

**N-heterocyclic carbene (NHC)-catalyzed oxidative [3+2]
annulation of dioxindoles and enals: mechanism, role of
NHC, role of a mixture of bases with different strength,
and origin of stereoselectivity**

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Table S1. Comparison of single point energies of the transition states in the stereoselectivity determining step.

[illegible]

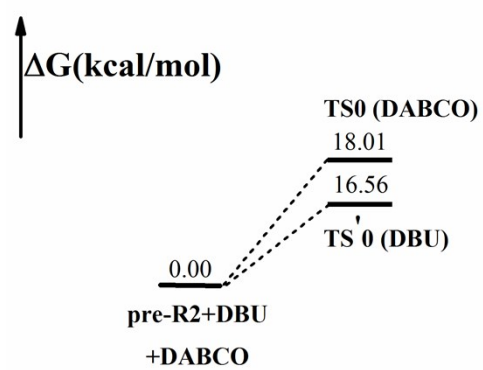
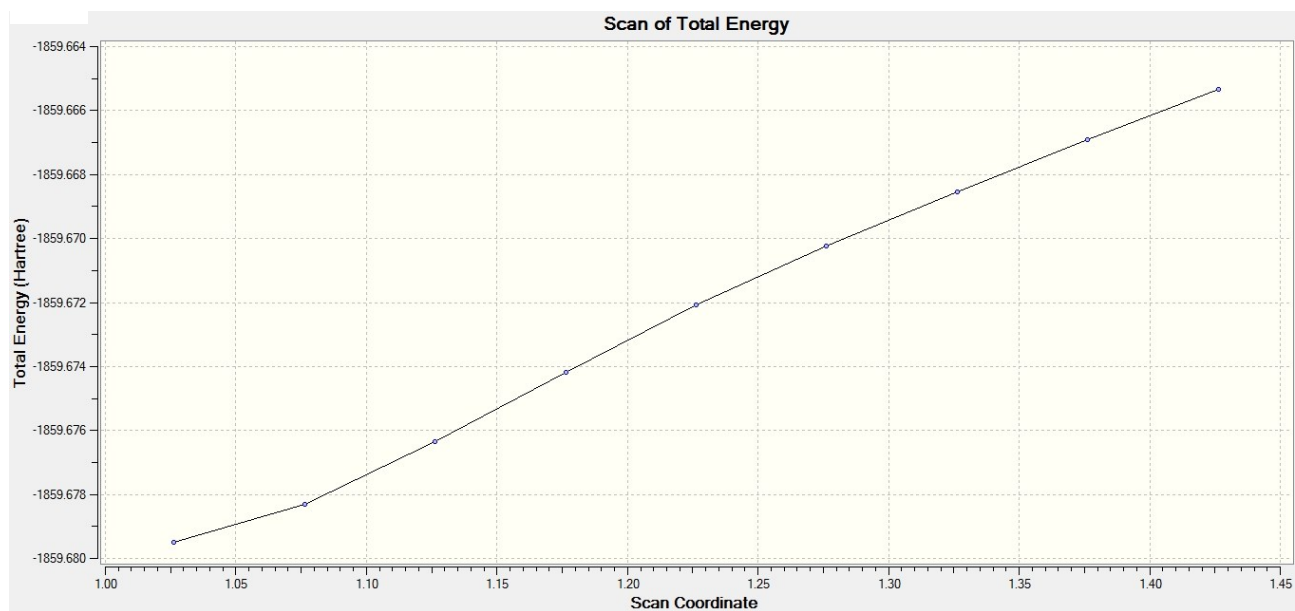


Fig. S1 The relative Gibbs free energy of the protonation of Pre-R2 using DBU and DABCO bases.

(a)



(b)

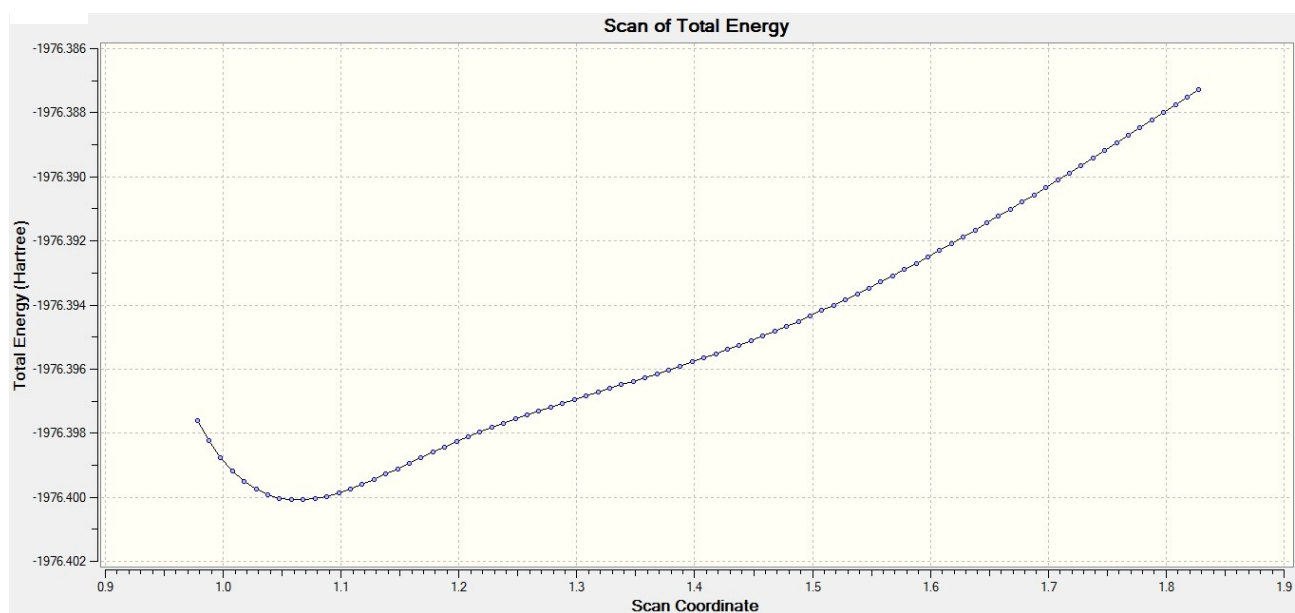


Fig. S2 The scanning curve of O²⁻ H⁷ (see scheme 2) for the generation of Int3d using (a) DABCO.H⁺, and (b) DBU.H⁺ species.

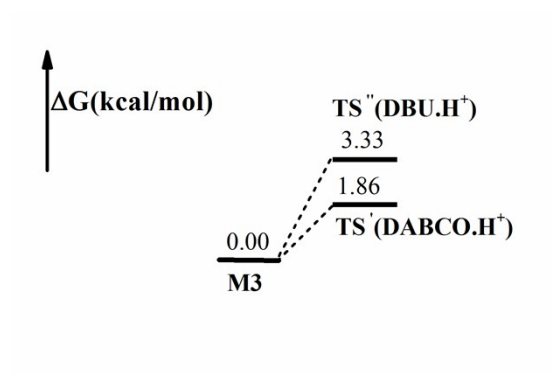


Fig. S3 The relative Gibbs free energy for the transformation of $[\text{NBH}]^-$ in M3 complex to NO and H_2O species using DBU.H^+ and DABCO.H^+ species.

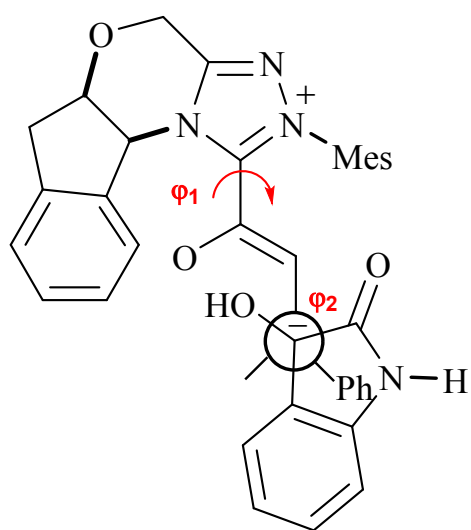


Fig. S4 Representation of dihedral angles in the critical region of the conformational space.

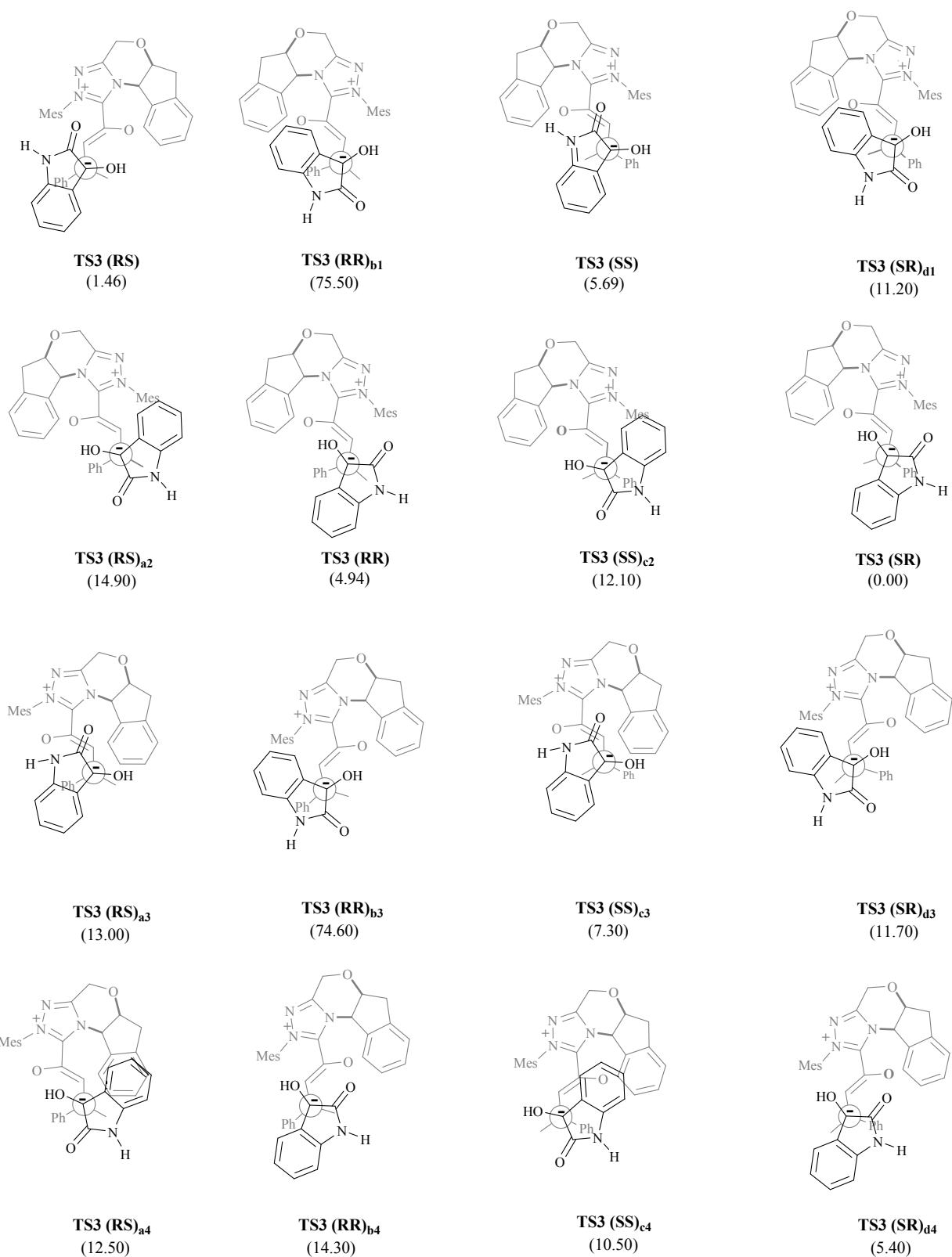


Fig. S5 Different conformers of transition states for stereoselectivity-determining step. The relative Gibbs free energies with respect to the lowest Gibbs free energy, TS3 (SR) transition state, are indicated in the parenthesis in kcal mol⁻¹.

The optimized structures, Gibbs free energies (GFE), and the imaginary frequency of all the transition states discussed in the main text.

NHC

GFE= -1051.82712243 a.u.

C	0.10036200	0.01880100	0.81332500
C	-0.53612900	-1.74682400	-0.44621100
C	-2.30244700	-0.71115700	0.99180500
H	-2.26124800	-0.96110100	2.05487200
N	0.72104900	-1.59971300	-0.72922300
N	1.07721700	-0.51627500	0.05164500
N	-0.94247400	-0.79877300	0.45675800
C	-1.48567500	-2.76605600	-0.99519200
H	-1.00215700	-3.74380200	-1.03220200
H	-1.77888600	-2.49592700	-2.01840500
C	-3.22746900	-1.67389800	0.20202800
O	-2.61342200	-2.89486400	-0.15221000
C	-3.79598600	0.56011200	-0.37305300
C	-2.93073400	0.63403000	0.72033600
C	-2.72302400	1.82972400	1.39703800
C	-3.41411100	2.96251200	0.97178900
C	-4.29197800	2.89083900	-0.11163100
C	-4.48750500	1.69101200	-0.79372600
C	-3.80518500	-0.83083300	-0.95625200
H	-2.02718600	1.87482000	2.22843100
H	-4.82794100	3.78075100	-0.42657900
H	-5.16806100	1.64205900	-1.63866100
H	-3.15732400	-0.87023800	-1.84021100
H	-4.79518400	-1.17858200	-1.26019800
C	2.42883400	-0.05002800	-0.00412800
C	2.68971200	1.19558500	-0.58186000
C	3.44278200	-0.86250800	0.50980200
C	4.01582300	1.62387200	-0.62978100
C	4.75397900	-0.39554000	0.43295900
C	5.05852500	0.84409700	-0.12933500
H	4.23898900	2.58934200	-1.07817900

H	5.55610400	-1.01530000	0.82732100
C	3.11911700	-2.19323500	1.13457900
H	2.74838000	-2.89742700	0.38495200
H	2.33327500	-2.08360600	1.88865000
H	4.00333700	-2.61971500	1.61178900
C	1.57362900	2.03909600	-1.13831100
H	0.87261300	2.32501200	-0.34966700
H	1.00130300	1.48018000	-1.88562600
H	1.97114400	2.94054400	-1.60829300
H	-4.04792600	-1.95288300	0.86817700
H	-3.27139200	3.90728800	1.48610700
C	6.48038100	1.34276500	-0.16887000
H	6.72109200	1.90267300	0.74080200
H	7.18841900	0.51391900	-0.24264800
H	6.64207100	2.01003900	-1.01887000

R1

GFE= -462.072664861 a.u.

C	-2.09986000	0.32504400	0.03704800
C	-0.94393500	1.00113900	0.18467100
C	0.39167300	0.35476600	0.08640200
C	1.40150000	0.92339800	-0.69997300
C	0.67865900	-0.80770900	0.81289100
C	2.65446900	0.32674300	-0.78198000
H	1.19806800	1.82503700	-1.26963700
C	1.93590000	-1.39918900	0.73761400
H	-0.08639600	-1.23269200	1.45637400
C	2.92528500	-0.83599900	-0.06342200
H	3.42165500	0.77004800	-1.40850300
H	2.14326200	-2.29758400	1.30973000
H	-3.04950800	0.83302800	0.18776900
H	3.90560300	-1.29730100	-0.12433500
C	-2.21128100	-1.07344800	-0.40408400
O	-3.27218200	-1.66420100	-0.44987600
H	-1.27701100	-1.56532600	-0.73309800
C	-0.94590000	2.47218700	0.49920400

H	-0.39666100	2.66463600	1.42594700
H	-0.43866200	3.03473100	-0.29160100
H	-1.96195400	2.85743700	0.59612700

DBU

GFE= -461.7888927 a.u.

C	-0.92155500	-1.55070700	-0.11051700
C	0.36475600	-0.73978500	-0.17603500
C	-2.00128900	-1.00796200	0.82708400
C	-0.84757700	1.50830000	-0.04804100
C	-2.90226400	0.00981800	0.12503100
C	-2.09060300	0.96930200	-0.74660500
H	-1.32865600	-1.66510900	-1.12315000
H	-1.10298800	1.81168800	0.98101300
H	-1.52054000	-0.54630700	1.69807200
H	-3.47225300	0.57846300	0.86852400
H	-0.59304000	-2.54430300	0.19649100
H	-2.60688100	-1.83398400	1.21136500
H	-0.52883700	2.42226500	-0.56595000
H	-3.63325000	-0.51346700	-0.50187300
H	-2.71342200	1.82261600	-1.03250000
H	-1.78448600	0.48565700	-1.68050400
C	1.54678300	1.38175200	0.26327400
H	1.79383200	2.02398300	-0.59488700
H	1.34322400	2.04754600	1.11315700
C	2.68421400	-0.68393100	-0.43487600
C	2.70763300	0.45468700	0.57790900
H	3.64597100	1.01532900	0.55161000
H	2.59218300	0.03384600	1.58220400
N	1.43934400	-1.42724500	-0.34363200
N	0.32427200	0.63510000	-0.03468000
H	2.80601000	-0.26815600	-1.44748600
H	3.51723800	-1.37389900	-0.27124100

DBU. H⁺

GFE= -462.2217659 a.u.

C	-5.97794872	-0.09576194	0.23525100
C	-4.69348372	0.71711106	0.16952800
C	-7.06150572	0.44751106	1.16790800
C	-5.90626772	2.96689806	0.30102200
C	-7.96015372	1.46602406	0.46352000
C	-7.14733672	2.42969106	-0.40305800
H	-6.38141672	-0.21626294	-0.77822000
H	-6.16699072	3.26915406	1.32971100
H	-6.58442272	0.90786706	2.04150000
H	-8.53469772	2.03249306	1.20523300
H	-5.64524772	-1.08667894	0.54587600
H	-7.66966472	-0.37769994	1.54993100
H	-5.58773872	3.88331006	-0.21339700
H	-8.68824372	0.94354406	-0.16735800
H	-7.77137472	3.28261406	-0.68781200
H	-6.83715372	1.94986206	-1.33743200
C	-3.51187872	2.84024806	0.60264200
H	-3.26713172	3.47798206	-0.26021600
H	-3.70854472	3.51213906	1.44980600
C	-2.37459272	0.76989906	-0.09012600
H	-1.54539972	0.07748606	0.08042100
H	-2.24813572	1.17833006	-1.10503100
C	-2.35034572	1.91371506	0.91778500
H	-1.41194972	2.47447306	0.88887700
H	-2.46499672	1.49676106	1.92373100
N	-3.62096772	0.03225806	0.00000000
N	-4.73600072	2.09498406	0.31504700
H	-3.64344272	-0.96524394	-0.06697200

DABCO

GFE= -345.1133379 a.u.

C	1.86064316	0.78866768	0.00000000
C	0.30189416	0.78867968	-0.00000500
H	2.26178916	0.79942368	-1.01901300

H	2.26192916	-0.09780632	0.50246600
H	-0.09924384	0.79946968	-1.01902100
H	-0.09940984	-0.09780032	0.50243500
C	1.86070016	3.17324668	0.02185700
H	2.26193116	4.05024868	0.54076700
H	2.26193816	3.18141768	-0.99713000
C	0.30184616	3.17325868	0.02188500
H	-0.09935284	4.05025468	0.54083000
H	-0.09942884	3.18146168	-0.99708800
C	0.30180916	1.96199668	2.07597200
H	-0.09943684	2.84040568	2.59245900
H	-0.09936284	1.07412668	2.57608300
C	1.86076416	1.96201368	2.07596100
H	2.26199816	2.84044468	2.59241900
H	2.26196316	1.07416468	2.57608900
N	2.36666016	1.97456868	0.69914600
N	-0.20410784	1.97457268	0.69916500

Re-TS1

GFE= -1513.87535609 a.u.

Frequency= -181.27 cm⁻¹

C	0.32538400	-0.10324600	0.13453600
C	-0.63790900	-1.29637900	1.74178300
C	-2.19219600	-0.01406100	0.32609700
H	-2.12418400	0.96504800	-0.15980800
N	0.62199100	-1.59449000	1.84087400
N	1.19170100	-0.84863100	0.82860400
N	-0.84944600	-0.39129000	0.73721800
C	-1.82783200	-1.68810100	2.55490300
H	-1.52503200	-2.05089400	3.53716700
H	-2.40383500	-2.47332900	2.04456400
C	-3.15530700	0.04940700	1.56445600
O	-2.60071900	-0.51502700	2.74604000
C	-4.06491900	-1.43645200	-0.12880100
C	-2.79887600	-1.06774100	-0.57517600

C	-2.21471900	-1.65534700	-1.69509300
C	-2.94752600	-2.62336500	-2.37927500
C	-4.22380600	-2.99158600	-1.94668900
C	-4.79105600	-2.40418500	-0.81793100
C	-4.44878200	-0.67134600	1.11383600
H	-1.20736200	-1.39117900	-2.02142500
H	-4.77546800	-3.75216900	-2.49031900
H	-5.77746000	-2.70433200	-0.47646700
H	-4.81875300	-1.31130400	1.92112700
H	-5.23397400	0.06094400	0.89698500
C	2.59787100	-0.94291000	0.56383100
C	3.05820500	-2.02904900	-0.18655300
C	3.44008400	0.05457200	1.05295600
C	4.42461400	-2.09383800	-0.44357500
C	4.80140200	-0.05090500	0.76390000
C	5.30762400	-1.11464900	0.01947800
H	4.80995400	-2.92715800	-1.02681100
H	5.47933500	0.71406500	1.13434500
C	2.89028700	1.20822900	1.84705200
H	2.24692100	0.85910200	2.66032500
H	2.28598900	1.85249400	1.19935600
H	3.69874300	1.80515900	2.27316500
C	6.77959300	-1.21805900	-0.28766900
H	7.34027300	-0.40469800	0.17747700
H	6.95555700	-1.17920100	-1.36680200
H	7.18857200	-2.16543000	0.07545600
C	2.09521900	-3.06289500	-0.70115400
H	1.38465300	-2.58162400	-1.38188100
H	1.53607800	-3.51986100	0.12087700
H	2.62763700	-3.84919300	-1.23937900
H	-3.34394300	1.09109700	1.82924900
C	1.54743000	1.58408100	-1.58996400
C	1.22278200	2.78776900	-1.10536100
C	-0.17020700	3.08592400	-0.64985400
C	-0.45759800	3.18997300	0.71628500
C	-1.20866800	3.27501100	-1.56880300

C	-1.75023200	3.47082300	1.15351600
H	0.33735500	3.04398700	1.44325900
C	-2.50238700	3.55568400	-1.13448000
H	-0.99300900	3.19563700	-2.63066900
C	-2.77700600	3.65464400	0.22851800
H	-1.95480100	3.54611900	2.21729800
H	-3.29460700	3.69938100	-1.86231200
H	2.57144500	1.36066900	-1.88652100
H	-3.78366000	3.87865400	0.56783200
C	0.58634100	0.43678300	-1.75810600
O	0.94518200	-0.59141300	-2.37573700
C	2.22791300	3.89421200	-0.92472100
H	1.94616300	4.77587700	-1.51046600
H	2.26844600	4.21268300	0.12395000
H	3.22643300	3.57187300	-1.22857200
H	-0.46956700	0.77222900	-1.82387500
H	-2.51767500	-3.10022900	-3.25407100

Si-TS1

GFE= 1513.87044898 a.u.

Frequency= -199.58 cm⁻¹

C	-0.29871700	-0.35622400	0.04150800
C	0.47711900	-0.44988100	2.11587500
C	2.17942100	-0.05375900	0.32483100
N	-0.80141500	-0.64487300	2.24208800
N	-1.25590400	-0.58034700	0.94488200
N	0.81684700	-0.27213500	0.79994800
C	1.53853600	-0.38249100	3.16907300
H	1.32843400	-1.09627700	3.96648900
H	1.57086400	0.63046900	3.59868000
C	3.14144300	0.13755300	1.52409700
O	2.78053800	-0.72345700	2.59508100
C	-2.64662700	-0.76663300	0.64858300
C	-3.54318400	0.24911200	0.99349800
C	-3.03783400	-1.93941500	0.00147100

C	-4.88218500	0.06696000	0.66204200
C	-4.39246100	-2.07472000	-0.30841500
C	-5.32305100	-1.08850000	0.01148900
H	-5.59797000	0.84703000	0.91131800
H	-4.72350600	-2.97655400	-0.81733900
C	-2.03644300	-2.99931100	-0.36694200
H	-1.36126000	-3.21268700	0.46745400
H	-1.44074500	-2.65120600	-1.21965300
H	-2.54722200	-3.92360300	-0.64373600
C	-6.78364500	-1.26758300	-0.31371100
H	-7.22586300	-0.33173300	-0.66497800
H	-7.34238000	-1.58192800	0.57380800
H	-6.92734900	-2.02678100	-1.08521200
C	-3.06257200	1.49727100	1.68152700
H	-2.21821000	1.92542200	1.13143600
H	-2.71982500	1.28163800	2.69769100
H	-3.85855800	2.24280700	1.73096000
C	4.49299900	-0.34757900	0.99258100
H	5.03077600	0.48691200	0.52727700
H	5.10648100	-0.73631700	1.80907200
C	4.10938800	-1.38428700	-0.03875100
C	2.77699000	-1.22680900	-0.42205400
C	4.88667800	-2.38505500	-0.60673800
C	2.18951700	-2.04759300	-1.37830700
C	4.30668700	-3.22327900	-1.55921100
H	5.92237200	-2.52017400	-0.30891900
C	2.97564200	-3.05508800	-1.94067500
H	1.15486100	-1.91837400	-1.69891800
H	4.89712600	-4.01643200	-2.00729900
H	2.54291300	-3.71514600	-2.68541000
H	3.15018000	1.17896300	1.87277700
H	2.17355200	0.85256800	-0.29197100
C	-1.44540600	1.13108100	-1.77224700
C	-1.15465000	2.37516500	-1.37217500
C	0.22700200	2.77095800	-0.95797200
C	1.26245100	2.87647800	-1.89398400

C	0.50408800	3.07193900	0.38166500
C	2.54274400	3.26190900	-1.50129600
H	1.05367300	2.65104600	-2.93590700
C	1.78335600	3.45546800	0.77737200
H	-0.28959800	2.99901100	1.12170100
C	2.80798400	3.54995700	-0.16356500
H	3.33220000	3.33972900	-2.24201600
H	1.97963200	3.68608400	1.82059600
H	-2.46715900	0.86997300	-2.04613400
H	3.80403400	3.85374400	0.14293400
C	-0.47597500	-0.02608200	-1.87788200
O	-0.82657500	-1.04853100	-2.51589500
H	0.58155900	0.31237600	-1.93312700
C	-2.19829500	3.45866600	-1.28071500
H	-2.21486900	3.90137600	-0.27773700
H	-1.97552000	4.27207000	-1.98007700
H	-3.19301800	3.06401000	-1.50151300

Re-M1

GFE= 1513.88229862 a.u.

