

Electronic Supplementary Information

Diastereoselectivity in Cyclic Secondary Amine Catalyzed Asymmetric Mannich Reaction: a Model Rationalization from DFT Studies

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1. Authors of Gaussian 09 in reference 14.

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, *revision, D.01*, Gaussian, Inc., Wallingford, CT, 2009

2. Strain energies of other 16 transition state structures.

Table S1. strain energies of other 16 transition state structures

	E_A	E_B	E_{dist}	E_{int}	$E_{\text{dist}}+E_{\text{int}}$
C1-trans-E-Re	6.4	72.8	79.2	-73.5	5.7
C1-cis-E-Re	7.3	80.1	87.4	-75.4	12.0
C2-trans-E-Re	7.3	73.4	80.7	-68.7	2.0
C2-cis-E-Re	8.8	48.5	57.3	-49.8	7.5
C3-trans-E-Re	7.1	83.5	90.6	-86.9	3.7
C3-cis-E-Re	7.0	63.1	70.1	-63.7	6.4
C4-trans-E-Re	5.3	60.4	65.7	-68.2	-2.5
C4-cis-E-Re	4.8	60.0	64.8	-67.3	-2.5
C5-trans-E-Re	7.8	71.0	78.8	-75.9	2.9
C5-cis-E-Re	8.1	82.9	91.0	-79.6	11.4
C6-trans-E-Re	10.1	97.9	108.0	-97.7	10.3
C6-cis-E-Re	8.9	79.1	88.0	-78.3	9.7

3. The prediction of catalysts C7 and C8.

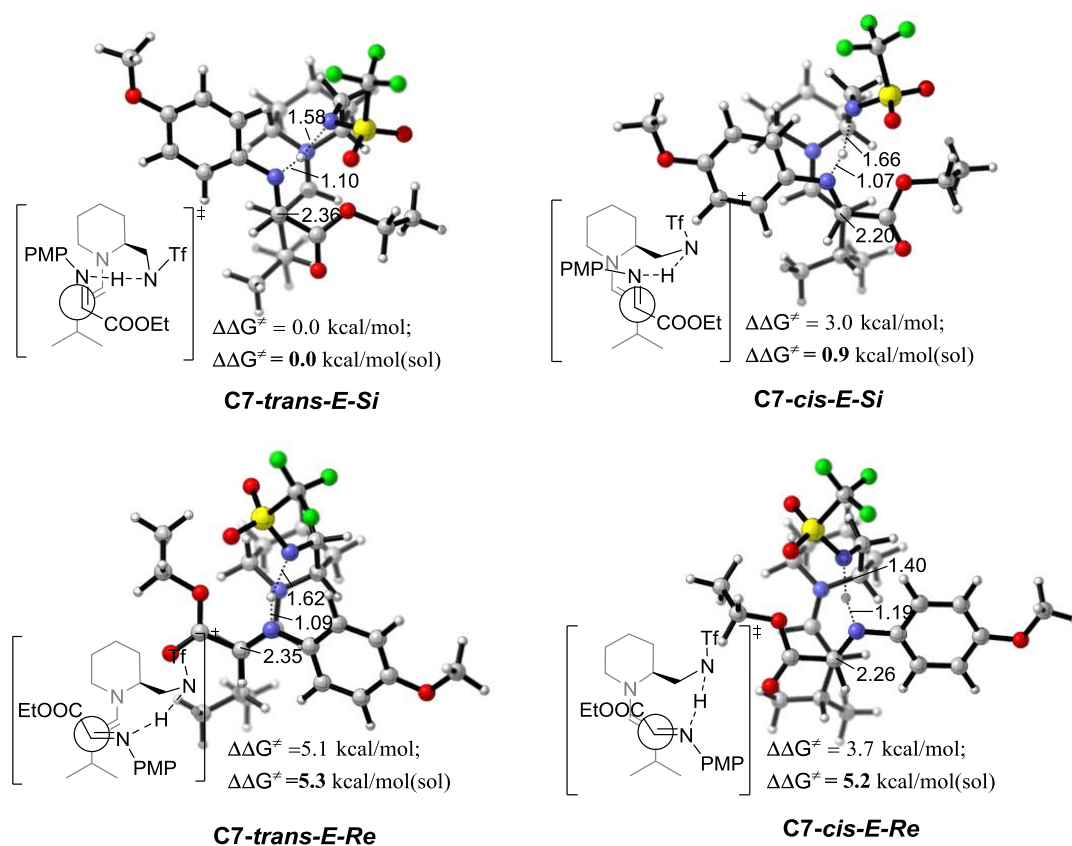


Fig. S1. Relative Free Energies in Gas Phase and Solvation of C7.

C7 bears acidic group -NHTf locates at 2-position in 6-membered piperidine ring. The free energy of **C7-trans-E-Si** is the most energy preferred in these four transition states, as shown in fig. S1. As an analog of C5, C7 is predicted to have a *d.e.* value of 64% for the Mannich reactions between N-PMP-protected α -imino ethyl glyoxylate and isovaleraldehyde. This is in agreement with our assumption that replacing the -COOH with -NHTf in 2-position would increase the *d.e.* values (17% for C5).

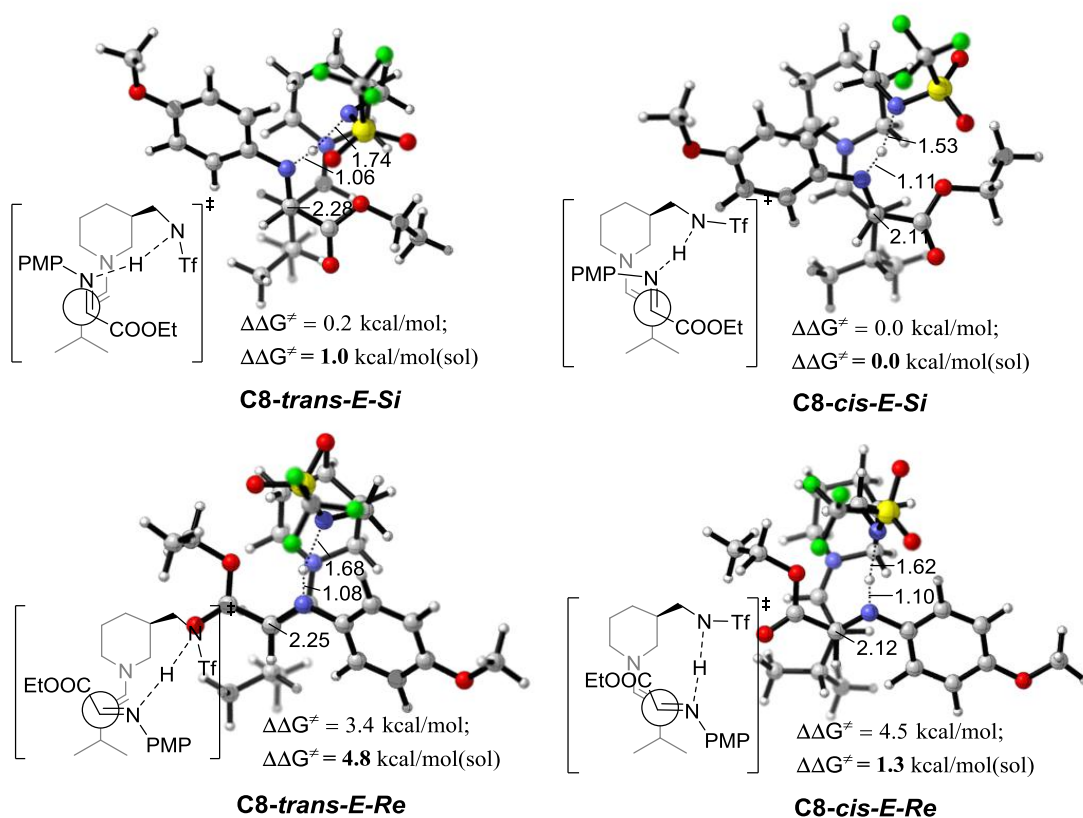


Fig S2. Relative Free Energies in Gas Phase and Solvation of **C8**.

Replaced the $-\text{COOH}$ with $-\text{NHTf}$ at 3-position of **C6**, **C8** is also predicted. **C8-cis-E-Si** is most energy preferred in these four transition states as shown in Fig. S2. The calculated *d.e.* value of **C8** is -54% , leading to the same diastereoselectivity of **C6** (-56%).

4. All optimized geometries and Cartesian coordinates for all the structures.

Cartesian coordinates of six catalysts and substrates

C1:

C	1.94186000	-0.75927200	-0.41988500
C	-0.09507000	-0.21161000	0.70894600
C	0.87999900	0.96871800	0.80996300

C	1.79838400	0.75939600	-0.39693700
N	0.57778300	-1.21303600	-0.14006600
H	-0.37047800	-0.61325700	1.69166300
H	1.45459900	0.88915000	1.73787000
H	0.35925400	1.92689800	0.79686100
H	1.29248800	1.09779700	-1.30606500
H	2.75536300	1.27745000	-0.30921200
H	2.66720000	-1.07539900	0.34755400
H	2.28210300	-1.14219000	-1.38644900
C	-1.37552900	0.17651000	-0.01415700
O	-1.56800100	1.20606800	-0.61144400
O	-2.29057000	-0.80686300	0.05132400
H	-3.04374600	-0.51987600	-0.48669300
H	0.52944000	-2.14541700	0.24830200

C2:

C	-3.63304000	-0.34720400	-0.96938200
C	-2.35073800	1.03533000	0.49383400
C	-2.54353500	-0.35535400	1.14816700
C	-2.90679300	-1.29059100	-0.01515900
N	-2.79686900	0.85483500	-0.90049400
H	-2.94425400	1.79232900	1.02590800
H	-3.37217700	-0.30953100	1.86124300
H	-1.65444000	-0.67897500	1.69670800
H	-4.66213200	-0.17181900	-0.61565300
H	-3.68168500	-0.71951600	-1.99661300
C	-0.89260500	1.50986500	0.48061000
N	-0.10010800	0.64223300	-0.39164700
H	-0.82431200	2.53016000	0.08882000
H	-0.46039100	1.49523600	1.48394900
S	0.88539400	-0.51694400	0.19461000
O	0.84809700	-0.53390200	1.64521300
O	0.73976700	-1.71391600	-0.61084900
C	2.53491000	0.17475700	-0.22443000
F	2.65594000	0.28988700	-1.53906000
F	3.47924300	-0.63113600	0.23730400
F	2.66248300	1.37175300	0.33556500
H	-0.62721600	0.34299000	-1.21535200
H	-3.26582600	1.67941200	-1.26264100
H	-2.00313800	-1.68482800	-0.49292200
H	-3.52299800	-2.13663800	0.29674800

C3:

C	0.72602500	-0.55275900	1.18125600
C	-0.19689500	0.56115000	0.66131600
C	0.70868500	1.30683200	-0.36314800
C	1.90821500	0.36122300	-0.59705100
N	1.43949200	-0.91838800	-0.04772800
H	2.79243600	0.73291900	-0.05891000
H	2.16938800	0.25028500	-1.65204200
H	1.03914300	2.26672600	0.03807900
H	0.16841300	1.50814000	-1.29148100
H	0.18403900	-1.41244400	1.58564500
H	1.39640400	-0.15729700	1.95992100
H	-0.56119900	1.21600400	1.45260700
C	-1.42212200	-0.02368600	-0.03711900
O	-2.53804400	0.38943700	0.13858300
O	-1.16285900	-1.02410800	-0.89167600
H	2.19411400	-1.58051200	0.11106300
H	-0.19540700	-1.23429900	-0.85755900

C4:

C	-3.17715500	0.91249500	-0.75018700
C	-2.43703800	1.01455700	0.58930500
C	-2.56012200	-0.42375100	1.13647000
C	-2.76059700	-1.31838400	-0.11321800
N	-2.70441800	-0.38165600	-1.25362600
H	-3.72646000	-1.83801500	-0.05769700
H	-1.97367500	-2.07142800	-0.21876900
H	-3.42723400	-0.49869200	1.79741600
H	-1.67993500	-0.71159100	1.71835300
H	-2.91797300	1.71594600	-1.44868100
H	-4.26632900	0.93800400	-0.58165500
H	-2.91940100	1.74309100	1.24865400
C	-0.97724200	1.45105800	0.41084800
N	-0.21078000	0.50429200	-0.41338200
H	-0.93162100	2.43362800	-0.07152700
H	-0.48763300	1.52863900	1.38504500
S	0.86005200	-0.52104000	0.26538200
O	0.84896000	-0.41070700	1.71335200
O	0.78298300	-1.79803400	-0.41839800
C	2.45512400	0.23461200	-0.24197600
F	2.55686900	0.24296400	-1.56309600

F	3.45646700	-0.46305100	0.27281700
F	2.50801100	1.48295400	0.21067700
H	-3.23978900	-0.71326800	-2.05047500
H	-0.78989100	0.03248100	-1.12837600

C5:

C	2.14545600	-0.15626300	-0.51347100
C	1.14152700	-1.30442900	-0.40895100
C	-0.37882300	0.08753000	0.91032700
C	0.55483700	1.29215700	0.77757300
C	1.40983900	1.18499000	-0.48550700
H	0.49240400	-1.29676900	-1.29526000
H	1.64199800	-2.27699300	-0.38750700
H	2.84991700	-0.21051300	0.32851800
H	2.73208000	-0.26272900	-1.43247300
H	-0.86221600	0.10281400	1.89634300
H	-0.04803600	2.20361300	0.76663400
H	1.20507500	1.32678200	1.66122900
H	0.75823600	1.26556700	-1.36550700
H	2.11782000	2.01816300	-0.53424000
N	0.26521300	-1.22508800	0.77048100
C	-1.53444100	0.16016900	-0.10445700
O	-1.96245700	1.19131500	-0.55039000
O	-2.04859800	-1.03473900	-0.41676300
H	0.79851800	-1.43597300	1.61064300
H	-1.48421300	-1.69587400	0.04239600

C6:

C	0.51546400	-0.89912400	1.17624100
C	-0.48294700	0.23277700	0.91199200
C	0.27442400	1.48820400	0.43727200
C	1.17646400	1.17397100	-0.75982300
C	2.09258900	-0.00670800	-0.44213400
H	-0.44406000	2.27611500	0.19230600
H	-1.02209900	0.46821100	1.83331100
H	1.17502700	-0.60534700	2.00968000
H	-0.00659300	-1.81707900	1.46447300
H	0.56559900	0.92572800	-1.63554400
H	1.78084400	2.04814800	-1.02103200
H	2.68772400	-0.28328000	-1.31673600
H	2.78739000	0.27704300	0.36759000

H	0.89161500	1.85219700	1.26966400
C	-1.56520400	-0.12756400	-0.11274500
O	-2.66067900	0.37023000	-0.07031800
O	-1.21578600	-0.98735200	-1.07652900
H	-0.26225100	-1.24323200	-0.95430700
N	1.27635700	-1.16333000	-0.05218500
H	1.85928400	-1.98754900	0.06583900

C7

C	4.24327100	0.67404800	0.32446300
C	3.02037600	1.34234600	-0.30572400
C	1.95568500	-0.83468900	-0.71484300
C	3.11911200	-1.54926700	-0.00984100
C	3.83924100	-0.64137700	0.99308700
H	2.31149000	1.63075000	0.48253200
H	3.29532400	2.26293300	-0.82879400
H	4.98633500	0.47394700	-0.46026900
H	4.71161300	1.35101400	1.04711700
H	1.62349700	-1.43867800	-1.56710000
H	2.75357300	-2.46007700	0.47958100
H	3.83688400	-1.86846400	-0.77683400
H	3.18633100	-0.42619700	1.84890600
H	4.71724800	-1.15690900	1.39542900
N	2.31012900	0.48312300	-1.25921400
C	0.74768000	-0.67804000	0.21743100
N	-0.24315400	0.13329700	-0.49340200
H	0.32314200	-1.66214200	0.43488800
H	1.02519600	-0.21323100	1.17014300
S	-1.52840500	0.74167000	0.31330600
O	-1.35993300	0.59572300	1.74587200
O	-1.91555800	1.99038900	-0.30970300
C	-2.81490400	-0.49098000	-0.13665700
F	-2.37100100	-1.70966900	0.16364000
F	-3.07863900	-0.42938400	-1.43256000
F	-3.91933400	-0.24624400	0.55176600
H	0.19473200	0.81487000	-1.12144100
H	2.88221500	0.35706300	-2.09119400

C8

C	-2.15437100	1.23028900	0.66182100
C	-2.91776300	1.25940600	-0.66803100

C	-3.16849800	-1.13508400	-0.75997400
C	-2.44204800	-1.34095300	0.56631200
C	-2.47412500	-0.06874000	1.42731400
H	-2.51587000	2.07412400	1.26460400
H	-4.25175300	-1.01528900	-0.57530100
H	-3.03181700	-2.00515700	-1.40832200
H	-2.91706800	-2.15995100	1.11635000
H	-1.41784400	-1.66264600	0.35989600
H	-3.48591700	0.03623800	1.84068500
H	-1.79006100	-0.17568300	2.27670900
N	-2.61862400	0.04576900	-1.43622600
H	-2.61796200	2.13325700	-1.25773600
H	-3.99962600	1.34875800	-0.46212200
C	-0.65802800	1.49500400	0.46409300
N	-0.00003200	0.50387600	-0.39693700
H	-0.51699700	2.48293300	0.01054300
H	-0.14961300	1.49540800	1.43227100
S	1.06486300	-0.56376700	0.21452400
O	1.05001000	-0.54951100	1.66639900
O	0.97805200	-1.79029300	-0.55384000
C	2.66311100	0.21827700	-0.24076000
F	2.78337500	0.28349100	-1.55829700
F	3.66393100	-0.49102200	0.25837000
F	2.69822500	1.44856300	0.26416700
H	-3.01898300	0.12550800	-2.36755000
H	-0.61764500	0.09520300	-1.11355800

