

Simple Descriptors for Accessing the Outcome of Aza-Diels-Alder Reactions - Supplementary Information

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Energies

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Table S.1: Energies involved in the formation of the *endo-3R*, *endo-3S*, *exo-3R* and *exo-3S* molecular complexes for the 16 alkyimines studied, in $\text{kJ} \cdot \text{mol}^{-1}$. The energies were calculated using X3LYP/6-311G(2df,2p) and include the zero-point vibrational energy correction. Zero-point corrections and the molecular geometry were obtained at the X3LYP/6-31G(d) level of theory.

Parent Imine	$\Delta E_{Endo-3R}$	$\Delta E_{Endo-3S}$	ΔE_{Exo-3R}	ΔE_{Exo-3S}
1	-40.1	-39.7	-42.2	-42.2
2	-38.2	-38.1	-41.5	-41.5
3	-36.8	-35.8	-38.4	-38.4
4	-33.1	-33.1	-36.6	-36.5
5	-36.9	-36.6	-39.5	-39.4
6	-34.9	-34.9	-38.0	-38.0
7	-33.3	-32.7	-34.6	-34.6
8	-29.8	-29.6	-32.7	-32.7
9	-31.1	-31.0	-33.7	-33.7
10	-28.8	-28.4	-32.8	-32.8
11	-25.4	-25.3	-28.8	-28.8
12	-23.2	-23.2	-27.6	-27.7
13	-28.0	-28.6	-29.9	-29.8
14	-26.5	-26.5	-28.4	-28.5
15	-24.7	-25.0	-25.6	-25.7
16	-23.6	-23.4	-23.3	-23.3

Table S.2: Enthalpies of formation at 298.15 K, $\Delta_f H_{298}$, of the *endo-3R*, *endo-3S*, *exo-3R* and *exo-3S* molecular complexes for the 16 alkylimines studied, in $\text{kJ}\cdot\text{mol}^{-1}$. The molecular geometries, as well as vibrational corrections, were obtained using X3LYP/6-31G(d), while the electronic energy was refined at the X3LYP/6-311G(2df,2p) level of theory.

Parent Imine	$\Delta_f H_{Endo-3R}$	$\Delta_f H_{Endo-3S}$	$\Delta_f H_{Exo-3R}$	$\Delta_f H_{Exo-3S}$
1	-38.4	-38.4	-41.6	-41.6
2	-36.2	-36.4	-40.1	-40.1
3	-34.7	-34.3	-37.7	-37.7
4	-31.6	-31.6	-35.5	-35.3
5	-35.4	-35.2	-38.5	-38.5
6	-33.3	-33.4	-36.8	-36.8
7	-32.0	-31.8	-34.4	-34.4
8	-28.7	-28.6	-32.1	-32.1
9	-29.2	-29.0	-32.3	-32.3
10	-28.8	-26.3	-31.1	-31.1
11	-24.3	-24.2	-28.5	-28.5
12	-21.9	-21.8	-26.8	-26.9
13	-25.7	-28.5	-27.5	-27.5
14	-24.3	-24.2	-26.3	-26.3
15	-22.9	-23.1	-24.3	-24.3
16	-24.0	-23.8	-22.1	-22.1

Table S.3: Enthalpies at 298.15 K, $\Delta_f H_{298}$, in $\text{kJ} \cdot \text{mol}^{-1}$, of the transition states of the *endo-3R*, *endo-3S*, *exo-3R* and *exo-3S* channels for the reaction between the 16 alkyimines studied and CP, taking the combined enthalpies of the isolated reactants as reference. The molecular geometries, as well as vibrational corrections, were obtained using X3LYP/6-31G(d), while the electronic energy was refined at the X3LYP/6-311G(2df,2p) level of theory.

Parent Imine	$\Delta_f H_{Endo-3R}$	$\Delta_f H_{Endo-3S}$	$\Delta_f H_{Exo-3R}$	$\Delta_f H_{Exo-3S}$
1	-18.9	-19.1	-24.9	-24.9
2	-16.1	-16.0	-22.1	-22.1
3	-13.6	-13.5	-19.3	-19.3
4	-9.9	-10.0	-16.6	-16.7
5	-13.7	-13.7	-18.0	-18.0
6	-10.7	-10.8	-15.4	-15.4
7	-8.6	-8.4	-12.6	-12.6
8	-4.8	-4.8	-9.8	-9.8
9	-5.9	-5.8	-11.7	-11.8
10	6.0	5.9	-9.3	-9.3
11	8.1	8.3	-6.7	-6.7
12	11.5	11.4	-4.2	-4.2
13	11.0	11.2	6.0	6.1
14	13.8	14.0	8.4	8.4
15	15.6	15.6	10.3	10.3
16	18.9	19.0	13.2	13.2

Table S.4: Apparent activation energies at 0 K, ΔE^\ddagger , and apparent activation enthalpies at 298.15 K, ΔH_{298}^\ddagger for the *endo-3R*, *endo-3S*, *exo-3R* and *exo-3S* reaction channels of the addition of CP to the 16 alkylimines studied. All values are given in $\text{kJ}\cdot\text{mol}^{-1}$. The molecular geometries, as well as vibrational corrections, were obtained using X3LYP/6-31G(d), while the electronic energy was refined at the X3LYP/6-311G(2df,2p) level of theory.

Parent Imine	<i>Endo-3R</i>		<i>Endo-3S</i>		<i>Exo-3R</i>		<i>Exo-3S</i>	
	ΔE^\ddagger	ΔH_{298}^\ddagger	ΔE^\ddagger	ΔH_{298}^\ddagger	ΔE^\ddagger	ΔH_{298}^\ddagger	ΔE^\ddagger	ΔH_{298}^\ddagger
1	23.6	19.5	23.1	19.4	20.1	16.7	20.1	16.7
2	23.7	20.1	23.9	20.3	21.6	18.0	21.6	18.0
3	25.3	21.2	22.8	20.8	21.9	18.4	21.8	18.4
4	25.2	21.6	25.3	21.6	21.3	18.8	21.0	18.7
5	25.4	21.7	25.1	21.5	24.2	20.5	24.2	20.5
6	26.1	22.6	26.3	22.7	24.8	21.4	24.8	21.4
7	25.6	23.4	26.8	23.3	25.4	21.8	25.4	21.8
8	27.4	23.8	27.3	23.7	25.2	22.3	25.2	22.3
9	28.1	23.3	28.1	23.3	25.0	20.6	24.8	20.5
10	38.1	34.8	36.7	32.2	26.5	21.8	26.5	21.8
11	37.8	32.4	37.2	32.6	26.1	21.8	26.0	21.8
12	38.3	33.4	38.2	33.3	25.5	22.6	25.5	22.6
13	43.3	36.7	43.9	39.7	39.8	33.6	39.7	33.6
14	44.9	38.1	44.7	38.2	40.9	34.7	40.9	34.8
15	44.7	38.4	45.0	38.7	41.0	34.5	41.0	34.6
16	47.6	42.9	47.4	42.8	39.4	35.3	39.3	35.4

Equilibrium Geometries at the X3LYP/6-31G(d) Level of Theory

Equilibrium geometry of **r01-endo-3r-mc**.

C 0.4408560000 1.0329770000 -0.3520420000
 N -0.3379020000 1.6602600000 0.4700940000
 H -0.1998220000 1.4061760000 1.4535630000
 H 0.4365850000 1.2706490000 -1.4094360000
 C 1.5156360000 0.1842150000 0.2703900000
 C -1.2532390000 2.7609700000 0.1579830000
 C -0.9973820000 -1.0948830000 -1.2413750000
 C -2.3082300000 -0.3537540000 -1.2150180000
 C -2.7186430000 -0.4450540000 0.2270350000
 C -1.8408490000 -1.2339100000 0.8990180000
 C -0.7924910000 -1.6553260000 -0.0128210000
 H -0.4229910000 -1.2911880000 -2.1393020000
 H -3.6230910000 -0.0016340000 0.6280340000
 H -3.0393260000 -0.8845310000 -1.8463040000
 H -2.2787520000 0.6669730000 -1.6180550000
 H -1.9067840000 -1.5292810000 1.9396550000
 H 0.0171880000 -2.3250100000 0.2550640000
 H -2.2261170000 2.5646720000 0.6087670000
 H -0.8409910000 3.6861280000 0.5721390000
 H -1.3521550000 2.8588380000 -0.9232510000
 O 2.3507680000 -0.2694070000 -0.6462230000
 O 1.5635060000 0.0281540000 1.4714020000
 C 3.4828740000 -1.0421940000 -0.1592040000
 H 4.0680190000 -1.2747970000 -1.0458570000
 H 4.0575940000 -0.4437030000 0.5493560000
 H 3.1243670000 -1.9513010000 0.3270840000

Equilibrium geometry of **r01-endo-3r-prod**.

C 0.0892060000 0.4247190000 -0.5816920000
 N -0.8642780000 1.0453100000 0.4306570000
 H -0.4154210000 0.8676840000 1.3456860000
 H 0.2815490000 1.1453720000 -1.3789990000
 C 1.3809280000 0.0933570000 0.1607040000
 C -1.0655200000 2.5190500000 0.2853990000
 C -0.7353160000 -0.7923630000 -1.1250390000
 C -2.1307130000 -0.1223470000 -1.2045930000
 C -2.1690030000 0.1758250000 0.3002320000
 C -1.8029420000 -1.1665540000 0.8951160000
 C -0.9499880000 -1.7479810000 0.0407510000
 H -0.3117680000 -1.2036900000 -2.0402520000
 H -3.0029940000 0.7313010000 0.7261090000
 H -2.9169420000 -0.8197040000 -1.4968720000
 H -2.1720120000 0.7631700000 -1.8471590000
 H -2.1301240000 -1.5214670000 1.8649180000
 H -0.4329020000 -2.6917630000 0.1701910000
 H -1.7208190000 2.8618750000 1.0876690000
 H -0.0966350000 3.0146560000 0.3655990000
 H -1.5183890000 2.7307350000 -0.6833920000
 O 2.3019790000 -0.3687650000 -0.6605190000
 O 1.4818570000 0.2459360000 1.3626340000
 C 3.5824290000 -0.7282180000 -0.0662530000
 H 4.2137200000 -1.0098650000 -0.9057690000
 H 3.9924820000 0.1298640000 0.4678370000
 H 3.4434700000 -1.5639130000 0.6212940000

Equilibrium geometry of **r01-endo-3r-ts**.

C 0.2505800000 0.7659700000 -0.4067600000
 N -0.5175500000 1.4658800000 0.4425200000
 H -0.3280400000 1.2704600000 1.4247700000
 H 0.3817200000 1.1772200000 -1.4032800000
 C 1.4546700000 0.1106000000 0.2301300000

C -1.1555600000 2.7463000000 0.1279100000
 C -0.7889000000 -0.8661400000 -1.0680800000
 C -2.1577400000 -0.2211300000 -1.1867600000
 C -2.6795500000 -0.3456000000 0.2047500000
 C -1.9303900000 -1.2638400000 0.9036900000
 C -0.8249600000 -1.6417900000 0.1043200000
 H -0.1933300000 -1.1445500000 -1.9316800000
 H -3.5769100000 0.1462900000 0.5640100000
 H -2.7697300000 -0.8593800000 -1.8457500000
 H -2.2031700000 0.7823900000 -1.6154600000
 H -2.1320400000 -1.6260200000 1.9045300000
 H -0.0731000000 -2.3666700000 0.3969100000
 H -2.0787200000 2.8524200000 0.6999600000
 H -0.4837900000 3.5751000000 0.3773000000
 H -1.3855000000 2.7931600000 -0.9379200000
 O 2.3309400000 -0.2719000000 -0.6870100000
 O 1.5422100000 -0.0283500000 1.4306300000
 C 3.5516900000 -0.8888900000 -0.1950000000
 H 4.0742400000 -1.2324600000 -1.0852600000
 H 4.1437600000 -0.1458700000 0.3419000000
 H 3.3091300000 -1.7196900000 0.4692500000

Equilibrium geometry of **r01-endo-3s-mc**.

