

Supporting information

for

Exploring fluoride effects in sterically enhanced cobalt ethylene polymerisation catalysts; a combined experimental and DFT study

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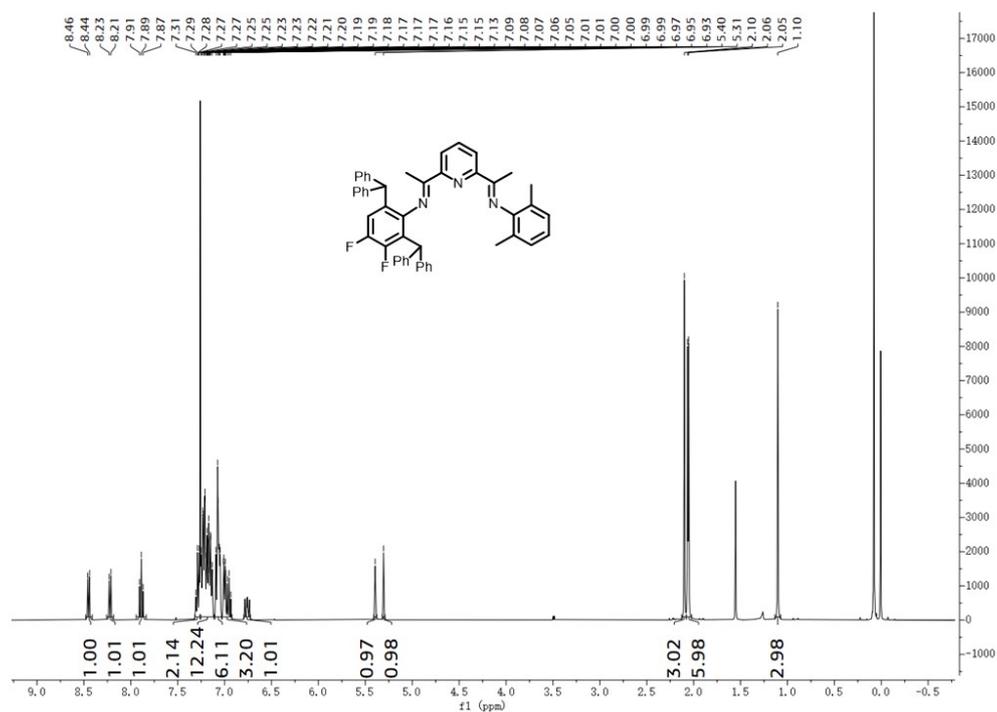