Imine

C	1.32448900	-1.39387900	-0.33359900
C	0.68954800	-0.19180800	0.00864200
C	1.47424300	0.90787300	0.36053700
C	2.86439800	0.82884000	0.34277000
C	3.48402400	-0.36261900	-0.04066100
C	2.70293500	-1.47598600	-0.37754200
H	0.70609300	-2.25144200	-0.57714100
H	1.00040000	1.82800900	0.68990800
H	3.44738000	1.69298900	0.63785500
H	3.20942600	-2.39376000	-0.65587800
O	4.82607800	-0.54474600	-0.10012300
C	5.65133600	0.55089900	0.22840200
H	6.67715000	0.20413600	0.10582500
H	5.47073000	1.40042000	-0.44146400
H	5.49612500	0.86960200	1.26637900

C	-1.34639800	0.87868300	-0.25412100
H	-0.87677300	1.82637500	-0.54147300
C	-2.84157800	0.94638800	-0.21387900
O	-3.43331800	1.97916400	-0.42653200
O	-3.42441800	-0.21607400	0.07236800
C	-4.85754500	-0.18139000	0.11780800
C	-5.32805900	-1.58785100	0.41580200
H	-5.23269100	0.18656400	-0.84202300
H	-5.16863900	0.53102600	0.88838800
H	-6.41998800	-1.61476700	0.46322600
H	-4.99512900	-2.27642100	-0.36474600
H	-4.92811100	-1.93198400	1.37272400
N	-0.71957800	-0.19034300	0.01539400

Isovaleraldehyde

C	2.10318200	-0.61669400	-0.27284700
C	0.72343200	0.03984700	-0.28485900
H	0.39659400	0.16636800	-1.32439800
H	2.09082600	-1.58935700	-0.77600200
H	2.84075000	0.01602000	-0.77651400
H	2.44751600	-0.77450800	0.75651000
C	0.77280800	1.42006700	0.37150900
H	-0.20302300	1.91017700	0.33536700
H	1.08282600	1.33329400	1.42048700
H	1.49679900	2.06469100	-0.13682200
C	-0.29862100	-0.85893900	0.40911800
H	-0.21516500	-1.89981100	0.05984200
H	-0.11488900	-0.90294700	1.49345800
C	-1.73534800	-0.45118300	0.19275200
H	-2.48710300	-1.05147100	0.74831100
O	-2.09098100	0.44112000	-0.53678500

Cartesian coordinates of *trans-E* enamine intermediates

C1-*trans-E*

C	-0.52576300	1.53860900	-0.79901100
C	-1.63531100	-0.00010900	0.68759300
C	-2.38854800	1.34037300	0.66272900
C	-2.00267900	1.91402400	-0.70353000
N	-0.47741300	0.20252000	-0.19878000
H	-1.32995100	-0.27172800	1.70317900

H	-2.01034900	1.98771900	1.46021300
H	-3.46052700	1.19730400	0.80993500
H	-2.57035000	1.41868800	-1.49945100
H	-2.16696500	2.99040400	-0.78394200
H	0.09717500	2.23681900	-0.21755000
H	-0.14117900	1.51323800	-1.82332900
C	-2.54452300	-1.13074500	0.17733100
O	-3.53720200	-1.46127100	0.76952900
O	-2.15785300	-1.68907600	-0.97218000
H	-1.33651200	-1.22024900	-1.23482500
C	0.76605300	-0.30816700	0.19694200
C	1.96462400	0.17797600	-0.13849300
H	0.69179800	-1.21101900	0.80255400
H	2.04179400	1.07172100	-0.75809300
C	3.26401300	-0.45606800	0.27913700
C	4.08249300	0.50775100	1.14555900
C	4.07503500	-0.89313500	-0.94615300
H	3.03217500	-1.34809500	0.87690800
H	3.52425200	0.80456900	2.03795500
H	5.02530200	0.04867200	1.46114700
H	4.32499900	1.41609100	0.58124800
H	3.51155300	-1.60153100	-1.56003200
H	4.32029900	-0.02547400	-1.57023800
H	5.01645600	-1.36504100	-0.64564300

C2-trans-E

C	-1.79874500	1.69651700	0.98252900
C	-0.70534400	1.17104100	-1.10263700
C	-0.15659600	2.50519400	-0.55251300
C	-0.49480500	2.48718800	0.94535600
N	-1.59569600	0.67580300	-0.03892200
H	-1.26285500	1.33944500	-2.03492900
H	-0.67921200	3.33436400	-1.03865900
H	0.91251900	2.62369100	-0.74846500
H	0.28222100	1.96799600	1.51633400
H	-0.60317100	3.48989500	1.36417400
H	-2.66556000	2.33182600	0.73293100
H	-1.99563300	1.22672800	1.95186700
C	0.37492200	0.12326400	-1.39304900
C	-2.67176400	-0.12994700	-0.40675200
C	-3.84534200	-0.23739400	0.22576000
H	-2.47950000	-0.73658300	-1.29237100
H	-4.04726200	0.36026000	1.11475700

C	-4.93901900	-1.17673600	-0.20642500
C	-6.22466300	-0.40378700	-0.52112600
C	-5.20487900	-2.23771700	0.86791500
H	-4.60942300	-1.68779000	-1.12170200
H	-6.57534800	0.12911500	0.37083000
H	-6.05746000	0.33545400	-1.30967200
H	-7.02363700	-1.08085500	-0.84154200
H	-4.30243100	-2.81813200	1.07967100
H	-5.52580500	-1.76150900	1.80204200
H	-5.99693700	-2.92620600	0.55413100
N	1.05003400	-0.28117800	-0.16047800
H	-0.07069300	-0.77267100	-1.83894800
H	1.12127200	0.51457500	-2.08839000
S	2.52387800	0.27910400	0.25776600
O	2.99191200	1.24535100	-0.71711900
O	2.54303200	0.52263800	1.68647700
C	3.56357600	-1.21144600	-0.01370600
F	3.14910600	-2.19635300	0.76990400
F	4.82565500	-0.92430200	0.26393100
F	3.46180000	-1.58632200	-1.28316500
H	0.42386600	-0.39583000	0.63648600

C3-trans-E

C	-1.22440800	-0.52236500	-1.17180300
C	-2.50922500	-0.73581300	-0.36358100
C	-1.97617500	-1.34594300	0.96353600
C	-0.47297300	-0.99410700	1.00054300
N	-0.28220800	-0.08928800	-0.13338700
H	0.14784800	-1.89513400	0.87508400
H	-0.16430500	-0.49994800	1.92630500
H	-2.11652500	-2.42875300	0.96262100
H	-2.51278000	-0.94827000	1.82838100
H	-1.31383500	0.24535700	-1.94709100
H	-0.90145700	-1.46343300	-1.64327400
H	-3.22016400	-1.39231500	-0.86519200
C	-3.23452500	0.57972000	-0.09471200
O	-4.42552300	0.70551200	-0.19685400
O	-2.44933200	1.59501400	0.30060500
H	-1.50939000	1.29843500	0.28996800
C	1.03138400	0.19919300	-0.53658900
C	2.14659400	-0.07734300	0.14346100
H	1.08229100	0.73606600	-1.48316300
H	2.09340800	-0.60690200	1.09488100

C	3.52215100	0.33208600	-0.30927500
C	4.42608200	-0.89562300	-0.46356600
C	4.14035300	1.33246000	0.67443100
H	3.42895500	0.82154900	-1.28818500
H	4.00894300	-1.60607700	-1.18287900
H	5.42640700	-0.60563100	-0.80130100
H	4.53452700	-1.41215800	0.49764000
H	3.52290300	2.23081600	0.76258800
H	4.22831200	0.88353200	1.67084200
H	5.14360400	1.63007700	0.35180900

C4-trans-E

C	-1.17728100	2.19486400	-1.08433100
C	0.09964300	2.64172500	-0.36613700
C	-0.23997300	2.36103700	1.11294400
C	-1.29471800	1.23105700	1.08403600
N	-1.55368700	0.99267300	-0.33862700
H	-2.22033500	1.53750000	1.59411400
H	-0.94302300	0.30549200	1.55441500
H	-0.66500300	3.25684500	1.57230900
H	0.64958100	2.08681100	1.68704400
H	-1.01972400	1.95243600	-2.14222500
H	-1.95241800	2.97615400	-1.02205400
H	0.29236600	3.70460700	-0.54258200
C	1.33624400	1.86867000	-0.83906000
C	-2.72646000	0.32608200	-0.70220800
C	-3.53332800	-0.36300400	0.11092700
H	-2.93341000	0.36702300	-1.77150800
H	-3.31850700	-0.41893700	1.17803600
C	-4.74031300	-1.12648800	-0.36324700
C	-6.01309800	-0.59644000	0.30619700
C	-4.57632800	-2.62566600	-0.08771700
H	-4.83366700	-0.98195300	-1.44849500
H	-6.16168100	0.46462800	0.08610900
H	-6.89588000	-1.14941200	-0.03201200
H	-5.94522600	-0.70834400	1.39488600
H	-3.68991200	-3.02372200	-0.58943200
H	-4.46177800	-2.80456100	0.98790100
H	-5.45280700	-3.18680000	-0.42906500
H	1.49061600	2.01707600	-1.91346500
H	2.22558000	2.22989500	-0.31594600
N	1.22314100	0.42502800	-0.58899200
S	2.06800500	-0.30085700	0.60434500

O	2.78661900	0.67573000	1.40228700
O	1.24113600	-1.33644900	1.19232700
C	3.37005500	-1.16628700	-0.35965300
F	2.81854000	-2.05241600	-1.17544400
F	4.19551300	-1.78346300	0.47168300
F	4.04653300	-0.27292200	-1.07374500
H	0.26700100	0.05673100	-0.65409500

C5-trans-E

C	0.66806000	1.75616400	1.14780700
C	0.58384500	0.25595400	1.43215300
C	1.45909900	-0.28174700	-0.77372800
C	1.64531300	1.20100000	-1.10296000
C	1.81734300	2.02803100	0.17250000
H	1.52221300	-0.07823600	1.89432700
H	-0.22078600	0.00437500	2.12735100
H	-0.27897800	2.09846800	0.71275900
H	0.81599300	2.29974300	2.08694200
H	1.19289900	-0.83095600	-1.68706200
H	2.51255100	1.30906100	-1.75922800
H	0.75679200	1.54116800	-1.64951700
H	2.77223300	1.76200200	0.64490400
H	1.86900200	3.09270900	-0.07554400
N	0.39664200	-0.53643200	0.20899400
C	2.76637000	-0.92595100	-0.28267600
O	3.85637500	-0.53088700	-0.59676700
O	2.58563900	-2.00452800	0.49139800
H	1.61945600	-2.08417900	0.63477000
C	-0.90128800	-0.57784500	-0.33606000
C	-2.04113200	-0.12918400	0.19590800
H	-0.93101500	-1.09040300	-1.29809300
H	-2.04615600	0.40493700	1.14579300
C	-3.38704900	-0.32967700	-0.44893700
C	-4.07060100	1.01991100	-0.69347700
C	-4.27655100	-1.23184300	0.41452600
H	-3.23310000	-0.82266200	-1.41848600
H	-3.45787500	1.66201900	-1.33272500
H	-5.04789800	0.88614800	-1.16877100
H	-4.23004400	1.54313500	0.25703200
H	-3.81616000	-2.21281700	0.56234100
H	-4.43349800	-0.78069700	1.40141300
H	-5.25869400	-1.37434300	-0.04854400

C6-trans-E

C	-0.96952900	-0.01858200	1.24194000
C	-2.43868300	0.19139200	0.87224700
C	-2.59716100	1.52465100	0.11986400
C	-1.65917300	1.57494700	-1.08539100
C	-0.21622500	1.29202700	-0.67351600
H	-3.64000900	1.65288100	-0.18482000
H	-3.03705100	0.22063300	1.78679100
H	-0.65621600	0.75790700	1.95923300
H	-0.82691100	-0.99194400	1.72405200
H	-1.97150800	0.83685200	-1.83361200
H	-1.70547600	2.55767400	-1.56494400
H	0.42061400	1.22745500	-1.56001500
H	0.17104800	2.11101300	-0.04084500
H	-2.34987600	2.34171100	0.81043100
C	-3.03400200	-0.94365800	0.03363000
O	-4.20534300	-1.21432400	0.07744600
O	-2.19308400	-1.59487600	-0.78320600
H	-1.29196000	-1.19616100	-0.71349500
N	-0.11551100	0.01958900	0.04321300
C	1.19755100	-0.43823100	0.29650200
C	2.34445300	0.13313700	-0.07627900
H	1.21380700	-1.38316900	0.83951400
H	2.34830300	1.08896900	-0.59888900
C	3.69636200	-0.48246000	0.16780000
C	4.55237200	0.43153600	1.05141700
C	4.40638100	-0.76125300	-1.16185300
H	3.55080700	-1.43726700	0.69059300
H	4.07613600	0.60244900	2.02107100
H	5.54189200	-0.00495300	1.22230300
H	4.69494500	1.40567400	0.56877500
H	3.81452500	-1.43095000	-1.79207100
H	4.56098000	0.17358300	-1.71383900
H	5.38785800	-1.21692100	-0.99481100

C7-trans-E

C	-1.59788000	1.96161000	1.46336000
C	-0.96678400	0.59762100	1.17148900
C	-0.57284300	1.17477600	-1.17016100
C	-1.13237900	2.58637200	-0.93747900
C	-1.00749100	3.02203600	0.52805600

H	0.11038900	0.63229600	1.38144700
H	-1.38001500	-0.19265300	1.80313800
H	-2.68137600	1.89654500	1.30664100
H	-1.43209600	2.23439900	2.51088200
H	-0.84877800	0.83210200	-2.17422900
H	-0.63074800	3.30061600	-1.60113400
H	-2.19312500	2.57361400	-1.21768200
H	0.04645200	3.18918700	0.78627300
H	-1.51427900	3.98186500	0.66987600
N	-1.14291500	0.20151700	-0.22661400
C	0.95789000	1.15102900	-1.09027600
N	1.37888100	-0.25143500	-1.12265600
H	1.37830700	1.66908900	-1.95533000
H	1.31599100	1.65881200	-0.18851300
S	2.92168000	-0.67244200	-0.82777400
O	3.07454900	-2.08593100	-1.08466400
O	3.78556400	0.34715400	-1.38031600
C	3.06978800	-0.51843600	1.00446100
F	2.13420500	-1.27202800	1.57936700
F	2.87318600	0.74860700	1.37534700
F	4.26388200	-0.91042600	1.41153100
H	0.67606100	-0.90218300	-0.76460900
C	-2.40339200	-0.29783900	-0.59610400
C	-3.43728500	-0.61636500	0.18874600
H	-2.48151200	-0.47347200	-1.66946800
H	-3.40331400	-0.43835300	1.26333200
C	-4.70105000	-1.25064600	-0.32879500
C	-5.91377300	-0.36734000	-0.01539300
C	-4.89160200	-2.65096800	0.26547400
H	-4.61430200	-1.34786700	-1.41973600
H	-5.80443800	0.62477900	-0.46307500
H	-6.83822500	-0.81840100	-0.39104800
H	-6.02117900	-0.23830200	1.06840800
H	-4.04672500	-3.30042800	0.01987600
H	-4.96774100	-2.59410800	1.35787400
H	-5.80954900	-3.11529400	-0.11026600

C8-trans-E

C	0.10337300	2.28915700	-0.98933000
C	-1.28151100	1.68725000	-1.23517800
C	-1.71858800	1.32424300	1.11495500
C	-0.38149600	1.94295100	1.51489600
C	0.18137000	2.87239900	0.43226000

H	0.22042700	3.11620400	-1.70240400
H	-2.52021600	2.08626400	1.11489600
H	-1.99427300	0.55309800	1.83926700
H	-0.52172500	2.50986000	2.44118200
H	0.31938900	1.13985800	1.75587400
H	-0.40352800	3.80144900	0.43811100
H	1.21638400	3.14087000	0.67128400
N	-1.63354300	0.70039200	-0.20448000
H	-1.30905300	1.18747100	-2.21106200
H	-2.03918000	2.49091700	-1.25702900
C	1.22395800	1.30573300	-1.34103800
N	1.21477000	0.08102300	-0.53159300
H	1.13783300	1.01404400	-2.39433700
H	2.19629700	1.78642000	-1.20626400
S	2.36738300	-0.19744300	0.58563600
O	3.16735600	0.99212800	0.81267100
O	1.78232800	-0.96673500	1.66571500
C	3.48274900	-1.34334100	-0.31839900
F	2.85332400	-2.47760800	-0.58559900
F	4.55248000	-1.59369100	0.42050400
F	3.85684600	-0.77055900	-1.45874200
H	0.28695600	-0.24477700	-0.24170100
C	-2.74232700	-0.08717900	-0.57676500
C	-3.81647900	-0.39624800	0.15365700
H	-2.64922500	-0.48847400	-1.58640600
H	-3.94735400	0.00661200	1.15715900
C	-4.90268000	-1.32032500	-0.32879800
C	-6.25679400	-0.60289900	-0.33404900
C	-4.96916000	-2.58143600	0.54027600
H	-4.66453200	-1.62159200	-1.35803700
H	-6.23238600	0.28384100	-0.97388600
H	-7.05105100	-1.26740000	-0.69009200
H	-6.52091600	-0.28008500	0.68007100
H	-4.01658400	-3.11848900	0.52842600
H	-5.19430400	-2.31682800	1.58020200
H	-5.75549300	-3.25834300	0.18961100