C 0.4440840000 1.0378020000 0.3607780000
 N -0.3361080000 1.6702270000 -0.4556690000
 C -1.2522390000 2.7677480000 -0.1347590000
 C 1.5129320000 0.1878910000 -0.2705980000
 H 0.4429600000 1.2687030000 1.4196220000
 H -0.2018330000 1.4202230000 -1.4407950000
 C -2.7066380000 -0.4528230000 -0.2509670000
 C -2.3220430000 -0.3553540000 1.1980710000
 C -1.0097780000 -1.0920350000 1.2502950000
 C -0.7801470000 -1.6544950000 0.0272970000
 C -1.8141630000 -1.2403350000 -0.9046390000
 H -3.6059490000 -0.0146890000 -0.6691710000
 H -0.4501740000 -1.2826250000 2.1586040000
 H -3.0623950000 -0.8864320000 1.8181820000
 H -2.3028300000 0.6666710000 1.5986090000
 H 0.0365100000 -2.3223880000 -0.2232490000
 H -1.8599570000 -1.5393230000 -1.9453140000
 H -2.2339690000 2.5595300000 -0.5604320000
 H -1.3261010000 2.8771830000 0.9474280000
 H -0.8566400000 3.6908010000 -0.5691540000
 O 2.3469050000 -0.2795310000 0.6400050000
 O 1.5569610000 0.0421070000 -1.4731100000
 C 3.4705740000 -1.0587920000 0.1439500000
 H 4.0557060000 -1.3038120000 1.0271910000
 H 3.1022920000 -1.9607090000 -0.3483590000
 H 4.0491010000 -0.4603730000 -0.5615090000

Equilibrium geometry of **r01-endo-3s-prod**.

C 0.0884940000 0.4185920000 0.5838570000
 N -0.8629310000 1.0467530000 -0.4257570000
 C -1.0609910000 2.5202540000 -0.2727020000
 C 1.3812850000 0.0914990000 -0.1586820000
 H 0.2805120000 1.1338250000 1.3861610000
 H -0.4139520000 0.8726660000 -1.3414330000
 C -2.1697970000 0.1793300000 -0.3010070000
 C -2.1324470000 -0.1285730000 1.2018850000
 C -0.7382870000 -0.8008770000 1.1183860000
 C -0.9545820000 -1.7482930000 -0.0536150000
 C -1.8063970000 -1.1598640000 -0.9043490000
 H -3.0024030000 0.7395810000 -0.7233400000

H -0.3159360000 -1.2190040000 2.0310460000
H -2.9201690000 -0.8262070000 1.4895350000
H -2.1721400000 0.7530220000 1.8498860000
H -0.4392940000 -2.6923080000 -0.1891460000
H -2.1339970000 -1.5080850000 -1.8764800000
H -1.7152980000 2.8688650000 -1.0732410000
H -1.5135530000 2.7278170000 0.6971660000
H -0.0910330000 3.0141520000 -0.3500250000
O 2.3038630000 -0.3678330000 0.6623800000
O 1.4820140000 0.2456680000 -1.3604070000
C 3.5864430000 -0.7203850000 0.0686610000
H 4.2185880000 -0.9994130000 0.9084600000
H 3.4522620000 -1.5561230000 -0.6197970000
H 3.9925960000 0.1403050000 -0.4644460000

Equilibrium geometry of **r01-endo-3s-ts**.

C 0.2514000000 0.7582900000 0.4131500000
N -0.5138700000 1.4651700000 -0.4325500000
C -1.1480500000 2.7459400000 -0.1115300000
C 1.4555400000 0.1043200000 -0.2242200000
H 0.3795700000 1.1615000000 1.4132800000
H -0.3268000000 1.2729200000 -1.4158500000
C -2.6837400000 -0.3335600000 -0.2078600000
C -2.1592500000 -0.2298000000 1.1844600000
C -0.7946800000 -0.8818200000 1.0558700000
C -0.8359600000 -1.6410900000 -0.1267600000
C -1.9403800000 -1.2463200000 -0.9198200000
H -3.5791100000 0.1677800000 -0.5589300000
H -0.1992400000 -1.1740100000 1.9150400000
H -2.7747000000 -0.8719800000 1.8363400000
H -2.1975500000 0.7687000000 1.6254000000
H -0.0888100000 -2.3661600000 -0.4305300000
H -2.1451900000 -1.5941100000 -1.9251100000
H -2.0692600000 2.8588300000 -0.6853600000
H -1.3808900000 2.7865300000 0.9539400000
H -0.4725900000 3.5739200000 -0.3534200000
O 2.3421700000 -0.2576700000 0.6911700000
O 1.5368600000 -0.0480600000 -1.4235600000
C 3.5616400000 -0.8743500000 0.1954600000
H 4.1627000000 -1.0663300000 1.0815200000
H 3.3209100000 -1.8023400000 -0.3263800000
H 4.0697700000 -0.1888900000 -0.4843100000

Equilibrium geometry of **r01-exo-3r-mc**.

C 0.3755460000 1.0228250000 -0.3262540000
N -0.3399400000 1.6056070000 0.5839670000
H -0.0752300000 1.3739480000 1.5457280000
H 0.2548130000 1.2765270000 -1.3714020000
C 1.5588110000 0.2359240000 0.1700350000
C -1.3657240000 2.6289340000 0.3663150000
C -2.4541390000 -0.8699260000 0.7829810000
C -1.1607780000 -1.6248400000 0.6771460000
C -0.7479080000 -1.3895090000 -0.7492110000
C -1.7465570000 -0.7043730000 -1.3868540000
C -2.7914740000 -0.3723650000 -0.4351700000
H -3.0406230000 -0.8020350000 1.6920810000
H 0.1115440000 -1.8478790000 -1.2237500000
H -1.3378460000 -2.7008720000 0.8362060000
H -0.4102560000 -1.3432480000 1.4269030000
H -1.7774450000 -0.4683720000 -2.4457810000
H -3.6985230000 0.1686750000 -0.6796410000
H -2.2203250000 2.4249430000 1.0105140000
H -0.9457090000 3.6092920000 0.6123520000

H -1.6773900000 2.6130280000 -0.6779960000
O 2.3530060000 -0.1146030000 -0.8240350000
O 1.7152930000 0.0348090000 1.3564890000
C 3.5771070000 -0.8104570000 -0.4551280000
H 4.1097020000 -0.9592030000 -1.3916850000
H 4.1541240000 -0.1940080000 0.2357620000
H 3.3286680000 -1.7640020000 0.0141200000

Equilibrium geometry of **r01-exo-3r-prod**.

C 0.0922300000 0.2947160000 -0.4580570000
N -0.7801770000 0.8723870000 0.6474630000
H -0.1772670000 0.8123250000 1.4883230000
H 0.1266830000 0.9805890000 -1.3053430000
C 1.4882730000 0.1088290000 0.1380940000
C -1.1996360000 2.2924150000 0.4666380000
C -1.9433620000 -0.1701600000 0.8034590000
C -1.1291430000 -1.4570270000 0.6194550000
C -0.6452500000 -1.0489110000 -0.7965110000
C -1.9641680000 -0.6448610000 -1.4383570000
C -2.7401770000 -0.1134580000 -0.4832550000
H -2.4507160000 0.0208380000 1.7481790000
H -0.0157070000 -1.7463810000 -1.3477320000
H -1.7685240000 -0.2339980000 0.6022500000
H -0.3312020000 -1.5918860000 1.3566320000
H -2.1799840000 -0.7202500000 -2.4981920000
H -3.7242360000 0.3269720000 -0.5857530000
H -1.7894040000 2.5953120000 1.3336580000
H -0.3075010000 2.9165220000 0.3929960000
H -1.7956940000 2.3729230000 -0.4420560000
O 2.3598120000 -0.2460170000 -0.7820310000
O 1.7030190000 0.2652600000 1.3263120000
C 3.7270650000 -0.4757220000 -0.3339300000
H 4.2981230000 -0.6382130000 -1.2452740000
H 4.0873160000 0.3983620000 0.2097340000
H 3.7557230000 -1.3561190000 0.3099510000

Equilibrium geometry of **r01-exo-3r-ts**.

C 0.2390100000 0.7183300000 -0.3381500000
N -0.4701700000 1.3793100000 0.5898200000
H -0.1404500000 1.2551000000 1.5448900000
H 0.2557400000 1.1289000000 -1.3415900000
C 1.5424300000 0.1448100000 0.1807600000
C -1.3168000000 2.5331000000 0.2915400000
C -2.3989400000 -0.7739700000 0.8046600000
C -1.0844100000 -1.4608300000 0.6683400000
C -0.6668500000 -1.0704300000 -0.7370800000
C -1.8273300000 -0.6073400000 -1.3818600000
C -2.8504800000 -0.3701800000 -0.4304500000
H -2.9465900000 -0.6923600000 1.7373900000
H 0.1277300000 -1.5753300000 -1.2774300000
H -1.2564300000 -2.5502700000 0.6774900000
H -0.3659300000 -1.2604400000 1.4673300000
H -1.9091100000 -0.4102000000 -2.4463600000
H -3.8158100000 0.0726100000 -0.6448700000
H -2.0235100000 2.6847700000 1.1080400000
H -0.7100100000 3.4370200000 0.1661600000
H -1.8726200000 2.3487100000 -0.6304500000
O 2.3617500000 -0.1647900000 -0.8110900000
O 1.7484600000 0.0129800000 1.3682500000
C 3.6639500000 -0.6889500000 -0.4300500000
H 4.1989800000 -0.8244900000 -1.3674600000
H 4.1737400000 0.0278100000 0.2151500000
H 3.5403300000 -1.6383900000 0.0938900000

Equilibrium geometry of **r01-exo-3s-mc**.

C 0.3750850000 1.0233310000 0.3259650000
 N -0.3407840000 1.6056100000 -0.5842630000
 C -1.3672960000 2.6282480000 -0.3667770000
 C 1.5586370000 0.2368610000 -0.1703690000
 H 0.2543210000 1.2770710000 1.3710970000
 H -0.0760630000 1.3738740000 -1.5460110000
 C -0.7467590000 -1.3898130000 0.7493540000
 C -1.1601310000 -1.6255860000 -0.6767790000
 C -2.4540420000 -0.8715460000 -0.7821140000
 C -2.7911330000 -0.3740370000 0.4361320000
 C -1.7455130000 -0.7051960000 1.3873780000
 H 0.1131640000 -1.8476430000 1.2235750000
 H -3.0410280000 -0.8042030000 -1.6909270000
 H -1.3365840000 -2.7017420000 -0.8356240000
 H -0.4101130000 -1.3436390000 -1.4269310000
 H -3.6984070000 0.1664720000 0.6809820000
 H -1.7760000000 -0.4689680000 2.4462760000
 H -2.2217880000 2.4235440000 -1.0108550000
 H -1.6789190000 2.6123010000 0.6775870000
 H -0.9479950000 3.6088310000 -0.6130950000
 O 2.3530710000 -0.1133130000 0.8236480000
 O 1.7150830000 0.0357260000 -1.3568250000
 C 3.5773590000 -0.8087620000 0.4546890000
 H 4.1098610000 -0.9576140000 1.3912720000
 H 3.3292800000 -1.7622420000 -0.0148790000
 H 4.1543060000 -0.1919360000 -0.2359780000

Equilibrium geometry of **r01-exo-3s-prod**.