C	0.25467100	-0.13515500	-0.06003700
C	-0.68140500	-0.76391200	1.82077400
C	-2.27494700	0.00901000	0.07630900
H	-2.21873400	0.88388600	-0.57815900
N	0.58527400	-0.99296000	1.99614900
N	1.15359100	-0.60183400	0.80964100
N	-0.92289000	-0.23606600	0.58371100
C	-1.84425800	-0.90650500	2.74548100
H	-1.51200900	-0.90438200	3.78345400
H	-2.38160500	-1.84430500	2.54344800
C	-3.27675700	0.27374100	1.26041600
O	-2.67181900	0.22328200	2.54349700
C	-4.01142000	-1.63812300	-0.05723300
C	-2.80784700	-1.22189000	-0.62002400
C	-2.20178600	-1.91019400	-1.67050800

C	-2.85872700	-3.03410600	-2.16634900
C	-4.07742600	-3.45145600	-1.62410900
C	-4.66077100	-2.76130000	-0.56449100
C	-4.42801600	-0.74938300	1.08740400
H	-1.22605800	-1.60830200	-2.06811700
H	-4.57052000	-4.33068400	-2.02722500
H	-5.60064900	-3.09829600	-0.13684700
H	-4.58056600	-1.30383100	2.01998200
H	-5.36796400	-0.23119500	0.87446100
C	2.55595600	-0.82755100	0.57763500
C	2.92582100	-2.04793200	0.00202900
C	3.47658100	0.13809700	0.98414600
C	4.28562700	-2.26175900	-0.20838300
C	4.82611600	-0.12647200	0.75039800
C	5.24472500	-1.31126800	0.14627700
H	4.60404200	-3.19887800	-0.65856500
H	5.56538500	0.60973400	1.05644700
C	3.03881500	1.41604500	1.64606300
H	2.26948300	1.22911200	2.40115900
H	2.62395300	2.10516100	0.90288800
H	3.88504800	1.90537000	2.13155700
C	6.70468700	-1.56334400	-0.12829800
H	7.34105600	-0.92687300	0.49030500
H	6.94001900	-1.35406100	-1.17674800
H	6.96728800	-2.60651900	0.06470800
C	1.88852400	-3.07051900	-0.36350800
H	1.23576200	-2.63346000	-1.13060300
H	1.28441000	-3.33991200	0.50967900
H	2.36153300	-3.97616600	-0.74738000
H	-3.64236600	1.29763500	1.18177800
C	1.50601300	1.34352700	-1.63396900
C	1.25874300	2.61901300	-1.31919800
C	-0.07894100	3.02235100	-0.77935400
C	-0.37051300	2.89267900	0.58313800
C	-1.06707500	3.53154900	-1.62990800
C	-1.61976100	3.25254000	1.08487300

H	0.38773300	2.49680600	1.25479100
C	-2.31708000	3.89174900	-1.13284600
H	-0.85216300	3.62794300	-2.69070300
C	-2.59641200	3.75420900	0.22630900
H	-1.83234100	3.12674700	2.14247600
H	-3.07390900	4.27936300	-1.80751700
H	2.48137000	1.03633400	-2.01056700
H	-3.56978300	4.03901100	0.61438000
C	0.47577600	0.21042500	-1.55694500
O	0.78226600	-0.89896400	-2.21614800
H	-0.50506700	0.68027400	-1.83152000
C	2.27013200	3.72543600	-1.46883200
H	1.90006000	4.49631500	-2.15457800
H	2.45248600	4.22065900	-0.50774700
H	3.21860200	3.34185700	-1.85184100
H	-2.41416500	-3.59487300	-2.98226100

Si-M1

GFE= -1513.87913095 a.u.

C	0.38552300	-0.25402800	-0.16948800
C	-0.51546600	-0.64237800	1.78407800
C	-2.16872400	-0.12447200	-0.01172300
H	-2.11718800	0.64012100	-0.78759900
N	0.75460600	-0.84109600	1.97503200
N	1.29791100	-0.60466100	0.74143500
N	-0.78624000	-0.28506800	0.49012400
C	-1.64126900	-0.66238600	2.76187200
H	-1.26444900	-0.50213400	3.77218300
H	-2.16492800	-1.62832900	2.72683600
C	-3.14056000	0.23952900	1.17412900
O	-2.49430400	0.41046700	2.42792100
C	-3.80946400	-1.87276800	0.17465000
C	-2.69215200	-1.44363800	-0.53616900
C	-2.17248000	-2.18303200	-1.59661000
C	-2.78112900	-3.39538800	-1.91035800
C	-3.88951600	-3.84609600	-1.18689700

C	-4.41752500	-3.08434900	-0.14790700
C	-4.22366300	-0.86836500	1.21712800
H	-1.34595100	-1.75855700	-2.16499200
H	-4.35163800	-4.79361900	-1.44637100
H	-5.29055500	-3.42769200	0.39965100
H	-4.29502800	-1.29499100	2.22369800
H	-5.20719600	-0.44670200	0.98873300
C	2.70204700	-0.78749200	0.50911500
C	3.11717500	-1.97067500	-0.10799900
C	3.58748400	0.20604000	0.93300500
C	4.48283300	-2.12471400	-0.33985200
C	4.94268900	0.00278900	0.68024600
C	5.40491300	-1.14687400	0.03692000
H	4.83458900	-3.03481100	-0.81898800
H	5.65476800	0.76052500	0.99727700
C	3.08676000	1.43168200	1.64661000
H	2.62012000	1.16256000	2.59889300
H	2.33294400	1.94153800	1.03859800
H	3.90603100	2.12517600	1.84305400
C	6.87179600	-1.32261300	-0.25843200
H	7.48877200	-0.80807200	0.48146300
H	7.11747500	-0.90785600	-1.24131300
H	7.14966600	-2.37883700	-0.26672000
C	2.12618300	-3.04191700	-0.48156500
H	1.47789900	-2.72059200	-1.30358100
H	1.48114800	-3.28934200	0.36688800
H	2.64549000	-3.94838600	-0.79578200
H	-3.57892800	1.21417400	0.96634300
C	1.47238500	1.44055800	-1.55835300
C	1.03246000	2.64261200	-1.17351200
C	-0.38030300	2.91158900	-0.76876100
C	-0.69383600	3.13659700	0.57501500
C	-1.39407300	3.01309500	-1.72810000
C	-1.99319600	3.46538700	0.95868000
H	0.08595200	3.04948700	1.32917000
C	-2.68795900	3.35607700	-1.34841600

H	-1.15725100	2.77969100	-2.75921100
C	-2.98946800	3.59101800	-0.00613600
H	-2.22480900	3.61902200	2.00798000
H	-3.46589300	3.43595500	-2.10131400
H	2.52594800	1.33957100	-1.82223700
H	-3.99986900	3.86112300	0.28660900
C	0.60803600	0.16083900	-1.66000800
C	1.94477700	3.84248900	-1.10400200
H	1.59034700	4.63621400	-1.77065000
H	1.95236000	4.26331500	-0.09128100
H	2.96930500	3.58081700	-1.38003600
H	-2.40049500	-3.99229400	-2.73323000
O	-0.53177200	0.24581500	-2.31827800
H	1.33037500	-0.62625300	-2.01032400

DABCO.H⁺

GFE= -345.521265 a.u.

C	0.72852000	-0.57535000	1.30665700
C	-0.81402400	-0.69627100	1.18825900
H	1.22658100	-1.53452100	1.45475800
H	1.04430500	0.11664800	2.08916000
H	-1.11198600	-1.74432400	1.11333300
H	-1.28937200	-0.27290600	2.07510700
C	0.72724300	-0.84958700	-1.14820200
H	1.23231600	-0.50239800	-2.05067800
H	1.03416300	-1.87570000	-0.93840800
C	-0.81425000	-0.67538800	-1.20061500
H	-1.10499100	-0.08647000	-2.07319300
H	-1.29574900	-1.65212700	-1.27714700
C	-0.80273400	1.38384800	0.01237500
H	-1.27755800	1.94374800	-0.79558900
H	-1.09275600	1.84579800	0.95860100
C	0.73942700	1.41395200	-0.15870900
H	1.05262000	1.74279800	-1.15100000
H	1.24606600	2.01890600	0.59463200

N	1.22151900	-0.00634700	0.00020100
N	-1.29186200	0.00707400	0.00005300
H	2.24367000	-0.01175700	0.00005500

TS2a

GFE= -1513.812818 a.u.

Frequency= -1738.05 cm⁻¹

C	0.39331800	0.13895800	0.32582000
C	1.50612200	0.72016500	-1.48810900
C	2.83393100	0.91581800	0.58034800
H	2.58190400	1.16876400	1.61042000
N	0.36345400	0.31840100	-1.94064600
N	-0.32307800	-0.06665100	-0.80721800
N	1.58525800	0.63033800	-0.12474400
C	2.65686300	1.35637900	-2.19258800
H	2.34030100	1.73988700	-3.16241300
H	3.47525200	0.63695800	-2.33793100
C	3.61071800	2.08512800	-0.13822200
O	3.05696800	2.45353800	-1.39261600
C	5.02558100	0.11712300	0.01708000
C	3.78502300	-0.26224000	0.52123600
C	3.52220300	-1.57373400	0.90528400
C	4.53326700	-2.51837600	0.74659500
C	5.77676600	-2.15076600	0.22554900
C	6.03493700	-0.83051600	-0.13521200
C	5.07221700	1.59510100	-0.27278100
H	2.55821000	-1.81211600	1.35029600
H	6.55199800	-2.90118100	0.10593300
H	7.00599500	-0.54522200	-0.52949000
H	5.45209100	1.83381100	-1.27149900
H	5.71517800	2.11251500	0.44680400
C	-1.46680300	-0.91645800	-0.94620000
C	-1.36529800	-2.23808800	-0.49064700
C	-2.61455500	-0.41133600	-1.55679700
C	-2.50097100	-3.03672700	-0.58907600

C	-3.72323100	-1.25676000	-1.63671900
C	-3.69215300	-2.55892100	-1.14205000
H	-2.45114700	-4.06448200	-0.23695700
H	-4.63396900	-0.88014900	-2.09665300
C	-2.64826500	0.97732500	-2.13410700
H	-2.20703100	1.70367800	-1.44574000
H	-3.67694200	1.27904700	-2.33879900
H	-2.07672000	1.01423100	-3.06630900
C	-4.91667000	-3.43600600	-1.18872500
H	-5.63692000	-3.07319400	-1.92514800
H	-5.41569300	-3.45372700	-0.21378200
H	-4.65544300	-4.46707600	-1.44029600
C	-0.07432000	-2.79684600	0.05511300
H	0.14035500	-2.45692000	1.07551100
H	0.77529000	-2.49797100	-0.56915800
H	-0.11721400	-3.88763900	0.06590500
H	3.54425700	2.99505200	0.45917500
C	-1.29881100	-0.51878300	2.10324900
C	-2.53045200	-0.00436200	1.91778500
C	-2.84453200	1.30109300	1.28114100
C	-1.91387000	2.35100400	1.20527100
C	-4.13235300	1.54458500	0.77602700
C	-2.25101100	3.57488100	0.63726900
H	-0.92068400	2.20838100	1.61351900
C	-4.46757900	2.76523000	0.19904800
H	-4.88388700	0.76363300	0.82011700
C	-3.52804200	3.78880800	0.12209600
H	-1.51041600	4.36818600	0.59947600
H	-5.46909600	2.91462800	-0.19319400
H	-1.23496400	-1.45449000	2.66284500
H	-3.78697500	4.74150400	-0.32865700
C	0.04182000	-0.05158000	1.70073400
O	1.13780200	-0.58761100	2.51935700
C	-3.71385700	-0.83644600	2.35502800
H	-4.43769800	-0.24737300	2.92793500
H	-4.23878700	-1.24844000	1.48337100

H	-3.38541300	-1.67885200	2.96649600
H	4.35696500	-3.54922400	1.03705300
H	0.64364200	0.63381300	2.44486300

Int2b

GFE= -1976.114755 a.u.

N	-2.86124400	-1.24647900	-0.30859900
C	-1.51888800	-1.07327700	-0.49912700
N	-1.05666200	-2.34290800	-0.76347200
C	-2.14945400	-3.16511400	-0.83334000
C	-0.73266900	0.11643200	-0.70583000
C	-1.46584700	1.40455000	-0.59953000
C	-0.82746600	2.52648600	-0.23367300
O	0.56762600	0.07929000	-0.49234200
H	-2.50235600	1.43951000	-0.93346100
H	0.22363400	2.41958500	0.03112400
N	-3.25727900	-2.55174600	-0.57102400
C	-3.77589600	-0.33546000	0.29885800
C	-3.46555700	0.19449700	1.56617100
C	-4.93555600	0.01855900	-0.40112300
C	-4.35218100	1.12593300	2.10518800
C	-5.79959300	0.94390100	0.18880100
C	-5.50878400	1.50162500	1.42564600
H	-4.14236600	1.56255100	3.07533700
H	-6.70220100	1.23160300	-0.34434900
H	-6.18184300	2.23007800	1.86647800
C	0.32170500	-2.77186000	-1.01531900
C	-1.98018600	-4.58529600	-1.27303400
C	0.31532600	-4.18935900	-1.64129300
O	-0.66575900	-5.00850200	-1.01472500
H	-2.66145800	-5.23658400	-0.72364700
H	-2.21295000	-4.65770700	-2.34727000
C	1.93200400	-4.12280500	0.09772200
H	0.13826200	-4.16426300	-2.72607200
H	0.77228700	-2.02932600	-1.67876000

C	1.16992600	-2.96201100	0.22531500
C	1.27801300	-2.14055900	1.33874600
C	2.80228600	-4.50467500	1.11140700
C	2.89126500	-3.70626200	2.25173500
C	2.14182000	-2.53388100	2.36114200
C	1.66674400	-4.78264600	-1.23711200
H	1.60548700	-5.87296200	-1.19451900
H	2.43612700	-4.51014800	-1.96854100
H	0.74638300	-1.19304100	1.35538800
H	2.24207800	-1.91431900	3.24701100
H	3.55761800	-3.99583200	3.05857500
H	3.39731700	-5.40909600	1.02204500
C	-1.40702300	3.87411100	-0.24062000
C	-0.55906000	4.99120200	-0.23702100
C	-2.79348300	4.09872200	-0.27213200
C	-1.06987300	6.28415400	-0.29821000
H	0.51612400	4.83365900	-0.19502000
C	-3.30377700	5.38943000	-0.33383200
H	-3.47374000	3.25134300	-0.22582600
C	-2.44623700	6.48986100	-0.35373600
H	-0.39210600	7.13248400	-0.30101200
H	-4.37900700	5.54085200	-0.35525500
H	-2.84857500	7.49684800	-0.39887000
C	-5.28889200	-0.56973900	-1.74551500
C	-6.29984200	-1.71530000	-1.62466400
H	-4.38634400	-0.93192900	-2.24458400
H	-5.70922600	0.22497400	-2.37237600
H	-6.56119800	-2.10858700	-2.61108500
H	-5.87668900	-2.52441300	-1.02609400
H	-7.21836000	-1.36993900	-1.14106600
C	-2.20766100	-0.22594800	2.29844500
C	-2.20628000	0.06325000	3.79682300
H	-1.34744100	0.27581700	1.83508100
H	-2.05368500	-1.29987100	2.13566200
H	-1.30911400	-0.36227900	4.25231500
H	-2.19860400	1.13713600	4.00136800

H	-3.07964000	-0.37311400	4.29047300
C	3.34106500	2.42098900	-0.29381100
C	4.05045400	1.08011700	-0.17649800
C	4.09719700	3.62472800	0.27042800
C	6.36207800	2.06488100	-0.66261600
C	5.03931000	4.24138400	-0.76555400
C	5.79422300	3.16682000	-1.55022200
H	3.08020300	2.60092400	-1.34452700
H	6.84566000	2.51498400	0.22117700
H	4.66490700	3.30910900	1.15405000
H	5.75509200	4.90678500	-0.26954600
H	2.39629300	2.26401500	0.22759200
H	3.38583200	4.38024400	0.61673300
H	7.15936400	1.55227500	-1.21711500
H	4.46613700	4.86020700	-1.46529600
H	6.62555500	3.62578300	-2.09448800
H	5.14835000	2.70696900	-2.30579400
C	6.13831400	-0.17974900	0.20437700
H	6.60834900	-0.67018400	-0.66145800
H	6.95177600	0.13183600	0.87444900
C	3.91533200	-1.23263400	0.10703300
H	3.21037600	-1.93164200	0.56584400
H	4.14191200	-1.61926000	-0.89896000
C	5.20611900	-1.14637600	0.91401200
H	5.69494800	-2.11851500	1.02293600
H	4.96893500	-0.77234400	1.91539500
N	3.28165500	0.06926000	0.01104000
N	5.43338100	1.01802000	-0.24841700
H	2.29014200	0.17435500	0.08757400

Int2c

GFE= -1859.415482 a.u.

N	-1.80155600	-1.91914600	-0.23852100
C	-0.69494000	-1.14289000	-0.44112200
N	0.31416900	-2.05550200	-0.65167500

C	-0.26272000	-3.29702700	-0.68190000
C	-0.55651300	0.26743100	-0.70209500
C	-1.81070000	1.06261800	-0.64928500
C	-1.78082100	2.36657900	-0.33477600
O	0.60482200	0.85462100	-0.49177600
H	-2.73611700	0.59271800	-0.98076700
H	-0.80752500	2.77714800	-0.06928800
N	-1.53319700	-3.26665200	-0.44258300
C	-3.04739100	-1.52170900	0.33199400
C	-3.04448000	-0.85785100	1.57398100
C	-4.22507600	-1.78285900	-0.37861900
C	-4.27398600	-0.43197200	2.07513600
C	-5.43266700	-1.34969700	0.17357900
C	-5.45951200	-0.67176000	1.38398900
H	-4.31078500	0.09043900	3.02465100
H	-6.35521900	-1.54177600	-0.36838600
H	-6.40345500	-0.32835200	1.79512000
C	1.73657600	-1.79565900	-0.88949900
C	0.56161800	-4.48713600	-1.06006100
C	2.40786400	-3.07344400	-1.45326100
O	1.91605600	-4.23188300	-0.78823900
H	0.25687500	-5.35970200	-0.48049600
H	0.40882800	-4.70339800	-2.12931000
C	3.77326600	-2.18503900	0.27551400
H	2.25859700	-3.17796900	-2.53747600
H	1.79682300	-0.95567900	-1.58616200
C	2.55303300	-1.51484300	0.35523000
C	2.24314100	-0.69524200	1.43152700
C	4.70321200	-2.07195800	1.30176200
C	4.38681600	-1.28057800	2.40600000
C	3.17260200	-0.59495500	2.46699900
C	3.87234100	-2.94491400	-1.02844500
H	4.32987100	-3.93329400	-0.93829900
H	4.43599100	-2.37216400	-1.77373000
H	1.32842900	-0.10916500	1.40885400
H	2.95461000	0.03386400	3.32475100

H	5.09699600	-1.19028300	3.22230800
H	5.65488700	-2.59313700	1.24968900
C	-2.92543000	3.28193300	-0.39823300
C	-2.70203100	4.66567500	-0.44616500
C	-4.25405200	2.82679100	-0.43459100
C	-3.75933900	5.56298000	-0.56167900
H	-1.67982300	5.03400600	-0.40114600
C	-5.30983900	3.72234100	-0.55052000
H	-4.45704200	1.76169300	-0.34911200
C	-5.06975200	5.09495700	-0.62124300
H	-3.55974800	6.62948600	-0.60372900
H	-6.32956800	3.34941500	-0.57471500
H	-5.89723000	5.79178700	-0.70867300
C	-4.23718500	-2.52145400	-1.69492500
C	-4.59320700	-4.00195400	-1.52085000
H	-3.26180100	-2.43636900	-2.18096100
H	-4.97072100	-2.04351000	-2.35424200
H	-4.62197500	-4.51104800	-2.48832300
H	-3.84992700	-4.49240100	-0.88918100
H	-5.57451000	-4.11000500	-1.04948300
C	-1.74944200	-0.60778300	2.31939700
C	-1.91007500	-0.29221900	3.80378000
H	-1.21799900	0.22053700	1.83164100
H	-1.10610200	-1.48872400	2.20289200
H	-0.92621700	-0.22732100	4.27416900
H	-2.41145500	0.66636900	3.96144000
H	-2.48437200	-1.06784500	4.31899800
C	3.01655000	3.46415000	-0.50482300
C	4.42590500	4.10785100	-0.59113000
H	2.38986400	3.67947100	-1.37137200
H	2.47701900	3.73659800	0.40378700
H	4.59444500	4.53039900	-1.58403500
H	4.51108600	4.91560300	0.13823600
C	4.06331100	1.52807000	-1.62617300
H	4.05375000	0.43730900	-1.64204900
H	3.57126200	1.90354000	-2.52507900

C	5.47917200	2.12753300	-1.41339600
H	6.19427300	1.34275800	-1.15745300
H	5.82050100	2.60844300	-2.33205700
C	5.18991500	2.43865600	0.93851000
H	6.03677500	1.80060600	1.19826500
H	5.08888800	3.19836100	1.71664600
C	3.89697800	1.58622600	0.83793100
H	4.09534100	0.51460600	0.78177300
H	3.18973700	1.77680500	1.64642600
N	3.22277900	1.97128600	-0.45516600
N	5.46037500	3.10928600	-0.33114000
H	2.31288100	1.50829400	-0.50563300

Int3d

GFE= -1514.326856 a.u.

C	0.37857100	-0.11194400	0.32265900
C	1.50995800	0.33216600	-1.49140600
C	2.77495800	0.78110000	0.56315800
H	2.52003600	1.02376800	1.59794500
N	0.38629500	-0.17093800	-1.90974300
N	-0.30645900	-0.45633900	-0.77002700
N	1.54674300	0.37461400	-0.12717600
C	2.64699600	0.98248700	-2.21262100
H	2.34555400	1.25646400	-3.22317300
H	3.51859500	0.31774800	-2.25787000
C	3.40727000	2.01668900	-0.17637200
O	2.91193400	2.17684700	-1.49796900
C	5.05187100	0.26466200	0.06098000
C	3.84062700	-0.29247200	0.46589200
C	3.70666700	-1.65606900	0.70630000
C	4.82660100	-2.46583600	0.53423100
C	6.04658400	-1.91496500	0.13567700
C	6.16921500	-0.54803600	-0.10318300
C	4.92590700	1.75293500	-0.14607500
H	2.75435600	-2.07395600	1.01906700
H	6.90780100	-2.56171600	0.00372800
H	7.11692400	-0.12647300	-0.42345800

H	5.38353600	2.10908600	-1.07312900
H	5.38912200	2.30249500	0.68037800
C	-1.60360600	-1.07757700	-0.88550800
C	-1.75333400	-2.39031600	-0.42776200
C	-2.62414700	-0.35016800	-1.50079700
C	-3.02426700	-2.94956800	-0.52261500
C	-3.87700100	-0.96171600	-1.56846500
C	-4.09964500	-2.24590700	-1.07243100
H	-3.17567300	-3.96785400	-0.17403500
H	-4.69555000	-0.41878800	-2.03425300
C	-2.39028600	1.00471400	-2.11343600
H	-1.77880500	1.64603800	-1.47172500
H	-3.34158300	1.50869000	-2.28740000
H	-1.87272100	0.89983100	-3.07130400
C	-0.58983700	-3.18287500	0.10784500
H	-0.26110600	-2.83150300	1.09030900
H	0.27100300	-3.11734500	-0.56596500
H	-0.86476900	-4.23440300	0.20046400
H	3.13772200	2.94554200	0.32794500
C	-1.37440200	-0.50071100	2.15802300
C	-2.49957600	0.20301500	1.95213500
C	-2.60723700	1.52897700	1.28438000
C	-1.55156200	2.45144800	1.21652200
C	-3.83056800	1.90615000	0.70693700
C	-1.70170800	3.67951600	0.57932600
H	-0.60700100	2.25435300	1.70646700
C	-3.98213000	3.13097300	0.06665700
H	-4.67716700	1.23010000	0.74477400
C	-2.91605900	4.02261500	-0.00744500
H	-0.86882000	4.37461900	0.55506600
H	-4.93950000	3.38846400	-0.37479800
H	-1.47083200	-1.47317900	2.63636300
H	-3.03355300	4.97986800	-0.50388300
C	0.05949800	-0.19863100	1.80071700
O	0.94316900	-1.19421900	2.28579300
C	-3.79943700	-0.44807100	2.36353600

H	-4.43475300	0.24646900	2.91968700
H	-4.35366800	-0.77313700	1.47583700
H	-3.61536400	-1.32911600	2.97944600
H	4.75080900	-3.53359100	0.70962000
H	0.36726300	0.76887600	2.21593600
C	-5.47087600	-2.86574300	-1.11982400
H	-5.41251600	-3.93509900	-1.33461900
H	-5.97499900	-2.75123800	-0.15437800
H	-6.09502100	-2.39296500	-1.88037100
H	0.88955000	-1.20548900	3.25113900

TS2b

GFE= -1975.616826 a.u.

Frequency= -1019.51 cm⁻¹

C	-0.22001400	-0.78617600	0.09482700
C	0.23984500	-2.93554600	-0.04410000
C	2.05022000	-1.48874800	-0.84679500
H	2.09796300	-0.48785600	-1.29036600
N	-0.92365900	-2.89775900	0.52596300
N	-1.19516900	-1.55267500	0.62764900
N	0.70352100	-1.68317000	-0.32387000
C	1.06483600	-4.07917700	-0.53710300
H	0.45005200	-4.97443300	-0.63157900
H	1.89831800	-4.28402900	0.14818100
C	2.37601300	-2.59340300	-1.91034300
O	1.51579500	-3.72644400	-1.83294800
C	4.09004500	-2.56463200	-0.20986000
C	3.08106800	-1.71725900	0.23889200
C	3.07008800	-1.21671600	1.53703100
C	4.10898900	-1.58098600	2.39095900
C	5.12938100	-2.42583700	1.94671700
C	5.12902400	-2.92274500	0.64482100
C	3.84932100	-2.96907300	-1.64361100
H	2.27648800	-0.53976700	1.84727300
H	5.92987200	-2.70242900	2.62563700

H	5.92037000	-3.58549700	0.30719500
H	4.00759100	-4.03391000	-1.83614900
H	4.50699900	-2.40960000	-2.31837100
C	-2.33499300	-1.12583000	1.38580300
C	-2.11614800	-0.37508700	2.54776200
C	-3.60863500	-1.49502100	0.94826200
C	-3.23902200	0.08674600	3.22943700
C	-4.69853300	-1.00997200	1.67322600
C	-4.53505200	-0.20333200	2.79751800
H	-3.09678800	0.67822700	4.13096200
H	-5.70101500	-1.27189800	1.34317300
C	-3.81139500	-2.40211200	-0.23501500
H	-3.15871400	-2.12630400	-1.06762000
H	-4.84521700	-2.34755500	-0.57993100
H	-3.58377300	-3.43699800	0.03655700
C	-0.72978800	-0.09792100	3.06987100
H	-0.20326300	0.66588800	2.48636000
H	-0.11659100	-1.00538500	3.03867700
H	-0.78483600	0.23704400	4.10743900
H	2.22554500	-2.20784100	-2.91955100
C	-1.29803100	1.49988000	0.17656200
C	-2.52390900	1.52747400	-0.38415200
C	-3.00161300	0.66413900	-1.49606300
C	-4.38251600	0.51100400	-1.71089700
C	-2.13926800	0.00566500	-2.39134500
C	-4.87793900	-0.26852500	-2.75039800
H	-5.08670000	0.99603400	-1.04376500
C	-2.63476400	-0.76484300	-3.43912800
H	-1.06599400	0.11032000	-2.29144400
C	-4.00677100	-0.91455300	-3.62265700
H	-5.95159200	-0.37084300	-2.87750600
H	-1.93843800	-1.24911800	-4.11699000
H	-1.11156400	2.23519700	0.96135000
H	-4.39029500	-1.52233800	-4.43580900
C	-0.08772000	0.66389700	-0.07132800
O	1.04895100	1.13412300	0.54386300

C	-3.53794500	2.48479800	0.20196000
H	-4.06380500	3.04780700	-0.57618300
H	-4.29252900	1.94322000	0.78664600
H	-3.04930800	3.19362700	0.87354700
H	4.12785700	-1.20461100	3.40861200
C	3.34393000	1.70601600	-0.42583400
C	1.88115500	2.15808600	-0.66829000
C	4.31540300	2.85646800	-0.15347700
C	1.70834200	3.82508800	1.16740600
C	4.22702200	3.37246700	1.29671800
C	2.85018800	3.16884700	1.93114900
H	3.39356000	0.98542200	0.39271500
H	1.82240400	4.91684900	1.22924400
H	4.10417700	3.66673000	-0.85691400
H	4.49992800	4.43408000	1.33399300
H	3.64613200	1.18303400	-1.33738400
H	5.33778100	2.51739500	-0.35388100
H	0.75872600	3.57229100	1.66948400
H	4.96221400	2.84244900	1.91429700
H	2.84835200	3.58479300	2.94542900
H	2.63632300	2.10067500	2.03050200
C	0.60283500	4.25849600	-0.92942600
H	-0.41281600	3.98152600	-0.58957200
H	0.75335500	5.31444300	-0.67362400
C	0.49815400	2.55296200	-2.67258400
C	0.71847400	4.03545000	-2.42400700
H	-0.01901400	4.63473200	-2.96679800
H	1.72008900	4.33549900	-2.75324800
N	1.36285500	1.70132500	-1.85268600
N	1.63846300	3.49801300	-0.25104200
H	-0.57025100	2.34467400	-2.48973800
H	0.68357500	2.30998900	-3.72660600
H	0.38061000	0.88992800	-1.25163600
C	-5.72697200	0.35731400	3.52876000
H	-5.56793500	0.34833800	4.60994100
H	-5.90523400	1.39666000	3.23243800

H	-6.63246900	-0.21184500	3.30799300
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TS2c

GFE= 1858.946221 a.u.

