	-1	3.06689800	-5.12938400	7.48975700	L
C-CT--0.149000	-1	3.44507700	-4.99699100	8.89407700	L
H-H-0.271900	-1	3.82599900	-5.04801100	6.82358200	L
H-H1-0.097600	-1	2.55844900	-5.09986900	9.51986600	L
H-H1-0.097600	-1	3.89410700	-4.01821000	9.05915500	L
H-H1-0.097600	-1	4.16368500	-5.77522200	9.15134300	L
C-CT--0.366200	-1	12.49061500	-4.27958700	6.32036800	L
C-C-0.597200	-1	12.28771500	-3.55483700	4.97124500	L
O-O--0.567900	-1	13.25512000	-3.34098500	4.23406400	L
H-HC-0.112300	-1	11.53126900	-4.37688800	6.82859500	L
H-HC-0.112300	-1	13.17395700	-3.70174200	6.94386700	L
H-HC-0.112300	-1	12.90969300	-5.26900800	6.14210800	L
N-N--0.415700	-1	11.05381300	-3.12405700	4.66979300	L
C-CT--0.023700	-1	10.77922900	-2.29762400	3.49663300	L
C-C-0.597300	-1	11.35279300	-0.87698900	3.63396000	L
O-O--0.567900	-1	12.08286300	-0.41356900	2.75601900	L
C-CT-0.034200	0	9.27405000	-2.20987900	3.23273500	L
C-CT-0.001800	0	9.03909500	-1.51113600	1.88664800	L
S-S--0.273700	0	7.48186900	-1.92114000	1.08292800	L
C-CT--0.053600	0	6.27731600	-1.11307200	2.16474500	L
H-H-0.271900	-1	10.28849000	-3.35078000	5.29847400	L
H-H1-0.088000	-1	11.24732600	-2.77814900	2.63580300	L
H-HC-0.024100	0	8.76985700	-1.65835400	4.02742800	L
H-HC-0.024100	0	8.86841800	-3.21655100	3.20682100	L
H-H1-0.044000	0	9.83144400	-1.80421100	1.19675000	L
H-H1-0.044000	0	9.09730500	-0.43008400	2.02099000	L
H-H1-0.068400	0	5.26759700	-1.37192000	1.84301800	L
H-H1-0.068400	0	6.38628800	-0.03064800	2.09650200	L
H-H1-0.068400	0	6.40937700	-1.43713000	3.19502100	L
N-N--0.415700	-1	11.08887800	-0.18879200	4.75015700	L
C-CT--0.149000	-1	11.64805300	1.14718100	4.98020600	L
H-H-0.271900	-1	10.50941500	-0.61803300	5.47098800	L
H-H1-0.097600	-1	12.23673600	1.44820500	4.11374900	L
H-H1-0.097600	-1	12.28616000	1.12657600	5.86326000	L
H-H1-0.097600	-1	10.83711100	1.85897500	5.13453200	L
C-CT--0.366200	-1	6.23131900	8.70388600	-5.56594500	L
C-C-0.597200	-1	6.54206800	7.50948500	-4.64233900	L
O-O--0.567900	-1	6.68811900	6.36086800	-5.08415300	L
H-HC-0.112300	-1	6.14405900	9.61240600	-4.96910200	L
H-HC-0.112300	-1	5.29266100	8.52353000	-6.09115200	L
H-HC-0.112300	-1	7.03654600	8.82205700	-6.29173300	L
N-N--0.415700	-1	6.68808500	7.82270300	-3.34468000	L
C-CT--0.001400	-1	6.72651600	6.82973100	-2.25572500	L
C-C-0.597300	-1	5.34866500	6.15607600	-2.11408400	L
O-O--0.567900	-1	4.47827100	6.63960600	-1.37286300	L
C-CT--0.001400	-1	7.24828400	7.45929400	-0.95095000	L
C-CA--0.001100	-1	7.93036400	6.48404000	0.00255400	L
C-CA--0.190600	-1	9.33798400	6.42727500	0.05151100	L

C-CA--0.190600	-1	7.18155800	5.66531800	0.87287100	L
C-CA--0.234100	-1	9.98572400	5.60276300	0.99048300	L
C-CA--0.234100	-1	7.83363400	4.83569800	1.81156300	L
C-C-0.322600	-1	9.23612400	4.82703500	1.88895700	L
O-OH--0.557900	-1	9.89412500	4.07725700	2.81986800	L
H-H-0.271900	-1	6.62855900	8.81460200	-3.10173900	L
H-H1-0.087600	-1	7.43383600	6.05476800	-2.53741100	L
H-HC-0.029500	-1	7.97707500	8.22763300	-1.21192600	L
H-HC-0.029500	-1	6.43880900	7.96955900	-0.42748300	L
H-HA-0.169900	-1	9.92611300	7.04920300	-0.60826700	L
H-HA-0.169900	-1	6.10053200	5.67608600	0.83056900	L
H-HA-0.165600	-1	11.06288200	5.56843300	1.03843300	L
H-HA-0.165600	-1	7.25694600	4.20484800	2.47206900	L
H-HO-0.399200	-1	9.39751700	3.85513900	3.62352900	L
N-N--0.415700	-1	5.13123300	5.13705700	-2.95021900	L
C-CT-0.033700	-1	3.81196200	4.64852500	-3.33629500	L
C-C-0.597300	-1	2.97351800	4.01431700	-2.21558900	L
O-O--0.567900	-1	1.75053200	4.12101400	-2.28266500	L
C-CT--0.182500	-1	3.99480700	3.65036400	-4.47444500	L
H-H-0.271900	-1	5.91224000	4.84124000	-3.53078100	L
H-H1-0.082300	-1	3.24937000	5.49641000	-3.72832700	L
H-HC-0.060300	-1	3.02195800	3.34472400	-4.85852700	L
H-HC-0.060300	-1	4.52876100	2.77905400	-4.09510300	L
H-HC-0.060300	-1	4.56646400	4.10979600	-5.28095200	L
N-N--0.415700	-1	3.58590000	3.36837700	-1.21254100	L H-HC 209
C-CT-0.021300	0	2.90137900	2.68663000	-0.10284500	H
C-C-0.597300	0	2.35708900	3.73067600	0.89036300	H
O-O--0.567900	0	3.12308700	4.58173800	1.34099400	H
C-CT--0.123100	0	3.98425100	1.81637300	0.55929800	H
S-S--1.036000	0	3.32192700	0.54333600	1.70701400	H
H-H-0.271900	-1	4.58961700	3.33920200	-1.20598100	L
H-H1-0.112400	0	2.10879600	2.06022000	-0.51685700	H
H-H1-0.111200	0	4.66291800	2.44984800	1.13973000	H
H-H1-0.111200	0	4.58055600	1.29822400	-0.19964700	H
N-N--0.415700	0	1.03842500	3.64189900	1.22987000	H
C-CT--0.051800	0	0.45446700	4.49570300	2.28207800	H
C-C-0.597300	0	0.83822500	3.98466400	3.70324400	H
O-O--0.567900	0	1.40329400	4.70315800	4.52696600	H
C-CT--0.110200	-1	-1.07945100	4.63890000	2.02681200	H
C-CT-0.353100	-1	-1.93344300	5.54547300	2.93942300	L H-HC 222
C-CT--0.412100	-1	-2.12493000	4.99756500	4.35514700	L
C-CT--0.412100	-1	-1.39697900	6.97700000	3.02909600	L
H-H-0.271900	0	0.53289900	2.79163000	0.95701100	H
H-H1-0.092200	0	0.93649000	5.47259300	2.21398700	H
H-HC-0.045700	0	-1.19560900	5.01693100	1.00439800	H
H-HC-0.045700	0	-1.54764500	3.64973000	2.04116400	H
H-HC--0.036100	-1	-2.92558000	5.59826700	2.49257200	L
H-HC-0.100000	-1	-1.22454000	5.13431500	4.95041000	L
H-HC-0.100000	-1	-2.37403200	3.93824300	4.31280100	L
H-HC-0.100000	-1	-2.94140800	5.53292700	4.83739600	L
H-HC-0.100000	-1	-0.43402500	6.98906800	3.54062300	L
H-HC-0.100000	-1	-2.10553200	7.59749600	3.57640800	L
H-HC-0.100000	-1	-1.27336900	7.38051600	2.02322900	L
N-N--0.415700	0	0.56230800	2.66927100	3.96173600	H

C-CT--0.087500	0	0.61540000	2.14927700	5.33312100	H
C-C-0.597300	0	2.01673600	2.10921700	5.96003700	H
O-O--0.567900	0	2.11482000	2.05102400	7.18217000	H
C-CT-0.298500	-1	-0.00204500	0.73362400	5.36530200	H
C-CT--0.319200	0	0.87922500	-0.36555100	4.74910300	L H-HC 241
C-CT--0.319200	0	-0.43981500	0.25899000	6.75080400	L H-HC 241
H-H-0.271900	0	0.01161000	2.14420100	3.28199700	H
H-H1-0.096900	0	0.04174000	2.82194400	5.98437500	H
H-HC--0.029700	0	-0.90705100	0.76210800	4.75867900	H
H-HC-0.079100	0	1.74352700	-0.57505800	5.37509100	L
H-HC-0.079100	0	1.22820400	-0.04516100	3.76497300	L
H-HC-0.079100	0	0.29019100	-1.27189400	4.62882000	L
H-HC-0.079100	0	0.42736800	0.10197300	7.39038600	L
H-HC-0.079100	0	-0.98797300	-0.67745700	6.64985400	L
H-HC-0.079100	0	-1.09601200	1.00498700	7.19591300	L
N-N--0.415700	0	3.03850600	1.92726800	5.09100400	H
C-CT-0.033700	0	4.40412300	1.76786200	5.54749000	H
C-C-0.597300	-1	5.12711900	3.09398700	5.81848500	L H-H1 254
O-O--0.567900	-1	6.30249900	3.06412500	6.17292000	L
C-CT--0.182500	-1	5.17656800	0.94868400	4.51031800	L H-H1 254
H-H-0.271900	0	2.88063500	2.08588100	4.10624400	H
H-H1-0.082300	0	4.38592200	1.22102300	6.49420200	H
H-HC-0.060300	-1	6.14283500	0.65110100	4.91492600	L
H-HC-0.060300	-1	5.33455700	1.55095100	3.61591200	L
H-HC-0.060300	-1	4.61435300	0.04926900	4.25595800	L
N-N--0.415700	-1	4.42872200	4.22529300	5.65700600	L
C-CT--0.087500	-1	4.81832500	5.58552500	6.05543400	L
C-C-0.597300	-1	3.98012400	6.03467300	7.25950900	L
O-O--0.567900	-1	4.53566000	6.48081200	8.26439500	L
C-CT-0.298500	-1	4.60632300	6.56392700	4.88275200	L
C-CT--0.319200	-1	5.00737200	8.00014000	5.23680200	L
C-CT--0.319200	-1	5.42012900	6.16681100	3.65149600	L
H-H-0.271900	-1	3.51637400	4.11578600	5.23189700	L
H-H1-0.096900	-1	5.86876700	5.60908400	6.33550700	L
H-HC--0.029700	-1	3.55347800	6.55680600	4.60833800	L
H-HC-0.079100	-1	6.05842800	8.03232400	5.51540100	L
H-HC-0.079100	-1	4.40392900	8.37849600	6.06118300	L
H-HC-0.079100	-1	4.84849300	8.64171300	4.37039000	L
H-HC-0.079100	-1	6.47025800	6.08317900	3.92540500	L
H-HC-0.079100	-1	5.30579000	6.91655500	2.86902200	L
H-HC-0.079100	-1	5.06287500	5.21213300	3.26541900	L
N-N--0.415700	-1	2.64785600	5.85024800	7.20730000	L
C-CT--0.149000	-1	1.74369300	6.19186800	8.31613200	L
H-H-0.271900	-1	2.23814800	5.47317100	6.35814000	L
H-H1-0.097600	-1	2.32434200	6.58252500	9.15186600	L
H-H1-0.097600	-1	1.20414800	5.29888000	8.63327500	L
H-H1-0.097600	-1	1.03151000	6.94754100	7.98480900	L
C-CT--0.366200	-1	4.10933200	10.29348100	-0.99035000	L
C-C-0.597200	-1	2.63268900	9.97427800	-1.23367700	L
O-O--0.567900	-1	1.82739100	10.89309300	-1.30348500	L
H-HC-0.112300	-1	4.68044000	9.36669400	-0.95698100	L
H-HC-0.112300	-1	4.21483300	10.82017700	-0.04210000	L
H-HC-0.112300	-1	4.48289600	10.92166500	-1.79866000	L
N-N--0.415700	-1	2.24782200	8.69324200	-1.29127800	L

C-CT--0.024900	-1	0.83293700	8.31792500	-1.13103400	L
C-C-0.597300	-1	0.25018200	8.81565800	0.19736700	L
O-O--0.567900	-1	-0.84157600	9.38832400	0.20780200	L
C-CT-0.211700	0	0.65798900	6.81909400	-1.27982600	L
O-OH--0.654600	0	0.94375700	6.51396400	-2.62484200	L
H-H-0.271900	-1	2.94672200	7.95740800	-1.35418700	L
H-H1-0.084300	-1	0.26151600	8.77217700	-1.93624100	L
H-H1-0.035200	0	-0.36611500	6.53312300	-1.04798800	L
H-H1-0.035200	0	1.34136800	6.28919400	-0.61417400	L
H-HO-0.427500	0	1.05387800	5.53913000	-2.63872900	L
N-N--0.415700	-1	1.01345000	8.67554100	1.29192100	L
C-CT-0.033700	-1	0.66360700	9.15600800	2.62989000	L
C-C-0.597300	-1	0.20570000	10.61936500	2.62459500	L
O-O--0.567900	-1	-0.88862300	10.94206200	3.08938200	L
C-CT--0.182500	-1	1.85028700	8.91181900	3.55968100	L
H-H-0.271900	-1	1.89949500	8.17526600	1.18458000	L
H-H1-0.082300	-1	-0.15343000	8.56695300	3.01960800	L
H-HC-0.060300	-1	1.62339400	9.28164100	4.55894700	L
H-HC-0.060300	-1	2.73761900	9.40997200	3.17123200	L
H-HC-0.060300	-1	2.04055700	7.84164500	3.61188800	L
N-N--0.415700	-1	1.00717600	11.49576600	2.00944200	L
C-CT--0.149000	-1	0.67301000	12.89526800	1.81961400	L
H-H-0.271900	-1	1.90780600	11.18420800	1.65397600	L
H-H1-0.097600	-1	-0.31156700	13.09413600	2.24436300	L
H-H1-0.097600	-1	0.66225600	13.12566100	0.75515500	L
H-H1-0.097600	-1	1.41597400	13.51743700	2.31964800	L
C-CT--0.366200	-1	-11.88270400	4.62581500	4.97773900	L
C-C-0.597200	-1	-12.32229400	3.20922100	4.60440700	L
O-O--0.567900	-1	-12.88966700	2.50246100	5.43979800	L
H-HC-0.112300	-1	-11.40221100	5.09487400	4.11902500	L
H-HC-0.112300	-1	-11.17769900	4.58076000	5.80795000	L
H-HC-0.112300	-1	-12.75352200	5.21116600	5.27129200	L
N-N--0.415700	-1	-11.99187400	2.76887000	3.39006900	L
C-CT--0.087500	-1	-11.99475300	1.34705400	3.02846800	L
C-C-0.597300	-1	-10.55090700	0.94636900	2.71217100	L
O-O--0.567900	-1	-9.83373000	1.58832600	1.93710200	L
C-CT-0.298500	-1	-12.99416000	0.96331900	1.90463300	L
C-CT--0.319200	-1	-13.74683400	-0.32419000	2.28887200	L
C-CT--0.319200	-1	-14.06802700	2.01667400	1.59859100	L
H-H-0.271900	-1	-11.57952600	3.41930600	2.71873300	L
H-H1-0.096900	-1	-12.28872700	0.78748300	3.91408800	L
H-HC--0.029700	-1	-12.43742400	0.77258700	0.99083000	L
H-HC-0.079100	-1	-14.37724100	-0.14099700	3.15970000	L
H-HC-0.079100	-1	-13.03421900	-1.12014300	2.50874800	L
H-HC-0.079100	-1	-14.38609300	-0.63498300	1.46272200	L
H-HC-0.079100	-1	-14.69980200	2.16239100	2.47131100	L
H-HC-0.079100	-1	-14.67821100	1.68487300	0.75994900	L
H-HC-0.079100	-1	-13.60712700	2.96731500	1.33923400	L
N-N--0.415700	-1	-10.09096500	-0.07697700	3.43466500	L
C-CT--0.038900	-1	-8.68450200	-0.48052400	3.51419700	L
C-C-0.597300	-1	-8.56299800	-2.00672900	3.62470400	L
O-O--0.567900	-1	-9.49609100	-2.66385100	4.10761700	L
C-CT-0.365400	-1	-7.96332600	0.16158400	4.72314900	L
O-OH--0.676100	-1	-8.13269000	-0.55427200	5.92502200	L

C-CT--0.243800	-1	-8.37511500	1.59933300	5.03363500	L
H-H-0.271900	-1	-10.72160800	-0.54813500	4.06716900	L
H-H1-0.100700	-1	-8.18404600	-0.14773100	2.60492900	L
H-H1-0.004300	-1	-6.90461000	0.15729300	4.48531200	L
H-HC-0.064200	-1	-8.41737200	2.16571400	4.11079200	L
H-HC-0.064200	-1	-7.64406500	2.05201100	5.70483600	L
H-HC-0.064200	-1	-9.35763700	1.62930000	5.50378600	L
H-HO-0.410200	-1	-8.38045800	0.08501800	6.62521300	L
N-N--0.254800	-1	-7.44010600	-2.60566700	3.18909100	L
C-CT--0.026600	-1	-7.19509600	-4.03305300	3.35627700	L
C-C-0.589600	-1	-6.58628600	-4.39218500	4.71298600	L
O-O--0.574800	-1	-6.60189800	-5.56358000	5.07401400	L
C-CT--0.007000	0	-6.22104200	-4.39074200	2.23724500	L
C-CT-0.018900	0	-5.38285700	-3.12719200	2.09312000	L
C-CT-0.019200	0	-6.37267400	-2.00177200	2.39987500	L
H-H1-0.064100	-1	-8.10763800	-4.59940500	3.21208600	L
H-HC-0.025300	0	-5.60607400	-5.25026700	2.49683600	L
H-HC-0.025300	0	-6.77253600	-4.57560500	1.31459300	L
H-HC-0.021300	0	-4.97700400	-3.04799200	1.08845500	L
H-HC-0.021300	0	-4.58126200	-3.13078700	2.83047600	L
H-H1-0.039100	0	-6.78098500	-1.61765700	1.46493400	L
H-H1-0.039100	0	-5.87150100	-1.20477300	2.95044800	L
N-N--0.415700	-1	-5.96283100	-3.43413400	5.40691200	L
C-CT--0.001400	-1	-4.97090500	-3.68067900	6.46496400	L
C-C-0.597300	-1	-5.52045800	-4.46364000	7.67184800	L
O-O--0.567900	-1	-6.70602300	-4.34295500	7.98454400	L
C-CT--0.001400	0	-4.44992300	-2.34479700	7.01268600	L H-HA 373
C-CA--0.001100	0	-4.11848800	-1.30230500	5.96856600	H
C-CA--0.190600	0	-3.34170600	-1.64216500	4.85875000	H
C-CA--0.190600	0	-4.60005600	0.00231300	6.10026400	H
C-CA--0.234100	0	-3.05075200	-0.69213900	3.89161200	H
C-CA--0.234100	0	-4.29525800	0.97088100	5.14720800	H
C-C-0.322600	0	-3.50537300	0.62803800	4.04521500	H
O-OH--0.557900	0	-3.20553800	1.59228800	3.14305100	H
H-H-0.271900	-1	-6.02689700	-2.49448400	5.04684200	L
H-H1-0.087600	-1	-4.14900700	-4.25193700	6.03199100	L
H-HC-0.029500	0	-5.20736200	-1.92952700	7.68001800	L
H-HC-0.029500	0	-3.55404900	-2.53082600	7.60634300	L
H-HA-0.169900	0	-2.96776600	-2.65269800	4.71112800	H
H-HA-0.169900	0	-5.21611600	0.27922500	6.95685300	H
H-HA-0.165600	0	-2.43887700	-0.95692700	3.04105800	H
H-HA-0.165600	0	-4.62976800	1.99924600	5.26293200	H
H-HO-0.399200	0	-2.36471400	1.34276100	2.68442300	H
N-N--0.415700	-1	-4.64352900	-5.15797800	8.42355200	L
C-CT--0.149000	-1	-5.02798600	-5.62474100	9.77208600	L
H-H-0.271900	-1	-3.64911000	-5.15464300	8.18252800	L
H-H1-0.097600	-1	-6.11136700	-5.57041800	9.87999300	L
H-H1-0.097600	-1	-4.55547100	-4.99360900	10.52399500	L
H-H1-0.097600	-1	-4.70067700	-6.65605800	9.90606300	L
C-CT--0.366200	-1	-0.49592400	-10.77961700	2.44687100	L
C-C-0.597200	-1	-0.67458100	-9.83660000	1.24377700	L
O-O--0.567900	-1	-1.78409800	-9.65725100	0.73670800	L
H-HC-0.112300	-1	0.55239700	-10.79818700	2.74131900	L
H-HC-0.112300	-1	-0.81380100	-11.78518000	2.17013800	L

H-HC-0.112300	-1	-1.10202200	-10.42476500	3.28043800	L
N-N--0.415700	-1	0.44106400	-9.29359600	0.73947200	L
C-CT-0.014300	-1	0.39975600	-8.27436500	-0.30848500	L H-HC 405
C-C-0.597300	-1	0.02236000	-8.77860300	-1.72015800	L
O-O--0.567900	-1	-0.18686600	-7.95372100	-2.60034400	L
C-CT--0.204100	0	1.71625400	-7.46320100	-0.32490700	H
C-C-0.713000	0	1.44503200	-5.95632500	-0.45411800	H
O-O--0.593100	0	0.84820000	-5.37087000	0.44717500	H
N-N--0.919100	0	1.95801800	-5.31671300	-1.53416500	H
H-H-0.271900	-1	1.32372400	-9.48540300	1.18420000	L
H-H1-0.104800	-1	-0.39989200	-7.59953300	-0.00258800	L
H-HC-0.079700	0	2.38008100	-7.85920600	-1.10265400	H
H-HC-0.079700	0	2.21530300	-7.57752700	0.64109400	H
H-H-0.419600	0	1.78916600	-4.31535000	-1.64727700	H
H-H-0.419600	0	2.28743700	-5.84102800	-2.33359900	H
N-N--0.415700	-1	-0.07948300	-10.09114300	-1.95956600	L
C-CT--0.149000	-1	-0.62347600	-10.63798800	-3.21472900	L
H-H-0.271900	-1	0.02882100	-10.74206500	-1.17370500	L
H-H1-0.097600	-1	-0.68580600	-9.84573200	-3.96004200	L
H-H1-0.097600	-1	-1.61828600	-11.04492400	-3.03324600	L
H-H1-0.097600	-1	0.03115500	-11.43038700	-3.57979400	L
C-CT--0.366200	-1	-3.89615700	-11.68505700	-1.44542100	L
C-C-0.597200	-1	-4.65776400	-10.35530000	-1.51476900	L
O-O--0.567900	-1	-5.79719500	-10.35235700	-1.98483900	L
H-HC-0.112300	-1	-2.91162900	-11.51649700	-1.00813900	L
H-HC-0.112300	-1	-3.78224300	-12.09144700	-2.44940700	L
H-HC-0.112300	-1	-4.45179900	-12.39004000	-0.82746300	L
N-N--0.415700	-1	-4.02491100	-9.23141200	-1.13862000	L
C-CT--0.087500	-1	-4.58299700	-7.86766200	-1.29931500	L
C-C-0.597300	-1	-4.84769600	-7.48214200	-2.76586900	L
O-O--0.567900	-1	-5.83371600	-6.80762100	-3.05954400	L
C-CT-0.298500	-1	-3.67034200	-6.79599000	-0.64740200	L
C-CT--0.319200	-1	-4.15124500	-5.35557400	-0.88552000	L
C-CT--0.319200	-1	-3.65418300	-6.93473100	0.87248600	L
H-H-0.271900	-1	-3.14297400	-9.34688700	-0.63744500	L
H-H1-0.096900	-1	-5.54327000	-7.84214900	-0.78558200	L
H-HC--0.029700	-1	-2.65561200	-6.89822100	-1.03255100	L
H-HC-0.079100	-1	-5.18635300	-5.25472700	-0.55835600	L
H-HC-0.079100	-1	-4.08302200	-5.10284600	-1.94099300	L
H-HC-0.079100	-1	-3.52047200	-4.65187200	-0.34028700	L
H-HC-0.079100	-1	-4.65974100	-6.79583000	1.25222600	L
H-HC-0.079100	-1	-2.98659600	-6.19260400	1.31263300	L
H-HC-0.079100	-1	-3.30927600	-7.91407700	1.17286900	L
N-N--0.415700	-1	-4.00370600	-7.88452200	-3.72422900	L
C-CT--0.149000	-1	-4.08885400	-7.46804100	-5.13479700	L
H-H-0.271900	-1	-3.28479100	-8.55121100	-3.46892900	L
H-H1-0.097600	-1	-4.90383900	-6.75376200	-5.25467400	L
H-H1-0.097600	-1	-4.27581800	-8.34097100	-5.76178200	L
H-H1-0.097600	-1	-3.15061300	-7.00128100	-5.43342900	L
C-CT--0.366200	-1	-12.08269100	3.73459900	-1.31862500	L
C-C-0.597200	-1	-10.98343100	2.66336700	-1.28443300	L
O-O--0.567900	-1	-11.28190900	1.48162000	-1.13046200	L
H-HC-0.112300	-1	-11.62981700	4.71568800	-1.46207800	L
H-HC-0.112300	-1	-12.63231500	3.72234800	-0.37702600	L

H-HC-0.112300	-1	-12.76767000	3.52648100	-2.14081600	L
N-N--0.415700	-1	-9.72489800	3.09834700	-1.35260700	L
C-CT--0.024900	-1	-8.54586900	2.27055600	-1.17488500	L
C-C-0.597300	-1	-7.42896300	3.13034900	-0.57773700	L
O-O--0.567900	-1	-6.77305600	3.91627100	-1.27574500	L
C-CT-0.211700	0	-8.11298300	1.60425100	-2.47850400	L
O-OH--0.654600	0	-7.11637500	0.66741600	-2.16429300	L
H-H-0.271900	-1	-9.59387300	4.09427600	-1.42190700	L
H-H1-0.084300	-1	-8.78652500	1.47852100	-0.46709400	L
H-H1-0.035200	0	-7.73147000	2.33610500	-3.18758200	L
H-H1-0.035200	0	-8.96297200	1.08009500	-2.91749600	L
H-HO-0.427500	0	-6.23101800	1.08362000	-2.26614900	L
N-N--0.415700	-1	-7.26603500	3.05449100	0.75200700	L
C-CT-0.021300	-1	-6.08761600	3.66375800	1.38725200	L
C-C-0.597300	-1	-4.80272100	3.01155600	0.85187600	L
O-O--0.567900	-1	-3.82478500	3.69547900	0.59139500	L
C-CT--0.123100	-1	-6.14472200	3.52624600	2.91024800	L
S-SH--0.311900	-1	-7.39258100	4.63776600	3.62002900	L
H-H-0.271900	-1	-7.92906300	2.51052300	1.30094500	L
H-H1-0.112400	-1	-6.05437000	4.72585900	1.13941100	L
H-H1-0.111200	-1	-5.17197900	3.79442600	3.32602900	L
H-H1-0.111200	-1	-6.36547800	2.49231400	3.17430300	L
H-HS-0.193300	-1	-8.43741300	4.19532500	2.91118800	L
N-N--0.415700	-1	-4.84735700	1.69314200	0.64461400	L H-HC 478
C-CT-0.021300	0	-3.73698800	0.95524000	0.03030500	H
C-C-0.597300	0	-3.66973500	1.32020500	-1.45182800	H
O-O--0.567900	0	-4.67475200	1.66104400	-2.07330700	H
C-CT--0.123100	0	-4.04517000	-0.52040100	0.29733100	H
S-SH--0.311900	0	-2.84343900	-1.77893600	-0.28943300	H
H-H-0.271900	-1	-5.70047100	1.20867900	0.85069400	L
H-H1-0.112400	0	-2.80651400	1.23664500	0.53168600	H
H-H1-0.111200	0	-5.00013700	-0.78408200	-0.17037400	H
H-H1-0.111200	0	-4.14811100	-0.65898800	1.37443300	H
H-HS-0.193300	0	-1.40020900	-1.16047000	-0.70777200	H
N-N--0.415700	0	-2.43283000	1.24066300	-2.03551600	H
C-CT--0.087500	0	-2.28398100	1.39049100	-3.47861600	H
C-C-0.597300	0	-2.28787700	0.04882300	-4.28991800	H
O-O--0.567900	0	-2.61345700	0.10138200	-5.47302200	H
C-CT-0.298500	-1	-1.09419000	2.30120500	-3.88171000	H
C-CT--0.319200	0	-1.22759200	3.70225600	-3.28481400	L H-HC 492
C-CT--0.319200	0	0.24902100	1.69599600	-3.42713600	L H-HC 492
H-H-0.271900	0	-1.64262400	0.94844100	-1.47255400	H
H-H1-0.096900	0	-3.21639800	1.85765600	-3.80866700	H
H-HC--0.029700	0	-1.08415200	2.37670000	-4.97252600	H
H-HC-0.079100	0	-1.11453000	3.66502700	-2.19938600	L
H-HC-0.079100	0	-2.20423000	4.10648200	-3.53343100	L
H-HC-0.079100	0	-0.46199800	4.35143800	-3.70502000	L
H-HC-0.079100	0	0.32312000	1.69773800	-2.33609400	L
H-HC-0.079100	0	1.07003800	2.27072400	-3.84575300	L
H-HC-0.079100	0	0.34658000	0.66913800	-3.77116200	L
N-N--0.415700	0	-1.89275500	-1.06694500	-3.62352500	H
C-CT--0.003100	0	-2.04093200	-2.44293200	-4.09571800	H
C-C-0.597300	0	-3.52249200	-2.86676300	-4.24309800	H
O-O--0.567900	0	-3.84466100	-3.57287700	-5.19999200	H

C-CT--0.003600	-1	-1.29709100	-3.44001800	-3.13155600	H
C-CT--0.064500	-1	-1.43663100	-4.89309700	-3.62343100	L H-HC 508
C-C-0.695100	-1	-0.56584200	-5.23403200	-4.81797800	L
O-O--0.608600	-1	-0.42155800	-4.48253000	-5.76731800	L
N-N--0.940700	-1	0.04291300	-6.40044300	-4.81478400	L
H-H-0.271900	0	-1.49250300	-0.96898100	-2.70196800	H
H-H1-0.085000	0	-1.65262400	-2.51637200	-5.11575800	H
H-HC-0.017100	0	-0.24148800	-3.18982500	-3.04520400	H
H-HC-0.017100	0	-1.75065900	-3.37939400	-2.14059100	H
H-HC-0.035200	-1	-2.46607500	-5.14351900	-3.86366700	L
H-HC-0.035200	-1	-1.15328600	-5.54307800	-2.80298200	L
H-H-0.425100	-1	0.64422500	-6.65036800	-5.58020300	L
H-H-0.425100	-1	-0.06853200	-7.02183100	-4.01550400	L
N-N--0.415700	0	-4.33566500	-2.52238300	-3.21518800	H
C-CT--0.023700	0	-5.73121600	-2.93696400	-3.24688000	H
C-C-0.597300	-1	-6.40921900	-2.29992000	-4.48189000	L H-H1 522
O-O--0.567900	-1	-6.23386600	-1.10506200	-4.73932100	L
C-CT-0.034200	-1	-6.46798000	-2.64334700	-1.91571500	L H-H1 522
C-CT-0.001800	-1	-7.93826100	-3.08648300	-1.97137800	L
S-S--0.273700	-1	-8.84005800	-3.05872500	-0.39477500	L
C-CT--0.053600	-1	-9.20143500	-1.28951100	-0.26070500	L
H-H-0.271900	0	-3.96566200	-2.03319500	-2.40931100	H
H-H1-0.088000	0	-5.71664600	-4.01924600	-3.35112600	H
H-HC-0.024100	-1	-6.39306800	-1.59756500	-1.65476800	L
H-HC-0.024100	-1	-5.97573000	-3.19887900	-1.12103700	L
H-H1-0.044000	-1	-7.96798500	-4.11149500	-2.34227000	L
H-H1-0.044000	-1	-8.47684400	-2.45698700	-2.68004600	L
H-H1-0.068400	-1	-9.80515600	-1.10340000	0.62747700	L
H-H1-0.068400	-1	-9.75149500	-0.95683900	-1.14119700	L
H-H1-0.068400	-1	-8.26918800	-0.73332700	-0.18954200	L
N-N--0.254800	-1	-7.16222500	-3.06513200	-5.29366400	L
C-CT--0.026600	-1	-7.55939400	-2.64496900	-6.63837500	L
C-C-0.589600	-1	-9.00720700	-2.15566400	-6.62729900	L
O-O--0.574800	-1	-9.89529200	-2.85324000	-6.13040100	L
C-CT--0.007000	-1	-7.35909200	-3.88832500	-7.51932300	L
C-CT-0.018900	-1	-6.84533900	-4.95443900	-6.54843200	L
C-CT-0.019200	-1	-7.37394000	-4.49411100	-5.21629900	L
H-H1-0.064100	-1	-6.90947800	-1.84998200	-7.00351700	L
H-HC-0.025300	-1	-8.29535100	-4.20483000	-7.97007100	L
H-HC-0.025300	-1	-6.62401700	-3.70549300	-8.30085600	L
H-HC-0.021300	-1	-5.75717100	-4.95053500	-6.52378500	L
H-HC-0.021300	-1	-7.22344400	-5.93517000	-6.76528700	L
H-H1-0.039100	-1	-6.85047700	-5.00523400	-4.42003200	L
H-H1-0.039100	-1	-8.44013000	-4.71076700	-5.14066700	L
N-N--0.415700	-1	-9.22687800	-0.95742200	-7.16199300	L
C-CT--0.149000	-1	-10.45728500	-0.18389700	-6.96909100	L
H-H-0.271900	-1	-8.42098800	-0.49035400	-7.57710700	L
H-H1-0.097600	-1	-11.21919200	-0.81971800	-6.51874200	L
H-H1-0.097600	-1	-10.81114100	0.18025600	-7.93357100	L
H-H1-0.097600	-1	-10.25435500	0.66218600	-6.31214100	L
C-CT--0.366200	-1	-10.30375900	8.89193400	-4.22354300	L
C-C-0.597200	-1	-9.75877400	7.60018500	-3.59991400	L
O-O--0.567900	-1	-10.20116800	7.18037300	-2.52923100	L
H-HC-0.112300	-1	-9.78598500	9.08915500	-5.16211900	L

H-HC-0.112300	-1	-10.14086500	9.72257200	-3.53734300	L
H-HC-0.112300	-1	-11.37108400	8.78158000	-4.41424600	L
N-N--0.415700	-1	-8.79113800	6.97503700	-4.26525900	L
C-CT--0.024900	-1	-7.84915000	6.05255500	-3.62793600	L
C-C-0.597300	-1	-6.51664400	6.77952800	-3.40775800	L
O-O--0.567900	-1	-6.25929200	7.78684900	-4.07427600	L
C-CT-0.211700	0	-7.63287900	4.79454500	-4.48174800	L
O-OH--0.654600	0	-7.24687300	5.09595300	-5.80913700	L
H-H-0.271900	-1	-8.52046600	7.34413600	-5.17585000	L
H-H1-0.084300	-1	-8.23479300	5.71336600	-2.66615700	L
H-H1-0.035200	0	-8.55875000	4.21852600	-4.50523400	L
H-H1-0.035200	0	-6.85688200	4.18274500	-4.01913900	L
H-HO-0.427500	0	-6.82832400	4.31221700	-6.18538900	L
N-N--0.415700	-1	-5.63946200	6.24352000	-2.54862500	L
C-CT-0.033700	-1	-4.26374300	6.74730200	-2.44670500	L
C-C-0.597300	-1	-3.51817500	6.75114400	-3.80027600	L
O-O--0.567900	-1	-2.61637600	7.56201300	-4.01760900	L
C-CT--0.182500	-1	-3.51147400	5.92177900	-1.41305800	L
H-H-0.271900	-1	-5.92430200	5.43857900	-1.98570400	L
H-H1-0.082300	-1	-4.30697400	7.77435900	-2.08272200	L
H-HC-0.060300	-1	-2.49638500	6.29946300	-1.30883100	L
H-HC-0.060300	-1	-3.48057900	4.87604800	-1.71712400	L
H-HC-0.060300	-1	-4.02527000	6.00569700	-0.45669300	L
N-N--0.415700	-1	-3.94402900	5.88729200	-4.73563200	L
C-CT--0.149000	-1	-3.43139300	5.83388000	-6.10355600	L
H-H-0.271900	-1	-4.67439000	5.24078900	-4.46835500	L
H-H1-0.097600	-1	-2.65545900	6.58923800	-6.23017400	L
H-H1-0.097600	-1	-4.24324700	6.02789700	-6.80438500	L
H-H1-0.097600	-1	-3.01258100	4.84619700	-6.29616600	L
C-CM--0.139000	0	0.65035500	-2.08383200	0.49509000	H
C-C-0.519000	0	0.62576600	-1.74817800	-0.95254900	H
O-O2--0.567000	0	-0.34478700	-0.97057600	-1.33527600	H
C-CM--0.117000	0	0.22852500	-1.28593800	1.48707600	H
O-O2--0.618000	0	1.45117300	-2.25670500	-1.73881600	H
C-C--0.553000	0	-0.13502300	0.18166100	1.41326500	H
O-O2--0.556000	0	0.38183000	0.90337900	0.51922900	H
O-O2--0.607000	0	-0.89713100	0.60626100	2.33635900	H
H-HC-0.049000	0	0.93636100	-3.10842600	0.71593900	H
H-HC-0.162000	0	0.11788400	-1.74721000	2.45998400	H
O-OW--0.834000	-1	6.46552700	2.93016000	-1.19152600	L
H-HW-0.417000	-1	6.83595800	3.07151300	-2.06196100	L
H-HW-0.417000	-1	7.14671500	3.22740900	-0.58871100	L
O-OW--0.834000	0	3.50703300	7.17256000	1.04246100	L
H-HW-0.417000	0	3.31968700	6.27382600	1.38436200	L
H-HW-0.417000	0	3.87829500	6.96437000	0.16806800	L
O-OW--0.834000	0	-1.85949500	-3.68229500	2.15631400	H
H-HW-0.417000	0	-1.24409200	-4.25809900	1.68003300	H
H-HW-0.417000	0	-2.28117800	-3.17113600	1.43695600	H
O-OW--0.834000	0	-5.22201100	1.00146400	-6.10833000	L
H-HW-0.417000	0	-4.27755500	0.78509200	-6.05108000	L
H-HW-0.417000	0	-5.62320500	0.30791200	-5.55473100	L
H-HS-0.193300	0	2.17825000	0.34579300	1.01424200	H

IC1'

C-CT--0.366200	-1	8.218875	4.633508	-8.133049	L
C-C-0.597200	-1	9.048382	3.888053	-7.092853	L
O-O--0.567900	-1	9.647517	2.849505	-7.373796	L
H-HC-0.112300	-1	7.776893	5.520177	-7.678714	L
H-HC-0.112300	-1	7.426672	3.981190	-8.502127	L
H-HC-0.112300	-1	8.859537	4.932310	-8.963588	L
N-N--0.415700	-1	9.044146	4.447035	-5.876185	L
C-CT--0.087500	-1	9.514767	3.771505	-4.659847	L
C-C-0.597300	-1	8.376192	2.875913	-4.167525	L
O-O--0.567900	-1	7.465870	3.337361	-3.464098	L
C-CT-0.298500	-1	9.998573	4.773632	-3.584617	L
C-CT--0.319200	-1	10.417444	4.074496	-2.285762	L
C-CT--0.319200	-1	11.214004	5.579814	-4.064996	L
H-H-0.271900	-1	8.460055	5.269979	-5.749298	L
H-H1-0.096900	-1	10.351527	3.129137	-4.913819	L
H-HC--0.029700	-1	9.202339	5.480393	-3.368485	L
H-HC-0.079100	-1	11.122344	3.274671	-2.514552	L
H-HC-0.079100	-1	9.546623	3.652678	-1.787702	L
H-HC-0.079100	-1	10.894997	4.782427	-1.610226	L
H-HC-0.079100	-1	12.073537	4.921951	-4.193436	L
H-HC-0.079100	-1	11.461179	6.350870	-3.333170	L
H-HC-0.079100	-1	10.996197	6.059091	-5.018442	L
N-N--0.415700	-1	8.391162	1.603036	-4.598604	L
C-CT--0.087500	-1	7.277015	0.652402	-4.423057	L
C-C-0.597300	-1	7.691510	-0.623342	-3.661300	L
O-O--0.567900	-1	8.836923	-1.076355	-3.785651	L
C-CT-0.298500	-1	6.623020	0.245493	-5.767954	L
C-CT--0.319200	-1	5.766639	1.372742	-6.356503	L
C-CT--0.319200	-1	7.615165	-0.207121	-6.844472	L
H-H-0.271900	-1	9.166024	1.295922	-5.192467	L
H-H1-0.096900	-1	6.506704	1.160538	-3.849975	L
H-HC--0.029700	-1	5.952894	-0.594452	-5.581225	L
H-HC-0.079100	-1	6.284983	2.328522	-6.281092	L
H-HC-0.079100	-1	4.831646	1.421800	-5.802922	L
H-HC-0.079100	-1	5.518027	1.157379	-7.396985	L
H-HC-0.079100	-1	8.216539	0.636576	-7.178939	L
H-HC-0.079100	-1	7.065118	-0.610015	-7.693884	L
H-HC-0.079100	-1	8.268592	-0.980718	-6.449262	L
N-N--0.254800	-1	6.754774	-1.228444	-2.893209	L
C-CT--0.026600	-1	6.885270	-2.581367	-2.345708	L
C-C-0.589600	-1	7.132278	-3.605652	-3.455073	L
O-O--0.574800	-1	6.385413	-3.652967	-4.435544	L
C-CT--0.007000	0	5.552291	-2.872324	-1.637534	L
C-CT-0.018900	0	4.981936	-1.489457	-1.342489	L
C-CT-0.019200	0	5.448338	-0.677744	-2.536864	L
H-H1-0.064100	-1	7.703687	-2.597151	-1.626808	L
H-HC-0.025300	0	4.864005	-3.396255	-2.302882	L
H-HC-0.025300	0	5.700337	-3.452539	-0.731361	L
H-HC-0.021300	0	5.416704	-1.070216	-0.441769	L
H-HC-0.021300	0	3.904156	-1.496514	-1.252201	L
H-H1-0.039100	0	5.504763	0.371110	-2.244859	L
H-H1-0.039100	0	4.748706	-0.807187	-3.364336	L
N-N--0.415700	-1	8.156192	-4.452614	-3.306021	L
C-CT--0.149000	-1	8.524886	-5.449597	-4.323858	L

H-H-0.271900	-1	8.755299	-4.330540	-2.490680	L
H-H1-0.097600	-1	7.781610	-5.449136	-5.120475	L
H-H1-0.097600	-1	8.565398	-6.438105	-3.865302	L
H-H1-0.097600	-1	9.501949	-5.201792	-4.738651	L
C-CT--0.366200	-1	5.223370	-7.430029	-4.078818	L
C-C-0.597200	-1	4.095191	-6.758622	-4.872050	L
O-O--0.567900	-1	3.196894	-7.476122	-5.321527	L
H-HC-0.112300	-1	5.935872	-6.674166	-3.749198	L
H-HC-0.112300	-1	5.731107	-8.157207	-4.712318	L
H-HC-0.112300	-1	4.803618	-7.936045	-3.209336	L
N-N--0.415700	-1	4.084870	-5.427869	-5.011952	L
C-CT-0.014300	-1	2.983906	-4.679526	-5.643183	L H-HC 69
C-C-0.597300	-1	2.790054	-5.020740	-7.155393	L
O-O--0.567900	-1	3.784856	-5.186479	-7.862785	L
C-CT--0.204100	0	3.283680	-3.176699	-5.428601	H
C-C-0.713000	0	2.209177	-2.248033	-6.001624	H
O-O--0.593100	0	2.151761	-1.973753	-7.195450	H
N-N--0.919100	0	1.370374	-1.706242	-5.076280	H
H-H-0.271900	-1	4.853456	-4.890907	-4.643861	L
H-H1-0.104800	-1	2.075798	-4.942104	-5.110196	L
H-HC-0.079700	0	4.218832	-2.953841	-5.954126	H
H-HC-0.079700	0	3.425221	-3.002434	-4.358660	H
H-H-0.419600	0	0.524798	-1.290289	-5.449177	H
H-H-0.419600	0	1.384866	-2.018095	-4.112314	H
N-N--0.415700	-1	1.536708	-5.118882	-7.649531	L
C-CT--0.149000	-1	1.185529	-5.379021	-9.075380	L
H-H-0.271900	-1	0.781108	-4.892408	-7.003826	L
H-H1-0.097600	-1	2.091441	-5.605141	-9.637202	L
H-H1-0.097600	-1	0.706048	-4.495681	-9.498067	L
H-H1-0.097600	-1	0.501723	-6.225973	-9.130769	L
C-CT--0.366200	-1	11.714932	-5.938526	-0.621969	L
C-C-0.597200	-1	10.698274	-6.063184	0.521021	L
O-O--0.567900	-1	11.014580	-5.907963	1.705752	L
H-HC-0.112300	-1	11.214642	-6.114152	-1.574177	L
H-HC-0.112300	-1	12.506130	-6.675369	-0.486119	L
H-HC-0.112300	-1	12.146708	-4.937480	-0.617708	L
N-N--0.415700	-1	9.461724	-6.366124	0.128849	L
C-CT--0.023700	-1	8.300604	-6.562170	0.991931	L
C-C-0.597300	-1	7.246039	-7.404984	0.287284	L
O-O--0.567900	-1	7.068521	-7.246419	-0.927365	L
C-CT-0.034200	0	7.694996	-5.203476	1.383504	L
C-CT-0.001800	0	6.776545	-5.221608	2.622028	L
S-S--0.273700	0	5.058180	-5.788178	2.409759	L
C-CT--0.053600	0	4.210425	-4.227071	2.009009	L
H-H-0.271900	-1	9.293772	-6.440139	-0.868456	L
H-H1-0.088000	-1	8.623942	-7.093994	1.875128	L
H-HC-0.024100	0	7.154838	-4.783424	0.535367	L
H-HC-0.024100	0	8.527325	-4.541636	1.603997	L
H-H1-0.044000	0	6.729842	-4.207984	3.020702	L
H-H1-0.044000	0	7.247658	-5.840914	3.385239	L
H-H1-0.068400	0	3.157090	-4.415629	1.795979	L
H-H1-0.068400	0	4.662015	-3.761754	1.136147	L
H-H1-0.068400	0	4.277327	-3.535175	2.849107	L
N-N--0.415700	-1	6.536602	-8.249674	1.046066	L

C-CT--0.149000	-1	5.314436	-8.954768	0.631483	L
H-H-0.271900	-1	6.851865	-8.381038	2.007173	L
H-H1-0.097600	-1	5.098189	-8.724465	-0.411229	L
H-H1-0.097600	-1	4.480352	-8.633483	1.255542	L
H-H1-0.097600	-1	5.459757	-10.028802	0.743731	L
C-CT--0.366200	-1	3.875519	-9.351236	4.911627	L
C-C-0.597200	-1	3.708443	-7.944946	5.521630	L
O-O--0.567900	-1	4.670766	-7.229581	5.815503	L
H-HC-0.112300	-1	2.893077	-9.791126	4.737081	L
H-HC-0.112300	-1	4.438542	-9.982010	5.599310	L
H-HC-0.112300	-1	4.412272	-9.275884	3.965800	L
N-N--0.415700	-1	2.447236	-7.529228	5.667719	L
C-CT--0.087500	-1	2.012074	-6.124240	5.614243	L
C-C-0.597300	-1	1.889848	-5.565390	7.038248	L
O-O--0.567900	-1	0.852373	-5.657359	7.709733	L
C-CT-0.298500	0	0.693139	-5.949109	4.832531	L
C-CT--0.319200	0	0.345860	-4.465174	4.672366	L
C-CT--0.319200	0	0.781722	-6.575126	3.433005	L
H-H-0.271900	-1	1.710903	-8.222369	5.511218	L
H-H1-0.096900	-1	2.778799	-5.552198	5.088190	L
H-HC--0.029700	0	-0.115526	-6.445531	5.370588	L
H-HC-0.079100	0	1.091372	-3.956412	4.057556	L
H-HC-0.079100	0	0.280643	-3.966737	5.638632	L
H-HC-0.079100	0	-0.624128	-4.367712	4.190052	L
H-HC-0.079100	0	1.623588	-6.141282	2.891307	L
H-HC-0.079100	0	-0.132343	-6.357100	2.878533	L
H-HC-0.079100	0	0.900513	-7.653584	3.498126	L
N-N--0.415700	-1	3.050119	-5.114008	7.514075	L
C-CT--0.149000	-1	3.426410	-4.979538	8.918703	L
H-H-0.271900	-1	3.809847	-5.031879	6.848705	L
H-H1-0.097600	-1	2.539244	-5.083448	9.543558	L
H-H1-0.097600	-1	3.873430	-3.999764	9.083344	L
H-H1-0.097600	-1	4.146160	-5.756181	9.177573	L
C-CT--0.366200	-1	12.473604	-4.247863	6.354853	L
C-C-0.597200	-1	12.270938	-3.524812	5.004783	L
O-O--0.567900	-1	13.238805	-3.309888	4.268522	L
H-HC-0.112300	-1	11.513847	-4.346446	6.862055	L
H-HC-0.112300	-1	13.155143	-3.668139	6.978581	L
H-HC-0.112300	-1	12.894725	-5.236677	6.178053	L
N-N--0.415700	-1	11.036591	-3.096620	4.701467	L
C-CT--0.023700	-1	10.761846	-2.271848	3.527176	L
C-C-0.597300	-1	11.332611	-0.850016	3.663778	L
O-O--0.567900	-1	12.062846	-0.386103	2.786235	L
C-CT-0.034200	0	9.256992	-2.189111	3.268235	L
C-CT-0.001800	0	9.017397	-1.494486	1.922630	L
S-S--0.273700	0	7.457532	-1.918540	1.136810	L
C-CT--0.053600	0	6.257676	-1.085414	2.205349	L
H-H-0.271900	-1	10.270955	-3.324147	5.329476	L
H-H1-0.088000	-1	11.231840	-2.752347	2.667366	L
H-HC-0.024100	0	8.752957	-1.637891	4.063245	L
H-HC-0.024100	0	8.854890	-3.197427	3.244344	L
H-H1-0.044000	0	9.806341	-1.788872	1.229352	L
H-H1-0.044000	0	9.071715	-0.412655	2.052157	L
H-H1-0.068400	0	5.245891	-1.337476	1.883982	L

H-H1-0.068400	0	6.378264	-0.005151	2.124257	L
H-H1-0.068400	0	6.384855	-1.399059	3.239491	L
N-N--0.415700	-1	11.066115	-0.161218	4.778988	L
C-CT--0.149000	-1	11.622541	1.176016	5.008378	L
H-H-0.271900	-1	10.486607	-0.590827	5.499564	L
H-H1-0.097600	-1	12.211677	1.477284	4.142314	L
H-H1-0.097600	-1	12.259653	1.157462	5.892196	L
H-H1-0.097600	-1	10.810100	1.886454	5.161058	L
C-CT--0.366200	-1	6.204128	8.712312	-5.551506	L
C-C-0.597200	-1	6.516013	7.519394	-4.626365	L
O-O--0.567900	-1	6.664711	6.370619	-5.066880	L
H-HC-0.112300	-1	6.114484	9.621252	-4.955657	L
H-HC-0.112300	-1	5.266420	8.529698	-6.077631	L
H-HC-0.112300	-1	7.009982	8.831265	-6.276469	L
N-N--0.415700	-1	6.659931	7.834156	-3.328845	L
C-CT--0.001400	-1	6.698932	6.842324	-2.238871	L
C-C-0.597300	-1	5.322168	6.166251	-2.098177	L
O-O--0.567900	-1	4.450013	6.648890	-1.358448	L
C-CT--0.001400	-1	7.218004	7.474133	-0.934107	L
C-CA--0.001100	-1	7.900777	6.501081	0.021150	L
C-CA--0.190600	-1	9.308442	6.446978	0.071806	L
C-CA--0.190600	-1	7.152474	5.681824	0.891396	L
C-CA--0.234100	-1	9.956613	5.624591	1.012343	L
C-CA--0.234100	-1	7.804992	4.854337	1.831663	L
C-C-0.322600	-1	9.207404	4.848355	1.910702	L
O-OH--0.557900	-1	9.865706	4.100711	2.843118	L
H-H-0.271900	-1	6.598280	8.826180	-3.086948	L
H-H1-0.087600	-1	7.408016	6.068400	-2.518971	L
H-HC-0.029500	-1	7.945673	8.243567	-1.194986	L
H-HC-0.029500	-1	6.406972	7.983407	-0.412087	L
H-HA-0.169900	-1	9.896188	7.069352	-0.587896	L
H-HA-0.169900	-1	6.071481	5.690544	0.847821	L
H-HA-0.165600	-1	11.033776	5.592309	1.061584	L
H-HA-0.165600	-1	7.228703	4.223065	2.492115	L
H-HO-0.399200	-1	9.368573	3.878460	3.646416	L
N-N--0.415700	-1	5.107605	5.146011	-2.933564	L
C-CT-0.033700	-1	3.789695	4.654652	-3.320700	L
C-C-0.597300	-1	2.951119	4.019987	-2.200351	L
O-O--0.567900	-1	1.728017	4.124347	-2.268959	L
C-CT--0.182500	-1	3.975723	3.655718	-4.457654	L
H-H-0.271900	-1	5.889838	4.851076	-3.512923	L
H-H1-0.082300	-1	3.225989	5.501106	-3.714221	L
H-HC-0.060300	-1	3.003892	3.347896	-4.842572	L
H-HC-0.060300	-1	4.510849	2.785773	-4.076834	L
H-HC-0.060300	-1	4.547469	4.115419	-5.263944	L
N-N--0.415700	-1	3.563527	3.376166	-1.195950	L H-HC 209
C-CT-0.021300	0	2.851291	2.666595	-0.113721	H
C-C-0.597300	0	2.321011	3.678534	0.916496	H
O-O--0.567900	0	3.110655	4.462394	1.442884	H
C-CT--0.123100	0	3.894173	1.748194	0.543777	H
S-S--1.036000	0	3.209223	0.515662	1.722333	H
H-H-0.271900	-1	4.567287	3.348863	-1.188194	L
H-H1-0.112400	0	2.051764	2.077388	-0.561664	H
H-H1-0.111200	0	4.590641	2.351435	1.135186	H

H-H1-0.111200	0	4.478931	1.207487	-0.205954	H
N-N--0.415700	0	0.993942	3.636662	1.228239	H
C-CT--0.051800	0	0.423487	4.493620	2.287591	H
C-C-0.597300	0	0.807672	3.987599	3.711660	H
O-O--0.567900	0	1.345735	4.719435	4.541256	H
C-CT--0.110200	-1	-1.107962	4.641185	2.036710	H
C-CT-0.353100	-1	-1.964696	5.547088	2.947417	L H-HC 222
C-CT--0.412100	-1	-2.156822	5.000205	4.363460	L
C-CT--0.412100	-1	-1.430996	6.979689	3.036317	L
H-H-0.271900	0	0.417307	2.888571	0.843092	H
H-H1-0.092200	0	0.908903	5.469235	2.218658	H
H-HC-0.045700	0	-1.226368	5.019331	1.014499	H
H-HC-0.045700	0	-1.577550	3.652448	2.053505	H
H-HC--0.036100	-1	-2.956408	5.597595	2.499363	L
H-HC-0.100000	-1	-1.257384	5.139211	4.959639	L
H-HC-0.100000	-1	-2.403910	3.940382	4.321864	L
H-HC-0.100000	-1	-2.974856	5.534523	4.844230	L
H-HC-0.100000	-1	-0.468666	6.994045	3.548955	L
H-HC-0.100000	-1	-2.141340	7.599404	3.582191	L
H-HC-0.100000	-1	-1.306959	7.382448	2.030199	L
N-N--0.415700	0	0.552186	2.669133	3.973468	H
C-CT--0.087500	0	0.598106	2.150056	5.347925	H
C-C-0.597300	0	1.993654	2.095580	5.979954	H
O-O--0.567900	0	2.091207	2.003042	7.199050	H
C-CT-0.298500	-1	-0.027207	0.741213	5.380276	H
C-CT--0.319200	0	0.773082	-0.332113	4.611774	L H-HC 241
C-CT--0.319200	0	-0.350820	0.179310	6.764208	L H-HC 241
H-H-0.271900	0	0.080993	2.115416	3.260212	H
H-H1-0.096900	0	0.023559	2.827139	5.993053	H
H-HC--0.029700	0	-0.985263	0.819253	4.863018	H
H-HC-0.079100	0	1.663807	-0.625965	5.162627	L
H-HC-0.079100	0	1.087204	0.048526	3.638209	L
H-HC-0.079100	0	0.144882	-1.203029	4.430689	L
H-HC-0.079100	0	0.565577	-0.057791	7.302707	L
H-HC-0.079100	0	-0.942885	-0.728463	6.649714	L
H-HC-0.079100	0	-0.928199	0.912047	7.325363	L
N-N--0.415700	0	3.015698	1.937491	5.105760	H
C-CT-0.033700	0	4.379988	1.783883	5.565093	H
C-C-0.597300	-1	5.097029	3.111531	5.837132	L H-H1 254
O-O--0.567900	-1	6.272048	3.084199	6.192968	L
C-CT--0.182500	-1	5.151988	0.965043	4.531132	L H-H1 254
H-H-0.271900	0	2.860806	2.198818	4.144276	H
H-H1-0.082300	0	4.356963	1.237095	6.510912	H
H-HC-0.060300	-1	6.118333	0.669651	4.937160	L
H-HC-0.060300	-1	5.309906	1.566726	3.636319	L
H-HC-0.060300	-1	4.591742	0.064337	4.276999	L
N-N--0.415700	-1	4.396724	4.241380	5.673726	L
C-CT--0.087500	-1	4.783337	5.602723	6.071273	L
C-C-0.597300	-1	3.942896	6.051493	7.273927	L
O-O--0.567900	-1	4.496427	6.499647	8.279021	L
C-CT-0.298500	-1	4.570891	6.579580	4.897384	L
C-CT--0.319200	-1	4.968860	8.016881	5.250492	L
C-CT--0.319200	-1	5.386871	6.182769	3.667470	L
H-H-0.271900	-1	3.485079	4.129762	5.247661	L

H-H1-0.096900	-1	5.833405	5.628506	6.352549	L
H-HC--0.029700	-1	3.518382	6.570235	4.621749	L
H-HC-0.079100	-1	6.019527	8.051290	5.530285	L
H-HC-0.079100	-1	4.363752	8.394924	6.073794	L
H-HC-0.079100	-1	4.809803	8.657309	4.383263	L
H-HC-0.079100	-1	6.436832	6.101356	3.942686	L
H-HC-0.079100	-1	5.272055	6.931532	2.884127	L
H-HC-0.079100	-1	5.031840	5.227051	3.281914	L
N-N--0.415700	-1	2.611035	5.864545	7.220343	L
C-CT--0.149000	-1	1.704944	6.205570	8.327783	L
H-H-0.271900	-1	2.203020	5.485875	6.371076	L
H-H1-0.097600	-1	2.283889	6.598124	9.163810	L
H-H1-0.097600	-1	1.166686	5.311894	8.645174	L
H-H1-0.097600	-1	0.991747	6.959596	7.994887	L
C-CT--0.366200	-1	4.073847	10.302447	-0.979955	L
C-C-0.597200	-1	2.598084	9.980264	-1.224692	L
O-O--0.567900	-1	1.791164	10.897513	-1.296342	L
H-HC-0.112300	-1	4.646634	9.376755	-0.945008	L
H-HC-0.112300	-1	4.177261	10.830267	-0.032100	L
H-HC-0.112300	-1	4.447189	10.930531	-1.788444	L
N-N--0.415700	-1	2.215662	8.698460	-1.281484	L
C-CT--0.024900	-1	0.801290	8.320673	-1.122523	L
C-C-0.597300	-1	0.216059	8.818626	0.204708	L
O-O--0.567900	-1	-0.876771	9.389273	0.213305	L
C-CT-0.211700	0	0.627542	6.821206	-1.272732	L
O-OH--0.654600	0	0.916591	6.516059	-2.617047	L
H-H-0.271900	-1	2.916000	7.963863	-1.342854	L
H-H1-0.084300	-1	0.229969	8.773075	-1.928842	L
H-H1-0.035200	0	-0.396994	6.534763	-1.043764	L
H-H1-0.035200	0	1.308696	6.290430	-0.605799	L
H-HO-0.427500	0	1.026163	5.540608	-2.632077	L
N-N--0.415700	-1	0.978306	8.680999	1.300289	L
C-CT-0.033700	-1	0.626007	9.162126	2.637376	L
C-C-0.597300	-1	0.165393	10.624625	2.630109	L
O-O--0.567900	-1	-0.930070	10.945745	3.093301	L
C-CT--0.182500	-1	1.812051	8.921052	3.568791	L
H-H-0.271900	-1	1.865403	8.182265	1.194474	L
H-H1-0.082300	-1	-0.190390	8.571938	3.026717	L
H-HC-0.060300	-1	1.583304	9.291432	4.567427	L
H-HC-0.060300	-1	2.698910	9.420472	3.180888	L
H-HC-0.060300	-1	2.004245	7.851285	3.622271	L
N-N--0.415700	-1	0.965960	11.501909	2.015031	L
C-CT--0.149000	-1	0.629420	12.900601	1.823439	L
H-H-0.271900	-1	1.867581	11.191676	1.660923	L
H-H1-0.097600	-1	-0.356020	13.098057	2.246843	L
H-H1-0.097600	-1	0.619483	13.129931	0.758742	L
H-H1-0.097600	-1	1.370642	13.524638	2.323728	L
C-CT--0.366200	-1	-11.914612	4.610949	4.975025	L
C-C-0.597200	-1	-12.351136	3.193175	4.602572	L
O-O--0.567900	-1	-12.918171	2.486182	5.437994	L
H-HC-0.112300	-1	-11.433985	5.080057	4.116413	L
H-HC-0.112300	-1	-11.210496	4.568017	5.806102	L
H-HC-0.112300	-1	-12.786857	5.194969	5.266988	L
N-N--0.415700	-1	-12.018479	2.752249	3.389053	L

C-CT--0.087500	-1	-12.018297	1.330076	3.028846	L
C-C-0.597300	-1	-10.573341	0.931763	2.714629	L
O-O--0.567900	-1	-9.856451	1.574291	1.939767	L
C-CT-0.298500	-1	-13.015676	0.943385	1.904223	L
C-CT--0.319200	-1	-13.766408	-0.345142	2.288847	L
C-CT--0.319200	-1	-14.091137	1.994444	1.595893	L
H-H-0.271900	-1	-11.606554	3.402792	2.717561	L
H-H1-0.096900	-1	-12.312267	0.770829	3.914672	L
H-HC--0.029700	-1	-12.457519	0.752792	0.991259	L
H-HC-0.079100	-1	-14.398172	-0.162267	3.158759	L
H-HC-0.079100	-1	-13.052575	-1.139555	2.510338	L
H-HC-0.079100	-1	-14.404123	-0.657930	1.462258	L
H-HC-0.079100	-1	-14.724201	2.139843	2.467732	L
H-HC-0.079100	-1	-14.699724	1.660689	0.756866	L
H-HC-0.079100	-1	-13.631699	2.945685	1.336141	L
N-N--0.415700	-1	-10.112346	-0.090019	3.438663	L
C-CT--0.038900	-1	-8.705231	-0.490875	3.520235	L
C-C-0.597300	-1	-8.581024	-2.016743	3.632383	L
O-O--0.567900	-1	-9.513461	-2.675123	4.114851	L
C-CT-0.365400	-1	-7.986661	0.153756	4.729396	L
O-OH--0.676100	-1	-8.156102	-0.561236	5.931773	L
C-CT--0.243800	-1	-8.401481	1.591040	5.037989	L
H-H-0.271900	-1	-10.742853	-0.561727	4.070894	L
H-H1-0.100700	-1	-8.204330	-0.158044	2.611224	L
H-H1-0.004300	-1	-6.927661	0.151197	4.492799	L
H-HC-0.064200	-1	-8.443709	2.156437	4.114540	L
H-HC-0.064200	-1	-7.672057	2.045733	5.709597	L
H-HC-0.064200	-1	-9.384605	1.619644	5.506962	L
H-HO-0.410200	-1	-8.405874	0.078278	6.631045	L
N-N--0.254800	-1	-7.456514	-2.614022	3.198669	L
C-CT--0.026600	-1	-7.209052	-4.040785	3.367542	L
C-C-0.589600	-1	-6.601163	-4.397456	4.725314	L
O-O--0.574800	-1	-6.615023	-5.568524	5.087473	L
C-CT--0.007000	0	-6.232610	-4.396055	2.248742	L
C-CT-0.018900	0	-5.393754	-3.132044	2.105985	L
C-CT-0.019200	0	-6.386638	-2.008499	2.413363	L
H-H1-0.064100	-1	-8.120371	-4.608972	3.222842	L
H-HC-0.025300	0	-5.617962	-5.255787	2.508284	L
H-HC-0.025300	0	-6.782866	-4.580508	1.325285	L
H-HC-0.021300	0	-4.982045	-3.048955	1.102808	L
H-HC-0.021300	0	-4.593942	-3.137071	2.845062	L
H-H1-0.039100	0	-6.792661	-1.622264	1.478241	L
H-H1-0.039100	0	-5.887383	-1.212419	2.967203	L
N-N--0.415700	-1	-5.980298	-3.437570	5.419025	L
C-CT--0.001400	-1	-4.989154	-3.681235	6.478476	L
C-C-0.597300	-1	-5.538663	-4.464033	7.685487	L
O-O--0.567900	-1	-6.724815	-4.345244	7.996680	L
C-CT--0.001400	0	-4.451793	-2.338761	6.992583	L H-HA 373
C-CA--0.001100	0	-4.083813	-1.326881	5.922608	H
C-CA--0.190600	0	-3.294311	-1.698056	4.829444	H
C-CA--0.190600	0	-4.538939	-0.009182	6.021587	H
C-CA--0.234100	0	-2.962487	-0.769101	3.850833	H
C-CA--0.234100	0	-4.195907	0.936769	5.059398	H
C-C-0.322600	0	-3.391112	0.561512	3.978095	H

O-OH--0.557900	0	-3.047081	1.514426	3.079699	H
H-H-0.271900	-1	-6.045687	-2.498393	5.057958	L
H-H1-0.087600	-1	-4.165692	-4.251391	6.047024	L
H-HC-0.029500	0	-5.211117	-1.894402	7.638527	L
H-HC-0.029500	0	-3.567907	-2.524007	7.604106	L
H-HA-0.169900	0	-2.941774	-2.718869	4.702393	H
H-HA-0.169900	0	-5.163400	0.296808	6.862038	H
H-HA-0.165600	0	-2.361016	-1.065028	3.000239	H
H-HA-0.165600	0	-4.510347	1.973519	5.153491	H
H-HO-0.399200	0	-2.251922	1.223583	2.574998	H
N-N--0.415700	-1	-4.661329	-5.156004	8.438895	L
C-CT--0.149000	-1	-5.046494	-5.622159	9.787437	L
H-H-0.271900	-1	-3.666635	-5.151059	8.199029	L
H-H1-0.097600	-1	-6.130100	-5.569741	9.894026	L
H-H1-0.097600	-1	-4.576031	-4.989414	10.539276	L
H-H1-0.097600	-1	-4.717429	-6.652733	9.922810	L
C-CT--0.366200	-1	-0.496313	-10.775787	2.472585	L
C-C-0.597200	-1	-0.675313	-9.834283	1.268358	L
O-O--0.567900	-1	-1.784568	-9.657491	0.759817	L
H-HC-0.112300	-1	0.551696	-10.792122	2.768275	L
H-HC-0.112300	-1	-0.812000	-11.782210	2.196469	L
H-HC-0.112300	-1	-1.104042	-10.421244	3.305094	L
N-N--0.415700	-1	0.439911	-9.289703	0.764822	L
C-CT-0.014300	-1	0.397937	-8.271582	-0.284183	L H-HC 405
C-C-0.597300	-1	0.023129	-8.777899	-1.695799	L
O-O--0.567900	-1	-0.186599	-7.954270	-2.577040	L
C-CT--0.204100	0	1.726577	-7.485732	-0.298593	H
C-C-0.713000	0	1.486547	-5.986639	-0.512812	H
O-O--0.593100	0	0.958962	-5.330800	0.385670	H
N-N--0.919100	0	1.937996	-5.441655	-1.665583	H
H-H-0.271900	-1	1.322406	-9.479434	1.210768	L
H-H1-0.104800	-1	-0.403318	-7.597932	0.020116	L
H-HC-0.079700	0	2.404408	-7.931227	-1.036581	H
H-HC-0.079700	0	2.192820	-7.558760	0.687159	H
H-H-0.419600	0	1.797016	-4.442589	-1.844685	H
H-H-0.419600	0	2.209907	-6.034164	-2.439085	H
N-N--0.415700	-1	-0.075999	-10.090860	-1.934038	L
C-CT--0.149000	-1	-0.617508	-10.639943	-3.189297	L
H-H-0.271900	-1	0.032594	-10.740810	-1.147412	L
H-H1-0.097600	-1	-0.680437	-9.848535	-3.935460	L
H-H1-0.097600	-1	-1.611772	-11.048548	-3.008576	L
H-H1-0.097600	-1	0.039019	-11.431484	-3.552819	L
C-CT--0.366200	-1	-3.890306	-11.691354	-1.422782	L
C-C-0.597200	-1	-4.654298	-10.363081	-1.494326	L
O-O--0.567900	-1	-5.793183	-10.362714	-1.965728	L
H-HC-0.112300	-1	-2.906605	-11.520537	-0.984518	L
H-HC-0.112300	-1	-3.774464	-12.098514	-2.426235	L
H-HC-0.112300	-1	-4.445362	-12.396761	-0.804782	L
N-N--0.415700	-1	-4.023972	-9.237653	-1.118543	L
C-CT--0.087500	-1	-4.584400	-7.875099	-1.281228	L
C-C-0.597300	-1	-4.848099	-7.491509	-2.748469	L
O-O--0.567900	-1	-5.835024	-6.819107	-3.043957	L
C-CT-0.298500	-1	-3.674498	-6.801096	-0.629303	L
C-CT--0.319200	-1	-4.157794	-5.361809	-0.869398	L