C 0.0921210000 0.2950480000 0.4580100000
 N -0.7807870000 0.8719450000 -0.6473410000
 C -1.2010440000 2.2918140000 -0.4665800000
 C 1.4881710000 0.1097730000 -0.1384220000
 H 0.1264110000 0.9810290000 1.3051910000
 H -0.1781390000 0.8120820000 -1.4883430000
 C -0.6443850000 -1.0490240000 0.7968060000
 C -1.1283100000 -1.4577190000 -0.6190390000
 C -1.9434280000 -0.1713430000 -0.8029810000
 C -2.7400770000 -0.1150850000 0.4837390000
 C -1.9635610000 -0.6458950000 1.4388070000
 H -0.0142470000 -1.7459880000 1.3480020000
 H -2.4509560000 0.0193680000 -1.7476670000
 H -1.7670860000 -2.3411800000 -0.6016770000
 H -0.3305050000 -1.5920780000 -1.3563320000
 H -3.7244690000 0.3245880000 0.5862930000
 H -2.1792390000 -0.7214480000 2.4986530000
 H -1.7910960000 2.5941380000 -1.3335960000
 H -1.7969640000 2.3720510000 0.4421640000
 H -0.3092080000 2.9164670000 -0.3931800000
 O 2.3601110000 -0.2441470000 0.7816480000
 O 1.7025570000 0.2655150000 -1.3268330000
 C 3.7273140000 -0.4738550000 0.3332050000
 H 4.2988090000 -0.6360020000 1.2442920000
 H 3.7558330000 -1.3544850000 -0.3104670000
 H 4.0873640000 0.4000200000 -0.2106920000

Equilibrium geometry of **r01-exo-3s-ts**.

C 0.2387000000 0.7180900000 0.3379800000
 N -0.4707000000 1.3789600000 -0.5899600000
 C -1.3180700000 2.5322000000 -0.2917900000
 C 1.5424700000 0.1453800000 -0.1810700000
 H 0.2555200000 1.1288400000 1.3413500000

H -0.1411100000 1.2548000000 -1.5450800000
 C -0.6662700000 -1.0705500000 0.7370300000
 C -1.0843600000 -1.4614400000 -0.6681400000
 C -2.3992900000 -0.7752800000 -0.8038800000
 C -2.8505400000 -0.3717300000 0.4314200000
 C -1.8267700000 -0.6081900000 1.3823700000
 H 0.1287300000 -1.5751700000 1.2770600000
 H -2.9473500000 -0.6938600000 -1.7364000000
 H -1.2558200000 -2.5509700000 -0.6770300000
 H -0.3663900000 -1.2607700000 -1.4675200000
 H -3.8160200000 0.0705600000 0.6462200000
 H -1.9081500000 -0.4110000000 2.4468900000
 H -2.0248500000 2.6834200000 -1.1083200000
 H -1.8737900000 2.3476600000 0.6302400000
 H -0.7118100000 3.4365100000 -0.1665600000
 O 2.3621700000 -0.1633900000 0.8106900000
 O 1.7483900000 0.0134900000 -1.3685700000
 C 3.6649100000 -0.6861500000 0.4295300000
 H 4.2003200000 -0.8206700000 1.3668700000
 H 3.5423200000 -1.6359400000 -0.0940100000
 H 4.1736900000 0.0309700000 -0.2160600000

Equilibrium geometry of **r02-endo-3r-mc**.

C 0.4350440000 1.0061880000 -0.3736500000
 N -0.3246470000 1.6506300000 0.4523330000
 H -0.1717680000 1.4044400000 1.4359830000
 H 0.4167230000 1.2301440000 -1.4338990000
 C 1.5110380000 0.1537320000 0.2461460000
 C -1.2334320000 2.7573930000 0.1438780000
 C -1.0482030000 -1.1161060000 -1.2293990000
 C -2.3498930000 -0.3597030000 -1.1903640000
 C -2.7388520000 -0.4315210000 0.2589910000
 C -1.8581030000 -1.2211380000 0.9255760000
 C -0.8279230000 -1.6631500000 0.0018360000
 H -0.4893750000 -1.3263630000 -2.1339570000
 H -3.6325930000 0.0252610000 0.6687880000
 H -3.0972370000 -0.8863030000 -1.8057380000
 H -2.3131680000 0.6569620000 -1.6031730000
 H -1.9097500000 -1.5040130000 1.9704700000
 H -0.0197000000 -2.3364610000 0.2648780000
 H -2.1900450000 2.5913710000 0.6392500000
 H -0.7896660000 3.6871840000 0.5130690000
 H -1.3748500000 2.8258010000 -0.9348220000
 O 2.3368050000 -0.3079970000 -0.6706770000
 O 1.5611300000 0.0102380000 1.4497750000
 C 3.4973240000 -1.0764730000 -0.1899200000
 C 4.3766520000 -1.3658230000 -1.3842770000
 H 3.9973390000 -0.4717540000 0.5705120000
 H 3.1130590000 -1.9821770000 0.2869890000
 H 5.2548200000 -1.9275840000 -1.0510370000
 H 3.8510130000 -1.9672410000 -2.1312870000
 H 4.7222910000 -0.4405010000 -1.8534890000

Equilibrium geometry of **r02-endo-3r-prod**.

C 0.0653500000 0.3866680000 -0.6021610000
 N -0.8506680000 1.0429660000 0.4221040000
 H -0.3826240000 0.8658190000 1.3282430000
 H 0.2569690000 1.0916710000 -1.4135520000
 C 1.3660670000 0.0343250000 0.1171990000
 C -1.0206500000 2.5188310000 0.2616730000
 C -0.7991520000 -0.8176640000 -1.1096370000
 C -2.1804350000 -0.1169720000 -1.1676100000
 C -2.1774320000 0.2028660000 0.3334060000

C -1.8294300000 -1.1395340000 0.9387920000
C -1.0093180000 -1.7518830000 0.0738670000
H -0.4060420000 -1.2516060000 -2.0279320000
H -2.9883470000 0.7838080000 0.7696790000
H -2.9890810000 -0.7996870000 -1.4321700000
H -2.2158190000 0.7604990000 -1.8212990000
H -2.1415140000 -1.4733540000 1.9209910000
H -0.5101370000 -2.7048780000 0.2060340000
H -1.6512670000 2.8877900000 1.0720690000
H -0.0387890000 2.9919240000 0.3159770000
H -1.4876370000 2.7292550000 -0.7007280000
O 2.2603270000 -0.4506510000 -0.7162730000
O 1.4875600000 0.1963930000 1.3173250000
C 3.5662630000 -0.8326020000 -0.1491140000
C 4.4678290000 -1.2112180000 -1.3010010000
H 3.9379880000 0.0216880000 0.4210960000
H 3.3900720000 -1.6602290000 0.5424520000
H 5.4463370000 -1.5017520000 -0.9061400000
H 4.0629360000 -2.0574880000 -1.8633900000
H 4.6127190000 -0.3700780000 -1.9848190000

Equilibrium geometry of **r02-endo-3r-ts**.

C 0.2425335692 0.7275107229 -0.4268851654
N -0.5063002795 1.4534310254 0.4187302294
H -0.3113829687 1.2662342793 1.4015743968
H 0.3703711518 1.1224568366 -1.4304734501
C 1.4437033573 0.0625036589 0.2088493542
C -1.1197558869 2.7425244946 0.0921300076
C -0.8284542055 -0.8959633031 -1.0429030649
C -2.1860809996 -0.2276684752 -1.1656064511
C -2.6975403088 -0.3109858944 0.2329506470
C -1.9623618871 -1.2307415165 0.9447895592
C -0.8714365023 -1.6476072429 0.1452553154
H -0.2459778161 -1.2050637846 -1.9050550449
H -3.5807928770 0.2080274831 0.5890578158
H -2.8161342265 -0.8680584826 -1.8050356281
H -2.2147847588 0.7672390057 -1.6151658794
H -2.1628318585 -1.5671721963 1.9548169958
H -0.1318680646 -2.3807799840 0.4480264892
H -2.0385723266 2.8741435178 0.6660381545
H -0.4307726176 3.5608556424 0.3286637674
H -1.3532849956 2.7812944883 -0.9733060475
O 2.3170390217 -0.3226755372 -0.7060775856
O 1.5248135916 -0.0760909843 1.4109768061
C 3.5468385492 -0.9622634490 -0.2162340255
C 4.4072830230 -1.2746262649 -1.4191358997
H 4.0243875989 -0.2673715046 0.4783815550
H 3.2546631795 -1.8567368476 0.3404648457
H 5.3306255794 -1.7559972990 -1.0824163063
H 3.8982931634 -1.9569422301 -2.1060918159
H 4.6759259545 -0.3638692298 -1.9617145512

Equilibrium geometry of **r02-endo-3s-mc**.

C 0.4385110000 1.0484020000 0.3606880000
N -0.3412500000 1.6684310000 -0.4647750000
C -1.2704990000 2.7588140000 -0.1588580000
C 1.5215900000 0.2044670000 -0.2586180000
H 0.4268320000 1.2854860000 1.4181990000
H -0.1973000000 1.4106180000 -1.4467910000
C -2.7137140000 -0.4604930000 -0.2411900000
C -2.3254220000 -0.3606830000 1.2067820000
C -1.0101730000 -1.0925610000 1.2558160000
C -0.7795000000 -1.6516840000 0.0321360000

C -1.8183350000 -1.2419740000 -0.8973840000
H -3.6163940000 -0.0268790000 -0.6567230000
H -0.4472150000 -1.2792880000 2.1629740000
H -3.0628530000 -0.8916650000 1.8303350000
H -2.3068600000 0.6625260000 1.6047330000
H 0.0413940000 -2.3131100000 -0.2216580000
H -1.8647520000 -1.5401810000 -1.9382890000
H -2.2468700000 2.5372050000 -0.5900640000
H -1.3538960000 2.8750780000 0.9218830000
H -0.8811910000 3.6826190000 -0.5969640000
O 2.3637700000 -0.2310410000 0.6560650000
O 1.5620760000 0.0453290000 -1.4605910000
C 3.5309180000 -0.9884410000 0.1736360000
C 4.4112640000 -1.2756960000 1.3677460000
H 3.1549930000 -1.8950640000 -0.3080320000
H 4.0267920000 -0.3760130000 -0.5833810000
H 5.2941040000 -1.8291870000 1.0330190000
H 4.7492210000 -0.3498230000 1.8414330000
H 3.8895340000 -1.8844940000 2.1115560000

Equilibrium geometry of **r02-endo-3s-prod**.

C 0.0773760000 0.4235510000 0.5981660000
N -0.8579690000 1.0478870000 -0.4288010000
C -1.0555990000 2.5222850000 -0.2873660000
C 1.3797200000 0.0860410000 -0.1256790000
H 0.2602970000 1.1439840000 1.3978660000
H -0.3925090000 0.8675540000 -1.3355790000
C -2.1673060000 0.1840510000 -0.3192100000
C -2.1546450000 -0.1144650000 1.1860440000
C -0.7606820000 -0.7894300000 1.1286880000
C -0.9605760000 -1.7447480000 -0.0400690000
C -1.7974230000 -1.1601590000 -0.9079810000
H -2.9923940000 0.7422940000 -0.7586350000
H -0.3533050000 -1.2023430000 2.0504690000
H -2.9483780000 -0.8085850000 1.4656270000
H -2.2025420000 0.7713330000 1.8276730000
H -0.4445250000 -2.6901850000 -0.1614900000
H -2.1098500000 -1.5133950000 -1.8831980000
H -1.6986150000 2.8674510000 -1.0985350000
H -1.5204090000 2.7368820000 0.6751720000
H -0.0836010000 3.0136680000 -0.3550890000
O 2.2864330000 -0.3780750000 0.7061380000
O 1.4917520000 0.2400430000 -1.3277800000
C 3.5937100000 -0.7459160000 0.1327010000
C 4.5023580000 -1.1228100000 1.2794810000
H 3.4224510000 -1.5710380000 -0.5630660000
H 3.9562930000 0.1147260000 -0.4338350000
H 5.4818230000 -1.4032740000 0.8798630000
H 4.6426890000 -0.2840460000 1.9671690000
H 4.1062170000 -1.9751330000 1.8388260000

Equilibrium geometry of **r02-endo-3s-ts**.