Frequency= -1337.17 cm⁻¹

C	-0.56030500	-0.56058400	0.23249600
C	-1.93026500	-1.23206400	1.84293300
C	-2.86976500	0.57244500	0.44564000
H	-2.41001300	1.43208600	-0.03663700
N	-0.93350500	-2.04543800	1.94431400
N	-0.08150800	-1.65118600	0.91945800
N	-1.77868700	-0.32245100	0.83130500
C	-3.13185600	-1.09217700	2.71509000
H	-2.94862700	-1.54465700	3.68965800
H	-4.00680900	-1.57436000	2.25506000
C	-3.73178300	0.96126900	1.70799800
O	-3.34268100	0.29503900	2.90000300
C	-5.14246100	-0.08936200	0.02722800
C	-3.85047800	-0.10062300	-0.48875800
C	-3.56124100	-0.65795000	-1.73086000
C	-4.60189800	-1.25809800	-2.43563300
C	-5.89764800	-1.28271900	-1.91094700
C	-6.18052600	-0.68785700	-0.68365600
C	-5.20560800	0.65914400	1.33391300
H	-2.54780000	-0.55572500	-2.11836900
H	-6.69572500	-1.75943400	-2.47202300
H	-7.19325500	-0.68883900	-0.29050600
H	-5.68560500	0.09372700	2.13995200
H	-5.77045700	1.59038100	1.22236800
C	0.85725000	-2.60454700	0.41103200
C	0.59166400	-3.18767500	-0.84084200
C	1.98113500	-2.94849100	1.16236800
C	1.54922700	-4.03926700	-1.37742500
C	2.91351900	-3.81254000	0.57809300
C	2.73196000	-4.34181800	-0.69440000

H	1.36437200	-4.49288000	-2.34888700
H	3.80294900	-4.07710600	1.14599200
C	2.19567800	-2.48486600	2.58077900
H	3.19263400	-2.05276500	2.69951200
H	2.11387100	-3.34016100	3.25900000
H	1.45607900	-1.74724000	2.89236000
C	-0.70481000	-2.93036700	-1.56688000
H	-0.72077700	-1.95005300	-2.05453400
H	-1.55417000	-2.95823600	-0.87571800
H	-0.86314500	-3.69431400	-2.33099900
H	-3.58794100	2.01877300	1.93609700
C	1.22371300	-0.28434300	-1.51615100
C	2.54831800	-0.22712300	-1.26314600
C	3.17161300	0.36058000	-0.05497400
C	2.55668400	0.34920400	1.20530800
C	4.43755400	0.97036800	-0.14590100
C	3.17211200	0.91623000	2.31949400
H	1.59751200	-0.13257600	1.32382000
C	5.04409900	1.55543000	0.96030100
H	4.95328000	0.99524500	-1.10029200
C	4.41603100	1.52819300	2.20533900
H	2.67191700	0.87117900	3.28306500
H	6.01661500	2.02595000	0.85117500
H	0.95338700	-0.66389500	-2.50586400
H	4.89516500	1.97079400	3.07270300
C	0.00092500	0.24053300	-0.81634300
O	-0.89205500	0.80157500	-1.66913500
C	3.50604200	-0.75904400	-2.30841900
H	4.04937700	0.04268700	-2.82342700
H	4.25340200	-1.41903800	-1.85417100
H	2.96377400	-1.32855100	-3.06563000
H	-4.41027100	-1.70350900	-3.40708700
H	0.51576200	1.46692500	-0.23458700
C	-0.62028600	3.38620700	-0.22725300
C	-0.48492400	4.92404700	-0.36613000
H	-1.22246700	2.92175500	-1.01049400

H	-1.02306800	3.09297200	0.74891500
H	-1.21900900	5.31016100	-1.07911400
H	-0.65219400	5.42778000	0.59123300
C	1.22541700	2.98712900	-1.73896000
H	2.25282500	2.61182600	-1.76422900
H	0.60177300	2.36618900	-2.38593200
C	1.15018900	4.50577000	-2.04927100
H	2.09448700	4.86316500	-2.47060700
H	0.36069800	4.71677400	-2.77681400
C	1.81950700	4.90051000	0.20691500
H	2.82683700	5.08606900	-0.17862600
H	1.66954000	5.55100300	1.07383800
C	1.65620000	3.40531400	0.60238700
H	2.60775500	2.87492800	0.55980500
H	1.23889600	3.28034200	1.60596900
N	0.72300500	2.76850700	-0.35596500
N	0.85918800	5.27596400	-0.83328900
C	3.77252100	-5.22715900	-1.32956500
H	4.34151800	-4.67343800	-2.08397200
H	4.47997800	-5.60547200	-0.58859700
H	3.31035500	-6.08134400	-1.83190800

TS2d

GFE= -1976.10951 a.u.

Frequency= -1185.51 cm⁻¹

N	0.53180500	-0.29794600	1.97736600
C	0.74686600	-0.60479000	0.68576400
N	1.54968500	-1.70043900	0.72037900
C	1.78282600	-1.98582400	2.04800500
C	0.13777000	0.04510500	-0.46224100
C	0.28342100	1.51780200	-0.55126300
C	0.57095300	2.17945300	-1.68142800
O	0.47117000	-0.64675200	-1.65035700
H	0.04841900	2.07313000	0.35197100
H	0.82595700	1.60865200	-2.57256800

C	-2.38492700	-2.52558100	-0.85553500
C	-3.16898300	-1.23474700	-0.78221000
N	-4.51181000	-1.31192900	-0.80677300
C	-2.57330800	-3.31817200	-2.18325400
C	-5.17617000	-2.59935800	-1.01736000
C	-3.71874300	-2.83758000	-3.08190000
C	-5.11297900	-3.04357800	-2.48205600
H	-1.33021100	-2.27061300	-0.72213600
H	-4.71005700	-3.34723800	-0.37184900
H	-2.71844400	-4.37693000	-1.94559400
H	-3.65880800	-3.36132200	-4.03986500
H	-2.66989700	-3.13724800	0.00694500
H	-1.64220000	-3.25387500	-2.75305200
H	-6.20860200	-2.49379000	-0.67646700
H	-3.57186900	-1.77461500	-3.30988500
H	-5.39645200	-4.10051100	-2.52768600
H	-5.84955500	-2.49091800	-3.07464300
C	-5.34298300	-0.10342600	-0.89788100
H	-5.77618300	0.10647600	0.08708200
H	-6.16570600	-0.31672800	-1.58673900
C	-4.52140900	1.07707700	-1.39364100
H	-4.28330900	0.94372200	-2.45404300
H	-5.09845400	1.99825300	-1.29147000
C	-3.22797400	1.15276700	-0.59330500
H	-3.44171000	1.37193500	0.46226200
H	-2.56810500	1.94200900	-0.96408600
N	-2.50933200	-0.11361400	-0.68882200
H	-1.23560200	-0.09024500	-0.40514900
N	1.18031400	-1.14939500	2.83109400
C	-0.33870900	0.72228700	2.49144500
C	0.21995400	1.97030100	2.80398500
C	-1.69022300	0.41267400	2.65316100
C	-0.65270500	2.95479800	3.26476900
C	-2.52461600	1.43037700	3.12577400
C	-2.01305400	2.68735200	3.41798700
H	-0.27152200	3.93977600	3.50924300

H	-3.58142000	1.22154000	3.27031400
H	-2.67464500	3.46776700	3.77943000
C	2.25481200	-2.39412000	-0.37300200
C	2.62061900	-3.16603400	2.43068700
C	2.94712400	-3.67414800	0.16142900
O	3.55823100	-3.42215400	1.41557900
H	3.16194600	-2.94895300	3.35199700
H	1.96975800	-4.03715700	2.59863700
C	4.44700000	-2.50016900	-1.26188200
H	2.24790900	-4.51703100	0.24813700
H	1.51347900	-2.65312500	-1.13150700
C	3.40457200	-1.61675200	-0.97863000
C	3.50469900	-0.26345400	-1.27165000
C	5.61529300	-2.03827700	-1.85321400
C	5.72704300	-0.67923500	-2.14596800
C	4.68391500	0.19979000	-1.85518100
C	4.08394000	-3.90494800	-0.83791700
H	4.90179300	-4.44919300	-0.36056300
H	3.72768800	-4.49702300	-1.68840500
H	2.69445200	0.42874900	-1.06015600
H	4.78868000	1.25531700	-2.08379200
H	6.63838200	-0.30021200	-2.59690300
H	6.43271300	-2.71911400	-2.07011900
C	0.61356700	3.64509600	-1.80513200
C	1.21003800	4.21496700	-2.93658600
C	0.08466200	4.50454200	-0.82932700
C	1.29748100	5.59567600	-3.08359700
H	1.61665800	3.56178600	-3.70420300
C	0.17475600	5.88322400	-0.97401600
H	-0.41175900	4.09509300	0.04733800
C	0.78332700	6.43607800	-2.10046700
H	1.76751600	6.01505800	-3.96730500
H	-0.23967600	6.53244400	-0.20905600
H	0.84885000	7.51325400	-2.21234800
C	-2.23184800	-0.97875100	2.43285800
C	-2.20509300	-1.79551700	3.73029400

H	-1.65289800	-1.49656900	1.66075600
H	-3.25967900	-0.90399800	2.05650300
H	-2.61357200	-2.79605900	3.56711200
H	-1.18035200	-1.89193200	4.09870900
H	-2.79840500	-1.30493200	4.50634900
C	1.70585400	2.19852900	2.62442300
C	2.16654500	3.63654900	2.83140800
H	1.99268700	1.87254200	1.61559600
H	2.23901100	1.53010600	3.31186900
H	3.24132800	3.71062900	2.65691300
H	1.66650100	4.31575300	2.13409700
H	1.97044400	3.98042600	3.85046200
H	-0.30480300	-0.59047800	-2.22671100

TS2e

GFE= -1859.413115 a.u.

Frequency= -987.62 cm⁻¹

C	0.82309300	-0.46783000	-0.21578600
C	0.55288300	-2.51313600	-1.01018100
C	-1.54439200	-1.40883600	-0.35201600
H	-1.82702200	-0.65262500	0.35925900
N	1.80262800	-2.28663200	-1.16934800
N	1.97250300	-0.96892800	-0.65983500
N	-0.08413800	-1.43072200	-0.44595100
C	-0.26372400	-3.73137800	-1.27405700
H	0.36240100	-4.60578000	-1.30735700
H	-0.80652400	-3.62841700	-2.20275800
C	-2.09376500	-2.81134800	0.09218400
O	-1.14588600	-3.87383000	-0.14916000
C	-3.21979200	-2.07919400	-1.92211100
C	-2.17174900	-1.19973400	-1.72105300
C	-1.79507600	-0.30369800	-2.70194100
C	-2.50825900	-0.27613400	-3.88990400
C	-3.57732200	-1.13907700	-4.08384600
C	-3.93652200	-2.04982400	-3.10293900
C	-3.38794400	-3.00415800	-0.73182000

H	-0.95238600	0.34414800	-2.56138500
H	-4.11913000	-1.11235800	-5.00779400
H	-4.74869800	-2.72988600	-3.26678700
H	-3.48740600	-4.04318600	-1.01247800
H	-4.25170900	-2.71765000	-0.14198400
C	3.28405500	-0.38392100	-0.71328100
C	3.64298400	0.35109600	-1.84182600
C	4.18617100	-0.64442200	0.30723100
C	4.91361600	0.89175600	-1.89118400
C	5.45277100	-0.08525400	0.21989500
C	5.82659900	0.68892700	-0.86399600
H	5.20334100	1.46599900	-2.74915900
H	6.15815500	-0.27372800	1.00434200
C	3.82053800	-1.54730400	1.46651300
H	3.02446500	-1.11225600	2.05636900
H	4.67709400	-1.70078800	2.10823500
H	3.49259200	-2.51188700	1.09779900
C	7.21928600	1.27899300	-0.96043300
H	7.17362100	2.33348700	-1.20655000
H	7.78452300	0.77530900	-1.73736100
H	7.75606700	1.16984100	-0.02746500
C	2.66630700	0.54580400	-2.98385100
H	1.81955100	1.12631400	-2.64308300
H	2.31701900	-0.41301800	-3.34836300
H	3.14201300	1.06817400	-3.80232100
H	-2.26836500	-2.83489900	1.14886200
C	1.10683100	0.98748700	1.78522500
C	0.74925900	0.40213900	2.91631400
C	-0.34740600	-0.59990800	3.09496700
C	-1.63816800	-0.17469300	3.38544300
C	-0.06428100	-1.95963800	3.14239900
C	-2.62697400	-1.08856000	3.71153300
H	-1.85494300	0.87533900	3.39731600
C	-1.04828000	-2.87357600	3.47882500
H	0.93185700	-2.30137000	2.94211500
C	-2.33232700	-2.44055100	3.76635300

H	-3.61397900	-0.74507800	3.95116900
H	-0.81182200	-3.91794200	3.52267000
H	1.90273700	1.71173000	1.85289100
H	-3.08892500	-3.14665900	4.04520200
C	0.55437600	0.88252100	0.38130900
O	1.24639500	1.87553800	-0.45434900
C	1.46027400	0.71808700	4.22560100
H	0.74900800	1.09012400	4.95554300
H	1.90674800	-0.18005000	4.63931400
H	2.23801100	1.45878800	4.08715300
H	-2.22597800	0.40447400	-4.66789400
H	-0.74427400	1.65535000	0.25072700
C	-2.92211000	2.24500100	0.46610800
C	-3.78201300	3.54835300	0.34933200
H	-3.23464900	1.49291200	-0.24399200
H	-2.95241600	1.82671500	1.46067100
H	-4.52956100	3.44563200	-0.42365600
H	-4.28456900	3.76089700	1.28163600
C	-1.41062200	3.16098800	-1.23823100
H	-0.36542100	3.31340500	-1.44328600
H	-1.80018600	2.41055400	-1.90791400
C	-2.26119600	4.46915000	-1.29071500
H	-1.63953700	5.32491400	-1.51043200
H	-3.02518200	4.40098300	-2.05148400
C	-1.89459700	4.88236400	1.05963300
H	-1.31264300	5.75917500	0.81653200
H	-2.39677300	5.05910700	1.99979400
C	-0.98504000	3.61732600	1.14150700
H	0.03904300	3.81398900	0.86725200
H	-1.00193900	3.16190800	2.11988200
N	-1.49835100	2.59877900	0.15735000
N	-2.91161000	4.68608600	0.01304500
H	2.20957000	1.84764500	-0.34718100

M2

GFE= -1513.900714 a.u.

C	-0.62066400	0.15494800	-1.02639100
C	-2.81015200	0.27138300	-1.37114600
C	-1.97194800	-2.03671300	-0.95559500
H	-1.44564600	-2.66399000	-1.67530400
N	-2.49112100	1.47922500	-1.07072000
N	-1.12526400	1.43507300	-0.79855100
N	-1.75264800	-0.61787600	-1.31573100
C	-4.15971200	-0.19281000	-1.83598700
H	-4.36300000	0.21920600	-2.82765100
H	-4.93729100	0.17012600	-1.15261500
C	-3.50618200	-2.28102600	-0.94368500
O	-4.18627700	-1.59782100	-1.97229400
C	-2.73613800	-2.24792500	1.30640300
C	-1.60519500	-2.32677500	0.48780800
C	-0.35947400	-2.63103200	1.02595100
C	-0.25049200	-2.80823200	2.40499500
C	-1.37239600	-2.69851100	3.22707500
C	-2.62669200	-2.43130100	2.68036500
C	-3.97234600	-1.96123000	0.49597900
H	0.50253700	-2.72525400	0.37513500
H	-1.27115600	-2.83909300	4.29878100
H	-3.50504400	-2.37401900	3.31665400
H	-4.26297200	-0.90947600	0.60231400
H	-4.83418400	-2.56651900	0.78744800
C	-0.57606200	2.47401100	0.00484100
C	-0.20946300	2.22129900	1.33183300
C	-0.43540300	3.74607600	-0.57239400
C	0.34424000	3.27322300	2.06588700
C	0.10128400	4.76582800	0.20607000
C	0.50515600	4.54649900	1.52602700
H	0.64161400	3.08944100	3.09591500
H	0.21939000	5.75534500	-0.23058400
C	-0.84104600	3.97634000	-2.00260900

H	-0.55711300	4.97860300	-2.32911500
H	-1.92091400	3.85571100	-2.12632400
H	-0.36451400	3.24188800	-2.66020300
C	1.08396400	5.67324200	2.34284000
H	0.33202000	6.44607000	2.53085100
H	1.91724200	6.15110800	1.81948100
H	1.44884400	5.31572900	3.30800800
C	-0.39054800	0.86433800	1.95478500
H	0.40053700	0.17672900	1.63493700
H	-1.34023700	0.40614600	1.65647300
H	-0.36593700	0.93573200	3.04402900
H	-3.66829000	-3.34347800	-1.14115900
C	1.79044000	0.65422400	-0.99013000
C	3.11778400	0.39052900	-0.89197400
C	3.68253100	-0.94156600	-0.57327000
C	3.06575100	-1.77054400	0.37743100
C	4.88180100	-1.38581100	-1.15125800
C	3.60102800	-3.01019600	0.70563200
H	2.16313800	-1.41752900	0.86859800
C	5.41888000	-2.62678500	-0.82307000
H	5.39153100	-0.75703900	-1.87546400
C	4.77854500	-3.44807900	0.10186600
H	3.10335800	-3.63316500	1.44352400
H	6.34156200	-2.95392100	-1.29259800
H	1.51428800	1.70186100	-1.09257000
H	5.19860800	-4.41546700	0.35781900
C	0.67723800	-0.25412200	-1.11687700
O	0.85969700	-1.58633500	-1.46528700
C	4.11159800	1.51226900	-1.07541600
H	4.86425100	1.50887800	-0.28003400
H	4.65139100	1.42640500	-2.02653900
H	3.60627000	2.48109900	-1.07499200
H	0.71714100	-3.03578000	2.84315600
H	1.72046400	-1.65635200	-1.89821700

M3SET

GFE= -1513.72361 a.u.

C	-0.04189300	-0.75813100	-0.69701900
C	0.70495000	-2.79059300	-1.03250000
C	2.51494300	-1.04347300	-1.03383800
H	2.64403700	-0.35917000	-1.86981000
N	-0.53400500	-2.94812800	-0.67304900
N	-0.99110100	-1.68755400	-0.44008900
N	1.08084500	-1.47255300	-1.01665400
C	1.63013000	-3.86968300	-1.51197100
H	1.14772000	-4.39914800	-2.33612000
H	1.82140300	-4.59295400	-0.71111600
C	3.37901900	-2.33121600	-1.16561800
O	2.80927300	-3.29647300	-2.01894900
C	3.60951400	-1.50021700	1.04481500
C	2.96491300	-0.49896700	0.31102800
C	2.86304900	0.79227800	0.82462600
C	3.36900700	1.05307300	2.09625400
C	3.98399700	0.04503300	2.83910100
C	4.11893300	-1.23631000	2.31103300
C	3.68095900	-2.79015200	0.27576600
H	2.42299500	1.58991000	0.24078200
H	4.37858600	0.26597600	3.82544600
H	4.62595300	-2.01519300	2.87210700
H	2.93552600	-3.50041500	0.64975800
H	4.65449200	-3.27999300	0.34497500
C	-2.29846300	-1.52106400	0.12963500
C	-2.38012400	-1.19695000	1.48735700
C	-3.41333200	-1.70105200	-0.69180200
C	-3.65536200	-1.02975900	2.02216600
C	-4.66467100	-1.52366700	-0.10565700
C	-4.80414800	-1.19034400	1.24405500
H	-3.75421900	-0.77438900	3.07394200
H	-5.55344100	-1.65048300	-0.71831700
C	-3.25629200	-2.05056600	-2.14691500

H	-4.22379100	-2.03996300	-2.65007200
H	-2.81611400	-3.04488100	-2.26342800
H	-2.59751300	-1.33876900	-2.65548100
C	-6.17150200	-1.03931800	1.85584500
H	-6.54162800	-2.00953000	2.20175000
H	-6.88895700	-0.65204800	1.12944600
H	-6.14942200	-0.36740300	2.71607300
C	-1.13868100	-1.00890700	2.31856400
H	-0.61457900	-0.08505200	2.04454900
H	-0.43766100	-1.83810700	2.17979000
H	-1.39237700	-0.94854800	3.37736300
H	4.31216300	-2.02963700	-1.64592400
C	-1.38945400	1.35880700	-0.51279200
C	-1.58496800	2.71448800	-0.50020100
C	-0.48099500	3.70198900	-0.47051500
C	0.55389600	3.55238500	0.46798200
C	-0.47209100	4.82288500	-1.31432800
C	1.58335100	4.48429300	0.54197300
H	0.52976500	2.70801500	1.15340000
C	0.56358500	5.74873200	-1.24114700
H	-1.26725500	4.95926900	-2.04074700
C	1.59220300	5.58215600	-0.31588000
H	2.37076200	4.36153100	1.27854800
H	0.56633200	6.60460200	-1.90741500
H	-2.26434600	0.74172700	-0.34911300
H	2.39374500	6.31067100	-0.25777300
C	-0.18740500	0.65935800	-0.81123400
O	0.89153300	1.22892000	-1.37938200
C	-2.98110100	3.26252200	-0.44098800
H	-3.08330900	3.96635500	0.39034400
H	-3.21070400	3.81966800	-1.35662800
H	-3.72051400	2.46651800	-0.33567100
H	3.29822800	2.05541100	2.50686700
H	0.76570700	2.18834100	-1.45910800

M3HAT

GFE= -1513.308456 a.u.

C	0.40668600	-0.61865600	-0.90718700
C	2.07718600	-2.04522900	-1.13121000
C	2.77926200	0.35675600	-1.01621200
H	2.63982800	1.06216600	-1.83342800
N	1.06909300	-2.79648500	-0.82218700
N	0.02161300	-1.91317000	-0.63989700
N	1.76583400	-0.71205200	-1.15171100
C	3.44724000	-2.51974000	-1.51911500
H	3.36558100	-3.16293500	-2.39804000
H	3.88849600	-3.11226500	-0.70856000
C	4.17382800	-0.32828500	-1.00731000
O	4.26124400	-1.42945400	-1.88677100
C	3.68722400	0.41539500	1.20092300
C	2.73304400	0.99585600	0.36029200
C	1.90577900	2.01648400	0.82176800
C	2.02240700	2.41770900	2.15218400
C	2.95741700	1.82216100	3.00002300
C	3.80519800	0.82339600	2.52532500
C	4.49112500	-0.63015100	0.47490400
H	1.19398400	2.48305800	0.14988900
H	3.03587000	2.14962000	4.03196700
H	4.54979400	0.37507500	3.17651900
H	4.16008400	-1.63392700	0.76473200
H	5.56305100	-0.57362100	0.67873100
C	-1.11972700	-2.35819600	0.09173000
C	-1.32094000	-1.88398900	1.39376700
C	-1.99528600	-3.26123900	-0.52288800
C	-2.46060300	-2.32102300	2.06908000
C	-3.11151100	-3.67664600	0.19823500
C	-3.36297300	-3.21398900	1.49200600
H	-2.64079200	-1.95895200	3.07851100
H	-3.80815000	-4.37122000	-0.26536200

C	-1.73927800	-3.73435600	-1.92809200
H	-2.57300200	-4.33844700	-2.28969600
H	-0.82373800	-4.32991500	-1.97855500
H	-1.60415100	-2.88346300	-2.60371700
C	-4.56766200	-3.69682800	2.25786400
H	-4.35091300	-4.64315900	2.76409100
H	-5.41652100	-3.86775700	1.59146300
H	-4.86789900	-2.97438800	3.01993200
C	-0.35666900	-0.92688300	2.04376800
H	-0.48860200	0.08991300	1.65714000
H	0.68404700	-1.20672700	1.84874100
H	-0.51262800	-0.90489900	3.12377500
H	4.89419900	0.40111200	-1.38406700
C	-1.83480500	0.45615600	-1.00126700
C	-2.70300300	1.47706200	-0.86889400
C	-2.30429000	2.88887900	-0.62973700
C	-1.41017100	3.21072300	0.39800300
C	-2.87320700	3.93118700	-1.36812700
C	-1.07547400	4.53278200	0.66348900
H	-0.98046100	2.40800000	0.99170900
C	-2.53259700	5.25658800	-1.10986800
H	-3.57229600	3.70411500	-2.16764100
C	-1.63339100	5.56258700	-0.09303900
H	-0.38152300	4.76480700	1.46610400
H	-2.97266100	6.05091000	-1.70457100
H	-2.25760300	-0.54246600	-1.07706900
H	-1.37172100	6.59545700	0.11299600
C	-0.37021800	0.55825500	-1.15655700
O	0.21816200	1.59948300	-1.54745800
C	-4.18781200	1.21501700	-0.89794300
H	-4.66830700	1.60713700	0.00430900
H	-4.65938500	1.71743700	-1.74997800
H	-4.39957000	0.14635700	-0.97570900
H	1.38328600	3.20998900	2.53069900

NB

GFE= -436.6191229 a.u.

O	2.27862700	1.07773800	-0.00006400
O	2.27862700	-1.07773900	0.00003100
N	1.71112300	0.00000000	-0.00006800
C	0.24002200	0.00000000	-0.00003100
C	-0.42316300	1.21992400	0.00001500
C	-0.42316300	-1.21992400	-0.00003800
C	-1.81325400	1.21026400	0.00006900
C	-1.81325500	-1.21026400	0.00001200
C	-2.50495400	0.00000000	0.00006900
H	0.14630000	2.14066100	0.00001500
H	0.14630000	-2.14066100	-0.00007700
H	-2.35601200	2.14893100	0.00011500
H	-2.35601300	-2.14893000	0.00000800
H	-3.58987400	0.00000000	0.00011100

[NB]⁻

GFE= -436.7110027 a.u.