C-CT--0.319200	-1	-3.659859	-6.938317	0.890738	L
H-H-0.271900	-1	-3.142409	-9.350999	-0.616226	L
H-H1-0.096900	-1	-5.545318	-7.850865	-0.768642	L
H-HC--0.029700	-1	-2.659130	-6.901820	-1.013167	L
H-HC-0.079100	-1	-5.193469	-5.262563	-0.543541	L
H-HC-0.079100	-1	-4.088806	-5.109989	-1.925038	L
H-HC-0.079100	-1	-3.528966	-4.656403	-0.324120	L
H-HC-0.079100	-1	-4.666115	-6.800912	1.269168	L
H-HC-0.079100	-1	-2.994164	-6.194520	1.330935	L
H-HC-0.079100	-1	-3.313486	-7.916726	1.192484	L
N-N--0.415700	-1	-4.002244	-7.893259	-3.705447	L
C-CT--0.149000	-1	-4.086516	-7.478320	-5.116522	L
H-H-0.271900	-1	-3.282392	-8.558362	-3.448653	L
H-H1-0.097600	-1	-4.902683	-6.765673	-5.238052	L
H-H1-0.097600	-1	-4.271126	-8.352209	-5.742867	L
H-H1-0.097600	-1	-3.148794	-7.010112	-5.414517	L
C-CT--0.366200	-1	-12.105583	3.713192	-1.320688	L
C-C-0.597200	-1	-11.004378	2.644037	-1.284162	L
O-O--0.567900	-1	-11.300841	1.461890	-1.129379	L
H-HC-0.112300	-1	-11.654363	4.694979	-1.464577	L
H-HC-0.112300	-1	-12.656283	3.700844	-0.379722	L
H-HC-0.112300	-1	-12.789212	3.502997	-2.143474	L
N-N--0.415700	-1	-9.746575	3.081286	-1.351294	L
C-CT--0.024900	-1	-8.566221	2.255861	-1.171383	L
C-C-0.597300	-1	-7.451612	3.118310	-0.573776	L
O-O--0.567900	-1	-6.796348	3.904765	-1.271790	L
C-CT-0.211700	0	-8.121570	1.585596	-2.468938	L
O-OH--0.654600	0	-7.089931	0.686957	-2.147985	L
H-H-0.271900	-1	-9.617317	4.077388	-1.421419	L
H-H1-0.084300	-1	-8.806233	1.464074	-0.463095	L
H-H1-0.035200	0	-7.768862	2.320666	-3.189757	L
H-H1-0.035200	0	-8.957475	1.028647	-2.894601	L
H-HO-0.427500	0	-6.221604	1.135297	-2.256884	L
N-N--0.415700	-1	-7.290097	3.044059	0.756231	L
C-CT-0.021300	-1	-6.113555	3.656135	1.392253	L
C-C-0.597300	-1	-4.826826	3.005795	0.859018	L
O-O--0.567900	-1	-3.849857	3.691278	0.599008	L
C-CT--0.123100	-1	-6.172186	3.520009	2.915315	L
S-SH--0.311900	-1	-7.422934	4.629907	3.622547	L
H-H-0.271900	-1	-7.952756	2.499399	1.304929	L
H-H1-0.112400	-1	-6.081989	4.718053	1.143408	L
H-H1-0.111200	-1	-5.200429	3.790403	3.331968	L
H-H1-0.111200	-1	-6.391331	2.485929	3.180128	L
H-HS-0.193300	-1	-8.466114	4.184832	2.912922	L
N-N--0.415700	-1	-4.868774	1.687103	0.652999	L H-HC 478
C-CT-0.021300	0	-3.782333	0.952491	0.016783	H
C-C-0.597300	0	-3.692455	1.362262	-1.447378	H
O-O--0.567900	0	-4.670881	1.760113	-2.079969	H
C-CT--0.123100	0	-4.100449	-0.536148	0.220627	H
S-SH--0.311900	0	-2.768668	-1.676487	-0.297346	H
H-H-0.271900	-1	-5.721227	1.201254	0.858558	L
H-H1-0.112400	0	-2.848230	1.200371	0.524590	H
H-H1-0.111200	0	-5.028282	-0.779086	-0.309457	H
H-H1-0.111200	0	-4.279711	-0.700772	1.285294	H

H-HS-0.193300	0	0.855740	0.196100	-0.927327	H
N-N--0.415700	0	-2.446791	1.246590	-2.005981	H
C-CT--0.087500	0	-2.263134	1.362310	-3.441596	H
C-C-0.597300	0	-2.107731	0.014316	-4.185448	H
O-O--0.567900	0	-2.043557	0.036476	-5.416251	H
C-CT-0.298500	-1	-1.111462	2.297688	-3.869531	H
C-CT--0.319200	0	-1.267179	3.695883	-3.268895	L H-HC 492
C-CT--0.319200	0	0.273284	1.759305	-3.479074	L H-HC 492
H-H-0.271900	0	-1.706849	0.865026	-1.425853	H
H-H1-0.096900	0	-3.209152	1.772775	-3.812247	H
H-HC--0.029700	0	-1.140921	2.372418	-4.958959	H
H-HC-0.079100	0	-1.132263	3.658831	-2.185829	L
H-HC-0.079100	0	-2.258155	4.074986	-3.498785	L
H-HC-0.079100	0	-0.524650	4.363992	-3.701128	L
H-HC-0.079100	0	0.393141	1.797631	-2.396119	L
H-HC-0.079100	0	1.044958	2.362525	-3.946965	L
H-HC-0.079100	0	0.406137	0.730823	-3.807511	L
N-N--0.415700	0	-1.946529	-1.091139	-3.418297	H
C-CT--0.003100	0	-2.053691	-2.425948	-4.001917	H
C-C-0.597300	0	-3.523963	-2.854834	-4.198578	H
O-O--0.567900	0	-3.833133	-3.513890	-5.192569	H
C-CT--0.003600	-1	-1.304562	-3.443147	-3.113994	H
C-CT--0.064500	-1	-1.440849	-4.896978	-3.604584	L H-HC 508
C-C-0.695100	-1	-0.568028	-5.237464	-4.797785	L
O-O--0.608600	-1	-0.424029	-4.486625	-5.747693	L
N-N--0.940700	-1	0.042886	-6.402738	-4.792735	L
H-H-0.271900	0	-2.186583	-1.048172	-2.418958	H
H-H1-0.085000	0	-1.641486	-2.389918	-5.011943	H
H-HC-0.017100	0	-0.246572	-3.192525	-3.046618	H
H-HC-0.017100	0	-1.717570	-3.400333	-2.102588	H
H-HC-0.035200	-1	-2.469541	-5.149544	-3.845782	L
H-HC-0.035200	-1	-1.157252	-5.545626	-2.783173	L
H-H-0.425100	-1	0.645555	-6.652297	-5.557205	L
H-H-0.425100	-1	-0.068339	-7.023550	-3.992975	L
N-N--0.415700	0	-4.354867	-2.530798	-3.176922	H
C-CT--0.023700	0	-5.744182	-2.952089	-3.231519	H
C-C-0.597300	-1	-6.417229	-2.313884	-4.471401	L H-H1 522
O-O--0.567900	-1	-6.243792	-1.118950	-4.729800	L
C-CT-0.034200	-1	-6.478350	-2.654894	-1.904961	L H-H1 522
C-CT-0.001800	-1	-7.947742	-3.100819	-1.961903	L
S-S--0.273700	-1	-8.851431	-3.073190	-0.386382	L
C-CT--0.053600	-1	-9.216248	-1.304519	-0.254473	L
H-H-0.271900	0	-3.980773	-2.169490	-2.301754	H
H-H1-0.088000	0	-5.731939	-4.035377	-3.333186	H
H-HC-0.024100	-1	-6.405686	-1.608725	-1.644953	L
H-HC-0.024100	-1	-5.986002	-3.208738	-1.109162	L
H-H1-0.044000	-1	-7.975130	-4.126247	-2.331823	L
H-H1-0.044000	-1	-8.486664	-2.473018	-2.671818	L
H-H1-0.068400	-1	-9.821351	-1.118660	0.632821	L
H-H1-0.068400	-1	-9.765894	-0.973733	-1.135933	L
H-H1-0.068400	-1	-8.285118	-0.746536	-0.182767	L
N-N--0.254800	-1	-7.167863	-3.081283	-5.283301	L
C-CT--0.026600	-1	-7.564239	-2.663177	-6.628887	L
C-C-0.589600	-1	-9.012969	-2.176550	-6.619982	L

O-O--0.574800	-1	-9.900338	-2.875286	-6.123435	L
C-CT--0.007000	-1	-7.360600	-3.907021	-7.508378	L
C-CT-0.018900	-1	-6.846005	-4.971226	-6.535842	L
C-CT-0.019200	-1	-7.377016	-4.510576	-5.204779	L
H-H1-0.064100	-1	-6.915372	-1.867342	-6.994051	L
H-HC-0.025300	-1	-8.295742	-4.225705	-7.959908	L
H-HC-0.025300	-1	-6.624951	-3.723590	-8.289232	L
H-HC-0.021300	-1	-5.757876	-4.965278	-6.509928	L
H-HC-0.021300	-1	-7.222035	-5.952871	-6.752174	L
H-H1-0.039100	-1	-6.853537	-5.019946	-4.407400	L
H-H1-0.039100	-1	-8.442891	-4.729136	-5.130180	L
N-N--0.415700	-1	-9.234237	-0.979242	-7.156107	L
C-CT--0.149000	-1	-10.466303	-0.207815	-6.965402	L
H-H-0.271900	-1	-8.428731	-0.511085	-7.570740	L
H-H1-0.097600	-1	-11.227555	-0.844607	-6.515320	L
H-H1-0.097600	-1	-10.819706	0.154736	-7.930652	L
H-H1-0.097600	-1	-10.265711	0.639287	-6.309047	L
C-CT--0.366200	-1	-10.332829	8.870973	-4.228592	L
C-C-0.597200	-1	-9.786177	7.580849	-3.603060	L
O-O--0.567900	-1	-10.229043	7.161266	-2.532482	L
H-HC-0.112300	-1	-9.814324	9.068235	-5.166757	L
H-HC-0.112300	-1	-10.172279	9.702584	-3.543019	L
H-HC-0.112300	-1	-11.399723	8.758449	-4.420433	L
N-N--0.415700	-1	-8.816606	6.956847	-4.266661	L
C-CT--0.024900	-1	-7.873653	6.036741	-3.627332	L
C-C-0.597300	-1	-6.542756	6.766402	-3.406313	L
O-O--0.567900	-1	-6.286495	7.773545	-4.073519	L
C-CT-0.211700	0	-7.653706	4.783031	-4.485775	L
O-OH--0.654600	0	-7.285338	5.097785	-5.815619	L
H-H-0.271900	-1	-8.545555	7.325556	-5.177297	L
H-H1-0.084300	-1	-8.259791	5.697779	-2.665671	L
H-H1-0.035200	0	-8.574970	4.199467	-4.503353	L
H-H1-0.035200	0	-6.867967	4.176206	-4.032909	L
H-HO-0.427500	0	-6.846210	4.330432	-6.199643	L
N-N--0.415700	-1	-5.665586	6.232866	-2.545631	L
C-CT-0.033700	-1	-4.290925	6.739301	-2.442599	L
C-C-0.597300	-1	-3.543784	6.743202	-3.795302	L
O-O--0.567900	-1	-2.643237	7.555530	-4.012379	L
C-CT--0.182500	-1	-3.538334	5.916190	-1.407265	L
H-H-0.271900	-1	-5.949591	5.427950	-1.982252	L
H-H1-0.082300	-1	-4.336487	7.766633	-2.079676	L
H-HC-0.060300	-1	-2.524071	6.295861	-1.302224	L
H-HC-0.060300	-1	-3.505144	4.870221	-1.710267	L
H-HC-0.060300	-1	-4.053403	6.000091	-0.451583	L
N-N--0.415700	-1	-3.966940	5.877644	-4.730306	L
C-CT--0.149000	-1	-3.452607	5.823843	-6.097578	L
H-H-0.271900	-1	-4.696411	5.230048	-4.463246	L
H-H1-0.097600	-1	-2.677927	6.580517	-6.224032	L
H-H1-0.097600	-1	-4.263999	6.015666	-6.799544	L
H-H1-0.097600	-1	-3.031737	4.836752	-6.288728	L
C-CM--0.139000	0	0.773930	-2.051282	0.030355	H
C-C-0.519000	0	1.336357	-1.656211	-1.278466	H
O-O2--0.567000	0	1.438106	-0.380837	-1.587520	H
C-CM--0.117000	0	0.073331	-1.326267	0.933545	H

O-O2--0.618000	0	1.741683	-2.524585	-2.072658	H
C-C--0.553000	0	-0.217829	0.149366	1.002869	H
O-O2--0.556000	0	0.095553	0.912126	0.017573	H
O-O2--0.607000	0	-0.737943	0.577160	2.063520	H
H-HC-0.049000	0	0.847527	-3.120378	0.210147	H
H-HC-0.162000	0	-0.341698	-1.886335	1.764864	H
O-OW--0.834000	-1	6.443935	2.943320	-1.171148	L
H-HW-0.417000	-1	6.815121	3.084508	-2.041288	L
H-HW-0.417000	-1	7.123865	3.242423	-0.567830	L
O-OW--0.834000	0	3.408267	7.067434	1.060348	L
H-HW-0.417000	0	3.253144	6.163698	1.405150	L
H-HW-0.417000	0	3.790066	6.874546	0.187043	L
O-OW--0.834000	0	-1.798835	-3.660094	2.052733	H
H-HW-0.417000	0	-1.231448	-4.272273	1.561076	H
H-HW-0.417000	0	-2.267135	-3.169594	1.338848	H
O-OW--0.834000	0	-4.813967	0.646101	-6.290349	L
H-HW-0.417000	0	-3.878487	0.435152	-6.156186	L
H-HW-0.417000	0	-5.268996	0.051068	-5.670957	L
H-HS-0.193300	0	2.555984	-0.238407	0.821363	H

TS2 '

C-CT--0.366200	-1	8.231073	4.645490	-8.131504	L
C-C-0.597200	-1	9.060723	3.900380	-7.091177	L
O-O--0.567900	-1	9.661584	2.862912	-7.372425	L
H-HC-0.112300	-1	7.787428	5.531163	-7.676847	L
H-HC-0.112300	-1	7.440126	3.992342	-8.501807	L
H-HC-0.112300	-1	8.872042	4.945873	-8.961236	L
N-N--0.415700	-1	9.054618	4.458375	-5.874063	L
C-CT--0.087500	-1	9.525126	3.782537	-4.657853	L
C-C-0.597300	-1	8.387396	2.884929	-4.167256	L
O-O--0.567900	-1	7.475796	3.344514	-3.464264	L
C-CT-0.298500	-1	10.006556	4.784486	-3.581391	L
C-CT--0.319200	-1	10.425277	4.084903	-2.282729	L
C-CT--0.319200	-1	11.221261	5.592785	-4.060047	L
H-H-0.271900	-1	8.469242	5.280385	-5.747030	L
H-H1-0.096900	-1	10.363025	3.141567	-4.911602	L
H-HC--0.029700	-1	9.209125	5.489939	-3.365394	L
H-HC-0.079100	-1	11.131516	3.286267	-2.511538	L
H-HC-0.079100	-1	9.554618	3.661444	-1.785777	L
H-HC-0.079100	-1	10.901224	4.792969	-1.606202	L
H-HC-0.079100	-1	12.081844	4.936251	-4.188257	L
H-HC-0.079100	-1	11.466691	6.363602	-3.327384	L
H-HC-0.079100	-1	11.003613	6.072519	-5.013301	L
N-N--0.415700	-1	8.404560	1.612423	-4.599345	L
C-CT--0.087500	-1	7.291613	0.660062	-4.425547	L
C-C-0.597300	-1	7.707253	-0.615703	-3.664450	L
O-O--0.567900	-1	8.853420	-1.066985	-3.788153	L
C-CT-0.298500	-1	6.639385	0.253305	-5.771347	L
C-CT--0.319200	-1	5.781918	1.379807	-6.359746	L
C-CT--0.319200	-1	7.633123	-0.197029	-6.847352	L
H-H-0.271900	-1	9.180381	1.306890	-5.192770	L
H-H1-0.096900	-1	6.520073	1.166638	-3.852737	L
H-HC--0.029700	-1	5.970292	-0.587743	-5.585886	L
H-HC-0.079100	-1	6.298834	2.336262	-6.283109	L

H-HC-0.079100	-1	4.846368	1.427087	-5.806952	L
H-HC-0.079100	-1	5.534532	1.164927	-7.400620	L
H-HC-0.079100	-1	8.233589	0.647792	-7.180610	L
H-HC-0.079100	-1	7.084400	-0.600022	-7.697573	L
H-HC-0.079100	-1	8.287302	-0.970012	-6.452187	L
N-N--0.254800	-1	6.770702	-1.222757	-2.897673	L
C-CT--0.026600	-1	6.902643	-2.575932	-2.351144	L
C-C-0.589600	-1	7.152089	-3.598973	-3.461114	L
O-O--0.574800	-1	6.406157	-3.646561	-4.442282	L
C-CT--0.007000	0	5.565318	-2.882795	-1.655044	L
C-CT-0.018900	0	4.945315	-1.514738	-1.397125	L
C-CT-0.019200	0	5.453016	-0.684111	-2.564206	L
H-H1-0.064100	-1	7.720446	-2.591131	-1.631534	L
H-HC-0.025300	0	4.901351	-3.442933	-2.315071	L
H-HC-0.025300	0	5.714685	-3.438946	-0.733860	L
H-HC-0.021300	0	5.322742	-1.093488	-0.470451	L
H-HC-0.021300	0	3.860405	-1.548807	-1.370358	L
H-H1-0.039100	0	5.501779	0.360410	-2.255244	L
H-H1-0.039100	0	4.778586	-0.798268	-3.414369	L
N-N--0.415700	-1	8.177076	-4.444595	-3.311838	L
C-CT--0.149000	-1	8.548088	-5.440231	-4.330149	L
H-H-0.271900	-1	8.775289	-4.322323	-2.495871	L
H-H1-0.097600	-1	7.805516	-5.440188	-5.127422	L
H-H1-0.097600	-1	8.589604	-6.429050	-3.872353	L
H-H1-0.097600	-1	9.525164	-5.190702	-4.743880	L
C-CT--0.366200	-1	5.249182	-7.425560	-4.089619	L
C-C-0.597200	-1	4.120748	-6.755122	-4.883306	L
O-O--0.567900	-1	3.223870	-7.473538	-5.334153	L
H-HC-0.112300	-1	5.960315	-6.668949	-3.758762	L
H-HC-0.112300	-1	5.758513	-8.151504	-4.723254	L
H-HC-0.112300	-1	4.829384	-7.932873	-3.220914	L
N-N--0.415700	-1	4.108654	-5.424272	-5.022147	L
C-CT-0.014300	-1	3.007183	-4.676990	-5.653749	L H-HC 69
C-C-0.597300	-1	2.815151	-5.017263	-7.166405	L
O-O--0.567900	-1	3.810812	-5.181016	-7.873050	L
C-CT--0.204100	0	3.315267	-3.181250	-5.418505	H
C-C-0.713000	0	2.174532	-2.253513	-5.828179	H
O-O--0.593100	0	1.958642	-1.959798	-6.999762	H
N-N--0.919100	0	1.460031	-1.735892	-4.792453	H
H-H-0.271900	-1	4.876149	-4.886513	-4.652947	L
H-H1-0.104800	-1	2.098979	-4.941289	-5.121775	L
H-HC-0.079700	0	4.191041	-2.928511	-6.026242	H
H-HC-0.079700	0	3.569432	-3.040743	-4.364203	H
H-H-0.419600	0	0.596521	-1.287434	-5.065981	H
H-H-0.419600	0	1.572408	-2.032431	-3.824579	H
N-N--0.415700	-1	1.562383	-5.116792	-7.661728	L
C-CT--0.149000	-1	1.212833	-5.376281	-9.088096	L
H-H-0.271900	-1	0.805892	-4.891913	-7.016508	L
H-H1-0.097600	-1	2.119561	-5.600659	-9.649298	L
H-H1-0.097600	-1	0.732467	-4.493286	-9.510495	L
H-H1-0.097600	-1	0.530284	-6.224163	-9.144769	L
C-CT--0.366200	-1	11.735560	-5.927598	-0.625839	L
C-C-0.597200	-1	10.718073	-6.054623	0.516153	L
O-O--0.567900	-1	11.033112	-5.899906	1.701287	L

H-HC-0.112300	-1	11.236361	-6.103170	-1.578629	L
H-HC-0.112300	-1	12.527687	-6.663423	-0.489882	L
H-HC-0.112300	-1	12.165906	-4.925942	-0.620391	L
N-N--0.415700	-1	9.482302	-6.359007	0.122645	L
C-CT--0.023700	-1	8.320702	-6.557401	0.984544	L
C-C-0.597300	-1	7.267960	-7.401149	0.278287	L
O-O--0.567900	-1	7.091289	-7.241859	-0.936390	L
C-CT-0.034200	0	7.714654	-5.197088	1.372996	L
C-CT-0.001800	0	6.779800	-5.215711	2.598854	L
S-S--0.273700	0	5.059477	-5.762520	2.354250	L
C-CT--0.053600	0	4.222768	-4.182397	2.007896	L
H-H-0.271900	-1	9.315336	-6.432459	-0.874868	L
H-H1-0.088000	-1	8.644017	-7.089476	1.867598	L
H-HC-0.024100	0	7.186650	-4.772616	0.519365	L
H-HC-0.024100	0	8.545488	-4.537406	1.605507	L
H-H1-0.044000	0	6.738032	-4.205056	3.005576	L
H-H1-0.044000	0	7.233195	-5.846756	3.363239	L
H-H1-0.068400	0	3.169698	-4.358154	1.781893	L
H-H1-0.068400	0	4.682512	-3.686005	1.156405	L
H-H1-0.068400	0	4.288011	-3.523596	2.874247	L
N-N--0.415700	-1	6.559058	-8.247458	1.035763	L
C-CT--0.149000	-1	5.338265	-8.953959	0.619535	L
H-H-0.271900	-1	6.873660	-8.379147	1.997043	L
H-H1-0.097600	-1	5.122610	-8.723124	-0.423182	L
H-H1-0.097600	-1	4.503174	-8.634364	1.243113	L
H-H1-0.097600	-1	5.485016	-10.027875	0.731047	L
C-CT--0.366200	-1	3.896138	-9.355922	4.898085	L
C-C-0.597200	-1	3.726521	-7.950360	5.509070	L
O-O--0.567900	-1	4.687564	-7.233864	5.804368	L
H-HC-0.112300	-1	2.914479	-9.797068	4.722318	L
H-HC-0.112300	-1	4.459452	-9.986445	5.585758	L
H-HC-0.112300	-1	4.433616	-9.279043	3.952793	L
N-N--0.415700	-1	2.464594	-7.536558	5.654380	L
C-CT--0.087500	-1	2.027477	-6.132148	5.601647	L
C-C-0.597300	-1	1.903200	-5.574619	7.025993	L
O-O--0.567900	-1	0.865266	-5.668607	7.696488	L
C-CT-0.298500	0	0.699134	-5.965512	4.834852	L
C-CT--0.319200	0	0.351289	-4.482738	4.662895	L
C-CT--0.319200	0	0.767971	-6.620565	3.448957	L
H-H-0.271900	-1	1.729388	-8.230620	5.496671	L
H-H1-0.096900	-1	2.793851	-5.558592	5.076733	L
H-HC--0.029700	0	-0.102817	-6.452516	5.391206	L
H-HC-0.079100	0	1.069530	-3.990374	4.004131	L
H-HC-0.079100	0	0.331370	-3.964754	5.620640	L
H-HC-0.079100	0	-0.640541	-4.391066	4.224477	L
H-HC-0.079100	0	1.611671	-6.209183	2.893551	L
H-HC-0.079100	0	-0.149739	-6.402089	2.900635	L
H-HC-0.079100	0	0.870602	-7.699226	3.534364	L
N-N--0.415700	-1	3.062406	-5.121969	7.503208	L
C-CT--0.149000	-1	3.437267	-4.988094	8.908276	L
H-H-0.271900	-1	3.822603	-5.038222	6.838576	L
H-H1-0.097600	-1	2.549698	-5.093770	9.532263	L
H-H1-0.097600	-1	3.882745	-4.007817	9.074099	L
H-H1-0.097600	-1	4.157894	-5.763920	9.167157	L

C-CT--0.366200	-1	12.485666	-4.241473	6.353008	L
C-C-0.597200	-1	12.283162	-3.517625	5.003341	L
O-O--0.567900	-1	13.251370	-3.300729	4.268108	L
H-HC-0.112300	-1	11.525604	-4.341831	6.859282	L
H-HC-0.112300	-1	13.165829	-3.661281	6.977804	L
H-HC-0.112300	-1	12.908352	-5.229543	6.175785	L
N-N--0.415700	-1	11.048474	-3.090947	4.699279	L
C-CT--0.023700	-1	10.773591	-2.265623	3.525408	L
C-C-0.597300	-1	11.342210	-0.843089	3.663657	L
O-O--0.567900	-1	12.072556	-0.377430	2.787133	L
C-CT-0.034200	0	9.267593	-2.186532	3.257294	L
C-CT-0.001800	0	9.031639	-1.517125	1.896613	L
S-S--0.273700	0	7.445305	-1.889770	1.128225	L
C-CT--0.053600	0	6.288188	-0.971865	2.173702	L
H-H-0.271900	-1	10.282610	-3.320070	5.326428	L
H-H1-0.088000	-1	11.245028	-2.744759	2.665628	L
H-HC-0.024100	0	8.760914	-1.620613	4.040156	L
H-HC-0.024100	0	8.863739	-3.194534	3.250093	L
H-H1-0.044000	0	9.800993	-1.859022	1.203177	L
H-H1-0.044000	0	9.132680	-0.435719	1.998427	L
H-H1-0.068400	0	5.264625	-1.152509	1.839501	L
H-H1-0.068400	0	6.489077	0.096334	2.095980	L
H-H1-0.068400	0	6.380134	-1.295059	3.208822	L
N-N--0.415700	-1	11.073749	-0.155569	4.779185	L
C-CT--0.149000	-1	11.628065	1.182270	5.010142	L
H-H-0.271900	-1	10.494217	-0.586582	5.498904	L
H-H1-0.097600	-1	12.217536	1.485074	4.144840	L
H-H1-0.097600	-1	12.264424	1.163912	5.894507	L
H-H1-0.097600	-1	10.814478	1.891429	5.162675	L
C-CT--0.366200	-1	6.208241	8.719341	-5.548465	L
C-C-0.597200	-1	6.521009	7.526126	-4.624008	L
O-O--0.567900	-1	6.671732	6.377918	-5.065315	L
H-HC-0.112300	-1	6.116776	9.627674	-4.951964	L
H-HC-0.112300	-1	5.271257	8.535817	-6.075564	L
H-HC-0.112300	-1	7.014563	8.840025	-6.272620	L
N-N--0.415700	-1	6.663333	7.840047	-3.326109	L
C-CT--0.001400	-1	6.702785	6.847394	-2.236899	L
C-C-0.597300	-1	5.326863	6.169249	-2.097965	L
O-O--0.567900	-1	4.453368	6.650050	-1.358618	L
C-CT--0.001400	-1	7.219806	7.478891	-0.931169	L
C-CA--0.001100	-1	7.903121	6.506044	0.023909	L
C-CA--0.190600	-1	9.310817	6.453905	0.075765	L
C-CA--0.190600	-1	7.155218	5.685022	0.892835	L
C-CA--0.234100	-1	9.959328	5.631685	1.016213	L
C-CA--0.234100	-1	7.808085	4.857708	1.833013	L
C-C-0.322600	-1	9.210434	4.853659	1.913285	L
O-OH--0.557900	-1	9.868978	4.106204	2.845680	L
H-H-0.271900	-1	6.600055	8.831788	-3.083468	L
H-H1-0.087600	-1	7.413218	6.074706	-2.516993	L
H-HC-0.029500	-1	7.946607	8.249571	-1.190786	L
H-HC-0.029500	-1	6.407588	7.986589	-0.409455	L
H-HA-0.169900	-1	9.898256	7.077645	-0.582917	L
H-HA-0.169900	-1	6.074252	5.692236	0.848312	L
H-HA-0.165600	-1	11.036492	5.600896	1.066380	L

H-HA-0.165600	-1	7.232112	4.225085	2.492447	L
H-HO-0.399200	-1	9.371452	3.882598	3.648361	L
N-N--0.415700	-1	5.114489	5.149376	-2.934359	L
C-CT-0.033700	-1	3.797624	4.656454	-3.323054	L
C-C-0.597300	-1	2.958964	4.019693	-2.203957	L
O-O--0.567900	-1	1.735775	4.122366	-2.273563	L
C-CT--0.182500	-1	3.986078	3.658701	-4.460646	L
H-H-0.271900	-1	5.897653	4.856022	-3.513263	L
H-H1-0.082300	-1	3.233060	5.502420	-3.716392	L
H-HC-0.060300	-1	3.015026	3.349806	-4.846670	L
H-HC-0.060300	-1	4.522106	2.789212	-4.080052	L
H-HC-0.060300	-1	4.557879	4.119864	-5.266061	L
N-N--0.415700	-1	3.571402	3.375939	-1.199538	L H-HC 209
C-CT-0.021300	0	2.782262	2.634366	-0.165148	H
C-C-0.597300	0	2.329022	3.634490	0.913130	H
O-O--0.567900	0	3.149726	4.380359	1.445908	H
C-CT--0.123100	0	3.664591	1.503171	0.407876	H
S-S--1.036000	0	2.874056	0.322129	1.602996	H
H-H-0.271900	-1	4.575193	3.350057	-1.190913	L
H-H1-0.112400	0	1.918917	2.181525	-0.658452	H
H-H1-0.111200	0	4.503858	1.944535	0.957765	H
H-H1-0.111200	0	4.089377	0.930645	-0.421736	H
N-N--0.415700	0	0.997065	3.648500	1.224142	H
C-CT--0.051800	0	0.433271	4.498852	2.286458	H
C-C-0.597300	0	0.811711	3.996686	3.716392	H
O-O--0.567900	0	1.356441	4.727418	4.543209	H
C-CT--0.110200	-1	-1.104731	4.631716	2.030005	H
C-CT-0.353100	-1	-1.963563	5.535640	2.940697	L H-HC 222
C-CT--0.412100	-1	-2.156157	4.987353	4.356125	L
C-CT--0.412100	-1	-1.431981	6.968935	3.031214	L
H-H-0.271900	0	0.394195	2.930064	0.822894	H
H-H1-0.092200	0	0.908078	5.481126	2.223320	H
H-HC-0.045700	0	-1.222205	5.010236	1.007341	H
H-HC-0.045700	0	-1.556856	3.636635	2.044023	H
H-HC--0.036100	-1	-2.954948	5.585104	2.491803	L
H-HC-0.100000	-1	-1.257445	5.127159	4.953210	L
H-HC-0.100000	-1	-2.401698	3.927213	4.313458	L
H-HC-0.100000	-1	-2.975376	5.520118	4.836601	L
H-HC-0.100000	-1	-0.470125	6.984249	3.544714	L
H-HC-0.100000	-1	-2.143689	7.587199	3.576959	L
H-HC-0.100000	-1	-1.307630	7.372681	2.025530	L
N-N--0.415700	0	0.529903	2.686125	3.978673	H
C-CT--0.087500	0	0.599720	2.145499	5.339603	H
C-C-0.597300	0	2.002703	2.114174	5.959666	H
O-O--0.567900	0	2.104820	2.090025	7.184022	H
C-CT-0.298500	-1	-0.021379	0.730574	5.371402	H
C-CT--0.319200	0	0.705770	-0.313072	4.499451	L H-HC 241
C-CT--0.319200	0	-0.208391	0.123643	6.762387	L H-HC 241
H-H-0.271900	0	0.045997	2.151755	3.259252	H
H-H1-0.096900	0	0.028987	2.805508	6.006664	H
H-HC--0.029700	0	-1.024147	0.823870	4.949736	H
H-HC-0.079100	0	1.683534	-0.555766	4.909382	L
H-HC-0.079100	0	0.846245	0.071196	3.489443	L
H-HC-0.079100	0	0.105051	-1.217278	4.420171	L

H-HC-0.079100	0	0.756685	-0.134270	7.196695	L
H-HC-0.079100	0	-0.815631	-0.777470	6.680263	L
H-HC-0.079100	0	-0.719725	0.840045	7.403385	L
N-N--0.415700	0	3.020189	1.923730	5.093872	H
C-CT-0.033700	0	4.383401	1.776979	5.559958	H
C-C-0.597300	-1	5.099075	3.107824	5.834685	L H-H1 254
O-O--0.567900	-1	6.273816	3.081878	6.191538	L
C-CT--0.182500	-1	5.158246	0.962469	4.527010	L H-H1 254
H-H-0.271900	0	2.857956	2.028998	4.101749	H
H-H1-0.082300	0	4.365056	1.230656	6.507259	H
H-HC-0.060300	-1	6.124649	0.668126	4.933654	L
H-HC-0.060300	-1	5.316094	1.565096	3.632820	L
H-HC-0.060300	-1	4.599506	0.061171	4.271658	L
N-N--0.415700	-1	4.397306	4.236805	5.671570	L
C-CT--0.087500	-1	4.781628	5.598377	6.070552	L
C-C-0.597300	-1	3.939487	6.044982	7.272823	L
O-O--0.567900	-1	4.491492	6.493115	8.278766	L
C-CT-0.298500	-1	4.568825	6.575876	4.897260	L
C-CT--0.319200	-1	4.964435	8.013456	5.251875	L
C-CT--0.319200	-1	5.386455	6.181217	3.667748	L
H-H-0.271900	-1	3.486195	4.124233	5.244610	L
H-H1-0.096900	-1	5.831408	5.625430	6.352776	L
H-HC--0.029700	-1	3.516575	6.565254	4.620689	L
H-HC-0.079100	-1	6.014805	8.049137	5.532624	L
H-HC-0.079100	-1	4.358064	8.389974	6.074946	L
H-HC-0.079100	-1	4.805231	8.654356	4.385022	L
H-HC-0.079100	-1	6.436287	6.101077	3.943827	L
H-HC-0.079100	-1	5.271263	6.930446	2.884907	L
H-HC-0.079100	-1	5.033126	5.225306	3.281112	L
N-N--0.415700	-1	2.607941	5.856181	7.217913	L
C-CT--0.149000	-1	1.700388	6.195025	8.324825	L
H-H-0.271900	-1	2.201216	5.477614	6.367982	L
H-H1-0.097600	-1	2.278036	6.587728	9.161678	L
H-H1-0.097600	-1	1.163124	5.300327	8.641022	L
H-H1-0.097600	-1	0.986413	6.948301	7.991906	L
C-CT--0.366200	-1	4.071663	10.302761	-0.977522	L
C-C-0.597200	-1	2.596578	9.978674	-1.223820	L
O-O--0.567900	-1	1.788415	10.894831	-1.295447	L
H-HC-0.112300	-1	4.645738	9.377858	-0.942812	L
H-HC-0.112300	-1	4.173489	10.829965	-0.029150	L
H-HC-0.112300	-1	4.444823	10.932028	-1.785175	L
N-N--0.415700	-1	2.216033	8.696373	-1.281980	L
C-CT--0.024900	-1	0.802061	8.316445	-1.124572	L
C-C-0.597300	-1	0.214949	8.812495	0.202541	L
O-O--0.567900	-1	-0.878699	9.381578	0.210631	L
C-CT-0.211700	0	0.628429	6.817279	-1.277402	L
O-OH--0.654600	0	0.924393	6.514035	-2.620794	L
H-H-0.271900	-1	2.917470	7.962825	-1.343322	L
H-H1-0.084300	-1	0.230807	8.768681	-1.931032	L
H-H1-0.035200	0	-0.397377	6.531132	-1.054025	L
H-H1-0.035200	0	1.305350	6.284785	-0.607736	L
H-HO-0.427500	0	1.025497	5.537908	-2.636565	L
N-N--0.415700	-1	0.976426	8.675072	1.298683	L
C-CT-0.033700	-1	0.622262	9.154620	2.635845	L

C-C-0.597300	-1	0.159571	10.616467	2.629347	L
O-O--0.567900	-1	-0.936756	10.935654	3.091830	L
C-CT--0.182500	-1	1.807825	8.914486	3.568114	L
H-H-0.271900	-1	1.864325	8.177688	1.193252	L
H-H1-0.082300	-1	-0.193636	8.562957	3.023990	L
H-HC-0.060300	-1	1.577671	9.283736	4.566845	L
H-HC-0.060300	-1	2.694314	9.415480	3.181396	L
H-HC-0.060300	-1	2.001496	7.844950	3.620904	L
N-N--0.415700	-1	0.959431	11.495384	2.015681	L
C-CT--0.149000	-1	0.621067	12.893751	1.824916	L
H-H-0.271900	-1	1.861804	11.186722	1.662122	L
H-H1-0.097600	-1	-0.365027	13.089462	2.247609	L
H-H1-0.097600	-1	0.611743	13.123923	0.760396	L
H-H1-0.097600	-1	1.360958	13.518440	2.326361	L
C-CT--0.366200	-1	-11.913918	4.583710	4.958757	L
C-C-0.597200	-1	-12.348093	3.165616	4.584779	L
O-O--0.567900	-1	-12.914858	2.457145	5.419131	L
H-HC-0.112300	-1	-11.433203	5.054193	4.100946	L
H-HC-0.112300	-1	-11.210476	4.541112	5.790421	L
H-HC-0.112300	-1	-12.787250	5.166252	5.250418	L
N-N--0.415700	-1	-12.013738	2.726141	3.371201	L
C-CT--0.087500	-1	-12.011211	1.304261	3.009850	L
C-C-0.597300	-1	-10.565413	0.908259	2.696590	L
O-O--0.567900	-1	-9.848755	1.552430	1.922878	L
C-CT-0.298500	-1	-13.007047	0.917055	1.884036	L
C-CT--0.319200	-1	-13.756280	-0.372848	2.266961	L
C-CT--0.319200	-1	-14.083730	1.966829	1.575601	L
H-H-0.271900	-1	-11.602148	3.377810	2.700594	L
H-H1-0.096900	-1	-12.305166	0.743882	3.894967	L
H-HC--0.029700	-1	-12.447814	0.727992	0.971412	L
H-HC-0.079100	-1	-14.389071	-0.191574	3.136461	L
H-HC-0.079100	-1	-13.041513	-1.166422	2.488443	L
H-HC-0.079100	-1	-14.392820	-0.685880	1.439558	L
H-HC-0.079100	-1	-14.717771	2.110625	2.446997	L
H-HC-0.079100	-1	-14.691101	1.632884	0.735769	L
H-HC-0.079100	-1	-13.625420	2.918933	1.317020	L
N-N--0.415700	-1	-10.103601	-0.113447	3.420209	L
C-CT--0.038900	-1	-8.695990	-0.512366	3.502702	L
C-C-0.597300	-1	-8.569708	-2.038145	3.613732	L
O-O--0.567900	-1	-9.501631	-2.698240	4.094848	L
C-CT-0.365400	-1	-7.979406	0.132314	4.713015	L
O-OH--0.676100	-1	-8.148889	-0.583886	5.914667	L
C-CT--0.243800	-1	-8.396546	1.568757	5.022397	L
H-H-0.271900	-1	-10.733994	-0.586562	4.051504	L
H-H1-0.100700	-1	-8.194763	-0.178091	2.594402	L
H-H1-0.004300	-1	-6.920196	0.131454	4.477352	L
H-HC-0.064200	-1	-8.438765	2.134838	4.099366	L
H-HC-0.064200	-1	-7.668362	2.023947	5.695014	L
H-HC-0.064200	-1	-9.380122	1.595584	5.490524	L
H-HO-0.410200	-1	-8.400188	0.054708	6.614232	L
N-N--0.254800	-1	-7.443966	-2.633472	3.180533	L
C-CT--0.026600	-1	-7.194620	-4.060019	3.348478	L
C-C-0.589600	-1	-6.587421	-4.416915	4.706499	L
O-O--0.574800	-1	-6.599933	-5.588294	5.067705	L

C-CT--0.007000	0	-6.202475	-4.398440	2.234621	L
C-CT-0.018900	0	-5.360849	-3.130054	2.110467	L
C-CT-0.019200	0	-6.368776	-2.017323	2.404243	L
H-H1-0.064100	-1	-8.105001	-4.629386	3.202516	L
H-HC-0.025300	0	-5.588645	-5.259920	2.490358	L
H-HC-0.025300	0	-6.742429	-4.574979	1.303547	L
H-HC-0.021300	0	-4.927530	-3.034998	1.115878	L
H-HC-0.021300	0	-4.574852	-3.130632	2.866092	L
H-H1-0.039100	0	-6.767346	-1.637622	1.463049	L
H-H1-0.039100	0	-5.882186	-1.213932	2.958813	L
N-N--0.415700	-1	-5.968538	-3.456705	5.401529	L
C-CT--0.001400	-1	-4.977983	-3.699812	6.461659	L
C-C-0.597300	-1	-5.527441	-4.484362	7.667554	L
O-O--0.567900	-1	-6.714035	-4.367513	7.977795	L
C-CT--0.001400	0	-4.455977	-2.367734	7.017077	L H-HA 373
C-CA--0.001100	0	-4.147508	-1.300792	5.990447	H
C-CA--0.190600	0	-3.279347	-1.569777	4.930944	H
C-CA--0.190600	0	-4.721446	-0.032222	6.106353	H
C-CA--0.234100	0	-2.995223	-0.583838	3.995388	H
C-CA--0.234100	0	-4.438770	0.965142	5.178395	H
C-C-0.322600	0	-3.569965	0.692072	4.117160	H
O-OH--0.557900	0	-3.325340	1.676213	3.223685	H
H-H-0.271900	-1	-6.034946	-2.517332	5.041160	L
H-H1-0.087600	-1	-4.153329	-4.268446	6.030478	L
H-HC-0.029500	0	-5.202610	-1.968836	7.706217	L
H-HC-0.029500	0	-3.549899	-2.557924	7.593748	L
H-HA-0.169900	0	-2.824592	-2.550424	4.812441	H
H-HA-0.169900	0	-5.397483	0.192539	6.932092	H
H-HA-0.165600	0	-2.303256	-0.775595	3.187913	H
H-HA-0.165600	0	-4.853491	1.964701	5.282287	H
H-HO-0.399200	0	-2.471885	1.504598	2.755692	H
N-N--0.415700	-1	-4.649786	-5.175690	8.421181	L
C-CT--0.149000	-1	-5.035477	-5.643478	9.769008	L
H-H-0.271900	-1	-3.654889	-5.169135	8.182199	L
H-H1-0.097600	-1	-6.119249	-5.592689	9.874682	L
H-H1-0.097600	-1	-4.566578	-5.010669	10.521771	L
H-H1-0.097600	-1	-4.705063	-6.673692	9.903843	L
C-CT--0.366200	-1	-0.471507	-10.784732	2.454038	L
C-C-0.597200	-1	-0.650785	-9.842514	1.250410	L
O-O--0.567900	-1	-1.759841	-9.666893	0.741033	L
H-HC-0.112300	-1	0.576263	-10.799812	2.750641	L
H-HC-0.112300	-1	-0.785516	-11.791381	2.176835	L
H-HC-0.112300	-1	-1.080475	-10.431724	3.286295	L
N-N--0.415700	-1	0.464107	-9.295943	0.748298	L
C-CT-0.014300	-1	0.421607	-8.277034	-0.299926	L H-HC 405
C-C-0.597300	-1	0.048766	-8.782751	-1.712278	L
O-O--0.567900	-1	-0.161357	-7.958713	-2.593041	L
C-CT--0.204100	0	1.734349	-7.460276	-0.308742	H
C-C-0.713000	0	1.446865	-5.954538	-0.418367	H
O-O--0.593100	0	0.844609	-5.394178	0.499006	H
N-N--0.919100	0	1.926121	-5.294453	-1.490361	H
H-H-0.271900	-1	1.346476	-9.484775	1.194870	L
H-H1-0.104800	-1	-0.380876	-7.604775	0.004207	L
H-HC-0.079700	0	2.397404	-7.841683	-1.094728	H

H-HC-0.079700	0	2.237175	-7.584767	0.654082	H
H-H-0.419600	0	1.769697	-4.277306	-1.571558	H
H-H-0.419600	0	2.317179	-5.801168	-2.272712	H
N-N--0.415700	-1	-0.048281	-10.095660	-1.951660	L
C-CT--0.149000	-1	-0.587899	-10.644503	-3.207838	L
H-H-0.271900	-1	0.060543	-10.746087	-1.165461	L
H-H1-0.097600	-1	-0.651297	-9.852584	-3.953420	L
H-H1-0.097600	-1	-1.581739	-11.054669	-3.028324	L
H-H1-0.097600	-1	0.070075	-11.434815	-3.571415	L
C-CT--0.366200	-1	-3.860753	-11.701995	-1.445061	L
C-C-0.597200	-1	-4.626574	-10.374754	-1.516212	L
O-O--0.567900	-1	-5.765041	-10.375630	-1.988619	L
H-HC-0.112300	-1	-2.877683	-11.530130	-1.005790	L
H-HC-0.112300	-1	-3.743446	-12.108182	-2.448738	L
H-HC-0.112300	-1	-4.415350	-12.408689	-0.828118	L
N-N--0.415700	-1	-3.998184	-9.248732	-1.138968	L
C-CT--0.087500	-1	-4.560408	-7.886847	-1.301053	L
C-C-0.597300	-1	-4.823358	-7.502452	-2.768216	L
O-O--0.567900	-1	-5.810980	-6.831219	-3.064036	L
C-CT-0.298500	-1	-3.652613	-6.812075	-0.647460	L
C-CT--0.319200	-1	-4.137747	-5.373285	-0.886826	L
C-CT--0.319200	-1	-3.639119	-6.950499	0.872483	L
H-H-0.271900	-1	-3.116903	-9.361227	-0.635963	L
H-H1-0.096900	-1	-5.521813	-7.864394	-0.789296	L
H-HC--0.029700	-1	-2.636764	-6.911044	-1.030508	L
H-HC-0.079100	-1	-5.173849	-5.275776	-0.561804	L
H-HC-0.079100	-1	-4.068187	-5.120517	-1.942201	L
H-HC-0.079100	-1	-3.510405	-4.667423	-0.340426	L
H-HC-0.079100	-1	-4.645904	-6.814830	1.250133	L
H-HC-0.079100	-1	-2.974874	-6.206110	1.313865	L
H-HC-0.079100	-1	-3.291619	-7.928655	1.173747	L
N-N--0.415700	-1	-3.976089	-7.902227	-3.724770	L
C-CT--0.149000	-1	-4.059707	-7.486271	-5.135585	L
H-H-0.271900	-1	-3.255516	-8.566511	-3.467875	L
H-H1-0.097600	-1	-4.876781	-6.774690	-5.257262	L
H-H1-0.097600	-1	-4.242518	-8.359919	-5.762794	L
H-H1-0.097600	-1	-3.122390	-7.016490	-5.432375	L
C-CT--0.366200	-1	-12.098055	3.690751	-1.337843	L
C-C-0.597200	-1	-10.995360	2.623136	-1.301203	L
O-O--0.567900	-1	-11.290276	1.440444	-1.147633	L
H-HC-0.112300	-1	-11.648107	4.673294	-1.480544	L
H-HC-0.112300	-1	-12.649567	3.676861	-0.397374	L
H-HC-0.112300	-1	-12.780658	3.480244	-2.161401	L
N-N--0.415700	-1	-9.738124	3.062229	-1.366873	L
C-CT--0.024900	-1	-8.556754	2.238341	-1.186582	L
C-C-0.597300	-1	-7.443902	3.101896	-0.587298	L
O-O--0.567900	-1	-6.789144	3.889844	-1.284100	L
C-CT-0.211700	0	-8.132104	1.588346	-2.501888	L
O-OH--0.654600	0	-7.221022	0.567193	-2.204021	L
H-H-0.271900	-1	-9.610224	4.058571	-1.436082	L
H-H1-0.084300	-1	-8.796263	1.445644	-0.479144	L
H-H1-0.035200	0	-7.679354	2.314112	-3.174400	L
H-H1-0.035200	0	-9.004120	1.143044	-2.982946	L
H-HO-0.427500	0	-6.298816	0.903237	-2.270349	L

N-N--0.415700	-1	-7.283455	3.026803	0.742791	L	
C-CT-0.021300	-1	-6.108348	3.640042	1.380344	L	
C-C-0.597300	-1	-4.820224	2.991964	0.847723	L	
O-O--0.567900	-1	-3.844003	3.679047	0.589128	L	
C-CT--0.123100	-1	-6.168128	3.502607	2.903244	L	
S-SH--0.311900	-1	-7.421081	4.610152	3.610263	L	
H-H-0.271900	-1	-7.945822	2.480758	1.290466	L	
H-H1-0.112400	-1	-6.078075	4.702203	1.132380	L	
H-H1-0.111200	-1	-5.197125	3.774048	3.320971	L	
H-H1-0.111200	-1	-6.386034	2.468002	3.167032	L	
H-HS-0.193300	-1	-8.462998	4.164163	2.899358	L	
N-N--0.415700	-1	-4.860112	1.673375	0.640608	L	H-HC 478
C-CT-0.021300	0	-3.658959	0.987934	0.091809	H	
C-C-0.597300	0	-3.638459	1.205068	-1.414987	H	
O-O--0.567900	0	-4.683936	1.252409	-2.068473	H	
C-CT--0.123100	0	-3.646826	-0.513196	0.449565	H	
S-SH--0.311900	0	-2.141856	-1.493877	-0.079487	H	
H-H-0.271900	-1	-5.712054	1.186153	0.845023	L	
H-H1-0.112400	0	-2.784042	1.459855	0.540856	H	
H-H1-0.111200	0	-4.448080	-1.040799	-0.083935	H	
H-H1-0.111200	0	-3.796825	-0.661887	1.518262	H	
H-HS-0.193300	0	0.444650	0.245970	-1.071389	H	
N-N--0.415700	0	-2.402847	1.292290	-1.977770	H	
C-CT--0.087500	0	-2.256455	1.386163	-3.418809	H	
C-C-0.597300	0	-2.191773	0.032795	-4.171987	H	
O-O--0.567900	0	-2.317975	0.052928	-5.394785	H	
C-CT-0.298500	-1	-1.099674	2.292960	-3.878113	H	
C-CT--0.319200	0	-1.232116	3.694713	-3.275735	L	H-HC 492
C-CT--0.319200	0	0.311668	1.788952	-3.583968	L	H-HC 492
H-H-0.271900	0	-1.589869	1.270051	-1.362880	H	
H-H1-0.096900	0	-3.195524	1.817137	-3.783858	H	
H-HC--0.029700	0	-1.188994	2.377719	-4.964576	H	
H-HC-0.079100	0	-1.061664	3.660336	-2.197192	L	
H-HC-0.079100	0	-2.228709	4.077242	-3.473366	L	
H-HC-0.079100	0	-0.504063	4.361568	-3.733859	L	
H-HC-0.079100	0	0.495299	1.840654	-2.511554	L	
H-HC-0.079100	0	1.035791	2.413249	-4.098029	L	
H-HC-0.079100	0	0.432206	0.765729	-3.930435	L	
N-N--0.415700	0	-1.951161	-1.082657	-3.436772	H	
C-CT--0.003100	0	-2.040108	-2.419703	-4.019769	H	
C-C-0.597300	0	-3.503056	-2.873838	-4.190715	H	
O-O--0.567900	0	-3.803944	-3.669250	-5.072621	H	
C-CT--0.003600	-1	-1.285286	-3.448767	-3.127344	H	
C-CT--0.064500	-1	-1.419049	-4.902381	-3.619242	L	H-HC 508
C-C-0.695100	-1	-0.544696	-5.240666	-4.811938	L	
O-O--0.608600	-1	-0.400930	-4.488859	-5.761115	L	
N-N--0.940700	-1	0.067872	-6.405073	-4.807284	L	
H-H-0.271900	0	-1.887581	-1.018720	-2.423252	H	
H-H1-0.085000	0	-1.625089	-2.384782	-5.030066	H	
H-HC-0.017100	0	-0.230294	-3.190193	-3.045422	H	
H-HC-0.017100	0	-1.711619	-3.408487	-2.121672	H	
H-HC-0.035200	-1	-2.447173	-5.156220	-3.861545	L	
H-HC-0.035200	-1	-1.135259	-5.551288	-2.798096	L	
H-H-0.425100	-1	0.671569	-6.653157	-5.571424	L	

H-H-0.425100	-1	-0.043175	-7.026685	-4.008123	L
N-N--0.415700	0	-4.342903	-2.486097	-3.165237	H
C-CT--0.023700	0	-5.723986	-2.946501	-3.248534	H
C-C-0.597300	-1	-6.398341	-2.325676	-4.488372	L H-H1 522
O-O--0.567900	-1	-6.226381	-1.130293	-4.745657	L
C-CT-0.034200	-1	-6.461245	-2.668849	-1.922262	L H-H1 522
C-CT-0.001800	-1	-7.929947	-3.116816	-1.980861	L
S-S--0.273700	-1	-8.835064	-3.091741	-0.406118	L
C-CT--0.053600	-1	-9.202517	-1.323698	-0.273107	L
H-H-0.271900	0	-4.257691	-1.519791	-2.887590	H
H-H1-0.088000	0	-5.658469	-4.023356	-3.365132	H
H-HC-0.024100	-1	-6.390299	-1.622782	-1.661349	L
H-HC-0.024100	-1	-5.968808	-3.222627	-1.126474	L
H-H1-0.044000	-1	-7.955549	-4.141984	-2.351629	L
H-H1-0.044000	-1	-8.469135	-2.489212	-2.690746	L
H-H1-0.068400	-1	-9.808667	-1.139415	0.613799	L
H-H1-0.068400	-1	-9.751856	-0.992986	-1.154787	L
H-H1-0.068400	-1	-8.272246	-0.764448	-0.200132	L
N-N--0.254800	-1	-7.147167	-3.093495	-5.301552	L
C-CT--0.026600	-1	-7.542951	-2.674870	-6.647151	L
C-C-0.589600	-1	-8.992379	-2.190314	-6.639133	L
O-O--0.574800	-1	-9.879190	-2.890713	-6.143934	L
C-CT--0.007000	-1	-7.336764	-3.917716	-7.527462	L
C-CT-0.018900	-1	-6.821510	-4.981969	-6.555325	L
C-CT-0.019200	-1	-7.354352	-4.523148	-5.224363	L
H-H1-0.064100	-1	-6.894897	-1.877819	-7.011101	L
H-HC-0.025300	-1	-8.271053	-4.237367	-7.980073	L
H-HC-0.025300	-1	-6.600688	-3.732608	-8.307518	L
H-HC-0.021300	-1	-5.733416	-4.974492	-6.528447	L
H-HC-0.021300	-1	-7.195952	-5.963974	-6.772779	L
H-H1-0.039100	-1	-6.830852	-5.032413	-4.426932	L
H-H1-0.039100	-1	-8.419980	-4.743284	-5.150881	L
N-N--0.415700	-1	-9.214880	-0.992890	-7.174493	L
C-CT--0.149000	-1	-10.448212	-0.223373	-6.984256	L
H-H-0.271900	-1	-8.409676	-0.523254	-7.588036	L
H-H1-0.097600	-1	-11.208952	-0.861611	-6.535357	L
H-H1-0.097600	-1	-10.801279	0.139451	-7.949525	L
H-H1-0.097600	-1	-10.249407	0.623485	-6.327043	L
C-CT--0.366200	-1	-10.330087	8.853389	-4.240033	L
C-C-0.597200	-1	-9.782149	7.563543	-3.615055	L
O-O--0.567900	-1	-10.225362	7.142468	-2.545207	L
H-HC-0.112300	-1	-9.811036	9.052145	-5.177581	L
H-HC-0.112300	-1	-10.171327	9.684676	-3.553651	L
H-HC-0.112300	-1	-11.396650	8.739502	-4.432906	L
N-N--0.415700	-1	-8.811105	6.941456	-4.278300	L
C-CT--0.024900	-1	-7.867407	6.022179	-3.638879	L
C-C-0.597300	-1	-6.537746	6.753556	-3.416098	L
O-O--0.567900	-1	-6.282332	7.761600	-4.082268	L
C-CT-0.211700	0	-7.644858	4.768463	-4.496956	L
O-OH--0.654600	0	-7.272334	5.080646	-5.826091	L
H-H-0.271900	-1	-8.539776	7.311283	-5.188401	L
H-H1-0.084300	-1	-8.253910	5.681893	-2.677832	L
H-H1-0.035200	0	-8.565232	4.183481	-4.515867	L
H-H1-0.035200	0	-6.859243	4.163308	-4.042141	L

H-HO-0.427500	0	-6.842683	4.307321	-6.209839	L
N-N--0.415700	-1	-5.660577	6.220578	-2.555070	L
C-CT-0.033700	-1	-4.286730	6.728886	-2.450417	L
C-C-0.597300	-1	-3.538403	6.734939	-3.802457	L
O-O--0.567900	-1	-2.638823	7.548725	-4.018083	L
C-CT--0.182500	-1	-3.533881	5.906014	-1.415080	L
H-H-0.271900	-1	-5.943931	5.414804	-1.992589	L
H-H1-0.082300	-1	-4.334074	7.755859	-2.086709	L
H-HC-0.060300	-1	-2.520253	6.287044	-1.308838	L
H-HC-0.060300	-1	-3.498933	4.860338	-1.718893	L
H-HC-0.060300	-1	-4.049911	5.988412	-0.459786	L
N-N--0.415700	-1	-3.959499	5.869533	-4.738529	L
C-CT--0.149000	-1	-3.443884	5.817565	-6.105388	L
H-H-0.271900	-1	-4.688283	5.220684	-4.472634	L
H-H1-0.097600	-1	-2.670173	6.575443	-6.230549	L
H-H1-0.097600	-1	-4.254929	6.008797	-6.807916	L
H-H1-0.097600	-1	-3.021440	4.831228	-6.296960	L
C-CM--0.139000	0	0.721602	-1.645520	0.307428	H
C-C-0.519000	0	1.034658	-1.579292	-1.102319	H
O-O2--0.567000	0	0.812434	-0.415875	-1.727292	H
C-CM--0.117000	0	-0.508755	-1.015708	0.907907	H
O-O2--0.618000	0	1.583796	-2.481848	-1.779024	H
C-C--0.553000	0	-0.564073	0.500446	1.032296	H
O-O2--0.556000	0	-0.232548	1.207152	0.022932	H
O-O2--0.607000	0	-1.005264	0.978560	2.112700	H
H-HC-0.049000	0	0.893546	-2.642869	0.704708	H
H-HC-0.162000	0	-0.676936	-1.474477	1.878205	H
O-OW--0.834000	-1	6.452402	2.947173	-1.172535	L
H-HW-0.417000	-1	6.824153	3.089589	-2.042233	L
H-HW-0.417000	-1	7.131372	3.246758	-0.568376	L
O-OW--0.834000	0	3.377469	7.006691	1.063062	L
H-HW-0.417000	0	3.235062	6.100490	1.405194	L
H-HW-0.417000	0	3.761199	6.824094	0.188760	L
O-OW--0.834000	0	-1.373517	-4.006800	1.832256	H
H-HW-0.417000	0	-0.654715	-4.488415	1.389521	H
H-HW-0.417000	0	-1.860351	-3.599407	1.099516	H
O-OW--0.834000	0	-4.973687	0.833221	-6.184211	L
H-HW-0.417000	0	-4.034715	0.617795	-6.070780	L
H-HW-0.417000	0	-5.414654	0.184641	-5.609272	L
H-HS-0.193300	0	1.861139	-0.673644	0.834813	H

IC2'

C-CT--0.366200	-1	8.243323	4.613958	-8.138787	L
C-C-0.597200	-1	9.071373	3.868890	-7.097155	L
O-O--0.567900	-1	9.670282	2.829828	-7.376674	L
H-HC-0.112300	-1	7.801310	5.501198	-7.685595	L
H-HC-0.112300	-1	7.451180	3.961753	-8.508190	L
H-HC-0.112300	-1	8.885000	4.911803	-8.968886	L
N-N--0.415700	-1	9.066147	4.428809	-5.880921	L
C-CT--0.087500	-1	9.535161	3.753980	-4.663574	L
C-C-0.597300	-1	8.395627	2.859335	-4.171753	L
O-O--0.567900	-1	7.484803	3.321776	-3.469631	L
C-CT-0.298500	-1	10.018346	4.756692	-3.588611	L
C-CT--0.319200	-1	10.435514	4.058346	-2.288783	L

C-CT--0.319200	-1	11.234680	5.561899	-4.068340	L
H-H-0.271900	-1	8.482334	5.252142	-5.755276	L
H-H1-0.096900	-1	10.371866	3.111000	-4.916180	L
H-HC--0.029700	-1	9.222241	5.464016	-3.373852	L
H-HC-0.079100	-1	11.140252	3.257995	-2.516222	L
H-HC-0.079100	-1	9.563963	3.637345	-1.791307	L
H-HC-0.079100	-1	10.912715	4.766558	-1.613293	L
H-HC-0.079100	-1	12.094019	4.903508	-4.195378	L
H-HC-0.079100	-1	11.481477	6.333393	-3.336849	L
H-HC-0.079100	-1	11.018107	6.040550	-5.022381	L
N-N--0.415700	-1	8.410411	1.586119	-4.601838	L
C-CT--0.087500	-1	7.295607	0.636176	-4.426724	L
C-C-0.597300	-1	7.708670	-0.639189	-3.663554	L
O-O--0.567900	-1	8.853986	-1.092868	-3.786362	L
C-CT-0.298500	-1	6.642812	0.228560	-5.771989	L
C-CT--0.319200	-1	5.787609	1.355782	-6.362296	L
C-CT--0.319200	-1	7.635854	-0.225377	-6.847123	L
H-H-0.271900	-1	9.185738	1.278163	-5.194656	L
H-H1-0.096900	-1	6.524953	1.145136	-3.854835	L
H-HC--0.029700	-1	5.972072	-0.610908	-5.585314	L
H-HC-0.079100	-1	6.306350	2.311361	-6.287078	L
H-HC-0.079100	-1	4.852063	1.405732	-5.809730	L
H-HC-0.079100	-1	5.539973	1.139744	-7.402872	L
H-HC-0.079100	-1	8.237996	0.617764	-7.181611	L
H-HC-0.079100	-1	7.086491	-0.628649	-7.696799	L
H-HC-0.079100	-1	8.288481	-0.998995	-6.450637	L
N-N--0.254800	-1	6.770832	-1.243234	-2.895977	L
C-CT--0.026600	-1	6.900081	-2.595799	-2.347301	L
C-C-0.589600	-1	7.147734	-3.621061	-3.455620	L
O-O--0.574800	-1	6.401870	-3.668756	-4.436833	L
C-CT--0.007000	0	5.560064	-2.900129	-1.653988	L
C-CT-0.018900	0	4.923539	-1.535710	-1.412591	L
C-CT-0.019200	0	5.451560	-0.701237	-2.568671	L
H-H1-0.064100	-1	7.717740	-2.611439	-1.627535	L
H-HC-0.025300	0	4.903629	-3.473146	-2.310558	L
H-HC-0.025300	0	5.708043	-3.446124	-0.726546	L
H-HC-0.021300	0	5.274107	-1.111121	-0.476306	L
H-HC-0.021300	0	3.837462	-1.581711	-1.414857	L
H-H1-0.039100	0	5.502366	0.341062	-2.251825	L
H-H1-0.039100	0	4.784920	-0.804610	-3.426264	L
N-N--0.415700	-1	8.171070	-4.468418	-3.304850	L
C-CT--0.149000	-1	8.540328	-5.466366	-4.321535	L
H-H-0.271900	-1	8.769387	-4.346015	-2.488978	L
H-H1-0.097600	-1	7.797883	-5.466147	-5.118928	L
H-H1-0.097600	-1	8.579868	-6.454541	-3.862179	L
H-H1-0.097600	-1	9.517946	-5.219367	-4.735498	L
C-CT--0.366200	-1	5.237569	-7.444963	-4.078418	L
C-C-0.597200	-1	4.110554	-6.773605	-4.873342	L
O-O--0.567900	-1	3.212368	-7.491001	-5.323206	L
H-HC-0.112300	-1	5.950104	-6.689203	-3.748636	L
H-HC-0.112300	-1	5.745603	-8.172881	-4.710829	L
H-HC-0.112300	-1	4.816658	-7.950101	-3.208986	L
N-N--0.415700	-1	4.101043	-5.442954	-5.014277	L
C-CT-0.014300	-1	3.001112	-4.694548	-5.647232	L H-HC 69

C-C-0.597300	-1	2.808666	-5.036828	-7.159380	L
O-O--0.567900	-1	3.804122	-5.203606	-7.865606	L
C-CT--0.204100	0	3.307992	-3.196587	-5.421852	H
C-C-0.713000	0	2.181764	-2.271333	-5.876540	H
O-O--0.593100	0	1.995780	-1.993469	-7.055467	H
N-N--0.919100	0	1.437090	-1.733860	-4.869098	H
H-H-0.271900	-1	4.869512	-4.906092	-4.645798	L
H-H1-0.104800	-1	2.092317	-4.956262	-5.114991	L
H-HC-0.079700	0	4.198550	-2.953674	-6.011340	H
H-HC-0.079700	0	3.539115	-3.043393	-4.364090	H
H-H-0.419600	0	0.578123	-1.296893	-5.175091	H
H-H-0.419600	0	1.521430	-2.029015	-3.902179	H
N-N--0.415700	-1	1.555787	-5.134724	-7.654751	L
C-CT--0.149000	-1	1.205966	-5.395784	-9.080764	L
H-H-0.271900	-1	0.799628	-4.907378	-7.010007	L
H-H1-0.097600	-1	2.112350	-5.622788	-9.641468	L
H-H1-0.097600	-1	0.727367	-4.512530	-9.504630	L
H-H1-0.097600	-1	0.521795	-6.242438	-9.136216	L
C-CT--0.366200	-1	11.726266	-5.954040	-0.615946	L
C-C-0.597200	-1	10.708354	-6.077312	0.526078	L
O-O--0.567900	-1	11.023503	-5.921339	1.711019	L
H-HC-0.112300	-1	11.226882	-6.130148	-1.568540	L
H-HC-0.112300	-1	12.516955	-6.691173	-0.478704	L
H-HC-0.112300	-1	12.158538	-4.953206	-0.612003	L
N-N--0.415700	-1	9.472064	-6.379937	0.132849	L
C-CT--0.023700	-1	8.309947	-6.574741	0.994871	L
C-C-0.597300	-1	7.255696	-7.417571	0.289770	L
O-O--0.567900	-1	7.079524	-7.259850	-0.925184	L
C-CT-0.034200	0	7.707328	-5.212345	1.381537	L
C-CT-0.001800	0	6.765972	-5.229695	2.602376	L
S-S--0.273700	0	5.043052	-5.761494	2.343097	L
C-CT--0.053600	0	4.221636	-4.170413	2.012812	L
H-H-0.271900	-1	9.305115	-6.454635	-0.864574	L
H-H1-0.088000	-1	8.632098	-7.106047	1.878813	L
H-HC-0.024100	0	7.185278	-4.784961	0.525654	L
H-HC-0.024100	0	8.539329	-4.555951	1.619137	L
H-H1-0.044000	0	6.729960	-4.220750	3.013984	L
H-H1-0.044000	0	7.209733	-5.868289	3.366168	L
H-H1-0.068400	0	3.171638	-4.335931	1.765626	L
H-H1-0.068400	0	4.699612	-3.661026	1.179180	L
H-H1-0.068400	0	4.277040	-3.528770	2.892698	L
N-N--0.415700	-1	6.545046	-8.261324	1.048461	L
C-CT--0.149000	-1	5.322963	-8.966126	0.633145	L
H-H-0.271900	-1	6.859241	-8.392105	2.009997	L
H-H1-0.097600	-1	5.107918	-8.736517	-0.409968	L
H-H1-0.097600	-1	4.488388	-8.643945	1.256085	L
H-H1-0.097600	-1	5.467629	-10.040146	0.746369	L
C-CT--0.366200	-1	3.879384	-9.358588	4.912088	L
C-C-0.597200	-1	3.712374	-7.951745	5.520836	L
O-O--0.567900	-1	4.674747	-7.236635	5.815164	L
H-HC-0.112300	-1	2.896905	-9.798122	4.736856	L
H-HC-0.112300	-1	4.441375	-9.989113	5.600843	L
H-HC-0.112300	-1	4.417161	-9.284230	3.966764	L
N-N--0.415700	-1	2.451224	-7.535287	5.665290	L