C 0.2472681032 0.7658470802 0.4202503193
N -0.5193266608 1.4688157851 -0.4289496398
C -1.1567390079 2.7487035180 -0.1121928572
C 1.4545267073 0.1141076630 -0.2178716091
H 0.3757266654 1.1750122250 1.4180802240
H -0.3254997729 1.2756957766 -1.4109083737
C -2.6747921423 -0.3418896485 -0.2155147710
C -2.1620418942 -0.2253953162 1.1801913465
C -0.7906893050 -0.8667607041 1.0650403491
C -0.8204995937 -1.6381209051 -0.1110529780
C -1.9215273057 -1.2569252211 -0.9145819268

H -3.5699168979 0.1520345872 -0.5778181549
H -0.2004289764 -1.1502347102 1.9307590818
H -2.7767292176 -0.8691035842 1.8311727512
H -2.2116718004 0.7755784250 1.6144579215
H -0.0661498124 -2.3604085667 -0.4036630617
H -2.1168690096 -1.6136529817 -1.9186944743
H -2.0776192858 2.8582762068 -0.6873459789
H -1.3911062832 2.7917174579 0.9528985063
H -0.4833060412 3.5780353670 -0.3553496359
O 2.3408303036 -0.2494722117 0.6933897620
O 1.5285313135 -0.0346134003 -1.4192914670
C 3.5737592068 -0.8794591331 0.1987096058
C 4.4430403601 -1.1824717894 1.3978253782
H 3.2863658364 -1.7774040384 -0.3551476123
H 4.0419883154 -0.1816785031 -0.4995982345
H 5.3670451702 -1.6599879184 1.0573301943
H 4.7098677086 -0.2681964297 1.9355464044
H 3.9419297308 -1.8651948060 2.0902874099

Equilibrium geometry of **r02-exo-3r-mc**.

C 0.3752960000 1.0246900000 -0.3296400000
N -0.3371320000 1.6052050000 0.5835340000
H -0.0678120000 1.3688810000 1.5432500000
H 0.2491400000 1.2779450000 -1.3743280000
C 1.5611120000 0.2364610000 0.1637770000
C -1.3659980000 2.6267010000 0.3739650000
C -2.4589430000 -0.8746390000 0.7827990000
C -1.1662540000 -1.6309230000 0.6757210000
C -0.7549790000 -1.3972060000 -0.7512520000
C -1.7510500000 -0.7082510000 -1.3873390000
C -2.7954880000 -0.3751030000 -0.4343400000
H -3.0451380000 -0.8071510000 1.6920960000
H 0.1057870000 -1.8540000000 -1.2249700000
H -1.3428950000 -2.7065440000 0.8375590000
H -0.4135700000 -1.3474460000 1.4227290000
H -1.7816760000 -0.4699060000 -2.4457610000
H -3.7015090000 0.1681300000 -0.6780600000
H -2.2184460000 2.4170220000 1.0192150000
H -0.9480320000 3.6067170000 0.6245070000
H -1.6803310000 2.6157120000 -0.6696130000
O 2.3591660000 -0.1023790000 -0.8274830000
O 1.7092400000 0.0324040000 1.3519880000
C 3.6123470000 -0.7866150000 -0.4628980000
C 4.4344720000 -0.9302290000 -1.7231030000
H 4.1051280000 -0.1795220000 0.3001120000
H 3.3399170000 -1.7475960000 -0.0186040000
H 5.3773130000 -1.4282080000 -1.4768000000
H 3.9150620000 -1.5343960000 -2.4722590000
H 4.6676400000 0.0469150000 -2.1551250000

Equilibrium geometry of **r02-exo-3r-prod**.

C 0.0808030000 0.2839840000 -0.4717620000
N -0.7728160000 0.8733450000 0.6422110000
H -0.1566080000 0.8111230000 1.4739200000
H 0.1119360000 0.9667210000 -1.3216710000
C 1.4827300000 0.0846040000 0.1100190000
C -1.1828590000 2.2957970000 0.4615500000
C -1.9415600000 -0.1582530000 0.8183740000
C -1.1414120000 -1.4529540000 0.6275510000
C -0.6732210000 -1.0531540000 -0.7961330000
C -1.9976020000 -0.6406260000 -1.4211630000
C -2.7561400000 -0.0998910000 -0.4573230000
H -2.4348200000 0.0396490000 1.7691880000

H -0.0571490000 -1.7578090000 -1.3533520000
H -1.7889860000 -2.3300480000 0.6218840000
H -0.3348580000 -1.5925530000 1.3542960000
H -2.2289540000 -0.7179500000 -2.4775700000
H -3.7378750000 0.3484120000 -0.5473630000
H -1.7584490000 2.6071300000 1.3350750000
H -0.2864060000 2.9119750000 0.3736220000
H -1.7900140000 2.3781320000 -0.4395930000
O 2.3368910000 -0.2919820000 -0.8138600000
O 1.7070470000 0.2513960000 1.2964210000
C 3.7254680000 -0.5431900000 -0.3854800000
C 4.5479100000 -0.7719820000 -1.6329220000
H 4.0546700000 0.3255480000 0.1884630000
H 3.7080750000 -1.4128350000 0.2762270000
H 5.5864280000 -0.9620280000 -1.3445940000
H 4.1862930000 -1.6373630000 -2.1954860000
H 4.5291230000 0.1066220000 -2.2836720000

Equilibrium geometry of **r02-exo-3r-ts**.

C 0.2355953914 0.7098652854 -0.3410127214
N -0.4709535836 1.3741873346 0.5874724428
H -0.1369127462 1.2508103781 1.5412899331
H 0.2526923343 1.1210476317 -1.3442860978
C 1.5417358898 0.1363460526 0.1775381749
C -1.3124155913 2.5315751580 0.2897751361
C -2.4021751770 -0.7685689779 0.8071872111
C -1.0895937222 -1.4590930093 0.6713646540
C -0.6717171141 -1.0708830851 -0.7347893633
C -1.8327027673 -0.6089370835 -1.3802106961
C -2.8545178109 -0.3678112922 -0.4287535421
H -2.9486521747 -0.6830902015 1.7402661450
H 0.1215401606 -1.5785607654 -1.2744869261
H -1.2645244334 -2.5480398479 0.6816261417
H -0.3697098065 -1.2592229498 1.4691687600
H -1.9148270935 -0.4135404918 -2.4449893030
H -3.8191787525 0.0764060314 -0.6432173545
H -2.0168448951 2.6874133472 1.1075565290
H -0.7020218680 3.4328393848 0.1622840239
H -1.8712164631 2.3490545815 -0.6308208314
O 2.3577577788 -0.1739783316 -0.8131287492
O 1.7433036210 0.0087720326 1.3672833241
C 3.6805298935 -0.7024128050 -0.4444678491
C 4.4692514524 -0.8709529009 -1.7234585170
H 4.1385768566 0.0093745378 0.2460987372
H 3.5218135202 -1.6454053943 0.0852964476
H 5.4639025119 -1.2589997758 -1.4835308799
H 3.9817400328 -1.5776330816 -2.4013696106
H 4.5908975797 0.0857647593 -2.2391538802

Equilibrium geometry of **r02-exo-3s-mc**.

C 0.3746720000 1.0258520000 0.3289870000
N -0.3383190000 1.6056100000 -0.5842360000
C -1.3679730000 2.6263140000 -0.3747580000
C 1.5608950000 0.2382160000 -0.1644440000
H 0.2485110000 1.2792580000 1.3736290000
H -0.0689390000 1.3692680000 -1.5438890000
C -0.7528110000 -1.3971840000 0.7515800000
C -1.1648750000 -1.6318430000 -0.6750120000
C -2.4584640000 -0.8769730000 -0.7814210000
C -2.7946330000 -0.3772600000 0.4357460000
C -1.7491100000 -0.7089610000 1.3880940000
H 0.1088040000 -1.8528520000 1.2248190000
H -3.0453910000 -0.8104550000 -1.6903070000

H -1.3404410000 -2.7076960000 -0.8364080000
H -0.4130460000 -1.3477220000 -1.4226070000
H -3.7010320000 0.1651370000 0.6799310000
H -1.7791720000 -0.4701910000 2.4464340000
H -2.2204300000 2.4156900000 -1.0196220000
H -1.6819350000 2.6155160000 0.6689440000
H -0.9508160000 3.6065500000 -0.6257840000
O 2.3591560000 -0.1002280000 0.8267900000
O 1.7090030000 0.0341130000 -1.3526490000
C 3.6123750000 -0.7843190000 0.4622060000
C 4.4344750000 -0.9279000000 1.7224390000
H 3.3400390000 -1.7453170000 0.0178290000
H 4.1051420000 -0.1771480000 -0.3007770000
H 5.3773930000 -1.4257890000 1.4761260000
H 4.6675630000 0.0492780000 2.1544950000
H 3.9150930000 -1.5321310000 2.4715770000

Equilibrium geometry of **r02-exo-3s-prod.**

C 0.0805660000 0.2785810000 0.4722180000
N -0.7717580000 0.8722910000 -0.6404760000
C -1.1768050000 2.2957610000 -0.4572640000
C 1.4823980000 0.0795500000 -0.1100730000
H 0.1126750000 0.9592020000 1.3237420000
H -0.1559580000 0.8092930000 -1.4724400000
C -0.6769470000 -1.0574800000 0.7935460000
C -1.1471250000 -1.4526480000 -0.6307510000
C -1.9435830000 -0.1551930000 -0.8182130000
C -2.7572720000 -0.0971660000 0.4580810000
C -1.9998410000 -0.6423930000 1.4202360000
H -0.0628220000 -1.7653740000 1.3488810000
H -2.4368840000 0.0460650000 -1.7683280000
H -1.7972150000 -2.3279300000 -0.6266960000
H -0.3413110000 -1.5929240000 -1.3582320000
H -3.7375240000 0.3540790000 0.5497450000
H -2.2308550000 -0.7213270000 2.4766250000
H -1.7512170000 2.6106370000 -1.3302530000
H -1.7836440000 2.3785550000 0.4440340000
H -0.2782610000 2.9086610000 -0.3680670000
O 2.3384310000 -0.2930840000 0.8136230000
O 1.7055020000 0.2451940000 -1.2969250000
C 3.7282120000 -0.5369110000 0.3846150000
C 4.5537370000 -0.7550250000 1.6319970000
H 3.7159020000 -1.4093640000 -0.2735690000
H 4.0510550000 0.3318050000 -0.1929990000
H 5.5932530000 -0.9388230000 1.3431560000
H 4.5294990000 0.1259290000 2.2793230000
H 4.1987670000 -1.6205830000 2.1983050000

Equilibrium geometry of **r02-exo-3s-ts.**

C 0.2353281426 0.7104263694 0.3407336682
N -0.4718759836 1.3740846056 -0.5877071039
C -1.3141376190 2.5308845528 -0.2900137468
C 1.5416826719 0.1375939745 -0.1780391659
H 0.2524271102 1.1218430609 1.3439110058
H -0.1380698239 1.2506726723 -1.5415997787
C -0.6707251171 -1.0708621528 0.7352598616
C -1.0886593106 -1.4598483055 -0.6706589774
C -2.4018304864 -0.7704171657 -0.8063816440
C -2.8541307551 -0.3695124028 0.4295177344
C -1.8318688061 -0.6095058576 1.3807963965
H 0.1230257246 -1.5777830326 1.2749397229
H -2.9486182591 -0.6857076913 -1.7393460762
H -1.2627138427 -2.5489383787 -0.6805499207