Cartesian coordinates of transition states

C1-trans-E-Si

C	-0.49434300	-0.51697100	2.10738900
C	1.32105800	-2.00877500	1.45841600

C	0.43646000	-2.68976300	2.50973300
C	-0.90458600	-1.97795900	2.29956000
N	0.84233700	-0.61771000	1.49196400
H	2.38538600	-2.03598000	1.70679800
H	0.81927300	-2.49475700	3.51819700
H	0.39906900	-3.76748300	2.34641900
H	-1.37739100	-2.34362500	1.38238000
H	-1.60325600	-2.09896200	3.12982600
H	-0.38556800	0.00917100	3.06495900
H	-1.19420700	0.04236000	1.48353400
C	1.12917900	-2.74749400	0.09309200
O	1.73028900	-3.81080600	0.01824900
O	0.32757100	-2.23996700	-0.76327000
H	0.15027500	-0.90937200	-0.92619100
C	1.62178900	0.42342000	1.24269300
C	1.18371900	1.71897500	0.99661600
H	2.67024900	0.18080100	1.06444800
H	0.15185600	1.95986200	1.26208900
C	2.15548200	2.88001300	1.02433700
C	2.41326200	3.30787300	2.47617500
C	1.64943600	4.06925300	0.20363500
H	3.10575400	2.54237500	0.58715400
H	1.48350000	3.65245300	2.94404600
H	2.80042400	2.47525000	3.07189400
H	3.13615800	4.12933600	2.51775900
H	1.67049600	3.85352000	-0.86708700
H	0.62577600	4.33457600	0.49918700
H	2.27908500	4.94742700	0.37612900
C	-3.55317800	1.68313800	-0.38790700
C	-2.18230900	1.59536600	-0.56586600
C	-1.58553500	0.36315500	-0.87310400
C	-2.39441000	-0.77285200	-0.97608900
C	-3.77068300	-0.68632600	-0.79331700
C	-4.35953300	0.54636700	-0.50259300
H	-4.02849800	2.63003900	-0.15484700
H	-1.58345000	2.49500600	-0.45757600
H	-1.92498200	-1.72691600	-1.19962800
H	-4.36859200	-1.58571700	-0.88263700
C	0.65261700	1.19300300	-1.05911400
N	-0.20097200	0.18731100	-1.04625000
C	2.04712500	0.96063900	-1.54938100
O	2.76368400	1.85221300	-1.94191800
O	2.39134000	-0.32173500	-1.47875600
C	3.69809500	-0.66493800	-1.98090000

C	3.84968400	-2.16160200	-1.83251500
H	4.44636200	-0.10292800	-1.41180100
H	3.75731900	-0.33710400	-3.02282800
H	4.80650700	-2.47759500	-2.25764000
H	3.81227900	-2.46612400	-0.78408200
H	3.03806200	-2.68309700	-2.34509900
H	0.29580900	2.20121300	-1.24816700
O	-5.68912700	0.74088300	-0.30946700
C	-6.53577800	-0.38034300	-0.44109900
H	-7.54864000	-0.01535000	-0.27213600
H	-6.46693800	-0.81531700	-1.44540200
H	-6.29703700	-1.15005400	0.30303600

C1-trans-E-Re

C	-2.11201200	-2.44887700	2.13116600
C	-0.72466700	-2.45690700	2.79344700
C	0.08129500	-1.59220000	1.81970600
C	-2.23553300	-1.03781100	1.52152200
N	-0.86337300	-0.51595200	1.52669000
H	1.00798400	-1.18733100	2.23387300
H	-0.76111200	-1.98614400	3.78207600
H	-0.29274600	-3.45441900	2.88396000
H	-2.92213500	-2.65738400	2.83316700
H	-2.14201400	-3.19581000	1.33426900
H	-2.62606100	-1.06530300	0.50124100
H	-2.85890500	-0.36939400	2.12675200
C	0.41346000	-2.46908100	0.56389500
O	1.30306300	-3.29357100	0.73290700
O	-0.30339800	-2.27855100	-0.48030400
C	-0.57950100	0.77715700	1.42045500
C	-1.43244600	1.74465600	0.92317000
H	0.46134200	1.03434400	1.62402800
H	-2.48712100	1.49537000	0.80867400
C	-1.12722600	3.21921500	1.07296500
C	-1.40225900	3.68203500	2.51147300
C	-1.94715400	4.06397400	0.09416700
H	-0.05674600	3.37986500	0.87368700
H	-0.79416100	3.12238000	3.22880200
H	-1.18599900	4.74946600	2.63065000
H	-2.45617100	3.51923200	2.76441300
H	-1.76159500	3.80501700	-0.95131600
H	-3.01757500	3.90853000	0.27080700
H	-1.73212500	5.12814300	0.23214100

C	4.18013800	0.55330700	-0.51959400
C	3.64312500	-0.68808000	-0.86757100
C	2.28247600	-0.80864200	-1.12276800
C	1.44039500	0.30324100	-1.02539100
C	1.98390200	1.54731600	-0.67150700
C	3.33995200	1.67015500	-0.42811700
H	4.26378700	-1.57319500	-0.93317200
H	1.86339800	-1.77637700	-1.38075000
H	1.35094900	2.42386200	-0.57339000
H	3.77728700	2.62286400	-0.14944100
O	5.48711500	0.77750100	-0.24559900
C	6.36503500	-0.32872200	-0.29603900
H	6.39945900	-0.76299000	-1.30216800
H	7.34977700	0.05695100	-0.03318000
H	6.06999200	-1.10193000	0.42292100
C	-0.80721900	1.08507600	-1.27796500
C	-2.22365900	0.78386900	-1.65690800
O	-3.06730100	1.62977100	-1.83055200
O	-2.40966900	-0.52690200	-1.78345000
C	-3.74688200	-0.97492100	-2.05029400
C	-3.67903100	-2.48449900	-2.12462400
H	-4.09386500	-0.51722800	-2.98120400
H	-4.39589600	-0.62252100	-1.24043700
H	-4.68120700	-2.90161500	-2.25238000
H	-3.05608300	-2.79693200	-2.96572400
H	-3.23165300	-2.88826600	-1.21220000
N	0.06348200	0.10735300	-1.25567100
H	-0.48496600	2.10593300	-1.45482900
H	-0.25820500	-0.94248100	-1.02954700

C1-*cis-E-Si*

C	-1.42910700	0.27433800	2.20937500
C	0.85945400	-0.56608900	2.31040200
C	-0.03771800	-1.32249500	3.30669800
C	-1.44832500	-1.15768400	2.73195900
N	-0.05965900	0.41574300	1.71318800
H	1.68382200	-0.03696000	2.80011300
H	0.02829100	-0.85236600	4.29398000
H	0.25891200	-2.36912900	3.40237200
H	-1.57670800	-1.84930700	1.89590000
H	-2.23872000	-1.32320200	3.46787900
H	-1.62024300	0.99557500	3.01757500
H	-2.14794400	0.45643200	1.40307400

C	1.47592300	-1.52246900	1.25699500
O	2.70307200	-1.56343500	1.18929000
O	0.62628300	-2.18119800	0.55146900
C	0.36000700	1.52628000	1.07555300
C	1.61049300	1.71849400	0.55514100
H	-0.42508300	2.26416800	0.91299100
H	2.38265600	0.98541800	0.79193300
C	2.09268100	3.02919000	-0.02126100
C	3.13838500	3.65182100	0.91407800
C	0.97243200	4.02920500	-0.30119200
H	2.60207300	2.80081900	-0.96635300
H	2.68612800	3.89982300	1.88108200
H	3.96326400	2.95608500	1.09322100
H	3.55283600	4.56862400	0.48123400
H	0.20219600	3.61345800	-0.96279300
H	0.48143900	4.34372500	0.62732800
H	1.37440800	4.92509900	-0.78297900
C	-3.30171500	1.25115600	-1.26770900
C	-1.92949600	1.08229300	-1.35101100
C	-1.36357500	-0.17212700	-1.09050700
C	-2.19141800	-1.24057400	-0.74162300
C	-3.56898600	-1.07467500	-0.65957000
C	-4.13242600	0.17699500	-0.92632800
H	-3.76193400	2.21304000	-1.46649900
H	-1.30993700	1.93157200	-1.62037900
H	-1.73622700	-2.20288900	-0.52427900
H	-4.18671700	-1.92239100	-0.38853200
C	0.94010000	0.41937100	-1.47095100
N	0.01622100	-0.43400500	-1.14295200
C	2.35633000	-0.06275900	-1.65709600
O	3.28549700	0.68834700	-1.83406200
O	2.40383600	-1.37976900	-1.64975200
C	3.71120800	-1.98394600	-1.56616200
C	3.47866900	-3.45655800	-1.32302400
H	4.23600500	-1.51559600	-0.73182800
H	4.24451300	-1.77458600	-2.49886700
H	4.43736700	-3.96651300	-1.19370200
H	2.88123900	-3.56504400	-0.41523700
H	2.94959000	-3.91350900	-2.16392000
H	0.70161400	1.38070900	-1.91640600
O	-5.45799600	0.44997700	-0.87977600
C	-6.33484300	-0.60970100	-0.55806600
H	-7.33935300	-0.18869300	-0.58799800
H	-6.25751700	-1.42337100	-1.28887800

H	-6.13310200	-1.00236100	0.44569600
H	0.33721200	-1.35256800	-0.56894400

C1-cis-E-Re

N	-2.54823700	1.15124100	0.96637200
C	-3.96950500	0.90891200	0.72714800
C	-4.25888500	-0.31361300	1.59888400
C	-3.31746500	-0.10555200	2.79027800
C	-2.03762300	0.44707500	2.14002100
C	-1.76709700	1.86093700	0.12708700
C	-0.40310300	1.92727100	0.13784100
C	-0.12474900	-0.06508200	-1.50529500
C	0.39628800	2.91923000	-0.67771000
N	0.56313700	-0.87490400	-0.76435700
C	4.67722100	-0.55892400	-0.01344200
C	3.81187500	-1.02106700	0.98026600
C	2.44826100	-1.12751400	0.72268200
C	1.95237000	-0.76244100	-0.52574000
C	2.81860000	-0.31430500	-1.53151700
C	4.17087300	-0.20799500	-1.27347600
O	6.01557100	-0.42407700	0.13490500
C	6.57476100	-0.78002900	1.38277900
C	-1.05592100	-0.68168200	1.76052700
O	-0.01431800	-0.77471900	2.41914800
O	-1.40138900	-1.40492500	0.76481200
C	-1.54406700	-0.44311600	-1.85879200
O	-1.67665500	-1.76016700	-1.87513800
O	-2.39709500	0.35546200	-2.15711600
C	-3.02409300	-2.26375300	-1.81876700
H	-4.15327500	0.73800400	-0.33754300
H	-4.57097800	1.77157300	1.05076900
H	-5.31096800	-0.38349700	1.88613400
H	-3.96554800	-1.22311500	1.06722300
H	-3.73423200	0.63828400	3.47838500
H	-3.12467600	-1.02163600	3.35342900
H	-1.50010800	1.14288000	2.79407000
H	-2.32415500	2.37954300	-0.64918500
H	1.28036500	2.39532000	-1.07824700
H	-0.08263200	-1.45182000	-0.10263000
H	4.18083500	-1.29491400	1.96115600
H	1.74822900	-1.43520500	1.49714600
H	2.43907000	-0.07965800	-2.52198300
H	4.86708500	0.12714300	-2.03441300

H	6.17283100	-0.15603400	2.18957300
H	6.38913200	-1.83560900	1.61312900
H	7.64711200	-0.61032700	1.29099000
H	0.35976400	0.71598500	-2.08308000
H	0.14253300	1.40336200	0.92327900
H	-3.62397300	-1.55944900	-1.23629600
H	-3.42199100	-2.30207600	-2.83752000
C	-2.95264300	-3.62146800	-1.15669300
H	-3.95626300	-4.04694700	-1.06835300
H	-2.33490200	-4.30720000	-1.74257700
H	-2.51662900	-3.50681800	-0.16126700
C	-0.38099600	3.50065300	-1.85956700
H	-1.18604000	4.15539200	-1.50658100
H	0.27622300	4.10272200	-2.49416000
H	-0.84192000	2.71790300	-2.47391800
C	0.92898000	4.04667800	0.21681200
H	1.51126500	3.64345500	1.05082700
H	1.56907200	4.73223800	-0.35004300
H	0.09306200	4.61826600	0.63472700

C2-trans-E-Si

C	0.51828800	1.15529800	2.28569400
C	0.47186300	-1.29038500	2.35499400
C	-0.73124700	-0.71370500	3.11927600
C	-0.91115900	0.70305400	2.56309900
N	1.19340000	-0.08375700	1.88777100
H	1.13317800	-1.85545300	3.02503000
H	-0.50699500	-0.67655800	4.19043000
H	-1.62057700	-1.32915900	2.97337900
H	-1.47435000	0.66258600	1.62733700
H	-1.42216500	1.37317800	3.25812300
H	1.00898100	1.55542100	3.18494800
H	0.57640700	1.91069200	1.49965300
C	0.09412100	-2.19565800	1.18268600
C	2.42673900	-0.13144600	1.38371700
C	3.11905500	0.92079900	0.82311100
H	2.86116300	-1.13280900	1.33477200
H	2.71382400	1.92445900	0.95653300
C	4.60414200	0.84500700	0.55165100
C	5.38283300	1.10024900	1.85155700
C	5.03452900	1.84714000	-0.52195100
H	4.84553500	-0.16563400	0.19612600
H	5.16606600	2.10301400	2.23782700

H	5.10955400	0.37614200	2.62534400
H	6.46192500	1.03132300	1.67759500
H	4.63529900	1.57820100	-1.50234600
H	4.70029900	2.85932900	-0.25946400
H	6.12515500	1.87253800	-0.60702500
C	-0.40933900	4.15476100	-0.68366600
C	0.41190700	3.04379200	-0.76358400
C	-0.14869800	1.76542700	-0.89799600
C	-1.53481000	1.62267000	-0.95510600
C	-2.36007800	2.73897800	-0.86992000
C	-1.80132600	4.01201200	-0.73257700
H	0.00392700	5.15151700	-0.57439700
H	1.48797400	3.17999000	-0.70107700
H	-1.96447800	0.63497700	-1.09595800
H	-3.43295800	2.59687300	-0.91894700
C	1.91941000	0.58882500	-1.19989600
N	0.63404300	0.59047800	-0.95930200
C	2.62763400	-0.67756900	-1.55919900
O	3.75126000	-0.68816900	-2.00488400
O	1.86470000	-1.74466100	-1.36266500
C	2.40298500	-3.01635000	-1.78424300
C	1.24195300	-3.97454700	-1.92295200
H	3.13054200	-3.33975000	-1.03130100
H	2.93596400	-2.86458500	-2.72603900
H	1.60902500	-4.94065800	-2.28101500
H	0.71915700	-4.12652000	-0.97628600
H	0.51234500	-3.58879500	-2.63949000
H	2.40136200	1.48969200	-1.56521500
O	-2.51443900	5.15941600	-0.63661500
C	-3.92260700	5.05835200	-0.69288100
H	-4.30159200	6.07614400	-0.60596000
H	-4.25166900	4.62539200	-1.64473400
H	-4.31001700	4.45226600	0.13462500
N	-0.66310500	-1.44637100	0.19707000
H	0.11697800	-0.33157200	-0.62659400
H	1.02242700	-2.59276500	0.74055500
H	-0.45705400	-3.05844300	1.57940500
S	-1.79926000	-2.19768000	-0.58850900
O	-2.07423800	-1.49264400	-1.84053000
O	-1.70969600	-3.65705100	-0.57454300
C	-3.32416500	-1.88031900	0.39523300
F	-3.20366200	-2.41497000	1.61919500
F	-4.40090300	-2.39826300	-0.18171100
F	-3.51880400	-0.56276900	0.54509000

C2-trans-E-Re

C	-2.98145600	1.24503000	2.04352800
C	-2.22330300	0.47730900	3.13364600
C	-0.76250900	0.44904400	2.65591800
C	-1.97166100	2.28389500	1.56574400
N	-0.66665900	1.65727000	1.80720500
H	-0.06890100	0.55839300	3.49983600
H	-2.28640100	1.01848600	4.08376900
H	-2.61460600	-0.53225100	3.27406300
H	-3.89515000	1.71090100	2.41918600
H	-3.24856000	0.58347600	1.21606200
H	-2.09053100	2.52725600	0.50887000
H	-2.02203900	3.21699900	2.14387900
C	-0.37622600	-0.82544800	1.88194100
C	0.46850900	2.18459000	1.36454200
C	0.58622700	3.20927500	0.44123400
H	1.37299800	1.67018700	1.70166900
H	-0.31398600	3.75688100	0.16755000
C	1.87587200	3.97965600	0.24748100
C	2.17678700	4.86478200	1.46523700
C	1.80162700	4.84488600	-1.01434100
H	2.70959900	3.26987900	0.14732900
H	2.27860300	4.26521600	2.37519400
H	3.10336700	5.43094100	1.31906200
H	1.36256600	5.58080600	1.62299600
H	1.52812000	4.27467200	-1.90676200
H	1.03324400	5.61620100	-0.88669100
H	2.75514500	5.34899400	-1.19751300
C	4.34230000	-1.66808900	-0.17221500
C	3.12996100	-2.35722100	-0.26187800
C	1.95543600	-1.66053100	-0.51959900
C	1.97052800	-0.27432500	-0.68478600
C	3.18659800	0.41360900	-0.58664500
C	4.35904900	-0.27855300	-0.33758400
H	3.08336300	-3.43237700	-0.13776700
H	1.01368100	-2.19347000	-0.59468100
H	3.22678200	1.49143900	-0.70127800
H	5.30930800	0.23820200	-0.25736300
O	5.54123100	-2.24726700	0.07377200
C	5.56942100	-3.65117200	0.23014400
H	5.21230600	-4.15758400	-0.67426300
H	6.61211100	-3.91342400	0.40658500