C-CT--0.087500	-1	2.016819	-6.130124	5.610280	L
C-C-0.597300	-1	1.893387	-5.570119	7.033728	L
O-O--0.567900	-1	0.855166	-5.661054	7.704200	L
C-CT-0.298500	0	0.695159	-5.957111	4.832140	L
C-CT--0.319200	0	0.342755	-4.473275	4.674211	L
C-CT--0.319200	0	0.781709	-6.586465	3.434171	L
H-H-0.271900	-1	1.714708	-8.228181	5.508553	L
H-H1-0.096900	-1	2.784377	-5.558868	5.084589	L
H-HC--0.029700	0	-0.110164	-6.455725	5.373137	L
H-HC-0.079100	0	1.081789	-3.963923	4.052688	L
H-HC-0.079100	0	0.284319	-3.974616	5.640696	L
H-HC-0.079100	0	-0.632285	-4.377272	4.199832	L
H-HC-0.079100	0	1.608558	-6.138717	2.881035	L
H-HC-0.079100	0	-0.144372	-6.389412	2.892273	L
H-HC-0.079100	0	0.919786	-7.662516	3.500781	L
N-N--0.415700	-1	3.053387	-5.118949	7.510418	L
C-CT--0.149000	-1	3.428280	-4.983587	8.915335	L
H-H-0.271900	-1	3.813848	-5.037710	6.845778	L
H-H1-0.097600	-1	2.540410	-5.086575	9.539343	L
H-H1-0.097600	-1	3.875616	-4.003910	9.079688	L
H-H1-0.097600	-1	4.147371	-5.760389	9.175551	L
C-CT--0.366200	-1	12.478506	-4.258393	6.360363	L
C-C-0.597200	-1	12.277609	-3.536279	5.009527	L
O-O--0.567900	-1	13.246351	-3.322403	4.274111	L
H-HC-0.112300	-1	11.518171	-4.356107	6.866639	L
H-HC-0.112300	-1	13.159683	-3.678529	6.984356	L
H-HC-0.112300	-1	12.899318	-5.247552	6.184762	L
N-N--0.415700	-1	11.043792	-3.107705	4.704594	L
C-CT--0.023700	-1	10.770685	-2.283699	3.529385	L
C-C-0.597300	-1	11.342017	-0.862047	3.665490	L
O-O--0.567900	-1	12.073398	-0.399173	2.788353	L
C-CT-0.034200	0	9.264488	-2.202038	3.258268	L
C-CT-0.001800	0	9.031198	-1.545173	1.890390	L
S-S--0.273700	0	7.435408	-1.899577	1.129770	L
C-CT--0.053600	0	6.298982	-0.940371	2.160752	L
H-H-0.271900	-1	10.277389	-3.334368	5.331980	L
H-H1-0.088000	-1	11.241335	-2.765093	2.670434	L
H-HC-0.024100	0	8.758919	-1.626955	4.035148	L
H-HC-0.024100	0	8.856745	-3.208541	3.260356	L
H-H1-0.044000	0	9.792598	-1.906906	1.198292	L
H-H1-0.044000	0	9.150062	-0.464410	1.979126	L
H-H1-0.068400	0	5.271176	-1.099206	1.827991	L
H-H1-0.068400	0	6.525470	0.121904	2.071591	L
H-H1-0.068400	0	6.382132	-1.253408	3.199657	L
N-N--0.415700	-1	11.074702	-0.172259	4.779892	L
C-CT--0.149000	-1	11.631556	1.164873	5.008835	L
H-H-0.271900	-1	10.494229	-0.601025	5.500193	L
H-H1-0.097600	-1	12.221746	1.465182	4.143155	L
H-H1-0.097600	-1	12.267736	1.146680	5.893332	L
H-H1-0.097600	-1	10.819311	1.875834	5.160122	L
C-CT--0.366200	-1	6.227922	8.695749	-5.562482	L
C-C-0.597200	-1	6.538247	7.503389	-4.636101	L
O-O--0.567900	-1	6.686831	6.354201	-5.075577	L
H-HC-0.112300	-1	6.138110	9.605193	-4.967425	L

H-HC-0.112300	-1	5.290672	8.513199	-6.089445	L
H-HC-0.112300	-1	7.034590	8.813744	-6.286695	L
N-N--0.415700	-1	6.680968	7.819075	-3.338672	L
C-CT--0.001400	-1	6.718337	6.828062	-2.247898	L
C-C-0.597300	-1	5.341089	6.152785	-2.108120	L
O-O--0.567900	-1	4.468405	6.636426	-1.369672	L
C-CT--0.001400	-1	7.236364	7.460615	-0.943078	L
C-CA--0.001100	-1	7.917654	6.487959	0.013638	L
C-CA--0.190600	-1	9.325239	6.433193	0.065804	L
C-CA--0.190600	-1	7.168036	5.669743	0.883732	L
C-CA--0.234100	-1	9.972017	5.611205	1.007649	L
C-CA--0.234100	-1	7.819159	4.842654	1.825315	L
C-C-0.322600	-1	9.221485	4.836033	1.905821	L
O-OH--0.557900	-1	9.878440	4.088779	2.839497	L
H-H-0.271900	-1	6.619561	8.811316	-3.097601	L
H-H1-0.087600	-1	7.427327	6.053570	-2.526662	L
H-HC-0.029500	-1	7.964688	8.229486	-1.203789	L
H-HC-0.029500	-1	6.425042	7.970694	-0.422295	L
H-HA-0.169900	-1	9.913983	7.054766	-0.593762	L
H-HA-0.169900	-1	6.087092	5.678968	0.839023	L
H-HA-0.165600	-1	11.049112	5.578424	1.058039	L
H-HA-0.165600	-1	7.241866	4.212178	2.485650	L
H-HO-0.399200	-1	9.380359	3.867393	3.642446	L
N-N--0.415700	-1	5.126889	5.132010	-2.942946	L
C-CT-0.033700	-1	3.809138	4.641010	-3.331079	L
C-C-0.597300	-1	2.969078	4.007624	-2.211119	L
O-O--0.567900	-1	1.746100	4.112541	-2.281083	L
C-CT--0.182500	-1	3.995853	3.641110	-4.467071	L
H-H-0.271900	-1	5.909577	4.836239	-3.521262	L
H-H1-0.082300	-1	3.246265	5.487442	-3.725838	L
H-HC-0.060300	-1	3.024270	3.333476	-4.852767	L
H-HC-0.060300	-1	4.530147	2.771191	-4.085025	L
H-HC-0.060300	-1	4.568668	4.099906	-5.273118	L
N-N--0.415700	-1	3.580116	3.364273	-1.205591	L H-HC 209
C-CT-0.021300	0	2.839129	2.684029	-0.110250	H
C-C-0.597300	0	2.331987	3.743631	0.870976	H
O-O--0.567900	0	3.090442	4.607313	1.306685	H
C-CT--0.123100	0	3.787200	1.687528	0.603169	H
S-S--1.036000	0	2.961941	0.562520	1.814168	H
H-H-0.271900	-1	4.583854	3.336473	-1.196761	L
H-H1-0.112400	0	2.009623	2.129605	-0.555786	H
H-H1-0.111200	0	4.566305	2.267985	1.114540	H
H-H1-0.111200	0	4.295610	1.085445	-0.162393	H
N-N--0.415700	0	1.011226	3.671794	1.228903	H
C-CT--0.051800	0	0.436958	4.509950	2.286208	H
C-C-0.597300	0	0.803544	4.007125	3.717731	H
O-O--0.567900	0	1.340942	4.739249	4.548721	H
C-CT--0.110200	-1	-1.094105	4.634118	2.021222	H
C-CT-0.353100	-1	-1.951344	5.541124	2.930347	L H-HC 222
C-CT--0.412100	-1	-2.145216	4.995434	4.346605	L
C-CT--0.412100	-1	-1.417019	6.973535	3.018699	L
H-H-0.271900	0	0.468081	2.874334	0.910661	H
H-H1-0.092200	0	0.910999	5.491623	2.223525	H
H-HC-0.045700	0	-1.210845	5.009010	0.997035	H

H-HC-0.045700	0	-1.546747	3.638859	2.038817	H
H-HC--0.036100	-1	-2.942559	5.591789	2.481216	L
H-HC-0.100000	-1	-1.246331	5.134449	4.943615	L
H-HC-0.100000	-1	-2.392789	3.935702	4.305565	L
H-HC-0.100000	-1	-2.963484	5.530528	4.826111	L
H-HC-0.100000	-1	-0.455215	6.987805	3.532330	L
H-HC-0.100000	-1	-2.127621	7.594023	3.563356	L
H-HC-0.100000	-1	-1.291732	7.375458	2.012402	L
N-N--0.415700	0	0.497694	2.705518	3.983898	H
C-CT--0.087500	0	0.605482	2.148806	5.331936	H
C-C-0.597300	0	2.019249	2.132612	5.931756	H
O-O--0.567900	0	2.121811	2.169166	7.159289	H
C-CT-0.298500	-1	-0.018795	0.736158	5.368918	H
C-CT--0.319200	0	0.688692	-0.305893	4.479339	L H-HC 241
C-CT--0.319200	0	-0.164595	0.128504	6.764738	L H-HC 241
H-H-0.271900	0	0.108579	2.139553	3.237914	H
H-H1-0.096900	0	0.047132	2.802713	6.015033	H
H-HC--0.029700	0	-1.032735	0.831968	4.974526	H
H-HC-0.079100	0	1.677443	-0.545278	4.864261	L
H-HC-0.079100	0	0.803513	0.078954	3.466768	L
H-HC-0.079100	0	0.088116	-1.211201	4.414423	L
H-HC-0.079100	0	0.814358	-0.116399	7.175129	L
H-HC-0.079100	0	-0.763716	-0.779318	6.698979	L
H-HC-0.079100	0	-0.667605	0.840277	7.417483	L
N-N--0.415700	0	3.030210	1.919111	5.071962	H
C-CT-0.033700	0	4.387655	1.772123	5.555840	H
C-C-0.597300	-1	5.106151	3.104277	5.829294	L H-H1 254
O-O--0.567900	-1	6.280784	3.076633	6.186377	L
C-CT--0.182500	-1	5.161403	0.956759	4.525000	L H-H1 254
H-H-0.271900	0	2.879614	1.828245	4.062754	H
H-H1-0.082300	0	4.371296	1.229344	6.507119	H
H-HC-0.060300	-1	6.127173	0.661197	4.932263	L
H-HC-0.060300	-1	5.320551	1.557675	3.629891	L
H-HC-0.060300	-1	4.600970	0.056138	4.270976	L
N-N--0.415700	-1	4.406580	4.234349	5.664289	L
C-CT--0.087500	-1	4.793458	5.595804	6.061193	L
C-C-0.597300	-1	3.951988	6.045918	7.262626	L
O-O--0.567900	-1	4.504694	6.494569	8.267952	L
C-CT-0.298500	-1	4.582724	6.571865	4.886334	L
C-CT--0.319200	-1	4.981041	8.009238	5.238752	L
C-CT--0.319200	-1	5.399789	6.173702	3.657577	L
H-H-0.271900	-1	3.495324	4.122858	5.237359	L
H-H1-0.096900	-1	5.843245	5.621280	6.343545	L
H-HC--0.029700	-1	3.530499	6.562833	4.609608	L
H-HC-0.079100	-1	6.031434	8.043338	5.519615	L
H-HC-0.079100	-1	4.375265	8.388215	6.061133	L
H-HC-0.079100	-1	4.823210	8.649079	4.370867	L
H-HC-0.079100	-1	6.449421	6.091977	3.933950	L
H-HC-0.079100	-1	5.286163	6.921919	2.873540	L
H-HC-0.079100	-1	5.044682	5.217865	3.272385	L
N-N--0.415700	-1	2.620089	5.859592	7.207796	L
C-CT--0.149000	-1	1.713016	6.201921	8.314027	L
H-H-0.271900	-1	2.212772	5.480473	6.358395	L
H-H1-0.097600	-1	2.291284	6.594828	9.150356	L

H-H1-0.097600	-1	1.173981	5.308758	8.631544	L
H-H1-0.097600	-1	1.000542	6.956045	7.979809	L
C-CT--0.366200	-1	4.093668	10.290461	-0.994378	L
C-C-0.597200	-1	2.618001	9.968824	-1.240408	L
O-O--0.567900	-1	1.811615	10.886421	-1.313604	L
H-HC-0.112300	-1	4.665957	9.364510	-0.958123	L
H-HC-0.112300	-1	4.196358	10.818957	-0.046821	L
H-HC-0.112300	-1	4.468167	10.917737	-1.802961	L
N-N--0.415700	-1	2.234998	8.687168	-1.296614	L
C-CT--0.024900	-1	0.820273	8.310209	-1.138838	L
C-C-0.597300	-1	0.233907	8.809473	0.187398	L
O-O--0.567900	-1	-0.858647	9.380671	0.194417	L
C-CT-0.211700	0	0.647325	6.810515	-1.285149	L
O-OH--0.654600	0	0.934273	6.502990	-2.629452	L
H-H-0.271900	-1	2.935033	7.952176	-1.356689	L
H-H1-0.084300	-1	0.250020	8.762275	-1.946100	L
H-H1-0.035200	0	-0.376463	6.523310	-1.053273	L
H-H1-0.035200	0	1.330917	6.282700	-0.618075	L
H-HO-0.427500	0	1.040086	5.527182	-2.641175	L
N-N--0.415700	-1	0.994943	8.672308	1.283880	L
C-CT-0.033700	-1	0.641490	9.154638	2.620228	L
C-C-0.597300	-1	0.181613	10.617361	2.611357	L
O-O--0.567900	-1	-0.914171	10.939383	3.073160	L
C-CT--0.182500	-1	1.826440	8.913690	3.553066	L
H-H-0.271900	-1	1.881899	8.173051	1.179373	L
H-H1-0.082300	-1	-0.175607	8.565157	3.009171	L
H-HC-0.060300	-1	1.596837	9.284951	4.551178	L
H-HC-0.060300	-1	2.713953	9.412369	3.165704	L
H-HC-0.060300	-1	2.018045	7.843868	3.607567	L
N-N--0.415700	-1	0.983260	11.493773	1.996442	L
C-CT--0.149000	-1	0.647617	12.892485	1.803424	L
H-H-0.271900	-1	1.885094	11.182818	1.643513	L
H-H1-0.097600	-1	-0.338165	13.090758	2.225648	L
H-H1-0.097600	-1	0.638906	13.121001	0.738542	L
H-H1-0.097600	-1	1.388630	13.516537	2.304007	L
C-CT--0.366200	-1	-11.903831	4.611512	4.948289	L
C-C-0.597200	-1	-12.340674	3.193670	4.576470	L
O-O--0.567900	-1	-12.908934	2.487602	5.411842	L
H-HC-0.112300	-1	-11.422075	5.079720	4.089818	L
H-HC-0.112300	-1	-11.200604	4.568867	5.780132	L
H-HC-0.112300	-1	-12.776088	5.196190	5.238893	L
N-N--0.415700	-1	-12.006973	2.751645	3.363638	L
C-CT--0.087500	-1	-12.007125	1.329196	3.004523	L
C-C-0.597300	-1	-10.562041	0.929921	2.692120	L
O-O--0.567900	-1	-9.844022	1.571496	1.917513	L
C-CT-0.298500	-1	-13.003523	0.942137	1.879157	L
C-CT--0.319200	-1	-13.755300	-0.345719	2.263988	L
C-CT--0.319200	-1	-14.078137	1.993495	1.568899	L
H-H-0.271900	-1	-11.594023	3.401466	2.692076	L
H-H1-0.096900	-1	-12.302298	0.770777	3.890471	L
H-HC--0.029700	-1	-12.444510	0.750565	0.966922	L
H-HC-0.079100	-1	-14.387879	-0.161860	3.133100	L
H-HC-0.079100	-1	-13.042094	-1.140317	2.486833	L
H-HC-0.079100	-1	-14.392308	-0.658824	1.436974	L

H-HC-0.079100	-1	-14.712038	2.139880	2.439965	L
H-HC-0.079100	-1	-14.686016	1.659398	0.729494	L
H-HC-0.079100	-1	-13.617954	2.944308	1.308895	L
N-N--0.415700	-1	-10.102311	-0.091534	3.417420	L
C-CT--0.038900	-1	-8.695483	-0.493029	3.500766	L
C-C-0.597300	-1	-8.572154	-2.018871	3.614216	L
O-O--0.567900	-1	-9.505422	-2.676415	4.096217	L
C-CT-0.365400	-1	-7.977853	0.152173	4.710182	L
O-OH--0.676100	-1	-8.148904	-0.561809	5.912929	L
C-CT--0.243800	-1	-8.392276	1.589902	5.017237	L
H-H-0.271900	-1	-10.733713	-0.562441	4.049355	L
H-H1-0.100700	-1	-8.193469	-0.161146	2.592023	L
H-H1-0.004300	-1	-6.918607	0.148906	4.474691	L
H-HC-0.064200	-1	-8.433260	2.154610	4.093310	L
H-HC-0.064200	-1	-7.663326	2.044747	5.689256	L
H-HC-0.064200	-1	-9.375875	1.619356	5.485162	L
H-HO-0.410200	-1	-8.399085	0.078367	6.611450	L
N-N--0.254800	-1	-7.447491	-2.617043	3.182135	L
C-CT--0.026600	-1	-7.200918	-4.043800	3.352362	L
C-C-0.589600	-1	-6.594623	-4.399731	4.711040	L
O-O--0.574800	-1	-6.609445	-5.570512	5.074085	L
C-CT--0.007000	0	-6.208712	-4.385855	2.239766	L
C-CT-0.018900	0	-5.364502	-3.119310	2.114702	L
C-CT-0.019200	0	-6.371062	-2.004368	2.404762	L
H-H1-0.064100	-1	-8.112369	-4.611644	3.207147	L
H-HC-0.025300	0	-5.596824	-5.248234	2.497107	L
H-HC-0.025300	0	-6.748345	-4.562455	1.308514	L
H-HC-0.021300	0	-4.929803	-3.027427	1.120508	L
H-HC-0.021300	0	-4.579496	-3.119368	2.871506	L
H-H1-0.039100	0	-6.768605	-1.626715	1.462321	L
H-H1-0.039100	0	-5.883653	-1.200049	2.957277	L
N-N--0.415700	-1	-5.974003	-3.439620	5.404661	L
C-CT--0.001400	-1	-4.984086	-3.682966	6.465332	L
C-C-0.597300	-1	-5.535245	-4.464561	7.672370	L
O-O--0.567900	-1	-6.721661	-4.344941	7.982235	L
C-CT--0.001400	0	-4.468231	-2.352031	7.030083	L H-HA 373
C-CA--0.001100	0	-4.169958	-1.277256	6.011156	H
C-CA--0.190600	0	-3.297976	-1.536022	4.953752	H
C-CA--0.190600	0	-4.754338	-0.014004	6.131409	H
C-CA--0.234100	0	-3.022855	-0.545445	4.021923	H
C-CA--0.234100	0	-4.480280	0.988551	5.206067	H
C-C-0.322600	0	-3.610337	0.723911	4.144546	H
O-OH--0.557900	0	-3.377920	1.708912	3.246613	H
H-H-0.271900	-1	-6.038547	-2.500689	5.042805	L
H-H1-0.087600	-1	-4.160459	-4.253863	6.035179	L
H-HC-0.029500	0	-5.214811	-1.961188	7.723989	L
H-HC-0.029500	0	-3.559350	-2.541124	7.602706	L
H-HA-0.169900	0	-2.831885	-2.511730	4.838527	H
H-HA-0.169900	0	-5.431168	0.202506	6.958480	H
H-HA-0.165600	0	-2.318583	-0.719177	3.222497	H
H-HA-0.165600	0	-4.902061	1.984679	5.313258	H
H-HO-0.399200	0	-2.515451	1.554655	2.796114	H
N-N--0.415700	-1	-4.659041	-5.156390	8.427224	L
C-CT--0.149000	-1	-5.045846	-5.621316	9.775722	L

H-H-0.271900	-1	-3.664096	-5.152125	8.188394	L
H-H1-0.097600	-1	-6.129535	-5.568276	9.881141	L
H-H1-0.097600	-1	-4.575851	-4.988228	10.527565	L
H-H1-0.097600	-1	-4.717437	-6.651950	9.912230	L
C-CT--0.366200	-1	-0.490613	-10.782833	2.469582	L
C-C-0.597200	-1	-0.667887	-9.842165	1.264446	L
O-O--0.567900	-1	-1.776522	-9.665211	0.754613	L
H-HC-0.112300	-1	0.557078	-10.799463	2.766377	L
H-HC-0.112300	-1	-0.806514	-11.789311	2.193910	L
H-HC-0.112300	-1	-1.099033	-10.427347	3.301184	L
N-N--0.415700	-1	0.448134	-9.298530	0.761655	L
C-CT-0.014300	-1	0.407763	-8.281189	-0.288176	L H-HC 405
C-C-0.597300	-1	0.034173	-8.788409	-1.699791	L
O-O--0.567900	-1	-0.174223	-7.965354	-2.581882	L
C-CT--0.204100	0	1.718734	-7.465648	-0.291810	H
C-C-0.713000	0	1.422605	-5.971896	-0.467474	H
O-O--0.593100	0	0.755844	-5.382826	0.386050	H
N-N--0.919100	0	1.963544	-5.341471	-1.528680	H
H-H-0.271900	-1	1.330068	-9.488357	1.208667	L
H-H1-0.104800	-1	-0.393474	-7.606911	0.014771	L
H-HC-0.079700	0	2.403010	-7.872513	-1.045253	H
H-HC-0.079700	0	2.195149	-7.552010	0.688581	H
H-H-0.419600	0	1.782949	-4.339646	-1.650409	H
H-H-0.419600	0	2.402996	-5.863536	-2.273857	H
N-N--0.415700	-1	-0.065361	-10.101503	-1.937125	L
C-CT--0.149000	-1	-0.605835	-10.651282	-3.192527	L
H-H-0.271900	-1	0.042087	-10.750902	-1.149887	L
H-H1-0.097600	-1	-0.667591	-9.860415	-3.939362	L
H-H1-0.097600	-1	-1.600491	-11.059252	-3.012529	L
H-H1-0.097600	-1	0.050675	-11.443428	-3.554755	L
C-CT--0.366200	-1	-3.880998	-11.699702	-1.428619	L
C-C-0.597200	-1	-4.644252	-10.371104	-1.501981	L
O-O--0.567900	-1	-5.782644	-10.370532	-1.974571	L
H-HC-0.112300	-1	-2.897670	-11.529039	-0.989460	L
H-HC-0.112300	-1	-3.764314	-12.107691	-2.431638	L
H-HC-0.112300	-1	-4.437050	-12.404358	-0.810657	L
N-N--0.415700	-1	-4.013757	-9.245701	-1.126405	L
C-CT--0.087500	-1	-4.573333	-7.882993	-1.290721	L
C-C-0.597300	-1	-4.835310	-7.500400	-2.758531	L
O-O--0.567900	-1	-5.821592	-6.827734	-3.055564	L
C-CT-0.298500	-1	-3.663576	-6.808944	-0.638673	L
C-CT--0.319200	-1	-4.145903	-5.369601	-0.880377	L
C-CT--0.319200	-1	-3.650591	-6.945004	0.881489	L
H-H-0.271900	-1	-3.132774	-9.359100	-0.623082	L
H-H1-0.096900	-1	-5.534773	-7.857887	-0.779157	L
H-HC--0.029700	-1	-2.647859	-6.910470	-1.021399	L
H-HC-0.079100	-1	-5.181867	-5.269589	-0.555677	L
H-HC-0.079100	-1	-4.075688	-5.118627	-1.936137	L
H-HC-0.079100	-1	-3.517292	-4.664089	-0.334985	L
H-HC-0.079100	-1	-4.657173	-6.806805	1.258763	L
H-HC-0.079100	-1	-2.984984	-6.201200	1.321808	L
H-HC-0.079100	-1	-3.305022	-7.923353	1.184348	L
N-N--0.415700	-1	-3.988659	-7.903307	-3.714317	L
C-CT--0.149000	-1	-4.071252	-7.489412	-5.125797	L

H-H-0.271900	-1	-3.269407	-8.568572	-3.456261	L
H-H1-0.097600	-1	-4.886937	-6.776451	-5.248726	L
H-H1-0.097600	-1	-4.255646	-8.363690	-5.751663	L
H-H1-0.097600	-1	-3.132986	-7.021899	-5.423173	L
C-CT--0.366200	-1	-12.088685	3.709011	-1.346930	L
C-C-0.597200	-1	-10.988052	2.639336	-1.308433	L
O-O--0.567900	-1	-11.285268	1.457456	-1.153051	L
H-HC-0.112300	-1	-11.636825	4.690462	-1.491101	L
H-HC-0.112300	-1	-12.640373	3.697661	-0.406528	L
H-HC-0.112300	-1	-12.771561	3.498524	-2.170266	L
N-N--0.415700	-1	-9.729962	3.075906	-1.374588	L
C-CT--0.024900	-1	-8.550209	2.250031	-1.192812	L
C-C-0.597300	-1	-7.435793	3.112384	-0.594705	L
O-O--0.567900	-1	-6.779408	3.897975	-1.292638	L
C-CT-0.211700	0	-8.128727	1.599279	-2.508943	L
O-OH--0.654600	0	-7.232611	0.564839	-2.213245	L
H-H-0.271900	-1	-9.600134	4.071890	-1.445343	L
H-H1-0.084300	-1	-8.791355	1.458909	-0.484167	L
H-H1-0.035200	0	-7.664567	2.321537	-3.177431	L
H-H1-0.035200	0	-9.004613	1.166984	-2.994827	L
H-HO-0.427500	0	-6.305445	0.887632	-2.275060	L
N-N--0.415700	-1	-7.275702	3.039075	0.735526	L
C-CT-0.021300	-1	-6.099518	3.651052	1.372304	L
C-C-0.597300	-1	-4.812559	2.999662	0.840912	L
O-O--0.567900	-1	-3.834978	3.684457	0.581395	L
C-CT--0.123100	-1	-6.159806	3.516127	2.895410	L
S-SH--0.311900	-1	-7.410737	4.627190	3.600482	L
H-H-0.271900	-1	-7.939205	2.495166	1.283950	L
H-H1-0.112400	-1	-6.067163	4.712763	1.122677	L
H-H1-0.111200	-1	-5.188349	3.786356	3.312867	L
H-H1-0.111200	-1	-6.379743	2.482360	3.160787	L
H-HS-0.193300	-1	-8.453397	4.182091	2.890112	L
N-N--0.415700	-1	-4.854951	1.680828	0.635863	L H-HC 478
C-CT-0.021300	0	-3.656003	0.988879	0.089468	H
C-C-0.597300	0	-3.638094	1.191018	-1.420425	H
O-O--0.567900	0	-4.684773	1.207455	-2.072779	H
C-CT--0.123100	0	-3.663028	-0.509187	0.457580	H
S-SH--0.311900	0	-2.214108	-1.535593	-0.116637	H
H-H-0.271900	-1	-5.707861	1.195567	0.840906	L
H-H1-0.112400	0	-2.779842	1.458942	0.536757	H
H-H1-0.111200	0	-4.489611	-1.022834	-0.048903	H
H-H1-0.111200	0	-3.776926	-0.653115	1.531449	H
H-HS-0.193300	0	0.603373	0.281497	-0.855454	H
N-N--0.415700	0	-2.405238	1.295243	-1.986919	H
C-CT--0.087500	0	-2.263800	1.391133	-3.430583	H
C-C-0.597300	0	-2.195550	0.034104	-4.180024	H
O-O--0.567900	0	-2.314129	0.045182	-5.402262	H
C-CT-0.298500	-1	-1.092609	2.286074	-3.883216	H
C-CT--0.319200	0	-1.221606	3.699771	-3.311363	L H-HC 492
C-CT--0.319200	0	0.291184	1.749478	-3.506815	L H-HC 492
H-H-0.271900	0	-1.589198	1.291186	-1.373653	H
H-H1-0.096900	0	-3.201297	1.823891	-3.797185	H
H-HC--0.029700	0	-1.140075	2.343771	-4.973304	H
H-HC-0.079100	0	-1.078470	3.684618	-2.228508	L

H-HC-0.079100	0	-2.208009	4.091306	-3.539670	L
H-HC-0.079100	0	-0.472797	4.347342	-3.763642	L
H-HC-0.079100	0	0.430935	1.830628	-2.428874	L
H-HC-0.079100	0	1.058762	2.330050	-4.009564	L
H-HC-0.079100	0	0.397770	0.708628	-3.802610	L
N-N--0.415700	0	-1.939829	-1.079564	-3.439330	H
C-CT--0.003100	0	-2.041417	-2.420514	-4.015573	H
C-C-0.597300	0	-3.505876	-2.869493	-4.185064	H
O-O--0.567900	0	-3.805651	-3.670596	-5.060830	H
C-CT--0.003600	-1	-1.289391	-3.454100	-3.123459	H
C-CT--0.064500	-1	-1.425869	-4.908226	-3.613087	L H-HC 508
C-C-0.695100	-1	-0.551980	-5.250066	-4.805111	L
O-O--0.608600	-1	-0.406616	-4.500029	-5.755444	L
N-N--0.940700	-1	0.058347	-6.415640	-4.798529	L
H-H-0.271900	0	-1.938804	-1.011703	-2.424790	H
H-H1-0.085000	0	-1.626382	-2.391435	-5.025700	H
H-HC-0.017100	0	-0.234330	-3.199663	-3.049731	H
H-HC-0.017100	0	-1.710738	-3.413467	-2.115916	H
H-HC-0.035200	-1	-2.454441	-5.160466	-3.855159	L
H-HC-0.035200	-1	-1.143459	-5.556385	-2.790879	L
H-H-0.425100	-1	0.661688	-6.666087	-5.562178	L
H-H-0.425100	-1	-0.054023	-7.035780	-3.998409	L
N-N--0.415700	0	-4.347171	-2.472678	-3.161209	H
C-CT--0.023700	0	-5.726933	-2.941844	-3.246021	H
C-C-0.597300	-1	-6.400057	-2.323315	-4.487074	L H-H1 522
O-O--0.567900	-1	-6.225755	-1.128672	-4.746210	L
C-CT-0.034200	-1	-6.464027	-2.662331	-1.920438	L H-H1 522
C-CT-0.001800	-1	-7.933580	-3.107564	-1.978571	L
S-S--0.273700	-1	-8.838898	-3.078272	-0.404017	L
C-CT--0.053600	-1	-9.202969	-1.309318	-0.273845	L
H-H-0.271900	0	-4.283459	-1.494535	-2.918015	H
H-H1-0.088000	0	-5.657809	-4.018526	-3.361833	H
H-HC-0.024100	-1	-6.391111	-1.615994	-1.661159	L
H-HC-0.024100	-1	-5.972785	-3.215804	-1.123702	L
H-H1-0.044000	-1	-7.961094	-4.133261	-2.347732	L
H-H1-0.044000	-1	-8.471448	-2.480039	-2.689530	L
H-H1-0.068400	-1	-9.808904	-1.122477	0.612673	L
H-H1-0.068400	-1	-9.751530	-0.978937	-1.156132	L
H-H1-0.068400	-1	-8.271635	-0.751745	-0.201598	L
N-N--0.254800	-1	-7.150228	-3.090969	-5.299168	L
C-CT--0.026600	-1	-7.544992	-2.673699	-6.645487	L
C-C-0.589600	-1	-8.993487	-2.186343	-6.638467	L
O-O--0.574800	-1	-9.881722	-2.884255	-6.142310	L
C-CT--0.007000	-1	-7.341057	-3.918321	-7.523810	L
C-CT-0.018900	-1	-6.828008	-4.982034	-6.549921	L
C-CT-0.019200	-1	-7.360177	-4.520097	-5.219767	L
H-H1-0.064100	-1	-6.895348	-1.878469	-7.010585	L
H-HC-0.025300	-1	-8.275887	-4.236885	-7.976070	L
H-HC-0.025300	-1	-6.604503	-3.735857	-8.304037	L
H-HC-0.021300	-1	-5.739903	-4.976608	-6.522877	L
H-HC-0.021300	-1	-7.204302	-5.963657	-6.765891	L
H-H1-0.039100	-1	-6.837784	-5.029114	-4.421450	L
H-H1-0.039100	-1	-8.426237	-4.738068	-5.146111	L
N-N--0.415700	-1	-9.213599	-0.989337	-7.175744	L

C-CT--0.149000	-1	-10.445476	-0.217150	-6.986916	L
H-H-0.271900	-1	-8.407426	-0.521901	-7.589894	L
H-H1-0.097600	-1	-11.207516	-0.853217	-6.537139	L
H-H1-0.097600	-1	-10.797693	0.144834	-7.952812	L
H-H1-0.097600	-1	-10.245147	0.630355	-6.331002	L
C-CT--0.366200	-1	-10.310324	8.863670	-4.256943	L
C-C-0.597200	-1	-9.764969	7.573756	-3.629849	L
O-O--0.567900	-1	-10.209161	7.155217	-2.559413	L
H-HC-0.112300	-1	-9.790743	9.059953	-5.194718	L
H-HC-0.112300	-1	-10.150074	9.695729	-3.571842	L
H-HC-0.112300	-1	-11.377074	8.751532	-4.449810	L
N-N--0.415700	-1	-8.795019	6.948761	-4.291960	L
C-CT--0.024900	-1	-7.853193	6.028677	-3.650942	L
C-C-0.597300	-1	-6.522162	6.757844	-3.429094	L
O-O--0.567900	-1	-6.264703	7.764346	-4.096806	L
C-CT-0.211700	0	-7.633087	4.773206	-4.507052	L
O-OH--0.654600	0	-7.260456	5.082490	-5.836844	L
H-H-0.271900	-1	-8.522833	7.316635	-5.202595	L
H-H1-0.084300	-1	-8.240502	5.690646	-2.689423	L
H-H1-0.035200	0	-8.554470	4.189767	-4.524653	L
H-H1-0.035200	0	-6.848341	4.167510	-4.051512	L
H-HO-0.427500	0	-6.834494	4.307052	-6.220336	L
N-N--0.415700	-1	-5.646158	6.224533	-2.567087	L
C-CT-0.033700	-1	-4.271351	6.730361	-2.463011	L
C-C-0.597300	-1	-3.522799	6.732850	-3.814937	L
O-O--0.567900	-1	-2.621620	7.544562	-4.031697	L
C-CT--0.182500	-1	-3.520252	5.907671	-1.426260	L
H-H-0.271900	-1	-5.931151	5.420191	-2.003387	L
H-H1-0.082300	-1	-4.316778	7.757994	-2.100924	L
H-HC-0.060300	-1	-2.505909	6.286917	-1.320453	L
H-HC-0.060300	-1	-3.487268	4.861453	-1.728424	L
H-HC-0.060300	-1	-4.036275	5.992563	-0.471180	L
N-N--0.415700	-1	-3.945410	5.866784	-4.749716	L
C-CT--0.149000	-1	-3.429679	5.811676	-6.116409	L
H-H-0.271900	-1	-4.675484	5.219758	-4.482920	L
H-H1-0.097600	-1	-2.654491	6.567866	-6.242636	L
H-H1-0.097600	-1	-4.240243	6.003364	-6.819368	L
H-H1-0.097600	-1	-3.009103	4.824229	-6.306362	L
C-CM--0.139000	0	0.563279	-1.820344	0.344870	H
C-C-0.519000	0	1.032504	-1.587566	-1.077962	H
O-O2--0.567000	0	1.059946	-0.357182	-1.519595	H
C-CM--0.117000	0	-0.694483	-1.110247	0.902801	H
O-O2--0.618000	0	1.472795	-2.501721	-1.789385	H
C-C--0.553000	0	-0.632188	0.414950	1.048991	H
O-O2--0.556000	0	-0.253453	1.104655	0.043830	H
O-O2--0.607000	0	-1.081230	0.898533	2.113449	H
H-HC-0.049000	0	0.468542	-2.893673	0.505897	H
H-HC-0.162000	0	-0.870158	-1.563755	1.876205	H
O-OW--0.834000	-1	6.460280	2.930007	-1.177446	L
H-HW-0.417000	-1	6.832444	3.070341	-2.047306	L
H-HW-0.417000	-1	7.139730	3.229236	-0.573649	L
O-OW--0.834000	0	3.506461	7.194729	1.041644	L
H-HW-0.417000	0	3.299904	6.297668	1.376871	L
H-HW-0.417000	0	3.873923	6.983366	0.166362	L

O-OW--0.834000	0	-1.442720	-4.088899	1.799959	H
H-HW-0.417000	0	-0.753406	-4.630393	1.380261	H
H-HW-0.417000	0	-1.983272	-3.786076	1.055669	H
O-OW--0.834000	0	-4.974362	0.831661	-6.189546	L
H-HW-0.417000	0	-4.036130	0.612629	-6.078692	L
H-HW-0.417000	0	-5.416659	0.185315	-5.613072	L
H-HS-0.193300	0	1.405576	-1.434009	0.956451	H

TS3'

C-CT--0.366200	-1	8.24716700	4.60817400	-8.13764700	L
C-C-0.597200	-1	9.07468800	3.86301600	-7.09565800	L
O-O--0.567900	-1	9.67327300	2.82367000	-7.37481300	L
H-HC-0.112300	-1	7.80537900	5.49567500	-7.68474900	L
H-HC-0.112300	-1	7.45486800	3.95618700	-8.50710100	L
H-HC-0.112300	-1	8.88915400	4.90560000	-8.96765600	L
N-N--0.415700	-1	9.06938200	4.42319500	-5.87954500	L
C-CT--0.087500	-1	9.53785100	3.74844900	-4.66194200	L
C-C-0.597300	-1	8.39786400	2.85433800	-4.17020400	L
O-O--0.567900	-1	7.48704500	3.31726900	-3.46839800	L
C-CT-0.298500	-1	10.02115500	4.75120900	-3.58707700	L
C-CT--0.319200	-1	10.43775000	4.05298200	-2.28700100	L
C-CT--0.319200	-1	11.23790700	5.55585700	-4.06668600	L
H-H-0.271900	-1	8.48584800	5.24677500	-5.75421400	L
H-H1-0.096900	-1	10.37437500	3.10510100	-4.91421100	L
H-HC--0.029700	-1	9.22526500	5.45887700	-3.37265900	L
H-HC-0.079100	-1	11.14224200	3.25231900	-2.51410100	L
H-HC-0.079100	-1	9.56592300	3.63241400	-1.78964400	L
H-HC-0.079100	-1	10.91505600	4.76116000	-1.61154700	L
H-HC-0.079100	-1	12.09702800	4.89711600	-4.19337900	L
H-HC-0.079100	-1	11.48481900	6.32741400	-3.33530000	L
H-HC-0.079100	-1	11.02174200	6.03438600	-5.02088100	L
N-N--0.415700	-1	8.41227200	1.58102500	-4.60001400	L
C-CT--0.087500	-1	7.29707000	0.63153700	-4.42496500	L
C-C-0.597300	-1	7.70947300	-0.64382000	-3.66142500	L
O-O--0.567900	-1	8.85464700	-1.09795600	-3.78386300	L
C-CT-0.298500	-1	6.64444400	0.22388000	-5.77029900	L
C-CT--0.319200	-1	5.78980600	1.35129800	-6.36105000	L
C-CT--0.319200	-1	7.63757200	-0.23065800	-6.84509900	L
H-H-0.271900	-1	9.18762500	1.27265200	-5.19258100	L
H-H1-0.096900	-1	6.52647100	1.14090800	-3.85336800	L
H-HC--0.029700	-1	5.97334500	-0.61529600	-5.58360600	L
H-HC-0.079100	-1	6.30888700	2.30669700	-6.28591200	L
H-HC-0.079100	-1	4.85414600	1.40171600	-5.80871900	L
H-HC-0.079100	-1	5.54233700	1.13513100	-7.40164000	L
H-HC-0.079100	-1	8.24011100	0.61218500	-7.17962300	L
H-HC-0.079100	-1	7.08826100	-0.63390500	-7.69482100	L
H-HC-0.079100	-1	8.28981300	-1.00443700	-6.44829300	L
N-N--0.254800	-1	6.77122300	-1.24735000	-2.89394400	L
C-CT--0.026600	-1	6.89983400	-2.59984700	-2.34494900	L
C-C-0.589600	-1	7.14736600	-3.62543800	-3.45299100	L
O-O--0.574800	-1	6.40171900	-3.67306100	-4.43437200	L
C-CT--0.007000	0	5.56258600	-2.91010800	-1.65209900	L
C-CT-0.018900	0	4.91673500	-1.55014900	-1.42036800	L
C-CT-0.019200	0	5.44964800	-0.70906000	-2.57007800	L

H-H1-0.064100	-1	7.71731400	-2.61564000	-1.62498500	L
H-HC-0.025300	0	4.91085000	-3.49179900	-2.30580200	L
H-HC-0.025300	0	5.71312600	-3.44921800	-0.72108500	L
H-HC-0.021300	0	5.25007900	-1.12354100	-0.47853000	L
H-HC-0.021300	0	3.83291700	-1.61214800	-1.43882800	L
H-H1-0.039100	0	5.49750000	0.33204800	-2.24877400	L
H-H1-0.039100	0	4.78702300	-0.80933700	-3.43106700	L
N-N--0.415700	-1	8.17034800	-4.47314700	-3.30179600	L
C-CT--0.149000	-1	8.53947500	-5.47144900	-4.31818100	L
H-H-0.271900	-1	8.76851600	-4.35079500	-2.48580700	L
H-H1-0.097600	-1	7.79722000	-5.47112100	-5.11575100	L
H-H1-0.097600	-1	8.57853300	-6.45954100	-3.85860500	L
H-H1-0.097600	-1	9.51728400	-5.22490600	-4.73196200	L
C-CT--0.366200	-1	5.23591600	-7.44875400	-4.07543300	L
C-C-0.597200	-1	4.10934200	-6.77714200	-4.87076900	L
O-O--0.567900	-1	3.21099500	-7.49429700	-5.32069500	L
H-HC-0.112300	-1	5.94865500	-6.69319200	-3.74564100	L
H-HC-0.112300	-1	5.74382700	-8.17699800	-4.70756800	L
H-HC-0.112300	-1	4.81460600	-7.95354900	-3.20599400	L
N-N--0.415700	-1	4.10036500	-5.44651800	-5.01198900	L
C-CT-0.014300	-1	3.00086500	-4.69783200	-5.64536600	L H-HC 69 0.0000
C-C-0.597300	-1	2.80865300	-5.04036400	-7.15748800	L
O-O--0.567900	-1	3.80421400	-5.20766500	-7.86344000	L
C-CT--0.204100	0	3.30286000	-3.19827600	-5.41943500	H
C-C-0.713000	0	2.18714800	-2.27428100	-5.90460100	H
O-O--0.593100	0	2.02564600	-2.00917700	-7.08987000	H
N-N--0.919100	0	1.42102900	-1.72352900	-4.92019800	H
H-H-0.271900	-1	4.86894700	-4.90986600	-4.64344100	L
H-H1-0.104800	-1	2.09184600	-4.95909300	-5.11328700	L
H-HC-0.079700	0	4.20490100	-2.95802100	-5.99226900	H
H-HC-0.079700	0	3.51327000	-3.04104400	-4.35787200	H
H-H-0.419600	0	0.56812100	-1.29230300	-5.25165800	H
H-H-0.419600	0	1.48641600	-2.00015000	-3.94696600	H
N-N--0.415700	-1	1.55585600	-5.13789400	-7.65313700	L
C-CT--0.149000	-1	1.20627700	-5.39912600	-9.07917800	L
H-H-0.271900	-1	0.79962800	-4.91012700	-7.00862300	L
H-H1-0.097600	-1	2.11271000	-5.62659000	-9.63961700	L
H-H1-0.097600	-1	0.72811200	-4.51578200	-9.50334700	L
H-H1-0.097600	-1	0.52180200	-6.24553500	-9.13461400	L
C-CT--0.366200	-1	11.72434300	-5.95953000	-0.61172600	L
C-C-0.597200	-1	10.70611200	-6.08217900	0.53008000	L
O-O--0.567900	-1	11.02103700	-5.92607100	1.71506300	L
H-HC-0.112300	-1	11.22512000	-6.13565500	-1.56440200	L
H-HC-0.112300	-1	12.51472300	-6.69693200	-0.47413900	L
H-HC-0.112300	-1	12.15699000	-4.95885900	-0.60789300	L
N-N--0.415700	-1	9.46980300	-6.38442300	0.13662000	L
C-CT--0.023700	-1	8.30740700	-6.57860700	0.99840600	L
C-C-0.597300	-1	7.25300700	-7.42119100	0.29323200	L
O-O--0.567900	-1	7.07718500	-7.26366300	-0.92179800	L
C-CT-0.034200	0	7.70594100	-5.21549300	1.38446200	L
C-CT-0.001800	0	6.76046200	-5.23235800	2.60202900	L
S-S--0.273700	0	5.03649600	-5.75630500	2.33426100	L
C-CT--0.053600	0	4.22162900	-4.15953700	2.01491800	L
H-H-0.271900	-1	9.30306400	-6.45926900	-0.86082700	L

H-H1-0.088000	-1	8.62914700	-7.10984600	1.88253700	L
H-HC-0.024100	0	7.18751800	-4.78647300	0.52724700	L
H-HC-0.024100	0	8.53821800	-4.56066600	1.62538500	L
H-H1-0.044000	0	6.72707600	-4.22438700	3.01623800	L
H-H1-0.044000	0	7.19874700	-5.87492900	3.36564700	L
H-H1-0.068400	0	3.17216400	-4.31950400	1.76186000	L
H-H1-0.068400	0	4.70476400	-3.64382700	1.18808700	L
H-H1-0.068400	0	4.27539300	-3.52614200	2.90082700	L
N-N--0.415700	-1	6.54186000	-8.26451600	1.05193200	L
C-CT--0.149000	-1	5.31961100	-8.96894700	0.63647400	L
H-H-0.271900	-1	6.85577600	-8.39521000	2.01357100	L
H-H1-0.097600	-1	5.10490100	-8.73947900	-0.40674000	L
H-H1-0.097600	-1	4.48500800	-8.64632000	1.25914600	L
H-H1-0.097600	-1	5.46384700	-10.04299700	0.74996100	L
C-CT--0.366200	-1	3.87486200	-9.35995700	4.91515500	L
C-C-0.597200	-1	3.70823400	-7.95292200	5.52356400	L
O-O--0.567900	-1	4.67080600	-7.23811100	5.81797000	L
H-HC-0.112300	-1	2.89226100	-9.79916000	4.73978100	L
H-HC-0.112300	-1	4.43645200	-9.99054700	5.60417800	L
H-HC-0.112300	-1	4.41289300	-9.28600200	3.96994400	L
N-N--0.415700	-1	2.44720800	-7.53595900	5.66762700	L
C-CT--0.087500	-1	2.01334200	-6.13064600	5.61221500	L
C-C-0.597300	-1	1.88978000	-5.57029200	7.03551400	L
O-O--0.567900	-1	0.85136600	-5.66069300	7.70575700	L
C-CT-0.298500	0	0.69192800	-5.95728100	4.83334500	L
C-CT--0.319200	0	0.33908400	-4.47358700	4.67509000	L
C-CT--0.319200	0	0.77890800	-6.58562000	3.43487200	L
H-H-0.271900	-1	1.71046800	-8.22861000	5.51086200	L
H-H1-0.096900	-1	2.78124000	-5.55979000	5.08658600	L
H-HC--0.029700	0	-0.11362600	-6.45620000	5.37372000	L
H-HC-0.079100	0	1.07966900	-3.96343600	4.05614800	L
H-HC-0.079100	0	0.27749900	-3.97566700	5.64178300	L
H-HC-0.079100	0	-0.63458800	-4.37776300	4.19766800	L
H-HC-0.079100	0	1.60595200	-6.13754900	2.88228600	L
H-HC-0.079100	0	-0.14695400	-6.38795700	2.89270600	L
H-HC-0.079100	0	0.91685300	-7.66172800	3.50091000	L
N-N--0.415700	-1	3.04983600	-5.11945600	7.51238600	L
C-CT--0.149000	-1	3.42444400	-4.98393500	8.91736300	L
H-H-0.271900	-1	3.81048600	-5.03864400	6.84791000	L
H-H1-0.097600	-1	2.53638700	-5.08645700	9.54118100	L
H-H1-0.097600	-1	3.87210900	-4.00439100	9.08161500	L
H-H1-0.097600	-1	4.14318100	-5.76095200	9.17791700	L
C-CT--0.366200	-1	12.47555300	-4.26268300	6.36440200	L
C-C-0.597200	-1	12.27524900	-3.54078100	5.01336400	L
O-O--0.567900	-1	13.24424700	-3.32742500	4.27813400	L
H-HC-0.112300	-1	11.51505900	-4.35992900	6.87046900	L
H-HC-0.112300	-1	13.15679700	-3.68294200	6.98843400	L
H-HC-0.112300	-1	12.89603400	-5.25203800	6.18911200	L
N-N--0.415700	-1	11.04166600	-3.11180800	4.70804500	L
C-CT--0.023700	-1	10.76915000	-2.28795000	3.53259500	L
C-C-0.597300	-1	11.34098300	-0.86648300	3.66853500	L
O-O--0.567900	-1	12.07274700	-0.40407100	2.79147400	L
C-CT-0.034200	0	9.26300000	-2.20565900	3.25964300	L
C-CT-0.001800	0	9.03209100	-1.55487300	1.88823200	L

S-S--0.273700	0	7.43214100	-1.89940000	1.13083100	L
C-CT--0.053600	0	6.30577500	-0.91802600	2.15178300	L
H-H-0.271900	-1	10.27502800	-3.33805000	5.33529600	L
H-H1-0.088000	-1	11.23982300	-2.76970400	2.67385900	L
H-HC-0.024100	0	8.75743800	-1.62628600	4.03332400	L
H-HC-0.024100	0	8.85369700	-3.21154300	3.26586000	L
H-H1-0.044000	0	9.78942500	-1.92700800	1.19719900	L
H-H1-0.044000	0	9.16040900	-0.47467400	1.97031600	L
H-H1-0.068400	0	5.27662600	-1.06414700	1.81687000	L
H-H1-0.068400	0	6.54800100	0.14032700	2.05763800	L
H-H1-0.068400	0	6.38183200	-1.22696100	3.19242300	L
N-N--0.415700	-1	11.07366000	-0.17635800	4.78272600	L
C-CT--0.149000	-1	11.63096200	1.16061300	5.01151800	L
H-H-0.271900	-1	10.49285500	-0.60475400	5.50298000	L
H-H1-0.097600	-1	12.22147100	1.46051600	4.14591500	L
H-H1-0.097600	-1	12.26692400	1.14236900	5.89617100	L
H-H1-0.097600	-1	10.81894700	1.87191200	5.16246000	L
C-CT--0.366200	-1	6.23268300	8.69126800	-5.56269200	L
C-C-0.597200	-1	6.54233800	7.49898900	-4.63598300	L
O-O--0.567900	-1	6.69059700	6.34965200	-5.07517900	L
H-HC-0.112300	-1	6.14307000	9.60087300	-4.96785000	L
H-HC-0.112300	-1	5.29548900	8.50895800	-6.08984000	L
H-HC-0.112300	-1	7.03956900	8.80880600	-6.28673700	L
N-N--0.415700	-1	6.68486900	7.81489800	-3.33858700	L
C-CT--0.001400	-1	6.72160400	6.82410300	-2.24759400	L
C-C-0.597300	-1	5.34407000	6.14937200	-2.10800100	L
O-O--0.567900	-1	4.47139000	6.63349800	-1.36986500	L
C-CT--0.001400	-1	7.23955700	7.45673900	-0.94278400	L
C-CA--0.001100	-1	7.92025300	6.48403000	0.01430100	L
C-CA--0.190600	-1	9.32780400	6.42874700	0.06681600	L
C-CA--0.190600	-1	7.17012000	5.66628100	0.88439000	L
C-CA--0.234100	-1	9.97404900	5.60671700	1.00899000	L
C-CA--0.234100	-1	7.82070600	4.83914800	1.82630500	L
C-C-0.322600	-1	9.22301100	4.83201800	1.90714700	L
O-OH--0.557900	-1	9.87946200	4.08471500	2.84113900	L
H-H-0.271900	-1	6.62377600	8.80721300	-3.09774200	L
H-H1-0.087600	-1	7.43037100	6.04928500	-2.52602300	L
H-HC-0.029500	-1	7.96823100	8.22528100	-1.20348500	L
H-HC-0.029500	-1	6.42830200	7.96723300	-0.42230400	L
H-HA-0.169900	-1	9.91694000	7.04995900	-0.59274200	L
H-HA-0.169900	-1	6.08919000	5.67590200	0.83942100	L
H-HA-0.165600	-1	11.05111900	5.57354200	1.05964500	L
H-HA-0.165600	-1	7.24301800	4.20903000	2.48663600	L
H-HO-0.399200	-1	9.38110700	3.86368800	3.64401600	L
N-N--0.415700	-1	5.12968600	5.12850100	-2.94266100	L
C-CT-0.033700	-1	3.81184300	4.63791200	-3.33100500	L
C-C-0.597300	-1	2.97127700	4.00508100	-2.21111100	L
O-O--0.567900	-1	1.74835500	4.11044100	-2.28139000	L
C-CT--0.182500	-1	3.99845400	3.63770100	-4.46674000	L
H-H-0.271900	-1	5.91240000	4.83231300	-3.52072700	L
H-H1-0.082300	-1	3.24938200	5.48447200	-3.72607900	L
H-HC-0.060300	-1	3.02684800	3.33035000	-4.85260300	L
H-HC-0.060300	-1	4.53233000	2.76766300	-4.08438100	L
H-HC-0.060300	-1	4.57163400	4.09611100	-5.27274700	L

N-N--0.415700	-1	3.58183700	3.36171300	-1.20530300	L H-H1 209	0.0000
C-CT-0.021300	0	2.83631900	2.69495400	-0.11355100	H	
C-C-0.597300	0	2.33400300	3.74702900	0.87840200	H	
O-O--0.567900	0	3.09943800	4.59638300	1.33065600	H	
C-CT--0.123100	0	3.77431200	1.68241200	0.58443600	H	
S-S--1.036000	0	2.90923800	0.53841800	1.74340500	H	
H-H-0.271900	-1	4.58555900	3.33353900	-1.19622500	L	
H-H1-0.112400	0	1.99256600	2.17117800	-0.56786700	H	
H-H1-0.111200	0	4.54331800	2.24892100	1.12542300	H	
H-H1-0.111200	0	4.29653600	1.09742900	-0.18518200	H	
N-N--0.415700	0	1.01199700	3.67790700	1.22601500	H	
C-CT--0.051800	0	0.43728800	4.51234300	2.28621800	H	
C-C-0.597300	0	0.80591500	4.00361900	3.71499600	H	
O-O--0.567900	0	1.35570200	4.72970700	4.54370400	H	
C-CT--0.110200	-1	-1.09268200	4.63400200	2.02012600	H	
C-CT-0.353100	-1	-1.94979800	5.54152100	2.92885100	L H-HC 222	0.0000
C-CT--0.412100	-1	-2.14421300	4.99620500	4.34517900	L	
C-CT--0.412100	-1	-1.41495500	6.97375000	3.01702700	L	
H-H-0.271900	0	0.45828800	2.88964900	0.89486900	H	
H-H1-0.092200	0	0.90996100	5.49511800	2.22832900	H	
H-HC-0.045700	0	-1.20939300	5.00849100	0.99583700	H	
H-HC-0.045700	0	-1.54457500	3.63842400	2.03752400	H	
H-HC--0.036100	-1	-2.94088500	5.59246200	2.47947300	L	
H-HC-0.100000	-1	-1.24541700	5.13500900	4.94237500	L	
H-HC-0.100000	-1	-2.39217300	3.93655700	4.30430500	L	
H-HC-0.100000	-1	-2.96239400	5.53170800	4.82437600	L	
H-HC-0.100000	-1	-0.45326800	6.98776800	3.53088500	L	
H-HC-0.100000	-1	-2.12545500	7.59462100	3.56138200	L	
H-HC-0.100000	-1	-1.28927700	7.37541200	2.01067400	L	
N-N--0.415700	0	0.49580100	2.70280100	3.98011100	H	
C-CT--0.087500	0	0.60111500	2.15038900	5.33059100	H	
C-C-0.597300	0	2.01469500	2.13599600	5.93104600	H	
O-O--0.567900	0	2.12012500	2.17257100	7.15767900	H	
C-CT-0.298500	-1	-0.01963500	0.73634900	5.36890700	H	
C-CT--0.319200	0	0.68967300	-0.30337100	4.47777600	L H-HC 241	0.0000
C-CT--0.319200	0	-0.15928900	0.12518400	6.76395800	L H-HC 241	0.0000
H-H-0.271900	0	0.06301000	2.14805400	3.24720300	H	
H-H1-0.096900	0	0.04172000	2.80398900	6.01346900	H	
H-HC--0.029700	0	-1.03397500	0.82840400	4.97546000	H	
H-HC-0.079100	0	1.67417100	-0.55007900	4.86873200	L	
H-HC-0.079100	0	0.81487900	0.08637100	3.46864600	L	
H-HC-0.079100	0	0.08482000	-1.20508300	4.40276700	L	
H-HC-0.079100	0	0.82140200	-0.11851800	7.17083100	L	
H-HC-0.079100	0	-0.75693200	-0.78364200	6.69804300	L	
H-HC-0.079100	0	-0.66170700	0.83447400	7.41983100	L	
N-N--0.415700	0	3.02719800	1.91825900	5.07178100	H	
C-CT-0.033700	0	4.38551200	1.77146100	5.55514700	H	
C-C-0.597300	-1	5.10608800	3.10264100	5.83000500	L H-H1 254	0.0000
O-O--0.567900	-1	6.28062700	3.07463300	6.18737400	L	
C-CT--0.182500	-1	5.16084700	0.95482600	4.52618000	L H-H1 254	0.0000
H-H-0.271900	0	2.87120000	1.84580700	4.06514600	H	
H-H1-0.082300	0	4.36718300	1.22855500	6.50608800	H	
H-HC-0.060300	-1	6.12640800	0.65898700	4.93373700	L	
H-HC-0.060300	-1	5.32043400	1.55549100	3.63098100	L	

H-HC-0.060300	-1	4.60013600	0.05436000	4.27221400	L
N-N--0.415700	-1	4.40698200	4.23294000	5.66459200	L
C-CT--0.087500	-1	4.79427600	5.59433400	6.06129900	L
C-C-0.597300	-1	3.95268800	6.04502000	7.26243500	L
O-O--0.567900	-1	4.50532300	6.49367700	8.26779700	L
C-CT-0.298500	-1	4.58418900	6.57022500	4.88618200	L
C-CT--0.319200	-1	4.98296200	8.00752400	5.23838900	L
C-CT--0.319200	-1	5.40139900	6.17149300	3.65770500	L
H-H-0.271900	-1	3.49578700	4.12170100	5.23746700	L
H-H1-0.096900	-1	5.84400600	5.61947700	6.34389600	L
H-HC--0.029700	-1	3.53202800	6.56152900	4.60920600	L
H-HC-0.079100	-1	6.03330100	8.04128800	5.51949600	L
H-HC-0.079100	-1	4.37713200	8.38690200	6.06054500	L
H-HC-0.079100	-1	4.82558000	8.64723900	4.37033100	L
H-HC-0.079100	-1	6.45093400	6.08943300	3.93434600	L
H-HC-0.079100	-1	5.28824100	6.91958600	2.87348200	L
H-HC-0.079100	-1	5.04602600	5.21570900	3.27263100	L
N-N--0.415700	-1	2.62073200	5.85918200	7.20732600	L
C-CT--0.149000	-1	1.71352400	6.20208800	8.31326700	L
H-H-0.271900	-1	2.21347600	5.48003600	6.35790800	L
H-H1-0.097600	-1	2.29173900	6.59495600	9.14965100	L
H-H1-0.097600	-1	1.17407700	5.30919500	8.63084500	L
H-H1-0.097600	-1	1.00141300	6.95640800	7.97871800	L
C-CT--0.366200	-1	4.09793600	10.28775300	-0.99543700	L
C-C-0.597200	-1	2.62220700	9.96661800	-1.24175200	L
O-O--0.567900	-1	1.81618300	10.88450200	-1.31533600	L
H-HC-0.112300	-1	4.66986800	9.36159500	-0.95884900	L
H-HC-0.112300	-1	4.20059700	10.81641300	-0.04796800	L
H-HC-0.112300	-1	4.47286300	10.91471700	-1.80406400	L
N-N--0.415700	-1	2.23873600	8.68509400	-1.29777700	L
C-CT--0.024900	-1	0.82383100	8.30870000	-1.14025900	L
C-C-0.597300	-1	0.23733700	8.80846600	0.18573000	L
O-O--0.567900	-1	-0.85500400	9.38007500	0.19236700	L
C-CT-0.211700	0	0.65023300	6.80911500	-1.28649200	L
O-OH--0.654600	0	0.93905700	6.50146300	-2.63032100	L
H-H-0.271900	-1	2.93851000	7.94982600	-1.35752800	L
H-H1-0.084300	-1	0.25394200	8.76080800	-1.94775400	L
H-H1-0.035200	0	-0.37404300	6.52248700	-1.05609700	L
H-H1-0.035200	0	1.33256000	6.28096800	-0.61840200	L
H-HO-0.427500	0	1.04367900	5.52548200	-2.64172100	L
N-N--0.415700	-1	0.99805900	8.67124800	1.28242300	L
C-CT-0.033700	-1	0.64446700	9.15399500	2.61858400	L
C-C-0.597300	-1	0.18514200	10.61688800	2.60929200	L
O-O--0.567900	-1	-0.91063200	10.93942100	3.07076500	L
C-CT--0.182500	-1	1.82910400	8.91280100	3.55175700	L
H-H-0.271900	-1	1.88485300	8.17163600	1.17823500	L
H-H1-0.082300	-1	-0.17294300	8.56490400	3.00745700	L
H-HC-0.060300	-1	1.59940100	9.28436100	4.54973500	L
H-HC-0.060300	-1	2.71689700	9.41106400	3.16450100	L
H-HC-0.060300	-1	2.02029400	7.84291900	3.60653100	L
N-N--0.415700	-1	0.98726500	11.49286900	1.99438300	L
C-CT--0.149000	-1	0.65219400	12.89166600	1.80098700	L
H-H-0.271900	-1	1.88906700	11.18150000	1.64173600	L
H-H1-0.097600	-1	-0.33361500	13.09039900	2.22293300	L

H-H1-0.097600	-1	0.64382300	13.11995800	0.73605500	L
H-H1-0.097600	-1	1.39332100	13.51554600	2.30161500	L
C-CT--0.366200	-1	-11.90311500	4.61607400	4.94461100	L
C-C-0.597200	-1	-12.34040100	3.19831800	4.57298900	L
O-O--0.567900	-1	-12.90912600	2.49264200	5.40837500	L
H-HC-0.112300	-1	-11.42097800	5.08391900	4.08615600	L
H-HC-0.112300	-1	-11.20010200	4.57334300	5.77663100	L
H-HC-0.112300	-1	-12.77522100	5.20114200	5.23488200	L
N-N--0.415700	-1	-12.00657600	2.75590900	3.36033100	L
C-CT--0.087500	-1	-12.00717600	1.33338500	3.00151800	L
C-C-0.597300	-1	-10.56216800	0.93350100	2.68954600	L
O-O--0.567900	-1	-9.84372300	1.57464100	1.91497400	L
C-CT-0.298500	-1	-13.00345000	0.94646000	1.87599600	L
C-CT--0.319200	-1	-13.75580300	-0.34103100	2.26092100	L
C-CT--0.319200	-1	-14.07759600	1.99815500	1.56525800	L
H-H-0.271900	-1	-11.59322100	3.40543200	2.68873000	L
H-H1-0.096900	-1	-12.30277100	0.77526400	3.88751400	L
H-HC--0.029700	-1	-12.44429200	0.75448400	0.96393600	L
H-HC-0.079100	-1	-14.38852100	-0.15675100	3.12984300	L
H-HC-0.079100	-1	-13.04294900	-1.13585000	2.48410600	L
H-HC-0.079100	-1	-14.39273000	-0.65407400	1.43382200	L
H-HC-0.079100	-1	-14.71165000	2.14496400	2.43614100	L
H-HC-0.079100	-1	-14.68540000	1.66410800	0.72577900	L
H-HC-0.079100	-1	-13.61699300	2.94873900	1.30516200	L
N-N--0.415700	-1	-10.10299400	-0.08797300	3.41517300	L
C-CT--0.038900	-1	-8.69633800	-0.48997800	3.49894100	L
C-C-0.597300	-1	-8.57360800	-2.01584200	3.61274500	L
O-O--0.567900	-1	-9.50723900	-2.67293300	4.09466200	L
C-CT-0.365400	-1	-7.97875400	0.15521100	4.70839100	L
O-OH--0.676100	-1	-8.15036100	-0.55845100	5.91124900	L
C-CT--0.243800	-1	-8.39271100	1.59316100	5.01504100	L
H-H-0.271900	-1	-10.73472400	-0.55850900	4.04705700	L
H-H1-0.100700	-1	-8.19398100	-0.15847700	2.59024700	L
H-H1-0.004300	-1	-6.91945300	0.15149700	4.47315400	L
H-HC-0.064200	-1	-8.43326200	2.15768700	4.09098400	L
H-HC-0.064200	-1	-7.66375000	2.04787500	5.68713800	L
H-HC-0.064200	-1	-9.37641100	1.62308300	5.48272500	L
H-HO-0.410200	-1	-8.40046800	0.08196800	6.60957400	L
N-N--0.254800	-1	-7.44906700	-2.61452900	3.18106000	L
C-CT--0.026600	-1	-7.20307000	-4.04134200	3.35164900	L
C-C-0.589600	-1	-6.59723400	-4.39721200	4.71054800	L
O-O--0.574800	-1	-6.61258200	-5.56790900	5.07383800	L
C-CT--0.007000	0	-6.21072000	-4.38388100	2.23929600	L
C-CT-0.018900	0	-5.36605400	-3.11763600	2.11409900	L
C-CT-0.019200	0	-6.37215900	-2.00227700	2.40404100	L
H-H1-0.064100	-1	-8.11470000	-4.60887400	3.20633700	L
H-HC-0.025300	0	-5.59914300	-5.24639700	2.49692400	L
H-HC-0.025300	0	-6.75022900	-4.56049800	1.30797900	L
H-HC-0.021300	0	-4.93126000	-3.02586100	1.11992300	L
H-HC-0.021300	0	-4.58108000	-3.11796500	2.87091200	L
H-H1-0.039100	0	-6.76927300	-1.62429600	1.46155500	L
H-H1-0.039100	0	-5.88451400	-1.19824200	2.95677000	L
N-N--0.415700	-1	-5.97641900	-3.43718500	5.40411300	L
C-CT--0.001400	-1	-4.98684800	-3.68067800	6.46507200	L

C-C-0.597300	-1	-5.53858800	-4.46180900	7.67214500	L		
O-O--0.567900	-1	-6.72503300	-4.34167800	7.98170000	L		
C-CT--0.001400	0	-4.47478300	-2.34969300	7.03302600	L	H-HA 373	0.0000
C-CA--0.001100	0	-4.17604000	-1.27457600	6.01536100	H		
C-CA--0.190600	0	-3.30805100	-1.53617200	4.95548600	H		
C-CA--0.190600	0	-4.75696900	-0.00981500	6.13628800	H		
C-CA--0.234100	0	-3.03296400	-0.54763700	4.02251000	H		
C-CA--0.234100	0	-4.48245500	0.99162100	5.20957100	H		
C-C-0.322600	0	-3.61535300	0.72472600	4.14555900	H		
O-OH--0.557900	0	-3.37782000	1.70691600	3.24823200	H		
H-H-0.271900	-1	-6.04052300	-2.49830800	5.04204200	L		
H-H1-0.087600	-1	-4.16333200	-4.25197500	6.03523800	L		
H-HC-0.029500	0	-5.22419700	-1.96012100	7.72459900	L		
H-HC-0.029500	0	-3.56719800	-2.53753500	7.60811100	L		
H-HA-0.169900	0	-2.84480700	-2.51325200	4.83938700	H		
H-HA-0.169900	0	-5.43155800	0.20872500	6.96480200	H		
H-HA-0.165600	0	-2.32885000	-0.72085700	3.22316900	H		
H-HA-0.165600	0	-4.90163500	1.98887400	5.31755900	H		
H-HO-0.399200	0	-2.51687300	1.53907400	2.79056800	H		
N-N--0.415700	-1	-4.66282400	-5.15380700	8.42735500	L		
C-CT--0.149000	-1	-5.05012600	-5.61830100	9.77585900	L		
H-H-0.271900	-1	-3.66782100	-5.14996600	8.18876200	L		
H-H1-0.097600	-1	-6.13382000	-5.56483000	9.88100800	L		
H-H1-0.097600	-1	-4.58007300	-4.98522900	10.52768000	L		
H-H1-0.097600	-1	-4.72213700	-6.64902900	9.91266500	L		
C-CT--0.366200	-1	-0.49508500	-10.78308100	2.47190700	L		
C-C-0.597200	-1	-0.67171800	-9.84260300	1.26652800	L		
O-O--0.567900	-1	-1.78016500	-9.66534100	0.75639300	L		
H-HC-0.112300	-1	0.55252800	-10.80004100	2.76895600	L		
H-HC-0.112300	-1	-0.81129800	-11.78950000	2.19637300	L		
H-HC-0.112300	-1	-1.10357100	-10.42719000	3.30328700	L		
N-N--0.415700	-1	0.44462700	-9.29949400	0.76388900	L		
C-CT-0.014300	-1	0.40488900	-8.28236300	-0.28616800	L	H-HC 405	0.0000
C-C-0.597300	-1	0.03144600	-8.78974100	-1.69776500	L		
O-O--0.567900	-1	-0.17643000	-7.96679500	-2.58008100	L		
C-CT--0.204100	0	1.70770900	-7.45207300	-0.29507600	H		
C-C-0.713000	0	1.39126900	-5.96169200	-0.48162800	H		
O-O--0.593100	0	0.75032300	-5.36696600	0.38585700	H		
N-N--0.919100	0	1.88328200	-5.33963700	-1.57462400	H		
H-H-0.271900	-1	1.32638200	-9.48955700	1.21115200	L		
H-H1-0.104800	-1	-0.39616700	-7.60771700	0.01644400	L		
H-HC-0.079700	0	2.39605400	-7.85587600	-1.04635000	H		
H-HC-0.079700	0	2.18337200	-7.52603200	0.68622400	H		
H-H-0.419600	0	1.67523400	-4.34841000	-1.71351400	H		
H-H-0.419600	0	2.29001800	-5.86772700	-2.33442100	H		
N-N--0.415700	-1	-0.06852400	-10.10284700	-1.93484300	L		
C-CT--0.149000	-1	-0.60890400	-10.65269100	-3.19025800	L		
H-H-0.271900	-1	0.03849200	-10.75212000	-1.14744200	L		
H-H1-0.097600	-1	-0.67018400	-9.86196000	-3.93727600	L		
H-H1-0.097600	-1	-1.60375500	-11.06025000	-3.01041100	L		
H-H1-0.097600	-1	0.04739400	-11.44516100	-3.55216000	L		
C-CT--0.366200	-1	-3.88488200	-11.69950700	-1.42691000	L		
C-C-0.597200	-1	-4.64762000	-10.37063700	-1.50073700	L		
O-O--0.567900	-1	-5.78589900	-10.36973900	-1.97359900	L		