H -0.3691449520 -1.2596452851 -1.4687138299
H -3.8190662240 0.0740613409 0.6440775313
H -1.9138649169 -0.4137750880 2.4455238162
H -2.0187433971 2.6861809417 -1.1077467931
H -1.8727327660 2.3480191566 0.6306394046
H -0.7043767489 3.4325917517 -0.1626255843
O 2.3582079642 -0.1718874646 0.8124738317
O 1.7429709681 0.0097901063 -1.3678066588
C 3.6812021788 -0.6995880552 0.4435740357
C 4.4702442543 -0.8676885147 1.7224180160
H 3.5229272464 -1.6426617773 -0.0861711476
H 4.1387372467 0.0124563229 -0.2470642173
H 5.4650428574 -1.2552437965 1.4823114096
H 4.5915091981 0.0890993379 2.2380665976
H 3.9832121595 -1.5745896516 2.4004369414

Equilibrium geometry of **r03-endo-3r-mc.**

C 0.4300260000 1.0699920000 -0.3559190000
N -0.3575720000 1.6758190000 0.4717340000
H -0.2098470000 1.4130160000 1.4521470000
H 0.4146330000 1.3104160000 -1.4126630000
C 1.5239440000 0.2344430000 0.2612230000
C -1.3053510000 2.7513190000 0.1713170000
C -1.0060890000 -1.0866370000 -1.2715670000
C -2.3324650000 -0.3768350000 -1.2064300000
C -2.7080400000 -0.4945430000 0.2438330000
C -1.7935470000 -1.2638080000 0.8871910000
C -0.7544080000 -1.6482270000 -0.0538310000
H -0.4462910000 -1.2551110000 -2.1842520000
H -3.6149990000 -0.0800090000 0.6693350000
H -3.0665260000 -0.9130810000 -1.8293850000
H -2.3321030000 0.6502630000 -1.5952030000
H -1.8254100000 -1.5695850000 1.9264550000
H 0.0812430000 -2.2951260000 0.1887370000
H -2.2794960000 2.5074340000 0.5955840000
H -0.9357780000 3.6782870000 0.6198490000
H -1.3857960000 2.8757940000 -0.9088140000
O 2.3671220000 -0.1865950000 -0.6555980000
O 1.5540600000 0.0725590000 1.4644960000
C 3.5682100000 -0.9477870000 -0.2031940000
C 3.9652480000 -1.8164600000 -1.3812990000
C 4.6308240000 0.0498860000 0.2303720000
H 3.2401850000 -1.5519910000 0.6462570000
H 4.8346900000 -2.4203540000 -1.1048630000
H 3.1559160000 -2.4943330000 -1.6676740000
H 4.2360880000 -1.2043430000 -2.2470910000
H 5.5234710000 -0.4934150000 0.5551680000
H 4.9121270000 0.7036140000 -0.6010950000
H 4.2846870000 0.6586020000 1.0699940000

Equilibrium geometry of **r03-endo-3r-prod.**

C 0.0892290000 0.4330990000 -0.5877720000
N -0.8444120000 1.0432700000 0.4488640000
H -0.3798240000 0.8400200000 1.3518530000
H 0.2790940000 1.1666410000 -1.3735000000
C 1.3863970000 0.0637910000 0.1326810000
C -1.0343990000 2.5206080000 0.3348370000
C -0.7561470000 -0.7649610000 -1.1414970000
C -2.1461440000 -0.0815510000 -1.1883380000
C -2.1586740000 0.1897970000 0.3220960000
C -1.7982050000 -1.1672620000 0.8864630000
C -0.9634710000 -1.7406340000 0.0092350000
H -0.3495780000 -1.1632870000 -2.0699600000

H -2.9810010000 0.7448310000 0.7706440000
H -2.9431740000 -0.7664860000 -1.4805890000
H -2.1884690000 0.8154170000 -1.8147140000
H -2.1134920000 -1.5357040000 1.8550740000
H -0.4523080000 -2.6905320000 0.1146310000
H -1.6726140000 2.8548450000 1.1543190000
H -0.0598260000 3.0060640000 0.4068880000
H -1.5017290000 2.7546360000 -0.6219550000
O 2.2917640000 -0.3723330000 -0.7118800000
O 1.4780300000 0.1645410000 1.3435970000
C 3.6035130000 -0.8323730000 -0.1686520000
C 4.1676900000 -1.7624980000 -1.2256090000
C 4.4728230000 0.3788940000 0.1254220000
H 3.3724840000 -1.3715740000 0.7536800000
H 5.1129480000 -2.1829200000 -0.8691010000
H 3.4839170000 -2.5899830000 -1.4353010000
H 4.3640220000 -1.2228910000 -2.1574460000
H 5.4392730000 0.0402670000 0.5122330000
H 4.6557210000 0.9588630000 -0.7849180000
H 4.0170210000 1.0234970000 0.8813600000

Equilibrium geometry of **r03-endo-3r-ts**.

C 0.2482916243 0.7640927538 -0.4066398338
N -0.5202130116 1.4632691636 0.4437233696
H -0.3314951695 1.2623479794 1.4250737115
H 0.3787193053 1.1789273275 -1.4018852564
C 1.4564719201 0.1071089944 0.2288691741
C -1.1557032391 2.7452391185 0.1326763790
C -0.7846511453 -0.8656259587 -1.0607641044
C -2.1541537759 -0.2231380091 -1.1904029360
C -2.6838596209 -0.3430905934 0.1986083912
C -1.9386881219 -1.2588139030 0.9046827690
C -0.8277666247 -1.6382893413 0.1136711866
H -0.1848410594 -1.1482219018 -1.9201041702
H -3.5829586215 0.1505200730 0.5511414325
H -2.7617166021 -0.8638582124 -1.8509304029
H -2.1974468009 0.7792977231 -1.6219732896
H -2.1455662268 -1.6171505158 1.9058395559
H -0.0764029867 -2.3601826090 0.4143381185
H -2.0776581887 2.8526644181 0.7065373925
H -0.4823431828 3.5730529281 0.3813131659
H -1.3881696549 2.7939943498 -0.9326017487
O 2.3394841298 -0.2435327582 -0.6873223616
O 1.5180432275 -0.0535518996 1.4306777558
C 3.6030486076 -0.8859856467 -0.2336776216
C 4.0646201642 -1.7377269892 -1.4014097666
C 4.5823554313 0.2050429467 0.1686803308
H 3.3392858226 -1.5007281523 0.6303791004
H 4.9895977884 -2.2554326845 -1.1299930964
H 3.3182351775 -2.4928519395 -1.6660587158
H 4.2647309040 -1.1181364956 -2.2811102156
H 5.5267675986 -0.2518364593 0.4805694996
H 4.7870830530 0.8715287703 -0.6751770436
H 4.1994009345 0.7920149147 1.0079404655

Equilibrium geometry of **r03-endo-3s-mc**.

C 0.4175080000 1.1390850000 0.2974090000
N -0.4085880000 1.6933820000 -0.5294520000
C -1.3824770000 2.7477600000 -0.2377590000
C 1.5294250000 0.3266490000 -0.3183340000
H 0.4181410000 1.4134440000 1.3459950000
H -0.2736780000 1.4080420000 -1.5051920000
C -2.6802870000 -0.5438000000 -0.1557640000

C -2.2557630000 -0.3639390000 1.2743610000
C -0.9035770000 -1.0257980000 1.3118350000
C -0.6792460000 -1.6220440000 0.1048160000
C -1.7644580000 -1.3043910000 -0.8077310000
H -3.6155700000 -0.1733760000 -0.5600230000
H -0.3045120000 -1.1444480000 2.2071690000
H -2.9466180000 -0.9036160000 1.9421180000
H -2.2775590000 0.6754440000 1.6280590000
H 0.1688830000 -2.2484550000 -0.1479340000
H -1.8248160000 -1.6465730000 -1.8342490000
H -2.3536690000 2.4706650000 -0.6481610000
H -1.4562060000 2.8881090000 0.8408440000
H -1.0425740000 3.6771260000 -0.7045420000
O 2.4065560000 -0.0326170000 0.5933160000
O 1.5419380000 0.1288190000 -1.5163810000
C 3.6292920000 -0.7590030000 0.1417140000
C 4.0572990000 -1.6073200000 1.3237660000
H 3.3192010000 -1.3775220000 -0.7038430000
C 4.6569470000 0.2720760000 -0.2976920000
H 4.9541500000 -2.1731380000 1.0542470000
H 4.2952040000 -0.9814800000 2.1894430000
H 3.2771100000 -2.3198460000 1.6074300000
H 5.5680040000 -0.2412440000 -0.6204010000
H 4.2898050000 0.8652930000 -1.1397660000
H 4.9149320000 0.9392650000 0.5306870000

Equilibrium geometry of **r03-endo-3s-prod**.

C 0.1085830000 0.5242050000 0.5610250000
N -0.8768520000 1.0489860000 -0.4747350000
C -1.1367930000 2.5187440000 -0.4136110000
C 1.4021730000 0.1789010000 -0.1777470000
H 0.2857750000 1.2994020000 1.3090990000
H -0.4237400000 0.8346340000 -1.3810010000
C -2.1462390000 0.1422920000 -0.2825230000
C -2.0876180000 -0.0640270000 1.2369790000
C -0.6687380000 -0.6840790000 1.1850520000
C -0.8551100000 -1.7163170000 0.0810820000
C -1.7359800000 -1.2205920000 -0.7984510000
H -3.0032380000 0.6389810000 -0.7346830000
H -0.2251270000 -1.0252240000 2.1194740000
H -2.8449150000 -0.7722700000 1.5758060000
H -2.1596470000 0.8552550000 1.8277610000
H -0.3022470000 -2.6453280000 0.0043390000
H -2.0561650000 -1.6434010000 -1.7429350000
H -1.8043730000 2.7888230000 -1.2334040000
H -1.5993800000 2.7676380000 0.5418100000
H -0.1892140000 3.0488880000 -0.5228740000
O 2.3349520000 -0.2151460000 0.6578900000
O 1.4684980000 0.2567470000 -1.3918290000
C 3.6446280000 -0.6590770000 0.0966820000
C 4.2370270000 -1.5804170000 1.1459880000
H 3.4074310000 -1.2030420000 -0.8211580000
C 4.4919010000 0.5636930000 -0.2124660000
H 5.1822530000 -1.9881620000 0.7750470000
H 4.4403660000 -1.0378270000 2.0745140000
H 3.5674760000 -2.4168760000 1.3660390000
H 5.4550810000 0.2386350000 -0.6183970000
H 4.0123020000 1.2026810000 -0.9585820000
H 4.6843200000 1.1458360000 0.6944600000

Equilibrium geometry of **r03-endo-3s-ts**.

C 0.2474783002 0.8525840062 0.3737303011
N -0.5602551497 1.4968060622 -0.4852554982

C -1.2523895606 2.7547894979 -0.1999558024
 C 1.4635348719 0.2187034689 -0.2723341978
 H 0.3894687337 1.3115351254 1.3479530060
 H -0.3788711563 1.2746556730 -1.4633047719
 C -2.6383562122 -0.4276137825 -0.1520905309
 C -2.1071502801 -0.1969065897 1.2217352192
 C -0.7050799562 -0.7707033826 1.1170499063
 C -0.7141469434 -1.6126494952 -0.0103052644
 C -1.8485716949 -1.3404016355 -0.8119932538
 H -3.5644781239 -0.0039998940 -0.5254780222
 H -0.0927110080 -0.9805604089 1.9884680956
 H -2.6735748303 -0.8293479126 1.9254179791
 H -2.2023521693 0.8257168861 1.5932274572
 H 0.0734326734 -2.3103153509 -0.2734782778
 H -2.0417563151 -1.7664221372 -1.7890142065
 H -2.2102482188 2.7814642049 -0.7225712041
 H -1.4258304639 2.8458611929 0.8738275924
 H -0.6440717294 3.6049651714 -0.5284249608
 O 2.3733654357 -0.0963377615 0.6304581847
 O 1.5063643103 0.0403623592 -1.4725252086
 C 3.6436204888 -0.7104441722 0.1557454566
 C 4.1386005717 -1.5622143897 1.3097836280
 H 3.3808654964 -1.3238212893 -0.7094913211
 C 4.5944087686 0.4034940193 -0.2510177310
 H 5.0680322666 -2.0617766133 1.0198815609
 H 4.3419228915 -0.9462609187 2.1913009047
 H 3.4103987030 -2.3330213667 1.5801936338
 H 5.5438901302 -0.0314332343 -0.5788768594
 H 4.1889607191 0.9886530620 -1.0812527761
 H 4.7967610028 1.0685811600 0.5946049902

Equilibrium geometry of **r03-exo-3r-mc**.