Figure S1 ^1H NMR spectrum of L1 in CDCl_3 at room temperature

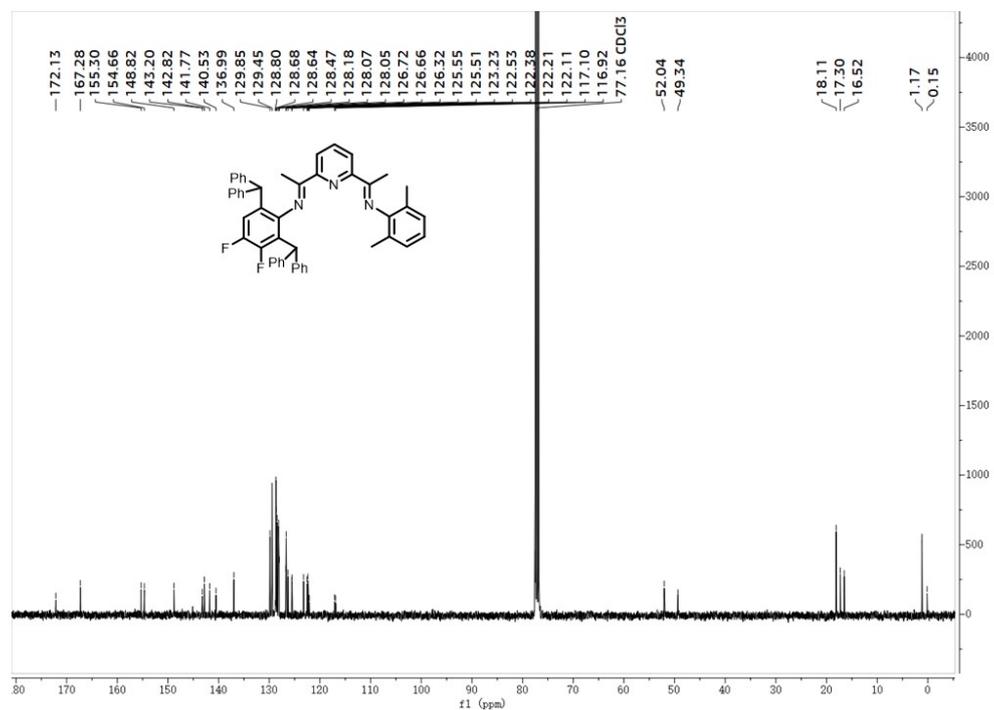


Figure S2 ^{13}C NMR spectrum of L1 in CDCl_3 at room temperature

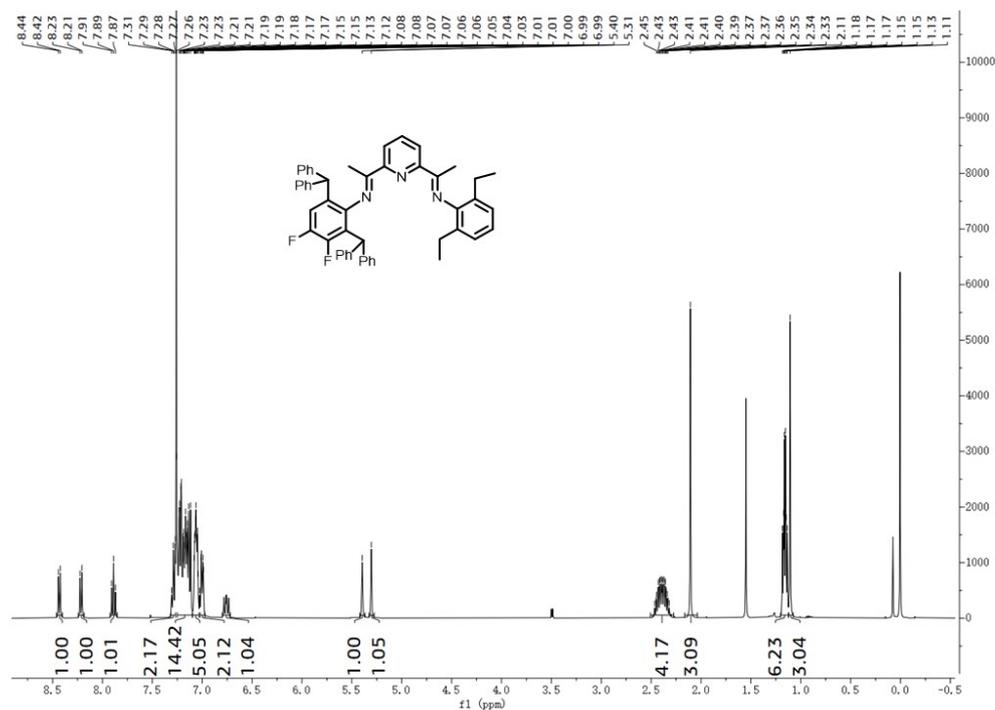


Figure S3 ^1H NMR spectrum of L2 in CDCl_3 at room temperature

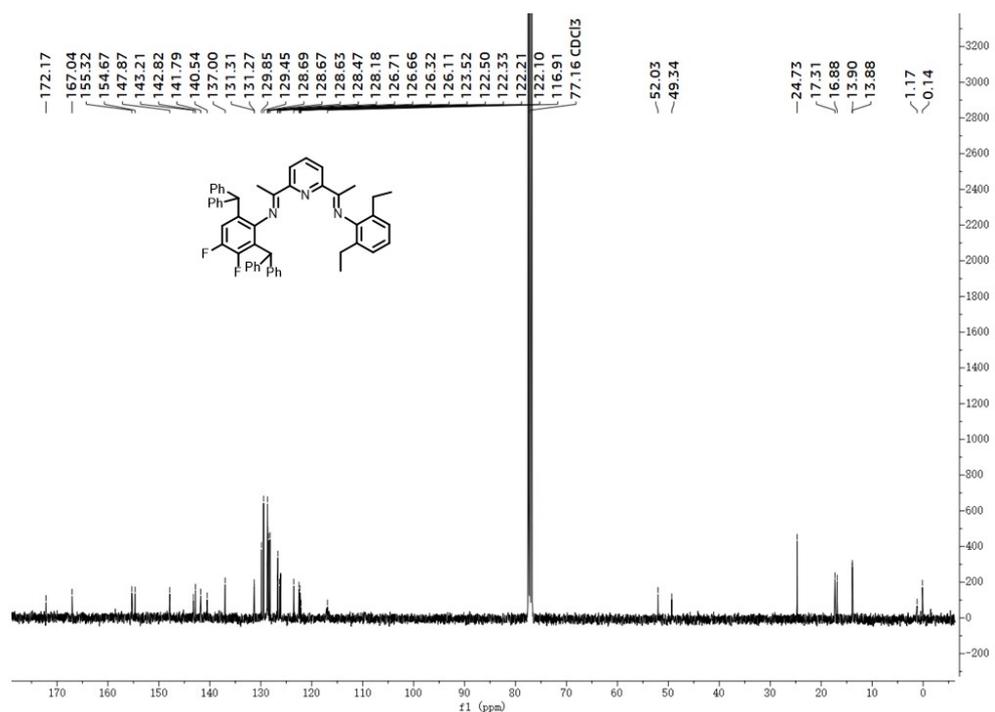


Figure S4 ^{13}C NMR spectrum of L2 in CDCl_3 at room temperature

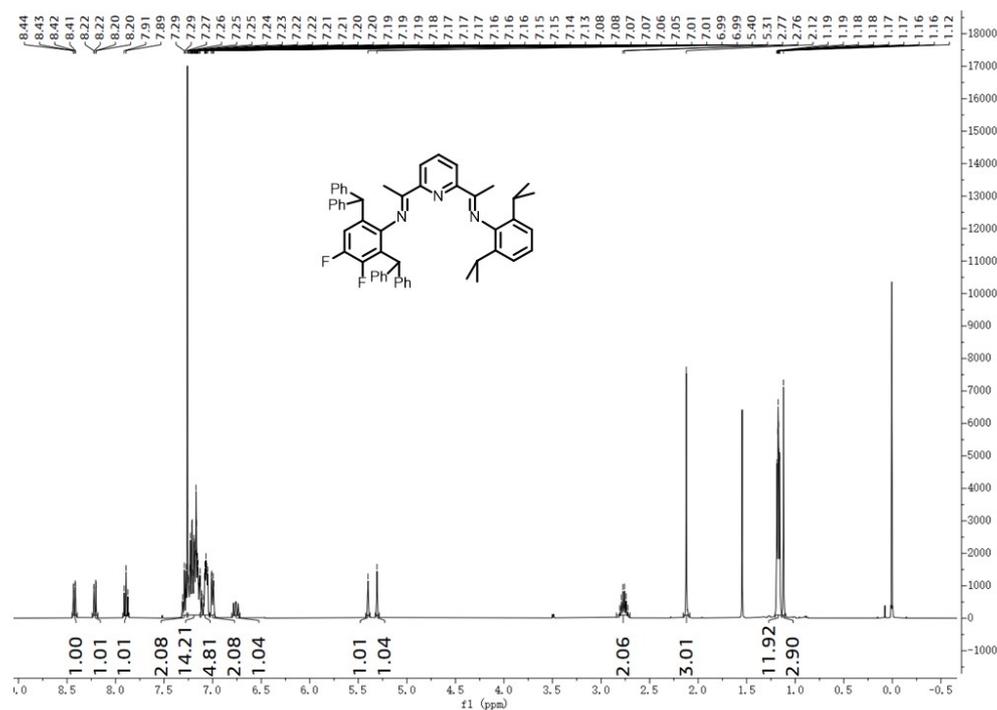


Figure S5 ^1H NMR spectrum of L3 in CDCl_3 at room temperature

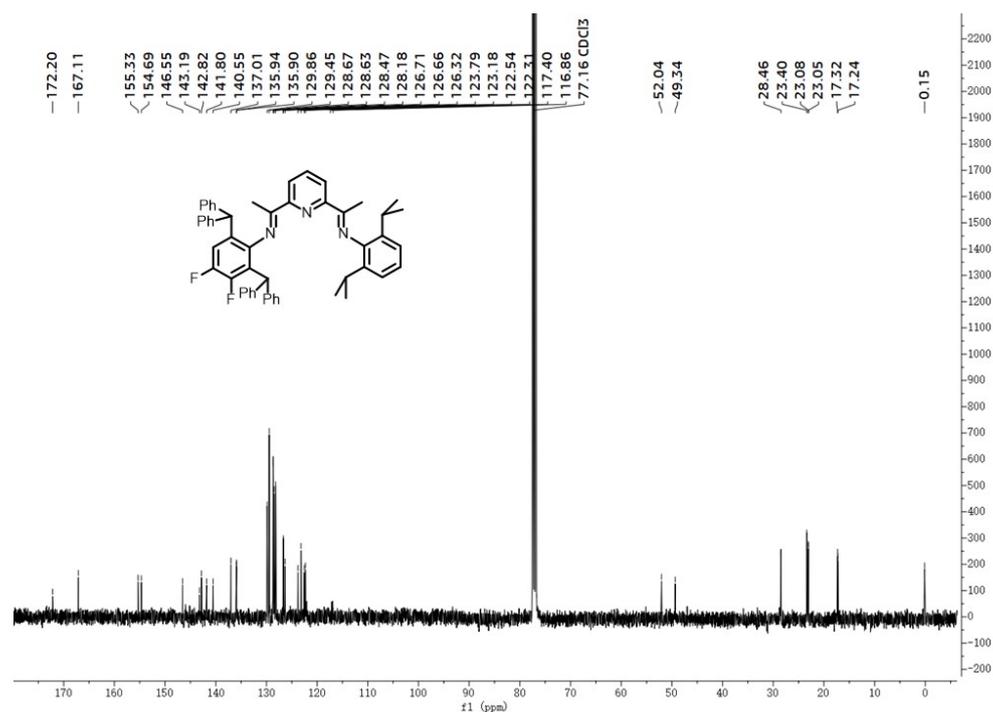


Figure S6 ^{13}C NMR spectrum of L3 in CDCl_3 at room temperature

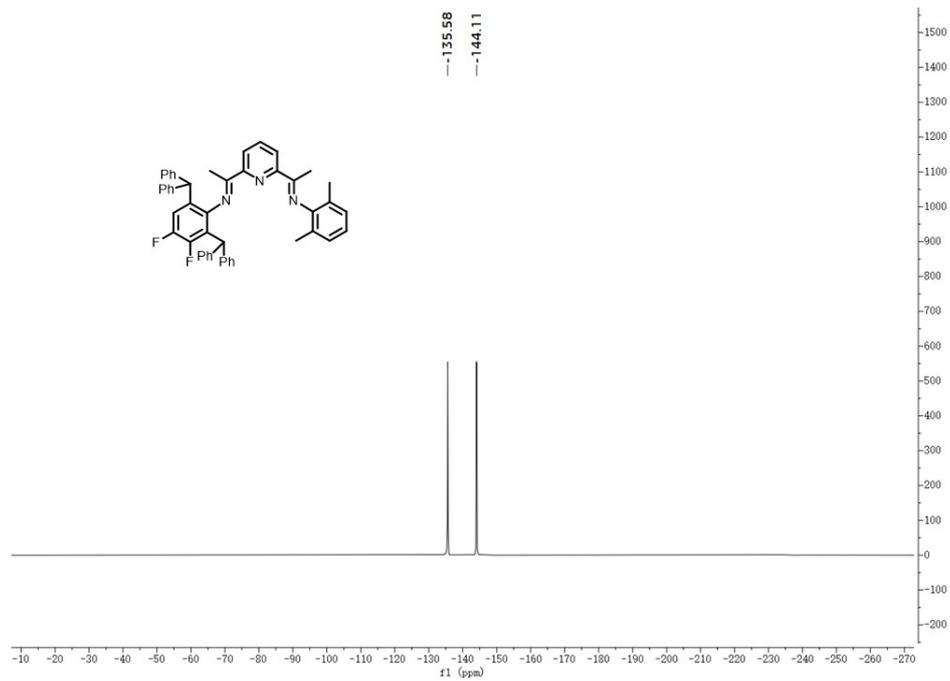


Figure S11 ^{19}F NMR spectrum of **L1** in CDCl_3 at room temperature

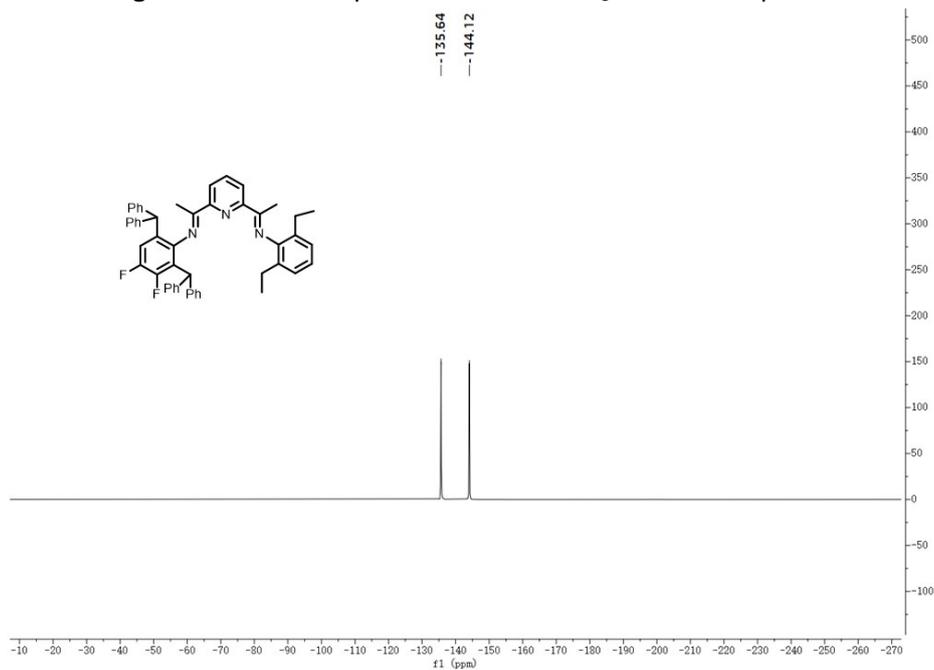


Figure S12 ^{19}F NMR spectrum of **L2** in CDCl_3 at room temperature

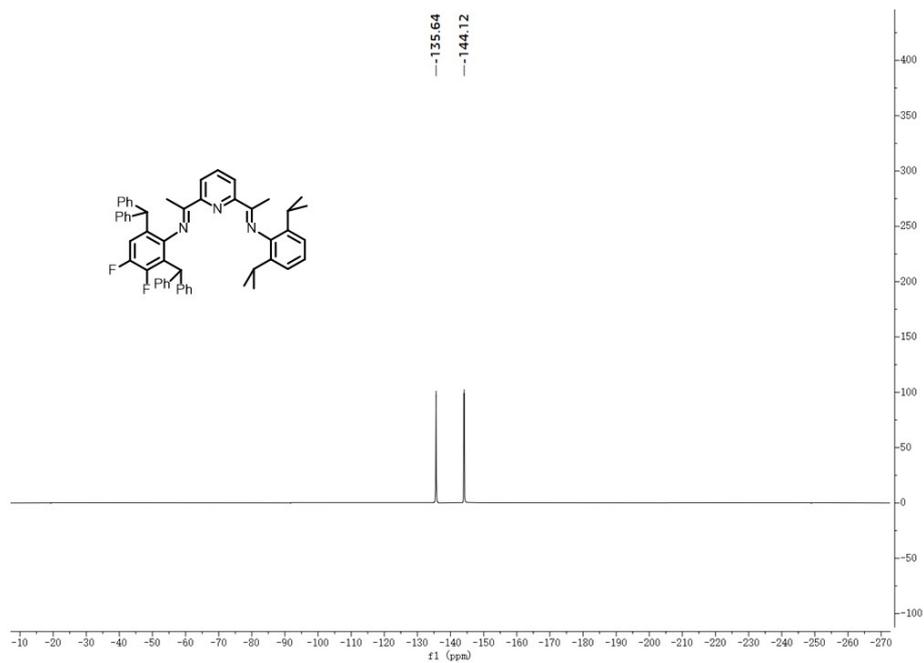


Figure S13 ^{19}F NMR spectrum of **L3** in CDCl_3 at room temperature

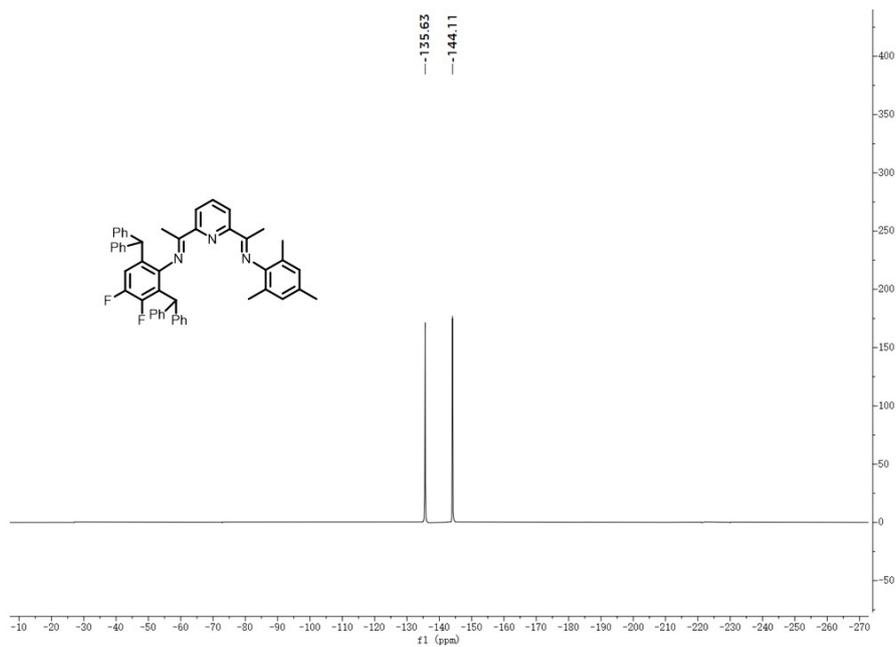


Figure S14 ^{19}F NMR spectrum of **L4** in CDCl_3 at room temperature

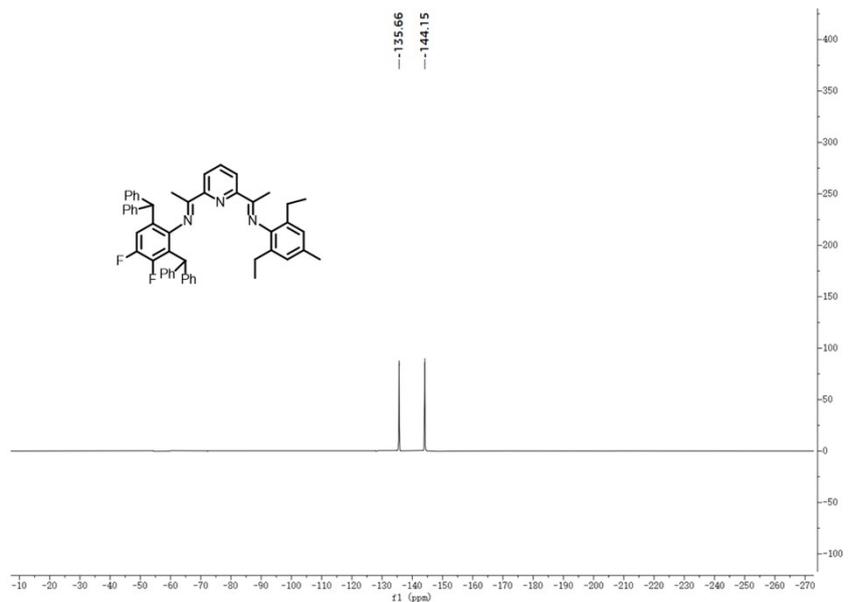


Figure S15 ^{19}F NMR spectrum of L5 in CDCl_3 at room temperature

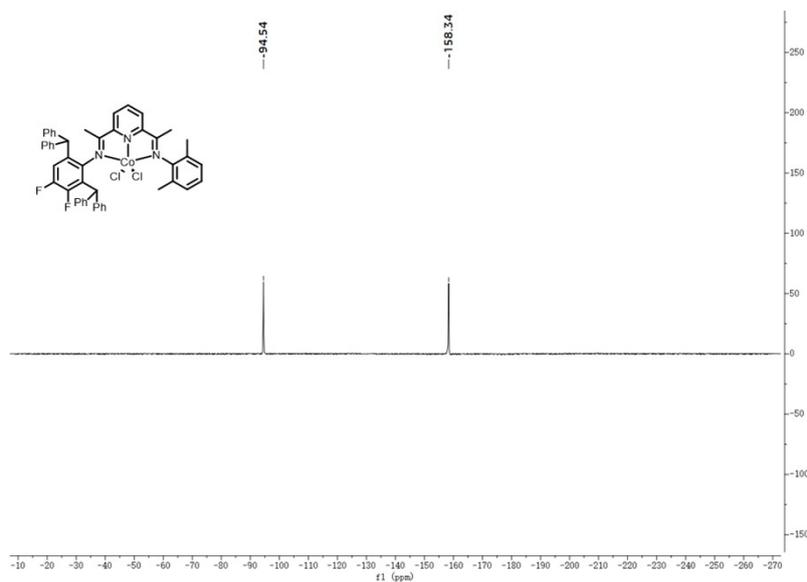


Figure S16 ^{19}F NMR spectrum of Co1 in CDCl_3 at room temperature

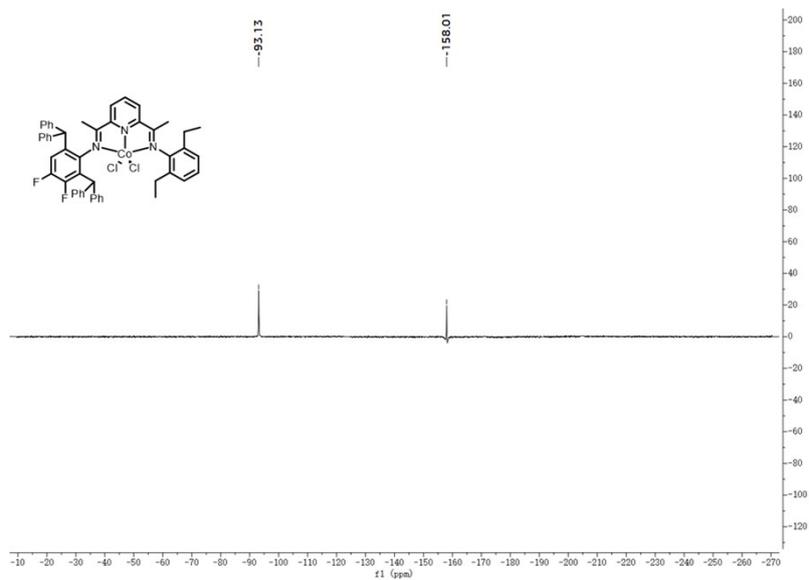


Figure S17 ^{19}F NMR spectrum of **Co2** in CDCl_3 at room temperature

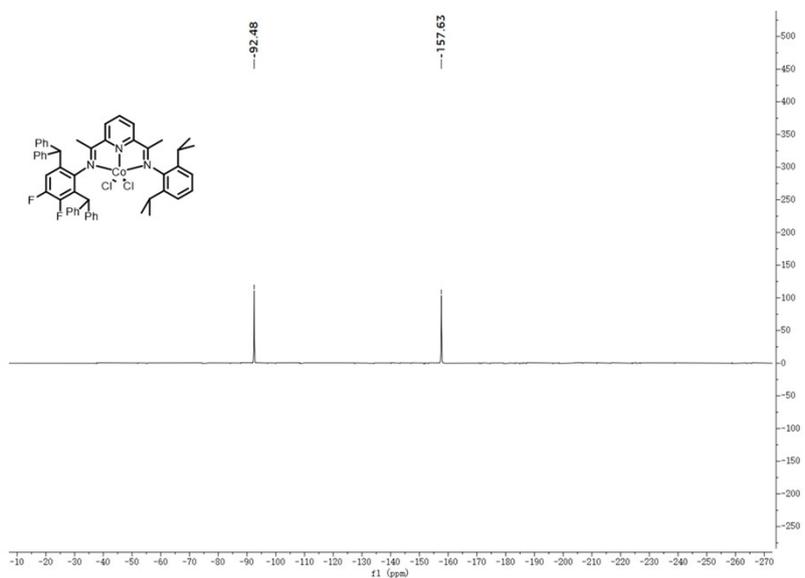


Figure S18 ^{19}F NMR spectrum of **Co3** in CDCl_3 at room temperature

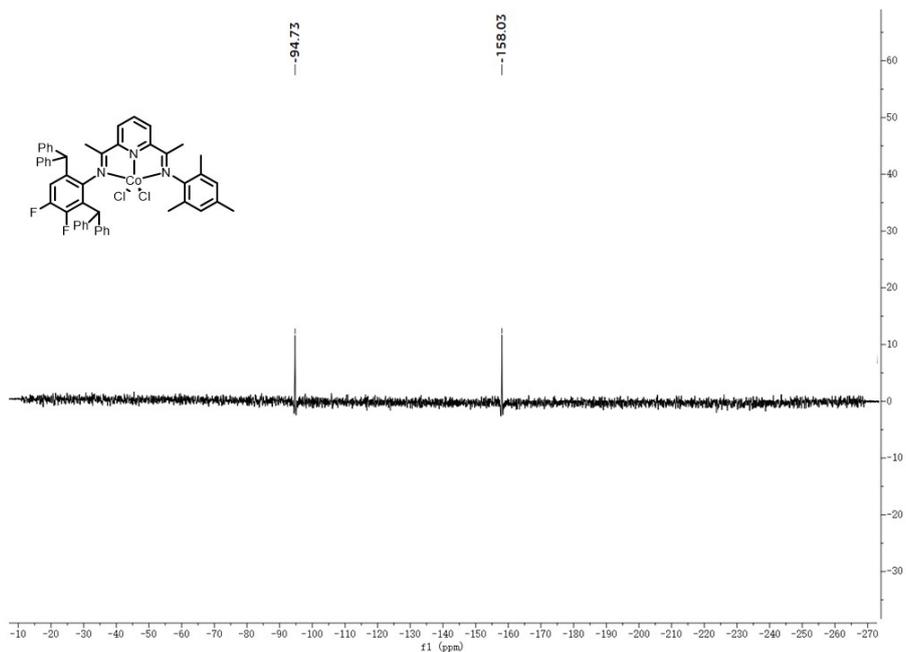


Figure S19 ^{19}F NMR spectrum of **Co4** in CDCl_3 at room temperature

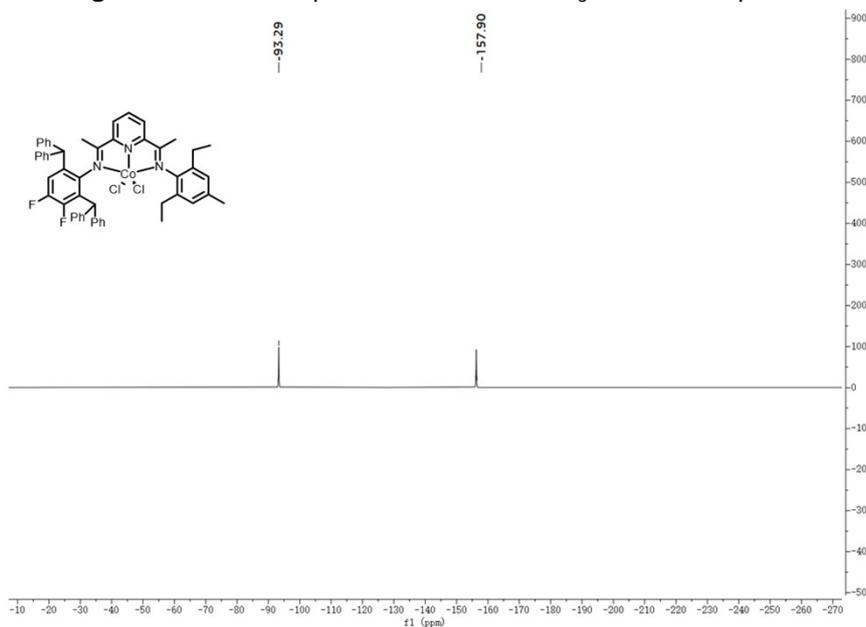


Figure S20 ^{19}F NMR spectrum of **Co5** in CDCl_3 at room temperature

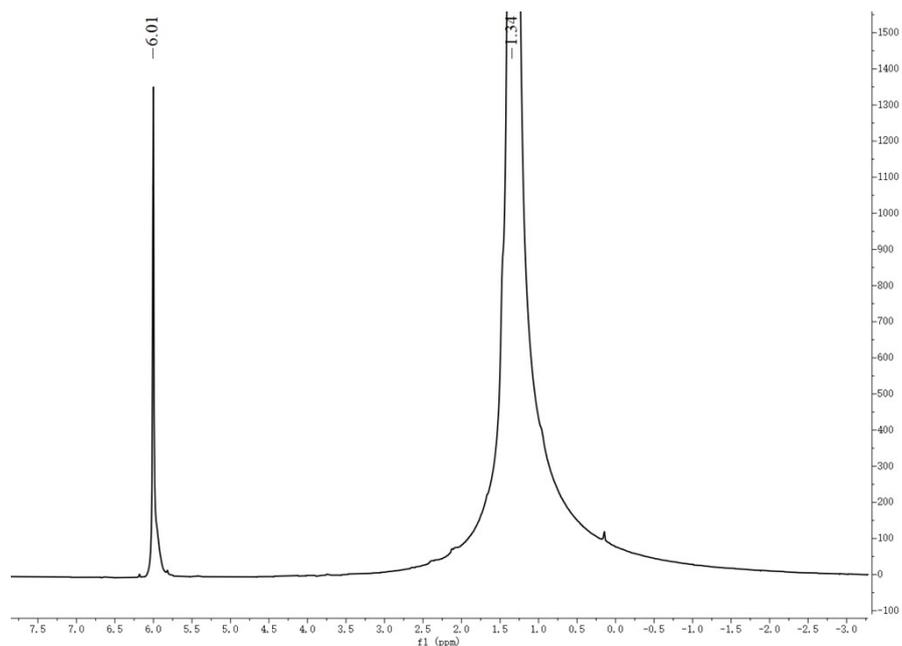


Figure S21 ¹H NMR spectrum of the polyethylene generated using **Co5**/MMAO at 30 °C (entry 8, Table 3); recorded in tetrachloroethane- *d*₂ at 100 °C.

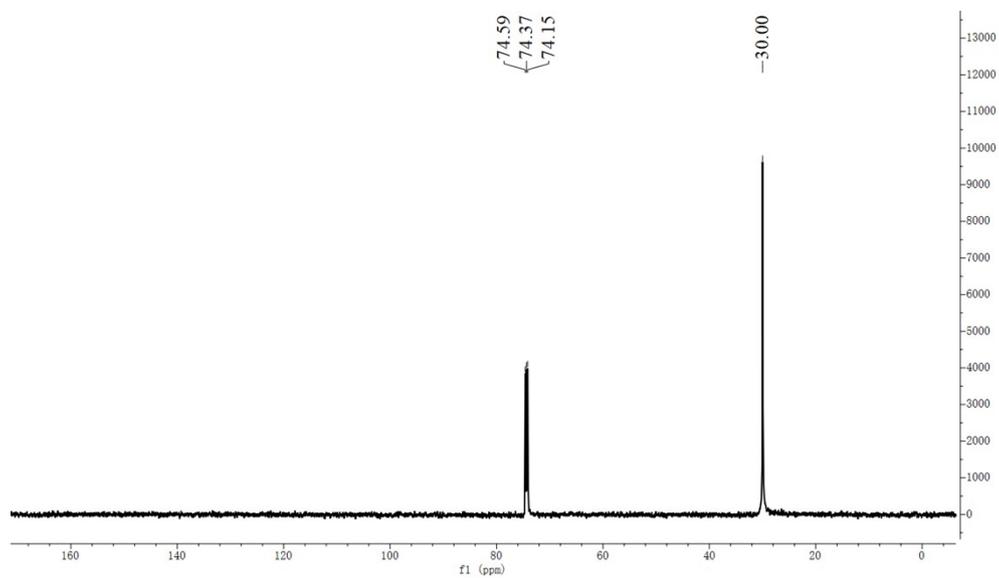


Figure S22 ¹³C NMR spectrum of the polyethylene generated using **Co5**/MMAO at 30 °C (entry 8, Table 3); recorded in tetrachloroethane- *d*₂ at 100 °C (δ C 74.37).

Coordinate of all optimized structures:

1-iPr

Doublet:

1

Atom	x	y	z
C	1.05873600	2.54137300	-1.36702800
C	1.06975500	3.73574400	-2.08325200
C	-0.14735600	4.36398000	-2.32842100
C	-1.33448500	3.79094800	-1.88253800
C	-1.26361800	2.58630000	-1.18693300
N	-0.08587600	2.01511100	-0.92968800
H	-0.17189400	5.29943800	-2.88029000
H	1.99929600	4.16576600	-2.44464300
H	-2.28813100	4.27022000	-2.08359700
C	2.25799400	1.73447000	-1.01458100
C	-2.42942800	1.79190300	-0.70996500
N	-2.12461700	0.63827800	-0.23014900
N	1.99913000	0.62385400	-0.41946400
C	-3.80126200	2.34545500	-0.86213600
H	-3.92978800	3.23599600	-0.23243200
H	-3.97534500	2.65754600	-1.89930500
H	-4.56012500	1.60924400	-0.58611700
C	3.60795300	2.24760500	-1.36664500
H	3.74270600	2.23314800	-2.45699800
H	3.72709600	3.28825000	-1.04283900
H	4.39649400	1.63994700	-0.91639100
C	-3.08311700	-0.28928300	0.26253100
C	-3.21936600	-1.49356900	-0.45757700
C	-3.71639500	-0.07956200	1.49872400
C	-4.06092000	-2.47268800	0.06170800

C	-4.53432100	-1.10358900	1.98335800
C	-4.71503800	-2.28105800	1.27401900
H	-4.19544900	-3.40797200	-0.47659400
H	-5.02892900	-0.97716400	2.94471300
H	-5.36034100	-3.06064900	1.67159000
C	3.01383600	-0.26075600	0.05083400
C	3.24787300	-0.28270900	1.43916100
C	3.64761500	-1.14591700	-0.83528500
C	4.15783300	-1.21637500	1.92896500
C	4.53937500	-2.07188100	-0.28889600
C	4.79554800	-2.10831900	1.07430100
H	4.36596000	-1.25214000	2.99624000
C	2.55632900	0.71261700	2.34921400
H	1.56023900	0.90119400	1.91069200
C	3.33819400	-1.15996700	-2.31919100
H	2.89874100	-0.18976500	-2.58985800
C	-3.45322500	1.14535500	2.35293300
H	-2.98961900	1.91796600	1.72434200
C	-2.46203300	-1.68726200	-1.75421700
H	-1.46486300	-1.23329800	-1.59445800
C	-0.13034800	-1.39296600	1.31751200
H	0.45755600	-1.29443300	2.24212500
H	-1.17774500	-1.51434900	1.64237600
C	0.31314700	-2.65454800	0.57520100
H	1.40676500	-2.64267400	0.43415200
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H	0.32410900	-3.96779200	2.30346400
H	-1.19235400	-3.98161500	1.39246200
H	0.23034200	-4.83555200	0.75840900

Co	-0.03537400	0.19016900	0.12123000
C	-3.14428000	-0.95145100	-2.90763500
H	-3.26724800	0.12093500	-2.71332700
H	-2.57267700	-1.06282600	-3.83729800
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H	-1.85460300	-3.74348100	-1.30577700
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H	4.32757700	1.88007300	2.79439000
H	3.43836300	2.47872700	1.38779800
H	2.80950000	2.76688400	3.02228900
C	4.58455600	-1.34050100	-3.17915900
H	4.33559100	-1.21130600	-4.23906400
H	5.36578500	-0.61430400	-2.92241000

H	5.01404300	-2.34439500	-3.07332600
C	2.30021500	-2.23517300	-2.63928600
H	2.08532100	-2.26354200	-3.71480200
H	2.66504100	-3.22693200	-2.34081800
H	1.35406000	-2.06305300	-2.10809300

2

Atom	x	y	z
C	1.06134200	2.56666200	-1.16157700
C	1.05817100	3.76888100	-1.86378000
C	-0.16790500	4.32867800	-2.21378300
C	-1.35317500	3.67373000	-1.89228700
C	-1.27902800	2.47649700	-1.18449200
N	-0.09187500	1.98268300	-0.80576300
H	-0.19817300	5.26706500	-2.75970600
H	1.98937500	4.25689700	-2.13746400
H	-2.31296700	4.08573300	-2.19107500
C	2.22602600	1.75003200	-0.78742600
C	-2.39061900	1.58887100	-0.81004700
N	-2.03245400	0.49934000	-0.19547400
N	1.93259300	0.62555300	-0.20226400
C	-3.77458500	1.97604300	-1.19600500
H	-3.80973300	2.26364500	-2.25355400
H	-4.49527700	1.17418600	-1.02603200
H	-4.08836600	2.85606000	-0.61790900
C	3.58612600	2.23103200	-1.14716200
H	3.83925200	3.11165400	-0.54048500
H	4.35011900	1.46789000	-0.98492700
H	3.61927100	2.54932000	-2.19578700
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C	4.74773700	-1.25622200	1.36370300
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H	0.79349700	2.44501500	1.79547400
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H	3.97963900	-1.22842800	-3.54653000
H	2.43627400	-0.71102500	-4.24862400
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H	-2.28123900	-1.08199000	-4.15437900
C	-4.97195000	1.59246500	2.27744300
H	-4.85321500	2.39896400	3.01147400
H	-5.17648400	2.04836000	1.30171000
H	-5.86229000	1.01786600	2.56330800
C	-3.47899200	0.13153100	3.65138300
H	-3.20516700	0.93235300	4.34916400
H	-4.37672000	-0.35646400	4.05095100
H	-2.67644400	-0.61656700	3.65553500

TS-2/3

Atom	x	y	z
C	-1.03946100	2.70301100	0.94435100
C	-1.01716400	3.95313900	1.55349000
C	0.20717000	4.49513700	1.93543700
C	1.37953900	3.77493800	1.72400500
C	1.30460100	2.53126000	1.10474300
N	0.11351600	2.04088800	0.69562500
H	0.24546000	5.46822400	2.41567900
H	-1.94279700	4.49175300	1.73625600
H	2.33887800	4.17444300	2.04078400
C	-2.21122700	1.91455600	0.58460600
C	2.39987700	1.60865500	0.83472800
N	2.02321500	0.48071000	0.29296100
N	-1.92277700	0.71784600	0.14362900