H-HC-0.112300	-1	-2.90159600	-11.52911900	-0.98755200	L
H-HC-0.112300	-1	-3.76811200	-12.10775200	-2.42981400	L
H-HC-0.112300	-1	-4.44134700	-12.40382200	-0.80893100	L
N-N--0.415700	-1	-4.01679200	-9.24539100	-1.12525000	L
C-CT--0.087500	-1	-4.57581700	-7.88250800	-1.28998900	L
C-C-0.597300	-1	-4.83729900	-7.50012900	-2.75794300	L
O-O--0.567900	-1	-5.82325800	-6.82715600	-3.05535500	L
C-CT-0.298500	-1	-3.66581200	-6.80866200	-0.63795200	L
C-CT--0.319200	-1	-4.14754200	-5.36919000	-0.88007700	L
C-CT--0.319200	-1	-3.65324300	-6.94440300	0.88224200	L
H-H-0.271900	-1	-3.13597200	-9.35901400	-0.62169200	L
H-H1-0.096900	-1	-5.53737000	-7.85693300	-0.77866000	L
H-HC--0.029700	-1	-2.65004300	-6.91065100	-1.02041300	L
H-HC-0.079100	-1	-5.18354600	-5.26871900	-0.55564600	L
H-HC-0.079100	-1	-4.07698000	-5.11846700	-1.93587400	L
H-HC-0.079100	-1	-3.51879600	-4.66379700	-0.33468500	L
H-HC-0.079100	-1	-4.65986200	-6.80574700	1.25924600	L
H-HC-0.079100	-1	-2.98746200	-6.20075600	1.32256200	L
H-HC-0.079100	-1	-3.30811300	-7.92281800	1.18539200	L
N-N--0.415700	-1	-3.99057200	-7.90355800	-3.71344100	L
C-CT--0.149000	-1	-4.07267200	-7.48993200	-5.12502900	L
H-H-0.271900	-1	-3.27163100	-8.56903800	-3.45507100	L
H-H1-0.097600	-1	-4.88805900	-6.77669100	-5.24830400	L
H-H1-0.097600	-1	-4.25724400	-8.36427300	-5.75075300	L
H-H1-0.097600	-1	-3.13415900	-7.02283400	-5.42228000	L
C-CT--0.366200	-1	-12.08680200	3.71230400	-1.35046000	L
C-C-0.597200	-1	-10.98658000	2.64222400	-1.31147200	L
O-O--0.567900	-1	-11.28427700	1.46048900	-1.15591000	L
H-HC-0.112300	-1	-11.63454000	4.69355500	-1.49473200	L
H-HC-0.112300	-1	-12.63871900	3.70136100	-0.41018700	L
H-HC-0.112300	-1	-12.76956000	3.50189800	-2.17391400	L
N-N--0.415700	-1	-9.72831100	3.07830800	-1.37741900	L
C-CT--0.024900	-1	-8.54891100	2.25202900	-1.19518600	L
C-C-0.597300	-1	-7.43431500	3.11409000	-0.59699500	L
O-O--0.567900	-1	-6.77746800	3.89928600	-1.29493800	L
C-CT-0.211700	0	-8.12774400	1.60008700	-2.51071600	L
O-OH--0.654600	0	-7.22643800	0.57011000	-2.21501100	L
H-H-0.271900	-1	-9.59809200	4.07422800	-1.44835500	L
H-H1-0.084300	-1	-8.79052400	1.46114800	-0.48643000	L
H-H1-0.035200	0	-7.66804700	2.32302100	-3.18160300	L
H-H1-0.035200	0	-9.00297400	1.16332800	-2.99374700	L
H-HO-0.427500	0	-6.30138600	0.89974000	-2.27485000	L
N-N--0.415700	-1	-7.27457000	3.04100400	0.73328900	L
C-CT-0.021300	-1	-6.09830800	3.65267500	1.37021900	L
C-C-0.597300	-1	-4.81146700	3.00068900	0.83927300	L
O-O--0.567900	-1	-3.83356700	3.68506100	0.57984400	L
C-CT--0.123100	-1	-6.15901000	3.51809700	2.89333900	L
S-SH--0.311900	-1	-7.40969300	4.62977900	3.59787500	L
H-H-0.271900	-1	-7.93840800	2.49746100	1.28167000	L
H-H1-0.112400	-1	-6.06549500	4.71432100	1.12037400	L
H-H1-0.111200	-1	-5.18755100	3.78805100	3.31097100	L
H-H1-0.111200	-1	-6.37939900	2.48446900	3.15888300	L
H-HS-0.193300	-1	-8.45235000	4.18492000	2.88735100	L
N-N--0.415700	-1	-4.85430400	1.68182800	0.63449400	L H-H1 478 0.0000

C-CT-0.021300	0	-3.66032800	0.99070800	0.08083400	H		
C-C-0.597300	0	-3.64089000	1.20316200	-1.42815000	H		
O-O--0.567900	0	-4.68818100	1.24089400	-2.07996600	H		
C-CT--0.123100	0	-3.67668500	-0.50857700	0.44028900	H		
S-SH--0.311900	0	-2.23170300	-1.53112800	-0.13932200	H		
H-H-0.271900	-1	-5.70744600	1.19693000	0.83943600	L		
H-H1-0.112400	0	-2.78116900	1.45423400	0.52840700	H		
H-H1-0.111200	0	-4.50827700	-1.01494800	-0.06555300	H		
H-H1-0.111200	0	-3.78755800	-0.65705600	1.51417600	H		
H-HS-0.193300	0	1.37358700	0.27442000	-0.44434800	H		
N-N--0.415700	0	-2.40713700	1.29350100	-1.99497000	H		
C-CT--0.087500	0	-2.27050700	1.39349600	-3.43930700	H		
C-C-0.597300	0	-2.19729500	0.03483500	-4.18815600	H		
O-O--0.567900	0	-2.30397400	0.04236500	-5.41175800	H		
C-CT-0.298500	-1	-1.09065600	2.28470100	-3.88381400	H		
C-CT--0.319200	0	-1.20984700	3.69957000	-3.31548700	L	H-HC 492	0.0000
C-CT--0.319200	0	0.26759700	1.70597200	-3.44730300	L	H-HC 492	0.0000
H-H-0.271900	0	-1.58524900	1.25783300	-1.38446100	H		
H-H1-0.096900	0	-3.20855200	1.82613600	-3.80438100	H		
H-HC--0.029700	0	-1.10576000	2.33389200	-4.97470300	H		
H-HC-0.079100	0	-1.08045400	3.68400600	-2.23088500	L		
H-HC-0.079100	0	-2.18839900	4.10292300	-3.55656200	L		
H-HC-0.079100	0	-0.44715300	4.33628600	-3.75949000	L		
H-HC-0.079100	0	0.36696000	1.75817000	-2.36203500	L		
H-HC-0.079100	0	1.07293900	2.27122000	-3.90688600	L		
H-HC-0.079100	0	0.36837100	0.66540600	-3.74652300	L		
N-N--0.415700	0	-1.94220200	-1.07801500	-3.44329300	H		
C-CT--0.003100	0	-2.04249400	-2.42127200	-4.01648800	H		
C-C-0.597300	0	-3.50646600	-2.87090400	-4.18602600	H		
O-O--0.567900	0	-3.80632800	-3.67284500	-5.06134300	H		
C-CT--0.003600	-1	-1.28977200	-3.45524300	-3.12288400	H		
C-CT--0.064500	-1	-1.42668100	-4.90941700	-3.61223500	L	H-HC 508	0.0000
C-C-0.695100	-1	-0.55263600	-5.25183900	-4.80397700	L		
O-O--0.608600	-1	-0.40676400	-4.50205800	-5.75443500	L		
N-N--0.940700	-1	0.05725200	-6.41764100	-4.79700100	L		
H-H-0.271900	0	-1.96068400	-1.00955300	-2.42810600	H		
H-H1-0.085000	0	-1.62755000	-2.39349200	-5.02665700	H		
H-HC-0.017100	0	-0.23785100	-3.19504000	-3.04558900	H		
H-HC-0.017100	0	-1.71197800	-3.41340500	-2.11593800	H		
H-HC-0.035200	-1	-2.45529000	-5.16132300	-3.85449900	L		
H-HC-0.035200	-1	-1.14471100	-5.55750700	-2.78982100	L		
H-H-0.425100	-1	0.66068200	-6.66847600	-5.56045300	L		
H-H-0.425100	-1	-0.05554200	-7.03756800	-3.99677600	L		
N-N--0.415700	0	-4.34763000	-2.47366800	-3.16277500	H		
C-CT--0.023700	0	-5.72745400	-2.94162900	-3.24674000	H		
C-C-0.597300	-1	-6.39968900	-2.32282500	-4.48796100	L	H-H1 522	0.0000
O-O--0.567900	-1	-6.22487700	-1.12830200	-4.74730900	L		
C-CT-0.034200	-1	-6.46440100	-2.66127000	-1.92126800	L	H-H1 522	0.0000
C-CT-0.001800	-1	-7.93410600	-3.10596400	-1.97965800	L		
S-S--0.273700	-1	-8.83978900	-3.07599700	-0.40532700	L		
C-CT--0.053600	-1	-9.20322700	-1.30688000	-0.27561800	L		
H-H-0.271900	0	-4.28207600	-1.49637200	-2.91725400	H		
H-H1-0.088000	0	-5.65910300	-4.01840200	-3.36213300	H		
H-HC-0.024100	-1	-6.39115300	-1.61490600	-1.66219400	L		

H-HC-0.024100	-1	-5.97355700	-3.21475900	-1.12429700	L
H-H1-0.044000	-1	-7.96191700	-4.13173000	-2.34860700	L
H-H1-0.044000	-1	-8.47156900	-2.47839000	-2.69087900	L
H-H1-0.068400	-1	-9.80930400	-1.11962200	0.61071500	L
H-H1-0.068400	-1	-9.75145400	-0.97648100	-1.15810600	L
H-H1-0.068400	-1	-8.27170100	-0.74964100	-0.20326700	L
N-N--0.254800	-1	-7.14995400	-3.09037000	-5.30007100	L
C-CT--0.026600	-1	-7.54424000	-2.67323900	-6.64657300	L
C-C-0.589600	-1	-8.99255400	-2.18533700	-6.64000300	L
O-O--0.574800	-1	-9.88116900	-2.88281000	-6.14391000	L
C-CT--0.007000	-1	-7.34056200	-3.91812400	-7.52458300	L
C-CT-0.018900	-1	-6.82814500	-4.98182100	-6.55034500	L
C-CT-0.019200	-1	-7.36045900	-4.51940200	-5.22041600	L
H-H1-0.064100	-1	-6.89421000	-1.87832900	-7.01168500	L
H-HC-0.025300	-1	-8.27540400	-4.23643300	-7.97699800	L
H-HC-0.025300	-1	-6.60375300	-3.73610200	-8.30467200	L
H-HC-0.021300	-1	-5.74004400	-4.97679900	-6.52304200	L
H-HC-0.021300	-1	-7.20475500	-5.96334900	-6.76619600	L
H-H1-0.039100	-1	-6.83844700	-5.02844500	-4.42186600	L
H-H1-0.039100	-1	-8.42661900	-4.73695800	-5.14696900	L
N-N--0.415700	-1	-9.21208800	-0.98836300	-7.17758700	L
C-CT--0.149000	-1	-10.44372000	-0.21567300	-6.98921800	L
H-H-0.271900	-1	-8.40563900	-0.52131700	-7.59164400	L
H-H1-0.097600	-1	-11.20610500	-0.85135800	-6.53948800	L
H-H1-0.097600	-1	-10.79556900	0.14623800	-7.95527500	L
H-H1-0.097600	-1	-10.24322900	0.63189700	-6.33343600	L
C-CT--0.366200	-1	-10.30581000	8.86567600	-4.26114300	L
C-C-0.597200	-1	-9.76109000	7.57569000	-3.63364500	L
O-O--0.567900	-1	-10.20569500	7.15754600	-2.56322600	L
H-HC-0.112300	-1	-9.78593100	9.06156500	-5.19883600	L
H-HC-0.112300	-1	-10.14541200	9.69782000	-3.57618100	L
H-HC-0.112300	-1	-11.37255600	8.75389800	-4.45424200	L
N-N--0.415700	-1	-8.79121600	6.95019100	-4.29539100	L
C-CT--0.024900	-1	-7.84988800	6.02989000	-3.65395200	L
C-C-0.597300	-1	-6.51863800	6.75860400	-3.43194100	L
O-O--0.567900	-1	-6.26064000	7.76486700	-4.09980500	L
C-CT-0.211700	0	-7.63013900	4.77433000	-4.50996200	L
O-OH--0.654600	0	-7.25850400	5.08371500	-5.84006000	L
H-H-0.271900	-1	-8.51867400	7.31776900	-5.20603900	L
H-H1-0.084300	-1	-8.23755500	5.69220800	-2.69245400	L
H-H1-0.035200	0	-8.55153700	4.19090500	-4.52697300	L
H-H1-0.035200	0	-6.84512300	4.16866500	-4.05479700	L
H-HO-0.427500	0	-6.83382000	4.30809000	-6.22441300	L
N-N--0.415700	-1	-5.64304000	6.22514800	-2.56961100	L
C-CT-0.033700	-1	-4.26806900	6.73048200	-2.46531400	L
C-C-0.597300	-1	-3.51919200	6.73240200	-3.81706100	L
O-O--0.567900	-1	-2.61765700	7.54373000	-4.03377800	L
C-CT--0.182500	-1	-3.51752600	5.90773100	-1.42820800	L
H-H-0.271900	-1	-5.92846900	5.42103200	-2.00580800	L
H-H1-0.082300	-1	-4.31319500	7.75820900	-2.10345600	L
H-HC-0.060300	-1	-2.50306500	6.28661700	-1.32223900	L
H-HC-0.060300	-1	-3.48486300	4.86143700	-1.73014200	L
H-HC-0.060300	-1	-4.03374500	5.99301900	-0.47327000	L
N-N--0.415700	-1	-3.94190500	5.86629600	-4.75175700	L

C-CT--0.149000	-1	-3.42586800	5.81070400	-6.11831500	L
H-H-0.271900	-1	-4.67228500	5.21960000	-4.48499800	L
H-H1-0.097600	-1	-2.65036600	6.56657600	-6.24451700	L
H-H1-0.097600	-1	-4.23619100	6.00254600	-6.82150900	L
H-H1-0.097600	-1	-3.00561700	4.82305900	-6.30795800	L
C-CM--0.139000	0	0.52744400	-1.82257000	0.35598900	H
C-C-0.519000	0	1.13203800	-1.51915100	-1.00283400	H
O-O2--0.567000	0	1.54263200	-0.29116300	-1.23830800	H
C-CM--0.117000	0	-0.73221000	-1.09512500	0.89443600	H
O-O2--0.618000	0	1.35396700	-2.39757000	-1.84532900	H
C-C--0.553000	0	-0.67242400	0.43665200	1.05911700	H
O-O2--0.556000	0	-0.31299800	1.13841400	0.07493400	H
O-O2--0.607000	0	-1.09808900	0.87606600	2.16302300	H
H-HC-0.049000	0	0.36015600	-2.89777200	0.41182600	H
H-HC-0.162000	0	-0.91804100	-1.55981800	1.86110300	H
O-OW--0.834000	-1	6.46182700	2.92637200	-1.17637500	L
H-HW-0.417000	-1	6.83425200	3.06638200	-2.04617500	L
H-HW-0.417000	-1	7.14124500	3.22547400	-0.57247900	L
O-OW--0.834000	0	3.50412700	7.18440000	1.04182300	L
H-HW-0.417000	0	3.30221900	6.28787200	1.38139200	L
H-HW-0.417000	0	3.87110200	6.97165600	0.16666400	L
O-OW--0.834000	0	-1.47577400	-4.08105200	1.80447200	H
H-HW-0.417000	0	-0.78721300	-4.61865400	1.37977500	H
H-HW-0.417000	0	-2.01113100	-3.76205500	1.06263900	H
O-OW--0.834000	0	-4.96626800	0.80245500	-6.22370100	L
H-HW-0.417000	0	-4.02780400	0.58916400	-6.10457000	L
H-HW-0.417000	0	-5.40913800	0.16718400	-5.63552000	L
H-HS-0.193300	0	1.33311600	-1.55351200	1.06074900	H

IC3'

C-CT--0.366200	-1	8.24768200	4.60580600	-8.14182300	L
C-C-0.597200	-1	9.07509000	3.85951900	-7.10055300	L
O-O--0.567900	-1	9.67282300	2.81989200	-7.38048700	L
H-HC-0.112300	-1	7.80670700	5.49338700	-7.68828800	L
H-HC-0.112300	-1	7.45477100	3.95457600	-8.51129700	L
H-HC-0.112300	-1	8.88954800	4.90320700	-8.97193500	L
N-N--0.415700	-1	9.07066900	4.41907100	-5.88414700	L
C-CT--0.087500	-1	9.53914600	3.74336000	-4.66708200	L
C-C-0.597300	-1	8.39871900	2.84980400	-4.17535100	L
O-O--0.567900	-1	7.48851200	3.31302000	-3.47294000	L
C-CT-0.298500	-1	10.02359500	4.74521700	-3.59189100	L
C-CT--0.319200	-1	10.44021300	4.04601900	-2.29234400	L
C-CT--0.319200	-1	11.24072600	5.54924700	-4.07157000	L
H-H-0.271900	-1	8.48777200	5.24300000	-5.75815500	L
H-H1-0.096900	-1	10.37511000	3.09954800	-4.92002100	L
H-HC--0.029700	-1	9.22829400	5.45334000	-3.37678700	L
H-HC-0.079100	-1	11.14404400	3.24497200	-2.52014200	L
H-HC-0.079100	-1	9.56828500	3.62581400	-1.79485600	L
H-HC-0.079100	-1	10.91829300	4.75350500	-1.61671500	L
H-HC-0.079100	-1	12.09932800	4.88996100	-4.19894900	L
H-HC-0.079100	-1	11.48848000	6.32024900	-3.33988300	L
H-HC-0.079100	-1	11.02451900	6.02842600	-5.02543000	L
N-N--0.415700	-1	8.41204900	1.57670400	-4.60582800	L
C-CT--0.087500	-1	7.29624100	0.62792000	-4.43082400	L

C-C-0.597300	-1	7.70804000	-0.64812700	-3.66811100	L
O-O--0.567900	-1	8.85284200	-1.10301300	-3.79124300	L
C-CT-0.298500	-1	6.64278600	0.22142600	-5.77610800	L
C-CT--0.319200	-1	5.78871400	1.34975800	-6.36593100	L
C-CT--0.319200	-1	7.63516000	-0.23326100	-6.85154100	L
H-H-0.271900	-1	9.18694500	1.26808700	-5.19886500	L
H-H1-0.096900	-1	6.52623300	1.13754300	-3.85865400	L
H-HC--0.029700	-1	5.97116400	-0.61736900	-5.58958100	L
H-HC-0.079100	-1	6.30850600	2.30475000	-6.29050500	L
H-HC-0.079100	-1	4.85331200	1.40055600	-5.81319800	L
H-HC-0.079100	-1	5.54067500	1.13430800	-7.40653300	L
H-HC-0.079100	-1	8.23816400	0.60932700	-7.18586900	L
H-HC-0.079100	-1	7.08522100	-0.63567500	-7.70125200	L
H-HC-0.079100	-1	8.28700900	-1.00771000	-6.45539800	L
N-N--0.254800	-1	6.76967000	-1.25138600	-2.90056700	L
C-CT--0.026600	-1	6.89753700	-2.60425900	-2.35232600	L
C-C-0.589600	-1	7.14389600	-3.62945000	-3.46099800	L
O-O--0.574800	-1	6.39782200	-3.67603400	-4.44210500	L
C-CT--0.007000	0	5.56710500	-2.92909000	-1.65933700	L
C-CT-0.018900	0	4.88181900	-1.58507000	-1.47023500	L
C-CT-0.019200	0	5.44421600	-0.71899100	-2.58777900	L
H-H1-0.064100	-1	7.71529500	-2.62100900	-1.63269700	L
H-HC-0.025300	0	4.93526800	-3.54931400	-2.29700800	L
H-HC-0.025300	0	5.72637100	-3.43550600	-0.71178900	L
H-HC-0.021300	0	5.14208800	-1.15374400	-0.50635800	L
H-HC-0.021300	0	3.80737300	-1.69241300	-1.56314300	L
H-H1-0.039100	0	5.49035100	0.31449600	-2.24201000	L
H-H1-0.039100	0	4.79847100	-0.79511300	-3.46378200	L
N-N--0.415700	-1	8.16633400	-4.47796600	-3.31065300	L
C-CT--0.149000	-1	8.53434200	-5.47600300	-4.32770400	L
H-H-0.271900	-1	8.76491600	-4.35646300	-2.49484100	L
H-H1-0.097600	-1	7.79176900	-5.47473300	-5.12497600	L
H-H1-0.097600	-1	8.57288200	-6.46436100	-3.86865600	L
H-H1-0.097600	-1	9.51216100	-5.22994100	-4.74174900	L
C-CT--0.366200	-1	5.22947300	-7.45108200	-4.08465700	L
C-C-0.597200	-1	4.10306000	-6.77825600	-4.87919300	L
O-O--0.567900	-1	3.20402200	-7.49453700	-5.32913100	L
H-HC-0.112300	-1	5.94288300	-6.69619800	-3.75475900	L
H-HC-0.112300	-1	5.73661300	-8.17935900	-4.71737300	L
H-HC-0.112300	-1	4.80815400	-7.95602800	-3.21531200	L
N-N--0.415700	-1	4.09497400	-5.44755200	-5.01971900	L
C-CT-0.014300	-1	2.99575500	-4.69775700	-5.65226700	L H-HC 69 0.0000
C-C-0.597300	-1	2.80269200	-5.03936400	-7.16448900	L
O-O--0.567900	-1	3.79785200	-5.20700900	-7.87092700	L
C-CT--0.204100	0	3.29531300	-3.19905700	-5.41562500	H
C-C-0.713000	0	2.16714500	-2.27434300	-5.86919100	H
O-O--0.593100	0	1.97601200	-2.01315000	-7.05143700	H
N-N--0.919100	0	1.42662500	-1.71823800	-4.86895400	H
H-H-0.271900	-1	4.86408500	-4.91163900	-4.65120100	L
H-H1-0.104800	-1	2.08676200	-4.95864500	-5.11995900	L
H-HC-0.079700	0	4.18614400	-2.94924500	-6.00186600	H
H-HC-0.079700	0	3.52575700	-3.05186500	-4.35655100	H
H-H-0.419600	0	0.57241500	-1.28057700	-5.18819100	H
H-H-0.419600	0	1.50471100	-1.97340200	-3.88955100	H

N-N--0.415700	-1	1.54962800	-5.13574600	-7.65968700 L
C-CT--0.149000	-1	1.19929200	-5.39598900	-9.08572300 L
H-H-0.271900	-1	0.79382000	-4.90777600	-7.01475100 L
H-H1-0.097600	-1	2.10533800	-5.62380700	-9.64664300 L
H-H1-0.097600	-1	0.72158600	-4.51208600	-9.50924100 L
H-H1-0.097600	-1	0.51419200	-6.24188200	-9.14132300 L
C-CT--0.366200	-1	11.72034700	-5.96827600	-0.62278000 L
C-C-0.597200	-1	10.70248600	-6.09079100	0.51937100 L
O-O--0.567900	-1	11.01799600	-5.93552300	1.70430900 L
H-HC-0.112300	-1	11.22061800	-6.14354900	-1.57534700 L
H-HC-0.112300	-1	12.51025600	-6.70631000	-0.48589100 L
H-HC-0.112300	-1	12.15370800	-4.96791400	-0.61860100 L
N-N--0.415700	-1	9.46580400	-6.39195100	0.12625000 L
C-CT--0.023700	-1	8.30361500	-6.58575500	0.98840000 L
C-C-0.597300	-1	7.24833500	-7.42722200	0.28321200 L
O-O--0.567900	-1	7.07213800	-7.26893800	-0.93166500 L
C-CT-0.034200	0	7.70363700	-5.22169500	1.37374400 L
C-CT-0.001800	0	6.75560800	-5.23641400	2.58922600 L
S-S--0.273700	0	5.03081000	-5.75534300	2.31678400 L
C-CT--0.053600	0	4.21869600	-4.15430700	2.01193700 L
H-H-0.271900	-1	9.29861300	-6.46616200	-0.87116900 L
H-H1-0.088000	-1	8.62533100	-7.11768100	1.87212800 L
H-HC-0.024100	0	7.18767400	-4.79183500	0.51556000 L
H-HC-0.024100	0	8.53650500	-4.56813300	1.61579300 L
H-H1-0.044000	0	6.72423400	-4.22840800	3.00357900 L
H-H1-0.044000	0	7.19032000	-5.88051700	3.35359800 L
H-H1-0.068400	0	3.16821600	-4.31020900	1.76078800 L
H-H1-0.068400	0	4.70052700	-3.63318100	1.18765100 L
H-H1-0.068400	0	4.27661400	-3.52775500	2.90243800 L
N-N--0.415700	-1	6.53689000	-8.27043400	1.04176000 L
C-CT--0.149000	-1	5.31397400	-8.97378000	0.62642600 L
H-H-0.271900	-1	6.85109800	-8.40185100	2.00320500 L
H-H1-0.097600	-1	5.09901100	-8.74361800	-0.41658100 L
H-H1-0.097600	-1	4.47985100	-8.65088200	1.24960000 L
H-H1-0.097600	-1	5.45749100	-10.04799100	0.73929800 L
C-CT--0.366200	-1	3.87066100	-9.36598200	4.90548300 L
C-C-0.597200	-1	3.70527900	-7.95914400	5.51468800 L
O-O--0.567900	-1	4.66847700	-7.24517100	5.80907900 L
H-HC-0.112300	-1	2.88767600	-9.80439300	4.73027500 L
H-HC-0.112300	-1	4.43207700	-9.99732800	5.59395400 L
H-HC-0.112300	-1	4.40836600	-9.29191900	3.96009500 L
N-N--0.415700	-1	2.44460600	-7.54136000	5.65947400 L
C-CT--0.087500	-1	2.01172100	-6.13570800	5.60496400 L
C-C-0.597300	-1	1.88912800	-5.57600500	7.02860400 L
O-O--0.567900	-1	0.85091700	-5.66601600	7.69921600 L
C-CT-0.298500	0	0.68985200	-5.95942900	4.82822600 L
C-CT--0.319200	0	0.35356600	-4.47338700	4.65730000 L
C-CT--0.319200	0	0.76639700	-6.60262300	3.43634000 L
H-H-0.271900	-1	1.70731200	-8.23340400	5.50264400 L
H-H1-0.096900	-1	2.77981400	-5.56512600	5.07932400 L
H-HC--0.029700	0	-0.11934200	-6.44479100	5.37537100 L
H-HC-0.079100	0	1.09765300	-3.97757900	4.03104700 L
H-HC-0.079100	0	0.30179100	-3.96628600	5.61987400 L
H-HC-0.079100	0	-0.62095600	-4.37088400	4.18359600 L

H-HC-0.079100	0	1.60057000	-6.17333200	2.87972800	L
H-HC-0.079100	0	-0.15686200	-6.39593800	2.89298800	L
H-HC-0.079100	0	0.88690000	-7.68014700	3.51326200	L
N-N--0.415700	-1	3.04969500	-5.12624300	7.50524400	L
C-CT--0.149000	-1	3.42496200	-4.99171900	8.91014100	L
H-H-0.271900	-1	3.81013600	-5.04562700	6.84050500	L
H-H1-0.097600	-1	2.53708100	-5.09393200	9.53426200	L
H-H1-0.097600	-1	3.87338900	-4.01257900	9.07472200	L
H-H1-0.097600	-1	4.14325000	-5.76938200	9.17000300	L
C-CT--0.366200	-1	12.47555800	-4.27558400	6.35392600	L
C-C-0.597200	-1	12.27522800	-3.55283800	5.00334300	L
O-O--0.567900	-1	13.24408300	-3.33979000	4.26783600	L
H-HC-0.112300	-1	11.51519900	-4.37240800	6.86032700	L
H-HC-0.112300	-1	13.15746600	-3.69665200	6.97798600	L
H-HC-0.112300	-1	12.89526600	-5.26514600	6.17795400	L
N-N--0.415700	-1	11.04182800	-3.12282900	4.69874100	L
C-CT--0.023700	-1	10.76942800	-2.29816700	3.52382900	L
C-C-0.597300	-1	11.34232700	-0.87717900	3.66027600	L
O-O--0.567900	-1	12.07406900	-0.41483200	2.78316200	L
C-CT-0.034200	0	9.26328100	-2.21253300	3.24821200	L
C-CT-0.001800	0	9.03560600	-1.55569700	1.87826200	L
S-S--0.273700	0	7.44117000	-1.89909100	1.10688300	L
C-CT--0.053600	0	6.30523800	-0.92458600	2.12309700	L
H-H-0.271900	-1	10.27528100	-3.34885100	5.32618200	L
H-H1-0.088000	-1	11.23941500	-2.77981000	2.66465400	L
H-HC-0.024100	0	8.75719000	-1.63517100	4.02304800	L
H-HC-0.024100	0	8.85244400	-3.21765900	3.25042500	L
H-H1-0.044000	0	9.79791900	-1.92159100	1.18937900	L
H-H1-0.044000	0	9.16079400	-0.47561700	1.96653500	L
H-H1-0.068400	0	5.27885500	-1.08502300	1.78783100	L
H-H1-0.068400	0	6.53461400	0.13617000	2.02342200	L
H-H1-0.068400	0	6.38360600	-1.22703700	3.16540100	L
N-N--0.415700	-1	11.07594300	-0.18744200	4.77493200	L
C-CT--0.149000	-1	11.63428700	1.14901400	5.00419400	L
H-H-0.271900	-1	10.49512000	-0.61579700	5.49519600	L
H-H1-0.097600	-1	12.22466400	1.44894600	4.13851100	L
H-H1-0.097600	-1	12.27059000	1.12985800	5.88858300	L
H-H1-0.097600	-1	10.82284000	1.86081100	5.15583000	L
C-CT--0.366200	-1	6.23713700	8.68899700	-5.56394300	L
C-C-0.597200	-1	6.54631500	7.49601700	-4.63797700	L
O-O--0.567900	-1	6.69357800	6.34680200	-5.07782800	L
H-HC-0.112300	-1	6.14841000	9.59835600	-4.96859300	L
H-HC-0.112300	-1	5.29960400	8.50762700	-6.09081000	L
H-HC-0.112300	-1	7.04381600	8.80633600	-6.28825000	L
N-N--0.415700	-1	6.68958900	7.81115000	-3.34047400	L
C-CT--0.001400	-1	6.72605700	6.81976300	-2.25001000	L
C-C-0.597300	-1	5.34809800	6.14594100	-2.11021500	L
O-O--0.567900	-1	4.47606000	6.63030500	-1.37147800	L
C-CT--0.001400	-1	7.24498200	7.45135300	-0.94508000	L
C-CA--0.001100	-1	7.92536900	6.47766400	0.01122800	L
C-CA--0.190600	-1	9.33290200	6.42135100	0.06314900	L
C-CA--0.190600	-1	7.17500200	5.65999700	0.88119300	L
C-CA--0.234100	-1	9.97893800	5.59837200	1.00463800	L
C-CA--0.234100	-1	7.82537700	4.83191200	1.82241700	L

C-C-0.322600	-1	9.22770800	4.82374200	1.90269400	L		
O-OH--0.557900	-1	9.88400100	4.07548800	2.83603500	L		
H-H-0.271900	-1	6.62930000	8.80338300	-3.09909000	L		
H-H1-0.087600	-1	7.43415900	6.04458600	-2.52912600	L		
H-HC-0.029500	-1	7.97410000	8.21951100	-1.20567400	L		
H-HC-0.029500	-1	6.43429900	7.96215400	-0.42401000	L		
H-HA-0.169900	-1	9.92221500	7.04248600	-0.59632200	L		
H-HA-0.169900	-1	6.09406100	5.67041100	0.83666200	L		
H-HA-0.165600	-1	11.05600400	5.56440500	1.05484300	L		
H-HA-0.165600	-1	7.24750600	4.20186200	2.48265300	L		
H-HO-0.399200	-1	9.38581000	3.85439800	3.63899700	L		
N-N--0.415700	-1	5.13265300	5.12565500	-2.94531900	L		
C-CT-0.033700	-1	3.81430600	4.63620700	-3.33338900	L		
C-C-0.597300	-1	2.97373900	4.00339200	-2.21348700	L		
O-O--0.567900	-1	1.75086400	4.10966100	-2.28322000	L		
C-CT--0.182500	-1	3.99975000	3.63645300	-4.46971700	L		
H-H-0.271900	-1	5.91492500	4.82921100	-3.52385200	L		
H-H1-0.082300	-1	3.25229000	5.48337200	-3.72779800	L		
H-HC-0.060300	-1	3.02777100	3.32999400	-4.85535000	L		
H-HC-0.060300	-1	4.53316000	2.76583600	-4.08802400	L		
H-HC-0.060300	-1	4.57293300	4.09487200	-5.27571600	L		
N-N--0.415700	-1	3.58423900	3.35906900	-1.20825400	L	H-H1 209	0.0000
C-CT-0.021300	0	2.85286000	2.68848600	-0.11201100	H		
C-C-0.597300	0	2.32832300	3.73859000	0.87106600	H		
O-O--0.567900	0	3.08975600	4.58909600	1.33087600	H		
C-CT--0.123100	0	3.83840800	1.74024300	0.60732000	H		
S-S--1.036000	0	2.98964500	0.52977000	1.71149000	H		
H-H-0.271900	-1	4.58794800	3.33017500	-1.19959600	L		
H-H1-0.112400	0	2.03816700	2.11049600	-0.55373500	H		
H-H1-0.111200	0	4.54330500	2.34013400	1.19421000	H		
H-H1-0.111200	0	4.42600000	1.18730900	-0.13705700	H		
N-N--0.415700	0	1.00917100	3.66148700	1.22031900	H		
C-CT--0.051800	0	0.44077200	4.50290300	2.28098400	H		
C-C-0.597300	0	0.81609000	3.99527900	3.70948100	H		
O-O--0.567900	0	1.36920000	4.72239800	4.53537100	H		
C-CT--0.110200	-1	-1.08807600	4.63300900	2.01970400	H		
C-CT-0.353100	-1	-1.94418200	5.54066800	2.92924500	L	H-HC 222	0.0000
C-CT--0.412100	-1	-2.13841800	4.99475500	4.34536800	L		
C-CT--0.412100	-1	-1.40828500	6.97247000	3.01794900	L		
H-H-0.271900	0	0.44320500	2.88794700	0.87147700	H		
H-H1-0.092200	0	0.91880600	5.48271600	2.21876200	H		
H-HC-0.045700	0	-1.20457300	5.00962100	0.99619900	H		
H-HC-0.045700	0	-1.54367200	3.63909500	2.03462800	H		
H-HC--0.036100	-1	-2.93541400	5.59254800	2.48029000	L		
H-HC-0.100000	-1	-1.23928600	5.13261000	4.94227400	L		
H-HC-0.100000	-1	-2.38715000	3.93530600	4.30404300	L		
H-HC-0.100000	-1	-2.95602600	5.53059200	4.82517000	L		
H-HC-0.100000	-1	-0.44638300	6.98553700	3.53142800	L		
H-HC-0.100000	-1	-2.11812400	7.59356300	3.56291100	L		
H-HC-0.100000	-1	-1.28272400	7.37456400	2.01175500	L		
N-N--0.415700	0	0.51632900	2.69127800	3.97426200	H		
C-CT--0.087500	0	0.60503300	2.14737200	5.33040300	H		
C-C-0.597300	0	2.01351600	2.12444100	5.94122900	H		
O-O--0.567900	0	2.11782800	2.13725600	7.16720300	H		

C-CT-0.298500	-1	-0.01646500	0.73285700	5.36603300	H		
C-CT--0.319200	0	0.72087500	-0.31589600	4.50804500	L	H-HC 241	0.0000
C-CT--0.319200	0	-0.21063700	0.14120300	6.76256200	L	H-HC 241	0.0000
H-H-0.271900	0	0.04880000	2.14547800	3.25198000	H		
H-H1-0.096900	0	0.04077400	2.80475900	6.00579900	H		
H-HC--0.029700	0	-1.01491400	0.82133200	4.93459300	H		
H-HC-0.079100	0	1.68419000	-0.57152700	4.94353800	L		
H-HC-0.079100	0	0.89358800	0.07011300	3.50312800	L		
H-HC-0.079100	0	0.10957900	-1.21114500	4.41028700	L		
H-HC-0.079100	0	0.75321300	-0.09642000	7.21084800	L		
H-HC-0.079100	0	-0.80511500	-0.76877200	6.68542200	L		
H-HC-0.079100	0	-0.73894500	0.85899400	7.38813100	L		
N-N--0.415700	0	3.02855300	1.91386800	5.08003800	H		
C-CT-0.033700	0	4.38998000	1.76517800	5.55292900	H		
C-C-0.597300	-1	5.11112800	3.09526100	5.82630300	L	H-H1 254	0.0000
O-O--0.567900	-1	6.28578800	3.06623000	6.18318800	L		
C-CT--0.182500	-1	5.16383400	0.94808300	4.52134400	L	H-H1 254	0.0000
H-H-0.271900	0	2.86624600	1.90893900	4.07739100	H		
H-H1-0.082300	0	4.37288000	1.22126800	6.50273600	H		
H-HC-0.060300	-1	6.12934800	0.65134700	4.92836000	L		
H-HC-0.060300	-1	5.32349000	1.54910000	3.62639300	L		
H-HC-0.060300	-1	4.60238100	0.04815000	4.26713500	L		
N-N--0.415700	-1	4.41275900	4.22614300	5.66175800	L		
C-CT--0.087500	-1	4.80118200	5.58705500	6.05901500	L		
C-C-0.597300	-1	3.96039600	6.03771600	7.26072200	L		
O-O--0.567900	-1	4.51375200	6.48545800	8.26609600	L		
C-CT-0.298500	-1	4.59131900	6.56370400	4.88448900	L		
C-CT--0.319200	-1	4.99125600	8.00053500	5.23728300	L		
C-CT--0.319200	-1	5.40775200	6.16502900	3.65547800	L		
H-H-0.271900	-1	3.50131400	4.11577400	5.23494100	L		
H-H1-0.096900	-1	5.85104100	5.61130300	6.34120500	L		
H-HC--0.029700	-1	3.53904000	6.55590100	4.60793100	L		
H-HC-0.079100	-1	6.04173100	8.03340700	5.51798600	L		
H-HC-0.079100	-1	4.38602500	8.37991900	6.05987800	L		
H-HC-0.079100	-1	4.83398100	8.64081300	4.36961900	L		
H-HC-0.079100	-1	6.45733900	6.08207800	3.93165600	L		
H-HC-0.079100	-1	5.29481300	6.91360900	2.87168900	L		
H-HC-0.079100	-1	5.05154400	5.20969700	3.27005100	L		
N-N--0.415700	-1	2.62828600	5.85285500	7.20605100	L		
C-CT--0.149000	-1	1.72176500	6.19583200	8.31253400	L		
H-H-0.271900	-1	2.22042000	5.47443900	6.35660000	L		
H-H1-0.097600	-1	2.30059500	6.58785300	9.14888900	L		
H-H1-0.097600	-1	1.18181000	5.30315800	8.62986500	L		
H-H1-0.097600	-1	1.01005700	6.95083200	7.97866200	L		
C-CT--0.366200	-1	4.10535700	10.28463000	-0.99500500	L		
C-C-0.597200	-1	2.62930100	9.96467300	-1.24089500	L		
O-O--0.567900	-1	1.82390200	10.88316900	-1.31367900	L		
H-HC-0.112300	-1	4.67664500	9.35804600	-0.95912600	L		
H-HC-0.112300	-1	4.20877500	10.81272400	-0.04730300	L		
H-HC-0.112300	-1	4.48040700	10.91174600	-1.80345700	L		
N-N--0.415700	-1	2.24489600	8.68345200	-1.29743100	L		
C-CT--0.024900	-1	0.82978700	8.30798300	-1.13954100	L		
C-C-0.597300	-1	0.24417900	8.80747800	0.18694200	L		
O-O--0.567900	-1	-0.84775200	9.37986200	0.19431300	L		

C-CT-0.211700	0	0.65501200	6.80865400	-1.28653300	L
O-OH--0.654600	0	0.94449900	6.50156700	-2.63032300	L
H-H-0.271900	-1	2.94412100	7.94771700	-1.35784400	L
H-H1-0.084300	-1	0.25989600	8.76091600	-1.94657200	L
H-H1-0.035200	0	-0.36965200	6.52274900	-1.05697500	L
H-H1-0.035200	0	1.33644900	6.27955300	-0.61831800	L
H-HO-0.427500	0	1.04818700	5.52544000	-2.64166200	L
N-N--0.415700	-1	1.00524200	8.66915000	1.28325900	L
C-CT-0.033700	-1	0.65253000	9.15145500	2.61981200	L
C-C-0.597300	-1	0.19424200	10.61468000	2.61146300	L
O-O--0.567900	-1	-0.90111600	10.93775200	3.07354200	L
C-CT--0.182500	-1	1.83736800	8.90893300	3.55238400	L
H-H-0.271900	-1	1.89163800	8.16896100	1.17845600	L
H-H1-0.082300	-1	-0.16514500	8.56274400	3.00870700	L
H-HC-0.060300	-1	1.60833000	9.28013800	4.55064700	L
H-HC-0.060300	-1	2.72536000	9.40676500	3.16503100	L
H-HC-0.060300	-1	2.02781800	7.83888700	3.60652700	L
N-N--0.415700	-1	0.99674300	11.49040800	1.99668600	L
C-CT--0.149000	-1	0.66259000	12.88954300	1.80415100	L
H-H-0.271900	-1	1.89818100	11.17858000	1.64351600	L
H-H1-0.097600	-1	-0.32290800	13.08875800	2.22659500	L
H-H1-0.097600	-1	0.65395500	13.11839400	0.73934000	L
H-H1-0.097600	-1	1.40436200	13.51263600	2.30480500	L
C-CT--0.366200	-1	-11.89734700	4.62126000	4.94851400	L
C-C-0.597200	-1	-12.33579200	3.20400800	4.57633200	L
O-O--0.567900	-1	-12.90468400	2.49830300	5.41158000	L
H-HC-0.112300	-1	-11.41522100	5.08920700	4.09010900	L
H-HC-0.112300	-1	-11.19403300	4.57759600	5.78023000	L
H-HC-0.112300	-1	-12.76892100	5.20679700	5.23943900	L
N-N--0.415700	-1	-12.00276800	2.76199200	3.36331100	L
C-CT--0.087500	-1	-12.00452500	1.33965400	3.00376100	L
C-C-0.597300	-1	-10.55992600	0.93890300	2.69100200	L
O-O--0.567900	-1	-9.84133500	1.57993400	1.91647500	L
C-CT-0.298500	-1	-13.00152500	0.95402300	1.87843800	L
C-CT--0.319200	-1	-13.75464000	-0.33313300	2.26299700	L
C-CT--0.319200	-1	-14.07504500	2.00664400	1.56867600	L
H-H-0.271900	-1	-11.58922000	3.41156900	2.69188100	L
H-H1-0.096900	-1	-12.30016200	0.78128500	3.88958600	L
H-HC--0.029700	-1	-12.44286800	0.76212300	0.96605400	L
H-HC-0.079100	-1	-14.38687800	-0.14885200	3.13226700	L
H-HC-0.079100	-1	-13.04226200	-1.12857400	2.48548300	L
H-HC-0.079100	-1	-14.39212100	-0.64529100	1.43599000	L
H-HC-0.079100	-1	-14.70864600	2.15345100	2.43988900	L
H-HC-0.079100	-1	-14.68342300	1.67346500	0.72926700	L
H-HC-0.079100	-1	-13.61387000	2.95703500	1.30888800	L
N-N--0.415700	-1	-10.10119000	-0.08327300	3.41591500	L
C-CT--0.038900	-1	-8.69478600	-0.48632300	3.49891000	L
C-C-0.597300	-1	-8.57309800	-2.01233300	3.61187300	L
O-O--0.567900	-1	-9.50700200	-2.66900900	4.09382400	L
C-CT-0.365400	-1	-7.97625900	0.15772800	4.70840700	L
O-OH--0.676100	-1	-8.14789200	-0.55643600	5.91096300	L
C-CT--0.243800	-1	-8.38906900	1.59581300	5.01596900	L
H-H-0.271900	-1	-10.73300200	-0.55368700	4.04780800	L
H-H1-0.100700	-1	-8.19255800	-0.15470800	2.59018700	L

H-H1-0.004300	-1	-6.91705600	0.15338100	4.47274400	L		
H-HC-0.064200	-1	-8.42958800	2.16084800	4.09222200	L		
H-HC-0.064200	-1	-7.65951600	2.04965900	5.68800900	L		
H-HC-0.064200	-1	-9.37256000	1.62619300	5.48406200	L		
H-HO-0.410200	-1	-8.39726400	0.08379800	6.60972100	L		
N-N--0.254800	-1	-7.44915600	-2.61159500	3.17942700	L		
C-CT--0.026600	-1	-7.20410700	-4.03867100	3.34917800	L		
C-C-0.589600	-1	-6.59798000	-4.39567700	4.70764800	L		
O-O--0.574800	-1	-6.61401600	-5.56655300	5.07033800	L		
C-CT--0.007000	0	-6.21268400	-4.38151400	2.23609200	L		
C-CT-0.018900	0	-5.36737000	-3.11577700	2.11066600	L		
C-CT-0.019200	0	-6.37226300	-1.99975700	2.40219900	L		
H-H1-0.064100	-1	-8.11619800	-4.60547900	3.20393600	L		
H-HC-0.025300	0	-5.60139500	-5.24442300	2.49312000	L		
H-HC-0.025300	0	-6.75288300	-4.55758700	1.30507600	L		
H-HC-0.021300	0	-4.93349500	-3.02366600	1.11610600	L		
H-HC-0.021300	0	-4.58169100	-3.11720800	2.86669900	L		
H-H1-0.039100	0	-6.76966000	-1.62063400	1.46029700	L		
H-H1-0.039100	0	-5.88353400	-1.19663600	2.95531800	L		
N-N--0.415700	-1	-5.97620400	-3.43645400	5.40146300	L		
C-CT--0.001400	-1	-4.98638100	-3.68120100	6.46189900	L		
C-C-0.597300	-1	-5.53819400	-4.46256600	7.66878700	L		
O-O--0.567900	-1	-6.72442900	-4.34175100	7.97888000	L		
C-CT--0.001400	0	-4.47392200	-2.34896300	7.02693100	L	H-HA 373	0.0000
C-CA--0.001100	0	-4.17060000	-1.27736800	6.00611100	H		
C-CA--0.190600	0	-3.30369400	-1.54565200	4.94677600	H		
C-CA--0.190600	0	-4.74460600	-0.00890800	6.12334200	H		
C-CA--0.234100	0	-3.02204500	-0.55935600	4.01387600	H		
C-CA--0.234100	0	-4.46334700	0.99001700	5.19534600	H		
C-C-0.322600	0	-3.59476500	0.71754000	4.13340700	H		
O-OH--0.557900	0	-3.34267400	1.69485800	3.23618000	H		
H-H-0.271900	-1	-6.03978500	-2.49734300	5.03990400	L		
H-H1-0.087600	-1	-4.16344500	-4.25286200	6.03143800	L		
H-HC-0.029500	0	-5.22455400	-1.95623700	7.71536400	L		
H-HC-0.029500	0	-3.56801000	-2.53632300	7.60479800	L		
H-HA-0.169900	0	-2.84720100	-2.52581300	4.82951900	H		
H-HA-0.169900	0	-5.41927400	0.21483100	6.95050200	H		
H-HA-0.165600	0	-2.31893400	-0.73803800	3.21579700	H		
H-HA-0.165600	0	-4.87756100	1.98954300	5.30197500	H		
H-HO-0.399200	0	-2.47648400	1.51742700	2.78425400	H		
N-N--0.415700	-1	-4.66262100	-5.15557800	8.42328700	L		
C-CT--0.149000	-1	-5.04971400	-5.62049600	9.77170500	L		
H-H-0.271900	-1	-3.66771100	-5.15232200	8.18429700	L		
H-H1-0.097600	-1	-6.13332700	-5.56631000	9.87731600	L		
H-H1-0.097600	-1	-4.57890900	-4.98815000	10.52366600	L		
H-H1-0.097600	-1	-4.72240300	-6.65152800	9.90784500	L		
C-CT--0.366200	-1	-0.50127700	-10.78472600	2.46324900	L		
C-C-0.597200	-1	-0.67772300	-9.84349700	1.25843000	L		
O-O--0.567900	-1	-1.78624700	-9.66518200	0.74883000	L		
H-HC-0.112300	-1	0.54644300	-10.80258600	2.75986900	L		
H-HC-0.112300	-1	-0.81831700	-11.79077600	2.18732000	L		
H-HC-0.112300	-1	-1.10917500	-10.42883300	3.29505800	L		
N-N--0.415700	-1	0.43880800	-9.30092200	0.75562400	L		
C-CT-0.014300	-1	0.39937300	-8.28321600	-0.29388900	L	H-HC 405	0.0000

C-C-0.597300	-1	0.02500400	-8.78959800	-1.70559900	L
O-O--0.567900	-1	-0.18264000	-7.96604700	-2.58740400	L
C-CT--0.204100	0	1.68830300	-7.42844700	-0.30446300	H
C-C-0.713000	0	1.33824700	-5.93724400	-0.45277000	H
O-O--0.593100	0	0.69427800	-5.37799900	0.43495100	H
N-N--0.919100	0	1.80513800	-5.27524400	-1.53570800	H
H-H-0.271900	-1	1.32060700	-9.49184500	1.20243500	L
H-H1-0.104800	-1	-0.40108100	-7.60816000	0.00939400	L
H-HC-0.079700	0	2.37190900	-7.80201600	-1.07543200	H
H-HC-0.079700	0	2.18046700	-7.51570200	0.66743900	H
H-H-0.419600	0	1.56104100	-4.28980200	-1.65648600	H
H-H-0.419600	0	2.20349200	-5.77643600	-2.31811800	H
N-N--0.415700	-1	-0.07599600	-10.10251000	-1.94331800	L
C-CT--0.149000	-1	-0.61727100	-10.65131700	-3.19880100	L
H-H-0.271900	-1	0.03087300	-10.75226600	-1.15629600	L
H-H1-0.097600	-1	-0.67828700	-9.86015400	-3.94538400	L
H-H1-0.097600	-1	-1.61234100	-11.05826000	-3.01876700	L
H-H1-0.097600	-1	0.03831900	-11.44406500	-3.56137800	L
C-CT--0.366200	-1	-3.89328700	-11.69671500	-1.43468300	L
C-C-0.597200	-1	-4.65510700	-10.36726500	-1.50751500	L
O-O--0.567900	-1	-5.79357400	-10.36531100	-1.97992100	L
H-HC-0.112300	-1	-2.90970300	-11.52725500	-0.99563100	L
H-HC-0.112300	-1	-3.77720900	-12.10452300	-2.43784600	L
H-HC-0.112300	-1	-4.45000500	-12.40095500	-0.81684700	L
N-N--0.415700	-1	-4.02332800	-9.24266300	-1.13169700	L
C-CT--0.087500	-1	-4.58144900	-7.87929700	-1.29550500	L
C-C-0.597300	-1	-4.84324700	-7.49597000	-2.76315600	L
O-O--0.567900	-1	-5.82884500	-6.82214200	-3.05982300	L
C-CT-0.298500	-1	-3.67041900	-6.80643800	-0.64327600	L
C-CT--0.319200	-1	-4.15122000	-5.36649700	-0.88446200	L
C-CT--0.319200	-1	-3.65733600	-6.94297700	0.87684200	L
H-H-0.271900	-1	-3.14238800	-9.35717400	-0.62855100	L
H-H1-0.096900	-1	-5.54277800	-7.85330300	-0.78377800	L
H-HC--0.029700	-1	-2.65487500	-6.90895100	-1.02619800	L
H-HC-0.079100	-1	-5.18702200	-5.26545800	-0.55956300	L
H-HC-0.079100	-1	-4.08090200	-5.11527700	-1.94015600	L
H-HC-0.079100	-1	-3.52175400	-4.66183600	-0.33895600	L
H-HC-0.079100	-1	-4.66370600	-6.80380000	1.25432100	L
H-HC-0.079100	-1	-2.99085000	-6.20003200	1.31728100	L
H-HC-0.079100	-1	-3.31278200	-7.92179400	1.17934600	L
N-N--0.415700	-1	-3.99718900	-7.89950500	-3.71920200	L
C-CT--0.149000	-1	-4.07956000	-7.48508900	-5.13054200	L
H-H-0.271900	-1	-3.27861900	-8.56563100	-3.46146600	L
H-H1-0.097600	-1	-4.89448900	-6.77120300	-5.25312100	L
H-H1-0.097600	-1	-4.26500600	-8.35897400	-5.75664600	L
H-H1-0.097600	-1	-3.14083400	-7.01850500	-5.42792700	L
C-CT--0.366200	-1	-12.08420000	3.72088800	-1.34695000	L
C-C-0.597200	-1	-10.98472500	2.65000500	-1.30895900	L
O-O--0.567900	-1	-11.28320100	1.46840200	-1.15389100	L
H-HC-0.112300	-1	-11.63129600	4.70189100	-1.49089400	L
H-HC-0.112300	-1	-12.63574800	3.70985000	-0.40646300	L
H-HC-0.112300	-1	-12.76743800	3.51139600	-2.17024000	L
N-N--0.415700	-1	-9.72617100	3.08522700	-1.37518400	L
C-CT--0.024900	-1	-8.54728800	2.25801400	-1.19385200	L

C-C-0.597300	-1	-7.43183800	3.11897200	-0.59566200	L		
O-O--0.567900	-1	-6.77471200	3.90406200	-1.29346000	L		
C-CT-0.211700	0	-8.12849400	1.60582400	-2.50988900	L		
O-OH--0.654600	0	-7.22318600	0.57883300	-2.21620900	L		
H-H-0.271900	-1	-9.59527200	4.08109100	-1.44565500	L		
H-H1-0.084300	-1	-8.78917900	1.46693800	-0.48541000	L		
H-H1-0.035200	0	-7.67283200	2.32947900	-3.18268700	L		
H-H1-0.035200	0	-9.00402500	1.16625900	-2.98987300	L		
H-HO-0.427500	0	-6.30034600	0.91575500	-2.27380000	L		
N-N--0.415700	-1	-7.27161200	3.04508200	0.73452100	L		
C-CT-0.021300	-1	-6.09466000	3.65558400	1.37129600	L		
C-C-0.597300	-1	-4.80849600	3.00295800	0.83949600	L		
O-O--0.567900	-1	-3.83021300	3.68676900	0.58003000	L		
C-CT--0.123100	-1	-6.15484900	3.52025900	2.89437000	L		
S-SH--0.311900	-1	-7.40445700	4.63246500	3.59998500	L		
H-H-0.271900	-1	-7.93561700	2.50172700	1.28288600	L		
H-H1-0.112400	-1	-6.06119100	4.71733600	1.12198800	L		
H-H1-0.111200	-1	-5.18303100	3.78930300	3.31175200	L		
H-H1-0.111200	-1	-6.37586700	2.48665000	3.15946600	L		
H-HS-0.193300	-1	-8.44771500	4.18871800	2.88964700	L		
N-N--0.415700	-1	-4.85235500	1.68423400	0.63405000	L	H-H1 478	0.0000
C-CT-0.021300	0	-3.66815900	0.99245600	0.06883700	H		
C-C-0.597300	0	-3.65071800	1.22204600	-1.43852200	H		
O-O--0.567900	0	-4.70047500	1.29001600	-2.08425700	H		
C-CT--0.123100	0	-3.69897400	-0.50972400	0.41224000	H		
S-SH--0.311900	0	-2.25064800	-1.52514000	-0.15924800	H		
H-H-0.271900	-1	-5.70575900	1.19983800	0.83908300	L		
H-H1-0.112400	0	-2.78392400	1.44565200	0.51592300	H		
H-H1-0.111200	0	-4.53161400	-1.00431200	-0.10348500	H		
H-H1-0.111200	0	-3.81977000	-0.66759300	1.48433200	H		
H-HS-0.193300	0	2.11103600	-0.02227500	0.19770700	H		
N-N--0.415700	0	-2.41695300	1.29334300	-2.00618100	H		
C-CT--0.087500	0	-2.27647400	1.39719000	-3.44924400	H		
C-C-0.597300	0	-2.20768400	0.03794700	-4.19953800	H		
O-O--0.567900	0	-2.32756000	0.04525800	-5.42224400	H		
C-CT-0.298500	-1	-1.09008800	2.28677200	-3.88545300	H		
C-CT--0.319200	0	-1.20379300	3.69762500	-3.30665100	L	H-HC 492	0.0000
C-CT--0.319200	0	0.26168000	1.69064400	-3.44139900	L	H-HC 492	0.0000
H-H-0.271900	0	-1.59622200	1.23060700	-1.39314300	H		
H-H1-0.096900	0	-3.21162200	1.83429700	-3.81633000	H		
H-HC--0.029700	0	-1.09810700	2.34312700	-4.97614700	H		
H-HC-0.079100	0	-1.07357800	3.67317200	-2.22221200	L		
H-HC-0.079100	0	-2.18090400	4.10660900	-3.54429400	L		
H-HC-0.079100	0	-0.43918500	4.33462100	-3.74665200	L		
H-HC-0.079100	0	0.35178900	1.70882300	-2.35296500	L		
H-HC-0.079100	0	1.07550100	2.26305900	-3.87649100	L		
H-HC-0.079100	0	0.36199700	0.65900400	-3.76886900	L		
N-N--0.415700	0	-1.94515100	-1.07419000	-3.45650700	H		
C-CT--0.003100	0	-2.04466900	-2.41983800	-4.02474500	H		
C-C-0.597300	0	-3.50931800	-2.86912000	-4.19190700	H		
O-O--0.567900	0	-3.81211500	-3.67065500	-5.06690400	H		
C-CT--0.003600	-1	-1.29298900	-3.45341700	-3.12741900	H		
C-CT--0.064500	-1	-1.43112700	-4.90724400	-3.61747100	L	H-HC 508	0.0000
C-C-0.695100	-1	-0.55780300	-5.24966900	-4.80974100	L		

O-O--0.608600	-1	-0.41177700	-4.49949900	-5.75986800	L		
N-N--0.940700	-1	0.05125700	-6.41590800	-4.80361400	L		
H-H-0.271900	0	-1.93570500	-1.00434500	-2.44150100	H		
H-H1-0.085000	0	-1.63088200	-2.39622800	-5.03568400	H		
H-HC-0.017100	0	-0.24380200	-3.18761400	-3.04202600	H		
H-HC-0.017100	0	-1.71901100	-3.41014500	-2.12237900	H		
H-HC-0.035200	-1	-2.46001200	-5.15829100	-3.85945300	L		
H-HC-0.035200	-1	-1.14928900	-5.55596100	-2.79550700	L		
H-H-0.425100	-1	0.65420200	-6.66677700	-5.56743800	L		
H-H-0.425100	-1	-0.06165800	-7.03617000	-4.00366600	L		
N-N--0.415700	0	-4.34899100	-2.47230400	-3.16703200	H		
C-CT--0.023700	0	-5.72997700	-2.93681600	-3.24947000	H		
C-C-0.597300	-1	-6.40264300	-2.31665800	-4.48986100	L	H-H1 522	0.0000
O-O--0.567900	-1	-6.22708300	-1.12212600	-4.74866000	L		
C-CT-0.034200	-1	-6.46656600	-2.65639000	-1.92331900	L	H-H1 522	0.0000
C-CT-0.001800	-1	-7.93661200	-3.10000700	-1.98135000	L		
S-S--0.273700	-1	-8.84164300	-3.07021300	-0.40664100	L		
C-CT--0.053600	-1	-9.20376900	-1.30090400	-0.27586800	L		
H-H-0.271900	0	-4.27772700	-1.49652200	-2.91798400	H		
H-H1-0.088000	0	-5.66366000	-4.01368400	-3.36541700	H		
H-HC-0.024100	-1	-6.39247100	-1.61021300	-1.66373100	L		
H-HC-0.024100	-1	-5.97579800	-3.21064100	-1.12683200	L		
H-H1-0.044000	-1	-7.96530100	-4.12556100	-2.35082000	L		
H-H1-0.044000	-1	-8.47391200	-2.47168000	-2.69203000	L		
H-H1-0.068400	-1	-9.80935800	-1.11367600	0.61080500	L		
H-H1-0.068400	-1	-9.75211300	-0.96965700	-1.15796500	L		
H-H1-0.068400	-1	-8.27181800	-0.74436600	-0.20360200	L		
N-N--0.254800	-1	-7.15377900	-3.08324700	-5.30206900	L		
C-CT--0.026600	-1	-7.54830700	-2.66513600	-6.64819600	L		
C-C-0.589600	-1	-8.99627000	-2.17620800	-6.64079200	L		
O-O--0.574800	-1	-9.88518300	-2.87330500	-6.14470500	L		
C-CT--0.007000	-1	-7.34586700	-3.90971000	-7.52693300	L		
C-CT-0.018900	-1	-6.83381800	-4.97427900	-6.55345200	L		
C-CT-0.019200	-1	-7.36526900	-4.51217000	-5.22307100	L		
H-H1-0.064100	-1	-6.89785700	-1.87050100	-7.01315600	L		
H-HC-0.025300	-1	-8.28111600	-4.22711900	-7.97913900	L		
H-HC-0.025300	-1	-6.60924100	-3.72780800	-8.30722300	L		
H-HC-0.021300	-1	-5.74570300	-4.97004400	-6.52658300	L		
H-HC-0.021300	-1	-7.21121400	-5.95542600	-6.76966200	L		
H-H1-0.039100	-1	-6.84330100	-5.02200000	-4.42499400	L		
H-H1-0.039100	-1	-8.43155400	-4.72900500	-5.14930900	L		
N-N--0.415700	-1	-9.21516700	-0.97879900	-7.17766700	L		
C-CT--0.149000	-1	-10.44617300	-0.20533000	-6.98840400	L		
H-H-0.271900	-1	-8.40855300	-0.51211300	-7.59180500	L		
H-H1-0.097600	-1	-11.20883100	-0.84070600	-6.53869800	L		
H-H1-0.097600	-1	-10.79815200	0.15733200	-7.95413200	L		
H-H1-0.097600	-1	-10.24481600	0.64175500	-6.33226300	L		
C-CT--0.366200	-1	-10.30070500	8.87450100	-4.25567400	L		
C-C-0.597200	-1	-9.75665200	7.58380300	-3.62906300	L		
O-O--0.567900	-1	-10.20112600	7.16541900	-2.55868300	L		
H-HC-0.112300	-1	-9.78106300	9.07050600	-5.19347300	L		
H-HC-0.112300	-1	-10.13944000	9.70617600	-3.57034400	L		
H-HC-0.112300	-1	-11.36760800	8.76358200	-4.44840300	L		
N-N--0.415700	-1	-8.78748900	6.95795600	-4.29152200	L		

C-CT--0.024900	-1	-7.84656100	6.03665300	-3.65093800	L
C-C-0.597300	-1	-6.51470200	6.76430400	-3.42908300	L
O-O--0.567900	-1	-6.25625600	7.77073000	-4.09652900	L
C-CT-0.211700	0	-7.62805300	4.78128800	-4.50754600	L
O-OH--0.654600	0	-7.25713900	5.09090100	-5.83781600	L
H-H-0.271900	-1	-8.51505000	7.32581300	-5.20208900	L
H-H1-0.084300	-1	-8.23408100	5.69874900	-2.68946000	L
H-H1-0.035200	0	-8.54984300	4.19847000	-4.52420400	L
H-H1-0.035200	0	-6.84318000	4.17491500	-4.05305400	L
H-HO-0.427500	0	-6.83326700	4.31504800	-6.22260500	L
N-N--0.415700	-1	-5.63913900	6.22977700	-2.56738100	L
C-CT-0.033700	-1	-4.26376600	6.73407800	-2.46337300	L
C-C-0.597300	-1	-3.51543000	6.73616700	-3.81541900	L
O-O--0.567900	-1	-2.61340400	7.54696500	-4.03207700	L
C-CT--0.182500	-1	-3.51339400	5.91025400	-1.42699500	L
H-H-0.271900	-1	-5.92491500	5.42557300	-2.00388100	L
H-H1-0.082300	-1	-4.30801700	7.76164900	-2.10096400	L
H-HC-0.060300	-1	-2.49862200	6.28836500	-1.32123700	L
H-HC-0.060300	-1	-3.48159700	4.86409300	-1.72948500	L
H-HC-0.060300	-1	-4.02917000	5.99541500	-0.47180600	L
N-N--0.415700	-1	-3.93913400	5.87084700	-4.75039500	L
C-CT--0.149000	-1	-3.42368400	5.81559700	-6.11718800	L
H-H-0.271900	-1	-4.66986800	5.22453400	-4.48367900	L
H-H1-0.097600	-1	-2.64769400	6.57098200	-6.24330900	L
H-H1-0.097600	-1	-4.23415200	6.00838100	-6.81995700	L
H-H1-0.097600	-1	-3.00421200	4.82775100	-6.30751100	L
C-CM--0.139000	0	0.46649600	-1.85183700	0.47105400	H
C-C-0.519000	0	1.19496800	-1.46552000	-0.81327000	H
O-O2--0.567000	0	1.86605600	-0.35609800	-0.81162400	H
C-CM--0.117000	0	-0.80089800	-1.08615300	0.92981300	H
O-O2--0.618000	0	1.20496100	-2.23022400	-1.79679000	H
C-C--0.553000	0	-0.70221400	0.44914400	1.06732800	H
O-O2--0.556000	0	-0.41216500	1.13812000	0.06232800	H
O-O2--0.607000	0	-1.02769200	0.89803800	2.21057600	H
H-HC-0.049000	0	0.23030000	-2.91447200	0.42393800	H
H-HC-0.162000	0	-1.04440700	-1.52432700	1.89557000	H
O-OW--0.834000	-1	6.46393400	2.92166300	-1.18070900	L
H-HW-0.417000	-1	6.83611000	3.06185900	-2.05058600	L
H-HW-0.417000	-1	7.14380700	3.21996900	-0.57693000	L
O-OW--0.834000	0	3.50681000	7.17466200	1.04110900	L
H-HW-0.417000	0	3.30091700	6.27809500	1.37849800	L
H-HW-0.417000	0	3.87400000	6.96249900	0.16584800	L
O-OW--0.834000	0	-1.57565500	-4.06566100	1.84221800	H
H-HW-0.417000	0	-0.88081100	-4.60067800	1.42500400	H
H-HW-0.417000	0	-2.08369400	-3.72355300	1.09074800	H
O-OW--0.834000	0	-4.98057500	0.79766100	-6.24477400	L
H-HW-0.417000	0	-4.04145000	0.58866700	-6.12196900	L
H-HW-0.417000	0	-5.42155500	0.16754200	-5.64957900	L
H-HS-0.193300	0	1.19126000	-1.71692200	1.28305300	H

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C-CT--0.366200	-1	8.20636100	4.68274400	-8.15779200	L
C-C-0.597200	-1	9.03959200	3.93912000	-7.11927200	L
O-O--0.567900	-1	9.64329200	2.90379700	-7.40233400	L

H-HC-0.112300	-1	7.76056300	5.56657600	-7.70167100	L
H-HC-0.112300	-1	7.41695900	4.02754200	-8.52778400	L
H-HC-0.112300	-1	8.84536500	4.98594400	-8.98801000	L
N-N--0.415700	-1	9.03328900	4.49584600	-5.90157800	L
C-CT--0.087500	-1	9.50739000	3.82021100	-4.68664600	L
C-C-0.597300	-1	8.37303700	2.91860300	-4.19556700	L
O-O--0.567900	-1	7.46090100	3.37466000	-3.49096700	L
C-CT-0.298500	-1	9.98707300	4.82252900	-3.60975900	L
C-CT--0.319200	-1	10.40956100	4.12289500	-2.31233600	L
C-CT--0.319200	-1	11.19869100	5.63505300	-4.08908700	L
H-H-0.271900	-1	8.44554600	5.31592100	-5.77296800	L
H-H1-0.096900	-1	10.34693000	3.18207800	-4.94210100	L
H-HC--0.029700	-1	9.18775100	5.52529800	-3.39203800	L
H-HC-0.079100	-1	11.11797200	3.32668000	-2.54284400	L
H-HC-0.079100	-1	9.54082800	3.69625800	-1.81474100	L
H-HC-0.079100	-1	10.88417000	4.83173000	-1.63567300	L
H-HC-0.079100	-1	12.06113000	4.98129700	-4.21904100	L
H-HC-0.079100	-1	11.44266400	6.40586500	-3.35592800	L
H-HC-0.079100	-1	10.97837900	6.11508700	-5.04156900	L
N-N--0.415700	-1	8.39357300	1.64659700	-4.62898700	L
C-CT--0.087500	-1	7.28377600	0.69063900	-4.45478800	L
C-C-0.597300	-1	7.70428500	-0.58462100	-3.69551700	L
O-O--0.567900	-1	8.85168400	-1.03225400	-3.82111200	L
C-CT-0.298500	-1	6.63112600	0.28326200	-5.80019700	L
C-CT--0.319200	-1	5.76946900	1.40772700	-6.38636000	L
C-CT--0.319200	-1	7.62490400	-0.16290500	-6.87789400	L
H-H-0.271900	-1	9.16959100	1.34405800	-5.22369400	L
H-H1-0.096900	-1	6.51140000	1.19425600	-3.88049100	L
H-HC--0.029700	-1	5.96484900	-0.56002800	-5.61477100	L
H-HC-0.079100	-1	6.28353400	2.36568900	-6.30938500	L
H-HC-0.079100	-1	4.83446800	1.45155900	-5.83235500	L
H-HC-0.079100	-1	5.52143900	1.19316000	-7.42715300	L
H-HC-0.079100	-1	8.22235400	0.68410100	-7.21102300	L
H-HC-0.079100	-1	7.07636000	-0.56671500	-7.72784800	L
H-HC-0.079100	-1	8.28195000	-0.93428200	-6.48433600	L
N-N--0.254800	-1	6.77056600	-1.19534600	-2.92821000	L
C-CT--0.026600	-1	6.90734400	-2.54867100	-2.38323300	L
C-C-0.589600	-1	7.15854500	-3.56979000	-3.49457200	L
O-O--0.574800	-1	6.41154600	-3.61866600	-4.47486200	L
C-CT--0.007000	0	5.57191400	-2.87205500	-1.69162000	L
C-CT-0.018900	0	4.82059900	-1.54910600	-1.59331800	L
C-CT-0.019200	0	5.44486400	-0.65815000	-2.64713300	L
H-H1-0.064100	-1	7.72608200	-2.56208300	-1.66465800	L
H-HC-0.025300	0	4.97758400	-3.56551200	-2.28829500	L
H-HC-0.025300	0	5.73429600	-3.30061100	-0.70665300	L
H-HC-0.021300	0	4.96674100	-1.10810200	-0.60801000	L
H-HC-0.021300	0	3.76161900	-1.67794100	-1.81010800	L
H-H1-0.039100	0	5.49711700	0.36000100	-2.25913700	L
H-H1-0.039100	0	4.83390500	-0.68767700	-3.55014000	L
N-N--0.415700	-1	8.18631300	-4.41241600	-3.34744000	L
C-CT--0.149000	-1	8.55911600	-5.40585500	-4.36723400	L
H-H-0.271900	-1	8.78516700	-4.28913500	-2.53209100	L
H-H1-0.097600	-1	7.81555400	-5.40728000	-5.16359300	L
H-H1-0.097600	-1	8.60424200	-6.39501400	-3.91051500	L