H	4.96319600	-3.96724700	1.08720100
C	0.61679100	1.61900700	-1.30713500
C	-0.71783900	2.08889100	-1.80630200
O	-0.84507100	3.08602000	-2.47599300
O	-1.67540800	1.25557700	-1.42836900
C	-3.01427500	1.49880800	-1.91142500
C	-3.21080400	0.78577300	-3.23268900
H	-3.16062700	2.57884200	-1.99552800
H	-3.65528100	1.07402600	-1.13944600
H	-4.23707900	0.92969300	-3.58207600
H	-2.52865200	1.18189000	-3.99037100
H	-3.03376000	-0.28282900	-3.09228800
N	0.73874400	0.36593200	-0.94132600
H	1.47592300	2.14807300	-1.70772100
N	-1.00388800	-0.89979500	0.57847200
H	-0.13970500	-0.16358600	-0.53970900
H	0.71422400	-0.81768600	1.73561900
H	-0.60980500	-1.68613200	2.52225400
S	-2.26626100	-1.80859600	0.37325500
O	-2.84855000	-2.31748800	1.61735100
O	-3.15109100	-1.25663700	-0.65291100
C	-1.60767400	-3.31967600	-0.44108900
F	-1.03913600	-3.00170600	-1.61074700
F	-2.55356400	-4.22259400	-0.66243900
F	-0.66015500	-3.87237200	0.32836900

C2-cis-E-Si

C	-2.07084900	0.05229300	2.17271800
C	0.34180300	0.37364300	2.45463500
C	-0.16227300	-0.78429700	3.33784700
C	-1.45737000	-1.25075300	2.66508100
N	-0.89873400	0.86525100	1.80604700
H	0.74906700	1.19941800	3.05454700
H	-0.37085900	-0.42008800	4.34949400
H	0.58341900	-1.58153600	3.39621400
H	-1.22518500	-1.89521800	1.81299900
H	-2.12342600	-1.78463100	3.34665700
H	-2.62902400	0.55975700	2.97116500
H	-2.72515400	-0.06856600	1.30420100
C	1.43304900	-0.09233000	1.48032400
C	-1.05824400	2.04369800	1.20835500
C	-0.06916000	2.84920000	0.66894900
H	-2.10168100	2.30627600	1.03539600

H	0.96187900	2.62609700	0.94350300
C	-0.31410800	4.28453800	0.24833100
C	0.29676300	5.23923800	1.28290100
C	-1.78818200	4.62127900	0.02711600
H	0.22144800	4.44366700	-0.69667600
H	-0.19573400	5.11965000	2.25449100
H	1.36510200	5.04284700	1.41719600
H	0.18231800	6.28059700	0.96468900
H	-2.26733400	3.94633100	-0.69213400
H	-2.35283500	4.57010300	0.96526700
H	-1.88635200	5.63824400	-0.36234100
C	-4.15402000	0.31249700	-1.25030600
C	-2.86763800	0.82768000	-1.29595100
C	-1.76391600	-0.02074200	-1.13793300
C	-1.97408900	-1.39067000	-0.94643500
C	-3.26447200	-1.90595700	-0.90014500
C	-4.36450000	-1.05567900	-1.05006200
H	-5.01933300	0.95491900	-1.37423200
H	-2.73901900	1.89207900	-1.46392500
H	-1.12210000	-2.05689300	-0.82048300
H	-3.39336600	-2.97122400	-0.74938600
C	-0.06896000	1.68598700	-1.28785300
N	-0.43087800	0.42999900	-1.14285000
C	1.36745600	2.01909400	-1.56758900
O	1.71306100	3.12171300	-1.92383800
O	2.16948800	0.97110800	-1.41565300
C	3.56813900	1.19555300	-1.69749700
C	4.25999500	1.80398600	-0.49436500
H	3.64028000	1.84376300	-2.57330600
H	3.95388700	0.20559900	-1.93292500
H	5.31745500	1.96896700	-0.71961400
H	3.80940900	2.76855900	-0.24285200
H	4.19142900	1.13094300	0.36365700
H	-0.76093800	2.40385000	-1.71788300
O	-5.65900500	-1.45550900	-1.02006800
C	-5.91244300	-2.83668100	-0.86366900
H	-6.99598800	-2.94879700	-0.88848200
H	-5.46567500	-3.41631500	-1.67990800
H	-5.52876100	-3.20612300	0.09465800
N	0.91464300	-1.05264600	0.52956300
H	0.26434400	-0.28203700	-0.66722900
H	1.85208000	0.76767200	0.94374700
H	2.24119800	-0.50612500	2.09817100
S	1.53660900	-2.49289800	0.49179400

O	2.10404200	-2.93740900	1.76513500
O	0.66073700	-3.38438200	-0.26467800
C	3.02323700	-2.32076600	-0.57965400
F	2.67814900	-1.91832800	-1.80543600
F	3.83398800	-1.38157100	-0.05967700
F	3.70793000	-3.45262100	-0.68251600

C2-cis-E-Re

C	-3.23250600	-1.10120200	2.55482500
C	-1.84404700	-0.97347400	3.22061100
C	-0.98907900	-0.04698900	2.32377800
C	-3.13550300	-0.30240900	1.25141300
N	-1.97866800	0.57507100	1.43742200
H	-0.53587800	0.75568700	2.91840100
H	-1.93565200	-0.53771800	4.21866300
H	-1.36853000	-1.95000600	3.31489700
H	-4.00913200	-0.68117700	3.19894400
H	-3.47467300	-2.14361000	2.34803700
H	-2.95834500	-0.94683600	0.38181200
H	-4.01897800	0.31215600	1.05191100
C	0.15659900	-0.77451200	1.56360100
C	-1.89863600	1.77328200	0.87244800
C	-0.76899300	2.56661900	0.71666200
H	-2.83758200	2.10902500	0.42836200
H	0.15055300	2.20501200	1.18232500
C	-0.85197300	4.07536900	0.56903700
C	-0.61025700	4.74637100	1.92725400
C	-2.16137800	4.56627700	-0.04929000
H	-0.03473200	4.39477400	-0.09693600
H	0.34084800	4.42650500	2.36540700
H	-0.58929800	5.83649000	1.82427600
H	-1.41092000	4.48348600	2.62752500
H	-2.36006200	4.09301000	-1.01562500
H	-3.00693300	4.36910400	0.62023500
H	-2.11575600	5.64801400	-0.20510700
C	4.69643200	1.14308700	-0.08568400
C	4.14349100	-0.09162900	-0.43444100
C	2.79508900	-0.17808000	-0.76112200
C	1.97847800	0.95607800	-0.74761700
C	2.53725400	2.18881500	-0.37837400
C	3.88158500	2.27921200	-0.05796600
H	4.74833900	-0.99021500	-0.45827800
H	2.36025800	-1.13608700	-1.03067300

H	1.92499500	3.08470500	-0.32985400
H	4.32797000	3.22571000	0.22798900
O	5.99764100	1.33996700	0.24639000
C	6.85282300	0.21745500	0.22642000
H	6.91005700	-0.22218600	-0.77669700
H	7.83708700	0.58245800	0.51907000
H	6.52167700	-0.54824700	0.93840200
C	-0.18848000	1.80109200	-1.26296700
H	0.21300400	2.78348200	-1.50855800
C	-1.49911900	1.53910300	-1.94948600
O	-2.01416400	2.36310600	-2.66976900
O	-1.96305400	0.31865100	-1.71641200
C	-3.05220000	-0.13097300	-2.55291400
C	-4.38564700	0.44836500	-2.11997700
H	-3.01399400	-1.21509500	-2.44916400
H	-2.82182400	0.15429800	-3.58288800
H	-5.17125400	0.07771500	-2.78511900
H	-4.63647600	0.13866600	-1.10290200
H	-4.37310100	1.53916000	-2.17824500
N	0.62266200	0.78124300	-1.08760200
N	-0.18024000	-1.21336400	0.22086800
S	-0.82029400	-2.63328200	-0.01621700
O	-1.42479200	-3.19218000	1.19464700
O	-1.55614300	-2.66607200	-1.27426500
C	0.62276700	-3.73193800	-0.31961500
F	1.28966700	-3.32816800	-1.40505500
F	0.24912500	-4.99198300	-0.49610600
F	1.45628200	-3.67031700	0.72279300
H	0.99166400	-0.07253200	1.45018500
H	0.51777700	-1.59523500	2.19454200
H	0.15554800	-0.26173100	-0.70528500

C3-trans-E-Si

C	1.46160800	-2.03523600	1.62356000
C	0.11516900	-2.73280300	1.72890700
C	-0.66846600	-1.80696100	2.67213900
C	-0.25083000	-0.40260700	2.21114600
N	1.07859100	-0.61515800	1.61977600
H	-0.17383300	0.32372700	3.02891500
H	-0.95074600	-0.00306100	1.46975200
H	-0.36866600	-1.96758300	3.71312900
H	-1.74211100	-1.97521100	2.57764300
H	1.96515600	-2.27713400	0.68742300

H	2.10928300	-2.25112600	2.48468100
H	0.19856800	-3.74403800	2.13629700
C	-0.61553800	-2.81269900	0.35753500
O	-1.78396700	-3.19571500	0.38324300
O	0.05043600	-2.44218800	-0.67571900
H	0.11625300	-1.01545300	-0.95576300
C	1.91787000	0.35883100	1.26714800
C	1.59042200	1.66725100	0.99682400
H	2.94141200	0.02740900	1.08097900
H	0.57883400	2.00668800	1.22900000
C	2.64997500	2.73423400	0.85338200
C	2.99602300	3.31808200	2.23155600
C	2.21870500	3.85434600	-0.09838500
H	3.55377900	2.26571800	0.43857100
H	3.33464100	2.53546100	2.91710600
H	3.78452600	4.07383100	2.14892500
H	2.11520100	3.79590100	2.67624200
H	2.19669400	3.51206000	-1.13609500
H	1.22680500	4.23640000	0.17691500
H	2.91914000	4.69362300	-0.04654800
C	-3.14048600	2.06897600	-0.40763500
C	-1.80355000	1.76979600	-0.59522600
C	-1.41624200	0.45730300	-0.90503100
C	-2.38269100	-0.54450400	-1.00755100
C	-3.72517800	-0.24362400	-0.80713100
C	-4.11230200	1.06467900	-0.51153600
H	-3.46200300	3.07514300	-0.16171300
H	-1.06701700	2.55915000	-0.47821700
H	-2.08316600	-1.56901100	-1.20996100
H	-4.44978500	-1.04569900	-0.87660200
C	0.90956700	0.93857700	-1.20190700
N	-0.06370600	0.08121400	-1.07716600
C	2.27658100	0.48297000	-1.58342800
O	3.12641100	1.23618400	-1.99743200
O	2.41770500	-0.82936800	-1.42810200
C	3.64829600	-1.40318500	-1.90325600
C	3.58605000	-2.88510600	-1.60186900
H	4.48604100	-0.90110000	-1.40946600
H	3.72273600	-1.20107800	-2.97602200
H	4.40204700	-3.40434200	-2.11125900
H	3.67934700	-3.07057200	-0.52883000
H	2.62881400	-3.29267000	-1.93631100
O	-5.38989900	1.45842700	-0.29540600
C	-6.39398200	0.46544500	-0.34560400

H	-7.33275300	0.97568300	-0.13166500
H	-6.44712600	0.00414000	-1.33873200
H	-6.21956800	-0.31293600	0.40622600
H	0.70181600	1.98237000	-1.40738400

C3-trans-E-Re

C	0.57034700	-0.84916700	2.31230200
C	0.09026000	-2.30223500	2.16499000
C	-1.41715000	-2.17884800	2.41788700
C	-1.80238800	-0.84463800	1.77105200
N	-0.55654300	-0.07199700	1.78426800
H	-2.57800100	-0.29834100	2.32091900
H	-2.12642200	-0.99645700	0.73815600
H	-1.62139600	-2.14736800	3.49370500
H	-1.97411000	-3.00869000	1.97890200
H	1.47817400	-0.64029800	1.73408400
H	0.75003500	-0.58766300	3.36371900
H	0.59602100	-2.94835900	2.88495300
C	0.43722000	-2.78805000	0.73714600
O	1.52332500	-3.34530800	0.58434400
O	-0.41552800	-2.48457500	-0.17317500
H	-0.32510300	-1.13240500	-0.83513500
C	-0.50300900	1.21487000	1.44719700
C	-1.51185200	1.91001500	0.81313100
H	0.47079600	1.68444800	1.58950300
H	-2.51973200	1.49958800	0.82320400
C	-1.40966300	3.40650900	0.60749000
C	-1.68873100	4.14579400	1.92515400
C	-2.37162700	3.90634700	-0.47332800
H	-0.37939800	3.65053400	0.30450900
H	-0.98769200	3.83889600	2.70734400
H	-1.60825900	5.23025600	1.79203500
H	-2.70269200	3.92094500	2.27462200
H	-2.19243100	3.44884900	-1.44923500
H	-3.40468200	3.66502700	-0.20021400
H	-2.29131500	4.99261900	-0.58070000
C	3.10461700	1.76422500	-0.68757600
C	1.74953600	1.52739500	-0.83942800
C	1.28058600	0.21366400	-0.98966100
C	2.18731900	-0.84997200	-0.98459500
C	3.54627100	-0.61075300	-0.82255000
C	4.01285100	0.69841400	-0.67460000
H	3.48999000	2.77088900	-0.56719500

H	1.06361600	2.36861700	-0.82897200
H	1.82922000	-1.87239700	-1.07400100
H	4.22032600	-1.45829800	-0.80379500
C	-1.02568100	0.80219900	-1.25962000
N	-0.08677400	-0.09635700	-1.10709000
C	-2.43139600	0.33935400	-1.51189700
O	-3.38019200	1.07962800	-1.60475300
O	-2.46934400	-0.98275200	-1.62074000
C	-3.76174900	-1.60920300	-1.64851700
C	-3.50479100	-3.09956100	-1.60230800
H	-4.28958800	-1.28968500	-2.55188300
H	-4.33023400	-1.25465900	-0.78158700
H	-4.45012100	-3.64170600	-1.51538100
H	-2.99271700	-3.42685700	-2.51020900
H	-2.85827800	-3.33723800	-0.75310000
O	5.31276900	1.03675100	-0.50569700
C	6.26261400	-0.00960500	-0.48483500
H	7.23203700	0.46684000	-0.34217200
H	6.07010400	-0.70381800	0.34138700
H	6.26278300	-0.56367600	-1.43074600
H	-0.77745400	1.79840900	-1.60739000

C3-cis-E-Si

C	1.18118100	-1.18022100	1.75291300
C	0.18654300	-2.31405600	1.96025300
C	-0.84874800	-1.69037800	2.90215600
C	-1.01008200	-0.28174900	2.32332500
N	0.31565600	0.00910100	1.75032600
H	-1.27530900	0.47521300	3.06748300
H	-1.76261400	-0.27298400	1.52336300
H	-0.46776000	-1.63925900	3.92782200
H	-1.78126600	-2.25368800	2.88121200
H	1.71264100	-1.28220600	0.80581500
H	1.90774700	-1.09370900	2.57381100
H	0.66624200	-3.19655400	2.39503800
C	-0.48922600	-2.74116300	0.62097800
O	-1.62096200	-3.21352100	0.68999700
O	0.19878700	-2.55215000	-0.44793800
H	0.28715100	-1.20974500	-0.89665300
C	0.73012600	1.22873000	1.41177600
C	1.93259100	1.50023600	0.79130200
H	-0.01358100	2.01257100	1.54708500
H	2.69188700	0.72048400	0.83448100

C	2.46535600	2.88716800	0.51292300
C	3.64203100	3.19508000	1.44849700
C	1.40885400	3.98565600	0.61535100
H	2.86240700	2.88337600	-0.51329500
H	4.42623200	2.43758600	1.35448200
H	4.08259000	4.16948800	1.21322800
H	3.30750500	3.21077800	2.49180500
H	0.55742200	3.80803900	-0.05128200
H	1.02575100	4.07014600	1.63893500
H	1.84201300	4.95249700	0.34381200
C	-2.96899000	1.92531900	-0.72733000
C	-1.62647300	1.60879900	-0.84943400
C	-1.22893400	0.27655200	-1.03002900
C	-2.20074700	-0.72731300	-1.08654700
C	-3.54793800	-0.40896200	-0.95816200
C	-3.94052900	0.91967300	-0.77918800
H	-3.29375100	2.95061600	-0.58602300
H	-0.89378700	2.40683900	-0.79661600
H	-1.89842500	-1.76441600	-1.20071400
H	-4.27389300	-1.21222600	-0.99295300
C	1.11079600	0.73536600	-1.26289000
N	0.12359400	-0.11271800	-1.12578600
C	2.47855400	0.23724800	-1.59973200
O	3.34093600	0.94261400	-2.06593300
O	2.60200300	-1.05613400	-1.32453000
C	3.84937200	-1.68788600	-1.65315800
C	3.72515700	-3.12581700	-1.19927100
H	4.65872900	-1.15015400	-1.14977700
H	4.00550500	-1.59986500	-2.73253700
H	4.61574400	-3.68996300	-1.48813200
H	3.61372200	-3.17644800	-0.11298300
H	2.84101200	-3.58523800	-1.64657000
O	-5.22500600	1.33068100	-0.64109100
C	-6.23091900	0.33965700	-0.67381100
H	-7.17647900	0.86470700	-0.54080500
H	-6.23794800	-0.18727600	-1.63536400
H	-6.09900300	-0.38788500	0.13563700
H	0.92086500	1.76104500	-1.56564600