C	3.79071800	1.98095400	1.21338800
H	3.81586300	2.34678200	2.24701800
H	4.47490000	1.13381400	1.12854800
H	4.16380700	2.79355700	0.57558900
C	-3.57539700	2.46746700	0.80560800
H	-3.77950500	3.26874800	0.08259600
H	-4.34780700	1.70188600	0.70267400
H	-3.65818800	2.91161900	1.80453600
C	2.99279600	-0.52081300	-0.02979000
C	2.99562600	-1.68953400	0.76222900
C	3.84095400	-0.38485400	-1.14604500
C	3.85919500	-2.72363700	0.40845600
C	4.67370600	-1.46170300	-1.46469100
C	4.68613100	-2.61902300	-0.70344900
H	3.88483600	-3.63026100	1.00848200
C	-2.95855600	-0.25810000	-0.02212100
C	-3.76247900	-0.31515400	-1.17360800
C	-3.08348700	-1.20416000	1.01879900
C	-4.70768300	-1.34197200	-1.25640300
C	-4.03874500	-2.20901300	0.88179900
C	-4.84624800	-2.28181300	-0.24690500
H	-5.34517900	-1.40231800	-2.13701700
H	-4.15562800	-2.94712600	1.67260000
H	-5.58685400	-3.07297100	-0.33651700
C	-3.65111600	0.67421000	-2.31732200
H	-2.78029500	1.31889800	-2.12583700
C	-2.24814300	-1.09673500	2.28127500
H	-1.29707500	-0.60850700	2.00917200
C	3.92643400	0.86920600	-1.99637800
H	3.22611700	1.61389500	-1.59245600

C	2.11994400	-1.79474200	1.99534000
H	1.21425900	-1.19530100	1.80597100
C	0.01319300	-1.52692800	-0.81806600
H	1.05659500	-1.85885200	-0.83457400
H	-0.32941000	-1.52636400	0.23982300
C	-0.85105300	-2.53109600	-1.55595900
H	-0.53233100	-2.60083100	-2.60608500
H	-1.89932900	-2.20178800	-1.56341400
C	-0.75196800	-3.90722600	-0.91543800
H	0.28632000	-4.26535900	-0.89839900
H	-1.12082500	-3.89515800	0.11909700
H	-1.34846500	-4.64290200	-1.46612200
Co	0.04223500	0.43998200	-0.19662100
C	0.01684800	-0.11189900	-2.20313100
H	-0.95345000	-0.37985900	-2.61692100
H	0.83780200	-0.64781200	-2.68444000
C	0.20729000	1.28777100	-1.95106400
H	1.19003300	1.72840000	-2.12623800
H	-0.62491400	1.96414500	-2.15716800
C	-4.89096400	1.56511800	-2.41070600
H	-4.77526600	2.30285000	-3.21422600
H	-5.78185600	0.96689600	-2.64136700
H	-5.09218800	2.10618800	-1.47978900
C	-3.43835600	-0.02289700	-3.66185900
H	-3.19771000	0.71203200	-4.43942600
H	-2.63143700	-0.76502800	-3.63439000
H	-4.34644800	-0.54850300	-3.98305800
C	-2.94320100	-0.20733400	3.31290800
H	-3.91743900	-0.63322200	3.58748300
H	-2.34192000	-0.12810900	4.22703600

H	-3.12071100	0.80789700	2.93846500
C	-1.91266900	-2.44214100	2.91208700
H	-1.48179900	-3.14719900	2.18953900
H	-1.18728800	-2.30149800	3.72357800
H	-2.79618600	-2.91740800	3.35708000
H	5.34571800	-3.44108300	-0.97079500
H	5.33353000	-1.38084200	-2.32709800
C	3.53569200	0.61248500	-3.45026800
H	2.51886200	0.21383200	-3.54382900
H	3.58304000	1.54387700	-4.02805300
H	4.21835900	-0.10264900	-3.92590500
C	5.33067700	1.47411600	-1.94246400
H	5.35404900	2.43665700	-2.46795400
H	5.67487400	1.63751500	-0.91462500
H	6.06193200	0.81863300	-2.43199900
C	2.82719900	-1.18876800	3.20762100
H	3.09190400	-0.13565600	3.05137200
H	2.18953300	-1.24597500	4.09883700
H	3.75490800	-1.73567600	3.42257300
C	1.68255200	-3.22018700	2.30810500
H	0.95088600	-3.22022600	3.12463600
H	1.22395400	-3.71307300	1.44080200
H	2.52449600	-3.84037700	2.64088000

3

Atom	x	y	z
C	-0.63521700	-3.25542000	-0.23358900
C	-0.45303900	-4.63456100	-0.23985500
C	0.84802100	-5.12780400	-0.32840300
C	1.93468200	-4.25569300	-0.38264500
C	1.68166900	-2.88815800	-0.36607800
N	0.42108100	-2.43243600	-0.32664400

H	1.01818900	-6.20041300	-0.33573600
H	-1.30087000	-5.31029000	-0.16662600
H	2.95206200	-4.63496900	-0.42027400
C	-1.88799400	-2.49063500	-0.12129700
C	2.64685200	-1.77840300	-0.32512700
N	2.10741600	-0.61048300	-0.10875600
N	-1.71348800	-1.20508800	0.00314400
C	4.09223100	-2.05574200	-0.52163800
H	4.52137600	-2.50082800	0.38726800
H	4.23020400	-2.77989800	-1.33294500
H	4.65423900	-1.14783300	-0.75273500
C	-3.19339500	-3.19503000	-0.18458100
H	-3.19730200	-3.92564700	-1.00186000
H	-3.36296500	-3.75274300	0.74703700
H	-4.02285600	-2.49857200	-0.32694600
C	2.93735100	0.55434800	-0.03194700
C	2.85853800	1.47586900	-1.09443000
C	3.73005000	0.78597900	1.10403600
C	3.65061200	2.61961400	-1.02180900
C	4.49008600	1.95821200	1.13212700
C	4.46513700	2.85851800	0.07923500
H	3.62314200	3.34543800	-1.83070200
C	-2.83128200	-0.30912700	-0.04677300
C	-3.63730900	-0.06969900	1.07476600
C	-3.00433100	0.38602200	-1.26032500
C	-4.65881500	0.87531300	0.94085800
C	-4.04803200	1.30313700	-1.34594000
C	-4.87074300	1.54867100	-0.25178900
H	-5.30076400	1.08202600	1.79560600
H	-4.21077700	1.84966600	-2.27172800
H	-5.67568500	2.27539100	-0.33084600
C	-3.45141700	-0.78122100	2.39987000
H	-2.59359500	-1.46332700	2.30690300
C	-2.05228600	0.14393300	-2.41526000
H	-1.06048100	-0.05779500	-1.96013100
C	3.75555500	-0.14036400	2.30458300
H	3.16431900	-1.03585500	2.06829900
C	1.92914200	1.21813200	-2.26447100
H	0.99083900	0.82595900	-1.82355500
C	-0.08674700	1.05368300	1.00047500
H	-0.83688000	0.82208800	1.77837100
H	0.84998200	1.30990100	1.52258600
C	-0.55449900	2.26237100	0.20805200
H	-1.41949500	2.00072600	-0.42048200

H	0.24326100	2.57980100	-0.48442700
C	-0.95882300	3.46107800	1.05666100
H	-1.74604000	3.15488900	1.76651900
H	-0.10484400	3.78900300	1.67185200
Co	0.15466500	-0.60948700	0.02122200
C	-1.46897700	4.62126200	0.21482900
H	-0.69236400	4.91134800	-0.51114000
H	-2.32687000	4.27327500	-0.38415100
C	-1.87190800	5.82399500	1.04920600
H	-2.23773900	6.65173500	0.43112800
H	-2.66821000	5.56266000	1.75820500
H	-1.02357800	6.19895800	1.63623800
C	-3.13969200	0.19590500	3.53185300
H	-3.96708400	0.89818800	3.69352500
H	-2.98285300	-0.34649700	4.47216900
H	-2.23886500	0.78633400	3.32802300
C	-4.68473800	-1.61182200	2.75514300
H	-5.55212700	-0.96510700	2.93875100
H	-4.95913400	-2.30913300	1.95477100
H	-4.51022300	-2.19181500	3.66942800
C	-2.45107700	-1.08237300	-3.23413400
H	-3.44326600	-0.93292900	-3.67998200
H	-1.73837600	-1.25121100	-4.05113800
H	-2.49586300	-1.99944700	-2.63400700
C	-1.89421900	1.34594800	-3.33571800
H	-1.10513300	1.14870600	-4.07221100
H	-2.81212800	1.54077400	-3.90485100
H	-1.63351600	2.25981000	-2.78575700
H	5.10780300	2.16972800	2.00358300
H	5.07130200	3.76034400	0.11876100
C	3.10443100	0.52263100	3.51762800
H	2.06408400	0.80489300	3.31655700
H	3.11266200	-0.15656800	4.37899600
H	3.64633500	1.43187700	3.80678300
C	5.17315200	-0.59475700	2.64836900
H	5.69154800	-1.02975200	1.78504000
H	5.78408400	0.24152000	3.01065200
H	5.15111200	-1.34617000	3.44693000
C	1.58509700	2.47545400	-3.05158700
H	0.82036400	2.25261900	-3.80386300
H	1.20339000	3.28219400	-2.41371000
H	2.45927800	2.85610200	-3.59547800
C	2.47429900	0.16094700	-3.22521800
H	3.42247900	0.49672600	-3.66523500

H	2.65635000	-0.80736400	-2.74361600
H	1.76625500	-0.00758600	-4.04750600

1-iPr

Quartet:

1

Atom	x	y	z
C	0.98538000	2.59989200	-1.26869100
C	0.99555500	3.86761500	-1.84568900
C	-0.22452300	4.46884000	-2.13574700
C	-1.41290000	3.79389200	-1.87503300
C	-1.33817300	2.52756700	-1.30060000
N	-0.16163900	1.98066600	-0.98795800
H	-0.24773100	5.45903600	-2.58229800
H	1.93012800	4.37219800	-2.07216300
H	-2.37083300	4.24183700	-2.12201300
C	2.19440500	1.79724800	-0.95152000
C	-2.50122100	1.64076500	-1.02675900
N	-2.18604000	0.47836000	-0.57894700
N	1.95316400	0.63499200	-0.45449400
C	-3.87125500	2.12750800	-1.33927400
H	-3.92327500	2.46147800	-2.38335300
H	-4.61870200	1.34653800	-1.18255000
H	-4.12727600	2.99275800	-0.71409000
C	3.53203400	2.36533100	-1.27310500
H	3.74699500	3.23725000	-0.64085400
H	4.32571400	1.62863800	-1.12831600
H	3.55351500	2.71014600	-2.31402100
C	-3.13456100	-0.53209200	-0.26338800
C	-3.13487500	-1.67448100	-1.08203200
C	-3.89947000	-0.44229100	0.91457300
C	-3.99488000	-2.71689000	-0.74090700
C	-4.72818200	-1.52239100	1.21920800
C	-4.78900300	-2.63964300	0.39547100
H	-4.03048600	-3.61034200	-1.35989900
C	2.98707500	-0.26092800	-0.06156600
C	3.76543200	0.00947600	1.07904000
C	3.09810900	-1.47044300	-0.77539000
C	4.67777600	-0.96836600	1.48201300
C	4.03397900	-2.40384400	-0.33752400
C	4.81740800	-2.15851100	0.78399800
H	5.28417200	-0.79501600	2.36880000
H	4.14605400	-3.34314200	-0.87389900

H	5.53605800	-2.90268100	1.11845600
C	3.57667200	1.25437800	1.92546300
H	3.07514000	2.02110200	1.32162800
C	2.24415600	-1.71314700	-2.00132300
H	1.25999500	-1.25846400	-1.79123900
C	-3.74186200	0.73246800	1.86286700
H	-3.70774000	1.65633200	1.26688600
C	-2.21319300	-1.74540500	-2.28303100
H	-1.28454000	-1.21871600	-1.99225500
C	-0.08857400	-1.72692100	0.76725000
H	-1.13587700	-2.01166500	0.97388100
H	0.23127200	-2.39105800	-0.06003100
C	0.74751300	-2.04042900	2.00209200
H	0.33505800	-1.50474500	2.87308900
H	1.77526600	-1.66415500	1.88360500
C	0.80864600	-3.52955100	2.31154500
H	-0.19797600	-3.94929000	2.44071200
H	1.28661900	-4.07419700	1.48497100
H	1.38161600	-3.74365800	3.22281200
Co	-0.12384400	0.06808700	-0.08244300
C	4.89801400	1.85551000	2.39366500
H	4.72282400	2.82230300	2.88030200
H	5.40199400	1.21665400	3.12916300
H	5.59236600	2.01554600	1.55924000
C	2.66202900	0.95925600	3.11375200
H	2.54889000	1.84927300	3.74534200
H	1.66097300	0.64422000	2.78846900
H	3.07415500	0.15352800	3.73548500
C	2.84106700	-1.02099200	-3.22608000
H	3.82631400	-1.44670300	-3.45804100
H	2.20083000	-1.16186300	-4.10592800
H	2.97658300	0.05711100	-3.07588600
C	2.00816300	-3.18581800	-2.30340000
H	1.62913000	-3.73239600	-1.43053800
H	1.27552600	-3.28914600	-3.11280600
H	2.92629200	-3.68341700	-2.64175900
H	-5.44874000	-3.46471300	0.65309800
H	-5.33540800	-1.49610500	2.12062200
C	-1.81887000	-3.16607800	-2.66097600
H	-1.39989700	-3.71445300	-1.80817700
H	-2.67255300	-3.73702000	-3.04816000
H	-1.06608700	-3.14534500	-3.45854700
C	-2.81938300	-1.02811300	-3.48786700
H	-3.74677000	-1.52846800	-3.79703800

H	-3.06774900	0.01877700	-3.27278600
H	-2.13053000	-1.04343200	-4.34159600
C	-4.89315300	0.88840000	2.84742400
H	-4.77903800	1.82309500	3.40821600
H	-5.86724100	0.91341500	2.34541900
H	-4.90982800	0.07474300	3.58347600
C	-2.42217300	0.62404300	2.63110700
H	-2.30237600	1.46750600	3.32209600
H	-2.40046300	-0.30275800	3.21968400
H	-1.54672000	0.60313000	1.96535300

2

Atom	x	y	z
C	1.02004000	2.55956900	-1.18578600
C	0.99586800	3.79269300	-1.83346000
C	-0.23587700	4.32396200	-2.20053300
C	-1.40050500	3.61042400	-1.94295800
C	-1.29953100	2.38481100	-1.28668200
N	-0.11172900	1.90342700	-0.90852100
H	-0.28673000	5.28608000	-2.70211200
H	1.91551000	4.32606700	-2.05626800
H	-2.36564300	4.00181100	-2.25046200
C	2.25406100	1.81812600	-0.82308700
C	-2.44678100	1.49597400	-0.97626100
N	-2.16871700	0.45138800	-0.27508200
N	2.06765800	0.70680300	-0.19971100
C	-3.79143600	1.86592800	-1.49957300
H	-3.74848900	2.06677500	-2.57664500
H	-4.52512200	1.07833200	-1.31383700
H	-4.14435300	2.78630700	-1.01497200
C	3.56735300	2.38257000	-1.24052400
H	3.74643500	3.32830500	-0.71088900
H	4.39083600	1.69966200	-1.02093300
H	3.57188200	2.61442500	-2.31210800
C	-3.17614100	-0.50075100	0.06977500
C	-3.19272800	-1.72022100	-0.63828600
C	-4.05472000	-0.25125900	1.13926000
C	-4.10995100	-2.69175700	-0.24393300
C	-4.94050000	-1.26917400	1.50329100
C	-4.97099600	-2.47729600	0.82539100
H	-4.15000000	-3.63684700	-0.78128900
C	3.14435500	-0.20764300	0.02385400
C	3.92026500	-0.12484900	1.18966700
C	3.31582400	-1.24094200	-0.91862300

C	4.91549500	-1.08667100	1.37870800
C	4.32243100	-2.17517400	-0.67984900
C	5.11988200	-2.10115800	0.45561600
H	5.53476600	-1.04206500	2.27313300
H	4.48423300	-2.97931700	-1.39509700
H	5.89836000	-2.84176100	0.62222000
C	3.70077600	0.94594200	2.23806600
H	2.77789900	1.48819500	1.98086200
C	2.46656100	-1.32221100	-2.17438900
H	1.52750200	-0.77657500	-1.98053800
C	-4.10305300	1.06532900	1.89198300
H	-3.37169700	1.75090600	1.44005100
C	-2.29550200	-1.93899500	-1.84109700
H	-1.39599700	-1.31620300	-1.70425600
C	0.05975700	-1.75220100	0.60454800
H	-0.96774700	-2.12372000	0.75400700
H	0.35011600	-2.06967800	-0.41600800
C	0.97818000	-2.44401400	1.59961700
H	0.63335500	-2.25067500	2.62818600
H	1.99876200	-2.03237300	1.54261100
C	1.04871000	-3.95194700	1.39581500
H	0.05517900	-4.41124900	1.49021200
H	1.42973500	-4.19877100	0.39457900
H	1.70953100	-4.43635300	2.12591300
Co	-0.02757100	0.25035500	0.34033900
C	-0.07216600	0.36818300	2.44837600
H	0.90560900	0.00972500	2.76738200
H	-0.91861000	-0.24922200	2.74828100
C	-0.23236000	1.64656500	1.97953800
H	-1.22069800	2.09788000	1.89153800
H	0.61507500	2.32894900	1.91487100
C	4.84488500	1.95860800	2.25135200
H	4.66527700	2.74132700	2.99886900
H	5.79456300	1.47088000	2.50647800
H	4.97683400	2.44311800	1.27623200
C	3.51396000	0.34535900	3.63093500
H	3.16458600	1.10932400	4.33640400
H	2.79055600	-0.48028600	3.63091900
H	4.45754700	-0.05187300	4.02537600
C	3.17698600	-0.64744500	-3.34818000
H	4.11875900	-1.16652500	-3.57102700
H	2.55724300	-0.67696200	-4.25298100
H	3.42510500	0.40048100	-3.14075800
C	2.08409000	-2.74735100	-2.55973200

H	1.62746700	-3.29471100	-1.72544200
H	1.36319400	-2.72743900	-3.38684400
H	2.94929600	-3.32430600	-2.90920600
H	-5.67092700	-3.25351700	1.12492800
H	-5.62386300	-1.10197200	2.33434400
C	-1.83182200	-3.38195200	-2.00330800
H	-1.39733300	-3.77948900	-1.07805200
H	-2.65251000	-4.04350100	-2.30881500
H	-1.06917900	-3.44543900	-2.78954100
C	-2.99806300	-1.47035800	-3.11576000
H	-3.91186000	-2.05485000	-3.28710600
H	-3.29054000	-0.41382300	-3.06623800
H	-2.34910000	-1.60060800	-3.99081000
C	-5.47763700	1.72430700	1.77463800
H	-5.46494300	2.72262900	2.22899700
H	-5.80022200	1.82820600	0.73185300
H	-6.24550600	1.14052500	2.29727900
C	-3.73096300	0.89743800	3.36311000
H	-3.74217700	1.86652300	3.87715900
H	-4.44506500	0.24314700	3.87860000
H	-2.73398800	0.45984800	3.49068100

TS-2/3

Atom	x	y	z
C	-0.99925900	2.70808600	0.94258200
C	-0.95977600	4.00773100	1.44055100
C	0.27562600	4.56137500	1.76073900
C	1.43457900	3.80619100	1.60222500
C	1.32545800	2.51534500	1.09234200
N	0.12932800	2.00383100	0.76562600
H	0.33489200	5.57522800	2.14561400
H	-1.87407800	4.57752700	1.57862800
H	2.40227700	4.21961000	1.87200500
C	-2.22382300	1.94170600	0.63440300
C	2.45086200	1.57941400	0.88384100
N	2.14819600	0.46893400	0.29489700
N	-2.03217400	0.80591000	0.04433700
C	3.80507500	1.97402200	1.36207700
H	3.76306300	2.31661400	2.40244100
H	4.51544800	1.14744900	1.28907300
H	4.18716400	2.81249100	0.76390600
C	-3.53717300	2.48310600	1.08159000
H	-3.69893000	3.48301800	0.65949400
H	-4.36610200	1.83796100	0.78220200

H	-3.55183900	2.59389700	2.17378600
C	3.12748600	-0.54224600	0.05987100
C	3.07384300	-1.69507500	0.87174800
C	4.04545200	-0.42703100	-0.99981000
C	3.97284500	-2.72618400	0.60778300
C	4.91340300	-1.49837700	-1.22838000
C	4.88472500	-2.63521500	-0.43700800
H	3.95926300	-3.61929900	1.22851500
C	-3.09886300	-0.13497000	-0.09826900
C	-3.74935700	-0.26554500	-1.33777200
C	-3.39330200	-0.97988700	0.98927500
C	-4.72373300	-1.25544200	-1.46541500
C	-4.36516900	-1.96492000	0.80182300
C	-5.02703900	-2.10563500	-0.40969700
H	-5.24949400	-1.36633800	-2.41199000
H	-4.61021600	-2.63023100	1.62865100
H	-5.78383100	-2.87696800	-0.53097800
C	-3.43486000	0.66196900	-2.49236900
H	-2.43881000	1.08993300	-2.30847400
C	-2.71806100	-0.85066900	2.34354800
H	-1.95930300	-0.05535500	2.28455900
C	4.14184200	0.79545500	-1.89196200
H	3.39676500	1.53050300	-1.55432100
C	2.10821000	-1.78325500	2.03787700
H	1.21582700	-1.18952100	1.77505500
C	-0.06377700	-1.69870200	-0.74018900
H	0.95802800	-2.09317000	-0.66688000
H	-0.44381300	-1.54349200	0.29651700
C	-0.98209300	-2.67980100	-1.43374100
H	-0.61716800	-2.87025900	-2.45411600
H	-1.98658800	-2.24311800	-1.53851200
C	-1.08325400	-4.00594700	-0.69328000
H	-0.09849200	-4.47984000	-0.58669600
H	-1.50564500	-3.87680400	0.31207300
H	-1.73080200	-4.70816900	-1.23110800
Co	0.05462600	0.37539500	-0.35757300
C	0.14533200	-0.36601100	-2.33507800
H	-0.79992100	-0.68510600	-2.77377100
H	0.98938100	-0.98089000	-2.65459800
C	0.34863900	1.05009900	-2.23446700
H	1.35213800	1.45742700	-2.35996900
H	-0.45524000	1.72140400	-2.53923500
C	-4.43427600	1.81722300	-2.54235300
H	-4.20046800	2.50177600	-3.36710200