H-H1-0.097600	-1	9.53490300	-5.15289400	-4.78192300	L
C-CT--0.366200	-1	5.26663900	-7.40157100	-4.12465300	L
C-C-0.597200	-1	4.13515700	-6.73379200	-4.91624600	L
O-O--0.567900	-1	3.23992700	-7.45450000	-5.36672100	L
H-HC-0.112300	-1	5.97585100	-6.64311400	-3.79389800	L
H-HC-0.112300	-1	5.77740700	-8.12529600	-4.75966700	L
H-HC-0.112300	-1	4.84948100	-7.91105600	-3.25595400	L
N-N--0.415700	-1	4.11879800	-5.40283900	-5.05369900	L
C-CT-0.014300	-1	3.01425000	-4.65831600	-5.68316700	L H-HC 69
C-C-0.597300	-1	2.82137600	-4.99761100	-7.19592900	L
O-O--0.567900	-1	3.81665300	-5.15757700	-7.90397800	L
C-CT--0.204100	0	3.33046000	-3.16384900	-5.44383700	H
C-C-0.713000	0	2.13956400	-2.23375700	-5.63755000	H
O-O--0.593100	0	1.80680800	-1.79698800	-6.72829100	H
N-N--0.919100	-1	1.51652500	-1.85134800	-4.47239900	H
H-H-0.271900	-1	4.88509500	-4.86310300	-4.68489800	L
H-H1-0.104800	-1	2.10752600	-4.92594000	-5.15033200	L
H-HC-0.079700	0	4.11250000	-2.87442300	-6.15265000	H
H-HC-0.079700	0	3.73104700	-3.04885400	-4.43212200	H
H-H-0.419600	0	0.59045600	-1.46648900	-4.60716200	H
H-H-0.419600	0	1.66567100	-2.36891800	-3.61977400	H
N-N--0.415700	-1	1.56830400	-5.10048200	-7.68979600	L
C-CT--0.149000	-1	1.21777700	-5.35958500	-9.11599700	L
H-H-0.271900	-1	0.81193300	-4.87859600	-7.04339900	L
H-H1-0.097600	-1	2.12448900	-5.58059700	-9.67855100	L
H-H1-0.097600	-1	0.73417600	-4.47763800	-9.53688500	L
H-H1-0.097600	-1	0.53776700	-6.20949200	-9.17269300	L
C-CT--0.366200	-1	11.75268700	-5.88722200	-0.66739800	L
C-C-0.597200	-1	10.73701500	-6.01854900	0.47572700	L
O-O--0.567900	-1	11.05306300	-5.86408400	1.66063100	L
H-HC-0.112300	-1	11.25284900	-6.06334900	-1.61974800	L
H-HC-0.112300	-1	12.54724100	-6.62074800	-0.53318700	L
H-HC-0.112300	-1	12.17996200	-4.88424700	-0.66145000	L
N-N--0.415700	-1	9.50170100	-6.32632600	0.08344500	L
C-CT--0.023700	-1	8.34179300	-6.52918100	0.94658000	L
C-C-0.597300	-1	7.29077500	-7.37543200	0.24076600	L
O-O--0.567900	-1	7.11209900	-7.21543900	-0.97353400	L
C-CT-0.034200	0	7.72870200	-5.17028700	1.33190800	L
C-CT-0.001800	0	6.88721700	-5.17300600	2.62235900	L
S-S--0.273700	0	5.19907100	-5.85013800	2.55799800	L
C-CT--0.053600	0	4.26483100	-4.41616000	1.93979000	L
H-H-0.271900	-1	9.33371500	-6.39927100	-0.91394000	L
H-H1-0.088000	-1	8.66783800	-7.06116700	1.82868500	L
H-HC-0.024100	0	7.12986200	-4.78515600	0.50649000	L
H-HC-0.024100	0	8.55398100	-4.48031600	1.48386900	L
H-H1-0.044000	0	6.79980900	-4.14241600	2.96681700	L
H-H1-0.044000	0	7.44207100	-5.71755900	3.38632100	L
H-H1-0.068400	0	3.19838300	-4.64174300	1.92251200	L
H-H1-0.068400	0	4.57791100	-4.16568200	0.92881900	L
H-H1-0.068400	0	4.42198600	-3.55191000	2.58569400	L
N-N--0.415700	-1	6.58542100	-8.22470300	0.99824500	L
C-CT--0.149000	-1	5.36628500	-8.93452300	0.58280800	L
H-H-0.271900	-1	6.90162100	-8.35641200	1.95900000	L
H-H1-0.097600	-1	5.14862000	-8.70328300	-0.45940200	L

H-H1-0.097600	-1	4.53099300	-8.61813500	1.20774800	L
H-H1-0.097600	-1	5.51648000	-10.00810100	0.69302700	L
C-CT--0.366200	-1	3.93074000	-9.34531500	4.86273300	L
C-C-0.597200	-1	3.75755900	-7.94091500	5.47537700	L
O-O--0.567900	-1	4.71676500	-7.22175900	5.77021900	L
H-HC-0.112300	-1	2.95021500	-9.78930000	4.68773200	L
H-HC-0.112300	-1	4.49684800	-9.97481000	5.54905100	L
H-HC-0.112300	-1	4.46679400	-9.26581200	3.91685400	L
N-N--0.415700	-1	2.49455400	-7.53114100	5.62267800	L
C-CT--0.087500	-1	2.05304500	-6.12802700	5.57193500	L
C-C-0.597300	-1	1.92883400	-5.57234600	6.99700900	L
O-O--0.567900	-1	0.89202800	-5.67021600	7.66869800	L
C-CT-0.298500	0	0.72512600	-5.96534900	4.80087500	L
C-CT--0.319200	0	0.42833300	-4.48338400	4.55007700	L
C-CT--0.319200	0	0.76379600	-6.70081800	3.45465400	L
H-H-0.271900	-1	1.76128700	-8.22729300	5.46517200	L
H-H1-0.096900	-1	2.81700600	-5.55157900	5.04666600	L
H-HC--0.029700	0	-0.09134000	-6.39387600	5.38333600	L
H-HC-0.079100	0	1.17769400	-4.04716000	3.88615100	L
H-HC-0.079100	0	0.40769600	-3.92339100	5.48423900	L
H-HC-0.079100	0	-0.54812100	-4.37867100	4.07830500	L
H-HC-0.079100	0	1.64970400	-6.39143100	2.89996600	L
H-HC-0.079100	0	-0.12199000	-6.43997000	2.87281900	L
H-HC-0.079100	0	0.77530200	-7.77748500	3.60334100	L
N-N--0.415700	-1	3.08723500	-5.11662700	7.47324900	L
C-CT--0.149000	-1	3.46343600	-4.98304500	8.87799000	L
H-H-0.271900	-1	3.84635100	-5.02985400	6.80776400	L
H-H1-0.097600	-1	2.57697000	-5.09208100	9.50297300	L
H-H1-0.097600	-1	3.90610400	-4.00156700	9.04427000	L
H-H1-0.097600	-1	4.18676300	-5.75691400	9.13517400	L
C-CT--0.366200	-1	12.50630300	-4.20596900	6.31224400	L
C-C-0.597200	-1	12.29989500	-3.48135700	4.96357700	L
O-O--0.567900	-1	13.26651000	-3.26073400	4.22736400	L
H-HC-0.112300	-1	11.54719000	-4.30979500	6.81960700	L
H-HC-0.112300	-1	13.18545300	-3.62433100	6.93679200	L
H-HC-0.112300	-1	12.93180600	-5.19255400	6.13347600	L
N-N--0.415700	-1	11.06351800	-3.05817100	4.66148800	L
C-CT--0.023700	-1	10.78464000	-2.23248200	3.48881500	L
C-C-0.597300	-1	11.34905100	-0.80835700	3.62782800	L
O-O--0.567900	-1	12.07687600	-0.33954800	2.75087100	L
C-CT-0.034200	0	9.27760700	-2.15274100	3.21531400	L
C-CT-0.001800	0	9.03204900	-1.40579700	1.89434500	L
S-S--0.273700	0	7.51054400	-1.83216800	1.02315400	L
C-CT--0.053600	0	6.23439700	-1.10245700	2.07899900	L
H-H-0.271900	-1	10.29914300	-3.29028600	5.28935300	L
H-H1-0.088000	-1	11.25647600	-2.70929400	2.62795300	L
H-HC-0.024100	0	8.76039200	-1.64022200	4.02758700	L
H-HC-0.024100	0	8.88979400	-3.16379700	3.14875900	L
H-H1-0.044000	0	9.85068600	-1.63457000	1.21077400	L
H-H1-0.044000	0	9.04650600	-0.33049100	2.07743000	L
H-H1-0.068400	0	5.24879800	-1.38840000	1.70789600	L
H-H1-0.068400	0	6.30498100	-0.01523900	2.04913800	L
H-H1-0.068400	0	6.33800900	-1.45422100	3.10361800	L
N-N--0.415700	-1	11.07986500	-0.12281000	4.74438900	L

C-CT--0.149000	-1	11.63035800	1.21649000	4.97604200	L
H-H-0.271900	-1	10.50256300	-0.55634700	5.46438700	L
H-H1-0.097600	-1	12.21781400	1.52200000	4.11031500	L
H-H1-0.097600	-1	12.26786900	1.19918400	5.85958800	L
H-H1-0.097600	-1	10.81479100	1.92299000	5.13031900	L
C-CT--0.366200	-1	6.17422700	8.74769500	-5.56804700	L
C-C-0.597200	-1	6.49182000	7.55449900	-4.64521100	L
O-O--0.567900	-1	6.64551900	6.40721800	-5.08788100	L
H-HC-0.112300	-1	6.08071500	9.65513600	-4.97049500	L
H-HC-0.112300	-1	5.23715900	8.56183700	-6.09416800	L
H-HC-0.112300	-1	6.97927600	8.87160200	-6.29307000	L
N-N--0.415700	-1	6.63479000	7.86752500	-3.34716500	L
C-CT--0.001400	-1	6.67865300	6.87387700	-2.25902600	L
C-C-0.597300	-1	5.30499100	6.19135700	-2.11908200	L
O-O--0.567900	-1	4.43095600	6.66871100	-1.37815700	L
C-CT--0.001400	-1	7.19536300	7.50562200	-0.95329400	L
C-CA--0.001100	-1	7.88285200	6.53390600	-0.00007200	L
C-CA--0.190600	-1	9.29076800	6.48604200	0.04998500	L
C-CA--0.190600	-1	7.13856500	5.70968600	0.86893900	L
C-CA--0.234100	-1	9.94297000	5.66485500	0.98877800	L
C-CA--0.234100	-1	7.79514500	4.88342700	1.80745000	L
C-C-0.322600	-1	9.19758900	4.88360300	1.88597600	L
O-OH--0.557900	-1	9.85959400	4.13721900	2.81678100	L
H-H-0.271900	-1	6.56876700	8.85881700	-3.10342200	L
H-H1-0.087600	-1	7.39111500	6.10367200	-2.54079800	L
H-HC-0.029500	-1	7.91946400	8.27879700	-1.21301800	L
H-HC-0.029500	-1	6.38223400	8.01028300	-0.43005000	L
H-HA-0.169900	-1	9.87546100	7.11225900	-0.60878100	L
H-HA-0.169900	-1	6.05752300	5.71362500	0.82577000	L
H-HA-0.165600	-1	11.02028800	5.63732500	1.03757300	L
H-HA-0.165600	-1	7.22193500	4.24835100	2.46695600	L
H-HO-0.399200	-1	9.36376200	3.91125800	3.61985400	L
N-N--0.415700	-1	5.09472000	5.17170900	-2.95626400	L
C-CT-0.033700	-1	3.77889700	4.67513200	-3.34382900	L
C-C-0.597300	-1	2.94358800	4.03463900	-2.22434500	L
O-O--0.567900	-1	1.72000800	4.13362400	-2.29232000	L
C-CT--0.182500	-1	3.96898900	3.67913000	-4.48268500	L
H-H-0.271900	-1	5.87806100	4.88134900	-3.53644400	L
H-H1-0.082300	-1	3.21124300	5.51976300	-3.73559300	L
H-HC-0.060300	-1	2.99842100	3.36765000	-4.86781500	L
H-HC-0.060300	-1	4.50817200	2.81090600	-4.10365200	L
H-HC-0.060300	-1	4.53836800	4.14287800	-5.28833000	L
N-N--0.415700	-1	3.55914000	3.39165300	-1.22128700	L H-H1 209
C-CT-0.021300	0	2.85307400	2.68128700	-0.12395700	H
C-C-0.597300	0	2.32289500	3.71788400	0.88223900	H
O-O--0.567900	0	3.09158400	4.55701600	1.35014200	H
C-CT--0.123100	0	3.89685300	1.74411600	0.53946600	H
S-S--1.036000	0	3.22141800	0.48663700	1.70422300	H
H-H-0.271900	-1	4.56313500	3.36894000	-1.21400000	L
H-H1-0.112400	0	2.03904000	2.09133600	-0.55870700	H
H-H1-0.111200	0	4.61477900	2.37490700	1.07778300	H
H-H1-0.111200	0	4.46404100	1.22888900	-0.24727400	H
N-N--0.415700	0	0.99980600	3.65630900	1.22636800	H
C-CT--0.051800	0	0.42016600	4.50900900	2.27826000	H

C-C-0.597300	0	0.80234800	4.01363200	3.71194700	H
O-O--0.567900	0	1.38589700	4.73628400	4.51905700	H
C-CT--0.110200	-1	-1.11653000	4.62979400	2.01533600	H
C-CT-0.353100	-1	-1.97718400	5.53017100	2.92794500	L H-HC 222
C-CT--0.412100	-1	-2.16630200	4.97982800	4.34308800	L
C-CT--0.412100	-1	-1.44987400	6.96499100	3.01932000	L
H-H-0.271900	0	0.40881900	2.90968100	0.85901100	H
H-H1-0.092200	0	0.89100500	5.49226800	2.21015500	H
H-HC-0.045700	0	-1.23377800	5.00988200	0.99314600	H
H-HC-0.045700	0	-1.56340700	3.63276900	2.02352600	H
H-HC--0.036100	-1	-2.96924900	5.57703400	2.48037300	L
H-HC-0.100000	-1	-1.26728000	5.12177900	4.93919400	L
H-HC-0.100000	-1	-2.40863600	3.91898200	4.29962400	L
H-HC-0.100000	-1	-2.98655200	5.50957600	4.82513400	L
H-HC-0.100000	-1	-0.48742500	6.98272900	3.53163400	L
H-HC-0.100000	-1	-2.16279400	7.58049400	3.56658100	L
H-HC-0.100000	-1	-1.32802100	7.37014100	2.01389600	L
N-N--0.415700	0	0.48275900	2.71606300	3.98864200	H
C-CT--0.087500	0	0.59003700	2.15358100	5.33733600	H
C-C-0.597300	0	2.00654100	2.13612200	5.93300100	H
O-O--0.567900	0	2.11594700	2.15287800	7.15878900	H
C-CT-0.298500	-1	-0.01725900	0.72858600	5.35130800	H
C-CT--0.319200	0	0.71170700	-0.26745200	4.43031600	L H-HC 241
C-CT--0.319200	0	-0.15183500	0.08306100	6.73033400	L H-HC 241
H-H-0.271900	0	-0.07302600	2.21206700	3.30066300	H
H-H1-0.096900	0	0.02691100	2.79063500	6.03334900	H
H-HC--0.029700	0	-1.03166400	0.81466300	4.95574600	H
H-HC-0.079100	0	1.68234600	-0.54475500	4.83602100	L
H-HC-0.079100	0	0.86788400	0.18508800	3.45143600	L
H-HC-0.079100	0	0.10198300	-1.15815300	4.28725400	L
H-HC-0.079100	0	0.83137600	-0.14922300	7.13760600	L
H-HC-0.079100	0	-0.72919800	-0.83660800	6.63856300	L
H-HC-0.079100	0	-0.67354300	0.76637200	7.39859800	L
N-N--0.415700	0	3.01930100	1.92641600	5.06899700	H
C-CT-0.033700	0	4.38402000	1.78605600	5.53746800	H
C-C-0.597300	-1	5.09651300	3.12112300	5.81068500	L H-H1 254
O-O--0.567900	-1	6.27177300	3.09840000	6.16604900	L
C-CT--0.182500	-1	5.16069200	0.97729200	4.50071000	L H-H1 254
H-H-0.271900	0	2.86500400	1.90938500	4.06525700	H
H-H1-0.082300	0	4.37439400	1.24060800	6.48663100	H
H-HC-0.060300	-1	6.12845600	0.68550100	4.90586700	L
H-HC-0.060300	-1	5.31552800	1.58131300	3.60695800	L
H-HC-0.060300	-1	4.60436500	0.07453800	4.24513900	L
N-N--0.415700	-1	4.39106900	4.24809300	5.64960400	L
C-CT--0.087500	-1	4.77170400	5.61042400	6.04950900	L
C-C-0.597300	-1	3.92969200	6.05320600	7.25329000	L
O-O--0.567900	-1	4.48156800	6.50200000	8.25900900	L
C-CT-0.298500	-1	4.55443100	6.58847600	4.87749200	L
C-CT--0.319200	-1	4.94606000	8.02689500	5.23310400	L
C-CT--0.319200	-1	5.37174400	6.19759800	3.64656600	L
H-H-0.271900	-1	3.47978600	4.13315400	5.22366100	L
H-H1-0.096900	-1	5.82174600	5.64042100	6.33046300	L
H-HC--0.029700	-1	3.50187800	6.57489400	4.60221800	L
H-HC-0.079100	-1	5.99666600	8.06552100	5.51257900	L

H-HC-0.079100	-1	4.33956400	8.40070000	6.05730900	L
H-HC-0.079100	-1	4.78381100	8.66819400	4.36711200	L
H-HC-0.079100	-1	6.42215800	6.12039700	3.92125600	L
H-HC-0.079100	-1	5.25326900	6.94727100	2.86464200	L
H-HC-0.079100	-1	5.02086800	5.24099600	3.25937800	L
N-N--0.415700	-1	2.59866800	5.86036400	7.19983800	L
C-CT--0.149000	-1	1.69145500	6.19527600	8.30823300	L
H-H-0.271900	-1	2.19204800	5.48142100	6.35002700	L
H-H1-0.097600	-1	2.26893800	6.58889200	9.14477000	L
H-H1-0.097600	-1	1.15734400	5.29860600	8.62417000	L
H-H1-0.097600	-1	0.97475000	6.94669800	7.97697300	L
C-CT--0.366200	-1	4.03849100	10.31983900	-0.99282100	L
C-C-0.597200	-1	2.56410400	9.99147700	-1.23761500	L
O-O--0.567900	-1	1.75304300	10.90521100	-1.30729400	L
H-HC-0.112300	-1	4.61545100	9.39667300	-0.95977600	L
H-HC-0.112300	-1	4.13988200	10.84637800	-0.04402800	L
H-HC-0.112300	-1	4.40870700	10.95107900	-1.80028800	L
N-N--0.415700	-1	2.18742600	8.70806700	-1.29662800	L
C-CT--0.024900	-1	0.77483500	8.32363500	-1.13785300	L
C-C-0.597300	-1	0.18785800	8.81651300	0.19050200	L
O-O--0.567900	-1	-0.90753100	9.38221700	0.20053500	L
C-CT-0.211700	0	0.60757700	6.82435600	-1.28878700	L
O-OH--0.654600	0	0.90020600	6.52263800	-2.63332700	L
H-H-0.271900	-1	2.89103900	7.97674000	-1.35959400	L
H-H1-0.084300	-1	0.20118500	8.77493600	-1.94313300	L
H-H1-0.035200	0	-0.41605100	6.53335800	-1.06115100	L
H-H1-0.035200	0	1.29058400	6.29676700	-0.62101100	L
H-HO-0.427500	0	1.00604000	5.54786000	-2.64854100	L
N-N--0.415700	-1	0.95111900	8.68030700	1.28555100	L
C-CT-0.033700	-1	0.59715100	9.15739000	2.62365500	L
C-C-0.597300	-1	0.12995900	10.61781300	2.61922900	L
O-O--0.567900	-1	-0.96676700	10.93314400	3.08340800	L
C-CT--0.182500	-1	1.78459900	8.91994600	3.55419900	L
H-H-0.271900	-1	1.84041100	8.18575600	1.17850900	L
H-H1-0.082300	-1	-0.21644400	8.56281500	3.01220200	L
H-HC-0.060300	-1	1.55456300	9.28745400	4.55359600	L
H-HC-0.060300	-1	2.66907000	9.42405300	3.16689600	L
H-HC-0.060300	-1	1.98162600	7.85095000	3.60564500	L
N-N--0.415700	-1	0.92634400	11.49981500	2.00548500	L
C-CT--0.149000	-1	0.58344000	12.89732600	1.81658200	L
H-H-0.271900	-1	1.82921800	11.19428700	1.65048500	L
H-H1-0.097600	-1	-0.40272400	13.08956400	2.24069500	L
H-H1-0.097600	-1	0.57208300	13.12856200	0.75231100	L
H-H1-0.097600	-1	1.32203700	13.52377300	2.31775200	L
C-CT--0.366200	-1	-11.92201900	4.54555000	4.95743300	L
C-C-0.597200	-1	-12.35229800	3.12651300	4.58252700	L
O-O--0.567900	-1	-12.91583800	2.41544800	5.41685400	L
H-HC-0.112300	-1	-11.44381800	5.01839400	4.09951200	L
H-HC-0.112300	-1	-11.21740500	4.50427000	5.78817100	L
H-HC-0.112300	-1	-12.79676600	5.12510800	5.25077600	L
N-N--0.415700	-1	-12.01810800	2.68932100	3.36808900	L
C-CT--0.087500	-1	-12.01166100	1.26782300	3.00526500	L
C-C-0.597300	-1	-10.56503800	0.87659100	2.68980200	L
O-O--0.567900	-1	-9.85132600	1.52375600	1.91586400	L

C-CT-0.298500	-1	-13.00769400	0.87871200	1.88029500	L
C-CT--0.319200	-1	-13.75248900	-0.41388200	2.26281600	L
C-CT--0.319200	-1	-14.08799000	1.92549300	1.57428200	L
H-H-0.271900	-1	-11.60935700	3.34293800	2.69764100	L
H-H1-0.096900	-1	-12.30278300	0.70563300	3.89017300	L
H-HC--0.029700	-1	-12.44902200	0.69231000	0.96677900	L
H-HC-0.079100	-1	-14.38474900	-0.23544700	3.13329500	L
H-HC-0.079100	-1	-13.03500400	-1.20548600	2.48259200	L
H-HC-0.079100	-1	-14.38908700	-0.72802300	1.43587900	L
H-HC-0.079100	-1	-14.72138400	2.06643400	2.44660700	L
H-HC-0.079100	-1	-14.69538000	1.59053900	0.73486300	L
H-HC-0.079100	-1	-13.63292500	2.87926000	1.31611400	L
N-N--0.415700	-1	-10.09919200	-0.14443100	3.41179300	L
C-CT--0.038900	-1	-8.69025500	-0.53910400	3.49212200	L
C-C-0.597300	-1	-8.55914500	-2.06460100	3.60141800	L
O-O--0.567900	-1	-9.48843200	-2.72805200	4.08301200	L
C-CT-0.365400	-1	-7.97415200	0.10653900	4.70220700	L
O-OH--0.676100	-1	-8.13993100	-0.61141400	5.90333300	L
C-CT--0.243800	-1	-8.39531500	1.54137700	5.01359300	L
H-H-0.271900	-1	-10.72733700	-0.62013500	4.04338600	L
H-H1-0.100700	-1	-8.19119400	-0.20235500	2.58354200	L
H-H1-0.004300	-1	-6.91522900	0.10917300	4.46522300	L
H-HC-0.064200	-1	-8.44042600	2.10826200	4.09119200	L
H-HC-0.064200	-1	-7.66769700	1.99810500	5.68577000	L
H-HC-0.064200	-1	-9.37839000	1.56469100	5.48296900	L
H-HO-0.410200	-1	-8.39232100	0.02568600	6.60386600	L
N-N--0.254800	-1	-7.43211800	-2.65601600	3.16621000	L
C-CT--0.026600	-1	-7.17817400	-4.08195800	3.33237000	L
C-C-0.589600	-1	-6.56819500	-4.43838100	4.68926900	L
O-O--0.574800	-1	-6.57665200	-5.61016100	5.04928600	L
C-CT--0.007000	0	-6.18554900	-4.41485400	2.21688600	L
C-CT-0.018900	0	-5.34893300	-3.14278200	2.09226600	L
C-CT-0.019200	0	-6.36154400	-2.03499200	2.38747900	L
H-H1-0.064100	-1	-8.08698200	-4.65397900	3.18696300	L
H-HC-0.025300	0	-5.56782300	-5.27402100	2.47102000	L
H-HC-0.025300	0	-6.72587400	-4.59291500	1.28633300	L
H-HC-0.021300	0	-4.91665600	-3.04439200	1.09738400	L
H-HC-0.021300	0	-4.56231800	-3.13996900	2.84728800	L
H-H1-0.039100	0	-6.76379900	-1.65775000	1.44692600	L
H-H1-0.039100	0	-5.87816200	-1.22852200	2.94027400	L
N-N--0.415700	-1	-5.95140000	-3.47699200	5.38451800	L
C-CT--0.001400	-1	-4.95877600	-3.71813700	6.44316700	L
C-C-0.597300	-1	-5.50431600	-4.50561500	7.64893900	L
O-O--0.567900	-1	-6.69087700	-4.39272500	7.96077300	L
C-CT--0.001400	0	-4.46140400	-2.39331700	7.04023100	L H-HA 373
C-CA--0.001100	0	-4.21565100	-1.28054100	6.05467200	H
C-CA--0.190600	0	-3.39091500	-1.50037400	4.95326000	H
C-CA--0.190600	0	-4.80704600	-0.02889800	6.24006500	H
C-CA--0.234100	0	-3.17414800	-0.48402700	4.03785700	H
C-CA--0.234100	0	-4.58323600	1.00322200	5.33341400	H
C-C-0.322600	0	-3.76468200	0.77660200	4.22308500	H
O-OH--0.557900	0	-3.58241100	1.78028100	3.33911100	H
H-H-0.271900	-1	-6.02113900	-2.53745800	5.02520600	L
H-H1-0.087600	-1	-4.13291500	-4.28378600	6.01037300	L

H-HC-0.029500	0	-5.19993400	-2.04004100	7.76259200	L
H-HC-0.029500	0	-3.53523100	-2.57799200	7.58595800	L
H-HA-0.169900	0	-2.91904600	-2.46710600	4.79343000	H
H-HA-0.169900	0	-5.45023400	0.15441300	7.10139700	H
H-HA-0.165600	0	-2.50777700	-0.62798600	3.20410500	H
H-HA-0.165600	0	-5.01083100	1.99129100	5.48562100	H
H-HO-0.399200	0	-2.70650600	1.66210500	2.88956100	H
N-N--0.415700	-1	-4.62360600	-5.19500800	8.40075300	L
C-CT--0.149000	-1	-5.00617300	-5.66537000	9.74857500	L
H-H-0.271900	-1	-3.62902700	-5.18514900	8.16054400	L
H-H1-0.097600	-1	-6.08996100	-5.61801900	9.85564700	L
H-H1-0.097600	-1	-4.53828200	-5.03189500	10.50141200	L
H-H1-0.097600	-1	-4.67242700	-6.69469300	9.88193800	L
C-CT--0.366200	-1	-0.43554000	-10.78503900	2.42264100	L
C-C-0.597200	-1	-0.61921300	-9.84214000	1.22021500	L
O-O--0.567900	-1	-1.72944200	-9.66940300	0.71239400	L
H-HC-0.112300	-1	0.61264300	-10.79719700	2.71792700	L
H-HC-0.112300	-1	-0.74679800	-11.79236600	2.14478800	L
H-HC-0.112300	-1	-1.04455500	-10.43476100	3.25602400	L
N-N--0.415700	-1	0.49336200	-9.29163200	0.71727800	L
C-CT-0.014300	-1	0.44646400	-8.27167300	-0.32985800	L H-HC 405
C-C-0.597300	-1	0.07337900	-8.77719000	-1.74224700	L
O-O--0.567900	-1	-0.14037000	-7.95290400	-2.62190400	L
C-CT--0.204100	0	1.79461700	-7.52110000	-0.34973300	H
C-C-0.713000	0	1.55228800	-6.01901600	-0.42038400	H
O-O--0.593100	0	1.11066500	-5.44607300	0.57353600	H
N-N--0.919100	0	1.86780000	-5.37592300	-1.56591500	H
H-H-0.271900	-1	1.37686600	-9.47820800	1.16255500	L
H-H1-0.104800	-1	-0.35773700	-7.60230700	-0.02402100	L
H-HC-0.079700	0	2.42021500	-7.90897400	-1.16331500	H
H-HC-0.079700	0	2.31518000	-7.68559700	0.59636100	H
H-H-0.419600	0	1.61477800	-4.38372300	-1.60153100	H
H-H-0.419600	0	2.05973400	-5.89674500	-2.41147100	H
N-N--0.415700	-1	-0.01992400	-10.09014100	-1.98286200	L
C-CT--0.149000	-1	-0.55942300	-10.63935700	-3.23894100	L
H-H-0.271900	-1	0.09188000	-10.74104000	-1.19747100	L
H-H1-0.097600	-1	-0.62618600	-9.84686700	-3.98362600	L
H-H1-0.097600	-1	-1.55177000	-11.05275800	-3.05860600	L
H-H1-0.097600	-1	0.10052800	-11.42726200	-3.60414600	L
C-CT--0.366200	-1	-3.82680500	-11.70871400	-1.47317800	L
C-C-0.597200	-1	-4.59679100	-10.38376700	-1.54200800	L
O-O--0.567900	-1	-5.73584500	-10.38765700	-2.01300800	L
H-HC-0.112300	-1	-2.84372100	-11.53428100	-1.03495800	L
H-HC-0.112300	-1	-3.70950800	-12.11350800	-2.47742600	L
H-HC-0.112300	-1	-4.37846100	-12.41774700	-0.85628100	L
N-N--0.415700	-1	-3.97140100	-9.25620900	-1.16438600	L
C-CT--0.087500	-1	-4.53800700	-7.89589300	-1.32437000	L
C-C-0.597300	-1	-4.80396700	-7.51079900	-2.79080900	L
O-O--0.567900	-1	-5.79401600	-6.84230200	-3.08471100	L
C-CT-0.298500	-1	-3.63270800	-6.81900500	-0.67079800	L
C-CT--0.319200	-1	-4.12256400	-5.38146700	-0.90807900	L
C-CT--0.319200	-1	-3.61689200	-6.95893900	0.84898800	L
H-H-0.271900	-1	-3.08914500	-9.36650700	-0.66259400	L
H-H1-0.096900	-1	-5.49884000	-7.87692200	-0.81139700	L

H-HC--0.029700	-1	-2.61703400	-6.91445300	-1.05521900	L
H-HC-0.079100	-1	-5.15855200	-5.28748300	-0.58167400	L
H-HC-0.079100	-1	-4.05509000	-5.12740000	-1.96327700	L
H-HC-0.079100	-1	-3.49671200	-4.67424200	-0.36173200	L
H-HC-0.079100	-1	-4.62361600	-6.82676400	1.22802300	L
H-HC-0.079100	-1	-2.95439600	-6.21296600	1.29030500	L
H-HC-0.079100	-1	-3.26601600	-7.93633500	1.14880900	L
N-N--0.415700	-1	-3.95666300	-7.90697700	-3.74882800	L
C-CT--0.149000	-1	-4.04331600	-7.48984100	-5.15910500	L
H-H-0.271900	-1	-3.23373800	-8.56931200	-3.49351200	L
H-H1-0.097600	-1	-4.86272700	-6.78064500	-5.27903400	L
H-H1-0.097600	-1	-4.22422400	-8.36339700	-5.78699300	L
H-H1-0.097600	-1	-3.10782300	-7.01687000	-5.45657800	L
C-CT--0.366200	-1	-12.11126100	3.65849700	-1.33985000	L
C-C-0.597200	-1	-11.00523900	2.59424100	-1.30568300	L
O-O--0.567900	-1	-11.29632300	1.41049800	-1.15296500	L
H-HC-0.112300	-1	-11.66450500	4.64257600	-1.48209500	L
H-HC-0.112300	-1	-12.66154900	3.64194500	-0.39871600	L
H-HC-0.112300	-1	-12.79423100	3.44674500	-2.16277300	L
N-N--0.415700	-1	-9.74944400	3.03727400	-1.37246500	L
C-CT--0.024900	-1	-8.56531600	2.21684100	-1.19449200	L
C-C-0.597300	-1	-7.45438000	3.08319900	-0.59570600	L
O-O--0.567900	-1	-6.80292100	3.87386400	-1.29250100	L
C-CT-0.211700	0	-8.15167300	1.57041300	-2.51495000	L
O-OH--0.654600	0	-7.24229500	0.54443800	-2.23347000	L
H-H-0.271900	-1	-9.62468800	4.03406900	-1.44080500	L
H-H1-0.084300	-1	-8.80151200	1.42268000	-0.48757300	L
H-H1-0.035200	0	-7.70215500	2.29825900	-3.18726100	L
H-H1-0.035200	0	-9.02872600	1.13071500	-2.99204200	L
H-HO-0.427500	0	-6.32284800	0.89068000	-2.29216700	L
N-N--0.415700	-1	-7.29204400	3.00723200	0.73411000	L
C-CT-0.021300	-1	-6.11803500	3.62342400	1.37083500	L
C-C-0.597300	-1	-4.82859400	2.97986000	0.83593900	L
O-O--0.567900	-1	-3.85481000	3.67020200	0.57684000	L
C-CT--0.123100	-1	-6.17550000	3.48424500	2.89366700	L
S-SH--0.311900	-1	-7.43096600	4.58719900	3.60337900	L
H-H-0.271900	-1	-7.95204600	2.45859000	1.28204800	L
H-H1-0.112400	-1	-6.09134100	4.68593100	1.12392800	L
H-H1-0.111200	-1	-5.20481400	3.75823300	3.31046300	L
H-H1-0.111200	-1	-6.38989500	2.44870000	3.15665900	L
H-HS-0.193300	-1	-8.47239500	4.13873700	2.89331800	L
N-N--0.415700	-1	-4.86468000	1.66138200	0.62750100	L H-H1 478
C-CT-0.021300	0	-3.70437500	0.98610800	0.01878700	H
C-C-0.597300	0	-3.70053800	1.24044900	-1.48109300	H
O-O--0.567900	0	-4.74506600	1.31280000	-2.13232200	H
C-CT--0.123100	0	-3.69214800	-0.52729100	0.31756400	H
S-SH--0.311900	0	-2.16392700	-1.43681900	-0.23307900	H
H-H-0.271900	-1	-5.71487200	1.17131300	0.83249100	L
H-H1-0.112400	0	-2.82250300	1.44913500	0.45025500	H
H-H1-0.111200	0	-4.49160500	-1.04057400	-0.23032200	H
H-H1-0.111200	0	-3.83041400	-0.72407900	1.38169200	H
H-HS-0.193300	0	2.87006500	-1.40992500	0.74738100	H
N-N--0.415700	0	-2.46248500	1.31388700	-2.04094100	H
C-CT--0.087500	0	-2.30742700	1.41229800	-3.48013900	H

C-C-0.597300	0	-2.25140100	0.04876400	-4.23065200	H
O-O--0.567900	0	-2.45008400	0.04644500	-5.44052200	H
C-CT-0.298500	-1	-1.11186900	2.29710500	-3.89521000	H
C-CT--0.319200	0	-1.23537700	3.70816000	-3.31723900	L H-HC 492
C-CT--0.319200	0	0.23404000	1.70142300	-3.43978400	L H-HC 492
H-H-0.271900	0	-1.65595800	1.27897400	-1.41090600	H
H-H1-0.096900	0	-3.23393600	1.85627900	-3.85980800	H
H-HC--0.029700	0	-1.10267200	2.35887900	-4.98623200	H
H-HC-0.079100	0	-1.11633600	3.68686500	-2.23145900	L
H-HC-0.079100	0	-2.21173700	4.11416100	-3.56399400	L
H-HC-0.079100	0	-0.47039300	4.34887100	-3.75127000	L
H-HC-0.079100	0	0.30334700	1.70511700	-2.34930700	L
H-HC-0.079100	0	1.04911200	2.28641700	-3.85646200	L
H-HC-0.079100	0	0.34247200	0.67908800	-3.79296900	L
N-N--0.415700	0	-1.90821200	-1.05725900	-3.49896000	H
C-CT--0.003100	0	-2.02859700	-2.41050400	-4.05331600	H
C-C-0.597300	0	-3.49579800	-2.86258300	-4.21141300	H
O-O--0.567900	0	-3.79280600	-3.66697500	-5.08532200	H
C-CT--0.003600	-1	-1.27880500	-3.44586500	-3.15016000	H
C-CT--0.064500	-1	-1.40873300	-4.89939500	-3.64338100	L H-HC 508
C-C-0.695100	-1	-0.53482800	-5.23376900	-4.83752100	L
O-O--0.608600	-1	-0.39455400	-4.48054300	-5.78609600	L
N-N--0.940700	-1	0.08132100	-6.39628200	-4.83482900	L
H-H-0.271900	0	-1.88372300	-0.98306300	-2.48242600	H
H-H1-0.085000	0	-1.62647900	-2.39859600	-5.07001800	H
H-HC-0.017100	0	-0.22816500	-3.18972600	-3.05789700	H
H-HC-0.017100	0	-1.69885000	-3.40158400	-2.14456500	H
H-HC-0.035200	-1	-2.43637600	-5.15614500	-3.88467600	L
H-HC-0.035200	-1	-1.12192200	-5.54827100	-2.82326100	L
H-H-0.425100	-1	0.68483000	-6.64172900	-5.59996900	L
H-H-0.425100	-1	-0.02682500	-7.01906000	-4.03617200	L
N-N--0.415700	0	-4.33706900	-2.47320700	-3.18467200	H
C-CT--0.023700	0	-5.71574000	-2.95325200	-3.26579000	H
C-C-0.597300	-1	-6.39700900	-2.33712900	-4.50366900	L H-H1 522
O-O--0.567900	-1	-6.22903500	-1.14096000	-4.75993500	L
C-CT-0.034200	-1	-6.45564800	-2.68312300	-1.93783900	L H-H1 522
C-CT-0.001800	-1	-7.92303800	-3.13554700	-1.99507000	L
S-S--0.273700	-1	-8.82627000	-3.11487500	-0.41917800	L
C-CT--0.053600	-1	-9.19898800	-1.34810700	-0.28388500	L
H-H-0.271900	0	-4.27996500	-1.49491700	-2.94093300	H
H-H1-0.088000	0	-5.63865700	-4.02907400	-3.38539700	H
H-HC-0.024100	-1	-6.38759300	-1.63712000	-1.67593600	L
H-HC-0.024100	-1	-5.96052400	-3.23620100	-1.14323500	L
H-H1-0.044000	-1	-7.94594900	-4.16041200	-2.36685700	L
H-H1-0.044000	-1	-8.46503800	-2.50887600	-2.70363800	L
H-H1-0.068400	-1	-9.80459600	-1.16660300	0.60396300	L
H-H1-0.068400	-1	-9.75044100	-1.01818500	-1.16453900	L
H-H1-0.068400	-1	-8.27035100	-0.78607200	-0.21149500	L
N-N--0.254800	-1	-7.14447700	-3.10640800	-5.31670200	L
C-CT--0.026600	-1	-7.54322200	-2.68761900	-6.66138000	L
C-C-0.589600	-1	-8.99411800	-2.20753000	-6.65106500	L
O-O--0.574800	-1	-9.87816100	-2.91116400	-6.15547900	L
C-CT--0.007000	-1	-7.33431500	-3.92892500	-7.54323100	L
C-CT-0.018900	-1	-6.81458200	-4.99258800	-6.57282800	L

C-CT-0.019200	-1	-7.34716400	-4.53676900	-5.24073900	L
H-H1-0.064100	-1	-6.89807900	-1.88821100	-7.02531500	L
H-HC-0.025300	-1	-8.26817700	-4.25098400	-7.99500500	L
H-HC-0.025300	-1	-6.59978300	-3.74075600	-8.32400600	L
H-HC-0.021300	-1	-5.72647600	-4.98178400	-6.54730000	L
H-HC-0.021300	-1	-7.18626600	-5.97551600	-6.79083700	L
H-H1-0.039100	-1	-6.82111400	-5.04524100	-4.44447600	L
H-H1-0.039100	-1	-8.41202700	-4.76025900	-5.16615600	L
N-N--0.415700	-1	-9.22097100	-1.01025100	-7.18490900	L
C-CT--0.149000	-1	-10.45642800	-0.24473000	-6.99234600	L
H-H-0.271900	-1	-8.41773000	-0.53772100	-7.59896900	L
H-H1-0.097600	-1	-11.21463500	-0.88576600	-6.54315800	L
H-H1-0.097600	-1	-10.81181300	0.11800100	-7.95680100	L
H-H1-0.097600	-1	-10.25940400	0.60206000	-6.33450900	L
C-CT--0.366200	-1	-10.36278900	8.82953200	-4.23891400	L
C-C-0.597200	-1	-9.81011000	7.54073400	-3.61595200	L
O-O--0.567900	-1	-10.25069400	7.11719900	-2.54598200	L
H-HC-0.112300	-1	-9.84551400	9.03084800	-5.17690000	L
H-HC-0.112300	-1	-10.20572500	9.66059300	-3.55187100	L
H-HC-0.112300	-1	-11.42923200	8.71256300	-4.43058200	L
N-N--0.415700	-1	-8.83797900	6.92232100	-4.28104300	L
C-CT--0.024900	-1	-7.89067000	6.00529800	-3.64374300	L
C-C-0.597300	-1	-6.56298700	6.74052600	-3.42185600	L
O-O--0.567900	-1	-6.31150000	7.75003400	-4.08730500	L
C-CT-0.211700	0	-7.66603400	4.75218600	-4.50203400	L
O-OH--0.654600	0	-7.29215700	5.06394500	-5.83089700	L
H-H-0.271900	-1	-8.56892700	7.29391500	-5.19109200	L
H-H1-0.084300	-1	-8.27492300	5.66282800	-2.68256900	L
H-H1-0.035200	0	-8.58588400	4.16640300	-4.52173300	L
H-H1-0.035200	0	-6.88039200	4.14774300	-4.04632400	L
H-HO-0.427500	0	-6.87756700	4.28465900	-6.21899600	L
N-N--0.415700	-1	-5.68311100	6.20936200	-2.56247200	L
C-CT-0.033700	-1	-4.31070100	6.72179200	-2.45900700	L
C-C-0.597300	-1	-3.56408700	6.73153700	-3.81196400	L
O-O--0.567900	-1	-2.66727500	7.54830200	-4.02787600	L
C-CT--0.182500	-1	-3.55404200	5.90017800	-1.42544800	L
H-H-0.271900	-1	-5.96328400	5.40214300	-2.00047300	L
H-H1-0.082300	-1	-4.36075400	7.74823900	-2.09418000	L
H-HC-0.060300	-1	-2.54144700	6.28421000	-1.32008100	L
H-HC-0.060300	-1	-3.51624800	4.85492300	-1.73038800	L
H-HC-0.060300	-1	-4.06912900	5.98000600	-0.46943900	L
N-N--0.415700	-1	-3.98368800	5.86580100	-4.74840300	L
C-CT--0.149000	-1	-3.46961300	5.81682300	-6.11595700	L
H-H-0.271900	-1	-4.71013000	5.21443800	-4.48227100	L
H-H1-0.097600	-1	-2.69839400	6.57720100	-6.24129800	L
H-H1-0.097600	-1	-4.28211600	6.00627800	-6.81727500	L
H-H1-0.097600	-1	-3.04437200	4.83198500	-6.30907000	L
C-CM--0.139000	0	0.57914400	-1.13015100	0.73923200	H
C-C-0.519000	0	1.27376800	-2.18510200	-0.05987500	H
O-O2--0.567000	0	2.56363200	-2.24851500	0.23422200	H
C-CM--0.117000	0	-0.90778100	-0.89775000	1.00840000	H
O-O2--0.618000	0	0.78362900	-2.84663000	-0.97420100	H
C-C--0.553000	0	-0.94873800	0.63532600	1.20400900	H
O-O2--0.556000	0	-0.62988500	1.35325300	0.22113500	H

O-O2--0.607000	0	-1.27204000	1.04662400	2.35368500	H
H-HC-0.049000	0	1.03835000	-1.15311600	1.72403600	H
H-HC-0.162000	0	-1.18143800	-1.43137400	1.91566900	H
O-OW--0.834000	-1	6.44159300	2.97181000	-1.19837800	L
H-HW-0.417000	-1	6.81182000	3.11626300	-2.06839000	L
H-HW-0.417000	-1	7.12039200	3.27287000	-0.59475100	L
O-OW--0.834000	0	3.43520000	7.15990700	1.03971300	L
H-HW-0.417000	0	3.25735900	6.26060200	1.38429500	L
H-HW-0.417000	0	3.80969700	6.95578500	0.16603300	L
O-OW--0.834000	0	-1.15728800	-3.98506400	1.57562300	H
H-HW-0.417000	0	-0.37830900	-4.41940600	1.18684000	H
H-HW-0.417000	0	-1.66942500	-3.69877100	0.80577300	H
O-OW--0.834000	0	-5.07949700	0.83600500	-6.23973500	L
H-HW-0.417000	0	-4.13879100	0.62581100	-6.13185600	L
H-HW-0.417000	0	-5.50980500	0.19156200	-5.65143700	L
H-HS-0.193300	0	0.98660300	-0.21481000	0.29810700	H

IC4'

C-CT--0.366200	-1	8.21064800	4.64676700	-8.14530600	L
C-C-0.597200	-1	9.04236500	3.90588400	-7.10361300	L
O-O--0.567900	-1	9.64545300	2.86913600	-7.38273600	L
H-HC-0.112300	-1	7.76518900	5.53246700	-7.69248900	L
H-HC-0.112300	-1	7.42102600	3.99100000	-8.51382000	L
H-HC-0.112300	-1	8.85062400	4.94669900	-8.97596200	L
N-N--0.415700	-1	9.03546900	4.46662900	-5.88777000	L
C-CT--0.087500	-1	9.50795700	3.79461300	-4.67020500	L
C-C-0.597300	-1	8.37243200	2.89556700	-4.17714000	L
O-O--0.567900	-1	7.46006300	3.35470000	-3.47484100	L
C-CT-0.298500	-1	9.98753800	4.80008100	-3.59621200	L
C-CT--0.319200	-1	10.40832300	4.10438000	-2.29612300	L
C-CT--0.319200	-1	11.20024400	5.61001900	-4.07716500	L
H-H-0.271900	-1	8.44829500	5.28760800	-5.76237500	L
H-H1-0.096900	-1	10.34719000	3.15494600	-4.92282400	L
H-HC--0.029700	-1	9.18861100	5.50422500	-3.38150400	L
H-HC-0.079100	-1	11.11627400	3.30682600	-2.52338800	L
H-HC-0.079100	-1	9.53880500	3.68010700	-1.79787800	L
H-HC-0.079100	-1	10.88293300	4.81505100	-1.62139000	L
H-HC-0.079100	-1	12.06225300	4.95512300	-4.20421400	L
H-HC-0.079100	-1	11.44422300	6.38304300	-3.34633900	L
H-HC-0.079100	-1	10.98115400	6.08709000	-5.03141400	L
N-N--0.415700	-1	8.39228800	1.62212100	-4.60634600	L
C-CT--0.087500	-1	7.28155000	0.66766100	-4.42995900	L
C-C-0.597300	-1	7.70034400	-0.60543600	-3.66612100	L
O-O--0.567900	-1	8.84747700	-1.05442700	-3.78924200	L
C-CT-0.298500	-1	6.62972700	0.25638800	-5.77458500	L
C-CT--0.319200	-1	5.76951300	1.37962500	-6.36519900	L
C-CT--0.319200	-1	7.62407000	-0.19415400	-6.84994000	L
H-H-0.271900	-1	9.16857100	1.31698300	-5.19937600	L
H-H1-0.096900	-1	6.50909400	1.17380700	-3.85799600	L
H-HC--0.029700	-1	5.96259200	-0.58573600	-5.58695700	L
H-HC-0.079100	-1	6.28430300	2.33741200	-6.29093900	L
H-HC-0.079100	-1	4.83406800	1.42605600	-5.81215500	L
H-HC-0.079100	-1	5.52220700	1.16182900	-7.40549400	L
H-HC-0.079100	-1	8.22250800	0.65125600	-7.18534200	L

H-HC-0.079100	-1	7.07592600	-0.60031100	-7.69903300	L
H-HC-0.079100	-1	8.28013200	-0.96477000	-6.45327000	L
N-N--0.254800	-1	6.76545400	-1.21285300	-2.89761700	L
C-CT--0.026600	-1	6.90063800	-2.56448700	-2.34806200	L
C-C-0.589600	-1	7.15195600	-3.58947100	-3.45580700	L
O-O--0.574800	-1	6.40576700	-3.64096400	-4.43658000	L
C-CT--0.007000	0	5.56268500	-2.87539800	-1.65909700	L
C-CT-0.018900	0	4.90637800	-1.51641400	-1.45111300	L
C-CT-0.019200	0	5.46071600	-0.65701700	-2.56761900	L
H-H1-0.064100	-1	7.71874500	-2.57620400	-1.62873500	L
H-HC-0.025300	0	4.91858900	-3.47297000	-2.30588400	L
H-HC-0.025300	0	5.71317200	-3.39733400	-0.71859500	L
H-HC-0.021300	0	5.18862900	-1.09717400	-0.48889500	L
H-HC-0.021300	0	3.83152500	-1.57256900	-1.54401700	L
H-H1-0.039100	0	5.53228200	0.37260500	-2.21511500	L
H-H1-0.039100	0	4.80209700	-0.71846000	-3.43520800	L
N-N--0.415700	-1	8.17889600	-4.43245700	-3.30500400	L
C-CT--0.149000	-1	8.55175900	-5.42956300	-4.32119400	L
H-H-0.271900	-1	8.77714600	-4.30698300	-2.48954600	L
H-H1-0.097600	-1	7.80888500	-5.43300000	-5.11818900	L
H-H1-0.097600	-1	8.59567100	-6.41724500	-3.86117800	L
H-H1-0.097600	-1	9.52811400	-5.17877600	-4.73586600	L
C-CT--0.366200	-1	5.25741900	-7.42174500	-4.07489400	L
C-C-0.597200	-1	4.12717800	-6.75564700	-4.86966800	L
O-O--0.567900	-1	3.23174100	-7.47709600	-5.31854000	L
H-HC-0.112300	-1	5.96697400	-6.66279000	-3.74602600	L
H-HC-0.112300	-1	5.76813700	-8.14798400	-4.70707300	L
H-HC-0.112300	-1	4.83908800	-7.92801800	-3.20488200	L
N-N--0.415700	-1	4.11204200	-5.42514300	-5.01152200	L
C-CT-0.014300	-1	3.00864700	-4.68176600	-5.64439800	L H-HC 69
C-C-0.597300	-1	2.81681100	-5.02591200	-7.15620300	L
O-O--0.567900	-1	3.81256900	-5.18903400	-7.86285600	L
C-CT--0.204100	0	3.31011500	-3.18205100	-5.42266500	H
C-C-0.713000	0	2.19815700	-2.25782500	-5.91030500	H
O-O--0.593100	0	2.09949500	-1.90346200	-7.07722900	H
N-N--0.919100	0	1.35885200	-1.79611000	-4.93103100	H
H-H-0.271900	-1	4.87846600	-4.88482600	-4.64383700	L
H-H1-0.104800	-1	2.10124900	-4.94690300	-5.11147500	L
H-HC-0.079700	0	4.21420000	-2.94122900	-5.99120800	H
H-HC-0.079700	0	3.51091000	-3.02354900	-4.35932500	H
H-H-0.419600	0	0.48423800	-1.42820600	-5.28645400	H
H-H-0.419600	0	1.34290800	-2.23658000	-4.02037800	H
N-N--0.415700	-1	1.56408200	-5.12937400	-7.65081600	L
C-CT--0.149000	-1	1.21457600	-5.39288900	-9.07645800	L
H-H-0.271900	-1	0.80733700	-4.90473300	-7.00581200	L
H-H1-0.097600	-1	2.12159400	-5.61650700	-9.63749400	L
H-H1-0.097600	-1	0.73207100	-4.51193500	-9.50067500	L
H-H1-0.097600	-1	0.53391300	-6.24242000	-9.13094300	L
C-CT--0.366200	-1	11.74172600	-5.90136200	-0.61701800	L
C-C-0.597200	-1	10.72495500	-6.02807900	0.52565300	L
O-O--0.567900	-1	11.04010600	-5.86996800	1.71031400	L
H-HC-0.112300	-1	11.24256700	-6.08021600	-1.56921500	L
H-HC-0.112300	-1	12.53555700	-6.63509900	-0.47970000	L
H-HC-0.112300	-1	12.16982600	-4.89872700	-0.61400500	L

N-N--0.415700	-1	9.48972700	-6.33612600	0.13331500	L
C-CT--0.023700	-1	8.32890400	-6.53517700	0.99610600	L
C-C-0.597300	-1	7.27779700	-7.38288200	0.29217000	L
O-O--0.567900	-1	7.10030400	-7.22674900	-0.92280400	L
C-CT-0.034200	0	7.71611400	-5.17369100	1.37434700	L
C-CT-0.001800	0	6.77677900	-5.18223100	2.59728200	L
S-S--0.273700	0	5.06376900	-5.75622500	2.36027800	L
C-CT--0.053600	0	4.20154700	-4.19527200	1.98326400	L
H-H-0.271900	-1	9.32254600	-6.41222300	-0.86397200	L
H-H1-0.088000	-1	8.65374500	-7.06451900	1.88024200	L
H-HC-0.024100	0	7.18886000	-4.75702100	0.51623600	L
H-HC-0.024100	0	8.54373200	-4.50856900	1.60223600	L
H-H1-0.044000	0	6.72050400	-4.16476100	2.98500400	L
H-H1-0.044000	0	7.23629800	-5.79308300	3.37422300	L
H-H1-0.068400	0	3.15327900	-4.38865900	1.74913400	L
H-H1-0.068400	0	4.65553700	-3.70194100	1.12751300	L
H-H1-0.068400	0	4.24599000	-3.52064300	2.83844200	L
N-N--0.415700	-1	6.57108300	-8.22906500	1.05183300	L
C-CT--0.149000	-1	5.35171800	-8.93924600	0.63768200	L
H-H-0.271900	-1	6.88634100	-8.35786600	2.01329500	L
H-H1-0.097600	-1	5.13514800	-8.71126500	-0.40547300	L
H-H1-0.097600	-1	4.51615000	-8.62010900	1.26085000	L
H-H1-0.097600	-1	5.50092900	-10.01257800	0.75157000	L
C-CT--0.366200	-1	3.91212900	-9.33473200	4.91769000	L
C-C-0.597200	-1	3.73958100	-7.92817700	5.52554900	L
O-O--0.567900	-1	4.69912500	-7.20884500	5.81884900	L
H-HC-0.112300	-1	2.93138700	-9.77848200	4.74330300	L
H-HC-0.112300	-1	4.47711900	-9.96243000	5.60657200	L
H-HC-0.112300	-1	4.44906800	-9.25879300	3.97201800	L
N-N--0.415700	-1	2.47678900	-7.51687800	5.67040000	L
C-CT--0.087500	-1	2.03649000	-6.11357100	5.61464800	L
C-C-0.597300	-1	1.91150400	-5.55309200	7.03777000	L
O-O--0.567900	-1	0.87403700	-5.64789200	7.70888100	L
C-CT-0.298500	0	0.71074200	-5.95685600	4.83866700	L
C-CT--0.319200	0	0.28922500	-4.48736300	4.73053300	L
C-CT--0.319200	0	0.82514900	-6.53203200	3.41907100	L
H-H-0.271900	-1	1.74308400	-8.21294000	5.51455500	L
H-H1-0.096900	-1	2.80137900	-5.53949300	5.08814400	L
H-HC--0.029700	0	-0.07447700	-6.50703600	5.35922800	L
H-HC-0.079100	0	1.01076800	-3.92205900	4.13618500	L
H-HC-0.079100	0	0.19492300	-4.02421000	5.71124700	L
H-HC-0.079100	0	-0.68219000	-4.42112000	4.24236800	L
H-HC-0.079100	0	1.63281600	-6.02921600	2.88460800	L
H-HC-0.079100	0	-0.10481800	-6.35080100	2.87773400	L
H-HC-0.079100	0	1.01058800	-7.60249100	3.44640800	L
N-N--0.415700	-1	3.06986900	-5.09676100	7.51351300	L
C-CT--0.149000	-1	3.44496300	-4.95885800	8.91813300	L
H-H-0.271900	-1	3.82963300	-5.01281200	6.84840600	L
H-H1-0.097600	-1	2.55786900	-5.06510100	9.54270200	L
H-H1-0.097600	-1	3.88830000	-3.97720300	9.08155900	L
H-H1-0.097600	-1	4.16742800	-5.73247200	9.17849600	L
C-CT--0.366200	-1	12.49068900	-4.19772000	6.35769600	L
C-C-0.597200	-1	12.28605100	-3.47739100	5.00646800	L
O-O--0.567900	-1	13.25348700	-3.25999500	4.27036900	L

H-HC-0.112300	-1	11.53105400	-4.29908100	6.86456300	L
H-HC-0.112300	-1	13.16978300	-3.61458500	6.98091000	L
H-HC-0.112300	-1	12.91553100	-5.18524000	6.18255100	L
N-N--0.415700	-1	11.05028800	-3.05418300	4.70191200	L
C-CT--0.023700	-1	10.77310900	-2.23213600	3.52627800	L
C-C-0.597300	-1	11.33858000	-0.80802500	3.66108500	L
O-O--0.567900	-1	12.06755400	-0.34271300	2.78321900	L
C-CT-0.034200	0	9.26419500	-2.15401000	3.25897000	L
C-CT-0.001800	0	9.01498600	-1.45832500	1.91216100	L
S-S--0.273700	0	7.44691600	-1.85123900	1.10960900	L
C-CT--0.053600	0	6.24117200	-0.99016100	2.15139900	L
H-H-0.271900	-1	10.28517700	-3.28359300	5.32987300	L
H-H1-0.088000	-1	11.24529700	-2.71217300	2.66740400	L
H-HC-0.024100	0	8.75582300	-1.60654500	4.05381400	L
H-HC-0.024100	0	8.86523400	-3.16340600	3.23488000	L
H-H1-0.044000	0	9.80061800	-1.75973000	1.21821400	L
H-H1-0.044000	0	9.08596100	-0.37758000	2.04219600	L
H-H1-0.068400	0	5.22826900	-1.19739200	1.79825300	L
H-H1-0.068400	0	6.40654700	0.08527400	2.09455300	L
H-H1-0.068400	0	6.32627100	-1.32693200	3.18280100	L
N-N--0.415700	-1	11.06899700	-0.11857900	4.77514500	L
C-CT--0.149000	-1	11.62039800	1.22102400	5.00286000	L
H-H-0.271900	-1	10.49071300	-0.54926100	5.49606600	L
H-H1-0.097600	-1	12.20885800	1.52319200	4.13663800	L
H-H1-0.097600	-1	12.25712800	1.20610600	5.88701100	L
H-H1-0.097600	-1	10.80528200	1.92870200	5.15409500	L
C-CT--0.366200	-1	6.17964300	8.72191400	-5.57074400	L
C-C-0.597200	-1	6.49544800	7.53150700	-4.64370300	L
O-O--0.567900	-1	6.64858200	6.38264800	-5.08245200	L
H-HC-0.112300	-1	6.08636800	9.63139900	-4.97627000	L
H-HC-0.112300	-1	5.24287900	8.53509500	-6.09706300	L
H-HC-0.112300	-1	6.98542200	8.84276500	-6.29547400	L
N-N--0.415700	-1	6.63755600	7.84869500	-3.34657300	L
C-CT--0.001400	-1	6.67965000	6.85860500	-2.25512600	L
C-C-0.597300	-1	5.30530600	6.17768700	-2.11412600	L
O-O--0.567900	-1	4.43102400	6.65820300	-1.37553800	L
C-CT--0.001400	-1	7.19575400	7.49422700	-0.95103600	L
C-CA--0.001100	-1	7.88161300	6.52509300	0.00598300	L
C-CA--0.190600	-1	9.28944400	6.47623100	0.05742000	L
C-CA--0.190600	-1	7.13589100	5.70435900	0.87705900	L
C-CA--0.234100	-1	9.94015100	5.65760600	0.99948300	L
C-CA--0.234100	-1	7.79097000	4.88065800	1.81885900	L
C-C-0.322600	-1	9.19334600	4.87993600	1.89860400	L
O-OH--0.557900	-1	9.85392600	4.13608000	2.83243900	L
H-H-0.271900	-1	6.57214300	8.84084100	-3.10615800	L
H-H1-0.087600	-1	7.39171900	6.08688600	-2.53373700	L
H-HC-0.029500	-1	7.92072100	8.26594400	-1.21267800	L
H-HC-0.029500	-1	6.38259300	8.00128100	-0.43016400	L
H-HA-0.169900	-1	9.87522500	7.09979000	-0.60289800	L
H-HA-0.169900	-1	6.05488800	5.70904900	0.83293900	L
H-HA-0.165600	-1	11.01740400	5.62934600	1.04930500	L
H-HA-0.165600	-1	7.21666500	4.24823400	2.47995900	L
H-HO-0.399200	-1	9.35721200	3.91317600	3.63582100	L
N-N--0.415700	-1	5.09491300	5.15545500	-2.94812200	L

C-CT-0.033700	-1	3.77901300	4.65869300	-3.33519200	L
C-C-0.597300	-1	2.94220600	4.02258600	-2.21432700	L
O-O--0.567900	-1	1.71876900	4.12235500	-2.28369100	L
C-CT--0.182500	-1	3.96926800	3.65878000	-4.47059100	L
H-H-0.271900	-1	5.87851400	4.86253700	-3.52666100	L
H-H1-0.082300	-1	3.21240000	5.50249500	-3.73023000	L
H-HC-0.060300	-1	2.99877400	3.34683600	-4.85553500	L
H-HC-0.060300	-1	4.50740300	2.79136700	-4.08822800	L
H-HC-0.060300	-1	4.53972800	4.11939800	-5.27726600	L
N-N--0.415700	-1	3.55651400	3.38252100	-1.20874400	L H-H1 209
C-CT-0.021300	0	2.79740300	2.68520100	-0.13326700	H
C-C-0.597300	0	2.32168100	3.72038400	0.89955300	H
O-O--0.567900	0	3.12661300	4.50213800	1.40469500	H
C-CT--0.123100	0	3.72374000	1.63258700	0.52047600	H
S-S--1.036000	0	2.88115500	0.48387500	1.69934600	H
H-H-0.271900	-1	4.56032400	3.35888200	-1.20038400	L
H-H1-0.112400	0	1.94032500	2.18178700	-0.59155200	H
H-H1-0.111200	0	4.51377100	2.16104200	1.06715200	H
H-H1-0.111200	0	4.22042900	1.05124200	-0.26652200	H
N-N--0.415700	0	0.99377600	3.70656900	1.21626700	H
C-CT--0.051800	0	0.41500900	4.53122900	2.28356700	H
C-C-0.597300	0	0.78856700	4.01184500	3.70780900	H
O-O--0.567900	0	1.33133100	4.73617200	4.54220500	H
C-CT--0.110200	-1	-1.12142300	4.63498600	2.01977800	H
C-CT-0.353100	-1	-1.98167400	5.53923400	2.92876400	L H-HC 222
C-CT--0.412100	-1	-2.17258300	4.99364900	4.34551300	L
C-CT--0.412100	-1	-1.45336400	6.97384400	3.01582900	L
H-H-0.271900	0	0.38413400	2.99607600	0.80603900	H
H-H1-0.092200	0	0.87231400	5.52301500	2.24106300	H
H-HC-0.045700	0	-1.24336600	5.00618000	0.99505700	H
H-HC-0.045700	0	-1.56481600	3.63668400	2.03897700	H
H-HC--0.036100	-1	-2.97342200	5.58537200	2.48014100	L
H-HC-0.100000	-1	-1.27396200	5.13682400	4.94192800	L
H-HC-0.100000	-1	-2.41575900	3.93286800	4.30533700	L
H-HC-0.100000	-1	-2.99280900	5.52566300	4.82509600	L
H-HC-0.100000	-1	-0.49134800	6.99247600	3.52891600	L
H-HC-0.100000	-1	-2.16624900	7.59173600	3.56043800	L
H-HC-0.100000	-1	-1.33030500	7.37557600	2.00918100	L
N-N--0.415700	0	0.49855700	2.70264900	3.96661600	H
C-CT--0.087500	0	0.58744400	2.16038600	5.32551100	H
C-C-0.597300	0	1.99549100	2.15103700	5.93704700	H
O-O--0.567900	0	2.09866400	2.17684600	7.16276200	H
C-CT-0.298500	-1	-0.02786200	0.74396200	5.36964300	H
C-CT--0.319200	0	0.68559400	-0.29821400	4.48302800	L H-HC 241
C-CT--0.319200	0	-0.17827800	0.13762000	6.76521200	L H-HC 241
H-H-0.271900	0	0.04771700	2.15119500	3.24142700	H
H-H1-0.096900	0	0.01969600	2.81934600	5.99605300	H
H-HC--0.029700	0	-1.04001900	0.83294100	4.97042000	H
H-HC-0.079100	0	1.67134800	-0.54014700	4.87374700	L
H-HC-0.079100	0	0.80875000	0.08478500	3.47068900	L
H-HC-0.079100	0	0.08602500	-1.20397500	4.40999600	L
H-HC-0.079100	0	0.79958000	-0.10516100	7.17931000	L
H-HC-0.079100	0	-0.77403700	-0.77223600	6.69665900	L
H-HC-0.079100	0	-0.68610300	0.84838800	7.41510800	L

N-N--0.415700	0	3.01222600	1.93939500	5.07890300	H
C-CT-0.033700	0	4.37363700	1.79941300	5.55352700	H
C-C-0.597300	-1	5.08741700	3.13377800	5.82554500	L H-H1 254
O-O--0.567900	-1	6.26234800	3.11127500	6.18199800	L
C-CT--0.182500	-1	5.15090500	0.98559200	4.52271700	L H-H1 254
H-H-0.271900	0	2.85123100	1.92250700	4.07714300	H
H-H1-0.082300	0	4.35947600	1.25616100	6.50373700	H
H-HC-0.060300	-1	6.11812000	0.69435000	4.92965500	L
H-HC-0.060300	-1	5.30706200	1.58654700	3.62709300	L
H-HC-0.060300	-1	4.59409800	0.08247200	4.26962000	L
N-N--0.415700	-1	4.38304200	4.26081100	5.66013100	L
C-CT--0.087500	-1	4.76446400	5.62413900	6.05587100	L
C-C-0.597300	-1	3.92177400	6.07158400	7.25745500	L
O-O--0.567900	-1	4.47315400	6.52323700	8.26216600	L
C-CT-0.298500	-1	4.54901600	6.59849700	4.88044600	L
C-CT--0.319200	-1	4.94152800	8.03775700	5.23165400	L
C-CT--0.319200	-1	5.36707100	6.20288700	3.65152600	L
H-H-0.271900	-1	3.47203500	4.14522200	5.23377800	L
H-H1-0.096900	-1	5.81428600	5.65419500	6.33763700	L
H-HC--0.029700	-1	3.49669000	6.58488100	4.60430500	L
H-HC-0.079100	-1	5.99192400	8.07644100	5.51191400	L
H-HC-0.079100	-1	4.33462800	8.41478300	6.05409300	L
H-HC-0.079100	-1	4.78055900	8.67633400	4.36341100	L
H-HC-0.079100	-1	6.41718100	6.12572600	3.92738400	L
H-HC-0.079100	-1	5.24989300	6.95007500	2.86703300	L
H-HC-0.079100	-1	5.01573600	5.24530500	3.26719100	L
N-N--0.415700	-1	2.59064000	5.87966700	7.20348200	L
C-CT--0.149000	-1	1.68274500	6.21898000	8.30997900	L
H-H-0.271900	-1	2.18444200	5.49825800	6.35457100	L
H-H1-0.097600	-1	2.25982900	6.61487800	9.14571400	L
H-H1-0.097600	-1	1.14761700	5.32380100	8.62840400	L
H-H1-0.097600	-1	0.96694800	6.96989900	7.97562200	L
C-CT--0.366200	-1	4.04125100	10.31090600	-1.00258400	L
C-C-0.597200	-1	2.56680700	9.98295500	-1.24757400	L
O-O--0.567900	-1	1.75656400	10.89712300	-1.32097100	L
H-HC-0.112300	-1	4.61741600	9.38737700	-0.96599400	L
H-HC-0.112300	-1	4.14225800	10.84048700	-0.05544600	L
H-HC-0.112300	-1	4.41268900	10.93917100	-1.81180600	L
N-N--0.415700	-1	2.18911800	8.69966900	-1.30268300	L
C-CT--0.024900	-1	0.77606700	8.31692700	-1.14386700	L
C-C-0.597300	-1	0.18834900	8.81467100	0.18234500	L
O-O--0.567900	-1	-0.90657800	9.38130900	0.18956000	L
C-CT-0.211700	0	0.60690000	6.81702700	-1.28928700	L
O-OH--0.654600	0	0.89874900	6.50935200	-2.63251300	L
H-H-0.271900	-1	2.89217600	7.96755900	-1.36262500	L
H-H1-0.084300	-1	0.20349100	8.76604700	-1.95113200	L
H-H1-0.035200	0	-0.41695700	6.52797400	-1.06026600	L
H-H1-0.035200	0	1.28901500	6.29070700	-0.61972400	L
H-HO-0.427500	0	1.00490400	5.53406800	-2.64188400	L
N-N--0.415700	-1	0.95055000	8.68144800	1.27849900	L
C-CT-0.033700	-1	0.59581700	9.16323200	2.61471500	L
C-C-0.597300	-1	0.12984200	10.62401900	2.60506800	L
O-O--0.567900	-1	-0.96702400	10.94178600	3.06725000	L
C-CT--0.182500	-1	1.78226200	8.92788000	3.54706600	L