O	2.29452000	1.11987700	-0.00012500
O	2.29451900	-1.11987700	0.00002300
N	1.67330600	0.00000000	-0.00004600
C	0.28665600	0.00000000	-0.00001200
C	-0.42959100	1.21897300	0.00003500
C	-0.42959000	-1.21897200	-0.00001800
C	-1.81416900	1.20379300	0.00007500
C	-1.81416900	-1.20379300	0.00001400
C	-2.52884600	0.00000000	0.00006300
H	0.13597400	2.14139100	0.00004600
H	0.13597400	-2.14139100	-0.00005600
H	-2.35252500	2.14893800	0.00011700
H	-2.35252400	-2.14893800	0.00000000
H	-3.61410000	0.00000000	0.00009200

[NBH]⁻

GFE= -437.2848703 a.u.

O	-2.24866900	1.15860200	0.07733400
O	-2.24726200	-1.12139500	0.21479800
N	-1.63018000	0.06836400	-0.40027700
C	-0.24486200	0.01057300	-0.14275700
C	0.47334700	1.21080200	-0.02796400
C	0.46222500	-1.20380100	-0.12457400
C	1.85896900	1.19255300	0.08675000
C	1.84605400	-1.20712200	-0.00718600
C	2.56194200	-0.01184000	0.09548700
H	-0.10762400	2.12404300	-0.01525300
H	-0.09930900	-2.12834800	-0.18966600
H	2.39804000	2.13274700	0.18212100
H	2.37605000	-2.15687100	0.01193900
H	3.64420200	-0.02178900	0.18419200
H	-2.57870100	-0.67297500	1.01301100

[NBH]⁻

GFE= -437.1956546 a.u.

O	2.27995900	-1.15424100	0.00001800
O	2.25901500	1.10226700	-0.00003100
N	1.59667000	-0.11164600	0.00000800
C	0.20376300	-0.03262700	-0.00000100
C	-0.51757600	-1.23288500	-0.00001000
C	-0.44383000	1.20795400	0.00000900
C	-1.90326000	-1.17916800	-0.00001200
C	-1.83264600	1.23215900	0.00000600
C	-2.56764600	0.04787900	-0.00000600
H	0.02234200	-2.17167400	-0.00001600
H	0.13417000	2.12268300	0.00002100
H	-2.47024400	-2.10413000	-0.00002300

H	-2.34454700	2.18881000	0.00001200
H	-3.65163100	0.08017000	-0.00001000
H	3.18859600	0.82158300	0.00015000

M3

GFE= -1950.508963 a.u.

C	0.42301100	-0.16625400	0.44948700
C	1.07245300	-0.55081600	2.55936000
C	1.44436500	-2.50222400	1.01102400
H	0.63109800	-3.23018700	0.99286000
N	0.55404600	0.62122000	2.64207000
N	0.00604100	0.88606900	1.35351700
N	0.90176000	-1.17616300	1.34562800
C	1.84463100	-1.21138400	3.66524200
H	1.26498800	-1.17607500	4.58984900
H	2.77637500	-0.65320000	3.82832500
C	2.52134200	-2.82843600	2.06955500
O	2.10638800	-2.57020900	3.39072600
C	3.61581600	-2.22643200	0.06957600
C	2.28070600	-2.49546100	-0.25162400
C	1.88561300	-2.69029400	-1.56810300
C	2.84497600	-2.57197700	-2.57649600
C	4.17136900	-2.26854100	-2.26184200
C	4.56855400	-2.10631900	-0.93306900
C	3.78055400	-2.09019500	1.56275300
H	0.85074800	-2.91075300	-1.80683300
H	4.90487600	-2.17630700	-3.05679400
H	5.60491600	-1.88995500	-0.69128900
H	3.75386900	-1.02816700	1.83905200
H	4.70677800	-2.51902800	1.95143000
C	-1.34669200	1.38027500	1.37923700
C	-1.57156100	2.66591400	0.86286500
C	-2.40492800	0.60366100	1.87408500
C	-2.88084600	3.13509700	0.78681400

C	-3.69917500	1.12039200	1.78649800
C	-3.96027600	2.37100900	1.23225900
H	-3.06273000	4.12237500	0.36667100
H	-4.52785000	0.51337000	2.14544700
C	-2.19610300	-0.76077200	2.47945600
H	-3.15846700	-1.25178600	2.63668700
H	-1.68615900	-0.67919000	3.44421500
H	-1.58878500	-1.40803600	1.84168300
C	-5.36818200	2.90042700	1.13075000
H	-5.54633700	3.68433400	1.87379200
H	-6.10325000	2.10944900	1.29861300
H	-5.55428000	3.33907100	0.14559800
C	-0.42963100	3.51910600	0.38130800
H	-0.77341300	4.53487700	0.17390500
H	0.02032700	3.10911900	-0.52813200
H	0.36663600	3.56076200	1.12879400
H	2.70609000	-3.90540800	2.02964300
C	-1.36282500	0.32230900	-1.37282300
C	-2.65442700	0.25737600	-1.75309400
C	-3.56375400	-0.90371600	-1.55897600
C	-3.26017500	-2.16126200	-2.09000300
C	-4.79321900	-0.72428100	-0.91128100
C	-4.15682700	-3.21736400	-1.96450500
H	-2.31477500	-2.30262500	-2.60070400
C	-5.67996200	-1.78610300	-0.76772200
H	-5.04179700	0.24759800	-0.49444200
C	-5.36560000	-3.03515900	-1.29781900
H	-3.90822300	-4.18615900	-2.38597200
H	-6.62090600	-1.63578800	-0.24780800
H	-0.82426200	1.24892400	-1.53784500
H	-6.06177600	-3.86143600	-1.19428900
C	-0.66077700	-0.67602600	-0.54613900
O	-0.89756300	-1.86917200	-0.53691100
C	-3.28541100	1.46422500	-2.39954900
H	-3.71309400	1.19713300	-3.37127700
H	-4.10505500	1.84038400	-1.77742300

H	-2.56026200	2.26985000	-2.52990300
H	2.55795100	-2.71930300	-3.61307200
O	1.64847800	0.22398800	-0.24114800
O	1.50012300	0.53967200	-2.44979100
N	1.48543200	1.20305800	-1.22117700
C	2.58163900	2.12368100	-1.09154700
C	2.96341600	2.53122200	0.18900200
C	3.18156600	2.66989000	-2.22309900
C	3.96442100	3.48519700	0.32558700
C	4.18529100	3.62391400	-2.06709400
C	4.58195200	4.03332200	-0.79829600
H	2.47024200	2.09770500	1.05309400
H	2.85945300	2.35178800	-3.20669400
H	4.26486600	3.80170600	1.31930600
H	4.65627200	4.04731100	-2.94849900
H	5.36298600	4.77735100	-0.68307900
H	2.27476800	-0.05723100	-2.41884300

M03

GFE= -1513.145737 a.u.

C	0.74045400	-0.42573800	-0.38930600
C	2.12893700	-1.88653400	-1.19438800
C	3.02417500	0.48766500	-1.09197700
H	2.66808900	1.13041100	-1.89789000
N	1.04726200	-2.56232100	-0.90899000
N	0.19480700	-1.63679600	-0.40642800
N	1.97791200	-0.56004400	-0.88837500
C	3.40071600	-2.41178600	-1.78860800
H	3.15864200	-3.07560900	-2.62031200
H	3.94968800	-2.99079500	-1.03573800
C	4.34043000	-0.26282100	-1.42286400
O	4.16148300	-1.34755300	-2.30530000
C	4.49085400	0.59084200	0.78002000
C	3.37877900	1.20193200	0.19063000
C	2.80250400	2.33995300	0.74850100

C	3.33645000	2.83864300	1.93549500
C	4.43028600	2.21724900	2.53863500
C	5.02208400	1.09513400	1.96068700
C	4.97663700	-0.56966500	-0.05046100
H	1.97399200	2.84320900	0.26296300
H	4.83793700	2.62444000	3.45794100
H	5.89144100	0.63288200	2.41752800
H	4.61093200	-1.51641100	0.36502600
H	6.06412400	-0.63919900	-0.11377500
C	-1.16535400	-1.97295100	-0.06119800
C	-1.37718700	-2.70689600	1.10859200
C	-2.19259900	-1.50291800	-0.88303800
C	-2.69948400	-2.96031300	1.46334000
C	-3.49621600	-1.79277200	-0.48186100
C	-3.76861900	-2.51151600	0.68335500
H	-2.89983300	-3.51993300	2.37304300
H	-4.31954800	-1.44636900	-1.10191200
C	-1.93657600	-0.68879600	-2.12492400
H	-2.74292800	-0.84283000	-2.84369600
H	-0.99539300	-0.95886400	-2.61155800
H	-1.90914600	0.38360600	-1.89612800
C	-5.18952900	-2.81450900	1.07808700
H	-5.54259600	-3.71638900	0.56837600
H	-5.85875800	-1.99648400	0.80043500
H	-5.27505700	-2.98515400	2.15299400
C	-0.22707300	-3.18558900	1.95366000
H	-0.59536100	-3.65474700	2.86633000
H	0.43187300	-2.35826800	2.23957800
H	0.38025400	-3.91566600	1.41156800
H	4.97706800	0.44392200	-1.95925400
C	-0.80886400	0.82667500	1.12418100
C	-2.08067300	1.27962100	1.24181300
C	-2.79527800	2.06282000	0.21110800
C	-2.22896600	3.19935900	-0.37935500
C	-4.09326200	1.67667600	-0.16188500
C	-2.93572200	3.91782700	-1.33930000

H	-1.24508600	3.52739100	-0.06906400
C	-4.78405900	2.38222800	-1.13792900
H	-4.55197100	0.80625300	0.29708900
C	-4.20605400	3.50540700	-1.72875700
H	-2.49107900	4.80324400	-1.78059900
H	-5.77820600	2.06305900	-1.43224300
H	-0.42782400	0.17227800	1.90600200
H	-4.75107500	4.06237300	-2.48362200
C	0.02333100	0.87595500	-0.07181700
O	0.19513100	1.76679300	-0.87859500
C	-2.87507900	0.87283900	2.45329200
H	-3.41014100	1.73059000	2.86813700
H	-3.62427400	0.12470900	2.16937500
H	-2.23637800	0.43252200	3.22027200
H	2.90758400	3.72790100	2.38446600

TS' (DABCO.H⁺)

GFE= -1950.505992 a.u.

Frequency= -313.65 cm⁻¹

C	0.07893100	-1.59891300	-0.99615700
C	1.39560000	-3.28227200	-1.37102400
C	1.90517600	-1.25405200	-2.79210100
H	1.23743800	-1.17258200	-3.65032100
N	0.54590100	-3.71017900	-0.48231900
N	-0.27357100	-2.65022200	-0.26558000
N	1.14267500	-1.97961600	-1.72708100
C	2.50775700	-4.08164700	-1.97500500
H	2.14018500	-5.08110500	-2.21290600
H	3.32841500	-4.18000100	-1.25324800
C	3.17335200	-2.10499600	-3.07183800
O	2.93052900	-3.48534100	-3.17623200
C	3.84585800	-0.17232500	-1.93271300
C	2.53952100	0.05830600	-2.37961900
C	2.06869200	1.35466200	-2.55660300

C	2.91167400	2.41878300	-2.23438200
C	4.19891900	2.19059600	-1.74394100
C	4.67750700	0.88808800	-1.59461100
C	4.17676500	-1.63917500	-1.99545300
H	1.07678100	1.53284100	-2.95574600
H	4.84004500	3.03132800	-1.50010900
H	5.69141700	0.70839300	-1.25121300
H	3.97921900	-2.11645200	-1.02746100
H	5.21147300	-1.84781000	-2.27293200
C	-1.39294400	-2.76890700	0.63307200
C	-1.12968500	-2.76635300	2.00234100
C	-2.67464900	-2.85867200	0.08319800
C	-2.23216100	-2.83748100	2.85496500
C	-3.73730500	-2.93446600	0.97952100
C	-3.53518300	-2.91821500	2.36387600
H	-2.06351600	-2.83288900	3.92864800
H	-4.74821800	-3.01899500	0.58766700
C	-2.89758700	-2.85046200	-1.40650700
H	-3.92551500	-3.13400500	-1.63729800
H	-2.22480600	-3.54850100	-1.91394900
H	-2.73733100	-1.85273900	-1.83408200
C	-4.71234700	-2.96223300	3.30257300
H	-5.48176700	-3.64607600	2.93699800
H	-5.16995200	-1.97114500	3.39450000
H	-4.41104100	-3.28245200	4.30156100
C	0.28094400	-2.69265700	2.52007000
H	0.74241500	-3.68552400	2.50866900
H	0.30149500	-2.31904200	3.54565200
H	0.89577200	-2.03437100	1.89990400
H	3.54412000	-1.79772600	-4.05238400
C	-1.35730500	0.16465200	0.10750600
C	-2.64783500	0.54996400	0.19884100
C	-3.60489900	0.65962000	-0.93144900
C	-3.30536700	1.36629600	-2.10288200
C	-4.87075900	0.06366300	-0.81099800
C	-4.23869300	1.45762500	-3.13206000

H	-2.33931300	1.84528000	-2.20483900
C	-5.79188000	0.13947800	-1.84789100
H	-5.12681300	-0.48310800	0.09118000
C	-5.47899400	0.83942900	-3.01208500
H	-3.99306800	2.01635500	-4.02900800
H	-6.75904400	-0.34140500	-1.74442500
H	-0.77775200	0.05048800	1.02029400
H	-6.20305800	0.90860300	-3.81711400
C	-0.65309700	-0.28904400	-1.10381700
O	-0.64356000	0.23612600	-2.20166400
C	-3.21852000	0.80271900	1.57244000
H	-3.76771800	1.74905100	1.59799600
H	-3.92846400	0.01182700	1.83748200
H	-2.43563500	0.80886900	2.33433800
H	2.57635100	3.43960800	-2.39196600
O	1.51784900	-0.16005600	0.36721300
O	2.42108400	1.95102300	0.98620600
N	1.46933200	0.63588600	1.38851800
C	2.28475200	0.13763100	2.49521800
C	3.38084600	-0.69199900	2.27810900
C	1.88579600	0.47647700	3.78000200
C	4.08709000	-1.18267900	3.36894700
C	2.59484900	-0.02162100	4.87237400
C	3.69420500	-0.85020700	4.66738700
H	3.64265400	-0.94256500	1.25490400
H	1.01448700	1.11160600	3.91234500
H	4.94503400	-1.82946100	3.21332700
H	2.28632000	0.23281900	5.88121500
H	4.24496400	-1.24082600	5.51681100
H	2.88942300	1.56734000	0.22417200
C	1.05720400	5.02222600	0.57450000
C	-0.18999800	5.91774100	0.33815800
H	1.52906600	5.20659100	1.54238800
H	1.81378900	5.13532200	-0.20555200
H	-0.18575300	6.76557200	1.02724400
H	-0.19838800	6.31581400	-0.68024300

C	-0.24801300	3.35847500	1.77643200
H	-0.65316000	2.35083200	1.66663400
H	0.41746000	3.36387300	2.64330900
C	-1.33605600	4.45661400	1.82966900
H	-2.30945400	4.01912400	2.06750600
H	-1.10936600	5.20153500	2.59753100
C	-1.53248300	4.13504900	-0.52160300
H	-2.34996800	3.45418100	-0.25911900
H	-1.79705600	4.62316300	-1.46347000
C	-0.19965700	3.36315700	-0.66595700
H	-0.32767500	2.28496700	-0.78100700
H	0.39523400	3.73037800	-1.50617500
N	0.59687400	3.60607400	0.56889500
N	-1.41927800	5.14272800	0.53753200
H	1.47939900	2.86904300	0.64532600

TS'' (DBU.H⁺)

GFE= -1950.503659 a.u.

Frequency= -549.73 cm⁻¹

C	0.50998800	-1.59258000	-0.65127100
C	2.33242100	-2.73962600	-0.42891100
C	2.35913000	-1.09947600	-2.35910300
H	1.77786800	-1.43683100	-3.21855700
N	1.52004100	-3.21026300	0.47851100
N	0.38381700	-2.48582300	0.32273000
N	1.73903700	-1.74850200	-1.16519100
C	3.72074000	-3.21151800	-0.72928700
H	3.76088700	-4.29660900	-0.62196200
H	4.42538300	-2.75948000	-0.02006500
C	3.84582900	-1.55388100	-2.40656900
O	4.03843200	-2.90464200	-2.06549900
C	3.80465500	0.73673900	-1.87441000
C	2.50702600	0.40534900	-2.28597400
C	1.62852800	1.39308800	-2.73184400

C	2.05336800	2.72167100	-2.71504800
C	3.33452100	3.05466900	-2.27278100
C	4.22087600	2.06303000	-1.85865700
C	4.60782000	-0.49988900	-1.57743000
H	0.64577000	1.13395700	-3.10916400
H	3.64799800	4.09312900	-2.26670400
H	5.22643700	2.31753900	-1.53877300
H	4.57886900	-0.71752100	-0.50316600
H	5.65513800	-0.42407900	-1.87654100
C	-0.83107700	-2.84954000	1.01447600
C	-0.92317000	-2.61302900	2.39039200
C	-1.86001500	-3.42319000	0.26121700
C	-2.13214200	-2.93005500	3.00449800
C	-3.04516000	-3.72457400	0.93237800
C	-3.20356900	-3.47758900	2.29515000
H	-2.23630300	-2.75017900	4.07155500
H	-3.86036500	-4.17412900	0.37053500
C	-1.73660100	-3.70659000	-1.21435500
H	-2.40282600	-4.52603900	-1.48905300
H	-0.71916400	-3.99554800	-1.49302600
H	-2.02756900	-2.84012200	-1.82005400
C	-4.48718100	-3.83019500	2.99991000
H	-4.72755100	-3.09779100	3.77434000
H	-4.40040700	-4.80633000	3.48719800
H	-5.32462800	-3.88358100	2.30053800
C	0.22366900	-2.04064400	3.17498700
H	-0.07232700	-1.87290000	4.21174100
H	0.55889600	-1.09497800	2.73706900
H	1.07206400	-2.73237900	3.17204700
H	4.15744200	-1.47398100	-3.45092300
C	-1.45905500	-0.11480700	-0.17275200
C	-2.81188400	-0.12833000	-0.18258100
C	-3.66553600	-0.61362400	-1.29228300
C	-3.45549500	-0.21917500	-2.62010500
C	-4.74030600	-1.47254500	-1.00764500
C	-4.27597100	-0.69793400	-3.63759500

H	-2.65348100	0.46999900	-2.84888500
C	-5.54512700	-1.96205300	-2.02754600
H	-4.92962000	-1.78115600	0.01554200
C	-5.31395500	-1.57671700	-3.34727900
H	-4.10247800	-0.37858400	-4.65977100
H	-6.36026500	-2.63875700	-1.79302600
H	-0.92508100	0.18323100	0.73094100
H	-5.94882300	-1.95285200	-4.14262400
C	-0.57948800	-0.69553900	-1.19009000
O	-0.62306100	-0.59023700	-2.40075200
C	-3.52266000	0.29934700	1.07550900
H	-4.29667100	1.04174400	0.85400100
H	-4.01810900	-0.55812400	1.54331800
H	-2.80940900	0.70366300	1.79476700
H	1.38506300	3.50115300	-3.06728400
O	1.24549700	0.19205700	1.11616200
O	2.12804200	2.43667600	0.58632000
N	2.03903000	1.00789200	1.67860400
C	3.42196300	0.55539200	1.63854600
C	3.64504400	-0.78554500	1.95702600
C	4.50085500	1.42688700	1.48002600
C	4.94971700	-1.25577700	2.10874100
C	5.79784400	0.93783300	1.59717800
C	6.03071800	-0.40149400	1.91384500
H	2.79337300	-1.43969900	2.10666200
H	4.30434600	2.46358300	1.23771000
H	5.11804600	-2.29225900	2.38809800
H	6.63589500	1.61256200	1.45217000
H	7.04538500	-0.76903500	2.02376100
H	2.03474200	1.96588600	-0.25691400
C	-0.93659200	3.34067700	-0.63215900
C	-1.12097900	3.36617400	0.87540300
C	-2.18453100	3.14529800	-1.48770000
C	-3.48913400	4.21588700	0.83242800
C	-2.99066400	4.43069900	-1.66020100
C	-3.17172100	5.15722200	-0.32645300

H	-0.40815400	4.25828800	-0.92176400
H	-4.21188400	3.44722600	0.52467300
H	-2.81011300	2.36529100	-1.03864600
H	-3.96891700	4.18999600	-2.08909200
H	-0.22917600	2.52313700	-0.80638000
H	-1.87786800	2.76127600	-2.46635400
H	-3.96542800	4.79149700	1.63235000
H	-2.49034200	5.09756800	-2.37038100
H	-3.98406100	5.88458300	-0.40879000
H	-2.27405600	5.73057300	-0.06766500
C	-2.50271900	3.34587200	2.90193900
H	-2.59880300	4.31675500	3.40499000
H	-3.45618500	2.81771000	3.02487500
C	-0.04461000	3.13715000	3.01447300
H	0.81622600	2.55087000	3.33987200
H	0.07497500	4.16557500	3.37919000
C	-1.35816000	2.55030200	3.50703700
H	-1.43035500	2.58582300	4.59642400
H	-1.40840000	1.49954000	3.20289300
N	-0.03957300	3.12818400	1.55938100
N	-2.31859500	3.58312200	1.46220800
H	0.99316700	2.82346900	1.01398800

Pre-R2

GFE= -514.1091614 a.u.

C	-0.27896400	0.54009900	0.17880500
C	-0.44811600	-0.83746900	-0.00219500
C	-1.70142300	-1.40848400	-0.15411300
C	-2.80586300	-0.55215400	-0.12916700
C	-2.65534100	0.82114400	0.04425000
C	-1.38021300	1.37516700	0.20281900
C	1.19650400	0.82780900	0.33366600
C	1.83776700	-0.56273900	0.11348800
H	-1.82173100	-2.47749800	-0.29358500
H	-3.79961300	-0.97149300	-0.24891500
H	-3.52952600	1.46259500	0.05666100

H	-1.25943600	2.44628900	0.33937100
O	3.01854100	-0.81180700	0.06167900
O	1.75912100	1.72177200	-0.59417500
H	1.57692200	2.61991500	-0.29760200
N	0.80463300	-1.46555200	-0.00030000
H	0.96497600	-2.44424600	-0.18678800
H	1.42858100	1.12335300	1.36761100

R2

GFE= -513.6090347 a.u.

C	-0.22323700	0.56370900	-0.00108000
C	-0.48493900	-0.85407400	-0.00114000
C	-1.77124400	-1.36274800	0.00033700
C	-2.85244600	-0.47002700	0.00182100
C	-2.61993400	0.91087600	0.00089000
C	-1.32994100	1.43478300	-0.00073200
C	1.17286800	0.70789700	-0.00099400
C	1.79438100	-0.55279200	-0.00039200
H	-1.93697700	-2.43804500	0.00057600
H	-3.86818700	-0.85339200	0.00318200
H	-3.46824200	1.59172200	0.00148900
H	-1.16997000	2.50911900	-0.00088100
O	3.01799100	-0.84514300	0.00280000
O	1.91366700	1.88364500	0.00024600
H	2.82613200	1.55744000	0.00417500
N	0.73729600	-1.49327700	-0.00572900
H	0.88986600	-2.48767200	0.01493100

TS0 (DABCO)

GFE= -859.1937871 a.u.

Frequency= -778.28 cm⁻¹

C	2.15434000	-0.11284800	0.54606900
C	2.60405600	0.44794800	-0.67410400
C	3.67877700	-0.08307700	-1.37152600

C	4.33371100	-1.18915900	-0.82140900
C	3.91707800	-1.73876000	0.39225900
C	2.82460100	-1.20860400	1.08107000
C	0.97098000	0.62963900	0.94104900
C	0.85834400	1.77310500	0.05025400
H	4.01001300	0.35485000	-2.30843800
H	5.18206800	-1.61870400	-1.34446500
H	4.44927000	-2.59053100	0.80457700
H	2.49627700	-1.63615400	2.02405300
O	0.04123400	2.70320700	0.04293300
O	0.45738500	0.64748400	2.24290300
H	0.95226200	1.29540900	2.76034400
N	1.79504800	1.54176000	-0.96384400
H	1.90273200	2.16430700	-1.74943200
H	-0.27650100	0.05839200	0.33163400
C	-1.69976000	0.23165900	-1.32672000
C	-3.14540800	-0.20192600	-1.68700000
H	-1.55355300	1.31444600	-1.34496400
H	-0.94468500	-0.22965900	-1.96909400
H	-3.69972200	0.63482000	-2.12033800
H	-3.14107300	-1.01480300	-2.41918500
C	-2.30249900	0.56482700	1.00455900
H	-2.11141400	0.17355200	2.00534600
H	-1.95688900	1.60043900	0.97444900
C	-3.77042700	0.36754400	0.54489800
H	-4.40230000	0.07266200	1.38711000
H	-4.17903000	1.29308700	0.12972300
C	-3.20652300	-1.89004700	-0.00089700
H	-3.69267100	-2.17999700	0.93493800
H	-3.37230000	-2.69142900	-0.72595400
C	-1.68624300	-1.65356900	0.21445200
H	-1.34431500	-1.95158800	1.20869100
H	-1.07240100	-2.16933100	-0.52875100
N	-1.43083400	-0.20155200	0.07002400
N	-3.85291100	-0.66959200	-0.49113100

TS0' (DBU)

GFE= -975.8716657 a.u.

Frequency= -942.98 cm⁻¹

C	2.33098700	-0.51354300	0.29367600
C	3.41605400	0.25856000	-0.18484200
C	4.57410500	-0.32666600	-0.67042500
C	4.66065000	-1.72303900	-0.65006100
C	3.61370500	-2.49832400	-0.15393000
C	2.44123100	-1.89942600	0.31661700
C	1.25870000	0.42092800	0.62213900
C	1.85138700	1.76077800	0.59391100
H	5.39618500	0.28010600	-1.03781500
H	5.56168300	-2.20389300	-1.01709300
H	3.71085200	-3.57926400	-0.13205100
H	1.62709600	-2.50282700	0.71094000
O	1.38839600	2.83936100	0.96461600
O	0.24281100	0.12377100	1.54195600
H	0.60192600	0.20707000	2.43447500
N	3.08567700	1.60349000	-0.04220200
H	3.70489500	2.38057600	-0.21301200
H	0.36259000	0.55159400	-0.53746800
C	-1.30345600	-1.45500700	-0.51260300
C	-1.67072900	0.00835300	-0.61646600
C	-1.92523500	-2.19237800	0.67123700
C	-4.06199300	-0.29477900	0.12239800
C	-3.32147600	-2.72492500	0.34353900
C	-4.14615600	-1.70581400	-0.44580900
H	-1.55542300	-1.94794300	-1.45991200
H	-4.15285500	-0.31977100	1.21813300
H	-1.95684800	-1.50716900	1.52503000
H	-3.84590200	-2.98343800	1.26989800
H	-0.21253800	-1.46763400	-0.45034600
H	-1.27075600	-3.01763700	0.96640100
H	-4.91101800	0.28962100	-0.24997700

H	-3.24157600	-3.64743100	-0.24204500
H	-5.19929500	-2.00223300	-0.44251200
H	-3.84041800	-1.68088000	-1.49745400
C	-3.06980400	1.92635400	-0.00303600
H	-3.75263300	2.31142900	-0.77174100
H	-3.57393100	2.02579400	0.96486700
C	-0.95379100	2.21444500	-1.20875000
H	0.01770700	2.70829700	-1.25588200
H	-1.49114700	2.41575900	-2.14438400
C	-1.75751200	2.68852300	-0.00797200
H	-1.95665600	3.76182300	-0.04969700
H	-1.17029400	2.47811700	0.89093900
N	-0.71714900	0.77928700	-1.08885600
N	-2.87157300	0.48588600	-0.23888700

TS3 (RS)

GFE= -2026.815876 a.u.