C3-cis-E-Re

C	-0.55675400	-0.68759300	2.08865600
C	-1.23043700	-2.05827000	2.03069800
C	-2.58011800	-1.77353300	2.69249500

C	-2.96945900	-0.42977500	2.06997400
N	-1.67520300	0.21169400	1.77625400
H	-3.56599900	0.20178100	2.73615300
H	-3.51590800	-0.58620500	1.13443300
H	-2.46895400	-1.67731300	3.77778400
H	-3.30989500	-2.54933200	2.46317800
H	0.25693200	-0.58932900	1.37153200
H	-0.17079300	-0.46666500	3.09359300
H	-0.64025500	-2.81353600	2.55938100
C	-1.42107300	-2.52535900	0.55847200
O	-2.51809900	-2.96383200	0.22588300
O	-0.37870100	-2.42182200	-0.18969700
H	-0.06567200	-1.21445800	-0.72716500
C	-1.59322000	1.39806800	1.17139800
C	-0.46085800	2.03244100	0.70831600
H	-2.56556000	1.85793700	0.99242100
H	0.50401900	1.62516700	1.01316700
C	-0.44187700	3.48719200	0.28657800
C	0.15131900	4.35626800	1.40315700
C	-1.80540900	4.02334000	-0.14988000
H	0.23384600	3.57931900	-0.58023100
H	1.14108600	3.99690600	1.70345900
H	0.24968500	5.39763400	1.07800100
H	-0.49764700	4.33122400	2.28531500
H	-2.25013200	3.40858000	-0.93895400
H	-2.49952900	4.06425800	0.69768300
H	-1.70129300	5.04251900	-0.53310200
C	3.90605800	1.00082400	-0.45865400
C	2.54931200	1.03144200	-0.72453700
C	1.81355200	-0.16324400	-0.76805800
C	2.46091000	-1.37497200	-0.51297100
C	3.82555600	-1.40592600	-0.24662000
C	4.55674700	-0.21620000	-0.22192300
H	4.49176100	1.91294600	-0.42213200
H	2.07042100	1.99202800	-0.88987700
H	1.87601300	-2.28957700	-0.51818500
H	4.30256600	-2.36037000	-0.05882300
C	-0.28251100	0.85091900	-1.29136700
N	0.42888800	-0.21093300	-1.02799500
C	-1.71162300	0.67420100	-1.71012200
O	-2.24135700	1.42704100	-2.49257800
O	-2.25421000	-0.39598400	-1.14884600
C	-3.46890600	-0.92428600	-1.73041400
C	-3.08772800	-1.92398700	-2.80173400

H	-4.06455900	-0.09098000	-2.10938800
H	-3.97019100	-1.42242300	-0.90169400
H	-3.98626400	-2.39672200	-3.20858900
H	-2.55597200	-1.43023400	-3.62114500
H	-2.45240400	-2.68865800	-2.34807300
O	5.88553100	-0.13241200	0.02855100
C	6.58249100	-1.33638200	0.27094000
H	7.62011000	-1.05413200	0.44728400
H	6.18929600	-1.85160300	1.15551800
H	6.52831000	-2.00805300	-0.59402800
H	0.18007100	1.75903300	-1.66824400

C4-trans-E-Si

C	1.07914900	-1.20989400	2.50439200
C	-0.35081000	-0.86088700	2.95740100
C	-0.46168600	0.68140900	2.84172000
C	0.93689700	1.19204800	2.48494200
N	1.59477000	0.02346100	1.90479900
H	1.49783900	1.51790400	3.37252800
H	0.91033700	2.02210200	1.77443500
H	-0.82769300	1.14052800	3.76271300
H	-1.16087300	0.93344500	2.03928100
H	1.07822000	-2.00172000	1.74859900
H	1.71042400	-1.50787700	3.35189900
H	-0.49237100	-1.17439500	3.99651400
C	-1.39740800	-1.57490000	2.09721500
C	2.70868600	0.04873600	1.16821200
C	3.17863000	1.09836400	0.41351600
H	3.19475100	-0.92070100	1.05826100
H	2.76086000	2.09229100	0.57509000
C	4.53477600	1.04668100	-0.25098000
C	5.61248600	1.55071500	0.72036900
C	4.56777200	1.86210600	-1.54735300
H	4.75567000	-0.00116500	-0.49976500
H	5.61872700	0.96271500	1.64306900
H	6.60605200	1.49172100	0.26378800
H	5.42551800	2.59710200	0.98873900
H	3.97762000	1.38720400	-2.33519800
H	4.18810700	2.87775000	-1.37400800
H	5.59380300	1.95402900	-1.91631500
C	-0.57585600	4.26470900	-0.59913100
C	0.19372200	3.11508200	-0.63863500
C	-0.41947700	1.85967300	-0.54179500

C	-1.80468500	1.77227000	-0.40089800
C	-2.57710100	2.92835000	-0.35854800
C	-1.96619500	4.18097400	-0.45894800
H	-0.12312300	5.24742100	-0.67305300
H	1.27189700	3.20037300	-0.74023300
H	-2.26741400	0.79162000	-0.33410000
H	-3.65182700	2.83552900	-0.25846100
C	1.48945000	0.55062700	-1.16546200
N	0.31827400	0.65282800	-0.59693400
C	2.07231800	-0.78698900	-1.49163900
O	2.91237400	-0.91505300	-2.35145400
O	1.56229900	-1.75560300	-0.74590000
C	1.90864100	-3.11127000	-1.11405500
C	3.22569800	-3.50459100	-0.47359000
H	1.95687000	-3.16372000	-2.20331000
H	1.06728100	-3.70499100	-0.75416900
H	3.47028900	-4.53857900	-0.73262500
H	4.03597200	-2.86053300	-0.82791900
H	3.16074100	-3.43847400	0.61755900
O	-2.62507300	5.36327400	-0.42953500
C	-4.03179700	5.32616800	-0.30245900
H	-4.36115200	6.36470100	-0.30097000
H	-4.49260100	4.79726000	-1.14491200
H	-4.33257400	4.84587900	0.63622300
H	1.85391000	1.36928100	-1.77627500
H	-1.30522200	-2.65888200	2.25011900
H	-2.39597500	-1.27995700	2.45281500
N	-1.21931600	-1.21424500	0.69359600
S	-1.51607400	-2.32395100	-0.37805400
O	-1.13088800	-1.83423400	-1.70209000
O	-1.14072700	-3.69008800	0.00715500
C	-3.35219900	-2.41399600	-0.46980000
F	-3.84963600	-2.73642900	0.72988900
F	-3.76162300	-3.31480800	-1.35505200
F	-3.85626600	-1.22443500	-0.81549300
H	-0.16520900	-0.18658400	-0.12803600

C4-trans-E-Re

C	-0.77852100	0.67354300	2.54880200
C	0.68230200	0.35668700	2.89559700
C	0.67161600	-1.16623800	3.10912200
C	-0.37077500	-1.68645500	2.11431700
N	-1.24689500	-0.53329500	1.86652500

H	-0.97176700	-2.51513400	2.51005000
H	0.09756500	-1.99992300	1.18260700
H	0.37490300	-1.40388200	4.13541600
H	1.65646100	-1.60249400	2.91628200
H	-0.88157600	1.54816900	1.89444900
H	-1.36823600	0.85028700	3.45914600
H	0.95782000	0.88200200	3.81655600
C	1.69564100	0.77855500	1.82345600
C	-2.43371000	-0.63404000	1.25721300
C	-2.85047300	-1.68120700	0.47400300
H	-3.05265600	0.26147000	1.32394800
H	-2.28204300	-2.61078000	0.50008700
C	-4.26762800	-1.76336900	-0.04778400
C	-5.21832300	-2.28355000	1.04032300
C	-4.35849500	-2.65736600	-1.28720000
H	-4.59795300	-0.74839000	-0.32123300
H	-5.20297500	-1.63493500	1.92144200
H	-6.24717700	-2.34253700	0.66866200
H	-4.91433600	-3.28770200	1.35698000
H	-3.74503100	-2.29791000	-2.11773000
H	-4.01422000	-3.67020000	-1.04548000
H	-5.39350700	-2.73165900	-1.63469700
C	-2.72640300	3.19810200	-0.63589000
C	-2.38997100	1.86247800	-0.77194100
C	-1.04312900	1.47367700	-0.78277200
C	-0.04730900	2.44608800	-0.66574900
C	-0.38401400	3.78851800	-0.52952100
C	-1.72822700	4.17153500	-0.51047000
H	-3.76255700	3.51847000	-0.62478800
H	-3.18076600	1.12454500	-0.86312600
H	0.99366100	2.14080200	-0.70212900
H	0.40878900	4.52241300	-0.44871200
C	-1.43169400	-0.80038000	-1.35340600
N	-0.64083000	0.12270800	-0.88893900
C	-0.90891400	-2.15765500	-1.72014300
O	-1.28452100	-2.70354700	-2.72905200
O	-0.02044300	-2.62502100	-0.86299900
C	0.72253200	-3.79810700	-1.26415300
C	1.47943100	-4.28242200	-0.04878700
H	1.39665900	-3.49283300	-2.06685900
H	0.01283700	-4.53809100	-1.64318800
H	0.78927900	-4.54194600	0.76032100
H	2.05214900	-5.17672900	-0.30944800
H	2.17773300	-3.51698900	0.30039200

O	-2.16156500	5.44678400	-0.37969200
C	-1.18561000	6.46560900	-0.29836200
H	-1.73505600	7.40324600	-0.22162800
H	-0.55299300	6.33993800	0.58840000
H	-0.55565700	6.48271000	-1.19519100
H	-2.32890700	-0.51169900	-1.89332300
N	1.54971600	0.06632200	0.55287300
H	1.59396200	1.86182800	1.65169100
H	2.69361600	0.61351700	2.24660000
S	2.81588700	-0.67745100	-0.01829400
O	3.63226000	-1.35755500	0.98817500
O	2.45465200	-1.38508800	-1.24448400
C	3.92516200	0.66592000	-0.61935000
F	3.28717200	1.41467900	-1.52664500
F	5.02751900	0.18078400	-1.17467100
F	4.27093300	1.46654300	0.39585600
H	0.33924100	-0.05865600	-0.35628800

C4-cis-E-Si

C	0.98002900	-0.83044900	2.21732700
C	-0.38933400	-0.50601300	2.84621900
C	-0.52287400	1.03034800	2.76076300
C	0.90235400	1.55599400	2.60054100
N	1.57361800	0.46884000	1.88745000
H	1.38734700	1.72486800	3.57156000
H	0.96174900	2.47539800	2.00829600
H	-1.01773800	1.45332500	3.63804500
H	-1.10910500	1.28720600	1.87482000
H	0.86304100	-1.42981200	1.31156300
H	1.64493000	-1.36715100	2.90761500
H	-0.39111500	-0.82019600	3.89544000
C	-1.52733800	-1.23210100	2.12036200
C	2.68704900	0.61407000	1.17270100
C	3.25726000	-0.38807500	0.41211400
H	3.05191400	1.63738000	1.10501400
H	2.96847500	-1.41052100	0.65304600
C	4.56870500	-0.26315300	-0.33071600
C	5.66224500	-1.05248400	0.40154800
C	5.01746900	1.17925200	-0.55766400
H	4.42747500	-0.73772000	-1.31287300
H	5.36547700	-2.09622500	0.54541600
H	6.59659600	-1.04189900	-0.16868900
H	5.85482000	-0.61502800	1.38754700

H	4.27227200	1.76603300	-1.10728100
H	5.22020400	1.68638200	0.39288600
H	5.94089600	1.19747800	-1.14303100
C	0.81454300	4.05866000	-0.84473500
C	1.17601500	2.72070000	-0.85978500
C	0.19771100	1.72796300	-0.72682400
C	-1.14329100	2.09369600	-0.59108500
C	-1.50459500	3.43568700	-0.57369000
C	-0.52649300	4.42718100	-0.69965900
H	1.55744000	4.84178600	-0.95051200
H	2.22189500	2.45751200	-0.97623900
H	-1.89669200	1.31596500	-0.50128800
H	-2.55253200	3.69157100	-0.47405500
C	1.62785900	-0.15132700	-1.19190500
N	0.50613900	0.35090300	-0.73250900
C	1.73587700	-1.61419500	-1.49660900
O	2.52276100	-2.02876900	-2.31429700
O	0.89841500	-2.34273000	-0.77457600
C	0.84183900	-3.75941700	-1.06345500
C	1.96159200	-4.47604500	-0.33423500
H	0.91507900	-3.88659300	-2.14523800
H	-0.14929800	-4.05559000	-0.71915100
H	2.93634800	-4.13257000	-0.69229500
H	1.88937000	-4.30041100	0.74356200
H	1.88997900	-5.55318800	-0.50906700
O	-0.77664600	5.75901100	-0.69637100
C	-2.12221900	6.17098200	-0.57258200
H	-2.10663700	7.26020200	-0.59669000
H	-2.73063900	5.79584300	-1.40390300
H	-2.55573100	5.83268600	0.37602700
H	2.27572800	0.47249600	-1.80028100
N	-1.50539000	-0.86295100	0.70857500
S	-2.20154200	-1.83674800	-0.30893600
O	-1.80517800	-1.47012900	-1.66892900
O	-2.20804500	-3.25400500	0.07085600
C	-3.98262000	-1.37808400	-0.25246500
F	-4.45439600	-1.52936700	0.99055000
F	-4.71151000	-2.12184300	-1.07683700
F	-4.13692700	-0.09498300	-0.59703400
H	-1.41133400	-2.31665900	2.25557400
H	-2.47673600	-0.94681600	2.59741900
H	-0.23503700	-0.26574700	-0.26544500

C4-cis-E-Re

C	-0.63112300	0.64881000	2.38833500
C	0.24856600	-0.51126700	2.87202700
C	-0.75934300	-1.65226900	3.10437900
C	-1.84477800	-1.43972000	2.04346700
N	-1.75455200	-0.00831900	1.71819100
H	-2.84946400	-1.67339100	2.41477000
H	-1.64464600	-2.02337500	1.14024000
H	-1.19155500	-1.57319400	4.10670500
H	-0.28650300	-2.63256300	3.00060100
H	-0.09226800	1.32005800	1.71224400
H	-1.01456500	1.25131700	3.22439700
H	0.74818800	-0.23250200	3.80613200
C	1.33521200	-0.88985500	1.85774600
C	-2.68181300	0.62095300	0.99441100
C	-2.59319300	1.89391500	0.47916200
H	-3.53484100	-0.00345700	0.73025800
H	-1.76845700	2.51573800	0.82534400
C	-3.73837100	2.62952100	-0.18588800
C	-3.98495500	3.95783100	0.54014100
C	-5.03056300	1.81651400	-0.26051000
H	-3.45087300	2.86765800	-1.22279100
H	-3.07607000	4.56835400	0.57664000
H	-4.76300100	4.53931800	0.03544400
H	-4.30760500	3.77378900	1.57069500
H	-4.89999400	0.90498800	-0.85012300
H	-5.37747200	1.54583800	0.74378100
H	-5.81542300	2.40801700	-0.74067700
C	1.76721300	3.94786800	-0.32085600
C	0.71741500	3.06472500	-0.50285400
C	0.96872000	1.69297500	-0.64833700
C	2.28420700	1.22958400	-0.60391000
C	3.34045700	2.11478800	-0.41904900
C	3.08629900	3.48150800	-0.27592100
H	1.59235600	5.01165400	-0.20321400
H	-0.29756000	3.44921400	-0.52415000
H	2.47698300	0.16888800	-0.72703000
H	4.35139200	1.72653500	-0.39486700
C	-1.23571700	1.07419100	-1.29445900
N	-0.06261600	0.73968100	-0.83592600
C	-2.21994400	0.03710800	-1.73087300
O	-3.12682300	0.30514400	-2.48523700
O	-1.94300900	-1.15299900	-1.22308500

C	-2.74589500	-2.26129400	-1.68578500
C	-4.06913000	-2.32068200	-0.94681600
H	-2.11621400	-3.12701200	-1.48992100
H	-2.89976400	-2.14256300	-2.76087500
H	-4.63508700	-3.19501500	-1.28080000
H	-3.90822300	-2.41643800	0.13115500
H	-4.67059200	-1.42968600	-1.14744600
O	4.03845400	4.42485300	-0.08887000
C	5.38403300	3.99648600	-0.03841100
H	5.98008700	4.89496900	0.11696300
H	5.54772800	3.30075900	0.79280300
H	5.68306100	3.51722400	-0.97781700
H	-1.38184800	2.04762800	-1.75472700
N	0.77581000	-1.30809900	0.57147200
H	1.98983200	-0.02020100	1.70291900
H	1.94741700	-1.68517600	2.29743800
S	1.00121200	-2.80681500	0.13810500
O	1.27227300	-3.71433900	1.25329900
O	0.04048400	-3.20010700	-0.88756000
C	2.60013300	-2.77141900	-0.77225800
F	2.99824300	-3.97975200	-1.14558100
F	2.49253500	-2.00186200	-1.86172800
F	3.54458200	-2.22939700	0.00925800
H	0.18125200	-0.27412700	-0.36829300

C5-trans-E-Si

C	-0.08957300	-1.85772500	2.92358000
C	-0.26615100	-0.96339600	1.69446000
C	1.87973100	-1.76102500	0.77421700
C	2.08601400	-2.68227000	1.97754900
C	0.74013000	-3.09497500	2.57228800
H	-0.82203600	-1.49905600	0.91771000
H	-0.81248200	-0.04903400	1.93176400
H	0.40995200	-1.28515900	3.71583200
H	-1.08025300	-2.14014200	3.29546200
H	2.84367500	-1.36298000	0.43713700
H	2.64547300	-3.55389700	1.63406000
H	2.68132000	-2.15531200	2.73509000
H	0.20141200	-3.70562500	1.83614700
H	0.89036200	-3.71744600	3.46008700
N	1.04797000	-0.61098000	1.14497500
C	1.30127300	-2.55772400	-0.45087000
O	1.80112900	-3.66096900	-0.62700400