H	-5.45246200	1.43761500	-2.70102600
H	-4.44064900	2.39803300	-1.61144700
C	-3.39078100	-0.05061500	-3.84045600
H	-2.97662400	0.61636600	-4.60628100
H	-2.77358200	-0.95780800	-3.81124800
H	-4.39258800	-0.34365800	-4.17960300
C	-3.72723400	-0.44982400	3.41917300
H	-4.47179500	-1.24090700	3.57450700
H	-3.22517100	-0.27884600	4.37929100
H	-4.27260800	0.46329200	3.15096300
C	-1.99106400	-2.12901900	2.75552900
H	-1.23237100	-2.42535600	2.01979700
H	-1.48841900	-1.98542900	3.72109500
H	-2.68560800	-2.97123500	2.86951800
H	5.57388000	-3.45343400	-0.63150500
H	5.62944200	-1.43089800	-2.04609600
C	3.82807300	0.45840300	-3.34857400
H	2.83957300	-0.00383900	-3.46103400
H	3.84741400	1.36534700	-3.96575900
H	4.56870900	-0.23653200	-3.76388900
C	5.52026800	1.44940800	-1.79444200
H	5.54570100	2.38242200	-2.37063200
H	5.79802900	1.67984200	-0.75889800
H	6.29849100	0.79283300	-2.20356600
C	2.71974300	-1.16025200	3.29268100
H	3.00035000	-0.11049100	3.14219600
H	2.01409100	-1.20279700	4.13214500
H	3.62635900	-1.70543100	3.58712800
C	1.64789400	-3.20466700	2.33683200
H	0.85077400	-3.19438000	3.08978500
H	1.26382800	-3.71202200	1.44268600
H	2.46059700	-3.81680800	2.74819800

3

Atom	x	y	z
C	-0.52658700	-3.24091900	0.16464500
C	-0.33542200	-4.61923900	0.12408500
C	0.96832500	-5.09677900	0.01995000
C	2.03749000	-4.21130400	-0.07972300
C	1.76765000	-2.84651400	-0.01450800
N	0.51929200	-2.41335200	0.16347800
H	1.15034500	-6.16719500	-0.01271100
H	-1.17639700	-5.30589200	0.15942900
H	3.05033600	-4.58110500	-0.20753000

C	-1.83788100	-2.53836900	0.13016500
C	2.76190700	-1.74939200	-0.14913900
N	2.26222000	-0.55821600	-0.16639900
N	-1.76030800	-1.25826900	-0.00889300
C	4.19582600	-2.10589200	-0.31610200
H	4.59508900	-2.58281700	0.58851000
H	4.30011300	-2.82960400	-1.13441200
H	4.80215500	-1.22749100	-0.54732300
C	-3.08774800	-3.34153400	0.15012700
H	-3.03114700	-4.14163200	-0.59897900
H	-3.23181200	-3.82532300	1.12581900
H	-3.96100700	-2.72502200	-0.07249300
C	3.06409000	0.61534600	-0.15971300
C	2.86558600	1.52786100	-1.21686400
C	3.90800600	0.91427800	0.92873500
C	3.59828400	2.71069800	-1.21049200
C	4.60456000	2.12427500	0.89070500
C	4.47088700	3.00507600	-0.16991900
H	3.47822700	3.42326600	-2.02215000
C	-2.90118100	-0.41286900	-0.11757400
C	-3.73653100	-0.14449900	0.98192700
C	-3.06348300	0.24285500	-1.35711900
C	-4.76782600	0.78006400	0.79404000
C	-4.11351500	1.14613000	-1.48923700
C	-4.96180500	1.41524700	-0.42135400
H	-5.42901100	1.00784200	1.62834800
H	-4.26609300	1.65997700	-2.43495400
H	-5.77267100	2.12990200	-0.53889100
C	-3.56801300	-0.78191000	2.34882800
H	-2.66425500	-1.40858100	2.33569100
C	-2.12103200	-0.05628000	-2.50505900
H	-1.11226500	-0.18263000	-2.06958400
C	4.03215100	0.04595400	2.16720700
H	3.48010600	-0.88920500	2.00577300
C	1.89125600	1.19812300	-2.32590100
H	1.02867300	0.70194300	-1.84323600
C	-0.13261100	1.22948000	1.27834800
H	-0.93323000	1.01410400	2.00372700
H	0.74152600	1.56597700	1.85407000
C	-0.58188100	2.31619200	0.30544100
H	-1.29030100	1.91518900	-0.44343400
H	0.28799000	2.67463800	-0.27076800
C	-1.26105500	3.51251400	0.96185400
H	-2.13604500	3.15841700	1.53327600

H	-0.57791800	3.96482700	1.69907200
Co	0.17500100	-0.40942500	0.21452000
C	-1.70861100	4.56098400	-0.04486800
H	-0.83664300	4.90044600	-0.62624400
H	-2.39044100	4.08762500	-0.77017300
C	-2.39087700	5.75107000	0.60514000
H	-2.71056300	6.49637400	-0.13183300
H	-3.28069800	5.43713900	1.16604200
H	-1.71965300	6.25321900	1.31362500
C	-3.37847600	0.26348000	3.44770500
H	-4.27451300	0.88573300	3.56400100
H	-3.19693100	-0.22817600	4.41097900
H	-2.53507700	0.93282200	3.24469100
C	-4.76327400	-1.66966300	2.70027800
H	-5.67128200	-1.06500800	2.82095700
H	-4.97458800	-2.42239700	1.93370600
H	-4.59057300	-2.18964900	3.65036400
C	-2.49408100	-1.36361000	-3.20450800
H	-3.50112800	-1.28723200	-3.63520500
H	-1.79561300	-1.57816900	-4.02299200
H	-2.48856000	-2.22579800	-2.52706300
C	-2.03468200	1.06083800	-3.53432300
H	-1.25568300	0.82609500	-4.27048600
H	-2.97283100	1.17162200	-4.09304900
H	-1.79229500	2.02952300	-3.07884900
H	5.25823100	2.38147600	1.72236200
H	5.03267900	3.93576700	-0.17851200
C	3.39146600	0.73039200	3.37369300
H	2.33105000	0.94774000	3.19877000
H	3.46467800	0.09076400	4.26182600
H	3.89325600	1.67818100	3.60446200
C	5.48335900	-0.31771000	2.47530300
H	5.99663700	-0.75630100	1.61144200
H	6.05799900	0.56429300	2.78389700
H	5.53010000	-1.03703900	3.30171200
C	1.37507200	2.41984700	-3.07158400
H	0.60660500	2.12402000	-3.79383200
H	0.93615000	3.16429500	-2.39499400
H	2.17328300	2.90804200	-3.64541200
C	2.49253900	0.19943600	-3.31473200
H	3.34039800	0.65294200	-3.84479800
H	2.85900000	-0.70869600	-2.81982000
H	1.74924700	-0.10033100	-4.06526200

CHPh2

Doublet:

1

Atom	x	y	z
C	-0.02164900	0.16397600	2.86407000
C	-0.03133000	0.30687000	4.24767300
C	1.10638600	-0.07815100	4.95463200
C	2.22122000	-0.57940700	4.28405500
C	2.15311600	-0.70126300	2.89983000
N	1.04626500	-0.34220200	2.24194800
H	1.12976700	0.02492600	6.03558300
H	-0.89625700	0.71922300	4.75955200
H	3.11736100	-0.86194400	4.82927900
C	-1.05785600	0.58048200	1.89866200
C	3.19852800	-1.17014500	1.97118400
N	2.84338500	-1.18503400	0.71846200
N	-0.77887600	0.29863900	0.65585200
C	4.53513500	-1.51151100	2.52112900
H	4.96661900	-0.62523700	3.00587000
H	4.44129300	-2.28022600	3.29902000
H	5.22781100	-1.86176500	1.75397700
C	-2.23602500	1.31690900	2.41683700
H	-2.79752000	0.67602500	3.11039400
H	-1.88649400	2.19266900	2.98065400
H	-2.90926200	1.65235500	1.62724300
C	3.80841100	-1.56277100	-0.27925800
C	3.84860000	-2.89144800	-0.73472400
C	4.65040300	-0.56204900	-0.80333500
C	4.71876100	-3.18802500	-1.78609900
C	5.49241500	-0.91408600	-1.85752300
C	5.51851400	-2.20988800	-2.35653800
H	4.77267900	-4.20841200	-2.15928900
H	6.14957000	-0.16401400	-2.29123600
H	6.18026000	-2.46090900	-3.18194500
C	-1.67948300	0.77066800	-0.35529200
C	-1.37421200	1.99708700	-0.96608900
C	-2.79820500	0.01316100	-0.72637300
C	-2.27134600	2.51320000	-1.89747700
C	-3.67913100	0.57418700	-1.65410100
C	-3.43289900	1.81946300	-2.21743700
H	-2.04412500	3.46027200	-2.38440500
C	-0.07397800	2.69318100	-0.60225400
H	0.64565200	1.86916700	-0.44980100

C	-3.01666900	-1.37552800	-0.14138700
H	-2.00889000	-1.79035900	0.02860700
C	4.63981600	0.85472600	-0.25545100
H	4.46025100	0.79651800	0.83064600
C	3.06020100	-4.00376900	-0.06933200
H	2.19408000	-3.55094800	0.43834500
C	0.89253000	-0.81892100	-1.54633700
H	0.20740600	-0.11907800	-2.05521000
H	1.87976400	-0.72819500	-2.03235300
C	0.37154600	-2.23647800	-1.74007300
H	-0.66223900	-2.32181300	-1.36982700
H	0.95703400	-2.94538100	-1.13569800
C	0.40326800	-2.69655700	-3.19178300
H	-0.17552000	-2.01471500	-3.83041700
H	1.43194800	-2.70094600	-3.57834400
H	-0.01208200	-3.70539700	-3.31818600
Co	0.99952600	-0.51086300	0.35626700
C	3.91297300	-4.70012200	0.99308000
H	4.25663200	-4.01529200	1.77602900
H	3.34858600	-5.50794900	1.47523300
H	4.80432000	-5.14586600	0.53180700
C	2.53783300	-5.05293500	-1.04823500
H	3.34398500	-5.70430000	-1.40818100
H	1.80912600	-5.70158400	-0.54775500
H	2.05141600	-4.60903900	-1.92391200
C	5.95925200	1.59044300	-0.44928100
H	6.13802600	1.83512800	-1.50387500
H	5.93972800	2.54051000	0.09693600
H	6.81488700	1.00845500	-0.08710800
C	3.49587700	1.66124900	-0.86361800
H	3.48678400	2.69241000	-0.48654000
H	3.58453900	1.70276000	-1.95749100
H	2.52651600	1.20009800	-0.63398500
C	0.47691600	3.53768800	-1.73985400
C	0.92186100	2.88546000	-2.89617600
C	0.55753100	4.92850600	-1.68611800
C	1.43080100	3.60370400	-3.96938900
H	0.86608900	1.79772800	-2.94914500
C	1.06535900	5.65145900	-2.76478900
H	0.22805800	5.45880700	-0.79488000
C	1.50303400	4.99411100	-3.90733000
H	1.77210100	3.07733900	-4.85811500
H	1.11944900	6.73620200	-2.70468600
H	1.90075300	5.55964000	-4.74678200

C	-0.15693900	3.43314800	0.71794400
C	0.90311100	3.35539800	1.62567600
C	-1.26303600	4.21912900	1.04791200
C	0.85137700	4.02653200	2.84378500
H	1.78560400	2.76549300	1.36525000
C	-1.31284200	4.90383600	2.25845300
H	-2.09615600	4.28850700	0.34830000
C	-0.25997800	4.80149500	3.16469900
H	1.68438800	3.95241400	3.54008300
H	-2.17993700	5.51528900	2.49814600
H	-0.30116000	5.33270900	4.11276700
C	-3.67588600	-1.33293000	1.22230200
C	-4.86310300	-0.62860600	1.43446200
C	-3.10677900	-2.02431500	2.29324400
C	-5.45814300	-0.60314200	2.69086200
H	-5.32139500	-0.09177600	0.60409600
C	-3.69349800	-1.99429700	3.55640300
H	-2.18961600	-2.59415900	2.13181100
C	-4.87104800	-1.28027200	3.75844800
H	-6.38449000	-0.05273400	2.83927800
H	-3.23400300	-2.53652400	4.38031400
H	-5.33580300	-1.25753500	4.74138500
C	-3.69032300	-2.32979700	-1.12036700
C	-3.17879400	-2.43831400	-2.41993200
C	-4.75505000	-3.15482500	-0.75848700
C	-3.70940200	-3.34467300	-3.32710300
H	-2.35477100	-1.79386000	-2.72531700
C	-5.29414600	-4.06095900	-1.67044000
H	-5.17062000	-3.09909100	0.24537300
C	-4.77473300	-4.16173200	-2.95445400
H	-3.28915300	-3.41228700	-4.32866500
H	-6.12740800	-4.69174400	-1.36837800
H	-5.19591000	-4.87108800	-3.66311000
H	-4.55609800	0.00503000	-1.95749900
H	-4.13445000	2.23615000	-2.93590200

2

Atom	x	y	z
C	1.99839900	-0.78479100	2.98885500
C	2.04281500	-0.59073300	4.36661800
C	0.91686600	-0.06952500	4.99827700
C	-0.20517200	0.27780800	4.25136900
C	-0.18183100	0.05530600	2.87713400
N	0.88690500	-0.50185500	2.29488700

H	0.92348200	0.09100800	6.07239100
H	2.93684900	-0.83187600	4.93503800
H	-1.07221900	0.72577800	4.72796900
C	3.10259900	-1.19488500	2.10793200
C	-1.19749800	0.46556900	1.89305400
N	-0.89637600	0.18864800	0.65679500
N	2.80684000	-1.19943200	0.84094400
C	-2.39542300	1.19380700	2.38522800
H	-2.08051800	2.06462700	2.97497300
H	-3.04387900	1.53270700	1.57621500
H	-2.97847900	0.53686300	3.04476500
C	4.43219700	-1.48795700	2.70675400
H	4.38086500	-2.42680400	3.27490700
H	5.21314100	-1.58019400	1.94966400
H	4.72051700	-0.70338600	3.41618100
C	-1.74723300	0.71676300	-0.36952500
C	-1.38118400	1.95210500	-0.93613700
C	-2.87595700	0.01104400	-0.80773700
C	-2.22518800	2.51248400	-1.89296600
C	-3.67879900	0.60041400	-1.78733600
C	-3.37379600	1.84925300	-2.30783800
H	-1.96293000	3.47217200	-2.33382800
C	3.86515200	-1.35236000	-0.11559700
C	4.33174200	-2.62136800	-0.49145800
C	4.36748100	-0.16591900	-0.68718900
C	5.33787900	-2.68142100	-1.45926300
C	5.36874400	-0.28522700	-1.64966600
C	5.85211300	-1.52997100	-2.03504800
H	5.71762200	-3.65360100	-1.77016800
H	5.77828400	0.61241500	-2.10777300
H	6.63241000	-1.60024300	-2.78913900
C	3.77273400	-3.90890200	0.08118500
H	2.92880400	-3.65059500	0.73937100
C	3.87482100	1.20128100	-0.24650500
H	2.82031300	1.08845600	0.05852900
C	-3.23782400	-1.34449300	-0.22389500
H	-2.30155600	-1.78759400	0.14570100
C	-0.09236400	2.63398900	-0.50194200
H	0.63300000	1.82047000	-0.32861100
C	1.00465500	-0.57980600	-1.52716300
H	0.01751000	-0.23324500	-1.87599800
H	1.65852500	0.31438100	-1.49971800
C	1.56635200	-1.53568400	-2.56549500
H	0.85702000	-2.35752700	-2.74902900

H	2.49378900	-2.00605000	-2.20890600
C	1.86105700	-0.84325800	-3.89074000
H	0.95811500	-0.37759500	-4.30904200
H	2.61617100	-0.05471600	-3.76263100
H	2.24627700	-1.54731100	-4.63865000
Co	0.85675800	-0.85804700	0.41951300
C	0.18935700	-2.81726700	-0.19177900
H	1.04497200	-3.29451400	-0.66292900
H	-0.67549700	-2.66788400	-0.83758300
C	0.08342900	-2.77496000	1.16614400
H	-0.86341100	-2.55757800	1.66090000
H	0.86195000	-3.19902000	1.80030300
H	-4.55127400	0.05742200	-2.14716000
H	-4.01973400	2.29810900	-3.05819400
C	-4.14412000	-1.23695300	0.99050400
C	-5.21691300	-0.34470000	1.04149900
C	-3.92310000	-2.07755100	2.08413500
C	-6.03647500	-0.28327400	2.16394900
H	-5.40909900	0.31745100	0.19827100
C	-4.73866100	-2.01751300	3.21069000
H	-3.10841400	-2.80270900	2.04095500
C	-5.79677500	-1.11406800	3.25513300
H	-6.86744700	0.41828900	2.18636200
H	-4.55043300	-2.68149000	4.05162100
H	-6.43701200	-1.06418600	4.13275400
C	-3.75874400	-2.30430700	-1.28723400
C	-4.97425300	-2.97616200	-1.16913100
C	-2.96940500	-2.54451600	-2.41851900
C	-5.39021400	-3.86809000	-2.15670400
H	-5.60363600	-2.80848800	-0.29768300
C	-3.37938000	-3.43606700	-3.40025600
H	-2.02744300	-2.00550200	-2.53538600
C	-4.59651800	-4.10258400	-3.27179100
H	-6.34331800	-4.38093900	-2.04744500
H	-2.75038600	-3.60959500	-4.27050700
H	-4.92294600	-4.79947700	-4.04013900
C	0.52009100	3.50283000	-1.59334200
C	0.79925700	2.91963100	-2.83572200
C	0.87646300	4.83555300	-1.39058000
C	1.42304200	3.64255800	-3.84249900
H	0.52729200	1.87819500	-3.00507500
C	1.50212500	5.56475100	-2.40191900
H	0.67467900	5.31429400	-0.43443200
C	1.78044300	4.97261800	-3.62705100

H	1.63535400	3.16342100	-4.79651500
H	1.77221100	6.60340100	-2.22397200
H	2.27121200	5.54207700	-4.41294500
C	-0.22828000	3.34772000	0.82736600
C	0.78021400	3.21861200	1.78578700
C	-1.31853100	4.17292500	1.10895400
C	0.69277500	3.87727000	3.00884900
H	1.64573800	2.58906300	1.56168100
C	-1.40582800	4.84084000	2.32639900
H	-2.10790900	4.28720300	0.36583600
C	-0.40439000	4.68915500	3.28346000
H	1.48352500	3.75737700	3.74708200
H	-2.26050900	5.48171100	2.53116700
H	-0.47587100	5.20919900	4.23592800
C	4.81243800	-4.65562100	0.91583800
H	4.38177800	-5.57031000	1.34154600
H	5.66938800	-4.95415900	0.29853000
H	5.20025900	-4.04785500	1.74087100
C	3.24268700	-4.82853100	-1.01949100
H	2.69429700	-5.67285200	-0.58391000
H	2.57346500	-4.30392900	-1.71277300
H	4.06396800	-5.24640000	-1.61483600
C	4.65887400	1.71533300	0.96266700
H	5.73461500	1.73233900	0.74289200
H	4.35638900	2.74100000	1.21022600
H	4.51350600	1.10101300	1.85973200
C	3.92215500	2.24634300	-1.35527300
H	3.46127700	1.88914300	-2.28418000
H	3.38377300	3.15167100	-1.04418900
H	4.95305700	2.54874100	-1.58157000

TS-2/3

Atom	x	y	z
C	1.58485600	-0.65191400	3.07979200
C	1.55169000	-0.35696600	4.43982200
C	0.42803000	0.27437800	4.96406700
C	-0.62134300	0.63013200	4.12125300
C	-0.53592500	0.31026400	2.77042600
N	0.53057100	-0.35883600	2.28974900
H	0.38214000	0.51384700	6.02231700
H	2.39480000	-0.60826100	5.07720700
H	-1.48569400	1.16532200	4.50393000
C	2.71690800	-1.18559200	2.32179500
C	-1.46070100	0.72771500	1.71345800

N	-1.09238600	0.37929100	0.51229800
N	2.51844700	-1.22519000	1.03414200
C	-2.63267700	1.56622000	2.08128200
H	-2.28558500	2.46287200	2.61179700
H	-3.20871200	1.88158600	1.20981600
H	-3.29866600	1.01443600	2.75742400
C	3.97602300	-1.54207000	3.03180100
H	3.81824300	-2.42505200	3.66527300
H	4.78869200	-1.75373500	2.33313100
H	4.29211200	-0.72568200	3.69277300
C	-1.82744500	0.89095700	-0.60197700
C	-1.32585100	2.05030900	-1.22318300
C	-2.97019000	0.23814300	-1.08898100
C	-2.06138400	2.61532900	-2.26340200
C	-3.66300600	0.82654500	-2.14923300
C	-3.23408500	2.02014900	-2.71224400
H	-1.69198900	3.51965500	-2.74297500
C	3.59295600	-1.53503900	0.14112000
C	3.98683000	-2.85895800	-0.12235200
C	4.18899300	-0.43780700	-0.51914800
C	5.00803700	-3.06132400	-1.05522700
C	5.20295000	-0.69830400	-1.43900100
C	5.61219800	-1.99881800	-1.70848200
H	5.33002500	-4.07865300	-1.27202000
H	5.68237900	0.12996900	-1.95577900
H	6.40425900	-2.18139300	-2.43076800
C	3.35464200	-4.06587400	0.54314300
H	2.50034300	-3.71780200	1.14225900
C	3.77436500	0.98759100	-0.20350700
H	2.69325500	0.97365700	0.02241900
C	-3.44443300	-1.06822500	-0.47556700
H	-2.55371600	-1.55329500	-0.04893200
C	0.00334800	2.63123600	-0.76481700
H	0.63843600	1.75736000	-0.53293400
C	0.64701200	-1.06297100	-1.52952000
H	-0.28920100	-0.65286400	-1.92966200
H	1.28913400	-0.20147400	-1.22793700
C	1.40710600	-1.80055000	-2.61650800
H	0.79813700	-2.63535100	-2.99499200
H	2.32160700	-2.24222400	-2.19446300
C	1.77599400	-0.88267800	-3.77164000
H	0.88397900	-0.43773300	-4.23336000
H	2.42773900	-0.06195900	-3.44067100
H	2.31247100	-1.43284300	-4.55240900