C 0.3717620000 1.0419300000 -0.3247810000
 N -0.3509170000 1.6153770000 0.5841540000
 H -0.0824310000 1.3813420000 1.5448200000
 H 0.2458850000 1.2911110000 -1.3705320000
 C 1.5666610000 0.2671790000 0.1748710000
 C -1.3928480000 2.6222810000 0.3697680000
 C -2.4564410000 -0.8919280000 0.7716920000
 C -1.1533930000 -1.6322390000 0.6769620000
 C -0.7343550000 -1.3983750000 -0.7477040000
 C -1.7320110000 -0.7214010000 -1.3929900000
 C -2.7884950000 -0.3986210000 -0.4489180000
 H -3.0509780000 -0.8297310000 1.6759140000
 H 0.1372160000 -1.8438430000 -1.2121550000
 H -1.3163950000 -2.7092920000 0.8432580000
 H -0.4092270000 -1.3342720000 1.4269390000
 H -1.7564860000 -0.4847320000 -2.4519370000
 H -3.6986700000 0.1336810000 -0.7012500000
 H -2.2442840000 2.4024090000 1.0129320000
 H -0.9890000000 3.6084310000 0.6194320000
 H -1.7041900000 2.6049590000 -0.6746980000
 O 2.3677840000 -0.0599950000 -0.8144060000
 O 1.7011170000 0.0653800000 1.3663920000
 C 3.6546700000 -0.7389710000 -0.4784290000
 C 4.0337750000 -1.5234970000 -1.7197290000
 C 4.6645760000 0.3243460000 -0.0758960000
 H 3.4356540000 -1.4008100000 0.3628940000
 H 4.9666690000 -2.0634620000 -1.5319440000
 H 3.2642670000 -2.2561520000 -1.9806200000
 H 4.1896000000 -0.8562070000 -2.5728940000
 H 5.6189100000 -0.1571000000 0.1588340000
 H 4.8303250000 1.0309280000 -0.8950890000
 H 4.3366260000 0.8698790000 0.8130580000

Equilibrium geometry of **r03-exo-3r-prod**.

C 0.0938750000 0.2911880000 -0.4605560000
 N -0.7591620000 0.8595810000 0.6649720000
 H -0.1457940000 0.7665780000 1.4965600000
 H 0.1408810000 0.9986540000 -1.2892760000
 C 1.4905410000 0.0546510000 0.1247690000
 C -1.1534790000 2.2901190000 0.5212810000
 C -1.9395470000 -0.1630440000 0.8081880000
 C -1.1541400000 -1.4611360000 0.5826390000
 C -0.6757990000 -1.0255490000 -0.8272280000
 C -1.9930590000 -0.5797090000 -1.4445770000
 C -2.7491620000 -0.0588860000 -0.4678960000
 H -2.4336850000 0.0134350000 1.7627330000
 H -0.0660650000 -1.7209910000 -1.4027270000
 H -1.8120710000 -2.3301080000 0.5497750000
 H -0.3512070000 -1.6309860000 1.3066330000
 H -2.2213490000 -0.6233420000 -2.5035710000
 H -3.7253670000 0.4032180000 -0.5478130000
 H -1.7281140000 2.5846290000 1.4012890000
 H -0.2508880000 2.8995820000 0.4511870000
 H -1.7575120000 2.4030320000 -0.3787360000
 O 2.3437980000 -0.2979500000 -0.8057610000
 O 1.6968020000 0.1732300000 1.3218620000
 C 3.7474480000 -0.6135870000 -0.4006440000
 C 4.2873790000 -1.5042540000 -1.5028620000
 C 4.5102260000 0.6874260000 -0.2161970000
 H 3.6702410000 -1.1521520000 0.5470220000
 H 5.3082350000 -1.8087770000 -1.2529910000
 H 3.6818000000 -2.4077330000 -1.6186780000
 H 4.3133550000 -0.9715870000 -2.4585680000
 H 5.5451560000 0.4605360000 0.0590000000
 H 4.5248760000 1.2657290000 -1.1454970000
 H 4.0773110000 1.2944320000 0.5831380000

Equilibrium geometry of **r03-exo-3r-ts**.

C 0.2353053948 0.7132150478 -0.3389183537
 N -0.4740756108 1.3752825318 0.5896781790
 H -0.1416292591 1.2496537643 1.5436573007
 H 0.2544184840 1.1278069015 -1.3408431360
 C 1.5441709762 0.1419092506 0.1812762701
 C -1.3175424514 2.5308848031 0.2923517265
 C -2.3999433711 -0.7722880650 0.8043735516
 C -1.0847873325 -1.4576118726 0.6683318953
 C -0.6664172108 -1.0636111438 -0.7362305375
 C -1.8287698298 -0.6047853113 -1.3819028257
 C -2.8524980167 -0.3700777855 -0.4310387754
 H -2.9476564800 -0.6908495481 1.7370857196
 H 0.1287085790 -1.5679115464 -1.2762200236
 H -1.2554186358 -2.5472347096 0.6757200686
 H -0.3661357535 -1.2564558447 1.4668661547
 H -1.9103761345 -0.4066615472 -2.4462018160
 H -3.8185034359 0.0713208489 -0.6452745443
 H -2.0207967897 2.6867153159 1.1111908345
 H -0.7091790287 3.4332274070 0.1624529083
 H -1.8779854425 2.3465773043 -0.6269621009
 O 2.3618502511 -0.1562613880 -0.8087695040
 O 1.7312245004 0.0053176985 1.3737843016
 C 3.7036311438 -0.7050222408 -0.4653306673
 C 4.1435340407 -1.4870831705 -1.6889883817
 C 4.6254036128 0.4455047249 -0.0972616127
 H 3.5494532593 -1.3635037853 0.3935005441
 H 5.1089788196 -1.9607786645 -1.4868366246
 H 3.4263160285 -2.2740303351 -1.9406817461
 H 4.2611552755 -0.8273349053 -2.5543364061

H 5.6166315496 0.0491402752 0.1445119122
H 4.7328649585 1.1422545287 -0.9348850761
H 4.2580009390 0.9869080396 0.7785467554

Equilibrium geometry of **r03-exo-3s-mc**.

C 0.3713130000 1.0425460000 0.3253100000
N -0.3517560000 1.6159510000 -0.5833190000
C -1.3945590000 2.6218420000 -0.3684140000
C 1.5667200000 0.2687760000 -0.1746790000
H 0.2452270000 1.2910650000 1.3711750000
H -0.0830650000 1.3826420000 -1.5441180000
C -0.7326370000 -1.3992170000 0.7469860000
C -1.1518310000 -1.6325600000 -0.6777090000
C -2.4555430000 -0.8933060000 -0.7716660000
C -2.7876220000 -0.4009020000 0.4493060000
C -1.7305970000 -0.7233370000 1.3929050000
H 0.1393840000 -1.8442190000 1.2109320000
H -3.0503650000 -0.8310980000 -1.6757170000
H -1.3139110000 -2.7096070000 -0.8446830000
H -0.4080990000 -1.3334550000 -1.4276880000
H -3.6981350000 0.1305130000 0.7022190000
H -1.7548790000 -0.4872100000 2.4519790000
H -2.2457860000 2.4015450000 -1.0116630000
H -1.7058830000 2.6037060000 0.6759950000
H -0.9915900000 3.6084990000 -0.6175230000
O 2.3678890000 -0.0586590000 0.8144670000
O 1.7013520000 0.0677260000 -1.3663170000
C 3.6547980000 -0.7374510000 0.4782920000
C 4.0339260000 -1.5222180000 1.7194300000
H 3.4358010000 -1.3991060000 -0.3631680000
C 4.6646480000 0.3259660000 0.0759600000
H 4.9668030000 -2.0621480000 1.5315280000
H 4.1897710000 -0.8550870000 2.5727160000
H 3.2644350000 -2.2549000000 1.9802040000
H 5.6190240000 -0.1553570000 -0.1588740000
H 4.3366470000 0.8716150000 -0.8128810000
H 4.8303720000 1.0324330000 0.8952990000

Equilibrium geometry of **r03-exo-3s-prod**.

C 0.0938710000 0.2915010000 0.4610230000
N -0.7596450000 0.8599240000 -0.6640670000
C -1.1554310000 2.2899530000 -0.5192010000
C 1.4907370000 0.0565190000 -0.1244200000
H 0.1401530000 0.9982610000 1.2903540000
H -0.1461710000 0.7681990000 -1.4957070000
C -0.6744600000 -1.0263680000 0.8265550000
C -1.1523100000 -1.4612770000 -0.5836880000
C -1.9389510000 -0.1638140000 -0.8082030000
C -2.7487750000 -0.0615570000 0.4678960000
C -1.9922020000 -0.5823880000 1.4441940000
H -0.0640630000 -1.7216380000 1.4015370000
H -2.4332240000 0.0129280000 -1.7626460000
H -1.8094300000 -2.3308700000 -0.5514870000
H -0.3492530000 -1.6297860000 -1.3078430000
H -3.7254100000 0.3996150000 0.5481750000
H -2.2204730000 -0.6269820000 2.5031600000
H -1.7302420000 2.5846270000 -1.3990360000
H -1.7596650000 2.4014560000 0.3808280000
H -0.2534450000 2.9002420000 -0.4485300000
O 2.3441810000 -0.2960820000 0.8059260000
O 1.6969010000 0.1758060000 -1.3214600000
C 3.7475660000 -0.6125280000 0.4006840000
C 4.2874940000 -1.5018620000 1.5040090000

H 3.6698560000 -1.1522850000 -0.5463000000
C 4.5108670000 0.6878710000 0.2141770000
H 5.3082810000 -1.8067450000 1.2545060000
H 4.3134790000 -0.9680050000 2.4590100000
H 3.6819230000 -2.4052990000 1.6209380000
H 5.5456450000 0.4600800000 -0.0606970000
H 4.0781560000 1.2938230000 -0.5860710000
H 4.5258090000 1.2675260000 1.1426190000

Equilibrium geometry of **r03-exo-3s-ts**.

C 0.2351191294 0.7132739074 0.3394919751
N -0.4746459274 1.3754119992 -0.5887555764
C -1.3188474398 2.5303189269 -0.2908145995
C 1.5443077829 0.1429833639 -0.1810082264
H 0.2539811666 1.1273352399 1.3416364944
H -0.1421474869 1.2504601687 -1.5428063294
C -0.6655475113 -1.0643338561 0.7358589141
C -1.0836465109 -1.4578537285 -0.6689170841
C -2.3992208135 -0.7732651710 -0.8046292310
C -2.8520492873 -0.3719803789 0.4309848330
C -1.8281919099 -0.6065562241 1.3817450144
H 0.1298747469 -1.5684306433 1.2756021996
H -2.9469647872 -0.6916786554 -1.7373105526
H -1.2536218412 -2.5475743012 -0.6768663437
H -0.3651119261 -1.2558514978 -1.4673418360
H -3.8183289878 0.0687144097 0.6454342228
H -1.9099443525 -0.4090412227 2.4461457272
H -2.0222480214 2.6861016861 -1.1095385799
H -1.8791146259 2.3451764598 0.6284382184
H -0.7110581735 3.4329901257 -0.1604987802
O 2.3621806104 -0.1552058273 0.8088693250
O 1.7314083290 0.0070736486 -1.3735873919
C 3.7041951774 -0.7031987619 0.4651175555
C 4.1446100424 -1.4854075871 1.6884987121
H 3.5502235787 -1.3615088946 -0.3938847606
C 4.6253942108 0.4478558871 0.0972765141
H 5.1102120311 -1.9586617116 1.4860672214
H 4.2621117759 -0.8258382395 2.5539996288
H 3.4277520382 -2.2727087984 1.9401060181
H 5.6167902372 0.0520027677 -0.1446560469
H 4.2576847445 0.9893102477 -0.7783780381
H 4.7325952520 1.1444519132 0.9350696142

Equilibrium geometry of **r04-endo-3r-mc**.