H-H-0.271900	-1	1.83952400	8.18581400	1.17386000	L
H-H1-0.082300	-1	-0.21860400	8.57061800	3.00451300	L
H-HC-0.060300	-1	1.55166700	9.29887300	4.54504700	L
H-HC-0.060300	-1	2.66748600	9.42997600	3.15887400	L
H-HC-0.060300	-1	1.97836100	7.85889500	3.60221000	L
N-N--0.415700	-1	0.92748900	11.50333600	1.98911000	L
C-CT--0.149000	-1	0.58590500	12.90049700	1.79530100	L
H-H-0.271900	-1	1.83041600	11.19589200	1.63590400	L
H-H1-0.097600	-1	-0.40046300	13.09494800	2.21792100	L
H-H1-0.097600	-1	0.57566400	13.12823200	0.73026400	L
H-H1-0.097600	-1	1.32459300	13.52798400	2.29504500	L
C-CT--0.366200	-1	-11.92918700	4.56946100	4.95281200	L
C-C-0.597200	-1	-12.36031600	3.14955000	4.58221400	L
O-O--0.567900	-1	-12.92516900	2.44170600	5.41839200	L
H-HC-0.112300	-1	-11.44985200	5.03907500	4.09375300	L
H-HC-0.112300	-1	-11.22532700	4.53033800	5.78429200	L
H-HC-0.112300	-1	-12.80370700	5.15070600	5.24348200	L
N-N--0.415700	-1	-12.02544000	2.70807800	3.36951400	L
C-CT--0.087500	-1	-12.01985600	1.28538500	3.01138500	L
C-C-0.597300	-1	-10.57328500	0.89192200	2.69847100	L
O-O--0.567900	-1	-9.85836500	1.53594200	1.92302300	L
C-CT-0.298500	-1	-13.01523600	0.89339300	1.88684000	L
C-CT--0.319200	-1	-13.76143000	-0.39732100	2.27297400	L
C-CT--0.319200	-1	-14.09439900	1.94004900	1.57643800	L
H-H-0.271900	-1	-11.61556300	3.35914300	2.69727100	L
H-H1-0.096900	-1	-12.31221000	0.72635800	3.89789000	L
H-HC--0.029700	-1	-12.45592900	0.70351500	0.97443000	L
H-HC-0.079100	-1	-14.39429800	-0.21549200	3.14231200	L
H-HC-0.079100	-1	-13.04479700	-1.18878500	2.49598300	L
H-HC-0.079100	-1	-14.39757600	-0.71365900	1.44652500	L
H-HC-0.079100	-1	-14.72843000	2.08438900	2.44774400	L
H-HC-0.079100	-1	-14.70133800	1.60283000	0.73760300	L
H-HC-0.079100	-1	-13.63832000	2.89258300	1.31552300	L
N-N--0.415700	-1	-10.10890700	-0.12709700	3.42423000	L
C-CT--0.038900	-1	-8.70036900	-0.52266600	3.50708400	L
C-C-0.597300	-1	-8.57062100	-2.04790400	3.62152300	L
O-O--0.567900	-1	-9.50087100	-2.70899400	4.10449500	L
C-CT-0.365400	-1	-7.98478100	0.12637200	4.71565400	L
O-OH--0.676100	-1	-8.15219400	-0.58747800	5.91899800	L
C-CT--0.243800	-1	-8.40502200	1.56257500	5.02194100	L
H-H-0.271900	-1	-10.73799500	-0.60019600	4.05684200	L
H-H1-0.100700	-1	-8.20024300	-0.18932900	2.59783300	L
H-H1-0.004300	-1	-6.92565100	0.12734900	4.47958200	L
H-HC-0.064200	-1	-8.44886700	2.12645500	4.09763800	L
H-HC-0.064200	-1	-7.67761100	2.02091700	5.69324000	L
H-HC-0.064200	-1	-9.38848400	1.58824900	5.49038400	L
H-HO-0.410200	-1	-8.40466200	0.05213700	6.61720500	L
N-N--0.254800	-1	-7.44370700	-2.64168100	3.18924800	L
C-CT--0.026600	-1	-7.19108800	-4.06727500	3.36033000	L
C-C-0.589600	-1	-6.58258200	-4.41972400	4.71892500	L
O-O--0.574800	-1	-6.59232000	-5.59030500	5.08279800	L
C-CT--0.007000	0	-6.19734600	-4.40438500	2.24748400	L
C-CT-0.018900	0	-5.35797400	-3.13411100	2.12321400	L
C-CT-0.019200	0	-6.36933900	-2.02374600	2.41286600	L

H-H1-0.064100	-1	-8.10024400	-4.63902300	3.21601800	L
H-HC-0.025300	0	-5.58224300	-5.26460900	2.50426200	L
H-HC-0.025300	0	-6.73626200	-4.58251700	1.31610600	L
H-HC-0.021300	0	-4.92242600	-3.03968500	1.12957400	L
H-HC-0.021300	0	-4.57394500	-3.13068900	2.88100300	L
H-H1-0.039100	0	-6.76783800	-1.64736300	1.47032800	L
H-H1-0.039100	0	-5.88535400	-1.21766100	2.96594300	L
N-N--0.415700	-1	-5.96559200	-3.45656100	5.41153700	L
C-CT--0.001400	-1	-4.97408500	-3.69503200	6.47183700	L
C-C-0.597300	-1	-5.52132200	-4.47807800	7.67972400	L
O-O--0.567900	-1	-6.70805800	-4.36317900	7.99015300	L
C-CT--0.001400	0	-4.46172400	-2.36133700	7.03168300	L H-HA 373
C-CA--0.001100	0	-4.15055700	-1.29895800	6.00344400	H
C-CA--0.190600	0	-3.26412100	-1.56932600	4.96038300	H
C-CA--0.190600	0	-4.73971500	-0.03606800	6.09766300	H
C-CA--0.234100	0	-2.97598700	-0.59540100	4.01445100	H
C-CA--0.234100	0	-4.45391500	0.95218000	5.16105700	H
C-C-0.322600	0	-3.56831400	0.67670300	4.11344200	H
O-OH--0.557900	0	-3.32489900	1.65514100	3.21420100	H
H-H-0.271900	-1	-6.03424000	-2.51815800	5.04906600	L
H-H1-0.087600	-1	-4.14831800	-4.26278500	6.04162700	L
H-HC-0.029500	0	-5.21495800	-1.96290800	7.71392500	L
H-HC-0.029500	0	-3.55888000	-2.54694000	7.61492700	L
H-HA-0.169900	0	-2.79122600	-2.54457100	4.87002200	H
H-HA-0.169900	0	-5.42825700	0.19115600	6.91247800	H
H-HA-0.165600	0	-2.25698600	-0.78595500	3.22861500	H
H-HA-0.165600	0	-4.87800200	1.94942300	5.24862800	H
H-HO-0.399200	0	-2.46245900	1.48044700	2.75086800	H
N-N--0.415700	-1	-4.64183400	-5.16571500	8.43457100	L
C-CT--0.149000	-1	-5.02595700	-5.63131200	9.78360400	L
H-H-0.271900	-1	-3.64704200	-5.15746800	8.19519600	L
H-H1-0.097600	-1	-6.10979900	-5.58271400	9.88957800	L
H-H1-0.097600	-1	-4.55819600	-4.99574300	10.53475600	L
H-H1-0.097600	-1	-4.69318400	-6.66046400	9.92065200	L
C-CT--0.366200	-1	-0.45322900	-10.77889000	2.47856700	L
C-C-0.597200	-1	-0.63508000	-9.83981000	1.27287900	L
O-O--0.567900	-1	-1.74472400	-9.66783500	0.76352600	L
H-HC-0.112300	-1	0.59468600	-10.79094000	2.77480100	L
H-HC-0.112300	-1	-0.76508000	-11.78687200	2.20376800	L
H-HC-0.112300	-1	-1.06267300	-10.42536200	3.31026000	L
N-N--0.415700	-1	0.47838800	-9.29188200	0.76909400	L
C-CT-0.014300	-1	0.43320800	-8.27546400	-0.28142500	L H-HC 405
C-C-0.597300	-1	0.06096300	-8.78520900	-1.69247800	L
O-O--0.567900	-1	-0.15134300	-7.96365400	-2.57503200	L
C-CT--0.204100	0	1.78127100	-7.52542300	-0.28842000	H
C-C-0.713000	0	1.57867300	-6.02867000	-0.51392200	H
O-O--0.593100	0	0.88018700	-5.39842300	0.27814600	H
N-N--0.919100	0	2.25553300	-5.45422300	-1.52858500	H
H-H-0.271900	-1	1.36134900	-9.47771800	1.21575300	L
H-H1-0.104800	-1	-0.37066900	-7.60431000	0.02149300	L
H-HC-0.079700	0	2.45997000	-7.99631300	-1.01011400	H
H-HC-0.079700	0	2.23684000	-7.59987000	0.70366700	H
H-H-0.419600	0	2.13609800	-4.44220700	-1.67137300	H
H-H-0.419600	0	2.69622400	-6.02212900	-2.23827600	H

N-N--0.415700	-1	-0.03321900	-10.09887000	-1.92884100	L
C-CT--0.149000	-1	-0.57208800	-10.65178100	-3.18357000	L
H-H-0.271900	-1	0.07736100	-10.74726700	-1.14121200	L
H-H1-0.097600	-1	-0.63754900	-9.86169900	-3.93092200	L
H-H1-0.097600	-1	-1.56493500	-11.06376300	-3.00273500	L
H-H1-0.097600	-1	0.08752600	-11.44143100	-3.54560100	L
C-CT--0.366200	-1	-3.84188400	-11.71261000	-1.41712800	L
C-C-0.597200	-1	-4.61071000	-10.38726000	-1.49099800	L
O-O--0.567900	-1	-5.74935900	-10.39176300	-1.96297100	L
H-HC-0.112300	-1	-2.85903700	-11.53754200	-0.97863400	L
H-HC-0.112300	-1	-3.72405200	-12.12080800	-2.41993600	L
H-HC-0.112300	-1	-4.39466100	-12.41914600	-0.79837700	L
N-N--0.415700	-1	-3.98471400	-9.25897800	-1.11655400	L
C-CT--0.087500	-1	-4.55005200	-7.89873100	-1.28151300	L
C-C-0.597300	-1	-4.81442700	-7.51825800	-2.74944200	L
O-O--0.567900	-1	-5.80366300	-6.84991800	-3.04640800	L
C-CT-0.298500	-1	-3.64442900	-6.82044200	-0.63071000	L
C-CT--0.319200	-1	-4.13288800	-5.38329100	-0.87315700	L
C-CT--0.319200	-1	-3.63004700	-6.95537600	0.88954200	L
H-H-0.271900	-1	-3.10298400	-9.36835100	-0.61363300	L
H-H1-0.096900	-1	-5.51131300	-7.87727600	-0.76943900	L
H-HC--0.029700	-1	-2.62850100	-6.91799600	-1.01393000	L
H-HC-0.079100	-1	-5.16907600	-5.28737300	-0.54796200	L
H-HC-0.079100	-1	-4.06428800	-5.13276000	-1.92912700	L
H-HC-0.079100	-1	-3.50692200	-4.67478100	-0.32860200	L
H-HC-0.079100	-1	-4.63698700	-6.82111800	1.26726200	L
H-HC-0.079100	-1	-2.96731100	-6.20849800	1.32897300	L
H-HC-0.079100	-1	-3.28023900	-7.93206500	1.19288800	L
N-N--0.415700	-1	-3.96661900	-7.91829200	-3.70541600	L
C-CT--0.149000	-1	-4.05170600	-7.50573700	-5.11713500	L
H-H-0.271900	-1	-3.24446500	-8.58037700	-3.44728800	L
H-H1-0.097600	-1	-4.87042400	-6.79626200	-5.24011500	L
H-H1-0.097600	-1	-4.23279500	-8.38121000	-5.74229700	L
H-H1-0.097600	-1	-3.11556300	-7.03452400	-5.41535300	L
C-CT--0.366200	-1	-12.11370800	3.66179700	-1.34167500	L
C-C-0.597200	-1	-11.00860300	2.59674800	-1.30303800	L
O-O--0.567900	-1	-11.30079700	1.41375600	-1.14666900	L
H-HC-0.112300	-1	-11.66601600	4.64503100	-1.48677500	L
H-HC-0.112300	-1	-12.66482600	3.64880500	-0.40097000	L
H-HC-0.112300	-1	-12.79614500	3.44789700	-2.16448700	L
N-N--0.415700	-1	-9.75238100	3.03852000	-1.37018800	L
C-CT--0.024900	-1	-8.56908900	2.21770000	-1.18848300	L
C-C-0.597300	-1	-7.45795400	3.08511000	-0.59159200	L
O-O--0.567900	-1	-6.80523500	3.87293500	-1.29042300	L
C-CT-0.211700	0	-8.15512300	1.57237600	-2.50993700	L
O-OH--0.654600	0	-7.28455700	0.51431100	-2.22724800	L
H-H-0.271900	-1	-9.62674200	4.03498000	-1.44170500	L
H-H1-0.084300	-1	-8.80655400	1.42607100	-0.47915400	L
H-H1-0.035200	0	-7.67323000	2.29207200	-3.16855100	L
H-H1-0.035200	0	-9.03791000	1.16490800	-3.00476800	L
H-HO-0.427500	0	-6.35093000	0.81893800	-2.28410600	L
N-N--0.415700	-1	-7.29683100	3.01339700	0.73861000	L
C-CT-0.021300	-1	-6.12286500	3.63071600	1.37431600	L
C-C-0.597300	-1	-4.83349400	2.98432600	0.84266600	L

O-O--0.567900	-1	-3.85891500	3.67300500	0.58213700	L
C-CT--0.123100	-1	-6.18176400	3.49660800	2.89755000	L
S-SH--0.311900	-1	-7.43693000	4.60293400	3.60253200	L
H-H-0.271900	-1	-7.95776200	2.46710900	1.28777900	L
H-H1-0.112400	-1	-6.09507700	4.69238000	1.12393000	L
H-H1-0.111200	-1	-5.21121300	3.77116800	3.31428300	L
H-H1-0.111200	-1	-6.39724300	2.46211100	3.16376800	L
H-HS-0.193300	-1	-8.47811400	4.15299100	2.89304600	L
N-N--0.415700	-1	-4.87052400	1.66520400	0.63860300	L H-H1 478
C-CT-0.021300	0	-3.68272600	0.99659100	0.06462900	H
C-C-0.597300	0	-3.68962400	1.16534700	-1.45029000	H
O-O--0.567900	0	-4.73757400	1.12743000	-2.10023800	H
C-CT--0.123100	0	-3.64400000	-0.48059700	0.48143800	H
S-SH--0.311900	0	-2.21484500	-1.49285600	-0.13367100	H
H-H-0.271900	-1	-5.72126800	1.17650800	0.84441300	L
H-H1-0.112400	0	-2.80894600	1.50012400	0.47285000	H
H-H1-0.111200	0	-4.47722200	-1.03286400	0.02797600	H
H-H1-0.111200	0	-3.70796600	-0.58429600	1.56310500	H
H-HS-0.193300	0	2.39270900	-1.13920800	0.81372300	H
N-N--0.415700	0	-2.46088700	1.30066500	-2.01914900	H
C-CT--0.087500	0	-2.30580700	1.39210900	-3.46040400	H
C-C-0.597300	0	-2.20674100	0.02917900	-4.20184200	H
O-O--0.567900	0	-2.26051300	0.03329100	-5.42876000	H
C-CT-0.298500	-1	-1.11310400	2.28300700	-3.88301200	H
C-CT--0.319200	0	-1.23476900	3.69205600	-3.29917600	L H-HC 492
C-CT--0.319200	0	0.24417000	1.69832300	-3.45068100	L H-HC 492
H-H-0.271900	0	-1.65206900	1.39274500	-1.39275700	H
H-H1-0.096900	0	-3.23473000	1.82277900	-3.85298800	H
H-HC--0.029700	0	-1.12038100	2.34640500	-4.97322200	H
H-HC-0.079100	0	-1.10471700	3.66687700	-2.21438500	L
H-HC-0.079100	0	-2.21408500	4.09674200	-3.53563600	L
H-HC-0.079100	0	-0.47504200	4.33591700	-3.73769200	L
H-HC-0.079100	0	0.33459700	1.71856300	-2.36347300	L
H-HC-0.079100	0	1.04686800	2.28613500	-3.88691200	L
H-HC-0.079100	0	0.35461500	0.67230200	-3.79327900	L
N-N--0.415700	0	-1.97130500	-1.08165700	-3.44409700	H
C-CT--0.003100	0	-2.04807400	-2.42912600	-4.01458100	H
C-C-0.597300	0	-3.50891300	-2.89074900	-4.18325300	H
O-O--0.567900	0	-3.80485300	-3.69228300	-5.06073100	H
C-CT--0.003600	-1	-1.28552300	-3.45750700	-3.11910200	H
C-CT--0.064500	-1	-1.41631700	-4.91247700	-3.60768900	L H-HC 508
C-C-0.695100	-1	-0.54162900	-5.25151700	-4.79994300	L
O-O--0.608600	-1	-0.39991000	-4.50153700	-5.75087600	L
N-N--0.940700	-1	0.07355700	-6.41452500	-4.79288500	L
H-H-0.271900	0	-2.08464400	-1.01903300	-2.43228700	H
H-H1-0.085000	0	-1.63710200	-2.39354400	-5.02608300	H
H-HC-0.017100	0	-0.23307300	-3.20131600	-3.01001400	H
H-HC-0.017100	0	-1.71975900	-3.41970300	-2.11671400	H
H-HC-0.035200	-1	-2.44393800	-5.16918100	-3.84901400	L
H-HC-0.035200	-1	-1.13072500	-5.55888900	-2.78516900	L
H-H-0.425100	-1	0.67752300	-6.66299000	-5.55668500	L
H-H-0.425100	-1	-0.03579800	-7.03457200	-3.99227300	L
N-N--0.415700	0	-4.34953400	-2.49748300	-3.16008100	H
C-CT--0.023700	0	-5.72763700	-2.96689200	-3.24024300	H

C-C-0.597300	-1	-6.40170400	-2.34894700	-4.48073600	L H-H1 522
O-O--0.567900	-1	-6.23250600	-1.15377000	-4.74080200	L
C-CT-0.034200	-1	-6.46287200	-2.68644500	-1.91381400	L H-H1 522
C-CT-0.001800	-1	-7.93055500	-3.13782700	-1.97084700	L
S-S--0.273700	-1	-8.83513200	-3.11121200	-0.39581900	L
C-CT--0.053600	-1	-9.20650700	-1.34370000	-0.26667600	L
H-H-0.271900	0	-4.28603600	-1.52344700	-2.90202100	H
H-H1-0.088000	0	-5.65791200	-4.04365500	-3.35401400	H
H-HC-0.024100	-1	-6.39414600	-1.63962500	-1.65532400	L
H-HC-0.024100	-1	-5.96886300	-3.23729300	-1.11698100	L
H-H1-0.044000	-1	-7.95399400	-4.16389500	-2.33927400	L
H-H1-0.044000	-1	-8.47142000	-2.51304900	-2.68194800	L
H-H1-0.068400	-1	-9.81273100	-1.15876800	0.62004200	L
H-H1-0.068400	-1	-9.75692200	-1.01623200	-1.14889100	L
H-H1-0.068400	-1	-8.27746500	-0.78219600	-0.19533200	L
N-N--0.254800	-1	-7.14909400	-3.12028800	-5.29188100	L
C-CT--0.026600	-1	-7.54632700	-2.70560600	-6.63827700	L
C-C-0.589600	-1	-8.99683500	-2.22428900	-6.63080700	L
O-O--0.574800	-1	-9.88188900	-2.92555200	-6.13367100	L
C-CT--0.007000	-1	-7.33768500	-3.94998700	-7.51584800	L
C-CT-0.018900	-1	-6.81967700	-5.01087200	-6.54149200	L
C-CT-0.019200	-1	-7.35303200	-4.55022300	-5.21137700	L
H-H1-0.064100	-1	-6.90020600	-1.90793900	-7.00428600	L
H-HC-0.025300	-1	-8.27142400	-4.27276300	-7.96737000	L
H-HC-0.025300	-1	-6.60232100	-3.76499900	-8.29660200	L
H-HC-0.021300	-1	-5.73158200	-5.00088600	-6.51505500	L
H-HC-0.021300	-1	-7.19198400	-5.99420600	-6.75658300	L
H-H1-0.039100	-1	-6.82809300	-5.05650000	-4.41298600	L
H-H1-0.039100	-1	-8.41814400	-4.77258600	-5.13698300	L
N-N--0.415700	-1	-9.22223100	-1.02859000	-7.16879200	L
C-CT--0.149000	-1	-10.45721900	-0.26141600	-6.97982800	L
H-H-0.271900	-1	-8.41824000	-0.55809200	-7.58370900	L
H-H1-0.097600	-1	-11.21634800	-0.90034200	-6.52918800	L
H-H1-0.097600	-1	-10.81146900	0.09842500	-7.94578100	L
H-H1-0.097600	-1	-10.26006300	0.58737700	-6.32461700	L
C-CT--0.366200	-1	-10.35844300	8.82179900	-4.25625300	L
C-C-0.597200	-1	-9.80737000	7.53460300	-3.62856600	L
O-O--0.567900	-1	-10.24923400	7.11496600	-2.55758800	L
H-HC-0.112300	-1	-9.84019100	9.01959000	-5.19445000	L
H-HC-0.112300	-1	-10.20128400	9.65499200	-3.57181800	L
H-HC-0.112300	-1	-11.42481600	8.70507500	-4.44846300	L
N-N--0.415700	-1	-8.83517900	6.91319700	-4.29076800	L
C-CT--0.024900	-1	-7.88918300	5.99750000	-3.64962700	L
C-C-0.597300	-1	-6.56108100	6.73236000	-3.42901200	L
O-O--0.567900	-1	-6.30818300	7.73945800	-4.09756700	L
C-CT-0.211700	0	-7.66495800	4.74261400	-4.50529900	L
O-OH--0.654600	0	-7.29502500	5.05305100	-5.83564800	L
H-H-0.271900	-1	-8.56503200	7.28156500	-5.20180400	L
H-H1-0.084300	-1	-8.27455100	5.65852100	-2.68766300	L
H-H1-0.035200	0	-8.58408500	4.15556600	-4.52158400	L
H-H1-0.035200	0	-6.87726800	4.14038300	-4.05034300	L
H-HO-0.427500	0	-6.87940800	4.27504700	-6.22461800	L
N-N--0.415700	-1	-5.68239000	6.20330400	-2.56711700	L
C-CT-0.033700	-1	-4.30964600	6.71494100	-2.46414800	L

C-C-0.597300	-1	-3.56185400	6.71960500	-3.81648000	L
O-O--0.567900	-1	-2.66417800	7.53491400	-4.03430800	L
C-CT--0.182500	-1	-3.55456600	5.89611300	-1.42723100	L
H-H-0.271900	-1	-5.96372000	5.39817600	-2.00270200	L
H-H1-0.082300	-1	-4.35916500	7.74262700	-2.10275200	L
H-HC-0.060300	-1	-2.54174400	6.27965500	-1.32225000	L
H-HC-0.060300	-1	-3.51737500	4.84983000	-1.72868800	L
H-HC-0.060300	-1	-4.07041300	5.97952200	-0.47193800	L
N-N--0.415700	-1	-3.98136100	5.85113000	-4.75042700	L
C-CT--0.149000	-1	-3.46614300	5.79721800	-6.11736300	L
H-H-0.271900	-1	-4.70857400	5.20125300	-4.48277900	L
H-H1-0.097600	-1	-2.69418600	6.55654200	-6.24454100	L
H-H1-0.097600	-1	-4.27788200	5.98503200	-6.82000900	L
H-H1-0.097600	-1	-3.04155100	4.81140000	-6.30686000	L
C-CM--0.139000	0	0.45020300	-0.85738000	-0.75468900	H
C-C-0.519000	0	1.44767700	-1.99216200	-0.72139200	H
O-O2--0.567000	0	2.23770000	-2.07479200	0.31389200	H
C-CM--0.117000	0	-0.54880900	-0.79754900	0.42559900	H
O-O2--0.618000	0	1.54574800	-2.76664600	-1.68977400	H
C-C--0.553000	0	-0.72240700	0.64111400	0.92323400	H
O-O2--0.556000	0	-0.55068100	1.56404500	0.07796000	H
O-O2--0.607000	0	-1.10200000	0.78818800	2.11725700	H
H-HC-0.049000	0	1.03435000	0.06583300	-0.69589300	H
H-HC-0.162000	0	-0.25211500	-1.45367100	1.24305200	H
O-OW--0.834000	-1	6.43844000	2.96025600	-1.18182200	L
H-HW-0.417000	-1	6.80954000	3.10153300	-2.05198300	L
H-HW-0.417000	-1	7.11696300	3.26274500	-0.57860400	L
O-OW--0.834000	0	3.40774300	7.11264700	1.04280000	L
H-HW-0.417000	0	3.24820200	6.21306100	1.39568600	L
H-HW-0.417000	0	3.78396400	6.90968600	0.16969500	L
O-OW--0.834000	0	-0.79262500	-3.65171000	1.78272800	H
H-HW-0.417000	0	-0.15773500	-4.19364100	1.28292900	H
H-HW-0.417000	0	-1.53244400	-3.53948900	1.16909400	H
O-OW--0.834000	0	-4.96949700	0.77352200	-6.22393000	L
H-HW-0.417000	0	-4.03254000	0.55280600	-6.11641500	L
H-HW-0.417000	0	-5.41340300	0.14146500	-5.63286600	L
H-HS-0.193300	0	-0.04975200	-0.87938000	-1.72187500	H

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C-CT--0.366200	-1	8.20752000	4.64427700	-8.15056600	L
C-C-0.597200	-1	9.03962800	3.90476700	-7.10821200	L
O-O--0.567900	-1	9.64303300	2.86793300	-7.38633200	L
H-HC-0.112300	-1	7.76181900	5.53029800	-7.69861500	L
H-HC-0.112300	-1	7.41807100	3.98785700	-8.51828900	L
H-HC-0.112300	-1	8.84728200	4.94356000	-8.98162000	L
N-N--0.415700	-1	9.03270200	4.46677900	-5.89295200	L
C-CT--0.087500	-1	9.50558300	3.79619500	-4.67475100	L
C-C-0.597300	-1	8.37043100	2.89727800	-4.18059400	L
O-O--0.567900	-1	7.45800000	3.35683300	-3.47865300	L
C-CT-0.298500	-1	9.98496400	4.80294800	-3.60187200	L
C-CT--0.319200	-1	10.40616200	4.10874700	-2.30111500	L
C-CT--0.319200	-1	11.19733000	5.61279700	-4.08383400	L
H-H-0.271900	-1	8.44526700	5.28768900	-5.76833700	L
H-H1-0.096900	-1	10.34500100	3.15655100	-4.92681400	L

H-HC--0.029700	-1	9.18582800	5.50704400	-3.38779200	L
H-HC-0.079100	-1	11.11435400	3.31119900	-2.52764100	L
H-HC-0.079100	-1	9.53685400	3.68469900	-1.80231000	L
H-HC-0.079100	-1	10.88061800	4.82028600	-1.62718600	L
H-HC-0.079100	-1	12.05954700	4.95806300	-4.21031500	L
H-HC-0.079100	-1	11.44114300	6.38666800	-3.35384800	L
H-HC-0.079100	-1	10.97795100	6.08879600	-5.03855100	L
N-N--0.415700	-1	8.39066300	1.62339100	-4.60847500	L
C-CT--0.087500	-1	7.28027600	0.66873700	-4.43094100	L
C-C-0.597300	-1	7.69960700	-0.60341900	-3.66583000	L
O-O--0.567900	-1	8.84687500	-1.05214600	-3.78863600	L
C-CT-0.298500	-1	6.62841200	0.25583800	-5.77505000	L
C-CT--0.319200	-1	5.76773700	1.37816500	-6.36672000	L
C-CT--0.319200	-1	7.62276500	-0.19548700	-6.85006800	L
H-H-0.271900	-1	9.16697200	1.31790000	-5.20129000	L
H-H1-0.096900	-1	6.50772200	1.17521600	-3.85940400	L
H-HC--0.029700	-1	5.96159000	-0.58631700	-5.58645300	L
H-HC-0.079100	-1	6.28221000	2.33620500	-6.29353000	L
H-HC-0.079100	-1	4.83234900	1.42485400	-5.81360100	L
H-HC-0.079100	-1	5.52036600	1.15919900	-7.40675400	L
H-HC-0.079100	-1	8.22087200	0.64977500	-7.18643300	L
H-HC-0.079100	-1	7.07464600	-0.60271800	-7.69866100	L
H-HC-0.079100	-1	8.27914300	-0.96546400	-6.45268100	L
N-N--0.254800	-1	6.76502500	-1.21035300	-2.89656600	L
C-CT--0.026600	-1	6.90074500	-2.56136600	-2.34562000	L
C-C-0.589600	-1	7.15226400	-3.58741900	-3.45232700	L
O-O--0.574800	-1	6.40596100	-3.64019100	-4.43294700	L
C-CT--0.007000	0	5.56319400	-2.86200400	-1.64600000	L
C-CT-0.018900	0	4.94442800	-1.49173900	-1.38943900	L
C-CT-0.019200	0	5.45112200	-0.66614300	-2.55877900	L
H-H1-0.064100	-1	7.71895000	-2.57205200	-1.62639100	L
H-HC-0.025300	0	4.89715100	-3.42288800	-2.30338400	L
H-HC-0.025300	0	5.71355200	-3.41493800	-0.72339200	L
H-HC-0.021300	0	5.32109300	-1.06639600	-0.46455000	L
H-HC-0.021300	0	3.86005400	-1.52198100	-1.36423500	L
H-H1-0.039100	0	5.50474900	0.37834300	-2.25017000	L
H-H1-0.039100	0	4.77374600	-0.77930000	-3.40659300	L
N-N--0.415700	-1	8.17951200	-4.42989700	-3.30078200	L
C-CT--0.149000	-1	8.55257800	-5.42793700	-4.31598000	L
H-H-0.271900	-1	8.77782700	-4.30336900	-2.48553500	L
H-H1-0.097600	-1	7.80959900	-5.43245900	-5.11287200	L
H-H1-0.097600	-1	8.59688800	-6.41512200	-3.85493900	L
H-H1-0.097600	-1	9.52879200	-5.17725000	-4.73104400	L
C-CT--0.366200	-1	5.25895100	-7.42098400	-4.06715800	L
C-C-0.597200	-1	4.12837700	-6.75610000	-4.86247600	L
O-O--0.567900	-1	3.23312600	-7.47832500	-5.31047400	L
H-HC-0.112300	-1	5.96829000	-6.66144300	-3.73917700	L
H-HC-0.112300	-1	5.76983300	-8.14770800	-4.69864600	L
H-HC-0.112300	-1	4.84091000	-7.92649100	-3.19656200	L
N-N--0.415700	-1	4.11276800	-5.42575200	-5.00571800	L
C-CT-0.014300	-1	3.00903400	-4.68341100	-5.63922100	L H-HC 69
C-C-0.597300	-1	2.81711500	-5.02920200	-7.15064000	L
O-O--0.567900	-1	3.81283300	-5.19272100	-7.85725600	L
C-CT--0.204100	0	3.30570000	-3.18147500	-5.42246700	H

C-C-0.713000	0	2.19495200	-2.26349900	-5.92869100	H
O-O--0.593100	0	2.08060100	-1.95889900	-7.10903200	H
N-N--0.919100	0	1.37616000	-1.75581500	-4.95866000	H
H-H-0.271900	-1	4.87905600	-4.88478900	-4.63869900	L
H-H1-0.104800	-1	2.10179800	-4.94830200	-5.10590000	L
H-HC-0.079700	0	4.21389100	-2.94243700	-5.98570600	H
H-HC-0.079700	0	3.49802400	-3.01547300	-4.35904100	H
H-H-0.419600	0	0.50886800	-1.37301100	-5.31432500	H
H-H-0.419600	0	1.38768000	-2.12270300	-4.01525400	H
N-N--0.415700	-1	1.56435300	-5.13360800	-7.64497600	L
C-CT--0.149000	-1	1.21474800	-5.39873000	-9.07029500	L
H-H-0.271900	-1	0.80761900	-4.90854900	-7.00010500	L
H-H1-0.097600	-1	2.12176600	-5.62262400	-9.63121900	L
H-H1-0.097600	-1	0.73188600	-4.51838400	-9.49536700	L
H-H1-0.097600	-1	0.53436800	-6.24854800	-9.12380300	L
C-CT--0.366200	-1	11.74320200	-5.89477900	-0.61174100	L
C-C-0.597200	-1	10.72662700	-6.02065000	0.53119800	L
O-O--0.567900	-1	11.04188400	-5.86119400	1.71565200	L
H-HC-0.112300	-1	11.24397800	-6.07480000	-1.56368400	L
H-HC-0.112300	-1	12.53730000	-6.62810300	-0.47376300	L
H-HC-0.112300	-1	12.17096000	-4.89199600	-0.60983200	L
N-N--0.415700	-1	9.49145200	-6.32952800	0.13934700	L
C-CT--0.023700	-1	8.33081200	-6.52807300	1.00250200	L
C-C-0.597300	-1	7.27990000	-7.37687200	0.29959100	L
O-O--0.567900	-1	7.10219100	-7.22206700	-0.91552000	L
C-CT-0.034200	0	7.72054500	-5.16880900	1.38853800	L
C-CT-0.001800	0	6.82661100	-5.18203400	2.64428700	L
S-S--0.273700	0	5.11774600	-5.78793600	2.47712100	L
C-CT--0.053600	0	4.24059400	-4.26088100	2.01425400	L
H-H-0.271900	-1	9.32416400	-6.40672300	-0.85783600	L
H-H1-0.088000	-1	8.65595200	-7.05638200	1.88714600	L
H-HC-0.024100	0	7.16030100	-4.76298900	0.54641500	L
H-HC-0.024100	0	8.54922800	-4.49468200	1.58556900	L
H-H1-0.044000	0	6.76524300	-4.16199200	3.02410400	L
H-H1-0.044000	0	7.32532900	-5.77642300	3.40978500	L
H-H1-0.068400	0	3.18436300	-4.47212000	1.84366500	L
H-H1-0.068400	0	4.65618000	-3.84189800	1.10134100	L
H-H1-0.068400	0	4.32205100	-3.51975200	2.80974400	L
N-N--0.415700	-1	6.57357600	-8.22250100	1.06023300	L
C-CT--0.149000	-1	5.35439700	-8.93352900	0.64698700	L
H-H-0.271900	-1	6.88900700	-8.35019000	2.02178600	L
H-H1-0.097600	-1	5.13761100	-8.70671200	-0.39637600	L
H-H1-0.097600	-1	4.51880400	-8.61402700	1.26993300	L
H-H1-0.097600	-1	5.50399100	-10.00669100	0.76197600	L
C-CT--0.366200	-1	3.91551500	-9.32503700	4.92759800	L
C-C-0.597200	-1	3.74256900	-7.91790600	5.53401100	L
O-O--0.567900	-1	4.70190900	-7.19794200	5.82643100	L
H-HC-0.112300	-1	2.93490300	-9.76930300	4.75380700	L
H-HC-0.112300	-1	4.48081200	-9.95182200	5.61705900	L
H-HC-0.112300	-1	4.45230300	-9.24990200	3.98177600	L
N-N--0.415700	-1	2.47965700	-7.50688700	5.67860300	L
C-CT--0.087500	-1	2.03887200	-6.10379000	5.62144500	L
C-C-0.597300	-1	1.91388600	-5.54186700	7.04399800	L
O-O--0.567900	-1	0.87654000	-5.63631900	7.71534600	L

C-CT-0.298500	0	0.71289500	-5.95076800	4.84286100	L
C-CT--0.319200	0	0.26793400	-4.48622900	4.75507100	L
C-CT--0.319200	0	0.83739200	-6.50031800	3.41298200	L
H-H-0.271900	-1	1.74616900	-8.20336200	5.52358300	L
H-H1-0.096900	-1	2.80349600	-5.53000000	5.09423900	L
H-HC--0.029700	0	-0.06574400	-6.52044400	5.35228400	L
H-HC-0.079100	0	1.00119400	-3.89548700	4.20133900	L
H-HC-0.079100	0	0.13175600	-4.05004400	5.74318600	L
H-HC-0.079100	0	-0.68565700	-4.42273500	4.23189800	L
H-HC-0.079100	0	1.61526700	-5.95409400	2.87734000	L
H-HC-0.079100	0	-0.10570000	-6.35354600	2.88438900	L
H-HC-0.079100	0	1.07089500	-7.56176000	3.42238500	L
N-N--0.415700	-1	3.07215900	-5.08464500	7.51910800	L
C-CT--0.149000	-1	3.44739300	-4.94514700	8.92353400	L
H-H-0.271900	-1	3.83180400	-5.00113300	6.85381200	L
H-H1-0.097600	-1	2.56041800	-5.05104100	9.54833000	L
H-H1-0.097600	-1	3.89041700	-3.96317100	9.08587500	L
H-H1-0.097600	-1	4.17015600	-5.71824300	9.18460600	L
C-CT--0.366200	-1	12.49251700	-4.18360100	6.36108900	L
C-C-0.597200	-1	12.28745200	-3.46475200	5.00913800	L
O-O--0.567900	-1	13.25471500	-3.24779400	4.27268300	L
H-HC-0.112300	-1	11.53298200	-4.28475900	6.86819100	L
H-HC-0.112300	-1	13.17149400	-3.59958200	6.98360400	L
H-HC-0.112300	-1	12.91767100	-5.17115700	6.18692000	L
N-N--0.415700	-1	11.05150300	-3.04228200	4.70430500	L
C-CT--0.023700	-1	10.77388700	-2.22155900	3.52785200	L
C-C-0.597300	-1	11.33889000	-0.79711600	3.66109500	L
O-O--0.567900	-1	12.06759000	-0.33247100	2.78264500	L
C-CT-0.034200	0	9.26619000	-2.14756400	3.26405700	L
C-CT-0.001800	0	9.01518200	-1.45623600	1.91696700	L
S-S--0.273700	0	7.44464800	-1.86087900	1.13053200	L
C-CT--0.053600	0	6.24734900	-0.99215700	2.17564200	L
H-H-0.271900	-1	10.28655500	-3.27129800	5.33260800	L
H-H1-0.088000	-1	11.24612400	-2.70233100	2.66941600	L
H-HC-0.024100	0	8.75741500	-1.60021100	4.05872100	L
H-HC-0.024100	0	8.87142000	-3.15867700	3.24088800	L
H-H1-0.044000	0	9.79804500	-1.75945100	1.22065000	L
H-H1-0.044000	0	9.08303900	-0.37475400	2.04258200	L
H-H1-0.068400	0	5.23174400	-1.19966500	1.83041700	L
H-H1-0.068400	0	6.41395100	0.08268500	2.11057500	L
H-H1-0.068400	0	6.33949800	-1.32241000	3.20853100	L
N-N--0.415700	-1	11.06922100	-0.10659900	4.77447100	L
C-CT--0.149000	-1	11.62019500	1.23343000	5.00071300	L
H-H-0.271900	-1	10.49118100	-0.53672500	5.49591900	L
H-H1-0.097600	-1	12.20843600	1.53489300	4.13409600	L
H-H1-0.097600	-1	12.25704900	1.21965200	5.88479400	L
H-H1-0.097600	-1	10.80485800	1.94098700	5.15131900	L
C-CT--0.366200	-1	6.17547000	8.72141900	-5.57998800	L
C-C-0.597200	-1	6.49180400	7.53208800	-4.65174600	L
O-O--0.567900	-1	6.64527000	6.38282400	-5.08931700	L
H-HC-0.112300	-1	6.08196300	9.63149100	-4.98645200	L
H-HC-0.112300	-1	5.23869800	8.53373200	-6.10598700	L
H-HC-0.112300	-1	6.98110800	8.84178700	-6.30495100	L
N-N--0.415700	-1	6.63397700	7.85068000	-3.35496900	L

C-CT--0.001400	-1	6.67655400	6.86174300	-2.26249200	L
C-C-0.597300	-1	5.30246200	6.18050400	-2.12059800	L
O-O--0.567900	-1	4.42811500	6.66149500	-1.38239500	L
C-CT--0.001400	-1	7.19261700	7.49890300	-0.95913800	L
C-CA--0.001100	-1	7.87893400	6.53100300	-0.00119900	L
C-CA--0.190600	-1	9.28678800	6.48267400	0.05010100	L
C-CA--0.190600	-1	7.13360800	5.71092500	0.87083400	L
C-CA--0.234100	-1	9.93790000	5.66525500	0.99293000	L
C-CA--0.234100	-1	7.78909500	4.88843000	1.81340600	L
C-C-0.322600	-1	9.19148100	4.88827000	1.89296300	L
O-OH--0.557900	-1	9.85244000	4.14561500	2.82748600	L
H-H-0.271900	-1	6.56825800	8.84305300	-3.11558000	L
H-H1-0.087600	-1	7.38884900	6.08997600	-2.54039500	L
H-HC-0.029500	-1	7.91728600	8.27059300	-1.22168200	L
H-HC-0.029500	-1	6.37935300	8.00622300	-0.43868500	L
H-HA-0.169900	-1	9.87226900	7.10574200	-0.61094600	L
H-HA-0.169900	-1	6.05259800	5.71520000	0.82685300	L
H-HA-0.165600	-1	11.01516900	5.63741500	1.04263800	L
H-HA-0.165600	-1	7.21509200	4.25650100	2.47524400	L
H-HO-0.399200	-1	9.35590800	3.92338200	3.63116800	L
N-N--0.415700	-1	5.09230600	5.15733000	-2.95349700	L
C-CT-0.033700	-1	3.77652300	4.65971500	-3.33987300	L
C-C-0.597300	-1	2.94008300	4.02449500	-2.21823200	L
O-O--0.567900	-1	1.71660400	4.12377200	-2.28753700	L
C-CT--0.182500	-1	3.96696800	3.65868300	-4.47425200	L
H-H-0.271900	-1	5.87593000	4.86407500	-3.53183600	L
H-H1-0.082300	-1	3.20957000	5.50291200	-3.73571500	L
H-HC-0.060300	-1	2.99652900	3.34600700	-4.85874100	L
H-HC-0.060300	-1	4.50545100	2.79185300	-4.09105600	L
H-HC-0.060300	-1	4.53716400	4.11865100	-5.28148400	L
N-N--0.415700	-1	3.55474500	3.38569000	-1.21206400	L H-H1 209
C-CT-0.021300	0	2.81139700	2.70888100	-0.11814200	H
C-C-0.597300	0	2.31849300	3.75883500	0.88594800	H
O-O--0.567900	0	3.10278000	4.57451400	1.36934500	H
C-CT--0.123100	0	3.75716800	1.69941300	0.57677100	H
S-S--1.036000	0	2.89867400	0.51099500	1.69781300	H
H-H-0.271900	-1	4.55856300	3.36240100	-1.20381300	L
H-H1-0.112400	0	1.96915800	2.16900200	-0.56149200	H
H-H1-0.111200	0	4.50633100	2.26939600	1.14114700	H
H-H1-0.111200	0	4.30713100	1.14044800	-0.19396900	H
N-N--0.415700	0	0.99241500	3.72126300	1.21411100	H
C-CT--0.051800	0	0.41127800	4.54101300	2.28044700	H
C-C-0.597300	0	0.78254700	4.02390500	3.70661300	H
O-O--0.567900	0	1.32117800	4.75030200	4.54233600	H
C-CT--0.110200	-1	-1.12319100	4.63992200	2.01577800	H
C-CT-0.353100	-1	-1.98362300	5.54483900	2.92393000	L H-HC 222
C-CT--0.412100	-1	-2.17415900	5.00066300	4.34127700	L
C-CT--0.412100	-1	-1.45579300	6.97971400	3.00942900	L
H-H-0.271900	0	0.39929200	2.99440700	0.81426600	H
H-H1-0.092200	0	0.86684900	5.53339400	2.23743600	H
H-HC-0.045700	0	-1.24627400	5.00923000	0.99040100	H
H-HC-0.045700	0	-1.56411600	3.64052000	2.03745900	H
H-HC--0.036100	-1	-2.97544900	5.59016400	2.47539400	L
H-HC-0.100000	-1	-1.27550900	5.14476800	4.93742000	L

H-HC-0.100000	-1	-2.41697900	3.93975900	4.30224000	L
H-HC-0.100000	-1	-2.99450400	5.53289700	4.82041200	L
H-HC-0.100000	-1	-0.49371400	6.99920800	3.52236700	L
H-HC-0.100000	-1	-2.16881600	7.59793200	3.55348800	L
H-HC-0.100000	-1	-1.33300600	7.38043600	2.00234600	L
N-N--0.415700	0	0.48526500	2.71765100	3.96770000	H
C-CT--0.087500	0	0.58735000	2.17016500	5.32160700	H
C-C-0.597300	0	1.99943700	2.16361500	5.92453900	H
O-O--0.567900	0	2.10443700	2.20184900	7.15110500	H
C-CT-0.298500	-1	-0.02785100	0.75277900	5.36955500	H
C-CT--0.319200	0	0.68865200	-0.28569500	4.48110700	L H-HC 241
C-CT--0.319200	0	-0.16909500	0.14948200	6.76751400	L H-HC 241
H-H-0.271900	0	0.06520200	2.15768300	3.23183100	H
H-H1-0.096900	0	0.02439900	2.82644200	5.99886500	H
H-HC--0.029700	0	-1.04136900	0.83985000	4.97398300	H
H-HC-0.079100	0	1.67615300	-0.52301300	4.87043800	L
H-HC-0.079100	0	0.80884100	0.09882800	3.46859000	L
H-HC-0.079100	0	0.09366300	-1.19445500	4.41073400	L
H-HC-0.079100	0	0.81166400	-0.08814600	7.17778600	L
H-HC-0.079100	0	-0.76184700	-0.76266300	6.70473700	L
H-HC-0.079100	0	-0.67621800	0.86035700	7.41797400	L
N-N--0.415700	0	3.01350100	1.94905600	5.06615100	H
C-CT-0.033700	0	4.37241500	1.80984000	5.54950600	H
C-C-0.597300	-1	5.08667400	3.14481400	5.82227700	L H-H1 254
O-O--0.567900	-1	6.26166000	3.12308300	6.17859600	L
C-CT--0.182500	-1	5.15072000	0.99529100	4.52168300	L H-H1 254
H-H-0.271900	0	2.85642500	1.87910700	4.06058100	H
H-H1-0.082300	0	4.35646600	1.26818900	6.50117500	H
H-HC-0.060300	-1	6.11808700	0.70480200	4.92879500	L
H-HC-0.060300	-1	5.30655100	1.59536300	3.62541100	L
H-HC-0.060300	-1	4.59418600	0.09171600	4.26960400	L
N-N--0.415700	-1	4.38189200	4.27143400	5.65578000	L
C-CT--0.087500	-1	4.76290100	5.63530400	6.05004500	L
C-C-0.597300	-1	3.92022000	6.08371600	7.25127300	L
O-O--0.567900	-1	4.47158000	6.53660500	8.25543800	L
C-CT-0.298500	-1	4.54696400	6.60836000	4.87363300	L
C-CT--0.319200	-1	4.93903200	8.04812100	5.22328400	L
C-CT--0.319200	-1	5.36499000	6.21174700	3.64501600	L
H-H-0.271900	-1	3.47086700	4.15508800	5.22967100	L
H-H1-0.096900	-1	5.81275100	5.66601200	6.33163900	L
H-HC--0.029700	-1	3.49460500	6.59409700	4.59764700	L
H-HC-0.079100	-1	5.98945100	8.08745400	5.50336300	L
H-HC-0.079100	-1	4.33211400	8.42579900	6.04541000	L
H-HC-0.079100	-1	4.77772900	8.68573400	4.35439500	L
H-HC-0.079100	-1	6.41516200	6.13523100	3.92081300	L
H-HC-0.079100	-1	5.24745100	6.95807500	2.85975800	L
H-HC-0.079100	-1	5.01392900	5.25364200	3.26172900	L
N-N--0.415700	-1	2.58914300	5.89128900	7.19768000	L
C-CT--0.149000	-1	1.68128100	6.23144800	8.30394200	L
H-H-0.271900	-1	2.18296300	5.50885600	6.34922200	L
H-H1-0.097600	-1	2.25834200	6.62841600	9.13918800	L
H-H1-0.097600	-1	1.14650000	5.33641900	8.62337600	L
H-H1-0.097600	-1	0.96518300	6.98177300	7.96889700	L
C-CT--0.366200	-1	4.03714600	10.31445100	-1.01320300	L

C-C-0.597200	-1	2.56278200	9.98574000	-1.25765300	L
O-O--0.567900	-1	1.75221600	10.89955600	-1.33189600	L
H-HC-0.112300	-1	4.61363100	9.39115600	-0.97572600	L
H-HC-0.112300	-1	4.13809800	10.84505400	-0.06663200	L
H-HC-0.112300	-1	4.40826200	10.94199800	-1.82313000	L
N-N--0.415700	-1	2.18552100	8.70227000	-1.31137100	L
C-CT--0.024900	-1	0.77262300	8.31921200	-1.15196500	L
C-C-0.597300	-1	0.18491300	8.81814000	0.17380300	L
O-O--0.567900	-1	-0.91020700	9.38441200	0.18057400	L
C-CT-0.211700	0	0.60492600	6.81897400	-1.29516700	L
O-OH--0.654600	0	0.89541300	6.51003700	-2.63835800	L
H-H-0.271900	-1	2.88882200	7.97033800	-1.37064300	L
H-H1-0.084300	-1	0.19978600	8.76729400	-1.95962400	L
H-H1-0.035200	0	-0.41829100	6.52890600	-1.06441400	L
H-H1-0.035200	0	1.28888900	6.29468600	-0.62579400	L
H-HO-0.427500	0	1.00258900	5.53480500	-2.64695500	L
N-N--0.415700	-1	0.94730500	8.68632200	1.26999400	L
C-CT-0.033700	-1	0.59258700	9.16938200	2.60575400	L
C-C-0.597300	-1	0.12611300	10.62999600	2.59464400	L
O-O--0.567900	-1	-0.97080000	10.94787200	3.05664100	L
C-CT--0.182500	-1	1.77923700	8.93540700	3.53819100	L
H-H-0.271900	-1	1.83643400	8.19088100	1.16575400	L
H-H1-0.082300	-1	-0.22158000	8.57689600	2.99628000	L
H-HC-0.060300	-1	1.54865000	9.30736200	4.53581600	L
H-HC-0.060300	-1	2.66423800	9.43739900	3.14935800	L
H-HC-0.060300	-1	1.97570900	7.86654600	3.59442500	L
N-N--0.415700	-1	0.92337700	11.50894200	1.97766100	L
C-CT--0.149000	-1	0.58129100	12.90578300	1.78243900	L
H-H-0.271900	-1	1.82636200	11.20143700	1.62465500	L
H-H1-0.097600	-1	-0.40508600	13.10033900	2.20498800	L
H-H1-0.097600	-1	0.57082900	13.13240300	0.71716500	L
H-H1-0.097600	-1	1.31983000	13.53404500	2.28142800	L
C-CT--0.366200	-1	-11.93053600	4.57378300	4.95032600	L
C-C-0.597200	-1	-12.36123200	3.15333900	4.58126800	L
O-O--0.567900	-1	-12.92573100	2.44617500	5.41826000	L
H-HC-0.112300	-1	-11.45147600	5.04266200	4.09071200	L
H-HC-0.112300	-1	-11.22655200	4.53576800	5.78175200	L
H-HC-0.112300	-1	-12.80521500	5.15503300	5.24050600	L
N-N--0.415700	-1	-12.02636700	2.71071500	3.36898400	L
C-CT--0.087500	-1	-12.02034600	1.28765100	3.01234000	L
C-C-0.597300	-1	-10.57368100	0.89435300	2.69964300	L
O-O--0.567900	-1	-9.85908500	1.53780800	1.92342800	L
C-CT-0.298500	-1	-13.01574100	0.89414600	1.88833900	L
C-CT--0.319200	-1	-13.76144400	-0.39641800	2.27592100	L
C-CT--0.319200	-1	-14.09530300	1.94010900	1.57699000	L
H-H-0.271900	-1	-11.61680100	3.36121700	2.69600800	L
H-H1-0.096900	-1	-12.31239100	0.72945000	3.89946800	L
H-HC--0.029700	-1	-12.45649200	0.70350500	0.97605300	L
H-HC-0.079100	-1	-14.39425700	-0.21389900	3.14515400	L
H-HC-0.079100	-1	-13.04451000	-1.18740500	2.49965900	L
H-HC-0.079100	-1	-14.39759200	-0.71383700	1.44988900	L
H-HC-0.079100	-1	-14.72926600	2.08514200	2.44822900	L
H-HC-0.079100	-1	-14.70224000	1.60180700	0.73858800	L
H-HC-0.079100	-1	-13.63958400	2.89252600	1.31502000	L

N-N--0.415700	-1	-10.10885900	-0.12374800	3.42640400	L
C-CT--0.038900	-1	-8.70017400	-0.51875000	3.50948200	L
C-C-0.597300	-1	-8.56989200	-2.04382300	3.62549700	L
O-O--0.567900	-1	-9.49985200	-2.70472500	4.10928400	L
C-CT-0.365400	-1	-7.98464600	0.13179300	4.71727900	L
O-OH--0.676100	-1	-8.15165400	-0.58085700	5.92138800	L
C-CT--0.243800	-1	-8.40533700	1.56817200	5.02212100	L
H-H-0.271900	-1	-10.73770100	-0.59640100	4.05959600	L
H-H1-0.100700	-1	-8.20028300	-0.18619100	2.59981800	L
H-H1-0.004300	-1	-6.92554900	0.13288600	4.48106300	L
H-HC-0.064200	-1	-8.44949800	2.13107300	4.09723600	L
H-HC-0.064200	-1	-7.67799200	2.02746400	5.69284500	L
H-HC-0.064200	-1	-9.38874400	1.59400000	5.49067000	L
H-HO-0.410200	-1	-8.40424900	0.05940200	6.61896300	L
N-N--0.254800	-1	-7.44283300	-2.63766700	3.19369200	L
C-CT--0.026600	-1	-7.18970500	-4.06299500	3.36622800	L
C-C-0.589600	-1	-6.58089700	-4.41381800	4.72510800	L
O-O--0.574800	-1	-6.59018800	-5.58402100	5.09020500	L
C-CT--0.007000	0	-6.19659400	-4.40131200	2.25326200	L
C-CT-0.018900	0	-5.35835900	-3.13062400	2.12626000	L
C-CT-0.019200	0	-6.37050500	-2.02057900	2.41397400	L
H-H1-0.064100	-1	-8.09868500	-4.63520300	3.22263400	L
H-HC-0.025300	0	-5.58079900	-5.26076300	2.51094000	L
H-HC-0.025300	0	-6.73609400	-4.58137600	1.32256500	L
H-HC-0.021300	0	-4.92338600	-3.03806000	1.13220200	L
H-HC-0.021300	0	-4.57430300	-3.12478400	2.88401900	L
H-H1-0.039100	0	-6.77089700	-1.64765100	1.47084000	L
H-H1-0.039100	0	-5.88694000	-1.21208900	2.96389100	L
N-N--0.415700	-1	-5.96414400	-3.44972100	5.41663200	L
C-CT--0.001400	-1	-4.97241200	-3.68674800	6.47704800	L
C-C-0.597300	-1	-5.51922100	-4.46871700	7.68582400	L
O-O--0.567900	-1	-6.70595400	-4.35390000	7.99629300	L
C-CT--0.001400	0	-4.46111500	-2.35142900	7.03508200	L H-HA 373
C-CA--0.001100	0	-4.15343600	-1.28684800	6.00752500	H
C-CA--0.190600	0	-3.25911900	-1.54933700	4.96947700	H
C-CA--0.190600	0	-4.75022600	-0.02724200	6.09958800	H
C-CA--0.234100	0	-2.97260700	-0.57191300	4.02646700	H
C-CA--0.234100	0	-4.46673500	0.96379700	5.16543600	H
C-C-0.322600	0	-3.57455800	0.69602000	4.12112000	H
O-OH--0.557900	0	-3.33610500	1.67368500	3.22234700	H
H-H-0.271900	-1	-6.03316000	-2.51172200	5.05319000	L
H-H1-0.087600	-1	-4.14650800	-4.25466800	6.04732000	L
H-HC-0.029500	0	-5.21356400	-1.95451600	7.71911700	L
H-HC-0.029500	0	-3.55710400	-2.53557600	7.61696300	L
H-HA-0.169900	0	-2.77887100	-2.52180600	4.88587600	H
H-HA-0.169900	0	-5.44335200	0.19518700	6.91167900	H
H-HA-0.165600	0	-2.24674800	-0.74853200	3.24400600	H
H-HA-0.165600	0	-4.89747300	1.95805400	5.25274500	H
H-HO-0.399200	0	-2.47147600	1.51132900	2.75807000	H
N-N--0.415700	-1	-4.63939900	-5.15526700	8.44127200	L
C-CT--0.149000	-1	-5.02318300	-5.61958600	9.79084100	L
H-H-0.271900	-1	-3.64464100	-5.14693100	8.20175500	L
H-H1-0.097600	-1	-6.10702600	-5.57124600	9.89691000	L
H-H1-0.097600	-1	-4.55553700	-4.98307300	10.54126600	L

H-H1-0.097600	-1	-4.69003800	-6.64847900	9.92891900	L
C-CT--0.366200	-1	-0.44967500	-10.77322900	2.49057000	L
C-C-0.597200	-1	-0.63200800	-9.83547200	1.28392700	L
O-O--0.567900	-1	-1.74177900	-9.66440600	0.77454400	L
H-HC-0.112300	-1	0.59828400	-10.78461400	2.78667700	L
H-HC-0.112300	-1	-0.76121800	-11.78160500	2.21686700	L
H-HC-0.112300	-1	-1.05912800	-10.41904100	3.32197600	L
N-N--0.415700	-1	0.48120600	-9.28769000	0.77942100	L
C-CT-0.014300	-1	0.43554000	-8.27238800	-0.27215300	L H-HC 405
C-C-0.597300	-1	0.06327800	-8.78373000	-1.68262200	L
O-O--0.567900	-1	-0.14942400	-7.96317000	-2.56600600	L
C-CT--0.204100	0	1.74125300	-7.45413800	-0.28561200	H
C-C-0.713000	0	1.45942100	-6.02500900	-0.76322200	H
O-O--0.593100	0	0.48980000	-5.40969700	-0.31598100	H
N-N--0.919100	0	2.35050600	-5.46279400	-1.60440700	H
H-H-0.271900	-1	1.36429100	-9.47275900	1.22615600	L
H-H1-0.104800	-1	-0.36852700	-7.60119000	0.03017100	L
H-HC-0.079700	0	2.50219400	-7.97591000	-0.87731800	H
H-HC-0.079700	0	2.11263700	-7.36022000	0.73993900	H
H-H-0.419600	0	2.21933700	-4.48061500	-1.86181200	H
H-H-0.419600	0	3.05751900	-6.01490500	-2.06624200	H
N-N--0.415700	-1	-0.03048600	-10.09766900	-1.91760000	L
C-CT--0.149000	-1	-0.56933500	-10.65207400	-3.17168100	L
H-H-0.271900	-1	0.08041900	-10.74520600	-1.12931100	L
H-H1-0.097600	-1	-0.63516400	-9.86279600	-3.91984900	L
H-H1-0.097600	-1	-1.56201700	-11.06420400	-2.99028100	L
H-H1-0.097600	-1	0.09050100	-11.44187700	-3.53297500	L
C-CT--0.366200	-1	-3.83853300	-11.71217200	-1.40369300	L
C-C-0.597200	-1	-4.60782100	-10.38716300	-1.47884400	L
O-O--0.567900	-1	-5.74653200	-10.39254700	-1.95066000	L
H-HC-0.112300	-1	-2.85568500	-11.53631300	-0.96551400	L
H-HC-0.112300	-1	-3.72069500	-12.12137800	-2.40609000	L
H-HC-0.112300	-1	-4.39098400	-12.41825100	-0.78413200	L
N-N--0.415700	-1	-3.98216000	-9.25827700	-1.10566200	L
C-CT--0.087500	-1	-4.54798300	-7.89839700	-1.27196600	L
C-C-0.597300	-1	-4.81268400	-7.51954600	-2.74025600	L
O-O--0.567900	-1	-5.80218700	-6.85185400	-3.03778800	L
C-CT-0.298500	-1	-3.64264100	-6.81911800	-0.62241100	L
C-CT--0.319200	-1	-4.13162200	-5.38238800	-0.86629300	L
C-CT--0.319200	-1	-3.62800900	-6.95246000	0.89798000	L
H-H-0.271900	-1	-3.10032400	-9.36682400	-0.60274600	L
H-H1-0.096900	-1	-5.50918300	-7.87673400	-0.75978600	L
H-HC--0.029700	-1	-2.62673100	-6.91672800	-1.00566400	L
H-HC-0.079100	-1	-5.16780000	-5.28648300	-0.54105800	L
H-HC-0.079100	-1	-4.06324800	-5.13293700	-1.92253300	L
H-HC-0.079100	-1	-3.50582500	-4.67309800	-0.32256100	L
H-HC-0.079100	-1	-4.63494400	-6.81815200	1.27569400	L
H-HC-0.079100	-1	-2.96546900	-6.20489700	1.33654100	L
H-HC-0.079100	-1	-3.27782700	-7.92871300	1.20229800	L
N-N--0.415700	-1	-3.96486700	-7.92029000	-3.69592500	L
C-CT--0.149000	-1	-4.05028300	-7.50923700	-5.10806100	L
H-H-0.271900	-1	-3.24245400	-8.58185700	-3.43720300	L
H-H1-0.097600	-1	-4.86926100	-6.80017100	-5.23167300	L
H-H1-0.097600	-1	-4.23115700	-8.38542400	-5.73228600	L

H-H1-0.097600	-1	-3.11434200	-7.03801700	-5.40689700	L
C-CT--0.366200	-1	-12.11559000	3.65948300	-1.34318600	L
C-C-0.597200	-1	-11.01011500	2.59485200	-1.30358500	L
O-O--0.567900	-1	-11.30188700	1.41192500	-1.14594100	L
H-HC-0.112300	-1	-11.66825200	4.64271800	-1.48937300	L
H-HC-0.112300	-1	-12.66657700	3.64728600	-0.40239400	L
H-HC-0.112300	-1	-12.79806400	3.44449100	-2.16568300	L
N-N--0.415700	-1	-9.75405400	3.03698100	-1.37136400	L
C-CT--0.024900	-1	-8.57045800	2.21675700	-1.18896000	L
C-C-0.597300	-1	-7.45953800	3.08516800	-0.59312500	L
O-O--0.567900	-1	-6.80718200	3.87248500	-1.29286600	L
C-CT-0.211700	0	-8.15414200	1.57053100	-2.50935800	L
O-OH--0.654600	0	-7.28698400	0.51066800	-2.22263200	L
H-H-0.271900	-1	-9.62876400	4.03341000	-1.44393900	L
H-H1-0.084300	-1	-8.80755800	1.42578800	-0.47877500	L
H-H1-0.035200	0	-7.66850000	2.28872300	-3.16687100	L
H-H1-0.035200	0	-9.03630800	1.16471500	-3.00663000	L
H-HO-0.427500	0	-6.35157900	0.80820600	-2.28385100	L
N-N--0.415700	-1	-7.29821300	3.01489900	0.73712900	L
C-CT-0.021300	-1	-6.12437300	3.63328200	1.37203300	L
C-C-0.597300	-1	-4.83485200	2.98677700	0.84088700	L
O-O--0.567900	-1	-3.86054400	3.67551600	0.57950800	L
C-CT--0.123100	-1	-6.18302100	3.50074400	2.89541500	L
S-SH--0.311900	-1	-7.43847100	4.60737800	3.59940900	L
H-H-0.271900	-1	-7.95888400	2.46896000	1.28695800	L
H-H1-0.112400	-1	-6.09698100	4.69469100	1.12053500	L
H-H1-0.111200	-1	-5.21250900	3.77607000	3.31173000	L
H-H1-0.111200	-1	-6.39811300	2.46645200	3.16274100	L
H-HS-0.193300	-1	-8.47959700	4.15633800	2.89053300	L
N-N--0.415700	-1	-4.87146400	1.66743300	0.63820700	L H-H1 478
C-CT-0.021300	0	-3.67073000	0.99308300	0.07673000	H
C-C-0.597300	0	-3.67791400	1.14754500	-1.44015200	H
O-O--0.567900	0	-4.72659500	1.08763200	-2.08799200	H
C-CT--0.123100	0	-3.61478100	-0.48444300	0.50425700	H
S-SH--0.311900	0	-2.15914300	-1.50874500	-0.07535900	H
H-H-0.271900	-1	-5.72200900	1.17865900	0.84464100	L
H-H1-0.112400	0	-2.80170300	1.50754500	0.48253600	H
H-H1-0.111200	0	-4.43018700	-1.05198600	0.03811100	H
H-H1-0.111200	0	-3.69597700	-0.58314300	1.58485600	H
H-HS-0.193300	0	1.36569000	-2.56364400	1.10469200	H
N-N--0.415700	0	-2.45291900	1.29919500	-2.01034200	H
C-CT--0.087500	0	-2.30519200	1.39140200	-3.45281800	H
C-C-0.597300	0	-2.21395300	0.02711100	-4.18994500	H
O-O--0.567900	0	-2.29981200	0.02502600	-5.41491700	H
C-CT-0.298500	-1	-1.11485400	2.28179100	-3.88455700	H
C-CT--0.319200	0	-1.23068700	3.69147700	-3.30198800	L H-HC 492
C-CT--0.319200	0	0.24394000	1.69322400	-3.45879100	L H-HC 492
H-H-0.271900	0	-1.64237800	1.39595300	-1.38577900	H
H-H1-0.096900	0	-3.23637900	1.82094400	-3.84096500	H
H-HC--0.029700	0	-1.12932800	2.34365000	-4.97480600	H
H-HC-0.079100	0	-1.09482000	3.66707900	-2.21797700	L
H-HC-0.079100	0	-2.21047900	4.09770100	-3.53385500	L
H-HC-0.079100	0	-0.47212900	4.33318200	-3.74567600	L
H-HC-0.079100	0	0.33849600	1.70049800	-2.37143400	L

H-HC-0.079100	0	1.04619400	2.28466900	-3.89089600	L
H-HC-0.079100	0	0.35329200	0.67077300	-3.81215100	L
N-N--0.415700	0	-1.95297500	-1.08007100	-3.43475100	H
C-CT--0.003100	0	-2.04403800	-2.42655700	-4.00558000	H
C-C-0.597300	0	-3.50611700	-2.88376900	-4.17394200	H
O-O--0.567900	0	-3.80091100	-3.68691500	-5.05020400	H
C-CT--0.003600	-1	-1.28521600	-3.45798000	-3.11462800	H
C-CT--0.064500	-1	-1.41557700	-4.91350400	-3.60168000	L H-HC 508
C-C-0.695100	-1	-0.54093300	-5.25349200	-4.79369600	L
O-O--0.608600	-1	-0.39959700	-4.50445600	-5.74542900	L
N-N--0.940700	-1	0.07465100	-6.41628100	-4.78550500	L
H-H-0.271900	0	-2.02429000	-1.01311400	-2.42118800	H
H-H1-0.085000	0	-1.63302100	-2.39469000	-5.01710100	H
H-HC-0.017100	0	-0.23068300	-3.20183500	-3.03178700	H
H-HC-0.017100	0	-1.70746400	-3.42045700	-2.10741000	H
H-HC-0.035200	-1	-2.44314200	-5.17081100	-3.84259800	L
H-HC-0.035200	-1	-1.12965600	-5.55896000	-2.77852300	L
H-H-0.425100	-1	0.67859900	-6.66533700	-5.54912700	L
H-H-0.425100	-1	-0.03438600	-7.03552900	-3.98423200	L
N-N--0.415700	0	-4.34898500	-2.49061000	-3.15198400	H
C-CT--0.023700	0	-5.72569700	-2.96649600	-3.23511700	H
C-C-0.597300	-1	-6.40195500	-2.35258800	-4.47673400	L H-H1 522
O-O--0.567900	-1	-6.23320000	-1.15762600	-4.73807000	L
C-CT-0.034200	-1	-6.46266500	-2.68742600	-1.90945200	L H-H1 522
C-CT-0.001800	-1	-7.93020200	-3.13936700	-1.96581800	L
S-S--0.273700	-1	-8.83457800	-3.11141600	-0.39069800	L
C-CT--0.053600	-1	-9.20653700	-1.34389600	-0.26335000	L
H-H-0.271900	0	-4.29116700	-1.51436600	-2.89914200	H
H-H1-0.088000	0	-5.65195100	-4.04313400	-3.34916000	H
H-HC-0.024100	-1	-6.39426200	-1.64031400	-1.65206600	L
H-HC-0.024100	-1	-5.96836200	-3.23727200	-1.11211000	L
H-H1-0.044000	-1	-7.95333900	-4.16582600	-2.33317000	L
H-H1-0.044000	-1	-8.47137500	-2.51551600	-2.67749900	L
H-H1-0.068400	-1	-9.81270700	-1.15824500	0.62325600	L
H-H1-0.068400	-1	-9.75718200	-1.01753800	-1.14583200	L
H-H1-0.068400	-1	-8.27767700	-0.78200100	-0.19271600	L
N-N--0.254800	-1	-7.14919100	-3.12502900	-5.28697200	L
C-CT--0.026600	-1	-7.54674600	-2.71188900	-6.63374700	L
C-C-0.589600	-1	-8.99741600	-2.23106000	-6.62658700	L
O-O--0.574800	-1	-9.88216500	-2.93210500	-6.12860000	L
C-CT--0.007000	-1	-7.33779600	-3.95711400	-7.51004700	L
C-CT-0.018900	-1	-6.81929500	-5.01680500	-6.53465300	L
C-CT-0.019200	-1	-7.35263000	-4.55494800	-5.20494900	L
H-H1-0.064100	-1	-6.90094600	-1.91438400	-7.00067700	L
H-HC-0.025300	-1	-8.27148600	-4.28068000	-7.96110700	L
H-HC-0.025300	-1	-6.60259900	-3.77269200	-8.29109100	L
H-HC-0.021300	-1	-5.73120200	-5.00642000	-6.50837300	L
H-HC-0.021300	-1	-7.19129700	-6.00049100	-6.74866700	L
H-H1-0.039100	-1	-6.82741100	-5.06021300	-4.40609900	L
H-H1-0.039100	-1	-8.41765700	-4.77759700	-5.13018000	L
N-N--0.415700	-1	-9.22329200	-1.03600000	-7.16579000	L
C-CT--0.149000	-1	-10.45851500	-0.26904900	-6.97746100	L
H-H-0.271900	-1	-8.41951700	-0.56566200	-7.58130400	L
H-H1-0.097600	-1	-11.21736700	-0.90776200	-6.52605300	L