Co	0.57632300	-0.84873500	0.51799100
C	0.03505200	-2.59301900	-0.51212700
H	0.84095500	-3.26044700	-0.81199800
H	-0.83529500	-2.68240100	-1.16741300
C	-0.23009000	-2.57737600	0.90372200
H	-1.26575000	-2.51553800	1.24486300
H	0.39756000	-3.20291400	1.54302000
H	-4.54608100	0.32556800	-2.54266700
H	-3.79641300	2.47197900	-3.52551000
C	-4.39367900	-0.85389900	0.68961800
C	-5.43606500	0.07390100	0.63560200
C	-4.25189600	-1.63280700	1.83960900
C	-6.30649400	0.22611400	1.71001800
H	-5.56481400	0.68852600	-0.25453700
C	-5.11783900	-1.48130700	2.91891100
H	-3.45801000	-2.37929600	1.88129700
C	-6.14761600	-0.54705700	2.85733900
H	-7.11366600	0.95294800	1.65095300
H	-4.99165800	-2.09833500	3.80589400
H	-6.82858500	-0.42625000	3.69656400
C	-3.98088600	-2.03921500	-1.52240600
C	-5.22834300	-2.65121100	-1.41096500
C	-3.17713000	-2.36441800	-2.62322300
C	-5.66081800	-3.56587300	-2.36993600
H	-5.87272400	-2.41975000	-0.56545600
C	-3.60407600	-3.27819900	-3.57723300
H	-2.20756000	-1.87597100	-2.74282400
C	-4.85253100	-3.88451900	-3.45315800
H	-6.63861200	-4.03041400	-2.26337600
H	-2.96323900	-3.51567600	-4.42363900
H	-5.19136200	-4.59883100	-4.19974600
C	0.73212200	3.38249500	-1.86989500
C	1.02369900	2.69711400	-3.05511400
C	1.17372700	4.69795900	-1.73858900
C	1.73834900	3.30250100	-4.07849600
H	0.68288500	1.66776000	-3.17138800
C	1.89291300	5.30985500	-2.76569300
H	0.96691400	5.25302500	-0.82585900
C	2.17963400	4.61703200	-3.93503100
H	1.95722600	2.74437300	-4.98723400
H	2.23061200	6.33675800	-2.64446200
H	2.74216800	5.09663400	-4.73258200
C	-0.10209000	3.41064100	0.53003300
C	0.84554600	3.20849900	1.53642900

C	-1.10301600	4.36282400	0.73299300
C	0.78914900	3.92728500	2.72681300
H	1.63667600	2.47024000	1.38217300
C	-1.15729900	5.09128400	1.91787800
H	-1.84557200	4.53292000	-0.04686300
C	-0.21578400	4.87106600	2.92099800
H	1.53198700	3.74958100	3.50230100
H	-1.93982300	5.83350500	2.05945400
H	-0.26142900	5.43906700	3.84728500
C	4.33660000	-4.76853300	1.48131800
H	3.85243600	-5.61710400	1.98013400
H	5.19403000	-5.16298600	0.92127600
H	4.73056000	-4.10046400	2.25503500
C	2.83475900	-5.07610700	-0.48137200
H	2.21195700	-5.83399800	0.00912800
H	2.24028700	-4.60797400	-1.27557700
H	3.66246500	-5.60477700	-0.97087600
C	4.49502000	1.51053600	1.04047300
H	5.58268200	1.46849700	0.89477300
H	4.22564900	2.55725500	1.23226400
H	4.25809500	0.93284900	1.94230400
C	3.99257300	1.95900500	-1.35613700
H	3.57784500	1.58651600	-2.30099700
H	3.50687300	2.91871700	-1.13619000
H	5.05907500	2.16632400	-1.51333400

3

Atom	x	y	z
C	1.07029800	-1.09801100	3.51099300
C	0.67475400	-1.30682500	4.82866300
C	-0.59937300	-0.88397400	5.20737000
C	-1.45543300	-0.28349900	4.28425500
C	-0.99546700	-0.10982000	2.98366900
N	0.24160000	-0.49368900	2.64903800
H	-0.93342900	-1.03684300	6.22962000
H	1.33316100	-1.79519200	5.54167100
H	-2.45798000	0.02617700	4.56638700
C	2.33160100	-1.47600000	2.84786900
C	-1.71341500	0.44276300	1.81805700
N	-1.07386800	0.29520700	0.69090900
N	2.34337800	-1.25766100	1.56267800
C	-3.02124100	1.10043700	2.03374400
H	-3.73476900	0.38138300	2.45792000
H	-2.89600300	1.91298300	2.76228100

H	-3.43919800	1.50791200	1.11263200
C	3.44455400	-2.03735600	3.65277900
H	3.56539600	-1.47083400	4.58354200
H	3.21551800	-3.07431100	3.93585400
H	4.38972000	-2.03010900	3.10522000
C	-1.61623000	0.80554900	-0.53028400
C	-1.17972000	2.06783200	-0.96727000
C	-2.45102500	-0.01047400	-1.31126700
C	-1.67819900	2.54804400	-2.17720400
C	-2.91869400	0.50950500	-2.51860300
C	-2.55496300	1.78287600	-2.93671500
H	-1.35031200	3.52079300	-2.53921200
C	3.53459900	-1.49444900	0.80006300
C	3.87539900	-2.78665100	0.37264800
C	4.28256900	-0.35850100	0.43097600
C	5.02328500	-2.92249900	-0.41394600
C	5.42250300	-0.55302800	-0.34573000
C	5.79429700	-1.82575000	-0.76400700
H	5.31241700	-3.91445300	-0.75742800
H	6.02440900	0.30305100	-0.64092600
H	6.68497300	-1.95826900	-1.37328700
C	3.06382300	-4.02138900	0.71181300
H	2.18221300	-3.70964000	1.29183700
C	3.84378000	1.02727100	0.86628600
H	2.73833500	1.04539200	0.77808300
C	-2.77677000	-1.42879700	-0.85602000
H	-1.84831300	-1.81540900	-0.40508000
C	-0.14152500	2.82689400	-0.14721500
H	0.60659700	2.06322900	0.14776900
C	0.95297800	-1.08639600	-1.01096700
H	1.44025100	-2.07320400	-0.92198000
H	-0.03219500	-1.24886000	-1.47090600
C	1.76916300	-0.22029300	-1.95521900
H	2.66265800	0.18492800	-1.44984000
H	1.16187200	0.64720400	-2.26083500
C	2.24959000	-0.93348100	-3.21249200
H	2.87533500	-1.79579600	-2.92177000
H	1.38486900	-1.35114100	-3.75527100
Co	0.69845100	-0.49945700	0.82993900
C	3.04355200	-0.01557400	-4.13021500
H	2.41907500	0.84956100	-4.40543500
H	3.89722600	0.39812700	-3.56708600
C	3.54265400	-0.71378000	-5.38246500
H	4.12187200	-0.04203800	-6.02615000

H	4.18623100	-1.56635700	-5.12911400
H	2.70607400	-1.10196300	-5.97758200
H	-3.55684200	-0.10770600	-3.14798800
H	-2.93149700	2.16989700	-3.88040900
C	-3.82940600	-1.47573100	0.23502700
C	-4.99849300	-0.71477400	0.16417300
C	-3.64563100	-2.31903800	1.33339800
C	-5.96473000	-0.80228300	1.16138900
H	-5.14395800	-0.03466700	-0.67533400
C	-4.60209500	-2.39848600	2.34154900
H	-2.73827600	-2.92309400	1.39007500
C	-5.76759500	-1.64072100	2.25587900
H	-6.87259800	-0.20767000	1.08850300
H	-4.44049400	-3.05964900	3.19038100
H	-6.52182900	-1.70711600	3.03660500
C	-3.09662300	-2.36410800	-2.01583500
C	-2.04592600	-3.00221300	-2.68139000
C	-4.40028300	-2.59551200	-2.45924900
C	-2.28773900	-3.83957600	-3.76421300
H	-1.02178000	-2.84300000	-2.34258800
C	-4.64503000	-3.43080700	-3.54563400
H	-5.23887000	-2.12711300	-1.94734600
C	-3.59076300	-4.05539000	-4.20244200
H	-1.45478100	-4.32860600	-4.26465200
H	-5.66840700	-3.59740200	-3.87472200
H	-3.78380400	-4.71129900	-5.04811200
C	-0.69604800	3.39449100	1.14512600
C	0.03876100	3.27242900	2.32670500
C	-1.91858800	4.06887800	1.18635900
C	-0.43522400	3.80139900	3.52314800
H	0.99895800	2.75134000	2.30258600
C	-2.38878700	4.61576700	2.37673300
H	-2.51120100	4.15628400	0.27532600
C	-1.65223500	4.47821900	3.55040300
H	0.14944700	3.69238100	4.43405700
H	-3.33846600	5.14600100	2.38863800
H	-2.02280900	4.90022000	4.48161700
C	0.60847200	3.86967000	-0.96414200
C	0.22698300	5.21190100	-1.00976600
C	1.70298400	3.46554300	-1.73187800
C	0.91960100	6.12010000	-1.80630600
H	-0.61333800	5.55950600	-0.41216900
C	2.40027400	4.36994000	-2.52391100
H	2.01658300	2.42326200	-1.70367600

C	2.00803100	5.70429400	-2.56560400
H	0.60721100	7.16179400	-1.82630000
H	3.25490000	4.02853900	-3.10561700
H	2.55030600	6.41724800	-3.18216700
C	2.55984500	-4.73043800	-0.54532100
H	3.39301600	-5.11463100	-1.14695400
H	1.93131300	-5.58749400	-0.27442000
H	1.96904600	-4.06545100	-1.18706700
C	3.87527600	-4.99906300	1.56286100
H	4.72962200	-5.39101200	0.99667600
H	4.27496800	-4.53337600	2.47196000
H	3.26036700	-5.85707000	1.86076800
C	4.20987600	1.31441600	2.32348200
H	5.28863700	1.17817800	2.47625200
H	3.96841900	2.35180700	2.58616900
H	3.68893200	0.66173800	3.03441800
C	4.38908900	2.14430900	-0.01313700
H	3.89749800	3.09144100	0.24015300
H	5.46633900	2.28553700	0.14409200
H	4.22270000	1.95531200	-1.08133300

Quartet:

1

Atom	x	y	z
C	-0.00184300	0.17396100	2.83835700
C	-0.04087300	0.25638200	4.22778500
C	1.08846800	-0.13211500	4.94038300
C	2.21811300	-0.58276800	4.26410900
C	2.17409200	-0.64743300	2.87416100
N	1.08406200	-0.26955900	2.20279500
H	1.09123900	-0.07859300	6.02532000
H	-0.92767900	0.61710000	4.74097000
H	3.10775900	-0.88042400	4.81100700
C	-1.09291100	0.60934600	1.92604700
C	3.28660400	-1.11237300	2.00271900
N	2.97590900	-1.25974700	0.76354400
N	-0.90477800	0.31987100	0.68457700
C	4.62556600	-1.33422300	2.61337100
H	5.00520300	-0.39703700	3.04101900
H	4.55950400	-2.05452900	3.43812600
H	5.34755700	-1.70428200	1.88199200
C	-2.23738400	1.35287600	2.50979400
H	-2.77596200	0.70585600	3.21603600

H	-1.86844300	2.22474500	3.06552800
H	-2.93896700	1.69096400	1.74544400
C	3.93394500	-1.63056300	-0.22844600
C	3.92044300	-2.95146700	-0.71247800
C	4.77168900	-0.63857300	-0.77370500
C	4.75491400	-3.25801700	-1.78688700
C	5.58254400	-1.00098900	-1.85019800
C	5.57073200	-2.29207500	-2.35961400
H	4.76764200	-4.27189900	-2.18009700
H	6.23804800	-0.25797100	-2.29909600
H	6.20766100	-2.54912300	-3.20255300
C	-1.79529900	0.81482200	-0.31245900
C	-1.46990800	2.03841000	-0.91989900
C	-2.89693400	0.05179400	-0.71743500
C	-2.35027300	2.55491600	-1.86736800
C	-3.76121100	0.61146200	-1.66024700
C	-3.50596100	1.86131600	-2.21081400
H	-2.11236700	3.49996800	-2.35312200
C	-0.15802000	2.71583500	-0.55343700
H	0.55288700	1.88138200	-0.39937500
C	-3.08590200	-1.34699200	-0.14963200
H	-2.06603700	-1.74650900	-0.00877200
C	4.75713500	0.79030400	-0.26137500
H	4.54479400	0.76723500	0.81865700
C	3.08874300	-4.02429900	-0.03905800
H	2.17953600	-3.54135000	0.35619000
C	0.88398700	-0.85947000	-1.82700900
H	0.15865000	-0.19790000	-2.33000600
H	1.85629300	-0.70686700	-2.32564200
C	0.44390000	-2.31331800	-1.99480900
H	-0.57035100	-2.45731800	-1.58494600
H	1.09048000	-2.98065500	-1.40473100
C	0.45975200	-2.79030100	-3.44036700
H	-0.15405000	-2.13771600	-4.07666900
H	1.48324700	-2.76573000	-3.84052000
H	0.07818800	-3.81493100	-3.54500400
Co	0.99339100	-0.52394200	0.11655200
C	3.84917900	-4.62202900	1.14646300
H	4.11299900	-3.86960700	1.89857200
H	3.25292800	-5.39894000	1.64083300
H	4.78396100	-5.08494600	0.80346000
C	2.65815900	-5.14710700	-0.97612200
H	3.50300900	-5.79610100	-1.23973500
H	1.91321500	-5.78192400	-0.48242600

H	2.21928700	-4.77261700	-1.90862300
C	6.08891100	1.50909600	-0.43571600
H	6.29912800	1.72914700	-1.48979500
H	6.06607000	2.47106700	0.08919700
H	6.92712500	0.92471400	-0.03817100
C	3.63799800	1.58630700	-0.93144200
H	3.62801800	2.62850000	-0.58671000
H	3.76933000	1.59362800	-2.02200400
H	2.65313900	1.14121700	-0.72794800
C	0.40659200	3.55039600	-1.69197000
C	0.86762300	2.88921900	-2.83643300
C	0.47935500	4.94212400	-1.65053000
C	1.38795400	3.59965300	-3.90957700
H	0.81485800	1.80090600	-2.88185300
C	0.99809400	5.65699300	-2.72918700
H	0.13645000	5.47873200	-0.76809900
C	1.45401900	4.99062800	-3.85952900
H	1.74268400	3.06639800	-4.78889400
H	1.04700600	6.74247200	-2.67878500
H	1.86143900	5.54983300	-4.69857000
C	-0.22361000	3.46162800	0.76358500
C	0.85596500	3.39644300	1.64855700
C	-1.32738000	4.24295600	1.11104100
C	0.82697500	4.07632300	2.86225800
H	1.73592100	2.81094000	1.37190500
C	-1.35408500	4.93778300	2.31666500
H	-2.17602800	4.30117700	0.42945100
C	-0.28120500	4.84866800	3.20038100
H	1.67375400	4.00945500	3.54242100
H	-2.21895500	5.54690900	2.56994200
H	-0.30467200	5.38775000	4.14459600
C	-3.71122400	-1.32269400	1.23034300
C	-4.89765800	-0.62694700	1.47541600
C	-3.10809900	-2.01037100	2.28469200
C	-5.45925600	-0.60845500	2.74728700
H	-5.38106400	-0.09190000	0.65802100
C	-3.66063000	-1.98614000	3.56315600
H	-2.19031100	-2.57124700	2.09763400
C	-4.83833200	-1.28183800	3.79764700
H	-6.38528800	-0.06499600	2.92149300
H	-3.17414600	-2.52446800	4.37424300
H	-5.27652100	-1.26354200	4.79285200
C	-3.76559500	-2.29664300	-1.12677600
C	-3.23477100	-2.42473700	-2.41697900

C	-4.85656400	-3.09139800	-0.77807900
C	-3.77308900	-3.32191400	-3.32843900
H	-2.39013200	-1.80102200	-2.71051900
C	-5.40300100	-3.98913500	-1.69436100
H	-5.28629200	-3.01954100	0.21877400
C	-4.86488500	-4.10992700	-2.96873200
H	-3.33908700	-3.40585400	-4.32280000
H	-6.25635500	-4.59776000	-1.40301100
H	-5.29150300	-4.81300400	-3.68037200
H	-4.62848600	0.03969600	-1.98574400
H	-4.19272600	2.27991500	-2.94228500

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Atom	x	y	z
C	1.96043300	-0.71661500	3.00108300
C	1.95812400	-0.59835100	4.38867300
C	0.79879200	-0.14517700	5.01050600
C	-0.30586100	0.20608600	4.24316900
C	-0.22404500	0.06492800	2.85837500
N	0.88042000	-0.40659500	2.27850800
H	0.76258600	-0.04837100	6.09177000
H	2.83845900	-0.85281100	4.97222400
H	-1.20485200	0.59339700	4.71310700
C	3.13325300	-1.10262600	2.17811900
C	-1.26597000	0.49724900	1.89313700
N	-1.03094900	0.19711600	0.66042200
N	2.90302600	-1.18927700	0.91487600
C	-2.41999000	1.27578700	2.41838800
H	-2.05678200	2.16231200	2.95508300
H	-3.09511900	1.59827700	1.62380700
H	-2.99169000	0.66272800	3.12804000
C	4.44715200	-1.29597000	2.85203900
H	4.42360400	-2.22083200	3.44471000
H	5.26649600	-1.36621700	2.13286600
H	4.65541000	-0.47676400	3.54985100
C	-1.86785400	0.74594000	-0.35958100
C	-1.47989900	1.97422300	-0.92720100
C	-2.99706500	0.04896000	-0.80796200
C	-2.32635100	2.55319400	-1.87075400
C	-3.80543800	0.65759400	-1.77026800
C	-3.49223300	1.91190400	-2.27430000
H	-2.05021000	3.50693300	-2.31620700
C	3.96947200	-1.33914500	-0.02462500
C	4.44170500	-2.60875000	-0.38646200

C	4.44576700	-0.15768100	-0.62766500
C	5.45658100	-2.67325000	-1.34520200
C	5.45836200	-0.27919200	-1.57686600
C	5.96707800	-1.52417000	-1.92970800
H	5.84548300	-3.64588600	-1.64278400
H	5.85068400	0.61552600	-2.05564200
H	6.75645600	-1.59738700	-2.67400000
C	3.87707600	-3.88464500	0.20347400
H	2.98907400	-3.61725800	0.79739000
C	3.87955300	1.19860100	-0.24876800
H	2.82255100	1.03722800	0.02739200
C	-3.31809700	-1.33209900	-0.26170900
H	-2.35221400	-1.77940800	0.01952400
C	-0.14781000	2.59756200	-0.53078300
H	0.54191500	1.74456800	-0.40127400
C	1.03989500	-0.52142900	-1.76407600
H	0.02599400	-0.24591100	-2.10965100
H	1.62625600	0.41583700	-1.79124700
C	1.64609800	-1.49449700	-2.76505800
H	0.98898200	-2.37091200	-2.88581300
H	2.60720400	-1.88861800	-2.39563500
C	1.87999100	-0.85821300	-4.12890300
H	0.94394700	-0.46191200	-4.54646000
H	2.58638700	-0.01929900	-4.04919800
H	2.29423800	-1.56978300	-4.85432500
Co	0.84696100	-0.89494600	0.20805500
C	0.23348600	-2.92240200	-0.27735600
H	1.12584000	-3.36268700	-0.72056200
H	-0.61665100	-2.79761400	-0.94915800
C	0.10209900	-2.81935500	1.07200900
H	-0.85364400	-2.57790600	1.53691700
H	0.88690200	-3.17053400	1.74047800
H	-4.68342700	0.12571500	-2.13363400
H	-4.14013000	2.37822100	-3.01223300
C	-4.13969900	-1.29617100	1.01362400
C	-5.18559300	-0.39023000	1.20147200
C	-3.86466800	-2.21848500	2.02692100
C	-5.92712900	-0.39734200	2.37930300
H	-5.41707400	0.33417300	0.42133100
C	-4.59928100	-2.22450200	3.20850500
H	-3.07292100	-2.95462400	1.87604800
C	-5.63222100	-1.30857900	3.38947500
H	-6.73860900	0.31547900	2.50856800
H	-4.37036200	-2.95001200	3.98608500

H	-6.21104900	-1.31045100	4.31017100
C	-3.89510400	-2.24907700	-1.33158500
C	-5.15111200	-2.84260700	-1.22472100
C	-3.12036700	-2.51895600	-2.46626100
C	-5.62189400	-3.68943000	-2.22754500
H	-5.76799300	-2.64915900	-0.34937900
C	-3.58599700	-3.36378700	-3.46404200
H	-2.14254300	-2.04344400	-2.57129000
C	-4.84325500	-3.95392000	-3.34658000
H	-6.60497800	-4.14415500	-2.12664700
H	-2.96846200	-3.56349200	-4.33690100
H	-5.21135700	-4.61691300	-4.12603000
C	0.46702300	3.45831200	-1.62912600
C	0.66014900	2.89768100	-2.89895500
C	0.91880100	4.75936000	-1.40610800
C	1.28852700	3.61143600	-3.90971700
H	0.32104500	1.88048900	-3.09095000
C	1.54908700	5.47872200	-2.42147700
H	0.78989000	5.22225400	-0.42981500
C	1.73906500	4.90888400	-3.67356300
H	1.43175800	3.14927900	-4.88465300
H	1.89345100	6.49176200	-2.22513500
H	2.23388800	5.46963000	-4.46318100
C	-0.19455800	3.29158300	0.81492400
C	0.81285800	3.05478700	1.75366600
C	-1.20261700	4.20467400	1.13078500
C	0.80900600	3.70118900	2.98673500
H	1.60932600	2.34519200	1.51412100
C	-1.20543500	4.86111600	2.35772000
H	-1.99108800	4.39997800	0.40381900
C	-0.20300400	4.60741800	3.29199400
H	1.60006600	3.49843300	3.70674200
H	-1.99421200	5.57437300	2.58613000
H	-0.20754800	5.12154000	4.25027900
C	4.88019100	-4.56447000	1.13388900
H	4.44889500	-5.47065200	1.57708600
H	5.78102700	-4.86437700	0.58296300
H	5.20068100	-3.90621700	1.94983600
C	3.43123800	-4.86240400	-0.88306400
H	2.86667200	-5.69380800	-0.44326500
H	2.80041500	-4.38074900	-1.64128100
H	4.29177600	-5.29692300	-1.40661000
C	4.59796400	1.79637100	0.96167100
H	5.67565100	1.87592400	0.76639300