O	0.39968300	-1.99713900	-1.16368900
H	0.12636100	-0.68211100	-1.15600400
C	1.55285500	0.61974000	1.12350900
C	0.87081000	1.82664400	1.07114000
H	2.63048000	0.65457700	0.95123100
H	-0.18931900	1.84647800	1.32784300
C	1.62033900	3.12476700	1.28197700
C	1.75129100	3.41444400	2.78420500
C	0.94433800	4.30064200	0.57172100
H	2.62771800	3.00794900	0.85939500
H	2.25664400	2.59403400	3.30299500
H	2.31879200	4.33515300	2.95576900
H	0.76099000	3.53975800	3.23743000
H	1.04240100	4.21873500	-0.51363300
H	-0.12021800	4.35453300	0.83577600
H	1.40530400	5.24580700	0.87440700
C	-4.49103900	0.27007100	-0.41835400
C	-3.80538600	-0.84981800	-0.89308000
C	-2.43503800	-0.77818900	-1.12266700
C	-1.72908000	0.40441100	-0.88362800
C	-2.42333500	1.52247900	-0.39665600
C	-3.78787400	1.45374000	-0.17188600
H	-4.32216100	-1.78099000	-1.09263800
H	-1.89095200	-1.64436000	-1.48955800
H	-1.90754100	2.45459000	-0.18633100
H	-4.33827900	2.31106800	0.20100500
O	-5.82342000	0.31109500	-0.16316800
C	-6.56866500	-0.86299500	-0.40246700
H	-6.21824500	-1.69224800	0.22402600
H	-7.60012400	-0.62420700	-0.14436100
H	-6.51644900	-1.15981300	-1.45693000
C	0.39926900	1.47507400	-1.05586700
C	1.81347400	1.43260700	-1.54143300
O	2.48227400	2.42346200	-1.72307200
O	2.23354200	0.18082700	-1.71346300
C	3.58442100	0.00221900	-2.17691400
C	3.72515700	-1.44312400	-2.60318400
H	4.26476300	0.26831900	-1.35882300
H	3.76276600	0.70071700	-2.99859800
H	4.73202500	-1.61206200	-2.99516700
H	3.55037500	-2.13651200	-1.77623100
H	2.99880500	-1.67605700	-3.38547800
N	-0.34209500	0.39030900	-1.12723700
H	-0.05610500	2.45820500	-1.12626100

C5-trans-E-Re

C	-2.63192700	-2.07394400	2.16649500
C	-2.27352100	-1.17985900	0.97576400
C	0.10350200	-1.72462000	1.24256900
C	-0.18991400	-2.62444100	2.44426000
C	-1.60497700	-3.19576400	2.33808100
H	-2.28937700	-1.74253300	0.03739300
H	-2.96667900	-0.34250900	0.88989700
H	-2.66639500	-1.45542100	3.07287200
H	-3.63596000	-2.48285500	2.00959000
H	1.07843100	-1.23394400	1.35223100
H	0.54857100	-3.42781500	2.44889900
H	-0.08602800	-2.03984000	3.36807300
H	-1.64018800	-3.86856500	1.47258200
H	-1.84411700	-3.79291300	3.22378000
N	-0.90945600	-0.66708600	1.15057900
C	0.17229200	-2.57443500	-0.08816900
O	0.66481300	-3.68857200	0.03108100
O	-0.26856200	-2.02420700	-1.15490900
H	-0.16143000	-0.59690400	-1.30987500
C	-0.62724400	0.61325300	1.36070300
C	-1.39113800	1.71765400	1.01031900
H	0.40590300	0.79175200	1.66655900
H	-2.45191400	1.58791600	0.80470000
C	-1.01453300	3.10479000	1.48755700
C	-1.33925800	3.27341000	2.97862200
C	-1.73782900	4.18172200	0.67430000
H	0.07138400	3.23748900	1.36865700
H	-0.79636500	2.54324000	3.58688700
H	-1.07603400	4.27841700	3.32617300
H	-2.41127400	3.12520300	3.15118900
H	-1.55070200	4.10056500	-0.39961000
H	-2.82137400	4.08973200	0.81300500
H	-1.43905500	5.18026700	1.00738000
C	4.30240700	0.56457800	-0.34635600
C	3.73517900	-0.54380900	-0.98027700
C	2.38136600	-0.54607100	-1.29554400
C	1.57340900	0.55168100	-0.98056400
C	2.14818500	1.65887700	-0.33966000
C	3.49811000	1.66575700	-0.03235900
H	4.33117100	-1.41219400	-1.23333600
H	1.93438700	-1.40700400	-1.78292300

H	1.54416900	2.51907300	-0.06909500
H	3.95681200	2.51355500	0.46502600
O	5.60685900	0.66534000	0.00758200
C	6.44381300	-0.43900600	-0.26622800
H	6.49669200	-0.64062200	-1.34269500
H	7.43276400	-0.16535000	0.10048100
H	6.09658600	-1.33929800	0.25450500
C	-0.63097300	1.47662500	-1.14795800
C	-2.03319600	1.31393800	-1.64416100
O	-2.79830700	2.23208700	-1.81592800
O	-2.30147300	0.02903000	-1.85576000
C	-3.61389600	-0.31938900	-2.31954300
C	-3.50607100	-1.70436000	-2.92111000
H	-3.94672800	0.43221100	-3.03972300
H	-4.29359900	-0.29166500	-1.45960100
H	-4.49650300	-2.06747500	-3.20810900
H	-2.86800000	-1.68381000	-3.80756200
H	-3.05822600	-2.40017600	-2.20706700
N	0.20247900	0.46801500	-1.29558100
H	-0.25743100	2.49602400	-1.14225300

C5-cis-E-Si

C	-0.66464300	-2.20349600	2.78722100
C	-0.92276000	-1.36214500	1.53746800
C	1.44258500	-1.46059900	0.88397500
C	1.77086400	-2.26761600	2.14490300
C	0.56311400	-3.09581300	2.58699600
H	-1.16049500	-1.99946700	0.67725100
H	-1.74879100	-0.65600600	1.66730300
H	-0.50372400	-1.52803900	3.63832200
H	-1.55514400	-2.80160200	3.00732600
H	2.28404000	-0.81665700	0.62263300
H	2.61455600	-2.91868800	1.91142800
H	2.06785000	-1.57348100	2.94265200
H	0.36036300	-3.84430000	1.81183900
H	0.79078300	-3.63702800	3.51088200
N	0.27872800	-0.60438400	1.17674400
C	1.23631400	-2.39507500	-0.36341600
O	1.87051900	-3.44343000	-0.34316200
O	0.47273600	-1.96521800	-1.29014500
H	0.26978000	-0.59011400	-1.40232400
C	0.34510200	0.70357400	1.40145800
C	1.35863700	1.55258100	0.96620500

H	-0.57779100	1.13443700	1.78735800
H	2.32666500	1.09606200	0.77250200
C	1.46436700	3.01217400	1.36100900
C	2.61620900	3.20271200	2.35580100
C	0.17494400	3.59744900	1.93410200
H	1.72979700	3.57126500	0.45103800
H	3.55939500	2.83465300	1.94050400
H	2.74580500	4.26151800	2.60216800
H	2.41521500	2.65598400	3.28397900
H	-0.67954400	3.46748000	1.26218400
H	-0.07537200	3.12394900	2.89070800
H	0.29535600	4.66883700	2.11640200
C	-4.27025100	0.44180300	-0.62974900
C	-3.62152500	-0.66664700	-1.18139800
C	-2.25387500	-0.62158700	-1.42544200
C	-1.50680700	0.52344500	-1.12250200
C	-2.16752200	1.63357600	-0.57796300
C	-3.53214100	1.59107100	-0.33520000
H	-4.16796500	-1.56905000	-1.42886600
H	-1.74114800	-1.48428500	-1.84059600
H	-1.62877800	2.54707600	-0.35299600
H	-4.05298200	2.44573200	0.08355800
O	-5.59732000	0.50043500	-0.34911300
C	-6.37402800	-0.64250200	-0.63452800
H	-6.03044300	-1.51189800	-0.06073000
H	-7.39437100	-0.39556100	-0.34216600
H	-6.35028000	-0.88389100	-1.70400000
C	0.68628200	1.49268300	-1.09941000
C	2.10387200	1.41524000	-1.57444400
O	2.79652700	2.38776200	-1.75503300
O	2.49269300	0.15138500	-1.71703800
C	3.84464500	-0.07666700	-2.15465400
C	4.01542100	-1.57555400	-2.26658100
H	4.52503400	0.37456100	-1.42458700
H	3.98836600	0.43662400	-3.10988400
H	5.02229700	-1.80714300	-2.62481700
H	3.85942600	-2.06872800	-1.30346400
H	3.28389200	-1.98944400	-2.96459200
N	-0.12177100	0.47744100	-1.35907600
H	0.29543100	2.50670500	-1.07186600

C5-cis-E-Re

C	3.91941400	-1.74574000	-2.07102900
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C	2.69137500	-1.31124000	-2.86636100
C	1.70125800	-0.52945800	-1.99663600
C	3.62785000	0.23037900	-0.57576700
C	4.59690800	-0.50522300	-1.49102700
H	0.97331200	-0.05009500	-2.65882300
H	3.01204300	-0.67869800	-3.70384900
H	2.15057000	-2.16707900	-3.28068400
H	3.61282800	-2.41206600	-1.25370300
H	4.61101800	-2.30409200	-2.71024400
H	4.05173900	1.17314800	-0.21359500
H	3.40835000	-0.40295800	0.29427800
H	4.91246100	0.15758200	-2.30714100
H	5.49025200	-0.77096000	-0.91581200
N	2.36618300	0.53990000	-1.25287700
C	0.88928900	-1.48417200	-1.08644800
O	-0.02056600	-2.11266300	-1.63649500
O	1.21651300	-1.50721500	0.14733000
C	1.62750500	1.56271900	-0.76557600
C	0.26323000	1.69898300	-0.78629000
H	-0.33911400	0.90747800	-1.23290600
C	-0.44728500	3.02211500	-0.59203100
H	-1.37639700	2.82588600	-0.03268800
H	2.22328900	2.32875700	-0.27314700
C	-0.10335400	0.77194700	1.49246300
H	-0.62381100	1.71732900	1.60940800
C	1.27852200	0.67056500	2.09356700
N	-0.75757800	-0.32354100	1.23896000
H	-0.09714600	-1.13374600	0.97389300
C	-2.12013200	-0.38085100	0.86944900
C	-3.05276600	0.51513800	1.40805500
C	-2.52316100	-1.36047100	-0.03467000
C	-4.37630500	0.44212700	1.02088900
H	-2.74902000	1.24744500	2.15070300
C	-3.85822600	-1.43231400	-0.42284600
H	-1.77950700	-2.02889900	-0.46804800
C	-4.78848600	-0.53085700	0.09896600
H	-5.12152300	1.11689500	1.42737600
H	-4.15294500	-2.19100200	-1.13773300
O	-6.10563400	-0.51821100	-0.21346500
C	-6.56942900	-1.48706800	-1.13128500
H	-6.40555200	-2.50255000	-0.75204500
H	-7.63857900	-1.30853600	-1.24249000
H	-6.07744500	-1.37877900	-2.10489700
O	2.07548300	1.57755700	2.08040500

O	1.43720700	-0.49700800	2.69588400
C	2.77064100	-0.85898900	3.10404800
H	3.48176900	-0.25390500	2.53747700
H	2.87252100	-0.60855100	4.16438600
C	0.37296300	4.04631200	0.19360400
H	1.23398400	4.38245200	-0.39532200
H	-0.23313300	4.92878700	0.41947400
H	0.75878800	3.63406600	1.13278900
C	-0.86978400	3.60298200	-1.94816300
H	-1.48358500	2.89175400	-2.50925800
H	-1.44666600	4.52536900	-1.81709700
H	0.01641200	3.83294300	-2.54951500
C	2.92691400	-2.33994000	2.83164400
H	2.71826200	-2.53585600	1.77634900
H	3.94458700	-2.65778700	3.07601800
H	2.22632800	-2.92019400	3.43764700

C6-trans-E-Si

C	3.97550200	-1.41251700	-0.54678800
C	3.63457100	-0.16824400	-1.08275400
C	2.29806900	0.17280500	-1.25475400
C	1.29357700	-0.72213000	-0.88428800
C	1.63362600	-1.97010700	-0.34855200
C	2.96597500	-2.31095000	-0.18370600
H	4.39271100	0.55497100	-1.35802900
H	2.03320700	1.16076000	-1.62389100
H	0.86485500	-2.67519600	-0.04392700
H	3.25431300	-3.26908100	0.23512200
O	5.24571200	-1.83619200	-0.33166700
C	6.29184500	-0.94484700	-0.65701100
H	6.21769800	-0.01699200	-0.07762300
H	7.21724100	-1.46092300	-0.40224000
H	6.29093100	-0.70384800	-1.72659000
C	-1.07468500	-1.11960700	-1.07551600
C	-2.37448000	-0.60811800	-1.61090800
O	-3.21568600	-1.31862500	-2.10731900
O	-2.45371000	0.70942100	-1.47600400
C	-3.56011500	1.38122500	-2.10150700
C	-3.43571700	2.84077700	-1.71979100
H	-4.49314900	0.92259900	-1.76003500
H	-3.48118800	1.22626900	-3.18178500
H	-4.13426100	3.44508600	-2.30439000
H	-3.66365600	2.98245200	-0.65916800

H	-2.41096200	3.17862300	-1.89688600
N	-0.04534200	-0.30508400	-1.05443500
H	-0.91085600	-2.18514400	-1.20128200
C	0.19127000	2.90609700	1.34837800
C	-1.07681700	2.10554200	1.60181300
C	0.32888100	0.14867400	2.31787800
C	1.57715900	1.01663200	2.17534700
C	1.27613300	2.50337600	2.34729400
H	-0.06061200	3.96556200	1.48648600
H	0.02549200	0.09555100	3.37495400
H	0.55273300	-0.86544000	1.98055700
H	2.30432900	0.66830700	2.91670500
H	2.02469600	0.86631200	1.18877800
H	0.94506600	2.71143300	3.37475500
H	2.17617600	3.08682100	2.14626500
N	-0.82559000	0.65230700	1.55645200
H	-1.80599500	2.32407500	0.82036400
H	-1.49468200	2.35758900	2.58863600
C	0.71065500	2.74493700	-0.11224800
O	1.88744800	3.04795800	-0.31927900
O	-0.13140200	2.29528200	-0.96343700
H	-0.18344100	0.77741200	-1.08621000
C	-1.85322800	-0.14696600	1.26028100
C	-1.83683100	-1.51153000	1.04158200
H	-2.77412900	0.38513600	1.02072300
H	-0.96201900	-2.08653600	1.34216000
C	-3.12729100	-2.29932500	0.96017500
C	-3.65526000	-2.58282300	2.37420000
C	-2.94147200	-3.61207400	0.19475600
H	-3.87592600	-1.69422200	0.42892300
H	-3.82691500	-1.65335900	2.92594500
H	-4.59655300	-3.14114200	2.33444600
H	-2.93129300	-3.18069700	2.93998800
H	-2.73797400	-3.43710800	-0.86428100
H	-2.11896100	-4.19532200	0.62829900
H	-3.84745700	-4.22223400	0.25748300

C6-trans-E-Re

C	0.02575900	-1.26573200	2.22660500
C	-0.07998600	-2.70167700	1.69569700
C	-1.50894200	-3.22301300	1.88462400
C	-2.53247400	-2.28770500	1.24652900
C	-2.37802000	-0.86471200	1.76945200

H	-1.59641300	-4.22517700	1.45347100
H	0.61016700	-3.29999500	2.29789500
H	-0.09545800	-1.27532300	3.32121400
H	1.00850100	-0.84522800	1.98813300
H	-2.37865500	-2.28969300	0.16750700
H	-3.55355500	-2.61701900	1.47255200
H	-3.03561000	-0.18727300	1.22747800
H	-2.64817600	-0.82646600	2.83673700
H	-1.71672200	-3.31560800	2.96133200
C	0.43409700	-2.79037800	0.23619900
O	1.53768700	-3.31241100	0.06712500
O	-0.31921200	-2.27270800	-0.66132200
N	-0.99723500	-0.36639200	1.66985900
C	-0.72139800	0.91839900	1.47356900
C	-1.51371100	1.88769600	0.87165100
H	0.31974100	1.18080200	1.67453000
H	-2.57835300	1.69272700	0.75151800
C	-1.16289900	3.35908000	0.98119700
C	-1.39358800	3.87295700	2.40865300
C	-1.98690400	4.18688500	-0.00928500
H	-0.09521300	3.48969600	0.75161900
H	-0.77636500	3.32855100	3.13022200
H	-1.15546100	4.93945100	2.48506200
H	-2.44313100	3.73854400	2.69375500
H	-1.88259100	3.84485400	-1.04298600
H	-3.05138000	4.11770200	0.24480200
H	-1.70082700	5.24178600	0.03731200
C	-0.74699400	1.25310800	-1.14649900
N	0.12811000	0.26628300	-1.13847000
C	4.25039100	0.65408200	-0.40032500
C	3.41788400	1.76859300	-0.24763800
C	2.05775000	1.66338800	-0.48484100
C	1.50745200	0.44085100	-0.89430700
C	2.33952200	-0.66878400	-1.05483800
C	3.70155700	-0.56654000	-0.79967100
O	5.56317400	0.85639900	-0.12761500
C	6.43041800	-0.25147100	-0.25432700
C	-2.12815000	0.94023100	-1.62511600
O	-2.47414800	-0.28517800	-1.23813800
O	-2.79891200	1.70956900	-2.26691800
C	-3.63460400	-0.90449500	-1.82452600
H	-0.39830500	2.26062200	-1.35125100
H	3.86121400	2.70564500	0.07174400
H	1.43212100	2.53945600	-0.34501100

H	1.91851800	-1.62883700	-1.33991500
H	4.31202800	-1.45496100	-0.90766800
H	6.14285600	-1.06120800	0.42655500
H	6.44186800	-0.63129200	-1.28274400
H	7.42343200	0.11161900	0.01000600
H	-4.19981900	-1.31793800	-0.98471800
H	-4.23258400	-0.13833800	-2.32184900
C	-3.15114900	-1.99033500	-2.76604700
H	-3.99332200	-2.59517400	-3.11373100
H	-2.66048300	-1.54512000	-3.63625000
H	-2.42497500	-2.62789900	-2.25265200
H	-0.19395000	-0.75610100	-1.04998600