C 0.4365390000 1.0578100000 -0.3468490000
N -0.3462060000 1.6712440000 0.4785460000
H -0.1953060000 1.4131390000 1.4599620000
H 0.4151810000 1.2893920000 -1.4055160000
C 1.5369840000 0.2234490000 0.2715390000
C -1.2953880000 2.7442620000 0.1737520000
C -1.0134290000 -1.1063400000 -1.2566730000
C -2.3357180000 -0.3860250000 -1.2229760000
C -2.7366830000 -0.4824430000 0.8221040000
C -1.8361890000 -1.2452600000 0.2912470000
C -0.7832340000 -1.6493120000 -0.0271260000
H -0.4397380000 -1.2895860000 -2.1577590000
H -3.6483230000 -0.0571980000 0.6265130000
H -3.0636560000 -0.9221080000 -1.8530140000
H -2.3187550000 0.6370380000 -1.6223320000
H -1.8867660000 -1.5352080000 1.9343380000
H 0.0456840000 -2.2950570000 0.2396620000
H -2.2687540000 2.5013440000 0.6004670000
H -0.9261560000 3.6741200000 0.6162860000

H -1.3774280000 2.8623680000 -0.9069300000
O 2.3753680000 -0.1733880000 -0.6554850000
O 1.5544100000 0.0654840000 1.4763550000
C 3.6560210000 -0.9203710000 -0.3309410000
C 4.2679950000 -1.1114840000 -1.7137130000
C 4.5209910000 -0.0308690000 0.5578090000
C 3.2956100000 -2.2501920000 0.3243330000
H 5.2200130000 -1.6417650000 -1.6203140000
H 3.6088050000 -1.7012600000 -2.3575250000
H 4.4581300000 -0.1472050000 -2.1938940000
H 5.4950530000 -0.5110170000 0.6938380000
H 4.6907610000 0.9422280000 0.0862910000
H 4.0741730000 0.1164650000 1.5428970000
H 4.2116680000 -2.8332210000 0.4621600000
H 2.8337050000 -2.1077750000 1.3035240000
H 2.6250330000 -2.8321970000 -0.3166290000

Equilibrium geometry of r04-endo-3r-prod.

C 0.0888160000 0.4384460000 -0.5818290000
N -0.8478660000 1.0340930000 0.4598890000
H -0.3855510000 0.8123290000 1.3603930000
H 0.2839230000 1.1843730000 -1.3543000000
C 1.3850750000 0.0512640000 0.1382660000
C -1.0314540000 2.5135580000 0.3709110000
C -0.7578650000 -0.7472300000 -1.1585720000
C -2.1454600000 -0.0585530000 -1.2018170000
C -2.1645290000 0.1890610000 0.3127870000
C -1.8127950000 -1.1786890000 0.8566860000
C -0.9749270000 -1.7405530000 -0.0249660000
H -0.3480930000 -1.1323060000 -2.0912780000
H -2.9873220000 0.7397840000 0.7658650000
H -2.9433030000 -0.7363450000 -1.5083030000
H -2.1816650000 0.8479550000 -1.8150000000
H -2.1346810000 -1.5611820000 1.8176600000
H -0.4667290000 -2.6932490000 0.0683150000
H -1.6693830000 2.8367650000 1.1950550000
H -0.0550720000 2.9940410000 0.4521880000
H -1.4965690000 2.7661700000 -0.5823570000
O 2.2857880000 -0.3485660000 -0.7239730000
O 1.4566940000 0.1235690000 1.3536680000
C 3.6580110000 -0.8451980000 -0.3083400000
C 4.3161540000 -1.1139780000 -1.6570270000
C 4.3776570000 0.2583710000 0.4621790000
C 3.4757410000 -2.1228890000 0.5048620000
H 5.3311250000 -1.4900950000 -1.4987080000
H 3.7576500000 -1.8635340000 -2.2255450000
H 4.3785610000 -0.1972270000 -2.2503340000
H 5.4115570000 -0.0549520000 0.6381620000
H 4.4045010000 1.1847130000 -0.1203310000
H 3.9097050000 0.4516900000 1.4287330000
H 4.4601400000 -2.5528910000 0.7144790000
H 2.9802970000 -1.9280530000 1.4585580000
H 2.9009510000 -2.8647180000 -0.0592880000

Equilibrium geometry of r04-endo-3r-ts.

C 0.2452412735 0.7662483160 -0.4076167415
N -0.5257675826 1.4639532552 0.4423517170
H -0.3332868833 1.2638155270 1.4233126846
H 0.3762740696 1.1831719124 -1.4019151655
C 1.4580316357 0.1123445858 0.2319765856
C -1.1600057338 2.7464107179 0.1318014985
C -0.7808802301 -0.8596679501 -1.0619593188
C -2.1532799270 -0.2225480457 -1.1902173226

C -2.6812481325 -0.3464430073 0.1990699317
C -1.9336921495 -1.2626414980 0.9020666174
C -0.8221683978 -1.6369637167 0.1097748401
H -0.1810825447 -1.1392608602 -1.9222297844
H -3.5811207425 0.1442731808 0.5536079869
H -2.7586253134 -0.8650818045 -1.8509719095
H -2.2006446588 0.7803189676 -1.6202359194
H -2.1391533508 -1.6237656012 1.9024932418
H -0.0679756675 -2.3571934164 0.4072042222
H -2.0804748906 2.8557841771 0.7078025398
H -0.4852036687 3.5739726114 0.3776510100
H -1.3953736764 2.7945949777 -0.9329278526
O 2.3339004557 -0.2279703846 -0.6901719144
O 1.5051847580 -0.0381537044 1.4367460899
C 3.6549538105 -0.8792352354 -0.3503370924
C 4.2873732436 -1.0526729257 -1.7271407950
C 4.4623162683 0.0736860025 0.5274316903
C 3.3833556141 -2.2232915802 0.3210850804
H 5.2715639108 -1.5180422983 -1.6210376656
H 3.6720559215 -1.6948225918 -2.3645614315
H 4.4161630463 -0.0862407950 -2.2230220892
H 5.4600383046 -0.3489510644 0.6819348607
H 4.5826614845 1.0447154727 0.0368723073
H 3.9970814893 0.2181229237 1.5042890918
H 4.3339044537 -2.7483669406 0.4576174227
H 2.9188214744 -2.1004565830 1.3015231552
H 2.7468114190 -2.8523764929 -0.3109742971

Equilibrium geometry of r04-endo-3s-mc.

C 0.4361020000 1.0603860000 0.3543200000
N -0.3468560000 1.6769110000 -0.4685470000
C -1.2997110000 2.7451460000 -0.1585930000
C 1.5404900000 0.2334960000 -0.2670320000
H 0.4119190000 1.2849240000 1.4143490000
H -0.1934780000 1.4256300000 -1.4513220000
C -2.7342340000 -0.4817450000 -0.2257760000
C -2.3316790000 -0.3978100000 1.2196090000
C -1.0078700000 -1.1157800000 1.2450940000
C -0.7781590000 -1.6470190000 0.0103220000
C -1.8330600000 -1.2366080000 -0.9030060000
H -3.6471720000 -0.0546210000 -0.6252150000
H -0.4329080000 -1.3061970000 2.1437020000
H -3.0577670000 -0.9412450000 1.8455200000
H -2.3165620000 0.6215390000 1.6283850000
H 0.0516610000 -2.2885970000 -0.2636140000
H -1.8844170000 -1.5170610000 -1.9486570000
H -2.2714830000 2.5024350000 -0.5890420000
H -1.3844430000 2.8556720000 0.9227190000
H -0.9321920000 3.6790160000 -0.5941680000
O 2.3795340000 -0.1640710000 0.6591010000
O 1.5599310000 0.0812910000 -1.4725390000
C 3.6640030000 -0.9036210000 0.3325620000
C 4.2762310000 -1.0964100000 1.7150010000
C 3.3100210000 -2.2328960000 -0.3273210000
C 4.5252960000 -0.0072030000 -0.5528050000
H 5.2309250000 -1.6215380000 1.6202850000
H 4.4612470000 -0.1328630000 2.1985920000
H 3.6196830000 -1.6916770000 2.3563820000
H 5.5014790000 -0.4826920000 -0.6899670000
H 4.0783400000 0.1414590000 -1.5376070000
H 4.6907100000 0.9650350000 -0.0779480000
H 4.2286990000 -2.8115830000 -0.4657860000
H 2.6410530000 -2.8196850000 0.3109020000
H 2.8487230000 -2.0893390000 -1.3066600000

Equilibrium geometry of **r04-endo-3s-prod.**

C 0.0972678884 0.4724552094 0.5707787198
 N -0.8570223097 1.0194665347 -0.4825920826
 C -1.0610525407 2.4984694025 -0.4451207582
 C 1.3924975689 0.0779423716 -0.1484702612
 H 0.2931870371 1.2518365081 1.3099375905
 H -0.3973844777 0.7794473554 -1.3795281993
 C -2.1591348290 0.1625103276 -0.2938722373
 C -2.1262414328 -0.0264915468 1.2290435435
 C -0.7296058241 -0.6969377493 1.2021699717
 C -0.9410123193 -1.7372259816 0.1101377007
 C -1.7924394072 -1.2214447393 -0.7866167805
 H -2.9934233700 0.6825764382 -0.7619864044
 H -0.3086833944 -1.0404642964 2.1460675140
 H -2.9119019524 -0.7039554872 1.5660000796
 H -2.1730562828 0.9014840471 1.8087724560
 H -0.4219190877 -2.6868772898 0.0528602928
 H -2.1176068179 -1.6456580075 -1.7287577814
 H -1.7074274302 2.7825650784 -1.2771243290
 H -1.5251579636 2.7798703233 0.5006301957
 H -0.0917362764 2.9885244387 -0.5494960117
 O 2.2783962647 -0.3568816645 0.7122147258
 O 1.4765972925 0.1787024216 -1.3609385885
 C 3.6580563440 -0.8357889886 0.3013265167
 C 4.2719722487 -1.2159625079 1.6439109758
 C 3.5019101802 -2.0449090232 -0.6162292669
 C 4.4029447342 0.3223791086 -0.3551258409
 H 5.2947271443 -1.5718401900 1.4892618946
 H 4.3066271048 -0.3533928949 2.3156353378
 H 3.7006353401 -2.0145731411 2.1261866162
 H 5.4372180178 0.0153576507 -0.5394302236
 H 3.9563167699 0.6043087451 -1.3104883356
 H 4.4266108830 1.1946932884 0.3057871282
 H 4.4932919415 -2.4606031838 -0.8223327592
 H 2.9078598095 -2.8265443976 -0.1315398775
 H 3.0406111466 -1.7750811599 -1.5679385215