H	4.22364600	2.80692100	1.17049600
H	4.47077300	1.19902300	1.87319900
C	3.90259100	2.20204200	-1.39512500
H	3.47109800	1.78873600	-2.31511500
H	3.32289200	3.09499800	-1.12493900
H	4.92387700	2.53697100	-1.61924200

TS-2/3

Atom	x	y	z
C	1.56176300	-1.01639200	2.97065500
C	1.40421500	-1.11059500	4.35028500
C	0.19577600	-0.70369100	4.91103700
C	-0.80670900	-0.18186700	4.09797900
C	-0.57920300	-0.11213800	2.72650400
N	0.57278400	-0.54283600	2.19878200
H	0.04122900	-0.77981800	5.98342100
H	2.20342800	-1.49459800	4.97818600
H	-1.74568400	0.16175500	4.52350800
C	2.78490700	-1.34460300	2.20811500
C	-1.49387900	0.47931400	1.72647500
N	-1.18466000	0.25116300	0.48745300
N	2.65754800	-1.29921900	0.92132900
C	-2.62245800	1.30804200	2.22732700
H	-2.23553600	2.10966300	2.87000800
H	-3.20210600	1.75355000	1.41740400
H	-3.29594500	0.69085000	2.83652200
C	4.03245900	-1.66701800	2.95444900
H	3.93144600	-2.65386200	3.42728400
H	4.90324900	-1.68964100	2.29477600
H	4.21017000	-0.94367100	3.75806800
C	-1.93686100	0.89029500	-0.54393700
C	-1.47748900	2.12574900	-1.03502200
C	-3.07080000	0.26112200	-1.08003500
C	-2.24481000	2.77648100	-1.99998700
C	-3.80431200	0.94483000	-2.05126900
C	-3.41264600	2.20285300	-2.48867900
H	-1.90681300	3.73649000	-2.38590100
C	3.78192100	-1.40377000	0.04707100
C	4.27441400	-2.65347500	-0.36169600
C	4.29953100	-0.19299900	-0.46134100
C	5.32121800	-2.66824800	-1.28791500
C	5.34411900	-0.26633500	-1.38056200
C	5.85328300	-1.49242100	-1.79395300
H	5.72240900	-3.62529300	-1.61779200

H	5.76499100	0.65130800	-1.78562500
H	6.66665900	-1.52785000	-2.51475900
C	3.71750400	-3.96361600	0.15845100
H	2.83380800	-3.73652400	0.77381200
C	3.75644100	1.14639100	0.00419900
H	2.67599800	1.01219300	0.19571800
C	-3.47703100	-1.12368200	-0.59784800
H	-2.54017500	-1.64696700	-0.34743300
C	-0.16180600	2.69715900	-0.52537900
H	0.50776100	1.82901700	-0.39357000
C	0.84336700	-0.74345800	-1.83198300
H	-0.09881200	-0.33796100	-2.22600700
H	1.40607800	0.10102300	-1.37481200
C	1.70678800	-1.32269200	-2.93212900
H	1.16285900	-2.12885200	-3.44708500
H	2.60270300	-1.78650000	-2.48951300
C	2.13633300	-0.28380400	-3.95745900
H	1.26909800	0.19313700	-4.43410400
H	2.74369000	0.50703500	-3.49651400
H	2.74073800	-0.73960300	-4.75025000
Co	0.61810800	-0.96707800	0.27381400
C	0.19075500	-2.56787500	-1.05589200
H	1.05407800	-3.08504900	-1.47111100
H	-0.64472600	-2.51526000	-1.75741500
C	-0.10470300	-2.84791600	0.31709300
H	-1.14332000	-2.86476700	0.64910800
H	0.56383600	-3.50626900	0.87435400
H	-4.68698900	0.47098200	-2.47744700
H	-4.00194600	2.72549100	-3.23799000
C	-4.27955100	-1.07194800	0.68893400
C	-5.34460300	-0.18262300	0.85062500
C	-3.97388000	-1.94472300	1.73523600
C	-6.07847200	-0.16010200	2.03190900
H	-5.59678600	0.50368200	0.04250400
C	-4.69777800	-1.91795700	2.92438600
H	-3.16140100	-2.66244800	1.61308300
C	-5.75263700	-1.02256800	3.07631500
H	-6.90723400	0.53628100	2.13876600
H	-4.44382900	-2.60530100	3.72863100
H	-6.32508000	-1.00238700	4.00081100
C	-4.13211800	-1.95193100	-1.69551100
C	-5.40565600	-2.50459100	-1.57417400
C	-3.41201900	-2.19060400	-2.87258600
C	-5.94582700	-3.27703500	-2.60171400

H	-5.98485600	-2.34061800	-0.66798300
C	-3.94621100	-2.96095900	-3.89592600
H	-2.42148600	-1.74699000	-2.99039000
C	-5.22085400	-3.50885200	-3.76293800
H	-6.94177400	-3.69922000	-2.48718500
H	-3.36895900	-3.13406800	-4.80153800
H	-5.64353500	-4.11224200	-4.56282800
C	0.53449200	3.58602700	-1.54634200
C	0.90122200	3.02201100	-2.77400700
C	0.87114300	4.91595300	-1.29905700
C	1.58939200	3.76125700	-3.72555000
H	0.64581700	1.98091800	-2.97777100
C	1.56343100	5.66119000	-2.25360600
H	0.60485000	5.37835300	-0.35083400
C	1.92684400	5.08870900	-3.46565800
H	1.86941600	3.29870700	-4.67040500
H	1.81960100	6.69687100	-2.04132600
H	2.46901700	5.67140700	-4.20670500
C	-0.27766500	3.33073000	0.84591100
C	0.68711200	3.05650600	1.81842700
C	-1.30840100	4.21963300	1.15635300
C	0.61653100	3.63969000	3.08022500
H	1.50225100	2.36825000	1.58082400
C	-1.37654500	4.81466000	2.41247600
H	-2.06578100	4.44309200	0.40476300
C	-0.41841300	4.52140800	3.38048600
H	1.37414800	3.40858600	3.82667000
H	-2.18331000	5.50844000	2.63815300
H	-0.47580900	4.98395100	4.36303300
C	4.73607900	-4.68749100	1.03924800
H	4.30730400	-5.60938700	1.45107200
H	5.62246300	-4.96952400	0.45634500
H	5.07960000	-4.06783700	1.87573600
C	3.27062500	-4.88974700	-0.97185700
H	2.72405900	-5.75091100	-0.56869400
H	2.62067000	-4.38346300	-1.69598600
H	4.13051200	-5.28347500	-1.52839800
C	4.40307400	1.58343500	1.31984900
H	5.49390200	1.63968100	1.20694000
H	4.04802000	2.57964800	1.61434200
H	4.19071300	0.89632000	2.14798000
C	3.90551500	2.26202400	-1.02207500
H	3.51821300	1.97917700	-2.00834200
H	3.35273700	3.15219000	-0.69376700

H 4.95425100 2.56318900 -1.14188600

3

Atom	x	y	z
C	0.96082900	-1.32922300	3.35980700
C	0.69717800	-1.32837700	4.72708800
C	-0.47206500	-0.71245600	5.16832200
C	-1.32617300	-0.08825100	4.26268800
C	-0.99814000	-0.14422800	2.91063000
N	0.08791400	-0.79991100	2.50229800
H	-0.70194600	-0.69183100	6.23010800
H	1.39124500	-1.77360000	5.43365100
H	-2.21245600	0.43782500	4.60574200
C	2.22591600	-1.77083100	2.71342300
C	-1.73391700	0.51847000	1.79718900
N	-1.13158300	0.46075500	0.65635700
N	2.34310600	-1.42488300	1.47627200
C	-3.00427400	1.21903300	2.10238200
H	-3.70548500	0.54608900	2.61139900
H	-2.78725500	2.05715200	2.78086600
H	-3.47714100	1.61856100	1.20401600
C	3.25619400	-2.44959600	3.54187000
H	3.44667800	-1.87542500	4.45690300
H	2.90126400	-3.44041600	3.85568200
H	4.19640600	-2.56518800	2.99807600
C	-1.72490200	0.94688300	-0.54401400
C	-1.31855400	2.19907200	-1.02890700
C	-2.57057600	0.09235000	-1.27690800
C	-1.86923100	2.64730400	-2.22885700
C	-3.08491900	0.57807500	-2.47802700
C	-2.76077800	1.85061800	-2.93589300
H	-1.57076600	3.61639200	-2.62365000
C	3.53612900	-1.62654200	0.72299600
C	3.90547700	-2.88246000	0.21394900
C	4.25790600	-0.45384100	0.41982400
C	5.05839600	-2.94043200	-0.57566600
C	5.40190800	-0.56929900	-0.36468400
C	5.80381900	-1.80598100	-0.85826600
H	5.37269200	-3.90173400	-0.97910000
H	5.98215100	0.31921800	-0.60380500
H	6.69797600	-1.88088800	-1.47272000
C	3.11205600	-4.15146800	0.46021400
H	2.19564700	-3.88515700	1.00871700
C	3.79817300	0.88105800	0.96905500

H	2.69140000	0.85299800	1.00442500
C	-2.80412100	-1.33032800	-0.77609300
H	-1.82531500	-1.65341200	-0.38345200
C	-0.25960300	2.97479600	-0.25867400
H	0.48715000	2.21649200	0.04271200
C	0.82143200	-1.36680200	-1.34069800
H	1.35853400	-2.32872800	-1.30410900
H	-0.08972400	-1.52064800	-1.93073100
C	1.69838800	-0.30252700	-1.99681200
H	2.41868700	0.12926000	-1.27528800
H	1.06367500	0.52965700	-2.34600400
C	2.53709100	-0.82646500	-3.15858200
H	3.21382700	-1.60902000	-2.77174900
H	1.88178200	-1.32234700	-3.89267500
Co	0.58378000	-0.72743000	0.50858600
C	3.35969500	0.25506200	-3.84153500
H	2.68283400	0.98946300	-4.30554500
H	3.92858000	0.80819900	-3.07459500
C	4.31754500	-0.30494100	-4.87796800
H	4.89466300	0.48244400	-5.37615000
H	5.03141900	-0.99797600	-4.41259700
H	3.77908200	-0.86292200	-5.65498000
C	-3.77805700	-1.42692600	0.38522800
C	-4.98637500	-0.72773100	0.40747900
C	-3.47919100	-2.27913600	1.45188900
C	-5.87460200	-0.87987300	1.46778800
H	-5.22550400	-0.04224400	-0.40567600
C	-4.35761500	-2.42394100	2.52098100
H	-2.54425400	-2.84253800	1.43349000
C	-5.56141000	-1.72378200	2.53061200
H	-6.81385300	-0.33110700	1.46728400
H	-4.10648900	-3.09183800	3.34240300
H	-6.25657000	-1.83974300	3.35895900
C	-3.16642200	-2.34235600	-1.85226200
C	-2.22323000	-3.29486200	-2.24286700
C	-4.43674300	-2.38953300	-2.43553800
C	-2.52615600	-4.25001400	-3.20890500
H	-1.23760800	-3.29219600	-1.77798200
C	-4.74071900	-3.33838500	-3.40514000
H	-5.20501800	-1.68561300	-2.11813400
C	-3.78456000	-4.27062600	-3.79848700
H	-1.77475400	-4.98182200	-3.49724900
H	-5.73367400	-3.35510000	-3.84905800
H	-4.02438500	-5.01503500	-4.55416000

C	-0.79409800	3.57379600	1.02744600
C	-0.05562500	3.46028200	2.20719400
C	-2.01619500	4.24871300	1.06627500
C	-0.52841600	3.99644400	3.40118100
H	0.90295600	2.93678600	2.18392900
C	-2.48543100	4.80200700	2.25397300
H	-2.61179600	4.32668000	0.15630900
C	-1.74621800	4.67227800	3.42690700
H	0.05722300	3.89291500	4.31240300
H	-3.43652100	5.32982800	2.26458100
H	-2.11582700	5.09908300	4.35642300
C	0.49099300	3.97531900	-1.12263800
C	0.15422400	5.32772300	-1.18733900
C	1.55119500	3.51285800	-1.90745300
C	0.85840000	6.19375400	-2.02043100
H	-0.65747300	5.71555500	-0.57456400
C	2.26124100	4.37606500	-2.73275600
H	1.82735300	2.45884300	-1.85646500
C	1.91369600	5.72287700	-2.79382000
H	0.58291500	7.24550500	-2.05695800
H	3.09214700	3.99712100	-3.32494600
H	2.46678400	6.40287700	-3.43757700
C	2.68747300	-4.82442700	-0.84533100
H	3.55728000	-5.18339600	-1.40963400
H	2.05568800	-5.69549700	-0.63286200
H	2.12504200	-4.14859800	-1.50014100
C	3.90465200	-5.14951700	1.30587900
H	4.79572100	-5.49480800	0.76637300
H	4.24421300	-4.72160000	2.25584600
H	3.29587100	-6.03397100	1.53039200
C	4.29756000	1.08882100	2.39945700
H	5.39549000	1.07895700	2.42168000
H	3.96457600	2.05808600	2.79148200
H	3.94506900	0.30884700	3.08626900
C	4.20178600	2.07046200	0.10758000
H	3.68693400	2.97670800	0.45112400
H	5.27950200	2.26914000	0.17215400
H	3.94737400	1.92136300	-0.94996300
H	-3.72440000	-0.06156100	-3.08162000
H	-3.17782100	2.20760500	-3.87437100

Co3

Doublet:

1

Atom	x	y	z
C	0.00200600	0.14433100	2.86422800
C	-0.00362800	0.28551900	4.24805900
C	1.14252600	-0.08463700	4.94925300
C	2.26085700	-0.56999200	4.27275200
C	2.18770700	-0.69331000	2.88884700
N	1.07338000	-0.34797100	2.23649100
H	1.16963200	0.01760000	6.03016600
H	-0.87257000	0.68338100	4.76459600
H	3.16319300	-0.84105100	4.81359100
C	-1.04068400	0.55646700	1.90460100
C	3.23318300	-1.15391600	1.95553200
N	2.87277000	-1.17137400	0.70453000
N	-0.76234600	0.28421600	0.65787600
C	4.57255800	-1.49181900	2.50047000
H	5.00464000	-0.60440500	2.98263600
H	4.48261000	-2.25996200	3.27949000
H	5.26290900	-1.84188500	1.73113000
C	-2.22244700	1.28302500	2.42988600
H	-2.77152400	0.64099200	3.13192200
H	-1.87660700	2.16514400	2.98610400
H	-2.90803400	1.60792500	1.64652200
C	3.83206800	-1.55295000	-0.29726400
C	3.85840900	-2.88170000	-0.75318500
C	4.67858900	-0.55887100	-0.82541100
C	4.72522900	-3.18726600	-1.80454700
C	5.51721900	-0.91943200	-1.87962900
C	5.53376500	-2.21652100	-2.37551300
H	4.76998900	-4.20824000	-2.17719300
H	6.17881600	-0.17492400	-2.31634800
H	6.19347300	-2.47406000	-3.20052400
C	-1.66841800	0.77096100	-0.34063300
C	-1.35111100	1.99289100	-0.95187000
C	-2.82105900	0.03846000	-0.66892700
C	-2.24916200	2.53476500	-1.86744800
C	-3.70749300	0.64297500	-1.55687400
C	-3.42680400	1.86970100	-2.14446200
H	-2.03915700	3.47467100	-2.37369800
C	-0.04133700	2.67740700	-0.60326100
H	0.67427300	1.84752200	-0.47353600
C	-3.06862300	-1.34392700	-0.08447500
H	-2.06535500	-1.72607800	0.16542100
C	4.67165400	0.86119500	-0.28723300

H	4.49255700	0.81203300	0.79944400
C	3.05438600	-3.98285600	-0.08864100
H	2.19122800	-3.51786400	0.41330900
C	0.90237000	-0.83116700	-1.54641900
H	0.24392400	-0.11096800	-2.06269300
H	1.88947900	-0.78779900	-2.03850600
C	0.31648400	-2.22715000	-1.71215700
H	-0.72135800	-2.25582300	-1.34563200
H	0.86456600	-2.95353800	-1.09210400
C	0.33122100	-2.71637100	-3.15419700
H	-0.20990800	-2.01868700	-3.80871500
H	1.36060000	-2.77990700	-3.53392500
H	-0.13518700	-3.70455000	-3.26171800
Co	1.02217400	-0.51561800	0.35134800
C	3.89422300	-4.68602500	0.97949500
H	4.24187500	-4.00257100	1.76210000
H	3.31863600	-5.48604500	1.46133200
H	4.78269800	-5.14300300	0.52365600
C	2.52131900	-5.02639400	-1.06711100
H	3.31998800	-5.68671100	-1.42738700
H	1.78514300	-5.66680700	-0.56689300
H	2.03991500	-4.57681400	-1.94273200
C	5.99148400	1.59405200	-0.48789400
H	6.16929300	1.83091000	-1.54438600
H	5.97365800	2.54804100	0.05148500
H	6.84684900	1.01371700	-0.12254100
C	3.52754100	1.66246500	-0.90229600
H	3.52191000	2.69815800	-0.53793100
H	3.61341300	1.69031300	-1.99680700
H	2.55809600	1.20585000	-0.66352100
C	0.48937700	3.53273200	-1.74171800
C	0.93672700	2.89072400	-2.90261900
C	0.53800200	4.92491200	-1.68664300
C	1.41733700	3.62139900	-3.98067000
H	0.90492300	1.80194800	-2.95596000
C	1.01706800	5.65986100	-2.77018900
H	0.20605100	5.44603600	-0.79090600
C	1.45735500	5.01292900	-3.91781400
H	1.76116000	3.10405100	-4.87360600
H	1.04640100	6.74546300	-2.71033500
H	1.83137900	5.58813100	-4.76149600
C	-0.09638600	3.40049200	0.72866000
C	0.98322200	3.30699000	1.61182300
C	-1.19189900	4.18574400	1.09346100

C	0.96086800	3.96198300	2.83940200
H	1.85893300	2.71991800	1.32424700
C	-1.21169700	4.85585600	2.31331100
H	-2.04069300	4.26809300	0.41448600
C	-0.13966200	4.73766300	3.19439300
H	1.80917600	3.87680500	3.51556800
H	-2.07054500	5.46825500	2.57875900
H	-0.15741200	5.25786000	4.14919100
C	-3.81846600	-1.28954200	1.23146700
C	-5.02902600	-0.60373900	1.35672400
C	-3.29862000	-1.94614100	2.34830800
C	-5.68977800	-0.55586200	2.57895200
H	-5.46158400	-0.11290000	0.48637800
C	-3.95906500	-1.90207500	3.57408000
H	-2.36501400	-2.50341000	2.25280100
C	-5.15390700	-1.19901400	3.69325900
H	-6.63155700	-0.01822000	2.66185100
H	-3.54244500	-2.42263700	4.43393500
H	-5.67414300	-1.16135300	4.64750100
C	-3.64068400	-2.34089700	-1.08835100
C	-3.13033300	-2.38210700	-2.39017600
C	-4.60824100	-3.27641400	-0.72458700
C	-3.57164300	-3.33199600	-3.30159600
H	-2.38327200	-1.65132500	-2.70040100
C	-5.05545900	-4.22742400	-1.63931600
H	-5.02282500	-3.26585000	0.28134600
C	-4.53939100	-4.26141000	-2.92869300
H	-3.15910800	-3.34182900	-4.30860100
H	-5.81495800	-4.94468300	-1.33615900
H	-4.89150000	-5.00328000	-3.64158800
F	-4.86319400	0.05461900	-1.86689700
F	-4.31143000	2.38727000	-2.99223300

2

Atom	x	y	z
C	2.00323800	-0.75711100	2.98256400
C	2.06349700	-0.55001400	4.35797800
C	0.94127100	-0.03339300	5.00019400
C	-0.19320600	0.29940800	4.26529200
C	-0.18368200	0.06975300	2.89220200
N	0.88147300	-0.48578500	2.30097100
H	0.96008500	0.13452200	6.07301400
H	2.96618300	-0.78034200	4.91707400
H	-1.05773300	0.74394900	4.74981600