C6-cis-E-Si

C	-3.81753000	1.15719400	-0.90029700
C	-3.43283900	-0.15064200	-1.21126800
C	-2.08664800	-0.47551200	-1.32259400
C	-1.10535000	0.49853800	-1.11417800
C	-1.49276400	1.80987000	-0.81035300
C	-2.83729000	2.13419600	-0.70534400
H	-4.16734800	-0.93229400	-1.36345300
H	-1.79405700	-1.50023600	-1.53787600
H	-0.75290300	2.58823300	-0.65553300
H	-3.15359600	3.14550200	-0.47293600
O	-5.10330900	1.57181900	-0.76767300
C	-6.11896200	0.61103800	-0.96602100
H	-6.04299100	-0.20460800	-0.23702200
H	-7.06343500	1.13643200	-0.82599900
H	-6.07970200	0.19390600	-1.97935500
C	1.26196700	0.93316100	-1.17688300
C	2.60934800	0.41783100	-1.58817500
O	3.45460400	1.10956900	-2.10177700
O	2.72407300	-0.87183800	-1.30586900
C	3.88940300	-1.56875200	-1.77471500
C	3.72440000	-3.00297400	-1.32023800
H	4.78039900	-1.08543900	-1.36191000
H	3.92652200	-1.47634000	-2.86426300
H	4.51844300	-3.62580000	-1.74038600
H	3.77135800	-3.06542200	-0.22938000
H	2.74798100	-3.37888300	-1.63523600
N	0.24313800	0.09772800	-1.20616100
H	1.10483600	1.98371000	-1.40760500
C	0.11194900	-2.52360100	1.58601400
C	0.97569400	-1.26642000	1.68954700

C	-1.06153600	0.00343100	2.48436900
C	-1.89052700	-1.26229300	2.32438900
C	-1.04046600	-2.50237600	2.58531500
H	0.78464400	-3.36340000	1.80645200
H	-0.79707400	0.13638200	3.54459500
H	-1.62818200	0.88228700	2.15884600
H	-2.73243300	-1.19960400	3.02216400
H	-2.29994500	-1.32226700	1.31152100
H	-0.65751500	-2.48892500	3.61602100
H	-1.64256900	-3.40200300	2.44920900
N	0.18793000	-0.01851800	1.70196300
H	1.64292200	-1.24611200	0.82642600
H	1.57845700	-1.28646900	2.61090900
C	-0.40711100	-2.77031800	0.13512000
O	-1.51874400	-3.28138600	0.00267000
O	0.39287600	-2.42280900	-0.80253300
H	0.40254500	-0.99359700	-1.11603200
C	0.76016200	1.15896700	1.44494000
C	1.99160700	1.36800600	0.84414700
H	0.11329600	2.01348900	1.63687700
H	2.69759600	0.54045600	0.87462900
C	2.63755700	2.73590700	0.72965200
C	3.77211600	2.86533000	1.75406800
C	1.65961200	3.90083200	0.87553600
H	3.09427500	2.79873600	-0.26902000
H	4.50851900	2.06517600	1.63113000
H	4.29103900	3.82248800	1.63950200
H	3.37565500	2.80855700	2.77400400
H	0.82865700	3.84050300	0.16329300
H	1.23837600	3.94189100	1.88666700
H	2.17598300	4.84784400	0.69640100

C6-cis-E-Re

C	-4.70153100	-0.56247400	0.03913400
C	-3.86774500	-1.68386600	0.02741000
C	-2.52765300	-1.55600000	0.37306900
C	-2.00678800	-0.31299700	0.74150500
C	-2.84176600	0.81393000	0.73443200
C	-4.17594500	0.68592700	0.39088800
H	-4.24548200	-2.65979700	-0.25279300
H	-1.86223800	-2.41338500	0.34727200
H	-2.45962700	1.79667000	0.99248100
H	-4.83722700	1.54552800	0.38136800

O	-6.01853300	-0.57835900	-0.28035400
C	-6.58781800	-1.81853400	-0.64267900
H	-6.50966800	-2.54588100	0.17411100
H	-7.63840500	-1.61838400	-0.85139600
H	-6.10923300	-2.22899500	-1.53995300
C	-0.00261600	0.83983400	1.39647800
C	1.43528400	0.73678300	1.84304300
O	2.09486100	1.70658300	2.13796000
O	1.82181500	-0.52192200	1.88030600
C	3.16754900	-0.82711600	2.30667400
C	3.12207400	-2.17650500	2.98622400
H	3.51130600	-0.02109300	2.95910600
H	3.78339300	-0.85910000	1.40473800
H	4.13425400	-2.47306100	3.27636100
H	2.50005600	-2.13525700	3.88472500
H	2.71928100	-2.90642000	2.28146300
N	-0.64264800	-0.25993800	1.08418300
H	-0.53763500	1.69775500	1.79359500
C	1.60326300	-1.76829400	-1.99152000
C	0.98979000	-0.36672900	-2.05109600
C	3.24742400	0.63670800	-1.93504700
C	3.88764700	-0.74220200	-1.86408500
C	3.01702500	-1.78052400	-2.56899900
H	0.94622700	-2.41237900	-2.58916100
H	3.22598600	0.98094900	-2.98196400
H	3.81565500	1.36823100	-1.35320100
H	4.88082400	-0.68488000	-2.32269500
H	4.00841800	-1.04577200	-0.82156400
H	2.98013700	-1.56239500	-3.64610600
H	3.45093200	-2.77427000	-2.43833700
N	1.86864600	0.63116600	-1.42895000
H	0.03403200	-0.38673500	-1.52584200
H	0.81602200	-0.06414800	-3.09610700
C	1.53892600	-2.32081200	-0.54035700
O	2.57382200	-2.74382000	-0.02309800
O	0.36699300	-2.29078200	-0.02856100
H	-0.07350100	-1.15615600	0.77655700
C	1.40039000	1.74357000	-0.84159500
C	0.10438700	2.06475100	-0.49462800
H	2.19025000	2.42997700	-0.54236700
H	-0.70822500	1.47459500	-0.91602000
C	-0.28732200	3.47281000	-0.08147700
C	-1.07571100	4.14294400	-1.21372100
C	0.88586600	4.34665900	0.36113900

H	-0.97292600	3.40432200	0.77940500
H	-1.94480800	3.54172600	-1.50181800
H	-1.43161700	5.13232000	-0.90738800
H	-0.44108500	4.26514600	-2.09828000
H	1.47192700	3.85925100	1.14639900
H	1.54694200	4.57170200	-0.48418500
H	0.51398800	5.30056700	0.74618900

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C	-1.63603500	0.64252600	3.51963600
C	-1.49662800	0.37712700	2.01932400
C	0.95182200	0.70081700	2.12227600
C	0.87221300	0.92746800	3.63936400
C	-0.35498300	0.24766600	4.26027000
H	-1.36380000	-0.69279000	1.82037100
H	-2.38553900	0.68875400	1.47039700
H	-1.83564100	1.71278200	3.66274100
H	-2.49746500	0.09141200	3.91131200
H	1.71737800	1.34311900	1.67516600
H	1.79353500	0.56600000	4.10927700
H	0.81629700	2.00827300	3.82355100
H	-0.23889500	-0.84241700	4.22437500
H	-0.43166600	0.51770700	5.31840200
N	-0.32905000	1.09520100	1.50797400
C	1.32834300	-0.74257900	1.75627600
C	-0.42813400	2.27688900	0.87941500
C	-1.48090900	2.75208900	0.13191300
H	0.50458200	2.84062100	0.85073500
H	-2.44924900	2.25556300	0.18959400
C	-1.50844500	4.18130700	-0.36211000
C	-2.02012100	5.11195800	0.74711600
C	-2.37619300	4.32518300	-1.61519300
H	-0.48187900	4.47978200	-0.61901100
H	-1.39328900	5.04338400	1.64165200
H	-2.02943400	6.15346700	0.40877800
H	-3.04348600	4.84036300	1.03165800
H	-1.92328100	3.82408100	-2.47391800
H	-3.37676800	3.90882800	-1.43912100
H	-2.50047100	5.38040300	-1.87668600
C	-3.90972800	-2.58647800	-0.68846500
C	-2.58683600	-3.01802800	-0.56671500
C	-1.54267600	-2.11136900	-0.72150700
C	-1.80932300	-0.76904600	-0.99711300

C	-3.13729400	-0.33675200	-1.11314400
C	-4.17518300	-1.23941400	-0.96241800
H	-2.35348700	-4.05548300	-0.35911200
H	-0.50950900	-2.43465200	-0.62853600
H	-3.37115800	0.70495600	-1.31261700
H	-5.20982500	-0.92531800	-1.04805900
O	-4.99638000	-3.38446800	-0.55520400
C	-4.77358500	-4.75522300	-0.29724100
H	-4.24515200	-4.90023200	0.65268300
H	-5.75978900	-5.21457000	-0.23671600
H	-4.20071300	-5.22339400	-1.10628800
C	-0.78528400	1.31539300	-1.60427100
C	0.44287400	2.10844900	-1.92367800
O	0.40493400	3.02657100	-2.70915400
O	1.50294500	1.68517100	-1.25087500
C	2.80114700	2.22431900	-1.59798900
C	3.39271600	2.89444700	-0.37707200
H	2.67380700	2.91632300	-2.43130900
H	3.39038700	1.35919000	-1.90499100
H	4.37678700	3.30313500	-0.62444000
H	2.75771900	3.71957200	-0.03611500
H	3.52225100	2.15971900	0.42138300
N	-0.70622300	0.10588000	-1.11809700
H	-1.66631100	1.61623300	-2.16149500
N	1.25287500	-0.98398500	0.32484400
H	2.33460700	-0.90823300	2.16073800
H	0.66570500	-1.45184400	2.26862500
S	2.61596900	-1.08944700	-0.45840400
O	2.37179300	-0.98827300	-1.89433100
O	3.72578900	-0.33044100	0.13204900
C	3.12872300	-2.84142000	-0.22898300
F	4.29283100	-3.09300000	-0.81653500
F	2.20728600	-3.65842000	-0.74227900
F	3.24213600	-3.11415900	1.07712200
H	0.20320900	-0.26349900	-0.61440100

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C	0.78092900	-2.47689700	3.12702900
C	0.71741100	-2.11745000	1.63921400
C	-0.12058000	0.13379800	2.14806300
C	-0.03385100	-0.13333000	3.65892600
C	0.99273900	-1.22751900	3.98731800
H	1.65732400	-1.67753000	1.28781600

H	0.51653800	-2.99163800	1.02247800
H	-0.16174100	-2.96824300	3.40349800
H	1.58894900	-3.19679900	3.29287700
H	-0.98161400	0.77300300	1.92142500
H	0.21868000	0.79748100	4.17994300
H	-1.02526700	-0.44488900	4.01234700
H	2.00916900	-0.85167400	3.82514100
H	0.92338700	-1.48523100	5.04911800
N	-0.35542500	-1.13674700	1.45177600
C	1.15935100	0.83398800	1.63203300
C	-1.57153100	-1.46735000	1.01197500
C	-1.92121000	-2.51066000	0.17906900
H	-2.33337500	-0.71163100	1.21672700
H	-1.20657700	-3.31318600	0.00280300
C	-3.36985500	-2.87233200	-0.06858300
C	-3.96681000	-3.60349800	1.14170400
C	-3.50806500	-3.73733300	-1.32424300
H	-3.94750000	-1.94593000	-0.21232700
H	-3.92187700	-2.98080100	2.04068800
H	-5.01227500	-3.87527800	0.95949400
H	-3.40739600	-4.52435400	1.34182500
H	-3.08268800	-3.26423600	-2.21396200
H	-2.97944000	-4.68741000	-1.18212000
H	-4.55921400	-3.96738600	-1.52200000
C	-3.18703600	3.44198600	-0.29077500
C	-1.80514000	3.55424700	-0.46520700
C	-1.04871900	2.42968400	-0.77644600
C	-1.66170800	1.18163600	-0.91630700
C	-3.04667400	1.07207100	-0.73473000
C	-3.80068200	2.19199400	-0.42895100
H	-1.30501000	4.51018600	-0.36713000
H	0.02595100	2.50898800	-0.90615000
H	-3.54396500	0.11137000	-0.82655900
H	-4.87361100	2.12474500	-0.28534300
O	-4.01027600	4.47284100	0.01565500
C	-3.43270100	5.75612800	0.13943100
H	-2.95718100	6.06914700	-0.79754300
H	-4.25253200	6.43384000	0.37534900
H	-2.69284900	5.78244700	0.94832600
C	-1.30635400	-1.09449500	-1.59870500
C	-0.35357900	-2.12782800	-2.11356000
O	-0.65765500	-2.84502800	-3.03608800
O	0.79954300	-2.12174300	-1.45981200
C	1.88560200	-2.87435600	-2.05918900

C	2.86213800	-3.25886900	-0.97240300
H	2.34869100	-2.21006000	-2.79163000
H	1.45871900	-3.74343800	-2.56335800
H	3.69904300	-3.79832600	-1.42571200
H	3.25831400	-2.37338100	-0.46877300
H	2.39349600	-3.92054500	-0.23704200
N	-0.84158100	0.07148400	-1.22033600
H	-2.31043100	-1.15800400	-2.00736800
N	1.31256000	0.70904500	0.19325100
H	0.16390200	0.18442800	-0.82186700
H	1.07228200	1.88787200	1.93640600
H	2.03538900	0.42943800	2.15324000
S	2.75965000	0.46716800	-0.36343700
O	3.65031600	-0.27121900	0.54200300
O	2.70022900	0.07487000	-1.76912700
C	3.51546000	2.14359100	-0.40437200
F	2.80884500	2.94854500	-1.20269600
F	3.49755000	2.66731100	0.82772300
F	4.77020200	2.11690800	-0.83694500

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C	-1.78918100	-0.09802900	3.58390600
C	-1.66102300	-0.40340300	2.08944600
C	0.46469300	0.84148400	1.91892300
C	0.37281300	1.21626600	3.40800500
C	-0.41856300	0.17628900	4.21333600
H	-1.12124200	-1.33910900	1.90820600
H	-2.63550600	-0.49928500	1.60073400
H	-2.42922400	0.78791400	3.69573800
H	-2.29076600	-0.92845100	4.09115000
H	0.92228400	1.64949200	1.34562000
H	1.38299700	1.32819800	3.81587800
H	-0.12113200	2.19383700	3.48548600
H	0.14949800	-0.75895600	4.27308600
H	-0.54632000	0.52756800	5.24228500
N	-0.92343200	0.67746600	1.43149300
C	1.34089900	-0.39628500	1.68576600
C	-1.61467400	1.67026800	0.86359400
C	-1.09288200	2.74093000	0.15556600
H	-2.68866900	1.49278600	0.82819200
H	-0.04801800	2.99216800	0.32680900
C	-1.92510700	3.90731600	-0.33741300
C	-1.64431100	5.14393800	0.52562600

C	-3.42484300	3.62429000	-0.38843900
H	-1.57920500	4.13779700	-1.35524500
H	-0.57749800	5.38860900	0.52605100
H	-2.19000900	6.01409700	0.14707200
H	-1.95431500	4.96723800	1.56193400
H	-3.66184000	2.73722100	-0.98640500
H	-3.83338100	3.47323800	0.61763300
H	-3.95200400	4.47178800	-0.83490800
C	-3.64573600	-2.61544100	-0.95052200
C	-2.30400900	-2.99001200	-0.82927200
C	-1.29921700	-2.03976200	-0.96990400
C	-1.61894600	-0.70305700	-1.22960600
C	-2.96327800	-0.33260600	-1.35699400
C	-3.96538400	-1.28143600	-1.21799500
H	-2.02663800	-4.01883400	-0.63243000
H	-0.25475700	-2.32045500	-0.86724500
H	-3.24219700	0.69233000	-1.57715900
H	-5.01107600	-1.01169500	-1.32071200
O	-4.69781100	-3.46329200	-0.82917200
C	-4.41350900	-4.82846000	-0.60732900
H	-3.88062800	-4.97611100	0.33987100
H	-5.37804100	-5.33360700	-0.56180100
H	-3.81872500	-5.24904400	-1.42678700
C	-0.69708800	1.49496900	-1.61558900
C	0.52499100	2.31093200	-1.92339800
O	0.46623600	3.34309300	-2.54877500
O	1.60667000	1.75686400	-1.40231000
C	2.89158500	2.36736600	-1.65797200
C	3.31724000	3.14027400	-0.42787200
H	2.80051900	3.00356400	-2.54001700
H	3.55459800	1.52509500	-1.85660800
H	4.29705200	3.59675200	-0.59417000
H	2.60017300	3.93821500	-0.20529800
H	3.39691700	2.45655200	0.42162400
N	-0.55582100	0.21516000	-1.32843900
H	-1.59170400	1.83070900	-2.13205600
N	1.35227900	-0.79114200	0.29129400
H	0.34687700	-0.12649100	-0.85540800
H	2.34011700	-0.11663300	2.04767600
H	1.00398500	-1.23029900	2.31600600
S	2.75808200	-0.94032700	-0.39812200
O	2.59634500	-0.98834100	-1.84826800
O	3.82279600	-0.10112600	0.16845100
C	3.28969600	-2.64435700	0.04350300