Frequency= -104.75 cm⁻¹

C	-1.81173700	0.63144500	-0.42374800
C	-3.82730400	1.48225700	-0.34414100
C	-3.76224300	-0.93660200	-0.89869000
H	-3.07189500	-1.49501300	-1.53294200
N	-3.04877200	2.46347200	0.00036000
N	-1.79288800	1.91958300	-0.05116600
N	-3.11460200	0.35425100	-0.63527200
C	-5.30754700	1.41783600	-0.52832700
H	-5.71739800	2.41485000	-0.68885300
H	-5.78404600	0.97174000	0.35704800
C	-5.16373000	-0.71455100	-1.57892800
O	-5.53745700	0.65129500	-1.69219500
C	-5.41987500	-1.97595800	0.48637700
C	-4.06948600	-1.65148500	0.39658400
C	-3.17245800	-1.97476200	1.41174900
C	-3.66052800	-2.63055800	2.53852100
C	-5.01541400	-2.95799400	2.63724900

C	-5.90275100	-2.63635800	1.61346500
C	-6.17426600	-1.53873600	-0.74311000
H	-2.11871000	-1.71492600	1.33089500
H	-5.37932900	-3.46966500	3.52256200
H	-6.95472100	-2.89363100	1.69463900
H	-7.05481700	-0.92912200	-0.51442900
H	-6.52590400	-2.40226700	-1.31610900
C	-0.63395200	2.74020300	0.16927100
C	-0.22698700	2.97182500	1.48338300
C	0.03386900	3.23841400	-0.95060200
C	0.93901400	3.71304500	1.66649700
C	1.19803800	3.96633000	-0.71362000
C	1.66870000	4.20133200	0.58037300
H	1.29017000	3.90145800	2.67784800
H	1.74843300	4.36236400	-1.56364400
C	2.95415800	4.95891200	0.79321500
H	3.81503300	4.34493800	0.50888200
H	3.07816300	5.24661100	1.83922700
H	2.98329800	5.86403400	0.18101800
C	-1.01485500	2.41638600	2.63980700
H	-1.11907200	1.32823500	2.55724900
H	-2.02346400	2.83990800	2.66301600
H	-0.52123300	2.64058900	3.58634000
H	-5.12281700	-1.06155200	-2.61114900
C	0.31002800	-0.28647800	0.32696000
C	1.35207000	-1.26396300	0.47700500
H	0.36086600	0.60692100	0.93513100
C	-0.71370000	-0.36082300	-0.59403500
O	-0.91442100	-1.20209400	-1.54208700
H	-2.98360300	-2.89290800	3.34483000
C	3.54509500	-1.94701000	-1.45211400
C	4.32396500	-0.78412300	-1.23665300
C	5.63909400	-0.86042800	-0.81108200
C	6.18351300	-2.13105600	-0.60281900
C	5.43125400	-3.28821600	-0.81654100
C	4.10402000	-3.20574100	-1.24023600

C	2.21393600	-1.50839000	-1.77458300
C	2.25568700	-0.04077900	-1.90764900
H	6.22368500	0.03696300	-0.63533300
H	7.21278300	-2.21572600	-0.26855600
H	5.88546100	-4.26053800	-0.65561000
H	3.51418500	-4.09946800	-1.42118400
O	1.36976800	0.73652500	-2.24562800
O	1.26886900	-2.28898100	-2.29369900
H	0.37128100	-1.84900700	-2.11149200
N	3.54498300	0.32621200	-1.53091500
H	3.80981300	1.28664800	-1.37842500
C	2.53839100	-0.88947800	1.25709400
C	3.38490700	-1.86376400	1.81475200
C	2.91087100	0.46033600	1.41231200
C	4.54505600	-1.50758100	2.49195200
H	3.13924200	-2.91449600	1.70904500
C	4.06119100	0.81553800	2.10490000
H	2.30490900	1.23856500	0.95437600
C	4.88944900	-0.16738200	2.64590400
H	5.18639100	-2.28377800	2.89817400
H	4.31685300	1.86618800	2.21379900
H	5.79331600	0.10926800	3.17960500
C	0.93730000	-2.71512100	0.47735900
H	0.68811700	-3.01315500	1.50443000
H	0.05806200	-2.86347600	-0.14879700
H	1.72971300	-3.37872200	0.11792800
C	-0.51160700	3.01845600	-2.33437300
H	-0.51350200	1.95470200	-2.58221800
H	-1.53212600	3.40817300	-2.40841700
H	0.11073200	3.52684800	-3.07194700

TS3 (RS)_{a2}

GFE= -2026.794299 a.u.

Frequency= -223.38 cm⁻¹

C	0.78107500	-1.06307300	-0.33872100
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C	2.46483500	-2.21419000	-1.15869400
C	2.78687500	0.20155700	-1.28253400
H	2.16636500	1.08371500	-1.43893900
N	1.76309100	-3.08934000	-0.51181600
N	0.71959700	-2.36304100	0.01010300
N	1.90769200	-0.96172100	-1.09951700
C	3.75238800	-2.35589300	-1.90777700
H	3.81955100	-3.34134200	-2.36974700
H	4.60294600	-2.22718700	-1.22282900
C	3.75031500	-0.04031100	-2.49560400
O	3.74987900	-1.39071700	-2.93792700
C	5.03118400	0.47520100	-0.50015600
C	3.70640500	0.35455700	-0.09064000
C	3.35408200	0.36168900	1.25600900
C	4.36654400	0.50386200	2.20118500
C	5.69792600	0.63392300	1.79841600
C	6.04071500	0.61826400	0.44825200
C	5.14063100	0.42642400	-2.00442200
H	2.31759900	0.24949800	1.56775400
H	6.47501500	0.74300400	2.54793500
H	7.07843000	0.70899300	0.14162400
H	5.91345600	-0.25926700	-2.36532800
H	5.37060700	1.41689800	-2.41063300
C	-0.38248900	-3.05290500	0.61879800
C	-0.43633900	-3.17111400	2.00656500
C	-1.33184900	-3.61468900	-0.24003100
C	-1.52707100	-3.85737400	2.54109000
C	-2.39790000	-4.29455700	0.34293900
C	-2.51687500	-4.41242100	1.73049000
H	-1.60134500	-3.96199200	3.62049900
H	-3.15011400	-4.74734600	-0.29945800
C	-1.18389800	-3.48068600	-1.73223100
H	-1.99634200	-3.99484800	-2.24875700
H	-0.23447800	-3.90670500	-2.07008800
H	-1.20906100	-2.42589400	-2.02938600
C	-3.70291600	-5.11771800	2.33461100

H	-3.96613300	-6.00965900	1.76062300
H	-4.57726100	-4.45930800	2.33982400
H	-3.50373300	-5.41613600	3.36585400
C	0.62888800	-2.57358400	2.88354400
H	0.49239500	-1.48970400	2.93873600
H	1.62738100	-2.76735000	2.48035300
H	0.57433800	-2.98982500	3.89088100
H	3.41665100	0.52409000	-3.36668100
C	-0.27846100	1.04477400	-0.85060800
C	-0.80862200	2.36417300	-0.73758800
C	-0.34547300	3.27564800	0.31897100
C	-0.53996200	4.66760400	0.20577400
C	0.35729600	2.82786500	1.45537100
C	-0.05951000	5.55128400	1.16345300
H	-1.07630500	5.07303100	-0.64312700
C	0.83563700	3.71453500	2.41223300
H	0.54263400	1.77265200	1.59735900
C	0.63378600	5.08481900	2.27703500
H	-0.23209700	6.61587800	1.03575700
H	1.37670200	3.32572400	3.27050700
H	-0.03352200	0.74243500	-1.87349900
H	1.01112500	5.77681100	3.02318800
C	-0.07923700	0.01760500	0.05393000
O	-0.55610500	-0.12521800	1.31746800
C	-1.15576200	2.97713800	-2.08129200
H	-0.26429700	3.37254400	-2.58970000
H	-1.61649400	2.22751900	-2.73257100
H	-1.86841700	3.79943000	-1.99474200
H	4.11926500	0.51364200	3.25743400
C	-3.30079000	0.69949400	-0.42826700
C	-4.07488100	1.32538300	-1.42463400
C	-4.69395600	0.59726400	-2.42690700
C	-4.55697800	-0.79458300	-2.39355200
C	-3.83061500	-1.42926300	-1.38721400
C	-3.18807300	-0.68466100	-0.39364300
C	-2.83599400	1.74687100	0.49972900

C	-3.46087500	3.04323600	-0.01679100
H	-5.28612200	1.08592500	-3.19364300
H	-5.04498300	-1.38950400	-3.15928300
H	-3.77373800	-2.51239500	-1.36574200
H	-2.63061200	-1.16992000	0.40396400
O	-3.40790700	4.15467300	0.46382200
O	-2.36098600	1.61281000	1.64559500
H	-1.29846300	0.54352300	1.51352500
N	-4.12329200	2.69688300	-1.18563000
H	-4.64995000	3.36433100	-1.72784100

TS3 (RS) _{a3}

GFE= -2026.797426 a.u.

Frequency= -209.09 cm⁻¹

C	1.75752000	-0.06757400	-0.25590300
C	3.22000700	1.44494000	-0.85602300
C	0.97505300	2.36124600	-0.56556500
H	-0.03884000	1.95921200	-0.62925500
N	3.90452600	0.34119500	-0.77516700
N	2.97816600	-0.58832700	-0.39597500
N	1.90645900	1.23914300	-0.54124300
C	3.58958600	2.80844000	-1.34311900
H	4.54207400	2.77107400	-1.87195700
H	3.66986200	3.50897600	-0.50158700
C	1.25125000	3.26207000	-1.80420500
O	2.59811700	3.20200000	-2.27387600
C	1.09052000	4.61747800	0.18084800
C	1.16398100	3.29259400	0.61204900
C	1.38837900	2.97888400	1.94730300
C	1.51628100	4.02293900	2.86331100
C	1.42391300	5.34917900	2.44090400
C	1.21416500	5.65617100	1.09631400
C	0.88036400	4.67586700	-1.31406500
H	1.47852700	1.94556400	2.27436500
H	1.53002000	6.15030100	3.16519800
H	1.16278100	6.69054900	0.76939800

H	1.49061300	5.42921300	-1.81867400
H	-0.17013800	4.88582100	-1.54753000
C	3.40086600	-1.93080200	-0.09313100
C	3.67789500	-2.23892600	1.23569700
C	3.52440900	-2.84171500	-1.14227700
C	4.12470000	-3.53230000	1.50828600
C	3.97565000	-4.11686600	-0.82021700
C	4.28374700	-4.47657700	0.49551100
H	4.34981900	-3.80494900	2.53607900
H	4.08008600	-4.85375900	-1.61295900
C	3.12825400	-2.44745400	-2.53674900
H	3.29933000	-3.26702300	-3.23621800
H	3.69243800	-1.57442900	-2.87843900
H	2.06422500	-2.18838200	-2.54300300
C	4.77826500	-5.86665200	0.80117900
H	5.75754500	-6.03950100	0.34438700
H	4.09334400	-6.61971600	0.40188500
H	4.87335100	-6.02692000	1.87689600
C	3.47275600	-1.22016700	2.32632300
H	2.40690300	-0.99340800	2.44804900
H	3.99046200	-0.28272600	2.09809900
H	3.84873100	-1.59587200	3.27902800
H	0.64142600	2.93069000	-2.64617400
C	-0.39695200	-0.17854400	0.86579300
C	-1.77128000	-0.31618000	1.18404600
C	-2.60994100	-1.53890000	1.04772600
C	-3.81554300	-1.63399900	1.76755300
C	-2.28680200	-2.60479300	0.19255500
C	-4.65796500	-2.73108200	1.63870100
H	-4.11756300	-0.84061000	2.43866900
C	-3.13051200	-3.70433700	0.06666400
H	-1.36059900	-2.57256100	-0.36663800
C	-4.32172800	-3.77498500	0.78291900
H	-5.58374500	-2.76132200	2.20474000
H	-2.84771800	-4.51501100	-0.59854800
H	0.00154000	0.77158000	1.20335600

H	-4.97793900	-4.63395100	0.67911700
C	0.49934100	-0.87766900	0.03381700
O	0.51780100	-2.00536300	-0.48377600
C	-2.21094400	0.63844500	2.28049800
H	-3.24081000	0.97676100	2.14625900
H	-2.14485000	0.12748900	3.24819700
H	-1.57230700	1.52109500	2.30415100
H	1.69499400	3.80178300	3.91032100
C	-4.07415700	0.60738400	-0.48215300
C	-4.16850100	-0.47010100	-1.40127700
C	-5.34659600	-1.17658900	-1.57559300
C	-6.46030600	-0.78619300	-0.82627400
C	-6.39259700	0.28826100	0.06374000
C	-5.20104700	0.99081600	0.24544700
C	-2.69770000	1.01208900	-0.47766900
C	-2.02615100	0.32619900	-1.56277400
H	-5.40085300	-2.00987300	-2.26910600
H	-7.39486800	-1.32482900	-0.94640400
H	-7.27759000	0.57819400	0.62139100
H	-5.14631700	1.82862800	0.93552100
O	-0.86603900	0.46745100	-1.97232500
O	-2.21032800	2.21129400	0.01047700
H	-2.58537000	2.92753300	-0.51891000
N	-2.93872600	-0.61434100	-2.02959900
H	-2.68704000	-1.34997400	-2.67096200

TS3 (RS)_{a4}

GFE= -2026.798278 a.u.

Frequency= -259.83 cm⁻¹

C	1.01386600	0.86003500	0.50282400
C	2.98950800	1.83124000	0.67898000
C	3.04539700	-0.49032800	1.38669800
H	2.33888100	-1.22067500	1.77712100
N	2.25511000	2.71859300	0.09122600

N	1.02401100	2.11703400	-0.01632000
N	2.29049100	0.68735600	0.96121800
C	4.40856500	1.89845700	1.14586600
H	4.70755900	2.93934600	1.27252200
H	5.07984100	1.41851100	0.42177600
C	4.10689800	-0.09855400	2.46431500
O	4.46466400	1.27918600	2.41716700
C	5.16228900	-1.35912400	0.69986100
C	3.88210500	-1.04170500	0.25187200
C	3.52029400	-1.18573800	-1.08083100
C	4.46221300	-1.69934600	-1.97119300
C	5.73735500	-2.04992200	-1.52431900
C	6.09937600	-1.87601300	-0.18859700
C	5.30632200	-1.02395800	2.16534700
H	2.53208600	-0.88356400	-1.42083600
H	6.46132000	-2.44568000	-2.22912700
H	7.10210500	-2.12412800	0.14623300
H	6.24443200	-0.51913200	2.41117500
H	5.24418700	-1.92823600	2.78132800
C	-0.05927100	2.87010900	-0.57611600
C	-0.15679500	2.94264000	-1.96690600
C	-0.97496000	3.47540100	0.28814900
C	-1.22694600	3.65898900	-2.49909700
C	-2.03192000	4.17306900	-0.29236400
C	-2.17505500	4.27169300	-1.67795200
H	-1.32873300	3.72966100	-3.57913200
H	-2.76357000	4.64982700	0.35552700
C	-0.85002900	3.32508100	1.77900600
H	-1.47473200	4.05689400	2.29342000
H	0.18471000	3.45737300	2.10742400
H	-1.17606100	2.32378500	2.08724600
C	-3.35107600	5.00317200	-2.27105500
H	-3.57061100	5.91597600	-1.71189200
H	-4.24759900	4.37564900	-2.24056600
H	-3.16649300	5.27228600	-3.31306600
C	0.82966800	2.21254400	-2.83904200

H	0.73955400	1.12820300	-2.69341900
H	1.85864200	2.49372200	-2.59774000
H	0.64612400	2.42770700	-3.89278000
H	3.71256800	-0.24518500	3.47075400
C	-1.28474800	0.18282400	0.03662000
C	-2.59751200	-0.33433600	0.21282800
C	-3.19230100	-0.51095500	1.55184200
C	-4.57606800	-0.73041400	1.69720500
C	-2.43771100	-0.41554200	2.73721200
C	-5.16707700	-0.85534800	2.94782200
H	-5.20774800	-0.81298400	0.82204500
C	-3.03217400	-0.54190800	3.98777800
H	-1.37340900	-0.22993700	2.69255800
C	-4.40037400	-0.76400000	4.10612400
H	-6.23703500	-1.02798300	3.01429700
H	-2.41519600	-0.46209100	4.87812000
H	-1.19751200	0.85415200	-0.81343800
H	-4.86234200	-0.86245400	5.08339100
C	-0.07247800	-0.05570800	0.66722200
O	0.23754700	-1.09076100	1.49221000
C	-3.53583400	0.09730700	-0.90220900
H	-3.89046300	1.12475300	-0.73974700
H	-3.01726900	0.06666700	-1.86599700
H	-4.41333700	-0.54506300	-0.99307700
H	4.20914900	-1.81848500	-3.02007600
C	-1.19083400	-2.46125200	-1.27496600
C	-2.10225500	-2.59107100	-2.33939000
C	-1.69401500	-2.48516600	-3.65901800
C	-0.33119700	-2.28197000	-3.90088700
C	0.58977900	-2.20452600	-2.85632000
C	0.16367400	-2.29425200	-1.52739600
C	-1.94460300	-2.60965200	-0.01618000
C	-3.36952500	-2.95377900	-0.44929100
H	-2.40151800	-2.57920400	-4.47617700
H	0.01604400	-2.20765900	-4.92654800
H	1.64588500	-2.09661100	-3.08266200

H	0.86509400	-2.25869600	-0.69828300
O	-4.31925600	-3.25150200	0.24185100
O	-1.50113300	-2.82461000	1.13551700
H	-0.45135100	-1.86024600	1.38790300
N	-3.37370600	-2.85053100	-1.83338800
H	-4.19443600	-3.04013400	-2.38802800

TS3 (RR)_{b1}

GFE= -2026.697776 a.u.

Frequency= -171.41 cm⁻¹

C	1.33079900	1.14032800	0.49492700
C	3.32348600	1.81558300	-0.12676000
C	3.36125600	-0.35354100	1.06616500
H	2.77152000	-0.68248200	1.91805200
N	2.52595400	2.76540400	-0.51062000
N	1.28911400	2.33534000	-0.12255800
N	2.64658600	0.81362500	0.50826300
C	4.81208100	1.75051100	-0.15269200
H	5.22913500	2.73457700	-0.36540400
H	5.16178900	1.03558700	-0.91099000
C	4.83285300	0.04019600	1.48074100
O	5.20351600	1.36968000	1.15027600
C	4.86546700	-1.82204100	-0.08386700
C	3.52741800	-1.46223200	0.05345000
C	2.52139100	-2.12953100	-0.64261200
C	2.88923500	-3.16573800	-1.49589200
C	4.23128900	-3.52273000	-1.64976400
C	5.22809200	-2.85561800	-0.94391400
C	5.75818200	-1.00594600	0.81297600
H	1.47775400	-1.85726600	-0.50687400
H	4.49746300	-4.33557000	-2.31806200
H	6.27004500	-3.14115000	-1.05539400
H	6.56430000	-0.49798200	0.27241700
H	6.23458200	-1.63450400	1.57145700
C	0.18539000	3.24578700	-0.28988100

C	-0.56316200	3.18163200	-1.46326500
C	-0.08159000	4.13875400	0.74917800
C	-1.63007700	4.06915500	-1.58625500
C	-1.15367400	5.00993000	0.57633400
C	-1.93386600	4.99038500	-0.58308200
H	-2.24399400	4.02863700	-2.48222000
H	-1.39091900	5.71461100	1.36945300
C	0.72455900	4.10738300	2.01916900
H	0.46665000	4.95136600	2.66034500
H	1.79806700	4.14405200	1.81174800
H	0.52161500	3.18372200	2.57317300
C	-3.07241500	5.96261100	-0.75131900
H	-3.81726100	5.58178100	-1.45323400
H	-2.70637200	6.91828600	-1.14022300
H	-3.56555700	6.16180700	0.20293700
C	-0.25246400	2.13575900	-2.49380300
H	-0.30595900	1.14682700	-2.02511200
H	0.75435300	2.26821300	-2.90230000
H	-0.97670700	2.16479500	-3.30860900
H	4.91282000	0.00510300	2.56736500
C	-1.05724100	0.66148300	0.86413600
C	-2.25943200	-0.01892200	1.23496800
C	-2.28616700	-1.43190200	1.65258600
C	-1.65327200	-2.34826800	0.67701200
C	-3.14012900	-1.98251800	2.54536400
C	-1.68987800	-3.88368600	0.77178700
H	-0.67164100	-2.00466300	0.36221700
C	-3.32455100	-3.44386900	2.60427200
H	-3.74457100	-1.36695800	3.20527500
C	-2.73134900	-4.31973300	1.77094400
H	-0.73038100	-4.37239500	0.98728700
H	-4.02474800	-3.81917900	3.34640100
H	-1.22258100	1.63998900	0.43577800
H	-2.94773700	-5.38157400	1.86457100
C	0.25163700	0.22822100	1.04248000
O	0.69221700	-0.81338500	1.59634200

C	-3.35097400	0.89288800	1.74097300
H	-4.33714300	0.42706900	1.71855300
H	-3.12245000	1.18943000	2.77208900
H	-3.37735400	1.80840300	1.14010900
H	2.11905900	-3.71282000	-2.02866200
C	-2.19325000	-1.31137100	-1.47471000
C	-2.58275500	-2.44119100	-0.57575000
C	-2.09459000	-3.88876500	-0.74680000
C	-0.92549800	-3.89357100	-1.70714100
C	-0.54031900	-2.80777900	-2.41124800
C	-1.14695900	-1.47731500	-2.31779100
C	-3.03708900	-0.25905900	-1.00418800
C	-4.26773900	-0.87837100	-0.51385000
H	-2.85760400	-4.62275100	-1.04094100
H	-0.41234300	-4.83977000	-1.86341600
H	0.28386500	-2.91481400	-3.11282500
H	-0.78343200	-0.68144800	-2.95607500
O	-5.31525100	-0.28293100	-0.27449700
O	-3.06191200	1.01434700	-1.46558400
H	-3.93878000	1.35760300	-1.22064400
N	-4.00485400	-2.22715500	-0.35969000
H	-4.47979300	-2.71018000	0.39443400

TS3 (RR)_{b2}

GFE= -2026.810308 a.u.

Frequency= -146.30 cm⁻¹

C	1.62903400	0.66762900	0.52790600
C	3.79359400	0.99299200	0.35977100
C	3.22534200	-1.33778100	0.91321900
H	2.44372900	-1.77254800	1.53022400
N	3.27158800	2.14642700	0.07694900
N	1.92573900	1.93443600	0.17873700
N	2.83763500	0.06402200	0.65817500
C	5.22520300	0.59816800	0.49783400
H	5.84928400	1.48472500	0.61104500

H	5.55864200	0.03111000	-0.38295100
C	4.63454200	-1.40969000	1.61313100
O	5.31484000	-0.16484600	1.68277000
C	4.64831200	-2.70368800	-0.44495200
C	3.40246800	-2.08555400	-0.38804800
C	2.48253500	-2.18592500	-1.42785000
C	2.85131000	-2.92040900	-2.55256200
C	4.10143600	-3.54064200	-2.62392200
C	5.00728100	-3.44136200	-1.57036000
C	5.43659900	-2.46906300	0.81826300
H	1.50251400	-1.71802500	-1.35781700
H	4.36947400	-4.10919600	-3.50902000
H	5.97659300	-3.92815100	-1.62754600
H	6.45340000	-2.10458300	0.63811400
H	5.52614100	-3.39198200	1.40029300
C	1.05669600	3.04780900	-0.09106800
C	0.64890100	3.26332400	-1.40684200
C	0.66931900	3.85440900	0.98110300
C	-0.19529100	4.35002800	-1.63631800
C	-0.17382500	4.92519300	0.69928400
C	-0.61233900	5.18765000	-0.60136400
H	-0.53644600	4.54298800	-2.65033000
H	-0.50079200	5.56633600	1.51411100
C	1.10431900	3.52262000	2.38213800
H	0.77578200	4.29229900	3.08180600
H	2.19253600	3.43167900	2.44903400
H	0.66826700	2.56640000	2.69439000
C	-1.50366100	6.37011400	-0.87843500
H	-2.00936500	6.26809800	-1.84069000
H	-0.91823200	7.29471800	-0.90416200
H	-2.26175700	6.48304600	-0.09961600
C	1.06604000	2.32448200	-2.50468800
H	0.62011500	1.33369700	-2.35169900
H	2.15348000	2.20477800	-2.52660900
H	0.74319700	2.70515500	-3.47534400
H	4.50791700	-1.70027200	2.65639300

C	-0.82509000	0.70618800	0.65492500
C	-2.20454200	0.27421000	0.73586300
C	-2.73109100	-0.52785500	1.85322400
C	-1.88984000	-1.19167500	2.76550000
C	-4.12075000	-0.64152500	2.05216200
C	-2.41540900	-1.93035000	3.81750500
H	-0.81631700	-1.13080500	2.64148700
C	-4.64238200	-1.37905400	3.10971400
H	-4.80815100	-0.14769800	1.37486400
C	-3.79351500	-2.03058600	3.99906300
H	-1.74054000	-2.43121200	4.50527800
H	-5.71919700	-1.44278800	3.23540200
H	-0.71295100	1.73457200	0.33985200
H	-4.19937600	-2.60635900	4.82502800
C	0.33026600	-0.04064800	0.71461800
O	0.47404400	-1.31245700	0.86586300
C	-3.16563700	1.26392100	0.11691000
H	-4.02014300	0.76795600	-0.35429700
H	-3.56450000	1.94497700	0.87929900
H	-2.66432500	1.85619800	-0.65195700
H	2.15364600	-3.01428900	-3.37845700
C	-3.58501700	-1.77471100	-1.00774900
C	-3.81074700	-0.93657000	-2.12433100
C	-5.07939800	-0.76799800	-2.65849500
C	-6.13258700	-1.46317700	-2.05701200
C	-5.92402300	-2.29469500	-0.95290300
C	-4.64744700	-2.45481700	-0.41512800
C	-2.18997200	-1.67937200	-0.66854500
C	-1.54928600	-0.88284600	-1.73688000
H	-5.24932000	-0.12330600	-3.51482600
H	-7.13380700	-1.35201900	-2.46110900
H	-6.76489200	-2.81943800	-0.51163100
H	-4.46525500	-3.09276100	0.44338200
O	-0.35863400	-0.67200500	-1.95201600
O	-1.56469600	-2.55193100	0.10898200
H	-0.68234600	-2.12647400	0.41643300

N	-2.59806800	-0.37423200	-2.50406700
H	-2.43779400	0.16605500	-3.33980400

TS3 (RR)_{b3}

GFE= -2026.69932 a.u.