C	3.09831400	-1.17334800	2.09179500
C	-1.20752000	0.47879900	1.91642200
N	-0.90970400	0.20843700	0.67675500
N	2.78779800	-1.19280800	0.82855200
C	-2.40714200	1.20102400	2.41468000
H	-2.09687200	2.07363800	3.00400400
H	-3.06261900	1.53647200	1.60950300
H	-2.98448800	0.54003000	3.07569800
C	4.43537500	-1.45889000	2.67752800
H	4.39114500	-2.38923500	3.26012400
H	5.20566500	-1.56330300	1.91096500
H	4.73416200	-0.66364500	3.37077900
C	-1.75694100	0.75712400	-0.33992100
C	-1.37355900	1.98743300	-0.90227700
C	-2.90761400	0.06925600	-0.75721800
C	-2.21032700	2.57319000	-1.85047400
C	-3.70516500	0.69567400	-1.70941600
C	-3.37092500	1.93373500	-2.23602600
H	-1.96072900	3.52580200	-2.31150200
C	3.83396600	-1.36009000	-0.14008300
C	4.28992400	-2.63492000	-0.50957100
C	4.33620400	-0.18245100	-0.72943100
C	5.28204800	-2.70988900	-1.49068100
C	5.32364800	-0.31648900	-1.70441600
C	5.79450200	-1.56724800	-2.08492600
H	5.65231400	-3.68717100	-1.79668500
H	5.73346600	0.57407000	-2.17575900
H	6.56400300	-1.64910600	-2.84887500
C	3.73699500	-3.91407400	0.08602900
H	2.90316800	-3.64611900	0.75256200
C	3.86018400	1.19230900	-0.29576800
H	2.80676100	1.09367900	0.01810400
C	-3.27045100	-1.29469400	-0.20003400
H	-2.33532700	-1.68881800	0.22310000
C	-0.06741000	2.64373500	-0.48353200
H	0.64655800	1.81521400	-0.34042200
C	0.94400700	-0.60296700	-1.52018400
H	-0.04984700	-0.26114400	-1.85663700
H	1.59655000	0.29327500	-1.51651300
C	1.48842700	-1.56918800	-2.55754400
H	0.78485700	-2.40269800	-2.70903600
H	2.43105400	-2.02246700	-2.21881200
C	1.73527100	-0.89120200	-3.89974000
H	0.81129500	-0.45182200	-4.30079000

H	2.47510900	-0.08421900	-3.80073300
H	2.11676100	-1.59718800	-4.64753900
Co	0.82964300	-0.85777900	0.42956300
C	0.15339800	-2.83308700	-0.14097800
H	1.00233900	-3.30498000	-0.62940300
H	-0.72873700	-2.69717100	-0.76633300
C	0.08144700	-2.77846500	1.21795400
H	-0.85455600	-2.56441400	1.73413700
H	0.87876800	-3.18746000	1.83833800
F	-4.83311600	0.12050500	-2.12847800
F	-4.18389200	2.48734600	-3.13149700
C	-4.23743600	-1.21710700	0.96746700
C	-5.37761000	-0.41024300	0.94790200
C	-3.98409300	-1.98892300	2.10379200
C	-6.22216600	-0.35568100	2.05192700
H	-5.61829600	0.17229800	0.06137200
C	-4.82994200	-1.94053200	3.20811100
H	-3.11468200	-2.64824900	2.11286700
C	-5.94859800	-1.11321100	3.18758200
H	-7.10405500	0.28023800	2.02264500
H	-4.61496400	-2.55032600	4.08295400
H	-6.61155300	-1.06764800	4.04834200
C	-3.66409200	-2.29005100	-1.28654200
C	-4.77465400	-3.12225700	-1.16898300
C	-2.84575400	-2.41685600	-2.41478900
C	-5.05812500	-4.06564100	-2.15423400
H	-5.42899500	-3.03741100	-0.30396100
C	-3.12615700	-3.35903500	-3.39623500
H	-1.98453500	-1.75539000	-2.53130200
C	-4.23634000	-4.18992900	-3.26772700
H	-5.93141300	-4.70526200	-2.04777200
H	-2.47835000	-3.44035300	-4.26635600
H	-4.45936000	-4.92740300	-4.03504900
C	0.52934300	3.52046200	-1.57662400
C	0.80616800	2.94069800	-2.82108800
C	0.86204900	4.85954500	-1.37698000
C	1.40522600	3.67493600	-3.83468800
H	0.55356100	1.89330500	-2.98694700
C	1.46434700	5.59922600	-2.39480100
H	0.66182900	5.33394800	-0.41838500
C	1.74011600	5.01136700	-3.62259600
H	1.61625600	3.20009400	-4.79096700
H	1.71776200	6.64253600	-2.22009800
H	2.21223000	5.58941100	-4.41353100

C	-0.16085700	3.33610400	0.86058500
C	0.87674800	3.18217700	1.78382700
C	-1.23407200	4.16567300	1.18953500
C	0.83630700	3.82374800	3.01808400
H	1.72662300	2.54573300	1.52309100
C	-1.27452200	4.81678500	2.41904200
H	-2.04571900	4.29946600	0.47411300
C	-0.24349600	4.64191200	3.33976900
H	1.64966600	3.68643500	3.72811200
H	-2.11587600	5.46238100	2.66068500
H	-0.27821700	5.15000400	4.30061600
C	4.78702200	-4.65095400	0.91647500
H	4.35770100	-5.55227000	1.37101700
H	5.62933100	-4.97025900	0.28952600
H	5.19570200	-4.02730900	1.71940400
C	3.19004900	-4.84579500	-0.99583400
H	2.64741100	-5.68466600	-0.54289200
H	2.51094000	-4.32795500	-1.68476000
H	4.00195000	-5.27083200	-1.59905300
C	4.65968700	1.70793500	0.90296200
H	5.73491200	1.69421900	0.68060900
H	4.38407900	2.74514500	1.13301100
H	4.50097500	1.11390400	1.81154700
C	3.91063500	2.22688900	-1.41404100
H	3.45235400	1.85967900	-2.34027300
H	3.37202500	3.13543700	-1.11312800
H	4.94232800	2.52585600	-1.64122600

TS-2/3

Atom	x	y	z
C	1.01994200	-1.08506300	3.54908300
C	0.60944000	-1.25611900	4.86764900
C	-0.67557000	-0.83974200	5.21706700
C	-1.52708400	-0.27874400	4.26524400
C	-1.04894800	-0.13089900	2.96804400
N	0.19798000	-0.50875700	2.66041600
H	-1.02151200	-0.96685600	6.23883200
H	1.26530400	-1.71332700	5.60356700
H	-2.53790600	0.02464900	4.52412600
C	2.29867100	-1.45610400	2.91466900
C	-1.74196800	0.41256700	1.78576600
N	-1.08401700	0.24771300	0.66809800
N	2.31261500	-1.28984600	1.62281900
C	-3.04398200	1.09748000	1.96786700

H	-3.77460200	0.39786800	2.39569400
H	-2.91998400	1.92362100	2.68121000
H	-3.44568400	1.49352500	1.03396600
C	3.43165800	-1.92822600	3.74831400
H	3.53364900	-1.30211300	4.64231400
H	3.24562800	-2.95495200	4.09312400
H	4.37371000	-1.91688500	3.19499600
C	-1.62040700	0.81889300	-0.52784700
C	-1.16666600	2.08859900	-0.91408800
C	-2.56213900	0.08822300	-1.26856700
C	-1.77331000	2.69488700	-2.01253300
C	-3.15484200	0.74602700	-2.34191200
C	-2.77450300	2.03366100	-2.69739200
H	-1.46860200	3.68136100	-2.35463400
C	3.51383100	-1.46301500	0.86095500
C	3.97496400	-2.73678000	0.50031200
C	4.12809200	-0.28171300	0.39806100
C	5.11276500	-2.80299200	-0.30987800
C	5.25692600	-0.40369000	-0.40713200
C	5.75143800	-1.65644900	-0.75518300
H	5.49591800	-3.77901300	-0.60316100
H	5.75351500	0.49077500	-0.77568900
H	6.63300200	-1.73457600	-1.38673300
C	3.27755500	-4.01852800	0.90958700
H	2.39125100	-3.75418000	1.50533800
C	3.56045800	1.07030400	0.78093500
H	2.45611200	0.95844000	0.73211900
C	-2.87615800	-1.35405200	-0.90725800
H	-1.96825700	-1.71246500	-0.39526700
C	-0.03478900	2.74706500	-0.13896100
H	0.65042800	1.91803200	0.12811500
C	0.94749900	-1.28694000	-0.94545400
H	1.67681600	-2.10403100	-0.83127700
H	0.01111700	-1.75674000	-1.29493800
C	1.46369200	-0.34148400	-2.01745000
H	2.23660000	0.32931700	-1.60070700
H	0.64593600	0.31600900	-2.36285300
C	2.08071000	-1.05094800	-3.21583600
H	2.88540900	-1.71640800	-2.85594600
H	1.33259600	-1.71252200	-3.68509800
Co	0.66713700	-0.58265500	0.84728200
C	2.64585000	-0.08635200	-4.24724300
H	1.84203400	0.57701900	-4.60555200
H	3.38077900	0.57004300	-3.75122300

C	3.29385000	-0.79381800	-5.42396200
H	3.69736100	-0.08774900	-6.15845900
H	4.12007100	-1.43548400	-5.09132400
H	2.57166600	-1.43600500	-5.94432200
F	-4.11427700	0.15590500	-3.05433200
F	-3.38172600	2.61548500	-3.72811700
C	-3.99339700	-1.46119900	0.10973400
C	-5.22682600	-0.83685100	-0.09218300
C	-3.79585200	-2.19824500	1.27865400
C	-6.22904400	-0.92811800	0.86668500
H	-5.40443000	-0.28521800	-1.01409300
C	-4.79614200	-2.28832600	2.24378900
H	-2.84334700	-2.70981500	1.42951600
C	-6.01442100	-1.64646900	2.04175000
H	-7.18500400	-0.43806100	0.69625800
H	-4.62451100	-2.86509100	3.15037700
H	-6.79966500	-1.71476900	2.79105500
C	-3.03397200	-2.26254500	-2.12232500
C	-2.09864400	-2.18547600	-3.16015600
C	-4.03358200	-3.23024400	-2.19743900
C	-2.16198500	-3.05160000	-4.24329600
H	-1.31470600	-1.42844000	-3.12284300
C	-4.09843700	-4.09988000	-3.28417700
H	-4.77172800	-3.31267500	-1.40272900
C	-3.16489000	-4.01571100	-4.30934400
H	-1.42519500	-2.97176900	-5.04001200
H	-4.88834000	-4.84666100	-3.32574000
H	-3.21718400	-4.69485700	-5.15701200
C	-0.50299000	3.32814200	1.18033600
C	0.23244600	3.08959800	2.34311900
C	-1.63516300	4.14149600	1.25726900
C	-0.16642800	3.62660900	3.56397900
H	1.12796100	2.46497400	2.28890100
C	-2.03139400	4.69022300	2.47295300
H	-2.20933700	4.34716900	0.35389600
C	-1.30287000	4.42787300	3.63128900
H	0.41296700	3.42160400	4.46187000
H	-2.91303500	5.32569300	2.51570800
H	-1.61633000	4.85403800	4.58138900
C	0.78672800	3.72853200	-0.96746000
C	1.10039900	5.01031300	-0.51321100
C	1.31788200	3.31291500	-2.19508300
C	1.92622200	5.84854400	-1.26137300
H	0.70702900	5.36551700	0.43671900

C	2.13918800	4.14603200	-2.94170400
H	1.09160700	2.31529600	-2.56709300
C	2.45060600	5.42095500	-2.47424600
H	2.15760200	6.84332700	-0.88725500
H	2.54090700	3.79365800	-3.88985400
H	3.09522800	6.07581200	-3.05577300
C	2.79201800	-4.79916200	-0.31186800
H	3.63501600	-5.15169700	-0.91931000
H	2.22124600	-5.68253200	-0.00083400
H	2.15002700	-4.18856000	-0.95861500
C	4.18263100	-4.89860700	1.76977800
H	5.05967000	-5.23326600	1.20154400
H	4.54974500	-4.37170900	2.65860400
H	3.64675400	-5.79608100	2.10175300
C	3.93286400	1.46146200	2.21125400
H	5.02467400	1.50709400	2.31606300
H	3.53541800	2.45500000	2.45624900
H	3.55836100	0.75515600	2.96248100
C	3.95416400	2.19713300	-0.16373000
H	3.37856900	3.10358100	0.06586000
H	5.01617700	2.45178000	-0.05170700
H	3.77392300	1.94554600	-1.21573800

3

Atom	x	y	z
C	1.99468800	-0.80034700	2.99426900
C	2.04220600	-0.61630600	4.37302200
C	0.92230600	-0.10659700	5.02276300
C	-0.20716300	0.23795600	4.28606600
C	-0.20040500	0.03161600	2.91029800
N	0.87057900	-0.51735000	2.30330300
H	0.93895100	0.04726200	6.09758600
H	2.94367900	-0.85837800	4.92927000
H	-1.07396300	0.67619800	4.77238500
C	3.10121500	-1.19842000	2.12181000
C	-1.23122400	0.45528100	1.95951100
N	-0.92904600	0.23006200	0.71048400
N	2.81546800	-1.15020300	0.85207400
C	-2.43724900	1.15858300	2.47434400
H	-2.12741600	2.04082300	3.05054900
H	-3.10404400	1.48454000	1.67434300
H	-3.00258500	0.50093800	3.14773400
C	4.42524700	-1.52767800	2.71718000
H	4.37260100	-2.48352500	3.25559700

H	5.20653400	-1.59705000	1.95672100
H	4.72148000	-0.76562400	3.44784700
C	-1.77972300	0.77349100	-0.29935800
C	-1.39941100	2.00671900	-0.85767600
C	-2.92423500	0.08128800	-0.73394600
C	-2.24017400	2.60491400	-1.79435800
C	-3.73274500	0.72388100	-1.66622700
C	-3.40574500	1.97229000	-2.17580000
H	-1.98878200	3.56045200	-2.24869800
C	3.83693900	-1.31417200	-0.13550200
C	4.29479300	-2.58231700	-0.53435600
C	4.30425500	-0.12834800	-0.74452600
C	5.24754700	-2.63770600	-1.55575100
C	5.25365600	-0.24353200	-1.75801600
C	5.72318300	-1.48710000	-2.16455500
H	5.61878000	-3.60887500	-1.87893300
H	5.63165500	0.65423000	-2.24160100
H	6.46268700	-1.55603800	-2.95881500
C	3.80289900	-3.87755900	0.08197600
H	2.97769200	-3.63650500	0.76863000
C	3.82307600	1.23402300	-0.27766000
H	2.76012200	1.12849900	0.00622200
C	-3.25401800	-1.30740300	-0.21644900
H	-2.30331200	-1.70126800	0.17022900
C	-0.08405600	2.64778900	-0.44631300
H	0.61814200	1.80772400	-0.30872300
C	0.75508900	-0.94010800	-1.55859700
H	-0.22602500	-0.55653300	-1.86801500
H	1.37410200	-0.06746400	-1.24868700
C	1.47389500	-1.57004200	-2.73780300
H	0.86480400	-2.38945300	-3.14887300
H	2.41924200	-2.01803300	-2.39834500
C	1.76816900	-0.55679100	-3.83314000
H	0.84904400	-0.08714500	-4.20924700
H	2.43314700	0.24028000	-3.47100500
H	2.26538300	-1.03573400	-4.68373800
Co	0.81872400	-0.86897300	0.49606600
C	0.29056400	-2.57389600	-0.60669100
H	1.10510400	-3.17019700	-1.01371600
H	-0.62020100	-2.66095600	-1.20525500
C	0.13699300	-2.66637200	0.82037400
H	-0.87029300	-2.68370000	1.24318200
H	0.84630100	-3.29249300	1.36688400
F	-4.86113700	0.15288600	-2.09119800

F	-4.22640000	2.53714100	-3.05728000
C	-4.19139400	-1.27901000	0.97638700
C	-5.37117400	-0.53039500	0.98070900
C	-3.87206700	-2.03373200	2.10693800
C	-6.19541500	-0.52034400	2.10087100
H	-5.65388100	0.04152300	0.09916600
C	-4.69816400	-2.03013100	3.22736800
H	-2.96276500	-2.63704500	2.10412700
C	-5.86025300	-1.26488600	3.22904900
H	-7.10917200	0.06949900	2.09037700
H	-4.43410700	-2.62658300	4.09799100
H	-6.50826900	-1.25517500	4.10236300
C	-3.66208900	-2.27935900	-1.31999500
C	-4.71609100	-3.17690600	-1.16245300
C	-2.91273300	-2.33116900	-2.50115900
C	-5.01301000	-4.10427500	-2.15882700
H	-5.31498900	-3.15573600	-0.25442500
C	-3.20602600	-3.25677300	-3.49461300
H	-2.09503400	-1.62333900	-2.65270100
C	-4.26067500	-4.15010900	-3.32591400
H	-5.84222700	-4.79397300	-2.01769500
H	-2.61254800	-3.27641600	-4.40624200
H	-4.49512800	-4.87401400	-4.10262500
C	0.51392700	3.50873200	-1.54826100
C	0.79367400	2.90168000	-2.77800800
C	0.83847900	4.85339900	-1.38047800
C	1.38597500	3.61245000	-3.81158100
H	0.54220100	1.84972000	-2.92039000
C	1.43562100	5.57071600	-2.41756900
H	0.63597900	5.34871800	-0.43292800
C	1.71330100	4.95549800	-3.63183900
H	1.59920700	3.11480300	-4.75609500
H	1.68416400	6.61918300	-2.26903700
H	2.18063500	5.51790300	-4.43664000
C	-0.15601600	3.33603000	0.90157100
C	0.87817100	3.15443400	1.82338700
C	-1.21756500	4.17676200	1.24071600
C	0.84707100	3.78353600	3.06435500
H	1.71818600	2.50590800	1.56093700
C	-1.24744400	4.81613700	2.47673700
H	-2.03001500	4.32818700	0.52993100
C	-0.21922000	4.61587900	3.39478200
H	1.65812100	3.62491800	3.77256800
H	-2.07900900	5.47174400	2.72516600

H	-0.24577700	5.11374600	4.36120100
C	4.90534200	-4.56705100	0.88713600
H	4.52179500	-5.47570100	1.36715100
H	5.73347700	-4.86682900	0.23213600
H	5.32291100	-3.92090300	1.66689300
C	3.27265800	-4.85170000	-0.97107200
H	2.76986100	-5.69876100	-0.48894300
H	2.56215000	-4.38454900	-1.66403700
H	4.08956800	-5.26266100	-1.57757000
C	4.58482000	1.69722300	0.96611800
H	5.66346600	1.72674600	0.76216900
H	4.27408500	2.70996600	1.25379000
H	4.42796100	1.04260800	1.83193500
C	3.91170700	2.31443300	-1.34724000
H	3.44775400	2.00799000	-2.29301300
H	3.39665700	3.22222000	-1.00667300
H	4.95329700	2.59357000	-1.55294000

Quartet:

1

Atom	x	y	z
C	0.00645800	0.17358400	2.85394700
C	-0.05630900	0.16419600	4.24374700
C	1.05814000	-0.28431600	4.94791500
C	2.18857100	-0.72132200	4.26469500
C	2.16107600	-0.71082900	2.87227000
N	1.09755000	-0.24793400	2.21174200
H	1.04266700	-0.29845900	6.03402000
H	-0.95045900	0.49290300	4.76598100
H	3.06173700	-1.07349500	4.80594100
C	-1.07086100	0.64951300	1.94451800
C	3.24745300	-1.18969800	1.97831700
N	2.89401500	-1.36077300	0.75162700
N	-0.88745700	0.36365100	0.69979500
C	4.60853400	-1.38165900	2.54317300
H	4.98537000	-0.43104100	2.94385100
H	4.58174700	-2.09001400	3.38083200
H	5.30964000	-1.75445700	1.79317900
C	-2.20546800	1.40255100	2.53602700
H	-2.74884300	0.75439400	3.23746400
H	-1.82589700	2.26566800	3.09820100
H	-2.91052700	1.74833300	1.77810800
C	3.83960500	-1.69932300	-0.26646100

C	3.90054400	-3.02958500	-0.72049500
C	4.58543600	-0.66852500	-0.86588500
C	4.74240900	-3.31061900	-1.79516900
C	5.40915000	-1.00628700	-1.94143300
C	5.48876200	-2.31040700	-2.40600600
H	4.81244100	-4.33183100	-2.16314600
H	5.99350200	-0.22460200	-2.42472800
H	6.13331800	-2.55100900	-3.24796500
C	-1.78944400	0.86255100	-0.28330900
C	-1.47856500	2.08188200	-0.90280400
C	-2.91006300	0.09776000	-0.63931700
C	-2.38006400	2.60189600	-1.82824200
C	-3.80570200	0.68108800	-1.53039300
C	-3.54520100	1.91572200	-2.11172200
H	-2.18084300	3.53988000	-2.34248900
C	-0.16056100	2.76620100	-0.57616300
H	0.56092600	1.93538500	-0.46036300
C	-3.08646200	-1.30134000	-0.07321900
H	-2.05798600	-1.65346800	0.11833700
C	4.51848700	0.77760100	-0.41094000
H	3.79998600	0.85176900	0.42131100
C	3.13084000	-4.13503300	-0.02653900
H	2.23458500	-3.68256300	0.42775200
C	0.92748000	-0.74456000	-1.81022900
H	0.18039000	-0.10747800	-2.30997000
H	1.88544700	-0.59490700	-2.33491800
C	0.50622700	-2.21369600	-1.91815400
H	-0.50455800	-2.35538900	-1.49693200
H	1.17048500	-2.84293800	-1.30357600
C	0.51995900	-2.74218400	-3.34543200
H	-0.10301700	-2.11626700	-3.99908700
H	1.54031600	-2.72347400	-3.75312200
H	0.14446400	-3.77194200	-3.41060100
Co	1.02849300	-0.47081900	0.14161300
C	3.96798600	-4.74389500	1.09924000
H	4.26796400	-3.99966200	1.84601800
H	3.41305700	-5.53707400	1.61544100
H	4.88590200	-5.18841800	0.69202900
C	2.66921000	-5.24026200	-0.97009700
H	3.50947300	-5.86101900	-1.30621600
H	1.97039700	-5.90779300	-0.45270100
H	2.16539400	-4.84591200	-1.86060800
C	5.87338400	1.26043800	0.10391400
H	6.61816300	1.27030100	-0.70184200