H-H1-0.097600	-1	-10.81301800	0.08966000	-7.94374300	L
H-H1-0.097600	-1	-10.26156300	0.58049300	-6.32316300	L
C-CT--0.366200	-1	-10.36247500	8.81703700	-4.26338500	L
C-C-0.597200	-1	-9.81087900	7.53068400	-3.63442900	L
O-O--0.567900	-1	-10.25245600	7.11201600	-2.56295300	L
H-HC-0.112300	-1	-9.84441600	9.01402500	-5.20185800	L
H-HC-0.112300	-1	-10.20550800	9.65099800	-3.57984200	L
H-HC-0.112300	-1	-11.42883300	8.69974900	-4.45532900	L
N-N--0.415700	-1	-8.83856400	6.90892000	-4.29611200	L
C-CT--0.024900	-1	-7.89217100	5.99421500	-3.65414200	L
C-C-0.597300	-1	-6.56428900	6.72975700	-3.43447200	L
O-O--0.567900	-1	-6.31182300	7.73624300	-4.10411100	L
C-CT-0.211700	0	-7.66748600	4.73827100	-4.50825400	L
O-OH--0.654600	0	-7.29656600	5.04679900	-5.83870600	L
H-H-0.271900	-1	-8.56866400	7.27642900	-5.20756800	L
H-H1-0.084300	-1	-8.27729400	5.65611000	-2.69177200	L
H-H1-0.035200	0	-8.58653700	4.15109800	-4.52435500	L
H-H1-0.035200	0	-6.88002800	4.13665900	-4.05211600	L
H-HO-0.427500	0	-6.87877100	4.26865900	-6.22536400	L
N-N--0.415700	-1	-5.68530300	6.20190400	-2.57214300	L
C-CT-0.033700	-1	-4.31272000	6.71411500	-2.46989200	L
C-C-0.597300	-1	-3.56511100	6.71762200	-3.82232900	L
O-O--0.567900	-1	-2.66774100	7.53300700	-4.04112900	L
C-CT--0.182500	-1	-3.55722100	5.89662700	-1.43222100	L
H-H-0.271900	-1	-5.96628400	5.39726700	-2.00684900	L
H-H1-0.082300	-1	-4.36254000	7.74216000	-2.10956300	L
H-HC-0.060300	-1	-2.54451600	6.28062400	-1.32777800	L
H-HC-0.060300	-1	-3.51971400	4.85004200	-1.73259000	L
H-HC-0.060300	-1	-4.07297000	5.98085800	-0.47694600	L
N-N--0.415700	-1	-3.98444500	5.84802900	-4.75531200	L
C-CT--0.149000	-1	-3.46939300	5.79286400	-6.12226000	L
H-H-0.271900	-1	-4.71140000	5.19818300	-4.48688800	L
H-H1-0.097600	-1	-2.69771000	6.55231800	-6.25033400	L
H-H1-0.097600	-1	-4.28128800	5.97966700	-6.82499300	L
H-H1-0.097600	-1	-3.04448900	4.80699500	-6.31078300	L
C-CM--0.139000	0	0.57707900	-0.93472100	-0.56134500	H
C-C-0.519000	0	1.32029100	-2.22346600	-0.77579300	H
O-O2--0.567000	0	1.80536500	-2.85557100	0.28798100	H
C-CM--0.117000	0	-0.50701500	-0.81409700	0.52442800	H
O-O2--0.618000	0	1.64714900	-2.62675500	-1.89614800	H
C-C--0.553000	0	-0.69573500	0.65099700	0.93537700	H
O-O2--0.556000	0	-0.52855700	1.52784300	0.04757700	H
O-O2--0.607000	0	-1.09862100	0.84274700	2.11720300	H
H-HC-0.049000	0	1.38428500	-0.26173300	-0.18040200	H
H-HC-0.162000	0	-0.26243900	-1.39236800	1.41189200	H
O-OW--0.834000	-1	6.43681800	2.96443500	-1.18508800	L
H-HW-0.417000	-1	6.80775500	3.10493100	-2.05544500	L
H-HW-0.417000	-1	7.11531800	3.26778500	-0.58227600	L
O-OW--0.834000	0	3.43651600	7.17290200	1.03249600	L
H-HW-0.417000	0	3.25928700	6.27575700	1.38360300	L
H-HW-0.417000	0	3.80734400	6.96197300	0.15873000	L
O-OW--0.834000	0	-0.45633400	-3.71745100	1.71456000	H
H-HW-0.417000	0	-0.12674600	-4.38995200	1.08874000	H
H-HW-0.417000	0	-1.30374800	-3.45158800	1.32460400	H

O-OW--0.834000	0	-4.98825500	0.80307500	-6.18580400 L
H-HW-0.417000	0	-4.05176800	0.57436700	-6.08784400 L
H-HW-0.417000	0	-5.43155600	0.15755900	-5.60879100 L
H-HS-0.193300	0	0.22242200	-0.58327700	-1.52826600 H

IC5'

C-CT--0.366200	-1	8.211946	4.639434	-8.153097 L
C-C-0.597200	-1	9.043664	3.899706	-7.110582 L
O-O--0.567900	-1	9.646463	2.862457	-7.388466 L
H-HC-0.112300	-1	7.766763	5.525827	-7.701351 L
H-HC-0.112300	-1	7.422117	3.983382	-8.520635 L
H-HC-0.112300	-1	8.851856	4.938152	-8.984246 L
N-N--0.415700	-1	9.037096	4.462019	-5.895459 L
C-CT--0.087500	-1	9.509628	3.791464	-4.677111 L
C-C-0.597300	-1	8.373977	2.893319	-4.182696 L
O-O--0.567900	-1	7.461837	3.353565	-3.480840 L
C-CT-0.298500	-1	9.989623	4.798208	-3.604489 L
C-CT--0.319200	-1	10.410461	4.104097	-2.303576 L
C-CT--0.319200	-1	11.202434	5.607243	-4.086689 L
H-H-0.271900	-1	8.450132	5.283294	-5.771030 L
H-H1-0.096900	-1	10.348680	3.151283	-4.929039 L
H-HC--0.029700	-1	9.190890	5.502817	-3.390563 L
H-HC-0.079100	-1	11.118186	3.306077	-2.529930 L
H-HC-0.079100	-1	9.540928	3.680658	-1.804639 L
H-HC-0.079100	-1	10.885348	4.815525	-1.629836 L
H-HC-0.079100	-1	12.064270	4.951991	-4.213037 L
H-HC-0.079100	-1	11.446710	6.381156	-3.356909 L
H-HC-0.079100	-1	10.983300	6.083140	-5.041523 L
N-N--0.415700	-1	8.393472	1.619319	-4.610261 L
C-CT--0.087500	-1	7.282543	0.665342	-4.432461 L
C-C-0.597300	-1	7.701170	-0.606865	-3.667055 L
O-O--0.567900	-1	8.848175	-1.056273	-3.789785 L
C-CT-0.298500	-1	6.630404	0.252484	-5.776445 L
C-CT--0.319200	-1	5.770349	1.375153	-6.368375 L
C-CT--0.319200	-1	7.624464	-0.199676	-6.851388 L
H-H-0.271900	-1	9.169585	1.313240	-5.203024 L
H-H1-0.096900	-1	6.510297	1.172401	-3.861030 L
H-HC--0.029700	-1	5.963109	-0.589245	-5.587621 L
H-HC-0.079100	-1	6.285374	2.332915	-6.295428 L
H-HC-0.079100	-1	4.835006	1.422517	-5.815238 L
H-HC-0.079100	-1	5.522827	1.156072	-7.408342 L
H-HC-0.079100	-1	8.223041	0.645162	-7.187982 L
H-HC-0.079100	-1	7.076090	-0.606798	-7.699866 L
H-HC-0.079100	-1	8.280414	-0.969928	-6.453834 L
N-N--0.254800	-1	6.766263	-1.213071	-2.897608 L
C-CT--0.026600	-1	6.901229	-2.564022	-2.346339 L
C-C-0.589600	-1	7.152132	-3.590503	-3.452797 L
O-O--0.574800	-1	6.405765	-3.643087	-4.433377 L
C-CT--0.007000	0	5.563975	-2.858247	-1.642780 L
C-CT-0.018900	0	4.961796	-1.482144	-1.373613 L
C-CT-0.019200	0	5.455958	-0.664410	-2.553100 L
H-H1-0.064100	-1	7.719454	-2.575010	-1.627130 L
H-HC-0.025300	0	4.890065	-3.406853	-2.302395 L
H-HC-0.025300	0	5.712746	-3.419843	-0.724966 L

H-HC-0.021300	0	5.361086	-1.057717	-0.458397	L
H-HC-0.021300	0	3.878195	-1.498481	-1.323478	L
H-H1-0.039100	0	5.512699	0.381844	-2.251270	L
H-H1-0.039100	0	4.770761	-0.783086	-3.393880	L
N-N--0.415700	-1	8.178905	-4.433523	-3.301079	L
C-CT--0.149000	-1	8.551370	-5.432029	-4.316044	L
H-H-0.271900	-1	8.777314	-4.307142	-2.485881	L
H-H1-0.097600	-1	7.808363	-5.436320	-5.112903	L
H-H1-0.097600	-1	8.595128	-6.419124	-3.854755	L
H-H1-0.097600	-1	9.527713	-5.182006	-4.731198	L
C-CT--0.366200	-1	5.256604	-7.423129	-4.066627	L
C-C-0.597200	-1	4.126389	-6.757797	-4.862074	L
O-O--0.567900	-1	3.230717	-7.479618	-5.309867	L
H-HC-0.112300	-1	5.966390	-6.663914	-3.738858	L
H-HC-0.112300	-1	5.767052	-8.150297	-4.697955	L
H-HC-0.112300	-1	4.838304	-7.928191	-3.195891	L
N-N--0.415700	-1	4.111536	-5.427477	-5.005645	L
C-CT-0.014300	-1	3.008213	-4.684631	-5.639283	L H-HC 69
C-C-0.597300	-1	2.816047	-5.030711	-7.150622	L
O-O--0.567900	-1	3.811650	-5.194972	-7.857230	L
C-CT--0.204100	0	3.310068	-3.184456	-5.420756	H
C-C-0.713000	0	2.181987	-2.266279	-5.882709	H
O-O--0.593100	0	2.016582	-1.965599	-7.058032	H
N-N--0.919100	0	1.406226	-1.755568	-4.879639	H
H-H-0.271900	-1	4.878146	-4.886860	-4.638784	L
H-H1-0.104800	-1	2.100837	-4.948900	-5.105883	L
H-HC-0.079700	0	4.201368	-2.940129	-6.008411	H
H-HC-0.079700	0	3.534562	-3.025657	-4.362596	H
H-H-0.419600	0	0.528200	-1.366856	-5.199148	H
H-H-0.419600	0	1.463014	-2.107645	-3.931871	H
N-N--0.415700	-1	1.563211	-5.134525	-7.644897	L
C-CT--0.149000	-1	1.213410	-5.399797	-9.070138	L
H-H-0.271900	-1	0.806621	-4.908877	-7.000064	L
H-H1-0.097600	-1	2.120283	-5.624345	-9.631041	L
H-H1-0.097600	-1	0.731034	-4.519279	-9.495414	L
H-H1-0.097600	-1	0.532540	-6.249247	-9.123417	L
C-CT--0.366200	-1	11.741834	-5.899780	-0.611782	L
C-C-0.597200	-1	10.725226	-6.024789	0.531215	L
O-O--0.567900	-1	11.040600	-5.865218	1.715618	L
H-HC-0.112300	-1	11.242472	-6.079748	-1.563665	L
H-HC-0.112300	-1	12.535519	-6.633520	-0.473644	L
H-HC-0.112300	-1	12.170163	-4.897246	-0.610137	L
N-N--0.415700	-1	9.489859	-6.333061	0.139476	L
C-CT--0.023700	-1	8.329131	-6.530725	1.002717	L
C-C-0.597300	-1	7.277708	-7.379101	0.300048	L
O-O--0.567900	-1	7.100054	-7.224492	-0.915089	L
C-CT-0.034200	0	7.720317	-5.171048	1.388758	L
C-CT-0.001800	0	6.819821	-5.184771	2.639745	L
S-S--0.273700	0	5.108887	-5.780988	2.459781	L
C-CT--0.053600	0	4.237000	-4.243303	2.022337	L
H-H-0.271900	-1	9.322498	-6.410401	-0.857676	L
H-H1-0.088000	-1	8.654001	-7.058999	1.887481	L
H-HC-0.024100	0	7.165449	-4.762162	0.544609	L
H-HC-0.024100	0	8.549914	-4.499838	1.591664	L

H-H1-0.044000	0	6.761993	-4.166144	3.023935 L
H-H1-0.044000	0	7.311091	-5.785275	3.405329 L
H-H1-0.068400	0	3.179437	-4.448482	1.852947 L
H-H1-0.068400	0	4.651537	-3.812109	1.114509 L
H-H1-0.068400	0	4.323732	-3.514807	2.828812 L
N-N--0.415700	-1	6.570926	-8.224135	1.060923 L
C-CT--0.149000	-1	5.351335	-8.934569	0.647885 L
H-H-0.271900	-1	6.886317	-8.351765	2.022492 L
H-H1-0.097600	-1	5.134647	-8.707885	-0.395526 L
H-H1-0.097600	-1	4.515940	-8.614439	1.270783 L
H-H1-0.097600	-1	5.500312	-10.007784	0.763139 L
C-CT--0.366200	-1	3.912351	-9.324201	4.928635 L
C-C-0.597200	-1	3.740233	-7.916819	5.534707 L
O-O--0.567900	-1	4.699991	-7.197341	5.826924 L
H-HC-0.112300	-1	2.931487	-9.767949	4.754981 L
H-HC-0.112300	-1	4.477311	-9.951137	5.618237 L
H-HC-0.112300	-1	4.449160	-9.249607	3.982780 L
N-N--0.415700	-1	2.477555	-7.505044	5.679239 L
C-CT--0.087500	-1	2.037579	-6.101714	5.621750 L
C-C-0.597300	-1	1.912952	-5.539370	7.044170 L
O-O--0.567900	-1	0.875574	-5.633060	7.715566 L
C-CT-0.298500	0	0.718163	-5.940911	4.833083 L
C-CT--0.319200	0	0.313440	-4.467469	4.703588 L
C-CT--0.319200	0	0.836297	-6.526142	3.416850 L
H-H-0.271900	-1	1.743664	-8.201144	5.524407 L
H-H1-0.096900	-1	2.802508	-5.528488	5.094375 L
H-HC--0.029700	0	-0.076546	-6.478863	5.351908 L
H-HC-0.079100	0	1.067196	-3.910026	4.143019 L
H-HC-0.079100	0	0.181159	-4.006288	5.681208 L
H-HC-0.079100	0	-0.632027	-4.389690	4.167009 L
H-HC-0.079100	0	1.629066	-6.010240	2.873015 L
H-HC-0.079100	0	-0.101298	-6.369639	2.881427 L
H-HC-0.079100	0	1.043051	-7.592574	3.451295 L
N-N--0.415700	-1	3.071505	-5.082688	7.519131 L
C-CT--0.149000	-1	3.446858	-4.943057	8.923507 L
H-H-0.271900	-1	3.831167	-4.999776	6.853786 L
H-H1-0.097600	-1	2.559844	-5.048298	9.548355 L
H-H1-0.097600	-1	3.890448	-3.961301	9.085592 L
H-H1-0.097600	-1	4.169188	-5.716502	9.184749 L
C-CT--0.366200	-1	12.492341	-4.187311	6.360603 L
C-C-0.597200	-1	12.287642	-3.468682	5.008482 L
O-O--0.567900	-1	13.255012	-3.252456	4.271946 L
H-HC-0.112300	-1	11.532758	-4.287799	6.867762 L
H-HC-0.112300	-1	13.171672	-3.603530	6.982954 L
H-HC-0.112300	-1	12.916922	-5.175153	6.186667 L
N-N--0.415700	-1	11.051930	-3.045578	4.703583 L
C-CT--0.023700	-1	10.774744	-2.224993	3.526936 L
C-C-0.597300	-1	11.340568	-0.800835	3.659807 L
O-O--0.567900	-1	12.069498	-0.336830	2.781228 L
C-CT-0.034200	0	9.267433	-2.150320	3.264808 L
C-CT-0.001800	0	9.017832	-1.462596	1.916193 L
S-S--0.273700	0	7.445807	-1.868891	1.135896 L
C-CT--0.053600	0	6.253541	-0.994721	2.182079 L
H-H-0.271900	-1	10.286872	-3.274009	5.331968 L

H-H1-0.088000	-1	11.246678	-2.706238	2.668605	L
H-HC-0.024100	0	8.759946	-1.599956	4.058186	L
H-HC-0.024100	0	8.871292	-3.161034	3.244616	L
H-H1-0.044000	0	9.799072	-1.769667	1.219735	L
H-H1-0.044000	0	9.087136	-0.380806	2.038186	L
H-H1-0.068400	0	5.236633	-1.201188	1.840306	L
H-H1-0.068400	0	6.422007	0.079631	2.113285	L
H-H1-0.068400	0	6.348023	-1.322033	3.215691	L
N-N--0.415700	-1	11.071329	-0.109890	4.773028	L
C-CT--0.149000	-1	11.623074	1.229879	4.998914	L
H-H-0.271900	-1	10.493062	-0.539504	5.494596	L
H-H1-0.097600	-1	12.211462	1.530787	4.132217	L
H-H1-0.097600	-1	12.259948	1.215950	5.882989	L
H-H1-0.097600	-1	10.808142	1.937935	5.149371	L
C-CT--0.366200	-1	6.182310	8.718374	-5.583458	L
C-C-0.597200	-1	6.497987	7.529090	-4.654934	L
O-O--0.567900	-1	6.650786	6.379624	-5.092233	L
H-HC-0.112300	-1	6.089338	9.628639	-4.990146	L
H-HC-0.112300	-1	5.245413	8.531087	-6.109385	L
H-HC-0.112300	-1	6.987993	8.838104	-6.308483	L
N-N--0.415700	-1	6.640384	7.847916	-3.358238	L
C-CT--0.001400	-1	6.682432	6.859230	-2.265524	L
C-C-0.597300	-1	5.307955	6.178813	-2.123416	L
O-O--0.567900	-1	4.433897	6.660481	-1.385304	L
C-CT--0.001400	-1	7.198889	7.496412	-0.962336	L
C-CA--0.001100	-1	7.884685	6.528351	-0.004178	L
C-CA--0.190600	-1	9.292512	6.479233	0.047086	L
C-CA--0.190600	-1	7.138914	5.708922	0.868077	L
C-CA--0.234100	-1	9.943191	5.661673	0.990097	L
C-CA--0.234100	-1	7.793958	4.886279	1.810834	L
C-C-0.322600	-1	9.196357	4.885339	1.890345	L
O-OH--0.557900	-1	9.856913	4.142537	2.825032	L
H-H-0.271900	-1	6.575240	8.840385	-3.119094	L
H-H1-0.087600	-1	7.394270	6.086983	-2.543258	L
H-HC-0.029500	-1	7.923994	8.267624	-1.225096	L
H-HC-0.029500	-1	6.385934	8.004326	-0.441984	L
H-HA-0.169900	-1	9.878334	7.101806	-0.614136	L
H-HA-0.169900	-1	6.057910	5.713800	0.824125	L
H-HA-0.165600	-1	11.020442	5.633234	1.039778	L
H-HA-0.165600	-1	7.219623	4.254847	2.472832	L
H-HO-0.399200	-1	9.360278	3.920789	3.628777	L
N-N--0.415700	-1	5.097185	5.155544	-2.956060	L
C-CT-0.033700	-1	3.781103	4.658588	-3.342270	L
C-C-0.597300	-1	2.944340	4.024127	-2.220452	L
O-O--0.567900	-1	1.720909	4.124088	-2.289746	L
C-CT--0.182500	-1	3.970949	3.657174	-4.476408	L
H-H-0.271900	-1	5.880621	4.861707	-3.534348	L
H-H1-0.082300	-1	3.214621	5.502010	-3.738306	L
H-HC-0.060300	-1	3.000312	3.344949	-4.860795	L
H-HC-0.060300	-1	4.508938	2.790126	-4.093019	L
H-HC-0.060300	-1	4.541380	4.116617	-5.283776	L
N-N--0.415700	-1	3.558591	3.385205	-1.214077	L H-HC 209
C-CT-0.021300	0	2.819089	2.712066	-0.117554	H
C-C-0.597300	0	2.319967	3.765216	0.878721	H

O-O--0.567900	0	3.098444	4.592129	1.352372	H
C-CT--0.123100	0	3.774946	1.718002	0.584411	H
S-S--1.036000	0	2.924987	0.518589	1.695975	H
H-H-0.271900	-1	4.562467	3.361359	-1.205922	L
H-H1-0.112400	0	1.982557	2.160061	-0.556641	H
H-H1-0.111200	0	4.513326	2.300099	1.150930	H
H-H1-0.111200	0	4.336831	1.165484	-0.182523	H
N-N--0.415700	0	0.995686	3.718342	1.213965	H
C-CT--0.051800	0	0.415421	4.541361	2.278248	H
C-C-0.597300	0	0.786839	4.026921	3.705486	H
O-O--0.567900	0	1.330051	4.753106	4.538432	H
C-CT--0.110200	-1	-1.118315	4.642943	2.013453	H
C-CT-0.353100	-1	-1.978353	5.548507	2.921520	L H-HC 222
C-CT--0.412100	-1	-2.169148	5.004831	4.338966	L
C-CT--0.412100	-1	-1.449693	6.983139	3.006612	L
H-H-0.271900	0	0.407592	2.982839	0.823236	H
H-H1-0.092200	0	0.873442	5.532330	2.231970	H
H-HC-0.045700	0	-1.240595	5.012699	0.988132	H
H-HC-0.045700	0	-1.560620	3.644034	2.034422	H
H-HC--0.036100	-1	-2.970159	5.594330	2.472969	L
H-HC-0.100000	-1	-1.270394	5.148572	4.935053	L
H-HC-0.100000	-1	-2.412574	3.944053	4.300209	L
H-HC-0.100000	-1	-2.989178	5.537651	4.817995	L
H-HC-0.100000	-1	-0.487588	7.002219	3.519522	L
H-HC-0.100000	-1	-2.162346	7.601905	3.550545	L
H-HC-0.100000	-1	-1.326704	7.383550	1.999428	L
N-N--0.415700	0	0.485439	2.722303	3.968990	H
C-CT--0.087500	0	0.589867	2.173638	5.322029	H
C-C-0.597300	0	2.002928	2.165936	5.923208	H
O-O--0.567900	0	2.108362	2.204362	7.149836	H
C-CT-0.298500	-1	-0.025285	0.755926	5.368199	H
C-CT--0.319200	0	0.694234	-0.280531	4.479503	L H-HC 241
C-CT--0.319200	0	-0.167214	0.151751	6.765725	L H-HC 241
H-H-0.271900	0	0.056128	2.165305	3.236109	H
H-H1-0.096900	0	0.028044	2.828653	6.001559	H
H-HC--0.029700	0	-1.038303	0.842611	4.971301	H
H-HC-0.079100	0	1.678103	-0.523291	4.874694	L
H-HC-0.079100	0	0.823547	0.108260	3.469500	L
H-HC-0.079100	0	0.096171	-1.186486	4.401111	L
H-HC-0.079100	0	0.813427	-0.084169	7.177257	L
H-HC-0.079100	0	-0.758099	-0.761501	6.701658	L
H-HC-0.079100	0	-0.676608	0.861287	7.415887	L
N-N--0.415700	0	3.016478	1.950733	5.064485	H
C-CT-0.033700	0	4.375523	1.810595	5.547793	H
C-C-0.597300	-1	5.090697	3.145230	5.820184	L H-H1 254
O-O--0.567900	-1	6.265649	3.122891	6.176497	L
C-CT--0.182500	-1	5.153439	0.995313	4.520164	L H-H1 254
H-H-0.271900	0	2.859710	1.878071	4.058758	H
H-H1-0.082300	0	4.359317	1.269247	6.499645	H
H-HC-0.060300	-1	6.120665	0.704378	4.927294	L
H-HC-0.060300	-1	5.309593	1.595080	3.623724	L
H-HC-0.060300	-1	4.596388	0.092000	4.268307	L
N-N--0.415700	-1	4.386528	4.272176	5.653456	L
C-CT--0.087500	-1	4.768322	5.635931	6.047378	L

C-C-0.597300	-1	3.925939	6.085116	7.248517	L
O-O--0.567900	-1	4.477587	6.537938	8.252553	L
C-CT-0.298500	-1	4.552910	6.608816	4.870734	L
C-CT--0.319200	-1	4.945812	8.048444	5.220010	L
C-CT--0.319200	-1	5.370666	6.211429	3.642185	L
H-H-0.271900	-1	3.475416	4.156247	5.227403	L
H-H1-0.096900	-1	5.818201	5.666102	6.328924	L
H-HC--0.029700	-1	3.500532	6.595089	4.594781	L
H-HC-0.079100	-1	5.996262	8.087239	5.500051	L
H-HC-0.079100	-1	4.339132	8.426667	6.042071	L
H-HC-0.079100	-1	4.784845	8.685931	4.350969	L
H-HC-0.079100	-1	6.420807	6.134389	3.917965	L
H-HC-0.079100	-1	5.253536	6.957633	2.856744	L
H-HC-0.079100	-1	5.019053	5.253438	3.259147	L
N-N--0.415700	-1	2.594745	5.893438	7.195014	L
C-CT--0.149000	-1	1.687117	6.234391	8.301213	L
H-H-0.271900	-1	2.188322	5.511030	6.346660	L
H-H1-0.097600	-1	2.264425	6.631236	9.136345	L
H-H1-0.097600	-1	1.151829	5.339746	8.620891	L
H-H1-0.097600	-1	0.971440	6.985039	7.966010	L
C-CT--0.366200	-1	4.045033	10.313751	-1.017000	L
C-C-0.597200	-1	2.570472	9.985818	-1.261332	L
O-O--0.567900	-1	1.760425	10.900084	-1.335771	L
H-HC-0.112300	-1	4.620992	9.390136	-0.979317	L
H-HC-0.112300	-1	4.146313	10.844532	-0.070568	L
H-HC-0.112300	-1	4.416485	10.940888	-1.827097	L
N-N--0.415700	-1	2.192480	8.702554	-1.314718	L
C-CT--0.024900	-1	0.779364	8.320341	-1.155177	L
C-C-0.597300	-1	0.191978	8.819930	0.170485	L
O-O--0.567900	-1	-0.902814	9.386833	0.177154	L
C-CT-0.211700	0	0.611062	6.820152	-1.297886	L
O-OH--0.654600	0	0.900868	6.510748	-2.641118	L
H-H-0.271900	-1	2.895363	7.970206	-1.373834	L
H-H1-0.084300	-1	0.206762	8.768551	-1.962925	L
H-H1-0.035200	0	-0.412166	6.530518	-1.066608	L
H-H1-0.035200	0	1.295215	6.295922	-0.628638	L
H-HO-0.427500	0	1.007978	5.535547	-2.649662	L
N-N--0.415700	-1	0.954326	8.687943	1.266691	L
C-CT-0.033700	-1	0.599925	9.171535	2.602332	L
C-C-0.597300	-1	0.134282	10.632415	2.590886	L
O-O--0.567900	-1	-0.962434	10.951037	3.052834	L
C-CT--0.182500	-1	1.786476	8.937112	3.534796	L
H-H-0.271900	-1	1.843168	8.191977	1.162539	L
H-H1-0.082300	-1	-0.214568	8.579615	2.993031	L
H-HC-0.060300	-1	1.556121	9.309451	4.532332	L
H-HC-0.060300	-1	2.671743	9.438510	3.145807	L
H-HC-0.060300	-1	1.982333	7.868162	3.591284	L
N-N--0.415700	-1	0.932034	11.510752	1.973655	L
C-CT--0.149000	-1	0.590747	12.907746	1.778101	L
H-H-0.271900	-1	1.834835	11.202650	1.620697	L
H-H1-0.097600	-1	-0.395508	13.102974	2.200637	L
H-H1-0.097600	-1	0.580379	13.134106	0.712773	L
H-H1-0.097600	-1	1.329651	13.535704	2.276911	L
C-CT--0.366200	-1	-11.925746	4.583680	4.948416	L

C-C-0.597200	-1	-12.357263	3.163391	4.579728	L
O-O--0.567900	-1	-12.922145	2.456754	5.416909	L
H-HC-0.112300	-1	-11.446448	5.052073	4.088672	L
H-HC-0.112300	-1	-11.221765	4.545459	5.779837	L
H-HC-0.112300	-1	-12.800093	5.165495	5.238484	L
N-N--0.415700	-1	-12.022685	2.720273	3.367537	L
C-CT--0.087500	-1	-12.017487	1.297122	3.011249	L
C-C-0.597300	-1	-10.571065	0.902921	2.698602	L
O-O--0.567900	-1	-9.856129	1.545777	1.922207	L
C-CT-0.298500	-1	-13.013152	0.903906	1.887369	L
C-CT--0.319200	-1	-13.759576	-0.386133	2.275297	L
C-CT--0.319200	-1	-14.092120	1.950404	1.575794	L
H-H-0.271900	-1	-11.612775	3.370377	2.694389	L
H-H1-0.096900	-1	-12.309830	0.739310	3.898515	L
H-HC--0.029700	-1	-12.454037	0.712722	0.975115	L
H-HC-0.079100	-1	-14.392258	-0.203039	3.144496	L
H-HC-0.079100	-1	-13.043088	-1.177471	2.499207	L
H-HC-0.079100	-1	-14.395933	-0.703389	1.449363	L
H-HC-0.079100	-1	-14.725974	2.096024	2.447023	L
H-HC-0.079100	-1	-14.699273	1.612247	0.737491	L
H-HC-0.079100	-1	-13.635871	2.902503	1.313572	L
N-N--0.415700	-1	-10.106800	-0.115271	3.425599	L
C-CT--0.038900	-1	-8.698343	-0.511056	3.508733	L
C-C-0.597300	-1	-8.568922	-2.036172	3.625125	L
O-O--0.567900	-1	-9.499250	-2.696426	4.109101	L
C-CT-0.365400	-1	-7.982400	0.139371	4.716350	L
O-OH--0.676100	-1	-8.149784	-0.572885	5.920634	L
C-CT--0.243800	-1	-8.402266	1.576066	5.020845	L
H-H-0.271900	-1	-10.735893	-0.587402	4.058921	L
H-H1-0.100700	-1	-8.198285	-0.179007	2.598972	L
H-H1-0.004300	-1	-6.923318	0.139807	4.480105	L
H-HC-0.064200	-1	-8.446131	2.138769	4.095828	L
H-HC-0.064200	-1	-7.674637	2.035113	5.691436	L
H-HC-0.064200	-1	-9.385641	1.602576	5.489416	L
H-HO-0.410200	-1	-8.401989	0.067689	6.618063	L
N-N--0.254800	-1	-7.442218	-2.630769	3.193426	L
C-CT--0.026600	-1	-7.189907	-4.056202	3.366309	L
C-C-0.589600	-1	-6.581249	-4.407040	4.725255	L
O-O--0.574800	-1	-6.591202	-5.577145	5.090636	L
C-CT--0.007000	0	-6.197140	-4.395686	2.253492	L
C-CT-0.018900	0	-5.358005	-3.125719	2.126327	L
C-CT-0.019200	0	-6.369191	-2.014660	2.414028	L
H-H1-0.064100	-1	-8.099216	-4.627919	3.222876	L
H-HC-0.025300	0	-5.582005	-5.255546	2.511407	L
H-HC-0.025300	0	-6.736769	-4.575542	1.322817	L
H-HC-0.021300	0	-4.923201	-3.033921	1.132150	L
H-HC-0.021300	0	-4.573747	-3.120483	2.883884	L
H-H1-0.039100	0	-6.769080	-1.641220	1.470863	L
H-H1-0.039100	0	-5.885041	-1.206702	2.964196	L
N-N--0.415700	-1	-5.963923	-3.443114	5.416522	L
C-CT--0.001400	-1	-4.972304	-3.680450	6.476964	L
C-C-0.597300	-1	-5.519522	-4.461807	7.685947	L
O-O--0.567900	-1	-6.706180	-4.346244	7.996426	L
C-CT--0.001400	0	-4.461803	-2.345685	7.037142	L H-HA 373

C-CA--0.001100	0	-4.157234	-1.278538	6.011939	H
C-CA--0.190600	0	-3.265140	-1.538815	4.971743	H
C-CA--0.190600	0	-4.754462	-0.019452	6.107786	H
C-CA--0.234100	0	-2.981559	-0.559582	4.030142	H
C-CA--0.234100	0	-4.473830	0.973441	5.174664	H
C-C-0.322600	0	-3.584212	0.707711	4.127778	H
O-OH--0.557900	0	-3.348974	1.685545	3.228386	H
H-H-0.271900	-1	-6.032424	-2.505167	5.052848	L
H-H1-0.087600	-1	-4.146739	-4.248954	6.047355	L
H-HC-0.029500	0	-5.213764	-1.950898	7.722936	L
H-HC-0.029500	0	-3.556776	-2.529864	7.617468	L
H-HA-0.169900	0	-2.785204	-2.511291	4.885946	H
H-HA-0.169900	0	-5.445833	0.200985	6.921855	H
H-HA-0.165600	0	-2.256555	-0.732287	3.246419	H
H-HA-0.165600	0	-4.905182	1.967203	5.264445	H
H-HO-0.399200	0	-2.481549	1.527025	2.768234	H
N-N--0.415700	-1	-4.640064	-5.148677	8.441545	L
C-CT--0.149000	-1	-5.024077	-5.612439	9.791241	L
H-H-0.271900	-1	-3.645313	-5.140969	8.201993	L
H-H1-0.097600	-1	-6.107892	-5.563458	9.897333	L
H-H1-0.097600	-1	-4.556046	-4.976010	10.541487	L
H-H1-0.097600	-1	-4.691513	-6.641498	9.929560	L
C-CT--0.366200	-1	-0.453733	-10.770499	2.492101	L
C-C-0.597200	-1	-0.635567	-9.832936	1.285226	L
O-O--0.567900	-1	-1.745252	-9.661364	0.775837	L
H-HC-0.112300	-1	0.594226	-10.782413	2.788175	L
H-HC-0.112300	-1	-0.765862	-11.778760	2.218655	L
H-HC-0.112300	-1	-1.062958	-10.415759	3.323431	L
N-N--0.415700	-1	0.477946	-9.285912	0.780555	L
C-CT-0.014300	-1	0.432794	-8.270780	-0.271249	L H-HC 405
C-C-0.597300	-1	0.060232	-8.782322	-1.681602	L
O-O--0.567900	-1	-0.152032	-7.961850	-2.565176	L
C-CT--0.204100	0	1.726996	-7.436707	-0.284317	H
C-C-0.713000	0	1.432952	-6.031591	-0.825528	H
O-O--0.593100	0	0.380050	-5.458541	-0.528738	H
N-N--0.919100	0	2.394147	-5.437298	-1.556003	H
H-H-0.271900	-1	1.360938	-9.471374	1.227311	L
H-H1-0.104800	-1	-0.370850	-7.599109	0.030917	L
H-HC-0.079700	0	2.507047	-7.964756	-0.844629	H
H-HC-0.079700	0	2.078288	-7.304758	0.744389	H
H-H-0.419600	0	2.279986	-4.445476	-1.791002	H
H-H-0.419600	0	3.218556	-5.938743	-1.849309	H
N-N--0.415700	-1	-0.034298	-10.096268	-1.916256	L
C-CT--0.149000	-1	-0.573493	-10.650666	-3.170175	L
H-H-0.271900	-1	0.076266	-10.743671	-1.127807	L
H-H1-0.097600	-1	-0.638894	-9.861536	-3.918536	L
H-H1-0.097600	-1	-1.566406	-11.062192	-2.988653	L
H-H1-0.097600	-1	0.085875	-11.440940	-3.531300	L
C-CT--0.366200	-1	-3.843246	-11.708466	-1.401837	L
C-C-0.597200	-1	-4.611781	-10.383032	-1.477291	L
O-O--0.567900	-1	-5.750502	-10.387883	-1.949064	L
H-HC-0.112300	-1	-2.860287	-11.533058	-0.963724	L
H-HC-0.112300	-1	-3.725668	-12.117986	-2.404128	L
H-HC-0.112300	-1	-4.396080	-12.414075	-0.782078	L

N-N--0.415700	-1	-3.985458	-9.254409	-1.104403	L
C-CT--0.087500	-1	-4.550514	-7.894245	-1.271024	L
C-C-0.597300	-1	-4.815039	-7.515607	-2.739403	L
O-O--0.567900	-1	-5.804174	-6.847423	-3.037063	L
C-CT-0.298500	-1	-3.644533	-6.815328	-0.621763	L
C-CT--0.319200	-1	-4.132698	-5.378378	-0.865981	L
C-CT--0.319200	-1	-3.629933	-6.948311	0.898656	L
H-H-0.271900	-1	-3.103677	-9.363337	-0.601488	L
H-H1-0.096900	-1	-5.511682	-7.871909	-0.758820	L
H-HC--0.029700	-1	-2.628696	-6.913614	-1.005016	L
H-HC-0.079100	-1	-5.168818	-5.281801	-0.540735	L
H-HC-0.079100	-1	-4.064222	-5.129231	-1.922286	L
H-HC-0.079100	-1	-3.506484	-4.669313	-0.322442	L
H-HC-0.079100	-1	-4.636783	-6.813326	1.276376	L
H-HC-0.079100	-1	-2.966949	-6.201017	1.337018	L
H-HC-0.079100	-1	-3.280297	-7.924687	1.203210	L
N-N--0.415700	-1	-3.967486	-7.917078	-3.694994	L
C-CT--0.149000	-1	-4.052711	-7.506319	-5.107234	L
H-H-0.271900	-1	-3.245436	-8.578990	-3.436133	L
H-H1-0.097600	-1	-4.871285	-6.796822	-5.230993	L
H-H1-0.097600	-1	-4.234104	-8.382560	-5.731229	L
H-H1-0.097600	-1	-3.116505	-7.035708	-5.406211	L
C-CT--0.366200	-1	-12.111513	3.667938	-1.344863	L
C-C-0.597200	-1	-11.006647	2.602685	-1.305032	L
O-O--0.567900	-1	-11.299095	1.419955	-1.147089	L
H-HC-0.112300	-1	-11.663625	4.650873	-1.491308	L
H-HC-0.112300	-1	-12.662483	3.656286	-0.404045	L
H-HC-0.112300	-1	-12.794138	3.453126	-2.167289	L
N-N--0.415700	-1	-9.750333	3.044073	-1.372956	L
C-CT--0.024900	-1	-8.567207	2.223214	-1.190388	L
C-C-0.597300	-1	-7.455773	3.091136	-0.594795	L
O-O--0.567900	-1	-6.802984	3.877916	-1.294757	L
C-CT-0.211700	0	-8.150488	1.576133	-2.510247	L
O-OH--0.654600	0	-7.282266	0.517356	-2.222231	L
H-H-0.271900	-1	-9.624481	4.040417	-1.445783	L
H-H1-0.084300	-1	-8.804732	1.432559	-0.480000	L
H-H1-0.035200	0	-7.665494	2.294068	-3.168503	L
H-H1-0.035200	0	-9.032332	1.169032	-3.006996	L
H-HO-0.427500	0	-6.347019	0.815308	-2.282936	L
N-N--0.415700	-1	-7.294450	3.021104	0.735464	L
C-CT-0.021300	-1	-6.120234	3.638973	1.370181	L
C-C-0.597300	-1	-4.831097	2.991601	0.839159	L
O-O--0.567900	-1	-3.856405	3.679723	0.577581	L
C-CT--0.123100	-1	-6.178909	3.506843	2.893595	L
S-SH--0.311900	-1	-7.433706	4.614370	3.597356	L
H-H-0.271900	-1	-7.955415	2.475679	1.285443	L
H-H1-0.112400	-1	-6.092240	4.700306	1.118421	L
H-H1-0.111200	-1	-5.208228	3.781725	3.309816	L
H-H1-0.111200	-1	-6.394583	2.472747	3.161182	L
H-HS-0.193300	-1	-8.475109	4.163757	2.888620	L
N-N--0.415700	-1	-4.868359	1.672150	0.636707	L H-HC 478
C-CT-0.021300	0	-3.667670	0.993445	0.082365	H
C-C-0.597300	0	-3.670707	1.148663	-1.434496	H
O-O--0.567900	0	-4.719833	1.089587	-2.081834	H

C-CT--0.123100	0	-3.624642	-0.484520	0.509980	H
S-SH--0.311900	0	-2.164946	-1.506640	-0.062432	H
H-H-0.271900	-1	-5.719285	1.183999	0.843380	L
H-H1-0.112400	0	-2.798215	1.503787	0.492394	H
H-H1-0.111200	0	-4.439082	-1.046642	0.035869	H
H-H1-0.111200	0	-3.714535	-0.584715	1.589825	H
H-HS-0.193300	0	0.837389	-3.087470	1.014890	H
N-N--0.415700	0	-2.446158	1.302334	-2.004745	H
C-CT--0.087500	0	-2.302238	1.395298	-3.448194	H
C-C-0.597300	0	-2.220126	0.030986	-4.186001	H
O-O--0.567900	0	-2.325444	0.028528	-5.409084	H
C-CT-0.298500	-1	-1.111767	2.283197	-3.886183	H
C-CT--0.319200	0	-1.226094	3.694368	-3.306894	L H-HC 492
C-CT--0.319200	0	0.246567	1.694431	-3.459775	L H-HC 492
H-H-0.271900	0	-1.634067	1.387828	-1.380840	H
H-H1-0.096900	0	-3.233957	1.827189	-3.832023	H
H-HC--0.029700	0	-1.128673	2.341593	-4.976539	H
H-HC-0.079100	0	-1.090159	3.672176	-2.222896	L
H-HC-0.079100	0	-2.205740	4.100750	-3.539171	L
H-HC-0.079100	0	-0.467184	4.334634	-3.752130	L
H-HC-0.079100	0	0.341202	1.703440	-2.372249	L
H-HC-0.079100	0	1.049279	2.284245	-3.893336	L
H-HC-0.079100	0	0.354178	0.671256	-3.811070	L
N-N--0.415700	0	-1.945962	-1.076032	-3.434380	H
C-CT--0.003100	0	-2.041359	-2.422412	-4.005267	H
C-C-0.597300	0	-3.504347	-2.877970	-4.173381	H
O-O--0.567900	0	-3.799519	-3.681288	-5.049102	H
C-CT--0.003600	-1	-1.285258	-3.455979	-3.114852	H
C-CT--0.064500	-1	-1.416500	-4.911732	-3.601537	L H-HC 508
C-C-0.695100	-1	-0.542061	-5.252498	-4.793523	L
O-O--0.608600	-1	-0.400328	-4.503787	-5.745447	L
N-N--0.940700	-1	0.072858	-6.415644	-4.785063	L
H-H-0.271900	0	-2.002017	-1.008130	-2.420465	H
H-H1-0.085000	0	-1.630582	-2.392086	-5.017069	H
H-HC-0.017100	0	-0.229110	-3.202648	-3.033782	H
H-HC-0.017100	0	-1.707206	-3.418140	-2.107802	H
H-HC-0.035200	-1	-2.444186	-5.168502	-3.842385	L
H-HC-0.035200	-1	-1.130899	-5.557138	-2.778262	L
H-H-0.425100	-1	0.676638	-6.665232	-5.548646	L
H-H-0.425100	-1	-0.036500	-7.034630	-3.983633	L
N-N--0.415700	0	-4.347736	-2.484562	-3.151204	H
C-CT--0.023700	0	-5.724627	-2.961396	-3.235287	H
C-C-0.597300	-1	-6.401417	-2.348154	-4.477123	L H-H1 522
O-O--0.567900	-1	-6.231985	-1.153371	-4.738734	L
C-CT-0.034200	-1	-6.462202	-2.682352	-1.909745	L H-H1 522
C-CT-0.001800	-1	-7.930035	-3.133464	-1.965946	L
S-S--0.273700	-1	-8.834343	-3.104606	-0.390804	L
C-CT--0.053600	-1	-9.205289	-1.336844	-0.263883	L
H-H-0.271900	0	-4.291461	-1.507330	-2.901338	H
H-H1-0.088000	0	-5.650477	-4.038029	-3.349580	H
H-HC-0.024100	-1	-6.393229	-1.635203	-1.652604	L
H-HC-0.024100	-1	-5.968222	-3.232281	-1.112272	L
H-H1-0.044000	-1	-7.953770	-4.159994	-2.333048	L
H-H1-0.044000	-1	-8.470876	-2.509478	-2.677764	L

H-H1-0.068400	-1	-9.811325	-1.150628	0.622695	L
H-H1-0.068400	-1	-9.755772	-1.010381	-1.146433	L
H-H1-0.068400	-1	-8.276107	-0.775465	-0.193413	L
N-N--0.254800	-1	-7.149112	-3.120389	-5.287131	L
C-CT--0.026600	-1	-7.546472	-2.707357	-6.633993	L
C-C-0.589600	-1	-8.996871	-2.225695	-6.626900	L
O-O--0.574800	-1	-9.881997	-2.926111	-6.128720	L
C-CT--0.007000	-1	-7.338260	-3.952910	-7.509987	L
C-CT-0.018900	-1	-6.820333	-5.012655	-6.534356	L
C-CT-0.019200	-1	-7.353373	-4.550172	-5.204740	L
H-H1-0.064100	-1	-6.900226	-1.910302	-7.001135	L
H-HC-0.025300	-1	-8.272149	-4.276052	-7.960943	L
H-HC-0.025300	-1	-6.602986	-3.769100	-8.291104	L
H-HC-0.021300	-1	-5.732239	-5.002891	-6.508104	L
H-HC-0.021300	-1	-7.192910	-5.996180	-6.748105	L
H-H1-0.039100	-1	-6.828412	-5.055539	-4.405789	L
H-H1-0.039100	-1	-8.418514	-4.772193	-5.129887	L
N-N--0.415700	-1	-9.222079	-1.030636	-7.166396	L
C-CT--0.149000	-1	-10.456853	-0.262932	-6.978218	L
H-H-0.271900	-1	-8.418047	-0.560853	-7.582051	L
H-H1-0.097600	-1	-11.216063	-0.901099	-6.526631	L
H-H1-0.097600	-1	-10.811179	0.095740	-7.944577	L
H-H1-0.097600	-1	-10.259399	0.586658	-6.324133	L
C-CT--0.366200	-1	-10.355538	8.823762	-4.266385	L
C-C-0.597200	-1	-9.804661	7.537256	-3.637121	L
O-O--0.567900	-1	-10.246440	7.119100	-2.565538	L
H-HC-0.112300	-1	-9.837400	9.020224	-5.204921	L
H-HC-0.112300	-1	-10.198080	9.657806	-3.583053	L
H-HC-0.112300	-1	-11.421975	8.707041	-4.458263	L
N-N--0.415700	-1	-8.832726	6.914770	-4.298686	L
C-CT--0.024900	-1	-7.886828	5.999677	-3.656518	L
C-C-0.597300	-1	-6.558522	6.734521	-3.437074	L
O-O--0.567900	-1	-6.305505	7.740699	-4.106969	L
C-CT-0.211700	0	-7.662818	4.743212	-4.510085	L
O-OH--0.654600	0	-7.290503	5.050671	-5.840359	L
H-H-0.271900	-1	-8.562637	7.281900	-5.210245	L
H-H1-0.084300	-1	-8.272120	5.662038	-2.694052	L
H-H1-0.035200	0	-8.582415	4.156906	-4.526611	L
H-H1-0.035200	0	-6.876273	4.141009	-4.053160	L
H-HO-0.427500	0	-6.872859	4.271868	-6.225998	L
N-N--0.415700	-1	-5.679812	6.206379	-2.574638	L
C-CT-0.033700	-1	-4.306936	6.717823	-2.472553	L
C-C-0.597300	-1	-3.559360	6.720572	-3.825020	L
O-O--0.567900	-1	-2.661540	7.535393	-4.044038	L
C-CT--0.182500	-1	-3.551865	5.900161	-1.434711	L
H-H-0.271900	-1	-5.961235	5.402043	-2.009138	L
H-H1-0.082300	-1	-4.356154	7.745988	-2.112477	L
H-HC-0.060300	-1	-2.538950	6.283609	-1.330385	L
H-HC-0.060300	-1	-3.514974	4.853482	-1.734820	L
H-HC-0.060300	-1	-4.067541	5.984920	-0.479431	L
N-N--0.415700	-1	-3.979218	5.850990	-4.757773	L
C-CT--0.149000	-1	-3.464245	5.795195	-6.124724	L
H-H-0.271900	-1	-4.706548	5.201626	-4.489168	L
H-H1-0.097600	-1	-2.692133	6.554180	-6.253009	L

H-H1-0.097600	-1	-4.276056	5.982291	-6.827480	L
H-H1-0.097600	-1	-3.039917	4.809036	-6.313017	L
C-CM--0.139000	0	0.591073	-0.991155	-0.460020	H
C-C-0.519000	0	1.273095	-2.305026	-0.695701	H
O-O2--0.567000	0	1.574202	-3.059239	0.357219	H
C-CM--0.117000	0	-0.519727	-0.838594	0.585612	H
O-O2--0.618000	0	1.729960	-2.610912	-1.803508	H
C-C--0.553000	0	-0.697306	0.638631	0.964685	H
O-O2--0.556000	0	-0.521289	1.495368	0.060672	H
O-O2--0.607000	0	-1.101172	0.857290	2.142015	H
H-HC-0.049000	0	1.428391	-0.377740	-0.020326	H
H-HC-0.162000	0	-0.300668	-1.396345	1.493447	H
O-OW--0.834000	-1	6.440494	2.962326	-1.187147	L
H-HW-0.417000	-1	6.811484	3.102393	-2.057550	L
H-HW-0.417000	-1	7.119188	3.265428	-0.584434	L
O-OW--0.834000	0	3.451480	7.187892	1.028571	L
H-HW-0.417000	0	3.267936	6.291355	1.378015	L
H-HW-0.417000	0	3.821302	6.975312	0.154797	L
O-OW--0.834000	0	-0.656912	-3.940855	1.535858	H
H-HW-0.417000	0	-0.433885	-4.646712	0.894649	H
H-HW-0.417000	0	-1.438123	-3.509648	1.147846	H
O-OW--0.834000	0	-5.000622	0.826249	-6.168924	L
H-HW-0.417000	0	-4.064185	0.594315	-6.076094	L
H-HW-0.417000	0	-5.442970	0.173736	-5.599012	L
H-HS-0.193300	0	0.299331	-0.570763	-1.420437	H

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C-CT--0.366200	-1	8.204670	4.663266	-8.149134	L
C-C-0.597200	-1	9.037493	3.922986	-7.107892	L
O-O--0.567900	-1	9.641346	2.886787	-7.387401	L
H-HC-0.112300	-1	7.758647	5.548537	-7.696019	L
H-HC-0.112300	-1	7.415455	4.006866	-8.517369	L
H-HC-0.112300	-1	8.844018	4.963848	-8.980043	L
N-N--0.415700	-1	9.030654	4.483586	-5.891979	L
C-CT--0.087500	-1	9.504265	3.811840	-4.674707	L
C-C-0.597300	-1	8.369737	2.911762	-4.181232	L
O-O--0.567900	-1	7.457293	3.370024	-3.478474	L
C-CT-0.298500	-1	9.983463	4.817603	-3.600809	L
C-CT--0.319200	-1	10.405428	4.122129	-2.300990	L
C-CT--0.319200	-1	11.195252	5.628639	-4.082216	L
H-H-0.271900	-1	8.442829	5.304044	-5.766232	L
H-H1-0.096900	-1	10.343944	3.172931	-4.927770	L
H-HC--0.029700	-1	9.184021	5.521038	-3.385669	L
H-HC-0.079100	-1	11.113961	3.325201	-2.528663	L
H-HC-0.079100	-1	9.536500	3.697040	-1.802402	L
H-HC-0.079100	-1	10.879729	4.833130	-1.626386	L
H-HC-0.079100	-1	12.057768	4.974508	-4.209726	L
H-HC-0.079100	-1	11.438888	6.401794	-3.351419	L
H-HC-0.079100	-1	10.975328	6.105635	-5.036319	L
N-N--0.415700	-1	8.390503	1.638385	-4.610590	L
C-CT--0.087500	-1	7.280668	0.682945	-4.433815	L
C-C-0.597300	-1	7.700902	-0.589876	-3.670313	L
O-O--0.567900	-1	8.848363	-1.037857	-3.793997	L
C-CT-0.298500	-1	6.628600	0.271259	-5.778193	L

C-CT--0.319200	-1	5.767149	1.393817	-6.368305	L
C-CT--0.319200	-1	7.622848	-0.178305	-6.854049	L
H-H-0.271900	-1	9.166781	1.333986	-5.204001	L
H-H1-0.096900	-1	6.508030	1.188357	-3.861455	L
H-HC--0.029700	-1	5.962278	-0.571463	-5.590362	L
H-HC-0.079100	-1	6.281149	2.352037	-6.294159	L
H-HC-0.079100	-1	4.831913	1.439382	-5.814838	L
H-HC-0.079100	-1	5.519573	1.175924	-7.408508	L
H-HC-0.079100	-1	8.220405	0.667658	-7.189627	L
H-HC-0.079100	-1	7.074678	-0.584836	-7.702944	L
H-HC-0.079100	-1	8.279751	-0.948397	-6.457762	L
N-N--0.254800	-1	6.766876	-1.198183	-2.901454	L
C-CT--0.026600	-1	6.903475	-2.549758	-2.352119	L
C-C-0.589600	-1	7.155188	-3.574411	-3.460086	L
O-O--0.574800	-1	6.408600	-3.626435	-4.440528	L
C-CT--0.007000	0	5.568605	-2.841429	-1.643450	L
C-CT-0.018900	0	4.985133	-1.459896	-1.360678	L
C-CT-0.019200	0	5.458803	-0.650161	-2.552185	L
H-H1-0.064100	-1	7.721916	-2.560860	-1.633156	L
H-HC-0.025300	0	4.886154	-3.377991	-2.303979	L
H-HC-0.025300	0	5.718287	-3.411002	-0.730747	L
H-HC-0.021300	0	5.411506	-1.036043	-0.458362	L
H-HC-0.021300	0	3.904565	-1.460614	-1.280907	L
H-H1-0.039100	0	5.513869	0.398647	-2.259954	L
H-H1-0.039100	0	4.765322	-0.780509	-3.384443	L
N-N--0.415700	-1	8.182924	-4.416519	-3.309841	L
C-CT--0.149000	-1	8.556192	-5.413192	-4.326310	L
H-H-0.271900	-1	8.781425	-4.290627	-2.494635	L
H-H1-0.097600	-1	7.812964	-5.417178	-5.122966	L
H-H1-0.097600	-1	8.601161	-6.400885	-3.866419	L
H-H1-0.097600	-1	9.532143	-5.161520	-4.741389	L
C-CT--0.366200	-1	5.263676	-7.408242	-4.078758	L
C-C-0.597200	-1	4.132508	-6.743030	-4.872952	L
O-O--0.567900	-1	3.237499	-7.465202	-5.321505	L
H-HC-0.112300	-1	5.972723	-6.648711	-3.750125	L
H-HC-0.112300	-1	5.774739	-8.133965	-4.711250	L
H-HC-0.112300	-1	4.846175	-7.914983	-3.208614	L
N-N--0.415700	-1	4.116161	-5.412529	-5.014652	L
C-CT-0.014300	-1	3.011846	-4.670002	-5.646936	L H-HC 69
C-C-0.597300	-1	2.819630	-5.014171	-7.158704	L
O-O--0.567900	-1	3.815212	-5.176352	-7.865823	L
C-CT--0.204100	0	3.317640	-3.173316	-5.413570	H
C-C-0.713000	0	2.156275	-2.254707	-5.776229	H
O-O--0.593100	0	1.904171	-1.939421	-6.933673	H
N-N--0.919100	0	1.458053	-1.764603	-4.710549	H
H-H-0.271900	-1	4.882283	-4.871588	-4.647250	L
H-H1-0.104800	-1	2.104911	-4.936010	-5.113651	L
H-HC-0.079700	0	4.172238	-2.909409	-6.046114	H
H-HC-0.079700	0	3.601825	-3.036610	-4.366673	H
H-H-0.419600	0	0.564025	-1.364245	-4.961419	H
H-H-0.419600	0	1.586921	-2.107305	-3.761333	H
N-N--0.415700	-1	1.566768	-5.118660	-7.652771	L
C-CT--0.149000	-1	1.216853	-5.382316	-9.078285	L
H-H-0.271900	-1	0.810115	-4.894745	-7.007409	L

H-H1-0.097600	-1	2.123812	-5.605085	-9.639757	L
H-H1-0.097600	-1	0.733395	-4.501731	-9.502189	L
H-H1-0.097600	-1	0.536897	-6.232434	-9.132564	L
C-CT--0.366200	-1	11.748216	-5.882650	-0.623609	L
C-C-0.597200	-1	10.732070	-6.010374	0.519498	L
O-O--0.567900	-1	11.047605	-5.852120	1.704035	L
H-HC-0.112300	-1	11.248781	-6.061829	-1.575603	L
H-HC-0.112300	-1	12.542742	-6.615715	-0.486724	L
H-HC-0.112300	-1	12.175449	-4.879651	-0.620678	L
N-N--0.415700	-1	9.496930	-6.319446	0.127676	L
C-CT--0.023700	-1	8.336663	-6.519590	0.990966	L
C-C-0.597300	-1	7.285969	-7.368128	0.287404	L
O-O--0.567900	-1	7.107801	-7.212010	-0.927465	L
C-CT-0.034200	0	7.726378	-5.161539	1.379461	L
C-CT-0.001800	0	6.828420	-5.177766	2.632225	L
S-S--0.273700	0	5.118966	-5.779258	2.456475	L
C-CT--0.053600	0	4.241319	-4.246036	2.014492	L
H-H-0.271900	-1	9.329370	-6.395572	-0.869537	L
H-H1-0.088000	-1	8.662362	-7.048750	1.874896	L
H-HC-0.024100	0	7.169253	-4.752792	0.536725	L
H-HC-0.024100	0	8.555462	-4.489461	1.581547	L
H-H1-0.044000	0	6.768190	-4.159321	3.016380	L
H-H1-0.044000	0	7.323171	-5.776612	3.396825	L
H-H1-0.068400	0	3.183492	-4.454771	1.852023	L
H-H1-0.068400	0	4.649354	-3.818734	1.101825	L
H-H1-0.068400	0	4.329741	-3.512463	2.816102	L
N-N--0.415700	-1	6.580327	-8.215002	1.047292	L
C-CT--0.149000	-1	5.361397	-8.926189	0.633602	L
H-H-0.271900	-1	6.896129	-8.343635	2.008592	L
H-H1-0.097600	-1	5.144164	-8.698279	-0.409429	L
H-H1-0.097600	-1	4.525828	-8.607847	1.257184	L
H-H1-0.097600	-1	5.511578	-9.999402	0.747308	L
C-CT--0.366200	-1	3.924053	-9.323398	4.914207	L
C-C-0.597200	-1	3.750569	-7.917057	5.522301	L
O-O--0.567900	-1	4.709622	-7.196941	5.815256	L
H-HC-0.112300	-1	2.943625	-9.767976	4.740207	L
H-HC-0.112300	-1	4.489894	-9.950683	5.602769	L
H-HC-0.112300	-1	4.460512	-9.246892	3.968306	L
N-N--0.415700	-1	2.487482	-7.506867	5.667767	L
C-CT--0.087500	-1	2.045956	-6.103940	5.612371	L
C-C-0.597300	-1	1.921117	-5.543728	7.035613	L
O-O--0.567900	-1	0.884034	-5.639494	7.707170	L
C-CT-0.298500	0	0.729798	-5.938774	4.819036	L
C-CT--0.319200	0	0.342070	-4.461881	4.677221	L
C-CT--0.319200	0	0.847298	-6.533777	3.406798	L
H-H-0.271900	-1	1.754309	-8.203551	5.512166	L
H-H1-0.096900	-1	2.810109	-5.529138	5.085585	L
H-HC--0.029700	0	-0.071700	-6.465292	5.339043	L
H-HC-0.079100	0	1.105786	-3.915971	4.118714	L
H-HC-0.079100	0	0.208078	-3.993951	5.651454	L
H-HC-0.079100	0	-0.598127	-4.376473	4.132273	L
H-HC-0.079100	0	1.651085	-6.033293	2.864880	L
H-HC-0.079100	0	-0.084515	-6.365652	2.864610	L
H-HC-0.079100	0	1.036806	-7.603143	3.448730	L

N-N--0.415700	-1	3.079306	-5.086446	7.510888	L
C-CT--0.149000	-1	3.454904	-4.948374	8.915353	L
H-H-0.271900	-1	3.838688	-5.001770	6.845446	L
H-H1-0.097600	-1	2.568183	-5.055462	9.540302	L
H-H1-0.097600	-1	3.897466	-3.966362	9.078690	L
H-H1-0.097600	-1	4.178153	-5.721395	9.175305	L
C-CT--0.366200	-1	12.498828	-4.179143	6.350960	L
C-C-0.597200	-1	12.292960	-3.458843	4.999907	L
O-O--0.567900	-1	13.259885	-3.240526	4.263401	L
H-HC-0.112300	-1	11.539500	-4.281392	6.858248	L
H-HC-0.112300	-1	13.177697	-3.595493	6.973938	L
H-HC-0.112300	-1	12.924440	-5.166276	6.175518	L
N-N--0.415700	-1	11.056700	-3.036663	4.695950	L
C-CT--0.023700	-1	10.778284	-2.214731	3.520533	L
C-C-0.597300	-1	11.342587	-0.790144	3.655242	L
O-O--0.567900	-1	12.070761	-0.324110	2.777110	L
C-CT-0.034200	0	9.270837	-2.141340	3.262609	L
C-CT-0.001800	0	9.017270	-1.444738	1.920026	L
S-S--0.273700	0	7.452202	-1.865784	1.136415	L
C-CT--0.053600	0	6.246325	-1.011378	2.183733	L
H-H-0.271900	-1	10.292071	-3.266811	5.324229	L
H-H1-0.088000	-1	11.250500	-2.694257	2.661395	L
H-HC-0.024100	0	8.763795	-1.597591	4.060857	L
H-HC-0.024100	0	8.876985	-3.152804	3.236245	L
H-H1-0.044000	0	9.802995	-1.736949	1.222181	L
H-H1-0.044000	0	9.073025	-0.363216	2.051089	L
H-H1-0.068400	0	5.233120	-1.226577	1.835813	L
H-H1-0.068400	0	6.404162	0.064859	2.121451	L
H-H1-0.068400	0	6.340316	-1.344254	3.215640	L
N-N--0.415700	-1	11.072909	-0.101055	4.769508	L
C-CT--0.149000	-1	11.623254	1.238998	4.997118	L
H-H-0.271900	-1	10.495317	-0.532313	5.490635	L
H-H1-0.097600	-1	12.211067	1.541765	4.130678	L
H-H1-0.097600	-1	12.260393	1.224524	5.880993	L
H-H1-0.097600	-1	10.807591	1.945951	5.148798	L
C-CT--0.366200	-1	6.171306	8.736376	-5.573202	L
C-C-0.597200	-1	6.488547	7.546136	-4.646436	L
O-O--0.567900	-1	6.642478	6.397452	-5.085391	L
H-HC-0.112300	-1	6.077507	9.645705	-4.978587	L
H-HC-0.112300	-1	5.234465	8.548802	-6.099126	L
H-HC-0.112300	-1	6.976652	8.858004	-6.298286	L
N-N--0.415700	-1	6.630963	7.863298	-3.349334	L
C-CT--0.001400	-1	6.674401	6.873128	-2.258021	L
C-C-0.597300	-1	5.300709	6.191009	-2.116480	L
O-O--0.567900	-1	4.426335	6.670685	-1.377446	L
C-CT--0.001400	-1	7.190530	7.509044	-0.954085	L
C-CA--0.001100	-1	7.877656	6.540391	0.002519	L
C-CA--0.190600	-1	9.285551	6.492742	0.053318	L
C-CA--0.190600	-1	7.133029	5.718925	0.873835	L
C-CA--0.234100	-1	9.937390	5.674570	0.994997	L
C-CA--0.234100	-1	7.789239	4.895677	1.815251	L
C-C-0.322600	-1	9.191661	4.896158	1.894365	L
O-OH--0.557900	-1	9.853294	4.152769	2.827823	L
H-H-0.271900	-1	6.564802	8.855359	-3.108780	L

H-H1-0.087600	-1	7.387003	6.102049	-2.537038	L
H-HC-0.029500	-1	7.914718	8.281417	-1.215968	L
H-HC-0.029500	-1	6.377168	8.015340	-0.432792	L
H-HA-0.169900	-1	9.870505	7.116881	-0.607196	L
H-HA-0.169900	-1	6.052008	5.722683	0.830194	L
H-HA-0.165600	-1	11.014686	5.647240	1.044334	L
H-HA-0.165600	-1	7.215782	4.262689	2.476524	L
H-HO-0.399200	-1	9.357130	3.929351	3.631397	L
N-N--0.415700	-1	5.090821	5.168678	-2.950499	L
C-CT-0.033700	-1	3.775174	4.670825	-3.337035	L
C-C-0.597300	-1	2.939423	4.033878	-2.215872	L
O-O--0.567900	-1	1.715864	4.132597	-2.284680	L
C-CT--0.182500	-1	3.965793	3.671212	-4.472630	L
H-H-0.271900	-1	5.874414	4.876510	-3.529420	L
H-H1-0.082300	-1	3.207658	5.514183	-3.731728	L
H-HC-0.060300	-1	2.995389	3.358466	-4.857181	L
H-HC-0.060300	-1	4.504838	2.804216	-4.090610	L
H-HC-0.060300	-1	4.535492	4.132411	-5.279513	L
N-N--0.415700	-1	3.554657	3.394217	-1.210567	L H-HC 209
C-CT-0.021300	0	2.778435	2.679124	-0.162043	H
C-C-0.597300	0	2.317429	3.683878	0.908266	H
O-O--0.567900	0	3.139196	4.421564	1.453679	H
C-CT--0.123100	0	3.689772	1.590067	0.435880	H
S-S--1.036000	0	2.821011	0.313684	1.440260	H
H-H-0.271900	-1	4.558561	3.371458	-1.202729	L
H-H1-0.112400	0	1.917554	2.201065	-0.638618	H
H-H1-0.111200	0	4.438277	2.064271	1.081452	H
H-H1-0.111200	0	4.238311	1.089545	-0.370207	H
N-N--0.415700	0	0.986797	3.697198	1.211850	H
C-CT--0.051800	0	0.416003	4.530860	2.279951	H
C-C-0.597300	0	0.795725	4.018133	3.705970	H
O-O--0.567900	0	1.338962	4.745118	4.537728	H
C-CT--0.110200	-1	-1.122705	4.642311	2.020043	H
C-CT-0.353100	-1	-1.983474	5.545659	2.929623	L H-HC 222
C-CT--0.412100	-1	-2.173273	4.999788	4.346358	L
C-CT--0.412100	-1	-1.456359	6.980748	3.016578	L
H-H-0.271900	0	0.364302	3.008153	0.779879	H
H-H1-0.092200	0	0.876831	5.521015	2.231311	H
H-HC-0.045700	0	-1.243466	5.015784	0.996148	H
H-HC-0.045700	0	-1.566092	3.644081	2.036815	H
H-HC--0.036100	-1	-2.975457	5.591026	2.481415	L
H-HC-0.100000	-1	-1.274507	5.143674	4.942392	L
H-HC-0.100000	-1	-2.415551	3.938799	4.306181	L
H-HC-0.100000	-1	-2.993750	5.531038	4.826365	L
H-HC-0.100000	-1	-0.494130	7.000161	3.529242	L
H-HC-0.100000	-1	-2.169534	7.597971	3.561579	L
H-HC-0.100000	-1	-1.334093	7.382705	2.009922	L
N-N--0.415700	0	0.519040	2.704577	3.966039	H
C-CT--0.087500	0	0.591488	2.169572	5.330069	H
C-C-0.597300	0	1.994765	2.140952	5.948554	H
O-O--0.567900	0	2.098875	2.109613	7.172660	H
C-CT-0.298500	-1	-0.024474	0.751789	5.369023	H
C-CT--0.319200	0	0.717864	-0.287215	4.500605	L H-HC 241
C-CT--0.319200	0	-0.215949	0.146026	6.759689	L H-HC 241

H-H-0.271900	0	0.035456	2.162494	3.250505	H
H-H1-0.096900	0	0.020889	2.831486	5.995384	H
H-HC--0.029700	0	-1.023654	0.838960	4.939367	H
H-HC-0.079100	0	1.680472	-0.546871	4.935229	L
H-HC-0.079100	0	0.894833	0.105494	3.498366	L
H-HC-0.079100	0	0.111326	-1.184441	4.391169	L
H-HC-0.079100	0	0.747988	-0.104149	7.200799	L
H-HC-0.079100	0	-0.815336	-0.759923	6.674459	L
H-HC-0.079100	0	-0.737069	0.859697	7.395777	L
N-N--0.415700	0	3.013071	1.955913	5.081522	H
C-CT-0.033700	0	4.376229	1.813356	5.549635	H
C-C-0.597300	-1	5.089020	3.146050	5.822917	L H-H1 254
O-O--0.567900	-1	6.264097	3.124496	6.178867	L
C-CT--0.182500	-1	5.153743	0.998029	4.519865	L H-H1 254
H-H-0.271900	0	2.852082	2.084747	4.092208	H
H-H1-0.082300	0	4.356368	1.268681	6.497646	H
H-HC-0.060300	-1	6.121402	0.707581	4.926313	L
H-HC-0.060300	-1	5.308988	1.599223	3.624223	L
H-HC-0.060300	-1	4.597609	0.094462	4.266898	L
N-N--0.415700	-1	4.383573	4.272458	5.657969	L
C-CT--0.087500	-1	4.763987	5.636076	6.053697	L
C-C-0.597300	-1	3.921455	6.082654	7.255702	L
O-O--0.567900	-1	4.472892	6.534671	8.260217	L
C-CT-0.298500	-1	4.547178	6.610374	4.878479	L
C-CT--0.319200	-1	4.938606	8.049940	5.229664	L
C-CT--0.319200	-1	5.365020	6.215606	3.649144	L
H-H-0.271900	-1	3.472467	4.156131	5.232011	L
H-H1-0.096900	-1	5.813912	5.667000	6.334988	L
H-HC--0.029700	-1	3.494738	6.595884	4.602804	L
H-HC-0.079100	-1	5.989092	8.089491	5.509463	L
H-HC-0.079100	-1	4.331746	8.426346	6.052426	L
H-HC-0.079100	-1	4.776694	8.688470	4.361563	L
H-HC-0.079100	-1	6.415322	6.139328	3.924518	L
H-HC-0.079100	-1	5.246851	6.962781	2.864783	L
H-HC-0.079100	-1	5.014346	5.257770	3.264861	L
N-N--0.415700	-1	2.590456	5.889596	7.202306	L
C-CT--0.149000	-1	1.682770	6.228004	8.309238	L
H-H-0.271900	-1	2.184210	5.507935	6.353531	L
H-H1-0.097600	-1	2.259880	6.624309	9.144763	L
H-H1-0.097600	-1	1.148550	5.332326	8.627811	L
H-H1-0.097600	-1	0.966178	6.978339	7.975291	L
C-CT--0.366200	-1	4.033581	10.323008	-1.003907	L
C-C-0.597200	-1	2.559311	9.993805	-1.248283	L
O-O--0.567900	-1	1.748243	10.907288	-1.321211	L
H-HC-0.112300	-1	4.610561	9.399971	-0.967683	L
H-HC-0.112300	-1	4.134550	10.852571	-0.056760	L
H-HC-0.112300	-1	4.404119	10.951685	-1.813228	L
N-N--0.415700	-1	2.182707	8.710204	-1.303362	L
C-CT--0.024900	-1	0.770055	8.326223	-1.143959	L
C-C-0.597300	-1	0.182498	8.823309	0.182567	L
O-O--0.567900	-1	-0.912910	9.389004	0.190341	L
C-CT-0.211700	0	0.600709	6.826477	-1.291875	L
O-OH--0.654600	0	0.896911	6.520453	-2.634503	L
H-H-0.271900	-1	2.886372	7.978709	-1.363705	L