Frequency= -162.30 cm⁻¹

C	-1.53525400	-0.13390200	0.22190400
C	-3.02109300	1.22346300	1.09159700
C	-0.87381200	2.31166500	0.66340400
H	0.16474800	1.97985700	0.58055400
N	-3.64252500	0.08769400	0.97394400
N	-2.70545000	-0.74422300	0.42771700
N	-1.73257500	1.13301600	0.64311400
C	-3.42371200	2.51481300	1.72638600
H	-4.30992500	2.36913500	2.34401400
H	-3.63496500	3.27356000	0.96169300
C	-1.09535900	3.13093200	1.97597400
O	-2.36346300	2.90132300	2.58270800
C	-1.23802700	4.58964800	0.06214900
C	-1.23033200	3.28842600	-0.43800400
C	-1.54332100	3.02130700	-1.76603900
C	-1.84158600	4.09335600	-2.60614600
C	-1.82929200	5.39993400	-2.11641900
C	-1.53206300	5.65710600	-0.77844300
C	-0.91044600	4.59680100	1.53463700
H	-1.57242300	2.00148800	-2.14216000
H	-2.06673900	6.22380300	-2.78155500
H	-1.54319100	6.67369300	-0.39720400
H	-1.54963800	5.25539900	2.12817600
H	0.12962200	4.90195700	1.69647400
C	-3.09199900	-2.07247800	0.02576400
C	-3.54532900	-2.24366700	-1.27893400
C	-3.02276600	-3.10250100	0.96349000
C	-3.96841300	-3.52269500	-1.64247300
C	-3.45765400	-4.35813600	0.55408600

C	-3.93631200	-4.58412000	-0.74018700
H	-4.32816900	-3.68947600	-2.65444400
H	-3.41225200	-5.18541400	1.25835800
C	-2.44471700	-2.84920600	2.32641800
H	-2.49425100	-3.74775400	2.94315300
H	-2.97636400	-2.04336500	2.84173400
H	-1.39677300	-2.55218200	2.21156800
C	-4.40339100	-5.95908800	-1.14236500
H	-4.68212300	-5.99097000	-2.19742900
H	-5.27298100	-6.26254400	-0.55167900
H	-3.61817000	-6.70128200	-0.97378500
C	-3.54491900	-1.09677600	-2.25540400
H	-2.51825800	-0.79844200	-2.49840000
H	-4.05944000	-0.22195900	-1.84443700
H	-4.04198100	-1.38137800	-3.18392300
H	-0.37190700	2.84099400	2.74020100
C	0.53225100	0.00586200	-1.05572800
C	1.83240300	-0.22242100	-1.58470900
C	2.64342600	-1.41250600	-1.26936300
C	2.76530100	-1.68230100	0.17935300
C	3.56597700	-1.98457100	-2.07700700
C	3.68118200	-2.75212600	0.79651900
H	1.80885400	-1.66514100	0.69158000
C	4.56690300	-2.91800100	-1.52808600
H	3.62928500	-1.73818800	-3.13298800
C	4.68674100	-3.22649300	-0.22231800
H	3.17272100	-3.61406800	1.24901600
H	5.27888200	-3.33932700	-2.23342300
H	0.12400100	0.97847800	-1.30991500
H	5.47628200	-3.90176500	0.09977400
C	-0.27689400	-0.82309600	-0.26917200
O	-0.18415700	-2.02321400	0.06003700
C	2.12491900	0.50712000	-2.87336300
H	3.19379600	0.63433400	-3.05162700
H	1.69183000	-0.05159700	-3.71212200
H	1.65011500	1.49397600	-2.86049400

H	-2.09001500	3.90868300	-3.64588600
C	2.80497300	0.57666500	1.11551700
C	3.69165900	-0.58719200	0.80456400
C	4.12243000	-1.64956700	1.82762100
C	3.19791600	-1.55120300	3.02331100
C	2.28839700	-0.56601700	3.18534500
C	2.05441200	0.53208700	2.24454800
C	2.87672400	1.32930600	-0.08829300
C	4.17755400	1.08322200	-0.69680200
H	5.18043100	-1.64502200	2.12320800
H	3.29968700	-2.31192500	3.79320200
H	1.67803300	-0.57820100	4.08499900
H	1.33125600	1.30171600	2.49218800
O	4.66885200	1.73233200	-1.61868200
O	2.20580200	2.48251200	-0.35346000
H	2.69560300	2.90385000	-1.08068900
N	4.71428300	-0.02127600	-0.05910400
H	5.30316400	-0.63293100	-0.61221600

TS3 (RR)_{b4}

GFE= -2026.79543 a.u.

Frequency= -170.60 cm⁻¹

C	-1.66909400	0.28318500	-0.20521700
C	-3.25217400	-0.98563200	-1.02267500
C	-1.23910800	-2.23692700	-0.42001600
H	-0.17562500	-2.01509600	-0.31819100
N	-3.75441900	0.21665500	-1.03416500
N	-2.75345700	0.99160400	-0.51796100
N	-1.98449800	-0.98785800	-0.51404100
C	-3.74555400	-2.28492900	-1.57733000
H	-4.58964700	-2.10934100	-2.24448000
H	-4.05891600	-2.95345400	-0.76496600
C	-1.44863500	-3.08814800	-1.70086700
O	-2.69743800	-2.83753800	-2.35279100
C	-1.78976600	-4.44785900	0.25179700

C	-1.74546600	-3.12521400	0.69401500
C	-2.13985200	-2.77362500	1.97836400
C	-2.56884900	-3.78354300	2.84003400
C	-2.60023600	-5.11022300	2.41058800
C	-2.21367000	-5.45189600	1.11386200
C	-1.33795000	-4.53503500	-1.18709000
H	-2.13437400	-1.73503300	2.30261800
H	-2.94076000	-5.88458500	3.09051000
H	-2.25613200	-6.48472500	0.78116800
H	-1.93400800	-5.21373300	-1.80199400
H	-0.28859400	-4.84675800	-1.23318200
C	-2.95313000	2.39350200	-0.27187200
C	-3.29089500	2.78458700	1.02260100
C	-2.79413100	3.28426300	-1.33367300
C	-3.50005100	4.14621400	1.24051100
C	-3.01591200	4.63147600	-1.06546100
C	-3.37350000	5.07722800	0.21008000
H	-3.76506400	4.48436200	2.23884000
H	-2.89482600	5.35403100	-1.86868900
C	-2.35200300	2.78814700	-2.68144400
H	-2.27760300	3.61214200	-3.39246300
H	-3.04953700	2.04552700	-3.07993900
H	-1.36937800	2.31611200	-2.57723500
C	-3.62485700	6.54210200	0.45728000
H	-4.58702000	6.84615800	0.03305200
H	-2.85142000	7.15618100	-0.01108600
H	-3.64267300	6.76707700	1.52544300
C	-3.39686900	1.77464800	2.13540400
H	-2.41253600	1.35103100	2.36826200
H	-4.05959100	0.94780700	1.85996100
H	-3.78727200	2.23976200	3.04162500
H	-0.68230700	-2.84596100	-2.43914700
C	0.35814400	0.05013300	1.09571700
C	1.75885800	-0.08239500	1.33956300
C	2.69847000	1.05598300	1.41911900
C	2.26501700	2.38410200	1.27701100

C	4.06557900	0.84163100	1.67083300
C	3.16251400	3.44316300	1.36357300
H	1.21956100	2.58651500	1.08585900
C	4.96197800	1.89982700	1.74457300
H	4.44777900	-0.16563800	1.78534800
C	4.51563100	3.20984900	1.59271700
H	2.79625000	4.45930200	1.25306600
H	6.01445000	1.69606600	1.91589900
H	-0.24187000	-0.75427900	1.51249800
H	5.21409700	4.03869500	1.65430500
C	-0.30329700	0.82242700	0.14660200
O	0.06589500	1.78493100	-0.58448000
C	2.08841100	-1.29060100	2.19323400
H	3.12882200	-1.60331000	2.10636600
H	1.89872800	-1.04893300	3.24644200
H	1.46340800	-2.14132600	1.90949400
H	-2.88503300	-3.53474300	3.84760600
C	3.51921800	-0.15187000	-1.19550700
C	4.53007700	-1.06252500	-0.80872900
C	5.87344600	-0.72990800	-0.86670200
C	6.20756500	0.55094200	-1.31633300
C	5.22017000	1.46760800	-1.68385000
C	3.86970600	1.12777700	-1.62024600
C	2.25845900	-0.80333700	-0.94900600
C	2.54149200	-2.18508500	-0.56937500
H	6.64033500	-1.44087900	-0.57500900
H	7.25325100	0.83646000	-1.37116300
H	5.50800800	2.46085800	-2.01241800
H	3.09983300	1.84986500	-1.87782800
O	1.75313600	-3.11490600	-0.38368900
O	1.08405900	-0.57413200	-1.59536200
H	0.92000000	0.38529400	-1.61230300
N	3.92076700	-2.24871000	-0.39441300
H	4.39727800	-3.10438600	-0.15614600

TS3 (SS)

GFE= -2026.809111 a.u.

Frequency= -180.67 cm⁻¹

C	-1.60074500	0.89589100	-0.50094800
C	-3.51296100	1.67844200	0.23657900
C	-3.78983300	-0.31404300	-1.16971800
H	-3.22657500	-0.70545500	-2.01380700
N	-2.62196900	2.48578300	0.72610400
N	-1.43580800	1.98936500	0.26546000
N	-2.94030800	0.70878700	-0.53506700
C	-5.00245300	1.74284100	0.27934600
H	-5.32642100	2.72374900	0.62668300
H	-5.41063100	0.96891700	0.94365100
C	-5.16517800	0.30451600	-1.61695200
O	-5.43875900	1.58157400	-1.05609800
C	-5.53552800	-1.64148700	-0.21467700
C	-4.16419500	-1.40252700	-0.19119800
C	-3.30560600	-2.11414200	0.63924700
C	-3.86268000	-3.08568300	1.46874700
C	-5.23707500	-3.33587700	1.45427000
C	-6.08377200	-2.61858800	0.61129900
C	-6.22589500	-0.74640100	-1.21291000
H	-2.23666900	-1.90966100	0.65132500
H	-5.65128100	-4.09432200	2.11127700
H	-7.15218400	-2.81355800	0.60542400
H	-7.11202100	-0.24359400	-0.81321900
H	-6.54548800	-1.31704500	-2.09136800
C	-0.24555300	2.74202600	0.57928500
C	0.38117200	2.51457100	1.80614500
C	0.20799200	3.67059200	-0.35990000
C	1.52971100	3.25853600	2.07337100
C	1.35146100	4.40023300	-0.03581800
C	2.02292300	4.20510800	1.17300700

H	2.04971200	3.09120000	3.01328600
H	1.73125100	5.12631100	-0.75007400
C	-0.47858900	3.82017800	-1.69014800
H	-0.07427700	4.67130600	-2.23975700
H	-1.55653800	3.96453400	-1.56981600
H	-0.32425600	2.91817200	-2.29399200
C	3.25173200	5.00935500	1.51145800
H	3.69320900	5.45530400	0.61729000
H	4.00682500	4.38585700	1.99733400
H	3.00365100	5.82189800	2.20186100
C	-0.15214300	1.49075300	2.76501700
H	-0.13880100	0.49934100	2.29872400
H	-1.18191400	1.73010800	3.04951300
H	0.46204900	1.45965800	3.66616100
H	-5.16036000	0.48191800	-2.69301500
C	0.73318800	0.28899200	-1.01711500
C	1.84153900	-0.54170600	-1.28397800
H	0.92733900	1.16246100	-0.42129900
C	-0.61620300	-0.04216200	-1.19022800
O	-1.15563000	-0.97176600	-1.82638500
H	-3.22040500	-3.65161400	2.13613000
C	3.13203700	-2.36294700	0.75496800
C	2.38712600	-3.54505400	0.50756500
C	3.00862900	-4.75439500	0.23466500
C	4.40551600	-4.78274700	0.22746200
C	5.15516700	-3.63226400	0.48963700
C	4.52680700	-2.41570300	0.75096200
C	0.85640700	-1.89860000	0.94612000
H	2.42870100	-5.65109000	0.04022300
H	4.91421600	-5.71893900	0.02132300
H	6.23891200	-3.68834400	0.49061200
H	5.10765800	-1.52086000	0.95573700
O	-0.23131300	-1.36642500	1.18728400
O	2.37389400	-0.10970800	1.54731800
H	3.08439400	0.38013900	1.10184100
N	1.03842500	-3.23690100	0.60399300

H	0.27181000	-3.88220400	0.49817300
C	3.19451300	0.07927100	-1.29284100
C	3.41753000	1.38928500	-0.82131400
C	4.31286700	-0.63187500	-1.76162800
C	4.69521700	1.94051500	-0.79043100
H	2.58711300	2.01108600	-0.50576000
C	5.58628600	-0.07235700	-1.74571700
H	4.19279900	-1.63885700	-2.14258000
C	5.78976200	1.21273700	-1.25015500
H	4.82620100	2.95320900	-0.41945800
H	6.42615100	-0.65227300	-2.11592300
H	6.78503000	1.64488500	-1.23256900
C	1.67732800	-1.79868100	-2.09911500
H	1.87600000	-1.57186800	-3.15390500
H	2.38494600	-2.57347700	-1.79138600
H	0.66310000	-2.18001500	-2.01841800
C	2.17830800	-1.29585500	0.90220400

TS3 (SS) c2

GFE= -2026.798882 a.u.

Frequency= -149.14 cm⁻¹

C	-1.61275400	0.44941800	-0.41758600
C	-3.41176600	0.44468000	-1.65700400
C	-2.87361400	-1.74270800	-0.62104300
H	-1.92635100	-2.25475800	-0.43981000
N	-3.04159900	1.69109100	-1.61694000
N	-1.92405700	1.67489200	-0.82872700
N	-2.55263900	-0.35080900	-0.94924200
C	-4.54328900	-0.23947600	-2.35348100
H	-4.86765400	0.33847000	-3.21863700
H	-5.39285400	-0.36619600	-1.66707400
C	-3.68890400	-2.40057200	-1.79391300
O	-4.04683100	-1.48032400	-2.81478700
C	-4.94708500	-2.52311500	0.28384900
C	-3.79843000	-1.79333500	0.57358600

C	-3.59657000	-1.19725500	1.81639000
C	-4.58783900	-1.35280300	2.78225200
C	-5.74391800	-2.08718400	2.50315100
C	-5.93274400	-2.67727500	1.25583700
C	-4.91787300	-3.06184600	-1.12406000
H	-2.69778400	-0.61862400	2.02885600
H	-6.50549100	-2.19699400	3.26848000
H	-6.83519700	-3.24254900	1.04335300
H	-5.82259300	-2.82998400	-1.69531400
H	-4.80959400	-4.15099000	-1.12625300
C	-1.19027700	2.87800000	-0.53856800
C	-1.62779600	3.66888000	0.52398400
C	-0.07142900	3.17375700	-1.31521900
C	-0.90474700	4.82884200	0.78708900
C	0.61865300	4.34482300	-1.01035100
C	0.21708800	5.17971800	0.03233300
H	-1.21689800	5.46640600	1.61017000
H	1.49971400	4.60124100	-1.59273000
C	0.39049200	2.23425400	-2.39455000
H	1.18659400	2.69032800	-2.98569500
H	-0.42688100	1.95875800	-3.06830500
H	0.78335800	1.32071500	-1.93218000
C	1.00765100	6.41778400	0.36622500
H	0.37899800	7.17306000	0.84312300
H	1.45526100	6.85441300	-0.52954500
H	1.82039500	6.17493600	1.05815500
C	-2.79883900	3.24099300	1.36333900
H	-2.55779900	2.28563200	1.84191900
H	-3.69937800	3.10677800	0.75606000
H	-3.00961000	3.98063800	2.13708500
H	-3.06850500	-3.13471900	-2.30798100
C	0.34681100	-0.88330200	0.11668900
C	1.43874900	-1.41839600	0.87709000
H	0.23048100	-1.18370800	-0.92125800
C	-0.53065800	0.09124600	0.56650400
O	-0.59386200	0.75215000	1.64836500

H	-4.46023100	-0.90015700	3.75984800
C	3.78709000	0.32807600	-0.15507200
C	4.76710300	-0.39514800	0.57081700
C	5.87346700	-0.94256000	-0.05413700
C	6.01195900	-0.74112200	-1.43160400
C	5.07035300	-0.00781500	-2.15612700
C	3.94535700	0.52385900	-1.52544900
C	2.74768200	0.65853600	0.77323100
C	3.24318300	0.35467600	2.11840900
H	6.61061900	-1.50870000	0.50616600
H	6.87525700	-1.15774800	-1.94097100
H	5.21318600	0.14343400	-3.22141400
H	3.20538700	1.09157900	-2.08189300
O	2.77325700	0.65558800	3.20846900
O	1.80239900	1.57595800	0.50629700
H	1.13393000	1.55740600	1.22150700
N	4.39592900	-0.41135600	1.90989800
H	4.97137800	-0.73217400	2.67282800
C	1.19142600	-1.60787800	2.35511800
H	0.66419200	-0.74877100	2.76642700
H	0.56732900	-2.50196900	2.48785500
H	2.10865400	-1.74384700	2.92831800
C	2.37427900	-2.33727700	0.21036700
C	2.58432700	-2.28402100	-1.18140000
C	3.13858800	-3.26630800	0.93921000
C	3.50266200	-3.11215600	-1.80912600
H	2.05091100	-1.55005200	-1.77562700
C	4.05309200	-4.10293500	0.30903100
H	3.01076900	-3.34453700	2.01267500
C	4.24549300	-4.02904200	-1.06787500
H	3.65542700	-3.02618200	-2.88067800
H	4.62226900	-4.81395300	0.90045600
H	4.96772400	-4.67498100	-1.55720300

TS3 (SS) c3

GFE= -2026.806508 a.u.

Frequency= -203.29 cm⁻¹

C	1.74679700	0.18329800	-0.17902100
C	2.63859700	1.95198600	-1.10781100
C	0.20638200	2.09340100	-0.95295700
H	-0.60776500	1.36565600	-0.92944600
N	3.64927100	1.17586600	-0.84377700
N	3.07507200	0.08193300	-0.26097200
N	1.45971400	1.38593900	-0.71399900
C	2.55196300	3.23924800	-1.86175300
H	3.48575400	3.42357300	-2.39314300
H	2.35566500	4.07385600	-1.17570900
C	0.22177200	2.77728600	-2.35046200
O	1.52973400	3.09069600	-2.82865900
C	-0.49868900	4.34738800	-0.66780100
C	-0.00193800	3.23702400	0.01513000
C	0.23337900	3.27506200	1.38497300
C	-0.06234000	4.44916500	2.07832300
C	-0.57506500	5.55712900	1.40328000
C	-0.79346900	5.51536900	0.02571200
C	-0.63063400	4.04543600	-2.14244900
H	0.65175700	2.41611300	1.90592400
H	-0.79566200	6.46547900	1.95455500
H	-1.17669000	6.38676000	-0.49704400
H	-0.28319000	4.85241100	-2.79250200
H	-1.67507400	3.83214500	-2.39720400
C	3.91598300	-0.97093800	0.24584500
C	4.33504900	-0.88642800	1.57307100
C	4.28658900	-1.99693100	-0.61903500
C	5.18603500	-1.88664500	2.03486100
C	5.14141200	-2.97330900	-0.11055000
C	5.60187300	-2.93126100	1.20568900

H	5.53058000	-1.85127800	3.06564900
H	5.44685500	-3.79143100	-0.75760100
C	3.73785500	-2.04673000	-2.01693800
H	4.13159800	-2.90903500	-2.55729400
H	3.99288800	-1.14076200	-2.57532500
H	2.64618100	-2.12098300	-1.96876000
C	6.53511700	-3.99002600	1.73407200
H	6.15052400	-4.42166800	2.66219700
H	7.51972800	-3.56550300	1.95328600
H	6.66858600	-4.79686200	1.01087600
C	3.85679600	0.23117200	2.46194800
H	2.77731400	0.15285100	2.63518900
H	4.05142700	1.20881500	2.00948400
H	4.35731300	0.19431900	3.43066600
H	-0.19919500	2.09722600	-3.09204600
C	-0.36662600	-0.42818500	0.89102300
C	-1.56842300	-1.15244800	1.03768800
H	-0.38748500	0.63713800	1.07083100
C	0.81195800	-0.91639800	0.29480600
O	1.21625400	-2.07022500	0.07746100
H	0.11531300	4.50261300	3.14727000
C	-3.61065700	-1.68523300	-1.09821300
C	-3.02432500	-2.80755200	-1.73957400
C	-3.71879400	-3.99532100	-1.90970700
C	-5.03290200	-4.05648600	-1.43903200
C	-5.63135300	-2.95636000	-0.81867900
C	-4.92643000	-1.76656700	-0.63989500
C	-1.44464300	-1.15175100	-1.77727700
H	-3.25677600	-4.84845000	-2.39633200
H	-5.59714000	-4.97504000	-1.56418600
H	-6.65746500	-3.02940800	-0.47304300
H	-5.39227300	-0.91283100	-0.15590200
O	-0.40742000	-0.54796300	-2.06714200
O	-2.75792900	0.66904000	-0.89736800
H	-3.26307000	0.86104600	-0.09168000
N	-1.73203700	-2.47125900	-2.11388100

H	-1.07336700	-3.06884000	-2.58747000
C	-2.68755100	-0.51947000	1.79206500
C	-2.74922700	0.87033500	2.02325000
C	-3.74790600	-1.29716800	2.28845400
C	-3.82071000	1.44594500	2.70055900
H	-1.95720100	1.52526400	1.67518000
C	-4.81240100	-0.72122700	2.97476900
H	-3.74551300	-2.37014600	2.14188500
C	-4.86012500	0.65427200	3.18135800
H	-3.83341600	2.52020600	2.85714100
H	-5.61086700	-1.35625600	3.34569000
H	-5.69245800	1.10395300	3.71280400
C	-1.52690000	-2.66115700	1.05000000
H	-1.34952900	-2.99868900	2.07874700
H	-2.46802600	-3.10062100	0.71254800
H	-0.71084800	-3.02818300	0.43291700
C	-2.57607000	-0.68812300	-0.98973800

TS3 (SS) _{c4}

GFE= -2026.801373 a.u.

Frequency= -158.01 cm⁻¹

C	1.86261100	0.52329300	-0.19117400
C	2.31003600	2.66303800	-0.31227800
C	-0.05850300	2.12714600	-0.67619000
H	-0.57270700	1.22055600	-1.01483700
N	3.46306100	2.09548800	-0.10656900
N	3.16212200	0.76272600	-0.03032400
N	1.30682000	1.73567800	-0.36205200
C	1.92392000	4.06186200	-0.67005700
H	2.80944000	4.65143400	-0.90548500
H	1.37711500	4.53690400	0.15420100
C	-0.05858800	3.21070800	-1.80045200
O	1.14353200	3.97756200	-1.85135400
C	-1.49839300	3.89470000	0.00864400
C	-0.76998900	2.80144600	0.47775200

C	-0.76654300	2.45938600	1.82551300
C	-1.54274900	3.21309600	2.70504200
C	-2.29636000	4.28987200	2.23632200
C	-2.27448600	4.64237300	0.88734700
C	-1.28806800	4.08231600	-1.47481100
H	-0.16188800	1.63558300	2.19664900
H	-2.89481500	4.86867600	2.93226800
H	-2.84439700	5.49579600	0.53239800
H	-1.10359600	5.12021500	-1.76382400
H	-2.15787100	3.72957100	-2.04163800
C	4.18139500	-0.21273400	0.24896500
C	4.35692200	-0.61038300	1.57326900
C	4.92874400	-0.71195700	-0.81762900
C	5.36295300	-1.54084600	1.82762500
C	5.92186200	-1.63793300	-0.51056800
C	6.15572500	-2.05612900	0.80152000
H	5.52584100	-1.87392500	2.84939100
H	6.51993100	-2.05275400	-1.31804400
C	4.62315600	-0.29050900	-2.22741600
H	5.31779000	-0.75473100	-2.92886100
H	4.69116800	0.79597300	-2.34007800
H	3.60252500	-0.60192900	-2.47506600
C	7.25795600	-3.03838300	1.10155400
H	8.22196200	-2.52464500	1.17544200
H	7.34382900	-3.78742200	0.31091500
H	7.08184300	-3.55395100	2.04793900
C	3.46982200	-0.07152200	2.66456400
H	2.43583800	-0.40529900	2.51712200
H	3.47087000	1.02317700	2.67222800
H	3.80408300	-0.42302600	3.64155500
H	-0.13374000	2.73915400	-2.78187100
C	0.05049200	-0.97207700	0.42073700
C	-0.85814500	-2.07263000	0.35695800
H	-0.21592400	-0.12012000	1.03426800
C	1.19285900	-0.82084200	-0.35721400
O	1.73351200	-1.54977700	-1.23259300

H	-1.55508300	2.96308400	3.76056300
C	-3.05323300	-0.77366600	-1.34378200
C	-3.98304600	-1.83778800	-1.21561300
C	-5.26822200	-1.62674000	-0.74951100
C	-5.64067500	-0.31806600	-0.42280100
C	-4.74876100	0.74488800	-0.56730500
C	-3.44790900	0.52345800	-1.02184400
C	-1.80800200	-1.36733000	-1.73583700
C	-2.07733500	-2.75428200	-2.11292500
H	-5.96592700	-2.45089600	-0.64053600
H	-6.64536900	-0.13080400	-0.05731800
H	-5.06407700	1.75244800	-0.31514100
H	-2.75631300	1.35500100	-1.12830800
O	-1.34941000	-3.55766200	-2.68349200
O	-0.79480000	-0.64253700	-2.27282900
H	-0.00673300	-1.21566600	-2.33114900
N	-3.36423700	-3.01151900	-1.63100900
H	-3.82317500	-3.89890800	-1.76560200
C	-0.27248900	-3.42540400	0.02735900
H	0.48969200	-3.33755900	-0.74434900
H	0.19960100	-3.82091500	0.93605700
H	-1.01876300	-4.14376500	-0.31088400
C	-2.05962200	-2.03985700	1.21696400
C	-2.60246900	-0.82662000	1.68040300
C	-2.73757900	-3.22017100	1.56493700
C	-3.75844800	-0.79487900	2.44686200
H	-2.14215900	0.11584900	1.40504300
C	-3.89138600	-3.19062800	2.34178500
H	-2.35789200	-4.17857100	1.23126700
C	-4.41195600	-1.97809800	2.78464000
H	-4.15761600	0.16288100	2.76726100
H	-4.38651000	-4.12224300	2.59858000
H	-5.31699900	-1.95510800	3.38352900

TS3 (SR)_{d1}

GFE= -2026.800368 a.u.