F	3.28471600	-2.77784400	1.37695900
F	4.50919200	-2.92069900	-0.40399800
F	2.43926000	-3.54010000	-0.46261500

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C	2.60570400	-0.21005000	3.45480700
C	2.58855700	-0.00680700	1.93738500
C	0.15066900	-0.30878300	1.84573100
C	0.09754900	-0.50526900	3.36953600
C	1.26599500	0.18963000	4.07948100
H	2.49286800	1.05231100	1.67078100
H	3.50995400	-0.37714700	1.48210500
H	2.80693000	-1.26981400	3.66133300
H	3.42379200	0.37159100	3.89198600
H	-0.60495100	-0.93889600	1.37105500
H	-0.86139700	-0.13504800	3.74957400
H	0.13403400	-1.58279300	3.57500200
H	1.15017700	1.27815400	4.02214900
H	1.25504900	-0.06695500	5.14367600
N	1.46245400	-0.74394900	1.35650900
C	-0.14145000	1.15471700	1.45405500
C	1.68236800	-1.90429500	0.72697600
C	0.77548300	-2.81901600	0.22763900
H	2.73940100	-2.08253800	0.53504800
H	-0.25642900	-2.75783000	0.57234900
C	1.20040000	-4.18996200	-0.27396200
C	0.60931000	-5.27387100	0.63610800
C	2.71270700	-4.37151500	-0.40246900
H	0.77965200	-4.33997300	-1.28061900
H	-0.47926700	-5.17886000	0.71660600
H	0.83412300	-6.27361400	0.25035700
H	1.02850800	-5.19279400	1.64524400
H	3.15390800	-3.63373700	-1.07935200
H	3.20076400	-4.29962000	0.57709400
H	2.93019800	-5.36340300	-0.80911500
C	-4.69835200	-1.05830600	-0.20929700
C	-4.10110100	0.19626900	-0.35400600
C	-2.75731800	0.28946600	-0.70001200
C	-1.99072100	-0.86087500	-0.90935100
C	-2.59459400	-2.11810800	-0.74794800
C	-3.93267600	-2.21235500	-0.40656400
H	-4.66818000	1.10775500	-0.20736300
H	-2.29082500	1.26313200	-0.81927800

H	-2.02789100	-3.03364000	-0.88909800
H	-4.41292400	-3.17705000	-0.28280900
O	-5.99810100	-1.25970200	0.11878600
C	-6.81012000	-0.11852200	0.29671700
H	-6.85029400	0.48658900	-0.61670500
H	-7.80729700	-0.49137600	0.52923200
H	-6.44999400	0.50132700	1.12666800
C	0.13197600	-1.68281200	-1.61127700
C	1.50595200	-1.42785500	-2.15058400
O	2.08560100	-2.25286500	-2.81891000
O	1.94303300	-0.22727000	-1.80700100
C	3.17112100	0.26154300	-2.38784900
C	4.13848900	0.58900500	-1.27135100
H	2.88618000	1.16029800	-2.93502700
H	3.56113200	-0.49753400	-3.06778300
H	5.05201100	1.02160900	-1.68942400
H	3.69520600	1.31732400	-0.58513500
H	4.41324200	-0.31614200	-0.71892800
N	-0.63406300	-0.68559700	-1.25557400
H	-0.30400000	-2.61311500	-1.96706800
N	0.08657600	1.38839200	0.03861200
H	-0.18652400	0.33337600	-0.83591600
H	-1.19352100	1.34298100	1.71462800
H	0.46284300	1.83631400	2.06212700
S	0.94459700	2.63590500	-0.39962600
O	1.98005200	3.01584500	0.56690300
O	1.28131400	2.55589500	-1.81399100
C	-0.24733000	4.03303000	-0.29395000
F	-1.28182300	3.82190600	-1.11052400
F	0.31801700	5.18906200	-0.61475300
F	-0.71905200	4.11524800	0.95623100

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C	-2.48171100	3.87505800	-0.45489200
C	-2.91254200	2.54646400	-0.40775900
C	-1.98529300	1.51275500	-0.47011100
C	-0.62423200	1.79641400	-0.57592300
C	-0.19171100	3.12655000	-0.62402700
C	-1.11569100	4.15658000	-0.56522400
H	-3.96483500	2.29989200	-0.33409800
H	-2.31100400	0.47769400	-0.45182600
H	0.86517500	3.36485500	-0.70622900
H	-0.80364600	5.19472000	-0.59910100

O	-3.30159400	4.95244100	-0.39919000
C	-4.69114000	4.71353100	-0.31271800
H	-4.94464900	4.16474900	0.60210700
H	-5.16425700	5.69494700	-0.28962500
H	-5.05244500	4.15379200	-1.18341200
C	1.44869900	0.77299400	-1.21962800
C	2.17490800	-0.47369500	-1.62051000
O	3.04067500	-0.45792200	-2.46409900
O	1.75754700	-1.53930600	-0.95055500
C	2.30075600	-2.81620800	-1.35953700
C	3.65301500	-3.04666700	-0.71295600
H	2.37420000	-2.81868100	-2.44892500
H	1.54320700	-3.53389600	-1.04303600
H	4.04276400	-4.02441500	-1.01003200
H	4.36839200	-2.28244300	-1.03036400
H	3.57151900	-3.03637800	0.37891500
N	0.27649300	0.70702600	-0.63959800
H	1.68043800	1.64188900	-1.82681000
C	0.11213300	-1.58642500	2.92462300
C	1.53024500	-1.14781400	2.55311400
C	0.84337500	1.24025800	2.42301200
C	-0.59536800	0.83628900	2.72283900
C	-0.64480700	-0.42451500	3.57992500
H	0.24937800	-2.35849000	3.69426400
H	1.35244300	1.54809100	3.35114900
H	0.85818900	2.08706000	1.73482700
H	-1.08353100	1.67374500	3.23277400
H	-1.12870300	0.65465600	1.78821200
H	-0.19409700	-0.21466900	4.56083500
H	-1.68365300	-0.72042200	3.76047300
N	1.60628800	0.13311800	1.83397800
H	2.00007700	-1.90614600	1.91953500
H	2.12136800	-1.04981600	3.47741500
C	-0.64436700	-2.30822000	1.80358300
C	2.68923200	0.34819000	1.07567300
C	2.99616300	1.45380900	0.31169300
H	3.32352600	-0.53073300	0.95307300
H	2.47310400	2.39167800	0.49251900
C	4.35576600	1.58302700	-0.34133200
C	5.36202600	2.15980100	0.66520900
C	4.30567300	2.45396700	-1.59967600
H	4.69394200	0.57954800	-0.63561800
H	5.42929800	1.53334300	1.56002500
H	6.35879100	2.23688100	0.21864800

H	5.05496100	3.16395100	0.98027600
H	3.76813100	1.95487700	-2.40931900
H	3.82591000	3.41807700	-1.38590200
H	5.31798800	2.66407000	-1.95793300
N	-0.89308600	-1.49724800	0.61129800
H	-0.05810600	-0.20061900	-0.19213100
H	-0.06905100	-3.21006500	1.54676100
H	-1.58949000	-2.66007100	2.24556400
S	-1.29297200	-2.31644500	-0.67152500
O	-1.20021500	-1.45050900	-1.84893400
O	-0.75098600	-3.67835300	-0.74823000
C	-3.10764200	-2.61038200	-0.53397600
F	-3.38611300	-3.28300500	0.58838200
F	-3.57216900	-3.30320700	-1.56720200
F	-3.76327300	-1.44380900	-0.48436900

C8-trans-E-Re

C	-2.22338400	3.98893900	-0.38057600
C	-0.84427600	3.76362500	-0.42571100
C	-0.35501700	2.47168700	-0.57674400
C	-1.22943100	1.38701400	-0.67420900
C	-2.61041500	1.61821400	-0.63085700
C	-3.10084000	2.90609700	-0.48794200
H	-0.13925500	4.58315500	-0.35512600
H	0.71433500	2.29629800	-0.62572200
H	-3.31088400	0.79335700	-0.70834800
H	-4.16740900	3.10007300	-0.45311100
O	-2.80075600	5.20609700	-0.23719900
C	-1.94714400	6.32669200	-0.13200000
H	-1.32939600	6.44085300	-1.03062400
H	-2.59946900	7.19328000	-0.02808000
H	-1.29725800	6.25071400	0.74788700
C	-1.37467200	-0.92960800	-1.28278800
C	-0.63509000	-2.17741600	-1.65862300
O	-1.05263900	-2.95330200	-2.48529400
O	0.49199600	-2.28772700	-0.97252100
C	1.37943100	-3.36815200	-1.35171700
C	2.08299300	-3.04550700	-2.65405600
H	0.78587600	-4.28444200	-1.41849000
H	2.08674200	-3.42155500	-0.52593900
H	2.82276200	-3.82235700	-2.86795800
H	1.37190900	-3.00638600	-3.48263600
H	2.60036700	-2.08953000	-2.55228500

N	-0.68090300	0.09481300	-0.82410600
H	-2.26336200	-0.72625800	-1.87348600
C	0.68416500	0.11703800	3.08661100
C	-0.80643600	-0.18798900	2.91288900
C	-0.34799900	-2.49156500	2.14800300
C	1.15056900	-2.27838600	2.31095700
C	1.47015100	-1.18066200	3.33199400
H	0.73771300	0.72464500	4.00106700
H	-0.77608300	-2.93597000	3.06056300
H	-0.54008200	-3.16813000	1.31629500
H	1.58428600	-3.22866300	2.64273400
H	1.57789600	-2.03555700	1.33808400
H	1.23212500	-1.54927300	4.33962100
H	2.54332000	-0.96026800	3.31001100
N	-1.07753200	-1.23344600	1.91832000
H	-1.35093800	0.71248000	2.60824500
H	-1.21657700	-0.53002800	3.87619500
C	1.28758900	0.99296700	1.97382300
C	-2.20394100	-1.19278800	1.21238700
C	-2.62023900	-2.05553300	0.21015700
H	-2.77778300	-0.27466400	1.35368900
H	-2.14717400	-3.03199800	0.12676200
C	-4.04827600	-2.01167200	-0.30044100
C	-5.01503400	-2.55932900	0.75913100
C	-4.19961900	-2.80545000	-1.60047400
H	-4.32920400	-0.96523400	-0.49322500
H	-4.96653300	-1.97547400	1.68379100
H	-6.04690800	-2.54058400	0.39253900
H	-4.76131300	-3.59719700	1.00214400
H	-3.53557400	-2.45538200	-2.39432200
H	-3.95614000	-3.85983500	-1.42525100
H	-5.23188800	-2.75434100	-1.95925700
N	1.53056000	0.28409000	0.72590300
H	0.27876000	-0.02889000	-0.34235900
H	0.60254200	1.83465000	1.78849200
H	2.21896200	1.41789400	2.36752600
S	3.02349400	0.00837400	0.32410100
O	4.01162700	0.38508100	1.33726700
O	3.17401600	-1.28281200	-0.35162400
C	3.32617400	1.18483400	-1.05607200
F	4.56042300	1.09727200	-1.53508400
F	2.46311100	0.94407900	-2.05275700
F	3.12039600	2.44369800	-0.64252900

C8-cis-E-Si

C	2.62170300	3.57212200	-0.95736800
C	1.22540900	3.50355300	-0.99398900
C	0.59119800	2.26828200	-1.04973500
C	1.33645600	1.08447800	-1.06075000
C	2.73502900	1.15956400	-1.03917900
C	3.36860600	2.39174500	-0.98633000
H	0.62050300	4.40257100	-0.99059800
H	-0.49338900	2.20518800	-1.08910800
H	3.33647800	0.25753800	-1.06337400
H	4.45082000	2.46641400	-0.97117200
O	3.33661500	4.72444400	-0.89866800
C	2.61775900	5.93933200	-0.90130900
H	1.95702500	6.01330700	-0.02902200
H	3.36449000	6.73193600	-0.85804500
H	2.02270300	6.04750800	-1.81600000
C	1.20277300	-1.29089100	-1.39989300
C	0.29638400	-2.44242000	-1.75044200
O	0.57331800	-3.22651400	-2.62500200
O	-0.76945000	-2.47419700	-0.96590200
C	-1.76595000	-3.49643300	-1.20593700
C	-2.42207300	-3.79938900	0.12262200
H	-1.26398700	-4.36618300	-1.63618400
H	-2.47781200	-3.07972100	-1.91885300
H	-3.18833800	-4.56731800	-0.01589500
H	-1.68612900	-4.17575400	0.84107500
H	-2.90251200	-2.90609000	0.52977200
N	0.63607500	-0.13576700	-1.08797300
H	2.11974000	-1.27497700	-1.98608400
C	-0.79213500	-0.06035100	2.55193100
C	0.17044300	-1.13588700	2.04702400
C	2.11867700	0.21283100	2.87389600
C	1.16836900	1.29892700	3.35421700
C	-0.18577200	0.69762800	3.73748900
H	-1.69234500	-0.59930900	2.87023800
H	2.38342000	-0.43479000	3.72357500
H	3.04155900	0.64613900	2.47691500
H	1.63102300	1.79229200	4.21524500
H	1.05797300	2.05787900	2.57365500
H	-0.04895900	0.01496000	4.58730200
H	-0.87090100	1.48577200	4.06833600
N	1.54087500	-0.64020100	1.82116400
H	-0.21907700	-1.53733500	1.10933500

H	0.22896400	-1.95473300	2.78204600
C	-1.23707600	0.93327300	1.46404900
C	2.39750900	-1.30871500	1.04705600
C	2.08876700	-2.36185300	0.19400600
H	3.40933000	-0.90587400	1.06026700
H	1.18313100	-2.91147600	0.44216100
C	3.16019000	-3.21183600	-0.47174900
C	3.33640700	-4.52539000	0.29957400
C	4.50810700	-2.51056700	-0.63559500
H	2.79076600	-3.47200700	-1.47393200
H	2.38645800	-5.06168400	0.38736200
H	4.04887400	-5.18210100	-0.20986000
H	3.71151200	-4.33061100	1.31074400
H	4.42603800	-1.56079300	-1.17639400
H	4.97735500	-2.31336600	0.33528000
H	5.19149400	-3.14812700	-1.20326700
N	-1.59301700	0.32514800	0.19145100
H	-2.05646800	1.52818300	1.88742500
H	-0.42470500	1.63756600	1.24940800
S	-3.08968500	-0.10076000	-0.03026200
O	-3.21600200	-0.93227200	-1.22343600
O	-3.78703200	-0.49724200	1.19640700
C	-3.94129200	1.45804700	-0.52329900
F	-5.21539700	1.24355700	-0.83034100
F	-3.88983000	2.35188700	0.47306300
F	-3.33514300	1.99661000	-1.58488500
H	-0.40079400	-0.07564400	-0.68610900

C8-cis-E-Re

C	4.84849000	-0.98182900	0.03895000
C	3.80954700	-1.89006800	0.25597100
C	2.50361800	-1.55268700	-0.07954000
C	2.21549300	-0.30365700	-0.63581600
C	3.26222500	0.60940600	-0.84771700
C	4.56261500	0.26933300	-0.51655000
H	3.99889000	-2.87010400	0.67721900
H	1.70182300	-2.27036600	0.06251400
H	3.07974500	1.59150200	-1.27407100
H	5.38046500	0.96331700	-0.67764500
O	6.15159300	-1.21546900	0.33071200
C	6.48043000	-2.47410800	0.88042300
H	6.21116800	-3.28868400	0.19787200
H	7.56011000	-2.46558700	1.02810400

H	5.98158900	-2.62996600	1.84442600
C	0.52328000	1.14500100	-1.49566500
C	-0.89054400	1.37535400	-1.92693300
O	-1.17258500	2.13048000	-2.82770500
O	-1.75284000	0.68236000	-1.19691100
C	-3.14343200	0.83112200	-1.54159500
C	-3.69662900	2.10249100	-0.92758000
H	-3.61636400	-0.06412600	-1.14053600
H	-3.23324100	0.83535800	-2.63000500
H	-4.76798600	2.18533300	-1.13009900
H	-3.55129900	2.08904600	0.15791000
H	-3.19716700	2.98003700	-1.34876900
N	0.87062900	-0.00468200	-0.94439500
H	1.23757900	1.64116400	-2.14608600
C	-1.00882900	-0.18416400	2.67281500
C	-0.09451000	0.94730600	2.19252300
C	-1.92915100	2.58440000	2.49788300
C	-2.84407200	1.50036800	3.05784200
C	-2.02007500	0.37119400	3.68166600
H	-0.36299900	-0.92134300	3.16349600
H	-1.43327800	3.10054900	3.33469300
H	-2.49375100	3.33375900	1.93525600
H	-3.49815400	1.96215700	3.80478600
H	-3.49032800	1.10876000	2.26592800
H	-1.48608600	0.75886700	4.56023500
H	-2.67957300	-0.42851600	4.03360800
N	-0.87491100	2.05438700	1.62102200
H	0.60082300	0.56912500	1.44313600
H	0.48739000	1.34282400	3.04012200
C	-1.71558400	-0.90033100	1.51626800
C	-0.42689100	2.81832400	0.62334100
C	0.76569000	2.70965100	-0.08803600
H	-1.12429700	3.60770500	0.34302000
H	1.55733600	2.13765200	0.39738800
C	1.27644400	3.90408100	-0.88950700
C	2.31650100	4.66974800	-0.06275300
C	0.18167600	4.84700400	-1.39075600
H	1.79597400	3.51990900	-1.78103400
H	3.12723500	4.01091300	0.26666200
H	2.75619500	5.48402100	-0.64796600
H	1.85053800	5.10295500	0.82947400
H	-0.59335800	4.30781400	-1.94385300
H	-0.28237400	5.39325000	-0.56107100
H	0.61726800	5.59210100	-2.06231600

N	-0.75564900	-1.50315900	0.60263000
H	-2.38309000	-1.65475200	1.95307400
H	-2.34459200	-0.17977500	0.97286300
S	-1.06048700	-2.97490800	0.13727000
O	0.07440900	-3.49216500	-0.62489300
O	-1.70479100	-3.82009400	1.14033100
C	-2.37700000	-2.81226100	-1.14272300
F	-3.48194400	-2.28445900	-0.58206800
F	-2.70330400	-3.97883300	-1.68298300
F	-1.99303400	-1.98527500	-2.12229700
H	0.12360400	-0.63004500	-0.44066400