H-H1-0.084300	-1	0.196734	8.774939	-1.950916	L
H-H1-0.035200	0	-0.424089	6.537907	-1.066876	L
H-H1-0.035200	0	1.279780	6.298297	-0.620942	L
H-HO-0.427500	0	1.001059	5.544977	-2.646050	L
N-N--0.415700	-1	0.945302	8.690618	1.278372	L
C-CT-0.033700	-1	0.590750	9.171949	2.614791	L
C-C-0.597300	-1	0.123508	10.632333	2.605525	L
O-O--0.567900	-1	-0.973425	10.949107	3.068230	L
C-CT--0.182500	-1	1.777822	8.937516	3.546589	L
H-H-0.271900	-1	1.834656	8.195771	1.173274	L
H-H1-0.082300	-1	-0.222984	8.578590	3.004888	L
H-HC-0.060300	-1	1.547343	9.308203	4.544712	L
H-HC-0.060300	-1	2.662430	9.440426	3.158055	L
H-HC-0.060300	-1	1.974863	7.868702	3.601523	L
N-N--0.415700	-1	0.920124	11.512407	1.989302	L
C-CT--0.149000	-1	0.577255	12.909300	1.795805	L
H-H-0.271900	-1	1.823161	11.205788	1.635657	L
H-H1-0.097600	-1	-0.409093	13.102856	2.218892	L
H-H1-0.097600	-1	0.566338	13.137143	0.730798	L
H-H1-0.097600	-1	1.315614	13.537365	2.295287	L
C-CT--0.366200	-1	-11.929232	4.567113	4.957969	L
C-C-0.597200	-1	-12.359301	3.146872	4.587410	L
O-O--0.567900	-1	-12.923172	2.438444	5.423759	L
H-HC-0.112300	-1	-11.450689	5.037236	4.098748	L
H-HC-0.112300	-1	-11.224973	4.528496	5.789137	L
H-HC-0.112300	-1	-12.804132	5.147564	5.249100	L
N-N--0.415700	-1	-12.024582	2.705821	3.374504	L
C-CT--0.087500	-1	-12.017930	1.283177	3.016218	L
C-C-0.597300	-1	-10.571166	0.890997	2.702611	L
O-O--0.567900	-1	-9.857154	1.535723	1.926917	L
C-CT-0.298500	-1	-13.013483	0.890449	1.892069	L
C-CT--0.319200	-1	-13.758386	-0.400948	2.278397	L
C-CT--0.319200	-1	-14.093683	1.936203	1.582267	L
H-H-0.271900	-1	-11.615573	3.357316	2.702153	L
H-H1-0.096900	-1	-12.309411	0.723801	3.902784	L
H-HC--0.029700	-1	-12.454418	0.701157	0.979390	L
H-HC-0.079100	-1	-14.391020	-0.219766	3.148031	L
H-HC-0.079100	-1	-13.040970	-1.191815	2.500994	L
H-HC-0.079100	-1	-14.394630	-0.717741	1.452198	L
H-HC-0.079100	-1	-14.727448	2.079907	2.453878	L
H-HC-0.079100	-1	-14.700702	1.598559	0.743662	L
H-HC-0.079100	-1	-13.638549	2.889167	1.321252	L
N-N--0.415700	-1	-10.105582	-0.127706	3.428047	L
C-CT--0.038900	-1	-8.696670	-0.522065	3.510228	L
C-C-0.597300	-1	-8.565549	-2.047202	3.624444	L
O-O--0.567900	-1	-9.495017	-2.709151	4.107756	L
C-CT-0.365400	-1	-7.981096	0.127448	4.718555	L
O-OH--0.676100	-1	-8.147360	-0.586679	5.921885	L
C-CT--0.243800	-1	-8.402445	1.563255	5.025184	L
H-H-0.271900	-1	-10.733978	-0.601412	4.060884	L
H-H1-0.100700	-1	-8.197233	-0.188195	2.600793	L
H-H1-0.004300	-1	-6.922081	0.129375	4.482013	L
H-HC-0.064200	-1	-8.447188	2.127207	4.100970	L
H-HC-0.064200	-1	-7.675128	2.022156	5.696213	L

H-HC-0.064200	-1	-9.385716	1.588033	5.494069	L
H-HO-0.410200	-1	-8.400066	0.052640	6.620284	L
N-N--0.254800	-1	-7.438317	-2.639960	3.191593	L
C-CT--0.026600	-1	-7.184400	-4.065357	3.362406	L
C-C-0.589600	-1	-6.574973	-4.417435	4.720686	L
O-O--0.574800	-1	-6.583543	-5.588062	5.084428	L
C-CT--0.007000	0	-6.192021	-4.402546	2.248447	L
C-CT-0.018900	0	-5.354596	-3.131461	2.121594	L
C-CT-0.019200	0	-6.366668	-2.021880	2.411925	L
H-H1-0.064100	-1	-8.093124	-4.637866	3.218427	L
H-HC-0.025300	0	-5.575517	-5.261798	2.505154	L
H-HC-0.025300	0	-6.732130	-4.582367	1.318061	L
H-HC-0.021300	0	-4.920947	-3.037559	1.127050	L
H-HC-0.021300	0	-4.569445	-3.126593	2.878153	L
H-H1-0.039100	0	-6.767879	-1.647537	1.469704	L
H-H1-0.039100	0	-5.882810	-1.214267	2.962833	L
N-N--0.415700	-1	-5.958506	-3.453805	5.413130	L
C-CT--0.001400	-1	-4.966326	-3.691544	6.472958	L
C-C-0.597300	-1	-5.512347	-4.475194	7.680998	L
O-O--0.567900	-1	-6.699042	-4.361365	7.991974	L
C-CT--0.001400	0	-4.452731	-2.355004	7.025981	L H-HA 373
C-CA--0.001100	0	-4.140313	-1.293621	5.994979	H
C-CA--0.190600	0	-3.252048	-1.562946	4.952771	H
C-CA--0.190600	0	-4.727075	-0.029282	6.088247	H
C-CA--0.234100	0	-2.959297	-0.587073	4.009471	H
C-CA--0.234100	0	-4.437430	0.959909	5.153828	H
C-C-0.322600	0	-3.548538	0.686524	4.107824	H
O-OH--0.557900	0	-3.299040	1.664195	3.212849	H
H-H-0.271900	-1	-6.028134	-2.515424	5.050792	L
H-H1-0.087600	-1	-4.140262	-4.258542	6.042320	L
H-HC-0.029500	0	-5.205664	-1.954516	7.707272	L
H-HC-0.029500	0	-3.550435	-2.539185	7.610506	L
H-HA-0.169900	0	-2.783806	-2.540797	4.864007	H
H-HA-0.169900	0	-5.417473	0.198413	6.901274	H
H-HA-0.165600	0	-2.242913	-0.772189	3.219956	H
H-HA-0.165600	0	-4.861163	1.957177	5.241999	H
H-HO-0.399200	0	-2.435740	1.492899	2.745993	H
N-N--0.415700	-1	-4.631925	-5.162161	8.435385	L
C-CT--0.149000	-1	-5.015047	-5.628236	9.784536	L
H-H-0.271900	-1	-3.637251	-5.153030	8.195563	L
H-H1-0.097600	-1	-6.098885	-5.580589	9.891003	L
H-H1-0.097600	-1	-4.547500	-4.992349	10.535542	L
H-H1-0.097600	-1	-4.681320	-6.657123	9.921318	L
C-CT--0.366200	-1	-0.441139	-10.771051	2.476878	L
C-C-0.597200	-1	-0.624340	-9.831995	1.271371	L
O-O--0.567900	-1	-1.734356	-9.660923	0.762536	L
H-HC-0.112300	-1	0.606917	-10.782235	2.772639	L
H-HC-0.112300	-1	-0.752243	-11.779269	2.202105	L
H-HC-0.112300	-1	-1.050515	-10.418144	3.308877	L
N-N--0.415700	-1	0.488432	-9.283047	0.767154	L
C-CT-0.014300	-1	0.441871	-8.266491	-0.283213	L H-HC 405
C-C-0.597300	-1	0.069469	-8.776460	-1.694177	L
O-O--0.567900	-1	-0.143942	-7.954983	-2.576539	L
C-CT--0.204100	0	1.730228	-7.421834	-0.296310	H

C-C-0.713000	0	1.423297	-6.010961	-0.826402	H
O-O--0.593100	0	0.346389	-5.469476	-0.557074	H
N-N--0.919100	0	2.394902	-5.381790	-1.509473	H
H-H-0.271900	-1	1.371753	-9.468170	1.213400	L
H-H1-0.104800	-1	-0.362421	-7.596123	0.020122	L
H-HC-0.079700	0	2.511612	-7.939229	-0.865493	H
H-HC-0.079700	0	2.087209	-7.296601	0.731448	H
H-H-0.419600	0	2.278657	-4.372182	-1.701744	H
H-H-0.419600	0	3.247682	-5.859103	-1.759487	H
N-N--0.415700	-1	-0.023691	-10.090180	-1.930648	L
C-CT--0.149000	-1	-0.562635	-10.643407	-3.185190	L
H-H-0.271900	-1	0.087805	-10.738566	-1.143138	L
H-H1-0.097600	-1	-0.629111	-9.853300	-3.932425	L
H-H1-0.097600	-1	-1.555046	-11.056272	-3.003967	L
H-H1-0.097600	-1	0.097494	-11.432452	-3.547610	L
C-CT--0.366200	-1	-3.830728	-11.707261	-1.417416	L
C-C-0.597200	-1	-4.600733	-10.382564	-1.490793	L
O-O--0.567900	-1	-5.739582	-10.387998	-1.962251	L
H-HC-0.112300	-1	-2.847837	-11.531394	-0.979335	L
H-HC-0.112300	-1	-3.712987	-12.115246	-2.420314	L
H-HC-0.112300	-1	-4.382615	-12.414344	-0.798492	L
N-N--0.415700	-1	-3.975539	-9.253781	-1.116500	L
C-CT--0.087500	-1	-4.542128	-7.894003	-1.281053	L
C-C-0.597300	-1	-4.807483	-7.513595	-2.748823	L
O-O--0.567900	-1	-5.797432	-6.846076	-3.045267	L
C-CT-0.298500	-1	-3.637144	-6.815008	-0.630534	L
C-CT--0.319200	-1	-4.126948	-5.378252	-0.872598	L
C-CT--0.319200	-1	-3.621966	-6.950107	0.889693	L
H-H-0.271900	-1	-3.093497	-9.362450	-0.613987	L
H-H1-0.096900	-1	-5.503175	-7.873437	-0.768546	L
H-HC--0.029700	-1	-2.621308	-6.911645	-1.014211	L
H-HC-0.079100	-1	-5.163081	-5.283263	-0.546925	L
H-HC-0.079100	-1	-4.059044	-5.127548	-1.928572	L
H-HC-0.079100	-1	-3.501356	-4.669265	-0.328242	L
H-HC-0.079100	-1	-4.628857	-6.816754	1.267886	L
H-HC-0.079100	-1	-2.959676	-6.202704	1.328916	L
H-HC-0.079100	-1	-3.271177	-7.926526	1.192778	L
N-N--0.415700	-1	-3.959763	-7.912798	-3.705217	L
C-CT--0.149000	-1	-4.045838	-7.500153	-5.116854	L
H-H-0.271900	-1	-3.236917	-8.574283	-3.447488	L
H-H1-0.097600	-1	-4.865222	-6.791378	-5.239387	L
H-H1-0.097600	-1	-4.226449	-8.375715	-5.742027	L
H-H1-0.097600	-1	-3.110232	-7.028099	-5.415435	L
C-CT--0.366200	-1	-12.115781	3.659997	-1.336536	L
C-C-0.597200	-1	-11.009741	2.595898	-1.298511	L
O-O--0.567900	-1	-11.300852	1.412629	-1.142145	L
H-HC-0.112300	-1	-11.669011	4.643626	-1.481728	L
H-HC-0.112300	-1	-12.666472	3.646423	-0.395580	L
H-HC-0.112300	-1	-12.798405	3.445593	-2.159070	L
N-N--0.415700	-1	-9.753929	3.038755	-1.366171	L
C-CT--0.024900	-1	-8.569856	2.218934	-1.185089	L
C-C-0.597300	-1	-7.459202	3.087235	-0.588591	L
O-O--0.567900	-1	-6.807473	3.875710	-1.287633	L
C-CT-0.211700	0	-8.151805	1.572313	-2.504567	L

O-OH--0.654600	0	-7.271986	0.523284	-2.215222	L
H-H-0.271900	-1	-9.629188	4.035336	-1.437635	L
H-H1-0.084300	-1	-8.806315	1.427024	-0.475743	L
H-H1-0.035200	0	-7.675799	2.293010	-3.166339	L
H-H1-0.035200	0	-9.031407	1.155235	-2.997030	L
H-HO-0.427500	0	-6.340303	0.832073	-2.278544	L
N-N--0.415700	-1	-7.297425	3.015513	0.741522	L
C-CT-0.021300	-1	-6.123706	3.633775	1.376774	L
C-C-0.597300	-1	-4.834013	2.988558	0.844481	L
O-O--0.567900	-1	-3.860147	3.678113	0.583594	L
C-CT--0.123100	-1	-6.181803	3.499444	2.900018	L
S-SH--0.311900	-1	-7.437611	4.604610	3.605686	L
H-H-0.271900	-1	-7.957637	2.468595	1.290922	L
H-H1-0.112400	-1	-6.096943	4.695490	1.126495	L
H-H1-0.111200	-1	-5.211306	3.774803	3.316350	L
H-H1-0.111200	-1	-6.396272	2.464739	3.166215	L
H-HS-0.193300	-1	-8.478722	4.153853	2.896612	L
N-N--0.415700	-1	-4.869889	1.669353	0.640188	L H-HC 478
C-CT-0.021300	0	-3.671024	0.992720	0.085103	H
C-C-0.597300	0	-3.669702	1.167524	-1.428555	H
O-O--0.567900	0	-4.719527	1.132135	-2.077207	H
C-CT--0.123100	0	-3.634743	-0.491709	0.489688	H
S-SH--0.311900	0	-2.140090	-1.467699	-0.072731	H
H-H-0.271900	-1	-5.720222	1.179983	0.846416	L
H-H1-0.112400	0	-2.798861	1.492973	0.503701	H
H-H1-0.111200	0	-4.441215	-1.046351	-0.007006	H
H-H1-0.111200	0	-3.747593	-0.607638	1.566268	H
H-HS-0.193300	0	0.744560	-3.172319	0.987014	H
N-N--0.415700	0	-2.444504	1.315356	-1.997704	H
C-CT--0.087500	0	-2.304764	1.404913	-3.440774	H
C-C-0.597300	0	-2.238962	0.039287	-4.180968	H
O-O--0.567900	0	-2.383321	0.042649	-5.400450	H
C-CT-0.298500	-1	-1.115250	2.290851	-3.882900	H
C-CT--0.319200	0	-1.225031	3.701601	-3.301121	L H-HC 492
C-CT--0.319200	0	0.243491	1.698007	-3.464920	L H-HC 492
H-H-0.271900	0	-1.628445	1.373189	-1.378257	H
H-H1-0.096900	0	-3.236374	1.840808	-3.819517	H
H-HC--0.029700	0	-1.136884	2.351390	-4.973280	H
H-HC-0.079100	0	-1.083392	3.677684	-2.217900	L
H-HC-0.079100	0	-2.205307	4.109614	-3.527969	L
H-HC-0.079100	0	-0.467636	4.341246	-3.749724	L
H-HC-0.079100	0	0.339062	1.695036	-2.377732	L
H-HC-0.079100	0	1.046119	2.291789	-3.893189	L
H-HC-0.079100	0	0.348839	0.678850	-3.827432	L
N-N--0.415700	0	-1.942606	-1.067390	-3.439258	H
C-CT--0.003100	0	-2.036991	-2.414582	-4.011363	H
C-C-0.597300	0	-3.500119	-2.871656	-4.178852	H
O-O--0.567900	0	-3.796952	-3.672113	-5.057380	H
C-CT--0.003600	-1	-1.282249	-3.449587	-3.119572	H
C-CT--0.064500	-1	-1.412037	-4.904799	-3.608262	L H-HC 508
C-C-0.695100	-1	-0.537564	-5.242936	-4.800972	L
O-O--0.608600	-1	-0.396920	-4.492735	-5.751884	L
N-N--0.940700	-1	0.078628	-6.405420	-4.794317	L
H-H-0.271900	0	-1.954489	-1.004062	-2.422222	H

H-H1-0.085000	0	-1.627652	-2.384574	-5.024186	H
H-HC-0.017100	0	-0.225844	-3.196718	-3.029922	H
H-HC-0.017100	0	-1.708100	-3.411751	-2.114372	H
H-HC-0.035200	-1	-2.439511	-5.162354	-3.849181	L
H-HC-0.035200	-1	-1.125498	-5.551046	-2.785975	L
H-H-0.425100	-1	0.682463	-6.653277	-5.558420	L
H-H-0.425100	-1	-0.029826	-7.025648	-3.993726	L
N-N--0.415700	0	-4.343566	-2.484857	-3.154838	H
C-CT--0.023700	0	-5.720914	-2.959485	-3.238240	H
C-C-0.597300	-1	-6.400003	-2.345448	-4.478845	L H-H1 522
O-O--0.567900	-1	-6.231951	-1.150114	-4.738827	L
C-CT-0.034200	-1	-6.459694	-2.683313	-1.911921	L H-H1 522
C-CT-0.001800	-1	-7.927049	-3.135950	-1.968340	L
S-S--0.273700	-1	-8.830941	-3.110291	-0.392905	L
C-CT--0.053600	-1	-9.203782	-1.343115	-0.263399	L
H-H-0.271900	0	-4.277836	-1.513223	-2.888257	H
H-H1-0.088000	0	-5.647009	-4.036057	-3.354288	H
H-HC-0.024100	-1	-6.391793	-1.636450	-1.653331	L
H-HC-0.024100	-1	-5.964887	-3.233820	-1.115360	L
H-H1-0.044000	-1	-7.949766	-4.161990	-2.336876	L
H-H1-0.044000	-1	-8.468774	-2.511559	-2.679130	L
H-H1-0.068400	-1	-9.809771	-1.158806	0.623610	L
H-H1-0.068400	-1	-9.754873	-1.016017	-1.145334	L
H-H1-0.068400	-1	-8.275194	-0.780820	-0.192404	L
N-N--0.254800	-1	-7.147083	-3.117363	-5.289725	L
C-CT--0.026600	-1	-7.545275	-2.702876	-6.635893	L
C-C-0.589600	-1	-8.996198	-2.222812	-6.627716	L
O-O--0.574800	-1	-9.880416	-2.924893	-6.130269	L
C-CT--0.007000	-1	-7.335951	-3.946972	-7.513693	L
C-CT-0.018900	-1	-6.816588	-5.007516	-6.539695	L
C-CT-0.019200	-1	-7.349757	-4.547482	-5.209281	L
H-H1-0.064100	-1	-6.900006	-1.904601	-7.002099	L
H-HC-0.025300	-1	-8.269614	-4.270502	-7.964838	L
H-HC-0.025300	-1	-6.601100	-3.761262	-8.294758	L
H-HC-0.021300	-1	-5.728499	-4.996600	-6.513737	L
H-HC-0.021300	-1	-7.188151	-5.991148	-6.754719	L
H-H1-0.039100	-1	-6.824017	-5.053395	-4.411189	L
H-H1-0.039100	-1	-8.414634	-4.770772	-5.134440	L
N-N--0.415700	-1	-9.222865	-1.027244	-7.165470	L
C-CT--0.149000	-1	-10.458425	-0.261155	-6.975867	L
H-H-0.271900	-1	-8.419465	-0.556000	-7.580693	L
H-H1-0.097600	-1	-11.216808	-0.900785	-6.524962	L
H-H1-0.097600	-1	-10.813416	0.098483	-7.941622	L
H-H1-0.097600	-1	-10.261713	0.587731	-6.320647	L
C-CT--0.366200	-1	-10.366273	8.821831	-4.251317	L
C-C-0.597200	-1	-9.813813	7.535047	-3.624014	L
O-O--0.567900	-1	-10.254829	7.114906	-2.552894	L
H-HC-0.112300	-1	-9.848616	9.020176	-5.189722	L
H-HC-0.112300	-1	-10.209534	9.655088	-3.566860	L
H-HC-0.112300	-1	-11.432637	8.704213	-4.443058	L
N-N--0.415700	-1	-8.841385	6.914553	-4.286726	L
C-CT--0.024900	-1	-7.894305	5.999595	-3.646109	L
C-C-0.597300	-1	-6.566740	6.735582	-3.426010	L
O-O--0.567900	-1	-6.315013	7.742975	-4.094563	L

C-CT-0.211700	0	-7.668967	4.744062	-4.500810	L
O-OH--0.654600	0	-7.294694	5.052437	-5.830248	L
H-H-0.271900	-1	-8.571955	7.283255	-5.197845	L
H-H1-0.084300	-1	-8.278954	5.660185	-2.684009	L
H-H1-0.035200	0	-8.588388	4.157542	-4.519133	L
H-H1-0.035200	0	-6.882942	4.141531	-4.043393	L
H-HO-0.427500	0	-6.874219	4.274288	-6.214500	L
N-N--0.415700	-1	-5.687209	6.207192	-2.564563	L
C-CT-0.033700	-1	-4.314864	6.719994	-2.462148	L
C-C-0.597300	-1	-3.567676	6.725458	-3.814820	L
O-O--0.567900	-1	-2.670809	7.541565	-4.032948	L
C-CT--0.182500	-1	-3.558605	5.901703	-1.425667	L
H-H-0.271900	-1	-5.967592	5.401757	-2.000112	L
H-H1-0.082300	-1	-4.365104	7.747598	-2.100615	L
H-HC-0.060300	-1	-2.546080	6.286111	-1.321089	L
H-HC-0.060300	-1	-3.520655	4.855486	-1.727254	L
H-HC-0.060300	-1	-4.074102	5.984558	-0.470124	L
N-N--0.415700	-1	-3.986847	5.856726	-4.748674	L
C-CT--0.149000	-1	-3.472201	5.803412	-6.115847	L
H-H-0.271900	-1	-4.713391	5.206190	-4.480775	L
H-H1-0.097600	-1	-2.700956	6.563419	-6.243285	L
H-H1-0.097600	-1	-4.284415	5.990605	-6.818111	L
H-H1-0.097600	-1	-3.046848	4.817982	-6.305643	L
C-CM--0.139000	0	0.660578	-1.006957	-0.414531	H
C-C-0.519000	0	1.301345	-2.277242	-0.646758	H
O-O2--0.567000	0	1.540617	-3.084818	0.412772	H
C-CM--0.117000	0	-0.415043	-0.806001	0.599152	H
O-O2--0.618000	0	1.821883	-2.604262	-1.741138	H
C-C--0.553000	0	-0.636074	0.658378	0.967199	H
O-O2--0.556000	0	-0.486691	1.524626	0.063643	H
O-O2--0.607000	0	-1.022481	0.888301	2.154249	H
H-HC-0.049000	0	1.765487	-0.327586	0.341006	H
H-HC-0.162000	0	-0.260072	-1.381846	1.508977	H
O-OW--0.834000	-1	6.437029	2.974452	-1.185044	L
H-HW-0.417000	-1	6.807619	3.116145	-2.055354	L
H-HW-0.417000	-1	7.115562	3.277450	-0.582098	L
O-OW--0.834000	0	3.359267	7.044409	1.045266	L
H-HW-0.417000	0	3.220844	6.141364	1.397103	L
H-HW-0.417000	0	3.741664	6.854850	0.171975	L
O-OW--0.834000	0	-0.778535	-3.988806	1.486131	H
H-HW-0.417000	0	-0.533975	-4.678112	0.835086	H
H-HW-0.417000	0	-1.494812	-3.496188	1.046198	H
O-OW--0.834000	0	-5.041316	0.868705	-6.140816	L
H-HW-0.417000	0	-4.103459	0.638044	-6.055855	L
H-HW-0.417000	0	-5.477240	0.202972	-5.581142	L
H-HS-0.193300	0	0.501982	-0.455311	-1.337075	H

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C-CT--0.366200	-1	8.186332	4.642815	-8.155031	L
C-C-0.597200	-1	9.019670	3.904239	-7.112993	L
O-O--0.567900	-1	9.622537	2.867016	-7.390829	L
H-HC-0.112300	-1	7.741363	5.529381	-7.703414	L
H-HC-0.112300	-1	7.396304	3.986156	-8.521054	L
H-HC-0.112300	-1	8.825067	4.941140	-8.987224	L

N-N--0.415700	-1	9.014415	4.467500	-5.898303	L
C-CT--0.087500	-1	9.488762	3.798090	-4.680031	L
C-C-0.597300	-1	8.354103	2.899874	-4.183474	L
O-O--0.567900	-1	7.442667	3.360300	-3.480822	L
C-CT-0.298500	-1	9.969708	4.805867	-3.608806	L
C-CT--0.319200	-1	10.392476	4.112945	-2.307885	L
C-CT--0.319200	-1	11.181579	5.615015	-4.093176	L
H-H-0.271900	-1	8.427276	5.288635	-5.773772	L
H-H1-0.096900	-1	10.327754	3.158051	-4.932521	L
H-HC--0.029700	-1	9.170962	5.510321	-3.394419	L
H-HC-0.079100	-1	11.100237	3.315034	-2.534512	L
H-HC-0.079100	-1	9.523748	3.689545	-1.807515	L
H-HC-0.079100	-1	10.867929	4.825092	-1.635304	L
H-HC-0.079100	-1	12.043520	4.960012	-4.220104	L
H-HC-0.079100	-1	11.426467	6.389597	-3.364312	L
H-HC-0.079100	-1	10.961043	6.090076	-5.048103	L
N-N--0.415700	-1	8.373572	1.625547	-4.610066	L
C-CT--0.087500	-1	7.263256	0.671261	-4.430112	L
C-C-0.597300	-1	7.683368	-0.600177	-3.664242	L
O-O--0.567900	-1	8.830398	-1.049218	-3.788075	L
C-CT-0.298500	-1	6.609581	0.257087	-5.772945	L
C-CT--0.319200	-1	5.748322	1.378945	-6.364662	L
C-CT--0.319200	-1	7.602461	-0.195512	-6.848793	L
H-H-0.271900	-1	9.149057	1.319318	-5.203573	L
H-H1-0.096900	-1	6.491529	1.178455	-3.858099	L
H-HC--0.029700	-1	5.942867	-0.584763	-5.582616	L
H-HC-0.079100	-1	6.263051	2.336972	-6.293117	L
H-HC-0.079100	-1	4.813661	1.426364	-5.810377	L
H-HC-0.079100	-1	5.499571	1.158950	-7.404142	L
H-HC-0.079100	-1	8.200268	0.649304	-7.186806	L
H-HC-0.079100	-1	7.053177	-0.603520	-7.696256	L
H-HC-0.079100	-1	8.259226	-0.965187	-6.451469	L
N-N--0.254800	-1	6.749683	-1.206159	-2.893137	L
C-CT--0.026600	-1	6.885894	-2.556623	-2.340983	L
C-C-0.589600	-1	7.135811	-3.583868	-3.446954	L
O-O--0.574800	-1	6.388223	-3.637521	-4.426546	L
C-CT--0.007000	0	5.551777	-2.834903	-1.625463	L
C-CT-0.018900	0	4.996211	-1.444014	-1.324406	L
C-CT-0.019200	0	5.450238	-0.647088	-2.530163	L
H-H1-0.064100	-1	7.705035	-2.566717	-1.622803	L
H-HC-0.025300	0	4.856327	-3.352103	-2.288261	L
H-HC-0.025300	0	5.699248	-3.416366	-0.720143	L
H-HC-0.021300	0	5.454116	-1.022112	-0.437312	L
H-HC-0.021300	0	3.919590	-1.423071	-1.212084	L
H-H1-0.039100	0	5.513663	0.403671	-2.246744	L
H-H1-0.039100	0	4.742535	-0.782720	-3.349608	L
N-N--0.415700	-1	8.163117	-4.426354	-3.295879	L
C-CT--0.149000	-1	8.534699	-5.425504	-4.310534	L
H-H-0.271900	-1	8.762507	-4.299093	-2.481539	L
H-H1-0.097600	-1	7.790685	-5.430719	-5.106447	L
H-H1-0.097600	-1	8.579442	-6.412220	-3.848529	L
H-H1-0.097600	-1	9.510414	-5.175411	-4.727121	L
C-CT--0.366200	-1	5.241059	-7.417739	-4.055383	L
C-C-0.597200	-1	4.109567	-6.753487	-4.849916	L

O-O--0.567900	-1	3.213621	-7.476020	-5.296008	L
H-HC-0.112300	-1	5.950952	-6.657981	-3.729108	L
H-HC-0.112300	-1	5.751001	-8.145195	-4.686788	L
H-HC-0.112300	-1	4.824068	-7.922289	-3.183722	L
N-N--0.415700	-1	4.093993	-5.423286	-4.994509	L
C-CT-0.014300	-1	2.989567	-4.681382	-5.627329	L H-HC 69
C-C-0.597300	-1	2.795626	-5.028723	-7.138151	L
O-O--0.567900	-1	3.790399	-5.193134	-7.845892	L
C-CT--0.204100	0	3.289075	-3.178023	-5.419183	H
C-C-0.713000	0	2.206104	-2.251477	-5.974258	H
O-O--0.593100	0	2.166408	-1.923016	-7.153408	H
N-N--0.919100	0	1.334616	-1.761513	-5.042147	H
H-H-0.271900	-1	4.860849	-4.882072	-4.629043	L
H-H1-0.104800	-1	2.082975	-4.945600	-5.092572	L
H-HC-0.079700	0	4.216117	-2.951664	-5.956923	H
H-HC-0.079700	0	3.443522	-3.002803	-4.351295	H
H-H-0.419600	0	0.470112	-1.393966	-5.424981	H
H-H-0.419600	0	1.304051	-2.172999	-4.118854	H
N-N--0.415700	-1	1.542207	-5.133430	-7.630756	L
C-CT--0.149000	-1	1.190707	-5.399959	-9.055345	L
H-H-0.271900	-1	0.786343	-4.907583	-6.985141	L
H-H1-0.097600	-1	2.096959	-5.624579	-9.617221	L
H-H1-0.097600	-1	0.707436	-4.519969	-9.480697	L
H-H1-0.097600	-1	0.510114	-6.249725	-9.107096	L
C-CT--0.366200	-1	11.730045	-5.889066	-0.609955	L
C-C-0.597200	-1	10.714937	-6.013591	0.534427	L
O-O--0.567900	-1	11.031748	-5.852965	1.718304	L
H-HC-0.112300	-1	11.229550	-6.069981	-1.561063	L
H-HC-0.112300	-1	12.524202	-6.622377	-0.472250	L
H-HC-0.112300	-1	12.157970	-4.886358	-0.609637	L
N-N--0.415700	-1	9.479200	-6.322669	0.144496	L
C-CT--0.023700	-1	8.319647	-6.520126	1.009362	L
C-C-0.597300	-1	7.267678	-7.369476	0.308691	L
O-O--0.567900	-1	7.088421	-7.215890	-0.906341	L
C-CT-0.034200	0	7.709162	-5.162938	1.398364	L
C-CT-0.001800	0	6.823772	-5.177044	2.660356	L
S-S--0.273700	0	5.116576	-5.792793	2.510710	L
C-CT--0.053600	0	4.232242	-4.278944	2.019239	L
H-H-0.271900	-1	9.310606	-6.400857	-0.852382	L
H-H1-0.088000	-1	8.645852	-7.047576	1.894127	L
H-HC-0.024100	0	7.143007	-4.758652	0.559474	L
H-HC-0.024100	0	8.538926	-4.488897	1.590687	L
H-H1-0.044000	0	6.759783	-4.156064	3.037147	L
H-H1-0.044000	0	7.331800	-5.765584	3.424216	L
H-H1-0.068400	0	3.173818	-4.494470	1.870062	L
H-H1-0.068400	0	4.634147	-3.885628	1.088922	L
H-H1-0.068400	0	4.324984	-3.516470	2.793075	L
N-N--0.415700	-1	6.562203	-8.214200	1.071122	L
C-CT--0.149000	-1	5.342378	-8.925450	0.660186	L
H-H-0.271900	-1	6.878865	-8.340950	2.032390	L
H-H1-0.097600	-1	5.124276	-8.699670	-0.383126	L
H-H1-0.097600	-1	4.507643	-8.605170	1.283893	L
H-H1-0.097600	-1	5.491936	-9.998514	0.776091	L
C-CT--0.366200	-1	3.908979	-9.312313	4.943061	L

C-C-0.597200	-1	3.737059	-7.904526	5.548250	L
O-O--0.567900	-1	4.696895	-7.184432	5.838687	L
H-HC-0.112300	-1	2.928075	-9.756593	4.770998	L
H-HC-0.112300	-1	4.475066	-9.938480	5.632436	L
H-HC-0.112300	-1	4.444558	-9.238242	3.996468	L
N-N--0.415700	-1	2.474399	-7.493149	5.694060	L
C-CT--0.087500	-1	2.033782	-6.090042	5.636031	L
C-C-0.597300	-1	1.910730	-5.526635	7.058168	L
O-O--0.567900	-1	0.874242	-5.620219	7.730951	L
C-CT-0.298500	0	0.723043	-5.920414	4.833195	L
C-CT--0.319200	0	0.354749	-4.440758	4.667604	L
C-CT--0.319200	0	0.842735	-6.529017	3.426631	L
H-H-0.271900	-1	1.740594	-8.189666	5.540703	L
H-H1-0.096900	-1	2.797809	-5.516920	5.107239	L
H-HC--0.029700	0	-0.088668	-6.431347	5.352787	L
H-HC-0.079100	0	1.144424	-3.906432	4.134501	L
H-HC-0.079100	0	0.194697	-3.967375	5.635609	L
H-HC-0.079100	0	-0.563557	-4.345871	4.087108	L
H-HC-0.079100	0	1.667712	-6.055098	2.892809	L
H-HC-0.079100	0	-0.075705	-6.340892	2.868150	L
H-HC-0.079100	0	1.004163	-7.602592	3.480453	L
N-N--0.415700	-1	3.069699	-5.069113	7.531302	L
C-CT--0.149000	-1	3.446775	-4.928231	8.935091	L
H-H-0.271900	-1	3.828483	-4.986415	6.864930	L
H-H1-0.097600	-1	2.560596	-5.033342	9.561146	L
H-H1-0.097600	-1	3.890172	-3.946170	9.095846	L
H-H1-0.097600	-1	4.169749	-5.701180	9.196022	L
C-CT--0.366200	-1	12.488695	-4.170836	6.360131	L
C-C-0.597200	-1	12.281991	-3.453349	5.007709	L
O-O--0.567900	-1	13.248339	-3.237308	4.269778	L
H-HC-0.112300	-1	11.529797	-4.271315	6.868585	L
H-HC-0.112300	-1	13.168578	-3.586294	6.981163	L
H-HC-0.112300	-1	12.913456	-5.158643	6.186430	L
N-N--0.415700	-1	11.045723	-3.030983	4.704046	L
C-CT--0.023700	-1	10.766713	-2.211431	3.527110	L
C-C-0.597300	-1	11.332128	-0.786941	3.658149	L
O-O--0.567900	-1	12.059756	-0.323330	2.778284	L
C-CT-0.034200	0	9.260502	-2.136037	3.273381	L
C-CT-0.001800	0	9.008240	-1.429775	1.936590	L
S-S--0.273700	0	7.460823	-1.881931	1.142253	L
C-CT--0.053600	0	6.234695	-1.075937	2.204193	L
H-H-0.271900	-1	10.281554	-3.259231	5.333579	L
H-H1-0.088000	-1	11.237754	-2.693157	2.668558	L
H-HC-0.024100	0	8.754791	-1.597189	4.075819	L
H-HC-0.024100	0	8.866855	-3.147324	3.240558	L
H-H1-0.044000	0	9.805376	-1.697102	1.241713	L
H-H1-0.044000	0	9.036857	-0.348692	2.079850	L
H-H1-0.068400	0	5.229205	-1.339585	1.870243	L
H-H1-0.068400	0	6.338502	0.006684	2.132273	L
H-H1-0.068400	0	6.355388	-1.394544	3.237592	L
N-N--0.415700	-1	11.064020	-0.095234	4.771170	L
C-CT--0.149000	-1	11.615508	1.244934	4.995308	L
H-H-0.271900	-1	10.486843	-0.524517	5.493806	L
H-H1-0.097600	-1	12.202675	1.545402	4.127631	L

H-H1-0.097600	-1	12.253508	1.231955	5.878586	L
H-H1-0.097600	-1	10.800481	1.952779	5.146244	L
C-CT--0.366200	-1	6.158302	8.722944	-5.586012	L
C-C-0.597200	-1	6.475638	7.534515	-4.656959	L
O-O--0.567900	-1	6.628348	6.384769	-5.093552	L
H-HC-0.112300	-1	6.065714	9.633636	-4.993295	L
H-HC-0.112300	-1	5.220815	8.534867	-6.110604	L
H-HC-0.112300	-1	6.963017	8.842432	-6.312152	L
N-N--0.415700	-1	6.619549	7.854413	-3.360695	L
C-CT--0.001400	-1	6.663383	6.866600	-2.267262	L
C-C-0.597300	-1	5.289363	6.185739	-2.122879	L
O-O--0.567900	-1	4.416046	6.667632	-1.384036	L
C-CT--0.001400	-1	7.181233	7.505011	-0.965228	L
C-CA--0.001100	-1	7.868635	6.537977	-0.007184	L
C-CA--0.190600	-1	9.276545	6.489468	0.042334	L
C-CA--0.190600	-1	7.124302	5.718930	0.866657	L
C-CA--0.234100	-1	9.928750	5.672910	0.985158	L
C-CA--0.234100	-1	7.780874	4.897290	1.809226	L
C-C-0.322600	-1	9.183373	4.896979	1.886960	L
O-OH--0.557900	-1	9.845414	4.155176	2.821389	L
H-H-0.271900	-1	6.554306	8.847043	-3.122245	L
H-H1-0.087600	-1	7.375181	6.094424	-2.545294	L
H-HC-0.029500	-1	7.905692	8.276310	-1.229511	L
H-HC-0.029500	-1	6.368732	8.013003	-0.444244	L
H-HA-0.169900	-1	9.861277	7.111760	-0.620117	L
H-HA-0.169900	-1	6.043241	5.723337	0.824072	L
H-HA-0.165600	-1	11.006075	5.644945	1.033496	L
H-HA-0.165600	-1	7.207634	4.266144	2.472445	L
H-HO-0.399200	-1	9.349888	3.933856	3.625936	L
N-N--0.415700	-1	5.077952	5.161734	-2.954454	L
C-CT-0.033700	-1	3.761583	4.663944	-3.338607	L
C-C-0.597300	-1	2.926500	4.030023	-2.215233	L
O-O--0.567900	-1	1.702941	4.129435	-2.283054	L
C-CT--0.182500	-1	3.950397	3.661719	-4.472201	L
H-H-0.271900	-1	5.860773	4.867761	-3.533505	L
H-H1-0.082300	-1	3.194258	5.506826	-3.734584	L
H-HC-0.060300	-1	2.979400	3.348801	-4.855112	L
H-HC-0.060300	-1	4.489223	2.795189	-4.088816	L
H-HC-0.060300	-1	4.519618	4.120760	-5.280650	L
N-N--0.415700	-1	3.542283	3.392136	-1.209136	L H-HC 209
C-CT-0.021300	0	2.827281	2.697484	-0.115670	H
C-C-0.597300	0	2.309678	3.717313	0.919244	H
O-O--0.567900	0	3.118403	4.467988	1.468164	H
C-CT--0.123100	0	3.875083	1.785345	0.541296	H
S-S--1.036000	0	3.207908	0.590340	1.765433	H
H-H-0.271900	-1	4.546180	3.368703	-1.202237	L
H-H1-0.112400	0	2.010873	2.112390	-0.548313	H
H-H1-0.111200	0	4.584144	2.399633	1.105756	H
H-H1-0.111200	0	4.444875	1.225044	-0.206580	H
N-N--0.415700	0	0.982098	3.700068	1.210351	H
C-CT--0.051800	0	0.404120	4.535917	2.278152	H
C-C-0.597300	0	0.790124	4.019014	3.700129	H
O-O--0.567900	0	1.328829	4.747254	4.533296	H
C-CT--0.110200	-1	-1.131034	4.650514	2.023334	H

C-CT-0.353100	-1	-1.990291	5.556436	2.931783	L H-HC 222
C-CT--0.412100	-1	-2.179067	5.013795	4.349894	L
C-CT--0.412100	-1	-1.462103	6.991350	3.015082	L
H-H-0.271900	0	0.367692	3.015863	0.750302	H
H-H1-0.092200	0	0.867754	5.524254	2.228863	H
H-HC-0.045700	0	-1.255011	5.021905	0.999291	H
H-HC-0.045700	0	-1.583080	3.655159	2.044135	H
H-HC--0.036100	-1	-2.982681	5.601509	2.484453	L
H-HC-0.100000	-1	-1.279617	5.158365	4.944728	L
H-HC-0.100000	-1	-2.422112	3.952888	4.312275	L
H-HC-0.100000	-1	-2.998705	5.546658	4.829545	L
H-HC-0.100000	-1	-0.499356	7.011220	3.526756	L
H-HC-0.100000	-1	-2.174317	7.610253	3.559433	L
H-HC-0.100000	-1	-1.340553	7.391022	2.007430	L
N-N--0.415700	0	0.531777	2.699918	3.959674	H
C-CT--0.087500	0	0.585091	2.181699	5.334465	H
C-C-0.597300	0	1.982574	2.142265	5.965914	H
O-O--0.567900	0	2.081621	2.069953	7.186889	H
C-CT-0.298500	-1	-0.032180	0.766566	5.379731	H
C-CT--0.319200	0	0.754440	-0.291787	4.575651	L H-HC 241
C-CT--0.319200	0	-0.301831	0.193475	6.770768	L H-HC 241
H-H-0.271900	0	0.057207	2.149208	3.243442	H
H-H1-0.096900	0	0.008297	2.855464	5.981427	H
H-HC--0.029700	0	-1.006723	0.842038	4.894921	H
H-HC-0.079100	0	1.676693	-0.563786	5.084628	L
H-HC-0.079100	0	1.017444	0.092114	3.588377	L
H-HC-0.079100	0	0.141073	-1.178599	4.426555	L
H-HC-0.079100	0	0.635135	-0.048582	7.270544	L
H-HC-0.079100	0	-0.898114	-0.713201	6.672925	L
H-HC-0.079100	0	-0.855169	0.922441	7.360451	L
N-N--0.415700	0	3.004895	1.974297	5.094789	H
C-CT-0.033700	0	4.369658	1.827445	5.555907	H
C-C-0.597300	-1	5.083402	3.158287	5.823361	L H-H1 254
O-O--0.567900	-1	6.258814	3.136702	6.178201	L
C-CT--0.182500	-1	5.145368	1.007379	4.524944	L H-H1 254
H-H-0.271900	0	2.849079	2.210235	4.126312	H
H-H1-0.082300	0	4.348970	1.284342	6.504160	H
H-HC-0.060300	-1	6.113226	0.717154	4.931075	L
H-HC-0.060300	-1	5.300142	1.606507	3.627838	L
H-HC-0.060300	-1	4.588364	0.103644	4.274501	L
N-N--0.415700	-1	4.378566	4.284818	5.656644	L
C-CT--0.087500	-1	4.760306	5.649035	6.049015	L
C-C-0.597300	-1	3.919265	6.098820	7.250869	L
O-O--0.567900	-1	4.472001	6.552651	8.253850	L
C-CT-0.298500	-1	4.543009	6.620912	4.871884	L
C-CT--0.319200	-1	4.935770	8.060971	5.219535	L
C-CT--0.319200	-1	5.359368	6.222894	3.642611	L
H-H-0.271900	-1	3.466962	4.168187	5.231837	L
H-H1-0.096900	-1	5.810529	5.679851	6.329206	L
H-HC--0.029700	-1	3.490288	6.606543	4.597276	L
H-HC-0.079100	-1	5.986559	8.100410	5.498214	L
H-HC-0.079100	-1	4.329980	8.439593	6.042069	L
H-HC-0.079100	-1	4.773444	8.697713	4.350201	L
H-HC-0.079100	-1	6.409889	6.146494	3.917119	L

H-HC-0.079100	-1	5.240940	6.968435	2.856735	L
H-HC-0.079100	-1	5.007658	5.264461	3.260768	L
N-N--0.415700	-1	2.588082	5.906562	7.199204	L
C-CT--0.149000	-1	1.681719	6.248014	8.306286	L
H-H-0.271900	-1	2.180739	5.523326	6.351665	L
H-H1-0.097600	-1	2.259924	6.645746	9.140374	L
H-H1-0.097600	-1	1.147199	5.353403	8.627342	L
H-H1-0.097600	-1	0.965313	6.998110	7.971403	L
C-CT--0.366200	-1	4.026169	10.321031	-1.018098	L
C-C-0.597200	-1	2.551432	9.992311	-1.260303	L
O-O--0.567900	-1	1.740921	10.906191	-1.334430	L
H-HC-0.112300	-1	4.602549	9.397679	-0.980422	L
H-HC-0.112300	-1	4.128433	10.852594	-0.072210	L
H-HC-0.112300	-1	4.396340	10.947684	-1.829155	L
N-N--0.415700	-1	2.173893	8.708853	-1.312206	L
C-CT--0.024900	-1	0.761135	8.326194	-1.150575	L
C-C-0.597300	-1	0.175228	8.826583	0.175440	L
O-O--0.567900	-1	-0.919785	9.393049	0.183053	L
C-CT-0.211700	0	0.591935	6.825843	-1.293952	L
O-OH--0.654600	0	0.882808	6.516031	-2.636758	L
H-H-0.271900	-1	2.876997	7.976743	-1.371640	L
H-H1-0.084300	-1	0.187328	8.773540	-1.957947	L
H-H1-0.035200	0	-0.431792	6.537167	-1.064116	L
H-H1-0.035200	0	1.274176	6.299980	-0.624293	L
H-HO-0.427500	0	0.991408	5.540628	-2.645000	L
N-N--0.415700	-1	0.939018	8.695763	1.270781	L
C-CT-0.033700	-1	0.586114	9.180257	2.606492	L
C-C-0.597300	-1	0.119865	10.640939	2.594493	L
O-O--0.567900	-1	-0.976393	10.959479	3.057582	L
C-CT--0.182500	-1	1.773941	8.947043	3.537634	L
H-H-0.271900	-1	1.827928	8.200074	1.165890	L
H-H1-0.082300	-1	-0.227643	8.588314	2.998686	L
H-HC-0.060300	-1	1.544700	9.320070	4.535169	L
H-HC-0.060300	-1	2.658511	9.448494	3.147130	L
H-HC-0.060300	-1	1.970303	7.878217	3.594709	L
N-N--0.415700	-1	0.916478	11.519115	1.975564	L
C-CT--0.149000	-1	0.574378	12.915817	1.779350	L
H-H-0.271900	-1	1.818956	11.211101	1.621703	L
H-H1-0.097600	-1	-0.411420	13.110977	2.202984	L
H-H1-0.097600	-1	0.562568	13.141339	0.713860	L
H-H1-0.097600	-1	1.313659	13.544464	2.276732	L
C-CT--0.366200	-1	-11.934713	4.589178	4.972042	L
C-C-0.597200	-1	-12.366122	3.168427	4.605013	L
O-O--0.567900	-1	-12.929656	2.462217	5.443462	L
H-HC-0.112300	-1	-11.456695	5.057091	4.111325	L
H-HC-0.112300	-1	-11.229664	4.551892	5.802600	L
H-HC-0.112300	-1	-12.808928	5.170866	5.262763	L
N-N--0.415700	-1	-12.032901	2.724495	3.392745	L
C-CT--0.087500	-1	-12.027578	1.301068	3.037565	L
C-C-0.597300	-1	-10.581394	0.907207	2.723392	L
O-O--0.567900	-1	-9.867703	1.549744	1.945589	L
C-CT-0.298500	-1	-13.024508	0.906570	1.915256	L
C-CT--0.319200	-1	-13.769917	-0.383467	2.305139	L
C-CT--0.319200	-1	-14.104293	1.952387	1.604230	L

H-H-0.271900	-1	-11.624108	3.374237	2.718570	L
H-H1-0.096900	-1	-12.318570	0.743832	3.925637	L
H-HC--0.029700	-1	-12.466472	0.714898	1.002443	L
H-HC-0.079100	-1	-14.401570	-0.199948	3.174996	L
H-HC-0.079100	-1	-13.052825	-1.174340	2.528759	L
H-HC-0.079100	-1	-14.407191	-0.701626	1.480261	L
H-HC-0.079100	-1	-14.737102	2.098433	2.476148	L
H-HC-0.079100	-1	-14.712372	1.613329	0.766963	L
H-HC-0.079100	-1	-13.648763	2.904465	1.340685	L
N-N--0.415700	-1	-10.115796	-0.110228	3.450597	L
C-CT--0.038900	-1	-8.707074	-0.505379	3.532254	L
C-C-0.597300	-1	-8.576888	-2.030351	3.649675	L
O-O--0.567900	-1	-9.506334	-2.690602	4.135347	L
C-CT-0.365400	-1	-7.989865	0.146283	4.738454	L
O-OH--0.676100	-1	-8.155433	-0.565098	5.943506	L
C-CT--0.243800	-1	-8.409926	1.583046	5.042357	L
H-H-0.271900	-1	-10.743894	-0.582117	4.085085	L
H-H1-0.100700	-1	-8.208304	-0.173840	2.621601	L
H-H1-0.004300	-1	-6.931083	0.146962	4.500866	L
H-HC-0.064200	-1	-8.455192	2.145007	4.116956	L
H-HC-0.064200	-1	-7.681634	2.042912	5.711665	L
H-HC-0.064200	-1	-9.392717	1.609525	5.512153	L
H-HO-0.410200	-1	-8.407014	0.075920	6.640752	L
N-N--0.254800	-1	-7.450491	-2.624830	3.217013	L
C-CT--0.026600	-1	-7.197384	-4.050025	3.390691	L
C-C-0.589600	-1	-6.586862	-4.399553	4.749139	L
O-O--0.574800	-1	-6.595878	-5.569376	5.115447	L
C-CT--0.007000	0	-6.218456	-4.403230	2.273061	L
C-CT-0.018900	0	-5.383980	-3.135853	2.126829	L
C-CT-0.019200	0	-6.383674	-2.016750	2.428419	L
H-H1-0.064100	-1	-8.106642	-4.622222	3.248859	L
H-HC-0.025300	0	-5.600915	-5.260305	2.534358	L
H-HC-0.025300	0	-6.767731	-4.592065	1.349843	L
H-HC-0.021300	0	-4.971961	-3.054405	1.123392	L
H-HC-0.021300	0	-4.584131	-3.132482	2.866803	L
H-H1-0.039100	0	-6.791930	-1.637817	1.491206	L
H-H1-0.039100	0	-5.889218	-1.214477	2.977663	L
N-N--0.415700	-1	-5.969051	-3.434837	5.438868	L
C-CT--0.001400	-1	-4.975992	-3.670942	6.498237	L
C-C-0.597300	-1	-5.521361	-4.451574	7.708524	L
O-O--0.567900	-1	-6.707671	-4.336247	8.020417	L
C-CT--0.001400	0	-4.441378	-2.322994	7.002599	L H-HA 373
C-CA--0.001100	0	-4.078531	-1.313121	5.927085	H
C-CA--0.190600	0	-3.240388	-1.666224	4.864421	H
C-CA--0.190600	0	-4.577243	-0.009333	5.994831	H
C-CA--0.234100	0	-2.902564	-0.738608	3.884755	H
C-CA--0.234100	0	-4.234071	0.935341	5.032622	H
C-C-0.322600	0	-3.381555	0.580304	3.978921	H
O-OH--0.557900	0	-3.048316	1.534231	3.087006	H
H-H-0.271900	-1	-6.038392	-2.497203	5.074548	L
H-H1-0.087600	-1	-4.150742	-4.239449	6.068027	L
H-HC-0.029500	0	-5.199886	-1.878010	7.649075	L
H-HC-0.029500	0	-3.555706	-2.502086	7.613398	L
H-HA-0.169900	0	-2.851646	-2.679037	4.780703	H

H-HA-0.169900	0	-5.236046	0.286478	6.812408	H
H-HA-0.165600	0	-2.257657	-1.009909	3.055876	H
H-HA-0.165600	0	-4.583285	1.962375	5.106046	H
H-HO-0.399200	0	-2.227006	1.282059	2.584026	H
N-N--0.415700	-1	-4.640668	-5.137497	8.463544	L
C-CT--0.149000	-1	-5.022782	-5.600357	9.814088	L
H-H-0.271900	-1	-3.646224	-5.129574	8.222725	L
H-H1-0.097600	-1	-6.106481	-5.551731	9.921515	L
H-H1-0.097600	-1	-4.554058	-4.963152	10.563242	L
H-H1-0.097600	-1	-4.689626	-6.629173	9.952790	L
C-CT--0.366200	-1	-0.459604	-10.762282	2.513196	L
C-C-0.597200	-1	-0.643347	-9.825737	1.305820	L
O-O--0.567900	-1	-1.753746	-9.655013	0.797704	L
H-HC-0.112300	-1	0.588734	-10.773540	2.807951	L
H-HC-0.112300	-1	-0.771671	-11.770883	2.240935	L
H-HC-0.112300	-1	-1.067918	-10.407137	3.345020	L
N-N--0.415700	-1	0.469304	-9.278659	0.799310	L
C-CT-0.014300	-1	0.422407	-8.264368	-0.253230	L H-HC 405
C-C-0.597300	-1	0.048265	-8.777165	-1.662709	L
O-O--0.567900	-1	-0.165451	-7.957471	-2.546655	L
C-CT--0.204100	0	1.730160	-7.456540	-0.276948	H
C-C-0.713000	0	1.466789	-6.076782	-0.890099	H
O-O--0.593100	0	0.428773	-5.471791	-0.621987	H
N-N--0.919100	0	2.453063	-5.545492	-1.641678	H
H-H-0.271900	-1	1.352936	-9.463414	1.245091	L
H-H1-0.104800	-1	-0.381125	-7.592786	0.049429	L
H-HC-0.079700	0	2.511320	-8.024536	-0.795895	H
H-HC-0.079700	0	2.062235	-7.282358	0.751580	H
H-H-0.419600	0	2.365703	-4.571386	-1.945990	H
H-H-0.419600	0	3.236283	-6.101742	-1.947875	H
N-N--0.415700	-1	-0.046030	-10.091332	-1.896215	L
C-CT--0.149000	-1	-0.586589	-10.646929	-3.149015	L
H-H-0.271900	-1	0.065796	-10.738073	-1.107401	L
H-H1-0.097600	-1	-0.653258	-9.858412	-3.897910	L
H-H1-0.097600	-1	-1.579104	-11.058714	-2.965913	L
H-H1-0.097600	-1	0.072641	-11.437219	-3.510358	L
C-CT--0.366200	-1	-3.853669	-11.704666	-1.375706	L
C-C-0.597200	-1	-4.622836	-10.379602	-1.451223	L
O-O--0.567900	-1	-5.762152	-10.385283	-1.921548	L
H-HC-0.112300	-1	-2.870227	-11.528518	-0.938977	L
H-HC-0.112300	-1	-3.737196	-12.114923	-2.377825	L
H-HC-0.112300	-1	-4.405431	-12.410013	-0.754695	L
N-N--0.415700	-1	-3.996498	-9.250435	-1.080012	L
C-CT--0.087500	-1	-4.562316	-7.890630	-1.246980	L
C-C-0.597300	-1	-4.828855	-7.513249	-2.715319	L
O-O--0.567900	-1	-5.818637	-6.845698	-3.012247	L
C-CT-0.298500	-1	-3.655950	-6.810839	-0.599713	L
C-CT--0.319200	-1	-4.145006	-5.374278	-0.844436	L
C-CT--0.319200	-1	-3.639369	-6.942626	0.920790	L
H-H-0.271900	-1	-3.114037	-9.358613	-0.578130	L
H-H1-0.096900	-1	-5.522843	-7.868282	-0.733576	L
H-HC--0.029700	-1	-2.640560	-6.909015	-0.984176	L
H-HC-0.079100	-1	-5.180752	-5.277865	-0.517952	L
H-HC-0.079100	-1	-4.077970	-5.125930	-1.901021	L

H-HC-0.079100	-1	-3.518391	-4.664535	-0.302246	L
H-HC-0.079100	-1	-4.645794	-6.807752	1.299681	L
H-HC-0.079100	-1	-2.976133	-6.194721	1.357726	L
H-HC-0.079100	-1	-3.288952	-7.918622	1.225664	L
N-N--0.415700	-1	-3.982352	-7.915125	-3.671669	L
C-CT--0.149000	-1	-4.069533	-7.505506	-5.084121	L
H-H-0.271900	-1	-3.259706	-8.576542	-3.413206	L
H-H1-0.097600	-1	-4.888551	-6.796437	-5.207397	L
H-H1-0.097600	-1	-4.251362	-8.382308	-5.707200	L
H-H1-0.097600	-1	-3.133897	-7.034751	-5.384653	L
C-CT--0.366200	-1	-12.128086	3.668435	-1.320278	L
C-C-0.597200	-1	-11.022739	2.603660	-1.281015	L
O-O--0.567900	-1	-11.314507	1.420936	-1.121776	L
H-HC-0.112300	-1	-11.680782	4.651436	-1.468060	L
H-HC-0.112300	-1	-12.677858	3.657297	-0.378753	L
H-HC-0.112300	-1	-12.811666	3.452703	-2.141670	L
N-N--0.415700	-1	-9.766691	3.045502	-1.350876	L
C-CT--0.024900	-1	-8.583002	2.225265	-1.169167	L
C-C-0.597300	-1	-7.471166	3.094102	-0.575662	L
O-O--0.567900	-1	-6.819583	3.880597	-1.277067	L
C-CT-0.211700	0	-8.152549	1.558095	-2.472718	L
O-OH--0.654600	0	-7.173225	0.605433	-2.156514	L
H-H-0.271900	-1	-9.641335	4.041840	-1.424642	L
H-H1-0.084300	-1	-8.819306	1.435070	-0.457860	L
H-H1-0.035200	0	-7.756109	2.287203	-3.176658	L
H-H1-0.035200	0	-9.007416	1.047701	-2.918638	L
H-HO-0.427500	0	-6.281093	1.008020	-2.258366	L
N-N--0.415700	-1	-7.308128	3.025176	0.754446	L
C-CT-0.021300	-1	-6.133359	3.644017	1.387190	L
C-C-0.597300	-1	-4.844634	2.996750	0.855040	L
O-O--0.567900	-1	-3.870553	3.685061	0.591689	L
C-CT--0.123100	-1	-6.190050	3.513055	2.910780	L
S-SH--0.311900	-1	-7.444402	4.620626	3.615265	L
H-H-0.271900	-1	-7.968175	2.479915	1.305689	L
H-H1-0.112400	-1	-6.106114	4.705163	1.134564	L
H-H1-0.111200	-1	-5.218953	3.788655	3.325555	L
H-H1-0.111200	-1	-6.404965	2.479082	3.179449	L
H-HS-0.193300	-1	-8.486520	4.169037	2.908202	L
N-N--0.415700	-1	-4.881616	1.677125	0.653667	L H-HC 478
C-CT-0.021300	0	-3.774764	0.941739	0.038859	H
C-C-0.597300	0	-3.717696	1.295990	-1.442740	H
O-O--0.567900	0	-4.732415	1.570972	-2.085316	H
C-CT--0.123100	0	-4.032042	-0.554925	0.305657	H
S-SH--0.311900	0	-2.677383	-1.687714	-0.205111	H
H-H-0.271900	-1	-5.732084	1.188793	0.861801	L
H-H1-0.112400	0	-2.847942	1.247452	0.524212	H
H-H1-0.111200	0	-4.954650	-0.857140	-0.205444	H
H-H1-0.111200	0	-4.191233	-0.687816	1.377844	H
H-HS-0.193300	0	0.842681	-3.257895	0.716161	H
N-N--0.415700	0	-2.471548	1.257261	-2.003351	H
C-CT--0.087500	0	-2.293367	1.363679	-3.437342	H
C-C-0.597300	0	-2.145300	0.006114	-4.167743	H
O-O--0.567900	0	-2.120020	0.010969	-5.399983	H
C-CT-0.298500	-1	-1.131010	2.286151	-3.874458	H

C-CT--0.319200	0	-1.257918	3.676965	-3.250233	L H-HC 492
C-CT--0.319200	0	0.257537	1.720526	-3.519873	L H-HC 492
H-H-0.271900	0	-1.667274	1.137056	-1.389552	H
H-H1-0.096900	0	-3.234973	1.772852	-3.821597	H
H-HC--0.029700	0	-1.179535	2.377786	-4.961954	H
H-HC-0.079100	0	-1.098564	3.623203	-2.170488	L
H-HC-0.079100	0	-2.249212	4.070855	-3.452655	L
H-HC-0.079100	0	-0.520078	4.344103	-3.691136	L
H-HC-0.079100	0	0.391959	1.691553	-2.438983	L
H-HC-0.079100	0	1.025426	2.351961	-3.956884	L
H-HC-0.079100	0	0.384895	0.716321	-3.917102	L
N-N--0.415700	0	-1.942256	-1.091996	-3.394476	H
C-CT--0.003100	0	-2.050005	-2.428769	-3.977262	H
C-C-0.597300	0	-3.517832	-2.865499	-4.174175	H
O-O--0.567900	0	-3.821950	-3.532693	-5.163879	H
C-CT--0.003600	-1	-1.301197	-3.452491	-3.098416	H
C-CT--0.064500	-1	-1.432467	-4.908675	-3.583799	L H-HC 508
C-C-0.695100	-1	-0.559402	-5.250022	-4.776624	L
O-O--0.608600	-1	-0.419179	-4.501999	-5.729312	L
N-N--0.940700	-1	0.055999	-6.412912	-4.768034	L
H-H-0.271900	0	-2.137967	-1.039652	-2.385746	H
H-H1-0.085000	0	-1.644934	-2.391339	-4.990538	H
H-HC-0.017100	0	-0.241365	-3.207089	-3.021535	H
H-HC-0.017100	0	-1.711781	-3.412356	-2.086191	H
H-HC-0.035200	-1	-2.460353	-5.166050	-3.823141	L
H-HC-0.035200	-1	-1.145561	-5.553322	-2.760380	L
H-H-0.425100	-1	0.658912	-6.662854	-5.532186	L
H-H-0.425100	-1	-0.052093	-7.031315	-3.965982	L
N-N--0.415700	0	-4.353800	-2.546260	-3.155281	H
C-CT--0.023700	0	-5.741051	-2.976609	-3.212579	H
C-C-0.597300	-1	-6.419528	-2.347799	-4.455068	L H-H1 522
O-O--0.567900	-1	-6.250912	-1.153153	-4.717828	L
C-CT-0.034200	-1	-6.476924	-2.680011	-1.887354	L H-H1 522
C-CT-0.001800	-1	-7.944644	-3.131761	-1.941341	L
S-S--0.273700	-1	-8.846966	-3.102035	-0.365077	L
C-CT--0.053600	-1	-9.218467	-1.334324	-0.239069	L
H-H-0.271900	0	-3.990355	-2.147768	-2.296373	H
H-H1-0.088000	0	-5.720126	-4.059954	-3.312889	H
H-HC-0.024100	-1	-6.408049	-1.632634	-1.631120	L
H-HC-0.024100	-1	-5.981710	-3.229117	-1.090078	L
H-H1-0.044000	-1	-7.968428	-4.158587	-2.307610	L
H-H1-0.044000	-1	-8.486639	-2.508551	-2.652961	L
H-H1-0.068400	-1	-9.823454	-1.147659	0.648131	L
H-H1-0.068400	-1	-9.770200	-1.008775	-1.121175	L
H-H1-0.068400	-1	-8.289424	-0.772515	-0.170216	L
N-N--0.254800	-1	-7.167936	-3.120970	-5.263523	L
C-CT--0.026600	-1	-7.567170	-2.709153	-6.610203	L
C-C-0.589600	-1	-9.017754	-2.228072	-6.601648	L
O-O--0.574800	-1	-9.901964	-2.928455	-6.101798	L
C-CT--0.007000	-1	-7.359564	-3.955307	-7.485485	L
C-CT-0.018900	-1	-6.839972	-5.014078	-6.509683	L
C-CT-0.019200	-1	-7.371513	-4.550770	-5.179754	L
H-H1-0.064100	-1	-6.921713	-1.912124	-6.978787	L
H-HC-0.025300	-1	-8.293893	-4.279179	-7.935004	L

H-HC-0.025300	-1	-6.625355	-3.771811	-8.267677	L
H-HC-0.021300	-1	-5.751849	-5.003854	-6.484818	L
H-HC-0.021300	-1	-7.212421	-5.997921	-6.722190	L
H-H1-0.039100	-1	-6.845335	-5.055300	-4.381075	L
H-H1-0.039100	-1	-8.436469	-4.773163	-5.103377	L
N-N--0.415700	-1	-9.244130	-1.033526	-7.141792	L
C-CT--0.149000	-1	-10.478975	-0.266174	-6.952650	L
H-H-0.271900	-1	-8.440816	-0.563744	-7.558834	L
H-H1-0.097600	-1	-11.237354	-0.904294	-6.499601	L
H-H1-0.097600	-1	-10.834671	0.091598	-7.918839	L
H-H1-0.097600	-1	-10.281037	0.584007	-6.299480	L
C-CT--0.366200	-1	-10.377904	8.822680	-4.248056	L
C-C-0.597200	-1	-9.825709	7.536889	-3.618485	L
O-O--0.567900	-1	-10.265960	7.119394	-2.546016	L
H-HC-0.112300	-1	-9.861036	9.018616	-5.187402	L
H-HC-0.112300	-1	-10.219918	9.657322	-3.565577	L
H-HC-0.112300	-1	-11.444536	8.705378	-4.438491	L
N-N--0.415700	-1	-8.854361	6.914279	-4.280794	L
C-CT--0.024900	-1	-7.907279	6.000071	-3.639111	L
C-C-0.597300	-1	-6.578994	6.735623	-3.421926	L
O-O--0.567900	-1	-6.327234	7.741379	-4.092928	L
C-CT-0.211700	0	-7.683579	4.743818	-4.492868	L
O-OH--0.654600	0	-7.317597	5.054015	-5.824424	L
H-H-0.271900	-1	-8.585577	7.280804	-5.192982	L
H-H1-0.084300	-1	-8.291214	5.663030	-2.675893	L
H-H1-0.035200	0	-8.602505	4.156456	-4.506808	L
H-H1-0.035200	0	-6.894879	4.142114	-4.038476	L
H-HO-0.427500	0	-6.884063	4.283254	-6.207998	L
N-N--0.415700	-1	-5.698978	6.208512	-2.560192	L
C-CT-0.033700	-1	-4.326181	6.720590	-2.460247	L
C-C-0.597300	-1	-3.580321	6.722583	-3.813663	L
O-O--0.567900	-1	-2.683109	7.537595	-4.034456	L
C-CT--0.182500	-1	-3.569464	5.904046	-1.422724	L
H-H-0.271900	-1	-5.979358	5.404505	-1.993706	L
H-H1-0.082300	-1	-4.375359	7.749017	-2.100914	L
H-HC-0.060300	-1	-2.556573	6.287985	-1.319982	L
H-HC-0.060300	-1	-3.532529	4.857147	-1.722061	L
H-HC-0.060300	-1	-4.083963	5.989344	-0.466858	L
N-N--0.415700	-1	-4.001008	5.852101	-4.745202	L
C-CT--0.149000	-1	-3.487746	5.795444	-6.112761	L
H-H-0.271900	-1	-4.727734	5.202654	-4.475167	L
H-H1-0.097600	-1	-2.716105	6.554641	-6.242618	L
H-H1-0.097600	-1	-4.300523	5.981662	-6.814633	L
H-H1-0.097600	-1	-3.063257	4.809310	-6.300820	L
C-CM--0.139000	0	0.797151	-1.108079	-0.677554	H
C-C-0.519000	0	1.490609	-2.383075	-0.885926	H
O-O2--0.567000	0	1.691663	-3.162484	0.179063	H
C-CM--0.117000	0	0.214692	-0.779798	0.493683	H
O-O2--0.618000	0	1.971480	-2.694097	-1.985729	H
C-C--0.553000	0	-0.340828	0.574843	0.822727	H
O-O2--0.556000	0	-0.283640	1.473317	-0.063182	H
O-O2--0.607000	0	-0.766059	0.723365	2.010968	H
H-HC-0.049000	0	2.436170	-0.113273	0.913997	H
H-HC-0.162000	0	0.235392	-1.463054	1.332670	H

O-OW--0.834000	-1	6.424390	2.970444	-1.185531	L
H-HW-0.417000	-1	6.794220	3.109980	-2.056513	L
H-HW-0.417000	-1	7.103725	3.274292	-0.583916	L
O-OW--0.834000	0	3.366467	7.076358	1.038058	L
H-HW-0.417000	0	3.226514	6.176571	1.399298	L
H-HW-0.417000	0	3.746383	6.875606	0.166040	L
O-OW--0.834000	0	-0.620729	-3.735670	1.298892	H
H-HW-0.417000	0	-0.621151	-4.512883	0.710000	H
H-HW-0.417000	0	-1.367036	-3.172414	0.976786	H
O-OW--0.834000	0	-4.864226	0.643616	-6.265815	L
H-HW-0.417000	0	-3.929315	0.429639	-6.132269	L
H-HW-0.417000	0	-5.319556	0.043476	-5.650888	L
H-HS-0.193300	0	0.744062	-0.448229	-1.534757	H