Frequency= -207.18 cm⁻¹

C	1.24907100	-1.06460900	-0.32147600
C	2.96787900	-2.23570500	0.37752400
C	3.58754600	-0.49787500	-1.27406800
H	3.04696400	-0.16453600	-2.15640000
N	1.94656400	-2.77629600	0.96852900
N	0.88155600	-2.03994700	0.53311200
N	2.59317200	-1.20245000	-0.43401800
C	4.38766400	-2.68516000	0.33632700
H	4.47735600	-3.68659400	0.75592900
H	5.03829500	-1.99650200	0.89318600
C	4.78676100	-1.45947200	-1.64291600
O	4.72689300	-2.73943800	-1.03419600
C	5.62132000	0.54264800	-0.54235600
C	4.23433000	0.66223400	-0.55497600
C	3.59454600	1.76963900	-0.00521300
C	4.37963400	2.75533000	0.58632000
C	5.77158600	2.63396800	0.62158400
C	6.40212900	1.53074100	0.05311300
C	6.07980800	-0.69775200	-1.26179200
H	2.51480500	1.86554200	-0.07116600
H	6.36734400	3.41338700	1.08593200
H	7.48462800	1.44501900	0.06738800
H	6.72198700	-1.33990600	-0.64926100
H	6.65241900	-0.44336300	-2.15868700
C	-0.43226500	-2.53930700	0.86259200
C	-1.02372600	-2.19997100	2.07755400
C	-1.03711500	-3.38999000	-0.07222100
C	-2.28922400	-2.73001800	2.33817300
C	-2.29392000	-3.89836000	0.24072100
C	-2.93887200	-3.57005800	1.43724100

H	-2.77774200	-2.46734800	3.27357300
H	-2.78638600	-4.55588600	-0.47109000
C	-0.37425100	-3.68724400	-1.38980300
H	-0.90607100	-4.48026700	-1.91691700
H	0.66635700	-3.99839500	-1.25614200
H	-0.38237800	-2.79223600	-2.02294100
C	-4.32158900	-4.08764900	1.73756900
H	-5.06320500	-3.29300200	1.60708700
H	-4.39563200	-4.43745900	2.77022600
H	-4.59046100	-4.91153400	1.07347500
C	-0.38148000	-1.27362700	3.07135400
H	-0.92410000	-0.32327000	3.07475400
H	0.66868200	-1.08226700	2.84306000
H	-0.43761200	-1.69836500	4.07655400
H	4.75008200	-1.67111500	-2.71156500
C	-0.90872200	-0.00882900	-0.85019700
C	-1.85442200	0.95532600	-1.30158000
H	-1.29550300	-0.80714400	-0.24179600
C	0.47101700	0.03896900	-1.02716200
O	1.18846300	0.81694300	-1.70269400
H	3.90460000	3.63586000	1.00812600
C	-1.21452000	2.44684200	1.15029800
C	-1.50997300	3.79056100	0.79228800
C	-0.56207100	4.79264000	0.88523600
C	0.70751100	4.45085200	1.36936900
C	1.01039200	3.13923000	1.73177100
C	0.06065600	2.12135500	1.60727000
C	-2.39328000	1.68394800	0.87312500
C	-3.46380600	2.62234400	0.54372100
H	-0.79922000	5.81495200	0.60872500
H	1.45999800	5.22621300	1.47363800
H	1.99455500	2.90295900	2.12346500
H	0.29852600	1.09993000	1.88250000
O	-4.65653000	2.37883800	0.39937200
O	-2.68656000	0.48177800	1.44006500
H	-3.57795800	0.24798800	1.12906500

N	-2.83965300	3.85909800	0.38342400
H	-3.35229700	4.70707500	0.19790900
C	-1.34859000	2.19219600	-1.99329100
H	-0.42876000	2.53628000	-1.52025400
H	-1.10545700	1.96537200	-3.03812400
H	-2.08258000	2.99933000	-1.97261700
C	-3.23380800	0.48994500	-1.57782000
C	-4.14653700	1.28783800	-2.28734200
C	-3.69224800	-0.76653900	-1.13074300
C	-5.44447900	0.85808100	-2.53833300
H	-3.84202900	2.26121700	-2.65416300
C	-4.99639700	-1.18560200	-1.36533500
H	-3.02353300	-1.44582200	-0.61520400
C	-5.88310100	-0.37747100	-2.07305100
H	-6.11979600	1.50088000	-3.09409000
H	-5.31168200	-2.16246000	-1.00876100
H	-6.89852800	-0.70902400	-2.26395900

TS3 (SR)

GFE= -2026.818187 a.u.

Frequency= -135.18 cm⁻¹

C	-1.70211400	0.83580300	-0.58725400
C	-3.69494300	1.60283600	-0.08149400
C	-3.75896300	-0.65612400	-1.06255300
H	-3.15848000	-1.13697200	-1.83042900
N	-2.88306500	2.54008500	0.30171500
N	-1.64525200	2.05257200	-0.01063200
N	-3.02610900	0.55317000	-0.64421500
C	-5.18605900	1.56444500	-0.09133500
H	-5.59041900	2.57022700	0.02154100
H	-5.56419900	0.92873800	0.72199600
C	-5.19622700	-0.28089200	-1.58496800
O	-5.56025600	1.07415100	-1.36215100
C	-5.35195400	-1.89417200	0.22572000
C	-4.00279300	-1.56759600	0.11898600

C	-3.05471000	-2.05292800	1.01628200
C	-3.50028400	-2.87718100	2.04720800
C	-4.85257500	-3.20796000	2.16704100
C	-5.78811100	-2.72306200	1.25576300
C	-6.15955000	-1.26750000	-0.88193200
H	-1.99991600	-1.80506200	0.91015300
H	-5.17783800	-3.85127000	2.97878300
H	-6.83831500	-2.98392400	1.34940000
H	-7.04557300	-0.73052600	-0.52741200
H	-6.50804200	-2.02658600	-1.58976400
C	-0.49672900	2.85107200	0.32085500
C	0.02857900	2.74858000	1.60835400
C	0.04239200	3.67584400	-0.67011500
C	1.17224300	3.50075600	1.88642200
C	1.18558100	4.39873800	-0.34471300
C	1.76901600	4.31342900	0.92300400
H	1.61056600	3.43726800	2.87942600
H	1.63897500	5.03539700	-1.10036100
C	-0.56189200	3.70832000	-2.04699400
H	-0.08170700	4.47008400	-2.66249900
H	-1.63463800	3.91837700	-2.00400400
H	-0.42998500	2.73657300	-2.53713800
C	3.03807600	5.06797700	1.22075000
H	3.88247500	4.60582700	0.69893500
H	3.25956700	5.06924400	2.28997600
H	2.96970100	6.10465500	0.88091100
C	-0.59001600	1.82978100	2.62541900
H	-0.44568000	0.78349900	2.32939600
H	-1.66450800	2.01365100	2.71697600
H	-0.13124300	1.98173900	3.60422200
H	-5.23070600	-0.38886500	-2.66933200
C	0.66475900	0.34550100	-1.04445700
C	1.80081200	-0.45525400	-1.41345100
H	0.86424900	1.32807400	-0.64902000
C	-0.63766500	-0.10424500	-1.03981500
O	-1.07813500	-1.27824000	-1.32634900

H	-2.78412300	-3.26886900	2.76225500
C	2.91775100	-2.79641400	0.02120900
C	3.43800100	-2.08775800	1.12978400
C	4.78067400	-2.13991700	1.46142900
C	5.61501900	-2.93213500	0.66747500
C	5.11580100	-3.64823700	-0.42266500
C	3.76277400	-3.58268500	-0.75823200
C	1.53342000	-2.41920400	-0.10919500
C	1.19114500	-1.62185700	1.08186700
H	5.17348300	-1.57886200	2.30332500
H	6.67194100	-2.99045400	0.90777000
H	5.78726300	-4.26225700	-1.01393500
H	3.36244900	-4.14012200	-1.59988300
O	0.09545400	-1.19372100	1.44452900
O	0.64560400	-3.08652800	-0.84763400
H	-0.12844400	-2.45136200	-1.01835300
N	2.39416500	-1.40034900	1.73800700
H	2.47537600	-0.79958800	2.54312000
C	1.70677300	-1.26198600	-2.68646900
H	2.33206000	-2.15940100	-2.65995200
H	0.67892100	-1.56563500	-2.87574100
H	2.04582500	-0.63704300	-3.52223900
C	3.13156400	0.04875900	-1.02907800
C	3.29514300	0.94362700	0.04593300
C	4.29524900	-0.40495800	-1.67391900
C	4.55576200	1.36673400	0.44827300
H	2.42520300	1.29196400	0.59574900
C	5.55671900	0.00840000	-1.26315600
H	4.21566900	-1.09959100	-2.50229300
C	5.69669400	0.89722100	-0.20057700
H	4.64581900	2.05563500	1.28409800
H	6.43618200	-0.37227100	-1.77344400
H	6.68240800	1.21951900	0.12008100

TS3 (SR)_{d3}

GFE= -2026.799435 a.u.

Frequency= -189.15 cm⁻¹

C	1.33204200	0.55563700	-0.14114200
C	1.78946600	2.48513800	-1.07802200
C	-0.60682400	2.00389600	-1.05753900
H	-1.22625200	1.10118300	-1.05364700
N	2.94223500	2.02408600	-0.69564900
N	2.63959900	0.82733500	-0.10916200
N	0.77545300	1.62256500	-0.76166700
C	1.43231900	3.69139200	-1.88277000
H	2.32058000	4.09235500	-2.37076900
H	0.98683200	4.46749200	-1.24619000
C	-0.69790200	2.72246200	-2.44736300
O	0.54257000	3.25535600	-2.89406400
C	-1.78861700	4.05634800	-0.75169700
C	-1.12071500	3.03700300	-0.07477100
C	-0.98333300	3.05450700	1.30963700
C	-1.55300700	4.11021600	2.01934400
C	-2.23636100	5.12563300	1.34835400
C	-2.35554700	5.10843800	-0.04055900
C	-1.76695500	3.81665900	-2.24102000
H	-0.44008300	2.26951600	1.83038600
H	-2.67170400	5.94308700	1.91396100
H	-2.87417800	5.90908000	-0.55909700
H	-1.51234400	4.70451200	-2.82603100
H	-2.74093200	3.45706200	-2.59006900
C	3.68460400	0.10307300	0.57138000
C	3.91281100	0.41379600	1.91017000
C	4.42722500	-0.83651800	-0.14166100
C	4.96001700	-0.25008600	2.54840700
C	5.46180000	-1.47141300	0.53956200
C	5.74490200	-1.18730700	1.87773200

H	5.16217100	-0.03121700	3.59385200
H	6.05460100	-2.21651700	0.01481800
C	4.06501900	-1.18037700	-1.55712400
H	4.79278600	-1.87047500	-1.98744600
H	4.02042200	-0.28577800	-2.18681100
H	3.07542100	-1.65202300	-1.55900300
C	6.89180500	-1.87091700	2.57628600
H	6.74857500	-1.87725000	3.65893000
H	7.83442500	-1.35447100	2.36744900
H	6.99973500	-2.90364300	2.23653100
C	3.03566200	1.39820400	2.63834400
H	2.02360100	0.99523600	2.76051000
H	2.95619600	2.34422200	2.09337600
H	3.43532300	1.60775300	3.63167700
H	-0.98794600	2.01370200	-3.22523700
C	-0.61121900	-0.59330200	0.78248500
C	-1.52175200	-1.63876400	1.06202100
H	-0.97686600	0.41965500	0.84143900
C	0.71478200	-0.74604200	0.34600200
O	1.47472300	-1.72966300	0.30721800
H	-1.45977700	4.14423800	3.09947400
C	-1.29922800	-2.05850400	-1.85933400
C	-1.17118400	-3.47294100	-1.89178600
C	-0.06408200	-4.08423500	-2.44853900
C	0.92408600	-3.26359200	-3.01173200
C	0.78123200	-1.87784100	-3.04763000
C	-0.33052600	-1.26256000	-2.46898100
C	-2.46571500	-1.77138900	-1.09249600
C	-3.17293500	-3.02790800	-0.85757700
H	0.03699700	-5.16469100	-2.45529400
H	1.80302500	-3.72331300	-3.45237500
H	1.54103800	-1.27251900	-3.53287300
H	-0.46387300	-0.18854100	-2.54223400
O	-4.26921800	-3.20438500	-0.33408500
O	-3.10906800	-0.56993600	-1.15419500
H	-3.86361600	-0.62661300	-0.54507500

N	-2.30055900	-4.02548700	-1.29921400
H	-2.47912100	-5.00822900	-1.16564700
C	-0.96623300	-3.02409800	1.27057100
H	-0.21398500	-3.24609700	0.51337300
H	-0.45918800	-3.06621000	2.24234100
H	-1.74070400	-3.79037700	1.24967500
C	-2.80336300	-1.28738200	1.72455800
C	-3.55208300	-2.25229300	2.41812000
C	-3.33109100	0.02048100	1.68026600
C	-4.75490300	-1.93266400	3.03778100
H	-3.19044500	-3.26991500	2.48973200
C	-4.53986900	0.33613600	2.28980900
H	-2.80575600	0.81047800	1.15519200
C	-5.26043700	-0.63859600	2.97598400
H	-5.30147600	-2.70650400	3.56728100
H	-4.91443900	1.35369400	2.23187600
H	-6.20154400	-0.39110200	3.45635100

TS3 (SR) _{d4}

GFE= -2026.809519 a.u.

Frequency= -140.98 cm⁻¹

C	-1.69748100	0.37867000	-0.40360100
C	-3.66546200	0.18643000	-1.33575000
C	-2.66190500	-1.96334700	-0.64381100
H	-1.64090700	-2.34730400	-0.66419600
N	-3.48421300	1.46727700	-1.20572300
N	-2.25736100	1.56826300	-0.61096800
N	-2.58812600	-0.51680300	-0.87426800
C	-4.79595400	-0.60248200	-1.91207500
H	-5.34358200	-0.00990800	-2.64492700
H	-5.48659000	-0.91516100	-1.11546500
C	-3.56852100	-2.64211200	-1.73434300
O	-4.22475700	-1.70937500	-2.57981600
C	-4.42095200	-3.12068600	0.49307300
C	-3.35681400	-2.24180000	0.66888800

C	-3.03637700	-1.71101100	1.91597700
C	-3.81546400	-2.09067800	3.00606300
C	-4.88194200	-2.97895900	2.84200800
C	-5.19365600	-3.49913700	1.58841100
C	-4.55694200	-3.53920300	-0.94926900
H	-2.21237200	-1.00817700	2.03725600
H	-5.47835200	-3.26227000	3.70330500
H	-6.02805200	-4.18334700	1.46698700
H	-5.56983300	-3.40997400	-1.34420800
H	-4.29596700	-4.59413800	-1.07955500
C	-1.68573300	2.86326400	-0.34574700
C	-1.98473400	3.47846800	0.86930400
C	-0.88137700	3.43307000	-1.32979000
C	-1.44392200	4.74356400	1.08285300
C	-0.36450600	4.69889900	-1.06648700
C	-0.63799500	5.36632400	0.12740700
H	-1.64879300	5.25051800	2.02237900
H	0.27769200	5.16708800	-1.80797600
C	-0.55711900	2.68493600	-2.59301300
H	-0.05548700	3.34017600	-3.30725500
H	-1.45898500	2.28465700	-3.06673000
H	0.12089600	1.85948800	-2.35089800
C	-0.08909400	6.74783800	0.37345000
H	0.04032100	6.93640200	1.44148000
H	-0.77065300	7.50995100	-0.01880100
H	0.87666800	6.88149500	-0.11896600
C	-2.81646400	2.77158600	1.90346700
H	-2.27328300	1.88516800	2.24922200
H	-3.77586400	2.44629100	1.48833400
H	-3.01335800	3.42583600	2.75417200
H	-2.95079400	-3.22672500	-2.41599800
C	0.43515800	-0.78057600	-0.28091500
C	1.63070100	-1.31071000	0.33476300
H	0.22401200	-1.01938400	-1.32075700
C	-0.42949600	0.09482500	0.33743800
O	-0.35965700	0.69253500	1.46737600

H	-3.59307900	-1.69262500	3.99045700
C	4.11774600	0.08818100	1.19231100
C	4.66824300	0.30286200	-0.09320500
C	5.92939100	-0.15961000	-0.42886200
C	6.65235400	-0.84562700	0.55186200
C	6.12706000	-1.05727400	1.82821900
C	4.85182900	-0.59436100	2.15804100
C	2.76949500	0.59714800	1.16717200
C	2.58839900	1.28715300	-0.12493200
H	6.33958400	-0.00200400	-1.42124500
H	7.64407700	-1.21695500	0.31311800
H	6.71755400	-1.58400200	2.57081900
H	4.43610800	-0.74222900	3.15036400
O	1.62994000	1.93213300	-0.53530400
O	2.05947300	0.85123900	2.26793400
H	1.08557000	0.91276600	1.99533500
N	3.75001000	1.02157800	-0.84721000
H	3.85482600	1.27113800	-1.81783900
C	1.47166700	-1.84857300	1.73761900
H	2.41119300	-1.82924900	2.29772100
H	0.73586600	-1.26723100	2.29182000
H	1.12686200	-2.88961600	1.68614700
C	2.62691400	-1.96272400	-0.52817300
C	2.75408000	-1.61685000	-1.88659900
C	3.53599000	-2.90601300	-0.01461900
C	3.73068100	-2.18969900	-2.69133300
H	2.09683100	-0.85972900	-2.30472900
C	4.51896100	-3.47170600	-0.81734000
H	3.47816100	-3.19721600	1.02805100
C	4.62334200	-3.11962200	-2.16036200
H	3.80274000	-1.90094900	-3.73593500
H	5.21253300	-4.18811000	-0.38771200
H	5.39168600	-3.56187200	-2.78672800

M4 (RS)

GFE= -2026.845390 a.u.

C	-1.83507900	0.61855300	-0.50726100
C	-3.85577800	1.43759300	-0.34912800
C	-3.76230300	-0.97949200	-0.92371500
H	-3.06679400	-1.51679900	-1.57298300
N	-3.07808200	2.43281300	-0.04156100
N	-1.81738400	1.90519100	-0.14351000
N	-3.13633800	0.32012300	-0.66247800
C	-5.33913400	1.34359100	-0.49174300
H	-5.77531200	2.33253400	-0.63072100
H	-5.78203100	0.87637300	0.39999600
C	-5.17867300	-0.77544700	-1.57807600
O	-5.58151300	0.58522300	-1.65955800
C	-5.37874600	-2.06004900	0.47870000
C	-4.03730600	-1.70595300	0.37205200
C	-3.11946700	-2.01034900	1.37377400
C	-3.57671000	-2.68103700	2.50467000
C	-4.92242300	-3.03955800	2.62040300
C	-5.83111900	-2.73452000	1.61023300
C	-6.15807800	-1.63321400	-0.73908900
H	-2.07356300	-1.72551600	1.27552400
H	-5.26238100	-3.56271800	3.50854000
H	-6.87587400	-3.01522900	1.70550600
H	-7.05174500	-1.04858600	-0.49670600
H	-6.49230900	-2.50124200	-1.31580100
C	-0.65672100	2.74169500	0.00171500
C	-0.30210700	3.16833000	1.28062900
C	0.06798100	3.05588100	-1.15182600
C	0.84757300	3.94941300	1.39451600
C	1.21459200	3.82738400	-0.98047900
C	1.61665800	4.28167500	0.27860700
H	1.15653400	4.28917300	2.37975200

H	1.81026300	4.07632400	-1.85503300
C	2.86545900	5.11398800	0.41774200
H	3.72221000	4.60845900	-0.03756100
H	3.09885100	5.30769000	1.46709800
H	2.74994100	6.07844900	-0.08616200
C	-1.11919800	2.77453300	2.48223700
H	-1.25718500	1.68825900	2.52479200
H	-2.11459900	3.22676900	2.44536800
H	-0.62560400	3.09147300	3.40197100
H	-5.14919900	-1.10234100	-2.61719400
C	0.28714000	-0.26439400	0.17132500
C	1.49280600	-1.17960300	0.30485300
H	0.18328600	0.48143600	0.95095900
C	-0.71406600	-0.33718600	-0.74386300
O	-0.90130600	-1.10117300	-1.76755000
H	-2.88279300	-2.93035700	3.30075600
C	3.50595100	-2.22723400	-0.91345500
C	4.55316100	-1.34082000	-1.18895100
C	5.88299200	-1.70567900	-1.05652600
C	6.15559500	-3.01950400	-0.66517000
C	5.12850500	-3.93276200	-0.44617300
C	3.79173400	-3.53849700	-0.58075600
C	2.18033800	-1.51275600	-1.09879000
C	2.65175000	-0.16582500	-1.72558700
H	6.68333100	-1.00271000	-1.26246900
H	7.18838600	-3.33429800	-0.55319100
H	5.36485900	-4.95749400	-0.17972500
H	2.98818000	-4.25492700	-0.44528800
O	1.95877300	0.71292200	-2.19437000
O	1.35496600	-2.24381200	-1.93745900
H	0.44031200	-1.80775200	-1.96062300
N	4.02386200	-0.12441000	-1.63161200
H	4.56418400	0.65191200	-1.98320200
C	2.51844700	-0.48460400	1.20928500
C	3.33608000	-1.19530100	2.09317600
C	2.68851700	0.90435700	1.13173700

C	4.28205500	-0.54210700	2.87943700
H	3.24744600	-2.27435000	2.16576000
C	3.63046600	1.56008900	1.91782300
H	2.08226600	1.48094200	0.43577200
C	4.43188400	0.83935800	2.79907500
H	4.90374000	-1.11913700	3.55715500
H	3.73145500	2.63956400	1.83906300
H	5.16693000	1.34739200	3.41567300
C	0.97876800	-2.50179700	0.90218100
H	0.53983100	-2.31141000	1.88645700
H	0.21151100	-2.90918000	0.24006800
H	1.76440500	-3.25121400	1.01702000
C	-0.37676400	2.57356700	-2.50574800
H	-0.21503300	1.49543900	-2.60474100
H	-1.43706400	2.79323400	-2.66867900
H	0.20314300	3.06463600	-3.28852500

M4 (RR)

GFE= -2026.845300 a.u.

C	1.67455100	0.68161000	0.49640800
C	3.82950400	1.09106500	0.47389600
C	3.29136800	-1.20147200	1.21184300
H	2.49247800	-1.59499500	1.83388700
N	3.29221200	2.16733000	-0.01234800
N	1.95242500	1.89876800	-0.00396800
N	2.88573800	0.16258000	0.81161200
C	5.26059300	0.78155400	0.76081500
H	5.83262600	1.70458000	0.85705200
H	5.69227500	0.17442100	-0.04814300
C	4.67656500	-1.17406900	1.95828500
O	5.28938000	0.10640400	1.99917700
C	4.81112800	-2.58947200	-0.01551900
C	3.53010400	-2.04462000	-0.02030700
C	2.63815000	-2.27395100	-1.06602000
C	3.07260800	-3.05812400	-2.13146100

C	4.36003800	-3.60175400	-2.14171400
C	5.23616100	-3.37781000	-1.08247300
C	5.55984900	-2.22496200	1.24139200
H	1.62588600	-1.87582600	-1.03830000
H	4.67895200	-4.20990500	-2.98254700
H	6.23371900	-3.80750200	-1.09009200
H	6.55463100	-1.80772200	1.05206500
H	5.70018700	-3.10188400	1.88134200
C	1.07193600	2.86812100	-0.59711500
C	0.69172100	2.67959600	-1.92669100
C	0.63896900	3.93644600	0.18822100
C	-0.17313500	3.62532300	-2.47516200
C	-0.22262800	4.85468700	-0.40763700
C	-0.63630000	4.71403100	-1.73417300
H	-0.49701600	3.50428800	-3.50588400
H	-0.58423200	5.69473700	0.18007600
C	1.05303000	4.04285300	1.63055500
H	0.65340000	4.95272800	2.08035600
H	2.14230000	4.05367300	1.72886200
H	0.67641600	3.18525000	2.19910000
C	-1.54812300	5.73592900	-2.36204200
H	-2.13056600	5.29845400	-3.17580500
H	-0.96706000	6.56555100	-2.77782200
H	-2.23981000	6.15292300	-1.62659200
C	1.14707200	1.47036900	-2.69600100
H	0.64407200	0.56907700	-2.32252900
H	2.22659100	1.31896600	-2.59687500
H	0.91186400	1.57995900	-3.75600400
H	4.52451000	-1.42684100	3.00770900
C	-0.76111500	0.59709700	0.35376800
C	-2.18691600	0.06719800	0.29636400
C	-2.82597600	0.16708400	1.68417700
C	-2.15021700	-0.37009800	2.78884500
C	-4.07703100	0.75245700	1.89489900
C	-2.72022800	-0.33802800	4.05598500
H	-1.17540900	-0.82394700	2.64184200

C	-4.64587900	0.79215200	3.16769200
H	-4.62929600	1.17610000	1.06283400
C	-3.97272500	0.24286700	4.25272400
H	-2.18333000	-0.76779000	4.89632800
H	-5.61990200	1.25205600	3.30508700
H	-0.69663100	1.65083400	0.12223100
H	-4.41554600	0.26971600	5.24359800
C	0.38750900	-0.06504100	0.65380900
O	0.56503000	-1.29213700	1.02409900
C	-2.90242600	0.96761700	-0.73030700
H	-3.92877100	0.64808900	-0.92704700
H	-2.92251900	2.00006400	-0.36769600
H	-2.35073500	0.96236000	-1.67576500
H	2.39641700	-3.25286200	-2.95769700
C	-3.72950500	-1.85908400	-0.42715200
C	-3.94489400	-2.03557200	-1.79767100
C	-5.17312700	-2.42103200	-2.30903200
C	-6.20540200	-2.65234200	-1.39437000
C	-6.00000800	-2.51202000	-0.02481500
C	-4.75035500	-2.11798000	0.46922300
C	-2.29093800	-1.44331800	-0.18937500
C	-1.70471600	-1.54262600	-1.63119300
H	-5.32538700	-2.55321900	-3.37522800
H	-7.17879800	-2.95969300	-1.76357200
H	-6.81158300	-2.71612700	0.66546500
H	-4.57522200	-2.02165600	1.53598600
O	-0.54067300	-1.43852200	-1.96645200
O	-1.68093700	-2.35744600	0.65671900
H	-0.73227500	-2.03433100	0.81143800
N	-2.75023500	-1.78702300	-2.49081400
H	-2.60087500	-1.98559200	-3.46943500

M4 (SS)

GFE= -2026.837369 a.u.

C	-1.78463800	0.94492200	-0.43392100
C	-3.82507400	1.39941700	0.20676700
C	-3.60839000	-0.57130300	-1.29370300
H	-2.94771900	-0.73134700	-2.15108300
N	-3.08897300	2.26508800	0.84017400
N	-1.81291400	1.96178900	0.43052400
N	-3.06938200	0.59663900	-0.59753700
C	-5.30205000	1.17981100	0.16215600
H	-5.83745300	2.07940400	0.46515700
H	-5.58406800	0.35123600	0.82803100
C	-5.10304100	-0.31010300	-1.70282300
O	-5.63052700	0.90632300	-1.18583600
C	-4.94918800	-2.29421200	-0.30454700
C	-3.66750900	-1.75422000	-0.35445100
C	-2.62526800	-2.26551600	0.41407900
C	-2.89233000	-3.34972900	1.24532200
C	-4.17343400	-3.90586600	1.29554000
C	-5.20933000	-3.38389500	0.52320700
C	-5.89201600	-1.55208600	-1.21826000
H	-1.62868600	-1.82822600	0.38827800
H	-4.36762600	-4.75050000	1.94943600
H	-6.20526100	-3.81439900	0.57444800
H	-6.81615100	-1.23594000	-0.72312000
H	-6.18356600	-2.17191500	-2.07222800
C	-0.69158300	2.76972600	0.82551100
C	-0.15671800	2.59628600	2.10513200
C	-0.16886900	3.65847300	-0.11443100
C	0.95079900	3.37190200	2.43911500
C	0.93517100	4.41920100	0.27385100
C	1.50636300	4.28717200	1.53904700
H	1.39556400	3.25357900	3.42438500
H	1.36387400	5.12023800	-0.43795000
C	-0.74534400	3.75048500	-1.50210000

H	-0.29559200	4.58167400	-2.04715400
H	-1.82880000	3.90351200	-1.47060000
H	-0.55636900	2.82875100	-2.06535100
C	2.71177700	5.10063700	1.93532500
H	3.02894400	5.76013800	1.12478900
H	3.55217700	4.44925200	2.19362500
H	2.49591200	5.71790500	2.81225900
C	-0.73008100	1.57711100	3.05364700
H	-0.54960900	0.55836400	2.68947300
H	-1.81007100	1.70588700	3.16474400
H	-0.26483200	1.66812500	4.03626100
H	-5.17380400	-0.18580900	-2.78335300
C	0.37697000	-0.02655200	-0.28466000
C	1.65450000	-0.72629300	-0.67271700
H	0.28884100	0.28415200	0.74702100
C	-0.62901400	0.29274900	-1.14997000
O	-0.82463500	0.10902500	-2.39265200
H	-2.09045300	-3.75059100	1.85675500
C	3.60266600	-2.03881200	0.41796700
C	3.38221400	-3.39622600	0.67680200
C	4.37548700	-4.34964500	0.52567800
C	5.63676700	-3.90486900	0.11911200
C	5.88434200	-2.55539100	-0.11476100
C	4.86206900	-1.61055200	0.03427700
C	1.39906000	-2.38241800	1.25586700
H	4.18534300	-5.39883500	0.72525200
H	6.43599900	-4.62822400	-0.00642900
H	6.87475200	-2.23255500	-0.41636600
H	5.05670600	-0.55821100	-0.15106800
O	0.30113600	-2.24370800	1.75207800
O	2.42543000	-0.27853700	1.64733500
H	2.98592800	0.42237100	1.28587900
N	2.06278100	-3.57678100	1.11285400
H	1.68286000	-4.44302200	1.46535300
C	2.63173400	0.28533600	-1.28926000
C	2.71978500	1.57704900	-0.74873900

C	3.47528600	-0.03552800	-2.35711100
C	3.64358100	2.50044900	-1.23095200
H	2.02792300	1.87284300	0.03673800
C	4.38803500	0.89302500	-2.85391600
H	3.42720600	-1.01963300	-2.81011700
C	4.48646000	2.16032300	-2.28626300
H	3.68696800	3.49239800	-0.78835200
H	5.02561700	0.62101600	-3.68955400
H	5.20100100	2.87983700	-2.67335800
C	1.35646300	-1.89582800	-1.62425700
H	0.95409700	-1.50090500	-2.55797800
H	2.24276200	-2.50644000	-1.82231800
H	0.58719100	-2.53707000	-1.18331300
C	2.31244300	-1.27653300	0.65715700

M4 (SR)

GFE= -2026.845390 a.u.