H	5.79865500	2.28334200	0.49266100
H	6.26554600	0.61863800	0.90264000
C	4.01176900	1.69339600	-1.52362200
H	3.89938600	2.72306800	-1.16007400
H	4.70915100	1.71756800	-2.37034500
H	3.03887400	1.36151100	-1.90756300
C	0.34801800	3.61695900	-1.72809400
C	0.85637700	2.96831700	-2.85874100
C	0.30182800	5.01018400	-1.71923700
C	1.31395800	3.69356500	-3.95091500
H	0.89136800	1.87802600	-2.87591900
C	0.75377800	5.73935800	-2.81788200
H	-0.08190800	5.53535900	-0.84653500
C	1.26149800	5.08558700	-3.93392200
H	1.71092300	3.17149300	-4.81867100
H	0.70997400	6.82589400	-2.79516900
H	1.61592700	5.65685100	-4.78868900
C	-0.18474700	3.49777700	0.75052700
C	0.92219600	3.42003200	1.59947100
C	-1.27487400	4.27710600	1.14292300
C	0.93821800	4.09250500	2.81744400
H	1.78951300	2.83252400	1.29030800
C	-1.25784300	4.96387200	2.35357100
H	-2.14683700	4.34321100	0.49221000
C	-0.15467000	4.86734400	3.19781000
H	1.80986500	4.02407400	3.46488600
H	-2.11192600	5.57360100	2.63976100
H	-0.14286600	5.40252400	4.14437800
C	-3.77766800	-1.27691300	1.27358700
C	-4.98883900	-0.60325100	1.45045100
C	-3.20379100	-1.92888000	2.36599500
C	-5.60082400	-0.56657600	2.69813700
H	-5.45693900	-0.11466100	0.59638500
C	-3.81152500	-1.88992500	3.61909800
H	-2.26892000	-2.47562200	2.23016700
C	-5.00975200	-1.20279700	3.78855000
H	-6.54533900	-0.04155600	2.82107700
H	-3.35063400	-2.40312500	4.46084300
H	-5.48925700	-1.17097100	4.76408900
C	-3.66386400	-2.29585800	-1.07245700
C	-3.10692500	-2.36650900	-2.35399000
C	-4.67963400	-3.18758800	-0.73576300
C	-3.55474600	-3.30289400	-3.27559800
H	-2.31719800	-1.66835200	-2.63492100

C	-5.13162600	-4.12699500	-1.66067400
H	-5.12704600	-3.15198500	0.25547700
C	-4.57250700	-4.18948200	-2.93074400
H	-3.10973000	-3.33869900	-4.26785600
H	-5.92933000	-4.81181900	-1.38155600
H	-4.92893200	-4.92191700	-3.65121700
F	-4.94438800	0.06475800	-1.84726400
F	-4.43287000	2.41829600	-2.96637600

2

Atom	x	y	z
C	1.97794700	-0.74268300	2.98831700
C	1.99171200	-0.62806100	4.37662200
C	0.84225300	-0.17058200	5.01298800
C	-0.26999100	0.18812300	4.25938800
C	-0.20457400	0.04975400	2.87383900
N	0.89108000	-0.42559600	2.27948000
H	0.81956400	-0.07579000	6.09475300
H	2.87732900	-0.88796200	4.94973300
H	-1.16119700	0.57972500	4.74077800
C	3.14025800	-1.13184900	2.15105100
C	-1.25642600	0.49042600	1.92279600
N	-1.01986100	0.21871100	0.68360000
N	2.89670600	-1.20945700	0.88949000
C	-2.42651000	1.23325300	2.46367100
H	-2.09287200	2.09678400	3.05212500
H	-3.09472800	1.57932200	1.67292500
H	-3.00173200	0.57533500	3.12969500
C	4.45986200	-1.33892700	2.80870800
H	4.43547600	-2.26630800	3.39742100
H	5.26961600	-1.41278500	2.07911200
H	4.68301500	-0.52428300	3.50726100
C	-1.85852400	0.77861800	-0.32511500
C	-1.45305600	1.99512600	-0.90289700
C	-3.01147200	0.09632500	-0.74163600
C	-2.28802400	2.58549000	-1.84944800
C	-3.80916600	0.72820600	-1.69011000
C	-3.46202900	1.96082700	-2.22159500
H	-2.02567100	3.52784500	-2.32433200
C	3.95126400	-1.36120200	-0.06414800
C	4.41225900	-2.63183700	-0.43687400
C	4.42556600	-0.17990600	-0.66937800
C	5.41180300	-2.69824900	-1.41145500
C	5.42336600	-0.30353800	-1.63389400

C	5.91928700	-1.54989300	-1.99967100
H	5.79078900	-3.67188000	-1.71840700
H	5.81362200	0.59044500	-2.11550200
H	6.69650300	-1.62450700	-2.75649600
C	3.85230300	-3.90739900	0.15776700
H	2.98215400	-3.63734300	0.77601200
C	3.87425900	1.17855600	-0.27687500
H	2.81735700	1.02573800	0.00494900
C	-3.35681500	-1.27351500	-0.18653900
H	-2.40483200	-1.66934100	0.19952400
C	-0.11586500	2.60725300	-0.51037100
H	0.56814800	1.74814500	-0.39346200
C	1.00597900	-0.52101200	-1.76837400
H	-0.00776600	-0.23344100	-2.10448000
H	1.60164000	0.41027200	-1.79985700
C	1.59329000	-1.49662100	-2.77876400
H	0.92715200	-2.36662100	-2.89700500
H	2.55416900	-1.90078200	-2.41909200
C	1.81874100	-0.85716300	-4.14252200
H	0.88096900	-0.45430200	-4.54994400
H	2.53041900	-0.02227800	-4.06741900
H	2.22179200	-1.56871200	-4.87411300
Co	0.84824600	-0.90707500	0.20580000
C	0.16985100	-2.91851800	-0.27724200
H	1.03862500	-3.36405500	-0.76039900
H	-0.70600100	-2.77166200	-0.91125900
C	0.09279900	-2.83323400	1.07690000
H	-0.84316500	-2.59176900	1.57959500
H	0.89638000	-3.20230600	1.71245700
F	-4.94531700	0.16320000	-2.10079000
F	-4.27309400	2.52236800	-3.11490300
C	-4.28303400	-1.20175400	1.01318300
C	-5.42964300	-0.40330900	1.02273600
C	-3.98556200	-1.95864500	2.14851900
C	-6.24062400	-0.34704000	2.15124900
H	-5.69909100	0.17143400	0.13905300
C	-4.79745300	-1.90767900	3.27827500
H	-3.10681500	-2.60587900	2.13992200
C	-5.92501000	-1.09236800	3.28421700
H	-7.12854000	0.28110300	2.14384700
H	-4.54978400	-2.50646900	4.15217300
H	-6.56189100	-1.04569900	4.16440900
C	-3.78361700	-2.25989100	-1.26822900
C	-4.91843600	-3.05801400	-1.14901000

C	-2.97199900	-2.40934100	-2.39868600
C	-5.23432500	-3.98868700	-2.13673500
H	-5.56582400	-2.95579400	-0.28075400
C	-3.28495600	-3.33815600	-3.38278100
H	-2.09091700	-1.77466100	-2.51526500
C	-4.42074900	-4.13382300	-3.25365000
H	-6.12660500	-4.60138500	-2.02947700
H	-2.64274300	-3.43727400	-4.25510700
H	-4.66985100	-4.86052100	-4.02320600
C	0.49240800	3.47740500	-1.60434400
C	0.68375600	2.92665500	-2.87870800
C	0.93456400	4.78030800	-1.37318300
C	1.30212100	3.65245900	-3.88713900
H	0.35312900	1.90768100	-3.07677100
C	1.55548200	5.51104300	-2.38599100
H	0.80614700	5.23469600	-0.39289700
C	1.74394600	4.95127900	-3.64292400
H	1.44437800	3.19853600	-4.86599200
H	1.89294700	6.52524600	-2.18421000
H	2.23095000	5.52151000	-4.43051100
C	-0.15428600	3.28614600	0.84371000
C	0.86460000	3.04425400	1.76872400
C	-1.16469100	4.18883900	1.18069200
C	0.87167400	3.67837200	3.00792200
H	1.66055200	2.33983900	1.51340500
C	-1.15889600	4.82975600	2.41597100
H	-1.96161800	4.39004600	0.46479100
C	-0.14352300	4.57339200	3.33507800
H	1.67225900	3.47331700	3.71657000
H	-1.95036300	5.53406000	2.66186400
H	-0.14063700	5.07653100	4.29913000
C	4.87191100	-4.59977300	1.06080900
H	4.44362000	-5.50439700	1.50994700
H	5.75757900	-4.90450400	0.48849500
H	5.21613600	-3.94735500	1.87167700
C	3.37424300	-4.87449700	-0.92434500
H	2.81799700	-5.70737200	-0.47688600
H	2.72600300	-4.38474300	-1.66231600
H	4.21965400	-5.30747700	-1.47327500
C	4.60635200	1.76194800	0.93245400
H	5.68302100	1.83444000	0.72919500
H	4.24144200	2.77389900	1.15085900
H	4.48180300	1.15987800	1.84114800
C	3.89917600	2.19054800	-1.41561000

H	3.45362600	1.79015900	-2.33474500
H	3.33348900	3.08859400	-1.13281500
H	4.92236600	2.51491200	-1.64628800

TS-2/3

Atom	x	y	z
C	1.97703700	-1.16285700	2.87278500
C	1.92863200	-1.34553100	4.25157400
C	0.74296700	-1.05161200	4.92047000
C	-0.34758600	-0.55200400	4.21381300
C	-0.22885900	-0.38886300	2.83636000
N	0.90567200	-0.71261300	2.20302900
H	0.67472700	-1.19663500	5.99467000
H	2.79677000	-1.70609300	4.79626600
H	-1.26868700	-0.29245100	4.72791900
C	3.16226100	-1.35750900	2.01124400
C	-1.24939500	0.20006700	1.94401400
N	-1.00278000	0.09558400	0.67308000
N	2.94536800	-1.22371100	0.74287700
C	-2.41092300	0.88586900	2.57179100
H	-2.05404300	1.68537900	3.23454000
H	-3.08932100	1.31694800	1.83382200
H	-2.97699900	0.17170600	3.18464400
C	4.47518100	-1.65342800	2.64822500
H	4.46912500	-2.67835200	3.04403500
H	5.29854500	-1.56558300	1.93526400
H	4.66326100	-0.98349700	3.49492200
C	-1.86944700	0.75706300	-0.24654800
C	-1.52819900	2.05362200	-0.66553600
C	-3.01078600	0.09161400	-0.72593100
C	-2.40821000	2.73219900	-1.50713900
C	-3.86926900	0.81999500	-1.54260600
C	-3.57716000	2.12378000	-1.91843500
H	-2.18864100	3.73777600	-1.85837000
C	4.01038700	-1.18406700	-0.20777100
C	4.55419200	-2.36143400	-0.74486800
C	4.41207200	0.09515900	-0.64854900
C	5.54042800	-2.23245200	-1.72686000
C	5.39756300	0.16556700	-1.63113500
C	5.96090200	-0.98711600	-2.16751900
H	5.98154700	-3.13174900	-2.15400500
H	5.73013200	1.13800900	-1.98770400
H	6.72804500	-0.91082500	-2.93440800
C	4.10552400	-3.74301200	-0.31387700

H	3.25227000	-3.62474700	0.37081700
C	3.81436600	1.35165400	-0.04098700
H	2.76469800	1.12057300	0.22059200
C	-3.27085200	-1.35880600	-0.35650000
H	-2.27591800	-1.77052000	-0.13030200
C	-0.21908600	2.67894700	-0.20888400
H	0.51146900	1.85108000	-0.18121500
C	0.91488200	-0.58811100	-1.83819900
H	-0.07667000	-0.21874000	-2.13506500
H	1.45393400	0.25854700	-1.35447100
C	1.73191900	-1.01788300	-3.03823600
H	1.20786600	-1.82237400	-3.57599200
H	2.68872700	-1.44358800	-2.69582600
C	2.00983600	0.12332100	-4.00536400
H	1.07822500	0.56548300	-4.38368300
H	2.59070000	0.92283700	-3.52585200
H	2.58534900	-0.22541400	-4.87052600
Co	0.85557900	-0.98108700	0.25466700
C	0.43606100	-2.49901800	-1.17405200
H	1.29793900	-2.92796200	-1.68225900
H	-0.44989600	-2.45262500	-1.81141100
C	0.25475600	-2.90248200	0.18973500
H	-0.75468700	-3.02764500	0.58431500
H	1.00252400	-3.55367100	0.64575800
F	-5.00932400	0.28326700	-1.97896300
F	-4.43851100	2.77061700	-2.70005900
C	-4.06464200	-1.48952900	0.92799800
C	-5.26077500	-0.79533800	1.12838900
C	-3.59386400	-2.32385500	1.94343500
C	-5.95517700	-0.91825800	2.32679200
H	-5.65512200	-0.16146200	0.33562800
C	-4.28515500	-2.44705800	3.14590100
H	-2.67396700	-2.88909900	1.78508300
C	-5.46620100	-1.73763300	3.34216100
H	-6.88537900	-0.37282100	2.46876200
H	-3.90405300	-3.10282800	3.92601200
H	-6.01120300	-1.83027900	4.27867600
C	-3.78994900	-2.19645700	-1.51898900
C	-4.89080000	-3.04137800	-1.40038300
C	-3.09831300	-2.16485400	-2.73488200
C	-5.29354000	-3.83410900	-2.47312600
H	-5.44315800	-3.08492900	-0.46405300
C	-3.49818500	-2.95427100	-3.80510700
H	-2.24046900	-1.49859900	-2.84829800

C	-4.60154000	-3.79448500	-3.67704000
H	-6.15759300	-4.48551400	-2.36244500
H	-2.94905800	-2.91211100	-4.74318300
H	-4.91886100	-4.41278900	-4.51336100
C	0.33799000	3.67574800	-1.21507000
C	0.63703300	3.21536800	-2.50294400
C	0.61166700	5.00620000	-0.90315700
C	1.20012400	4.05654700	-3.45175500
H	0.42978500	2.17450400	-2.75688300
C	1.17852500	5.85373400	-1.85519200
H	0.39482400	5.38856900	0.09214000
C	1.47673800	5.38377900	-3.12780500
H	1.42971400	3.67451300	-4.44483100
H	1.38794000	6.88854000	-1.59353900
H	1.92078300	6.04684500	-3.86648100
C	-0.28440100	3.21190800	1.20825200
C	0.75852000	2.93790300	2.09635900
C	-1.34889100	4.00168400	1.64744600
C	0.73407100	3.42403400	3.40029500
H	1.60018400	2.32891400	1.75717400
C	-1.37246100	4.49898500	2.94698800
H	-2.16757800	4.22719100	0.96382500
C	-0.33500800	4.20587900	3.82950300
H	1.55356600	3.19520400	4.07893700
H	-2.20630000	5.11654000	3.27314200
H	-0.35731000	4.59207400	4.84581700
C	5.21414000	-4.48322000	0.43370900
H	4.86649000	-5.46978500	0.76414000
H	6.08293100	-4.64190400	-0.21806100
H	5.56158400	-3.93249400	1.31533900
C	3.63880100	-4.58554900	-1.50082300
H	3.15362100	-5.50549700	-1.15269600
H	2.92955700	-4.04794500	-2.14227800
H	4.48430700	-4.88350700	-2.13381100
C	4.53527900	1.73647100	1.25192600
H	5.60414300	1.89534600	1.05644200
H	4.13042900	2.67182600	1.65988400
H	4.45285800	0.96815400	2.02996900
C	3.80172000	2.54858300	-0.98338100
H	3.36743300	2.30897800	-1.96168100
H	3.20890700	3.36406000	-0.54820200
H	4.81265700	2.94298100	-1.14841300

Atom	x	y	z
C	1.05353100	-1.30638200	3.33690800
C	0.80765800	-1.31398000	4.70782300
C	-0.36996100	-0.72968300	5.16660000
C	-1.25398700	-0.12947600	4.27330500
C	-0.94199900	-0.17182500	2.91759100
N	0.15868900	-0.79300300	2.49180000
H	-0.58697700	-0.71707700	6.23103500
H	1.52044800	-1.74429000	5.40497400
H	-2.14966000	0.36963000	4.63074400
C	2.31180400	-1.74415400	2.67418800
C	-1.71814800	0.47198200	1.82116100
N	-1.13416100	0.43508000	0.67049500
N	2.41229900	-1.40500500	1.43372500
C	-3.00764900	1.12409100	2.15289700
H	-3.68301400	0.41907400	2.65266600
H	-2.81265000	1.95072000	2.85154100
H	-3.50335700	1.52923000	1.26967800
C	3.35105700	-2.43156800	3.48319500
H	3.57280500	-1.85492300	4.38971200
H	2.99150100	-3.41551900	3.81234200
H	4.27582400	-2.56204000	2.91658600
C	-1.73914300	0.92850600	-0.51748600
C	-1.31190700	2.17549500	-0.99809500
C	-2.61626900	0.08465400	-1.23203500
C	-1.83977200	2.63491700	-2.20293100
C	-3.13014600	0.60484100	-2.41436100
C	-2.74857000	1.85529100	-2.88808600
H	-1.54077000	3.59114600	-2.62601600
C	3.57553400	-1.66183600	0.64883300
C	3.86650400	-2.94538300	0.15427000
C	4.34427900	-0.53152100	0.29785200
C	4.97587000	-3.07203900	-0.68776400
C	5.44090900	-0.71680200	-0.53903700
C	5.75733700	-1.97911400	-1.03006600
H	5.22557800	-4.05403300	-1.08670100
H	6.05278900	0.13838700	-0.81796100
H	6.61403600	-2.10744000	-1.68728800
C	3.03827900	-4.17593700	0.47250900
H	2.17528600	-3.86859900	1.08229100
C	3.98562000	0.83203000	0.85417800
H	2.88196000	0.86934900	0.90248200
C	-2.93046500	-1.30700000	-0.68960500
H	-2.03101200	-1.57525600	-0.11499400

C	-0.26985700	2.95435900	-0.20871000
H	0.49186300	2.20864200	0.08050900
C	0.85849500	-1.22139400	-1.39994700
H	1.39052900	-2.18474200	-1.43524400
H	-0.06733200	-1.35378300	-1.97282500
C	1.72186200	-0.13823800	-2.04568700
H	2.42879700	0.30517300	-1.31854600
H	1.07801700	0.69099700	-2.38435400
C	2.55716800	-0.64682300	-3.21547400
H	3.22775000	-1.44206300	-2.84501200
H	1.89423100	-1.12740500	-3.95280600
Co	0.63380900	-0.70353500	0.48824800
C	3.38385600	0.43510700	-3.89208100
H	2.71054100	1.19291900	-4.32245800
H	3.98535900	0.95911200	-3.13022000
C	4.30143000	-0.11845100	-4.96778600
H	4.87870700	0.67028800	-5.46338700
H	5.01579400	-0.83584300	-4.54170000
H	3.73082800	-0.64669000	-5.74241300
F	-4.02417500	-0.07117200	-3.13356900
F	-3.27953700	2.28557200	-4.03019500
C	-4.07591100	-1.30104900	0.30683100
C	-5.22677100	-0.53324800	0.12167800
C	-3.98593200	-2.11777600	1.43687800
C	-6.26115500	-0.57634700	1.05168900
H	-5.31412600	0.10785400	-0.75530100
C	-5.01455400	-2.15754400	2.37198300
H	-3.09603800	-2.73526700	1.57479700
C	-6.15657000	-1.38257800	2.18173200
H	-7.15387000	0.02401300	0.89197400
H	-4.93001800	-2.79937100	3.24627800
H	-6.96560800	-1.41305500	2.90771000
C	-3.08085000	-2.44711500	-1.69438400
C	-1.99190800	-3.29361500	-1.91640600
C	-4.28875800	-2.74393100	-2.33068600
C	-2.08491000	-4.37471600	-2.78759300
H	-1.05536100	-3.11013400	-1.39022800
C	-4.38601200	-3.82250200	-3.20042400
H	-5.16710600	-2.13127400	-2.14147200
C	-3.28262400	-4.63729200	-3.44089700
H	-1.21951900	-5.01477800	-2.94625900
H	-5.33436000	-4.03168800	-3.69043700
H	-3.36293600	-5.48036200	-4.12312300
C	-0.81110000	3.51822900	1.09119700

C	-0.05285900	3.40477900	2.25917000
C	-2.04415200	4.17058900	1.15449200
C	-0.51156300	3.93137200	3.46250700
H	0.91229600	2.89412700	2.21756900
C	-2.50147300	4.70959300	2.35360600
H	-2.65691700	4.24629200	0.25576200
C	-1.73880400	4.58875800	3.51217400
H	0.09185000	3.83430900	4.36258900
H	-3.46048200	5.22193500	2.38376900
H	-2.09787400	5.00787600	4.44918400
C	0.46378000	3.99224000	-1.04131200
C	0.02909900	5.31338000	-1.15996200
C	1.60944100	3.60133800	-1.73719800
C	0.72335000	6.21639100	-1.96069400
H	-0.85229200	5.64659000	-0.61473800
C	2.31003600	4.50221600	-2.53058000
H	1.95813900	2.57230100	-1.64778400
C	1.86520600	5.81564700	-2.64664500
H	0.37110900	7.24224100	-2.04177400
H	3.20663800	4.17713200	-3.05548800
H	2.40865400	6.52574300	-3.26538300
C	2.48968600	-4.84240400	-0.78918600
H	3.29811900	-5.24408500	-1.41222300
H	1.83812400	-5.68312200	-0.52134500
H	1.91039700	-4.14945900	-1.41068100
C	3.85104300	-5.19548100	1.27229300
H	4.68999200	-5.57468900	0.67544100
H	4.27179900	-4.77291800	2.19208400
H	3.22988000	-6.05672300	1.54706100
C	4.51674700	1.00352400	2.27741300
H	5.61321000	0.94953100	2.28173100
H	4.22795200	1.98061800	2.68497600
H	4.14697100	0.23044300	2.96222000
C	4.45170400	1.99645900	-0.00835300
H	4.03068100	2.93595600	0.37079800
H	5.54357600	2.10402700	0.01105700
H	4.14103500	1.88713900	-1.05551800

C₂H₄

Atom	x	y	z
C	0.66343500	0.00000600	0.00030100
H	1.23805800	-0.92465000	-0.00091400
H	1.23828100	0.92451300	-0.00094800
C	-0.66335800	0.00000500	0.00034000

H	-1.23837700	0.92437000	-0.00097700
H	-1.23842400	-0.92430200	-0.00101000