C	-1.81618200	0.74164000	-0.69657500
C	-3.87108600	1.40848000	-0.31851800
C	-3.73326200	-0.94405400	-1.06601000
H	-3.12012400	-1.41991100	-1.82611500
N	-3.13501800	2.41376900	0.04380700
N	-1.85838100	1.98627300	-0.18851300
N	-3.11653700	0.37217800	-0.79131700
C	-5.35660600	1.27001000	-0.33399500
H	-5.82576400	2.25335500	-0.37275100
H	-5.70068400	0.74413600	0.56863300
C	-5.23240300	-0.77512300	-1.51465700
O	-5.69182500	0.56862300	-1.51069900
C	-5.10406700	-2.13180400	0.50106500
C	-3.79771000	-1.74837800	0.21155100
C	-2.73293200	-2.08007700	1.04632100
C	-3.01245000	-2.79887600	2.20547600
C	-4.32171900	-3.18123500	2.51076200
C	-5.37511200	-2.85690100	1.65912300

C	-6.06178600	-1.68556600	-0.57369700
H	-1.71073200	-1.80736300	0.79451700
H	-4.52053000	-3.74089200	3.41951800
H	-6.39050200	-3.16147700	1.89593900
H	-6.92563600	-1.13473500	-0.18608100
H	-6.45703500	-2.54286700	-1.12752000
C	-0.77294100	2.83474600	0.21937500
C	-0.25371900	2.65204500	1.50233000
C	-0.27322100	3.76411000	-0.69195900
C	0.82692100	3.45302900	1.86617900
C	0.81133100	4.53651700	-0.28177700
C	1.37938200	4.38467500	0.98474700
H	1.26372500	3.32774500	2.85445100
H	1.23385500	5.25957700	-0.97464300
C	-0.84934200	3.85982600	-2.07814300
H	-0.39320000	4.68238200	-2.63065300
H	-1.93164900	4.01454100	-2.04928900
H	-0.65957500	2.93059400	-2.62747800
C	2.60573000	5.16724700	1.37223900
H	3.50461100	4.60835200	1.08841100
H	2.64494300	5.33700500	2.45075000
H	2.63899000	6.13454900	0.86605200
C	-0.78839100	1.57001200	2.40023000
H	-0.52869300	0.58172100	1.99662300
H	-1.87800800	1.62427100	2.48647700
H	-0.35875700	1.65386500	3.39991500
H	-5.33031800	-1.08382700	-2.55551400
C	0.58836700	0.31751300	-0.85080100
C	1.86436300	-0.45018600	-1.15304300
H	0.72744500	1.32650400	-0.50005400
C	-0.67110600	-0.14716700	-1.06781900
O	-1.04082200	-1.30634300	-1.50444100
H	-2.19817000	-3.06716200	2.87080900
C	3.27019000	-2.50861100	-0.49518300
C	3.74862900	-2.51100500	0.81959000
C	5.02256300	-2.94634600	1.14322400

C	5.82314700	-3.42460000	0.10199800
C	5.34554200	-3.48186000	-1.20389300
C	4.05640700	-3.02841800	-1.50707300
C	1.87140300	-1.92273000	-0.51835800
C	1.56924300	-1.80976700	1.00630100
H	5.38020400	-2.93225600	2.16741700
H	6.82635000	-3.77449600	0.32407200
H	5.97302600	-3.88843700	-1.98986000
H	3.66907500	-3.10485800	-2.51762700
O	0.50529700	-1.54226200	1.53329700
O	0.99320100	-2.78049700	-1.16243600
H	0.12426000	-2.28184900	-1.30297000
N	2.73857800	-2.05998900	1.68007600
H	2.78465400	-2.08549500	2.68812600
C	1.95566300	-0.60820900	-2.68076600
H	2.80945700	-1.21681900	-2.98685200
H	1.04529900	-1.08799700	-3.04202200
H	2.04857100	0.37862900	-3.14286400
C	3.03967300	0.34724700	-0.57584600
C	2.92481100	0.93517200	0.69057000
C	4.25099800	0.49933700	-1.25658200
C	3.97395100	1.65585300	1.25259900
H	1.99476700	0.82962500	1.24497300
C	5.30414600	1.22043500	-0.69912000
H	4.38200400	0.05028000	-2.23547000
C	5.17082000	1.80522800	0.55733500
H	3.85096200	2.10498000	2.23474000
H	6.23284900	1.32467600	-1.25162000
H	5.99156900	2.36862200	0.99062300

TS4-D

GFE= -2026.804177 a.u.

Frequency= -144.77 cm⁻¹

C	-2.09302700	0.67356300	-0.49147400
C	-4.16801300	1.17844300	-0.04580200

C	-3.83264100	-1.07442800	-1.14761300
H	-3.57656400	-1.07206900	-2.20655600
N	-3.47206900	2.17910100	0.41696700
N	-2.18134300	1.84217900	0.13784400
N	-3.35949600	0.22612200	-0.59917500
C	-5.65898100	1.03123600	-0.05007300
H	-6.10869900	1.97502100	-0.36356900
H	-6.01846200	0.80231800	0.96060900
C	-5.35573000	-1.17766300	-0.86418500
O	-6.04014300	0.05341900	-0.98846800
C	-4.20823800	-2.69230200	0.57060100
C	-3.27263200	-2.23932000	-0.36410600
C	-2.01549200	-2.82581000	-0.46457800
C	-1.68579700	-3.85170200	0.41794500
C	-2.61712700	-4.30654200	1.35116700
C	-3.88928800	-3.74007600	1.42575500
C	-5.48607300	-1.89687600	0.49596800
H	-1.30503100	-2.48992600	-1.21077100
H	-2.34764500	-5.11026800	2.02890600
H	-4.61403100	-4.10429300	2.14786500
H	-5.54079200	-1.18691200	1.32918800
H	-6.38829400	-2.51126600	0.53825000
C	-1.10591100	2.72372900	0.51573200
C	-0.48445800	2.51252300	1.74952000
C	-0.74290000	3.73423700	-0.37585300
C	0.59005500	3.34299500	2.05920900
C	0.31836000	4.55649600	-0.00107500
C	1.00609900	4.35992400	1.19824900
H	1.12309400	3.17454100	2.99078500
H	0.62898400	5.35213700	-0.67371900
C	-1.44544100	3.88943300	-1.69835700
H	-1.08432800	4.77554800	-2.22182600
H	-2.52726100	3.98284900	-1.56507300
H	-1.26235100	3.02041800	-2.34032100
C	2.20472900	5.20203700	1.54723200
H	2.27838700	6.07820900	0.89907000

H	3.12120400	4.61431400	1.42968400
H	2.16129300	5.54108900	2.58536000
C	-0.91441200	1.40787400	2.67747100
H	-0.40276600	0.47392200	2.41920300
H	-1.99548200	1.25023100	2.64260000
H	-0.63465400	1.65416100	3.70315600
H	-5.77547400	-1.81605600	-1.64448400
C	0.24769000	-0.15705900	-0.38846700
C	1.62519300	-0.61710200	-0.86999100
H	0.30712800	0.55764400	0.42764200
C	-0.90106600	0.00306800	-1.19411100
O	-1.20437500	-0.40336900	-2.32060700
H	-0.68428900	-4.26539000	0.38900100
C	3.21571700	-2.39667400	0.24641700
C	4.32157900	-1.87556800	0.93201500
C	5.56531100	-2.48573900	0.90152700
C	5.68489900	-3.67404300	0.17456100
C	4.58825400	-4.23058700	-0.47788800
C	3.34264900	-3.59278900	-0.43708500
C	2.02732500	-1.48414100	0.44671800
C	2.59267900	-0.47226000	1.49056700
H	6.41275500	-2.06281700	1.43134900
H	6.64720800	-4.17469600	0.13284400
H	4.69872100	-5.16644400	-1.01554100
H	2.48022600	-4.03016300	-0.93032000
O	1.98538000	0.40584200	2.07687300
O	0.86227900	-2.07938400	0.84726200
H	0.14867000	-1.18127200	0.28339100
N	3.93771000	-0.72115200	1.62429800
H	4.52938700	-0.19676600	2.25145300
C	1.49007500	-1.56865400	-2.06453700
H	2.45939100	-1.97208700	-2.36249100
H	0.84259700	-2.40812600	-1.79154400
H	1.04280600	-1.05206200	-2.91404200
C	2.62126700	0.49323900	-1.16974000
C	2.32414500	1.84016000	-0.94703000

C	3.90034600	0.17754200	-1.65123300
C	3.26017400	2.83870600	-1.20537000
H	1.34529800	2.11948800	-0.57522700
C	4.84129000	1.17184800	-1.90035500
H	4.17387700	-0.85975300	-1.82327400
C	4.52536600	2.51074400	-1.68222700
H	2.98919300	3.87768500	-1.03469800
H	5.82468800	0.89692600	-2.26978200
H	5.25663700	3.28729400	-1.88414900

TS4-B

GFE= -2834.139809 a.u.

Frequency= -1241.24 cm⁻¹

C	-2.57942800	0.47645500	-0.05961400
C	-4.33526800	1.71325300	-0.48832800
C	-2.36232100	3.05738500	0.11350000
H	-1.56574000	2.92077600	0.83916400
N	-4.71410900	0.49834300	-0.75208500
N	-3.61396500	-0.26110500	-0.49227500
N	-3.04252500	1.74952100	-0.05253300
C	-5.11511400	2.98604500	-0.52483900
H	-6.18210200	2.77361800	-0.45477100
H	-4.91602400	3.53165200	-1.45858500
C	-3.38474100	4.16507700	0.57121200
O	-4.72950500	3.72128700	0.61379500
C	-2.31527900	4.80940800	-1.51557300
C	-1.83962300	3.53370300	-1.22298400
C	-1.00044700	2.84481800	-2.09666900
C	-0.65606200	3.46633500	-3.29465000
C	-1.13201800	4.74433700	-3.59977600
C	-1.95953500	5.42675000	-2.71219400
C	-3.17660700	5.34970600	-0.40270200
H	-0.59970100	1.86397800	-1.84810600
H	-0.85307700	5.21117300	-4.53896800
H	-2.32420700	6.42110600	-2.95145900
H	-4.14669200	5.72552200	-0.74450400

H	-2.68025000	6.17967800	0.10967100
C	-3.70739400	-1.65798100	-0.85531100
C	-3.56969300	-1.96593500	-2.21153800
C	-4.04029500	-2.60131600	0.11600500
C	-3.71762800	-3.30066600	-2.57382400
C	-4.15499200	-3.92674500	-0.29786600
C	-3.98543400	-4.29562800	-1.63210600
H	-3.60736700	-3.57537700	-3.61986600
H	-4.39357100	-4.68739200	0.44075900
C	-4.24449500	-2.21117900	1.55442700
H	-3.27867300	-2.04507400	2.04626600
H	-4.83324900	-1.29254100	1.64046700
C	-4.06442100	-5.73705200	-2.05573200
H	-3.05676100	-6.13431200	-2.21557700
H	-4.61417500	-5.84300100	-2.99394200
H	-4.55314800	-6.35130600	-1.29733800
C	-3.27458900	-0.89807400	-3.23133700
H	-2.39269100	-0.30543000	-2.95962000
H	-4.11829800	-0.20777400	-3.32730800
H	-3.09076500	-1.34534600	-4.20944100
H	-3.16991000	4.45084200	1.60160300
C	-0.84732100	-1.22517600	0.71146600
C	0.45460300	-2.05651000	0.52522700
H	-1.68606800	-1.87766100	0.48064600
C	-1.12142900	0.13483200	0.35748800
O	-0.45351400	1.14666900	0.53677400
H	-0.00498200	2.95053400	-3.99331300
C	3.01706800	-2.01684800	0.30792700
C	3.54001900	-2.00101700	-0.98617600
C	4.67248900	-2.71786700	-1.33967000
C	5.31182600	-3.44742700	-0.33475900
C	4.84694400	-3.42156600	0.97850900
C	3.69872900	-2.69155500	1.30712000
C	1.74790200	-1.16841100	0.36699400
C	1.73457300	-0.56656400	-1.08911000
H	5.05386000	-2.70692800	-2.35537300

H	6.19764500	-4.02365400	-0.58094100
H	5.37880500	-3.96710500	1.75039900
H	3.34756500	-2.64878100	2.33352000
O	0.93544400	0.19999600	-1.59202500
O	1.76934700	-0.25175200	1.40866100
H	2.19381200	0.61580300	1.06905100
N	2.76386200	-1.15131000	-1.78032300
H	2.88654900	-0.99757300	-2.76999200
C	0.33715400	-2.97804000	-0.70456000
C	-0.39040500	-2.58208000	-1.82992400
C	1.03581300	-4.19024700	-0.78107400
C	-0.42594100	-3.35863800	-2.98425300
H	-0.91261700	-1.63167900	-1.81169300
C	0.99555800	-4.97579500	-1.92929200
H	1.64631300	-4.52935500	0.04775900
C	0.26245900	-4.56559700	-3.03864900
H	-0.99119500	-3.01263600	-3.84529300
H	1.54933900	-5.90870500	-1.95554400
H	0.23749800	-5.17474300	-3.93648600
C	-2.17223600	0.57362200	3.31108100
C	-2.50150300	1.03210900	4.75891100
H	-3.02096100	0.07914600	2.82456500
H	-2.61712000	2.11880800	4.79934700
H	-3.43597200	0.58600800	5.11202600
C	0.17879200	0.36419200	3.79079000
H	0.99228000	-0.35829700	3.88547900
H	0.45259900	1.03925900	2.97905100
C	-0.14646600	1.08632900	5.12768500
H	0.63221800	0.89883300	5.87183600
H	-0.20693200	2.16925300	4.98285800
C	-1.41456600	-0.82873000	5.75603400
H	-0.54766800	-1.12326000	6.35392600
H	-2.31154300	-1.16493100	6.28359200
C	-1.34373200	-1.45144300	4.33485700
H	-0.56957700	-2.21691000	4.25879400
H	-2.29600400	-1.90411300	4.03996500

N	-1.03504400	-0.38041100	3.35327100
N	-1.43109400	0.63059200	5.66863700
H	-0.91811800	-0.86991000	2.08500900
H	-1.85562500	1.40971000	2.68178700
H	-4.76572500	-3.00204600	2.09588900
C	0.58403700	-2.88664600	1.81525200
H	1.34514400	-3.66227500	1.75993200
H	0.85052200	-2.21721800	2.63734400
H	-0.37338900	-3.36985500	2.03901900
C	4.98976400	0.81201500	1.02994600
C	4.23524600	1.80083700	0.16208600
C	6.15661500	0.10030700	0.34326300
C	6.35142300	2.71660300	-0.91667500
C	7.46011900	0.88912100	0.48152100
C	7.23527400	2.38891400	0.28122500
H	5.34000100	1.33348900	1.92958400
H	6.66424100	2.11874800	-1.78708400
H	5.91294600	-0.04714100	-0.71632300
H	8.19449900	0.52485600	-0.24507100
H	4.23941900	0.09828600	1.37247500
H	6.27091800	-0.90234600	0.76536800
H	6.51487500	3.76623500	-1.18832200
H	7.89216400	0.72322600	1.47459000
H	8.19786100	2.88572500	0.12629900
H	6.79928000	2.84656000	1.17539100
C	4.16520200	3.35850400	-1.74358600
H	4.25344100	4.42725100	-1.50311000
H	4.66306400	3.20436300	-2.70910600
C	2.17200100	2.81203000	-0.40381500
H	1.13234800	2.48263600	-0.40090500
H	2.22498800	3.78644600	0.10539600
C	2.70562300	2.94924500	-1.82141300
H	2.14331300	3.69372500	-2.39225600
H	2.59699100	1.98324100	-2.32557600
N	2.95063900	1.83416300	0.34052000
N	4.90076800	2.58755300	-0.73489300

M5

GFE= -2026.836182 a.u.

C	1.10165400	0.74264800	0.12731100
C	2.92395200	0.95272000	1.33563000
C	2.82406900	-1.16124800	0.10275900
H	2.02520100	-1.77450000	-0.31481500
N	2.31301100	2.08785600	1.48182900
N	1.18223200	1.94617400	0.70984700
N	2.22740900	0.11110200	0.51645500
C	4.13296400	0.38593000	2.00618100
H	4.36549000	0.95343400	2.90736400
H	5.00069600	0.40016400	1.33413600
C	3.50232400	-1.84163400	1.34120800
O	3.78312800	-0.92903700	2.40094700
C	5.08365900	-1.69061300	-0.47381500
C	3.96818300	-0.95466200	-0.86930000
C	3.97956300	-0.16519200	-2.01451500
C	5.15722100	-0.11330200	-2.75850600
C	6.28275900	-0.84201900	-2.36757100
C	6.25358500	-1.64052600	-1.22531300
C	4.79269000	-2.47473100	0.78232000
H	3.07487500	0.36195200	-2.30708900
H	7.19043700	-0.78845500	-2.96069500
H	7.12965200	-2.20790000	-0.92495500
H	5.58855200	-2.42744100	1.53113200
H	4.62257400	-3.53148000	0.54758800
C	0.28180200	3.06086900	0.61223000
C	0.23013200	3.76654800	-0.59577000
C	-0.45852800	3.42210600	1.73981300
C	-0.67032900	4.82644500	-0.67420000
C	-1.34494400	4.49115600	1.60598200
C	-1.47545900	5.19117900	0.40730800
H	-0.73836700	5.38608200	-1.60366100
H	-1.94366200	4.78388900	2.46502800
C	-0.28658200	2.73479000	3.06861100

H	-1.20456600	2.80463000	3.65583700
H	0.52018800	3.21070600	3.63448000
H	-0.02412500	1.68091600	2.96034600
C	-2.47150900	6.31354400	0.27592900
H	-2.66748600	6.78407200	1.24187200
H	-3.42404500	5.93674200	-0.11020300
H	-2.11399400	7.07891300	-0.41660500
C	1.11862300	3.39851500	-1.75363500
H	0.88566100	2.40457200	-2.15526500
H	2.16654500	3.37249400	-1.43431100
H	1.02178300	4.13731400	-2.55079000
H	2.83486200	-2.57921500	1.78920200
C	-1.25922800	0.67835900	-1.09819200
C	-2.14126400	-0.17424800	-0.17922800
H	-1.49964700	0.50509700	-2.14866900
C	0.18743700	0.13468900	-0.99832500
O	0.91128200	0.15964500	-2.05774600
H	5.19743900	0.49538100	-3.65613500
C	-1.69077500	-2.62306600	0.67685300
C	-2.40630500	-3.66802100	0.07733300
C	-2.82308300	-4.77738300	0.79622300
C	-2.47920600	-4.83790600	2.14973800
C	-1.73020900	-3.82980200	2.75085700
C	-1.32558900	-2.71460100	2.00816400
C	-1.41428900	-1.55822500	-0.35702000
C	-1.94184700	-2.23434800	-1.66084000
H	-3.38310800	-5.57623200	0.32198700
H	-2.79086500	-5.69690500	2.73539200
H	-1.45603400	-3.91075000	3.79706000
H	-0.72734200	-1.93300600	2.46653300
O	-1.85437300	-1.81629400	-2.79196800
O	-0.04903800	-1.25312100	-0.43095600
N	-2.57527100	-3.39849500	-1.28252000
H	-3.00186500	-4.02175700	-1.95196400
C	-2.00197200	0.31931600	1.26695500
H	-2.59569200	-0.27374000	1.96578100

H	-0.95723400	0.27118500	1.58963700
H	-2.33491100	1.36028900	1.32856000
C	-3.61742700	-0.22575900	-0.55590200
C	-4.13890500	0.48612300	-1.63843900
C	-4.49985300	-1.00511000	0.20572600
C	-5.49482500	0.42101000	-1.95352600
H	-3.48729600	1.10172800	-2.24792900
C	-5.85189700	-1.07783400	-0.11124000
H	-4.12532700	-1.57123400	1.05487000
C	-6.35712500	-0.36192000	-1.19402300
H	-5.87390600	0.98561200	-2.79977600
H	-6.51148300	-1.69408000	0.49193800
H	-7.41276100	-0.41332300	-1.44118100
H	-1.34669400	1.74604900	-0.88283500

TS5

GFE= -2026.82719 a.u.

Frequency= -154.71 cm⁻¹

C	1.65251300	-0.91664000	-0.22716400
C	3.57476400	-2.03672100	-0.36363900
C	3.71094700	0.38377400	-1.00261100
H	3.30850400	0.62118600	-1.98731600
N	2.71673900	-2.92577500	0.03268700
N	1.54669400	-2.21143300	0.11244300
N	2.98115600	-0.80863700	-0.51735500
C	5.02485700	-2.27245100	-0.65220500
H	5.13399500	-3.20881700	-1.20221700
H	5.58802400	-2.36339600	0.28572400
C	5.22651100	0.05427700	-1.01069200
O	5.53582400	-1.24370700	-1.46874300
C	4.81286400	1.56280700	0.76059700
C	3.66347200	1.54664100	-0.03644600
C	2.69913200	2.54093500	0.07575100
C	2.88431000	3.53812500	1.03315900
C	4.01894600	3.54596300	1.84491900

C	4.99743900	2.56161000	1.70848200
C	5.73113000	0.42353300	0.40130300
H	1.82517000	2.52583600	-0.56369400
H	4.14862000	4.33277200	2.58164000
H	5.89155300	2.58122900	2.32470600
H	5.60409300	-0.40614700	1.10722300
H	6.78961200	0.69402800	0.39987700
C	0.35426100	-2.89161100	0.52567400
C	-0.20391800	-2.56767200	1.76342200
C	-0.21740300	-3.81977500	-0.34855400
C	-1.40092500	-3.19185000	2.10751400
C	-1.40945700	-4.42570400	0.04605200
C	-2.01920500	-4.11364300	1.26290500
H	-1.87296100	-2.93015400	3.05114800
H	-1.87942600	-5.14471300	-0.62105700
C	0.41936300	-4.12188100	-1.67864600
H	-0.23934200	-4.74156100	-2.28950600
H	1.37108400	-4.64394200	-1.54681900
H	0.63528800	-3.19830700	-2.22666600
C	-3.33268500	-4.73730800	1.65875700
H	-3.68249100	-5.44399200	0.90278000
H	-4.09828000	-3.96587400	1.78715200
H	-3.24391100	-5.27149500	2.60931200
C	0.45914700	-1.56485700	2.66727000
H	0.47609400	-0.58133200	2.19041500
H	1.49131800	-1.85972200	2.88342700
H	-0.08907600	-1.47917700	3.60649000
H	5.69017300	0.73190800	-1.73185200
C	-0.89081300	-0.52864300	-1.37291600
C	-2.01705400	0.51510500	-1.31645300
H	-0.99006500	-1.21262700	-0.53096500
C	0.33002700	0.35737500	-1.17797000
O	1.03340400	0.79684000	-2.08389900
H	2.13835100	4.31913900	1.14145500
C	-1.82272800	2.88417700	-0.15864200
C	-2.64514000	3.16264900	0.93916800

C	-3.14915500	4.43189000	1.17415400
C	-2.78074400	5.44585600	0.28553900
C	-1.92615700	5.19521100	-0.78523000
C	-1.43570400	3.90443300	-1.00947400
C	-1.45510700	1.42033300	-0.13620300
C	-2.06549800	0.95567500	1.21380400
H	-3.79079200	4.63602600	2.02469000
H	-3.15954500	6.45020000	0.44590100
H	-1.63713100	6.00505500	-1.44599900
H	-0.75340500	3.70127000	-1.82953200
O	-1.93373600	-0.13158100	1.72882600
O	-0.04809400	1.23629100	-0.12148900
N	-2.80798400	2.00174000	1.70617000
H	-3.29629200	1.94813900	2.58774000
C	-2.07854300	1.27481100	-2.65106100
H	-2.78225700	2.10897700	-2.61318500
H	-1.09116700	1.64995600	-2.93121300
H	-2.41323900	0.58185300	-3.42853000
C	-3.39198900	-0.06395400	-1.00746500
C	-3.60909500	-1.43676800	-0.87190200
C	-4.48626300	0.79869400	-0.87005200
C	-4.88332800	-1.93379700	-0.60639600
H	-2.78455300	-2.13607000	-0.96824400
C	-5.75734200	0.30498300	-0.59448500
H	-4.34047200	1.87186300	-0.97294200
C	-5.96178500	-1.06666700	-0.46359700
H	-5.02855500	-3.00626600	-0.51323600
H	-6.58954100	0.99373600	-0.48695300
H	-6.95377800	-1.45492600	-0.25538900
H	-0.84889300	-1.07214100	-2.31953200

P

GFE= -975.0394982 a.u.

C	1.49553700	2.08833700	-0.35306800
C	0.78775000	0.78370200	-0.74596900

H	2.07146800	1.98277700	0.56977800
C	0.34818400	3.02133500	-0.03131500
O	0.32890100	4.21740700	-0.00446400
C	-1.66083800	0.04403100	-0.08352800
C	-1.80129800	-0.89974300	0.94251300
C	-2.80553200	-1.85338300	0.92459500
C	-3.69972100	-1.82673700	-0.14931500
C	-3.59554700	-0.87199400	-1.15767700
C	-2.56882800	0.07662000	-1.12738200
C	-0.45639000	0.89083700	0.21287400
C	-0.05357300	0.41482400	1.63609400
H	-2.90337400	-2.58417600	1.71978800
H	-4.49885400	-2.55998100	-0.18671900
H	-4.31623200	-0.86066000	-1.96755100
H	-2.49187300	0.83267500	-1.90172800
O	0.78906400	0.92256000	2.34140100
O	-0.76463300	2.28233800	0.24764700
N	-0.81855400	-0.68513900	1.91884400
H	-0.75217700	-1.17875600	2.79716900
C	0.34583400	0.89067900	-2.21297500
H	-0.23813100	0.02324800	-2.52511300
H	-0.25484400	1.79121500	-2.38089100
H	1.23392300	0.94927900	-2.84768000
C	1.57921100	-0.49758100	-0.52706900
C	2.88725200	-0.49119500	-0.03970700
C	0.98831500	-1.73300500	-0.82658700
C	3.58523000	-1.68200700	0.15175300
H	3.38125900	0.44622100	0.19035600
C	1.68060100	-2.92247300	-0.62789200
H	-0.02668100	-1.76997000	-1.21315000
C	2.98395800	-2.90172700	-0.13710900
H	4.60247500	-1.65013100	0.52841000
H	1.20021700	-3.86763200	-0.86021700
H	3.52606800	-3.82946000	0.01458000
H	2.12911500	2.50975000	-1.13503700