Equilibrium geometry of **r04-endo-3s-ts.**

C 0.2458093289 0.7655882583 0.4134031804
 N -0.5250059587 1.4680497150 -0.4327186978
 C -1.1612954459 2.7475845144 -0.1144777587
 C 1.4614922222 0.1190957284 -0.2280517415
 H 0.3737371634 1.1751702403 1.4111394961
 H -0.3317173371 1.2741412628 -1.4147631229
 C -2.6796225063 -0.3433577185 -0.2033307013
 C -2.1513090468 -0.2325316599 1.1869968272
 C -0.7788971475 -0.8684454248 1.0524558942
 C -0.8202740201 -1.6344447333 -0.1266475563
 C -1.9321501866 -1.2527596791 -0.9151173713
 H -3.5795803665 0.1507833017 -0.5529188394
 H -0.1785905150 -1.1558126229 1.9098192551
 H -2.7566868974 -0.8811107491 1.8418237963
 H -2.1984686970 0.7664456089 1.6260740660
 H -0.0661474961 -2.3517722100 -0.4312166619
 H -2.1378305222 -1.6043659929 -1.9188943059
 H -2.0813337968 2.8594583368 -0.6906610999
 H -1.3977897522 2.7884358904 0.9503011620
 H -0.4873497073 3.5776157150 -0.3542197802
 O 2.3386557934 -0.2196448588 0.6934566163
 O 1.5098619424 -0.0271081327 -1.4333263105
 C 3.6640148665 -0.8612602679 0.3520377115
 C 4.2976117606 -1.0342110386 1.7283955068
 C 3.4011090300 -2.2053071351 -0.3229048855
 C 4.4652729689 0.0993566308 -0.5230625417

H 5.2848653366 -1.4928333109 1.6208782683
 H 4.4201920827 -0.0682817084 2.2268739726
 H 3.6866612819 -1.6821801739 2.3641910654
 H 5.4656489268 -0.3165497440 -0.6788792592
 H 3.9990178337 0.2438293009 -1.4994415029
 H 4.5796002570 1.0696731506 -0.0296260660
 H 4.3549824654 -2.7241704416 -0.4602822084
 H 2.7681702093 -2.8399158548 0.3072390374
 H 2.9362595348 -2.0829179568 -1.3032584881

Equilibrium geometry of **r04-exo-3r-mc.**

C 0.3772500000 1.0682990000 -0.3260810000
 N -0.3496720000 1.6344220000 0.5824270000
 H -0.0714360000 1.4051820000 1.5420390000
 H 0.2405600000 1.3063750000 -1.3730860000
 C 1.5842940000 0.3051600000 0.1763850000
 C -1.4127430000 2.6194070000 0.3718770000
 C -2.4417230000 -0.9157600000 0.7727680000
 C -1.1284690000 -1.6383450000 0.6791490000
 C -0.7124740000 -1.4017170000 -0.7460230000
 C -1.7156200000 -0.7348760000 -1.3911490000
 C -2.7778090000 -0.4253800000 -0.4472730000
 H -3.0379770000 -0.8619540000 1.6763940000
 H 0.1667220000 -1.8340890000 -1.2081380000
 H -1.2747480000 -2.7169240000 0.8503670000
 H -0.3882360000 -1.3251270000 1.4270720000
 H -1.7418520000 -0.4968770000 -2.4497530000
 H -3.6940200000 0.0960770000 -0.7004890000
 H -2.2571160000 2.3812150000 1.0179970000
 H -1.0289010000 3.6136510000 0.6209660000
 H -1.7273900000 2.5961120000 -0.6713900000
 O 2.3754150000 -0.0123550000 -0.8188990000
 O 1.7078300000 0.1208220000 1.3731380000
 C 3.7183700000 -0.6887640000 -0.6031540000
 C 4.2342270000 -0.8382340000 -2.0290650000
 C 4.5953920000 0.2443280000 0.2270620000
 C 3.4849330000 -2.0431760000 0.0614400000
 H 5.2152640000 -1.3217110000 -2.0077620000
 H 3.5608970000 -1.4574440000 -2.6292640000
 H 4.3433640000 0.1359130000 -2.5144640000
 H 5.5920910000 -0.1985250000 0.3183580000
 H 4.7040860000 1.2163690000 -0.2639410000
 H 4.1959960000 0.3882350000 1.2328740000
 H 4.4403260000 -2.5741960000 0.1166180000
 H 3.0947710000 -1.9393920000 1.0754740000
 H 2.7995540000 -2.6572890000 -0.5321460000

Equilibrium geometry of **r04-exo-3r-prod.**

C 0.0884610000 0.3150100000 -0.4678820000
 N -0.7669950000 0.8597280000 0.6670820000
 H -0.1470610000 0.7606330000 1.4939570000
 H 0.1281150000 1.0336780000 -1.2870720000
 C 1.4909300000 0.0772830000 0.1130630000
 C -1.1764160000 2.2875250000 0.5443760000
 C -1.9354090000 -0.1765950000 0.8022670000
 C -1.1380980000 -1.4636960000 0.5561860000
 C -0.6696200000 -1.0038820000 -0.8494510000
 C -1.9943620000 -0.5644860000 -1.4554000000
 C -2.7519920000 -0.0650350000 -0.4688060000
 H -2.4271980000 -0.0179070000 1.7611530000
 H -0.0550740000 -1.6850610000 -1.4366550000
 H -1.7877780000 -2.3384810000 0.5141130000
 H -0.3306320000 -1.6352390000 1.2744990000

H -2.2270120000 -0.5968170000 -2.5138350000
H -3.7336330000 0.3871410000 -0.5381900000
H -1.7496000000 2.5648550000 1.4309590000
H -0.2802900000 2.9068590000 0.4781540000
H -1.7859240000 2.4067100000 -0.3511320000
O 2.3345220000 -0.2420000000 -0.8334150000
O 1.6806250000 0.1731170000 1.3163260000
C 3.7793550000 -0.6173390000 -0.5533220000
C 4.3233900000 -0.8550290000 -1.9570030000
C 4.4746300000 0.5546550000 0.1333960000
C 3.7843070000 -1.8936890000 0.2828840000
H 5.3747560000 -1.1500710000 -1.8921740000
H 3.7741850000 -1.6549930000 -2.4622360000
H 4.2598890000 0.0530600000 -2.5638050000
H 5.5408700000 0.3244640000 0.2245680000
H 4.3808160000 1.4674010000 -0.4636010000
H 4.0773680000 0.7339650000 1.1336690000
H 4.8171360000 -2.2345020000 0.4048060000
H 3.3640950000 -1.7284150000 1.2773090000
H 3.2268700000 -2.6906770000 -0.2198210000

Equilibrium geometry of **r04-exo-3r-ts**.

C 0.2325344745 0.7306609914 -0.3384172584
N -0.4827266602 1.3805561816 0.5945660998
H -0.1446177076 1.2524565648 1.5464282649
H 0.2490337239 1.1530430309 -1.3371516518
C 1.5510023429 0.1688740503 0.1830312286
C -1.3371828964 2.5297097734 0.3060604030
C -2.3874230009 -0.7921096582 0.7962285864
C -1.0637945792 -1.4595563249 0.6514580860
C -0.6515246031 -1.0449782050 -0.7492823086
C -1.8207638325 -0.5947409543 -1.3887209271
C -2.8464831919 -0.3830132216 -0.4343996306
H -2.9346498306 -0.7267371388 1.7305452895
H 0.1480498871 -1.5352721667 -1.2954577390
H -1.2205717679 -2.5513113646 0.6477755046
H -0.3473050785 -1.2565279210 1.4513079373
H -1.9061405542 -0.3860096596 -2.4507468443
H -3.8181093936 0.0487572609 -0.6429110127
H -2.0369987686 2.6771871789 1.1295195173
H -0.7376461517 3.4379516481 0.1756234685
H -1.9018005341 2.3441219983 -0.6105181246
O 2.3589231485 -0.1201615341 -0.8129249769
O 1.7248489391 0.0468395187 1.3802802038
C 3.7535455905 -0.6663405349 -0.5898364584
C 4.2671218448 -0.8262798273 -2.0165380627
C 4.5628607246 0.3646808598 0.1917907343
C 3.6436929024 -2.0110064777 0.1253781388
H 5.2835042303 -1.2302590711 -1.9929010088
H 3.6380394357 -1.5165045308 -2.5868726931
H 4.2940807933 0.1358796493 -2.5365961229
H 5.5982301565 0.0175378203 0.2676183311
H 4.5695563161 1.3275064328 -0.3290812389
H 4.1748284441 0.5023766782 1.2026270171
H 4.6383723947 -2.4639897401 0.1846473525
H 3.2595430390 -1.8998239933 1.1409061301
H 3.0003384173 -2.6982569054 -0.4346600987

Equilibrium geometry of **r04-exo-3s-mc**.

C 0.3766900000 1.0669040000 0.3258590000
N -0.3501150000 1.6317770000 -0.5835690000
C -1.4126320000 2.6176780000 -0.3745730000
C 1.5842850000 0.3038820000 -0.1755520000

H 0.2399450000 1.3065710000 1.3724490000
H -0.0716850000 1.4012850000 -1.5428170000
C -0.7152730000 -1.4005310000 0.7501090000
C -1.1293210000 -1.6395220000 -0.6752670000
C -2.4418330000 -0.9160650000 -0.7721970000
C -2.7794870000 -0.4233680000 0.4464990000
C -1.7190180000 -0.7319670000 1.3925450000
H 0.1628580000 -1.8327020000 1.2143780000
H -3.0366500000 -0.8634090000 -1.6768960000
H -1.2763280000 -2.7182870000 -0.8445030000
H -0.3877640000 -1.3284760000 -1.4227550000
H -3.6957520000 0.0991450000 0.6973890000
H -1.7467480000 -0.4920740000 2.4506880000
H -2.2565360000 2.3798800000 -1.0214340000
H -1.7283660000 2.5951030000 0.6683460000
H -1.0277560000 3.6114820000 -0.6237690000
O 2.3760260000 -0.0111180000 0.8200400000
O 1.7077830000 0.1177580000 -1.3720340000
C 3.7211750000 -0.6833940000 0.6045550000
C 4.2369710000 -0.8318890000 2.0305850000
C 3.4925990000 -2.0382350000 -0.0608020000
C 4.5953180000 0.2532160000 -0.2248190000
H 5.2195020000 -1.3123310000 2.0094440000
H 4.3429410000 0.1423310000 2.5165010000
H 3.5653440000 -1.4534570000 2.6302160000
H 5.5934610000 -0.1862950000 -0.3165370000
H 4.1954660000 0.3966990000 -1.2305280000
H 4.7008150000 1.2251540000 0.2670800000
H 4.4497790000 -2.5660860000 -0.1157060000
H 2.8089480000 -2.6548670000 0.5321210000
H 3.1026260000 -1.9352580000 -1.0749550000

Equilibrium geometry of **r04-exo-3s-prod**.

C 0.0884670000 0.3176790000 0.4681990000
N -0.7676540000 0.8593880000 -0.6677220000
C -1.1798180000 2.2865540000 -0.5469340000
C 1.4913230000 0.0809470000 -0.1121870000
H 0.1268460000 1.0375470000 1.2863730000
H -0.1473820000 0.7602580000 -1.4943450000
C -0.6674030000 -1.0019700000 0.8514920000
C -1.1346300000 -1.4646400000 -0.5536220000
C -1.9341640000 -0.1793260000 -0.8018350000
C -2.7513670000 -0.0674520000 0.4687600000
C -1.9931910000 -0.5641100000 1.4563680000
H -0.0518280000 -1.6811290000 1.4398950000
H -2.4258870000 -0.0228750000 -1.7611120000
H -1.7827010000 -2.3404810000 -0.5104000000
H -0.3266960000 -1.6358540000 -1.2714820000
H -3.7338390000 0.3830280000 0.5370400000
H -2.2261790000 -0.5954180000 2.5147560000
H -1.7533060000 2.5616750000 -1.4339770000
H -1.7898290000 2.4058050000 0.3482050000
H -0.2848630000 2.9076120000 -0.4812140000
O 2.3350090000 -0.2365350000 0.8348190000
O 1.6810480000 0.1753910000 -1.3155390000
C 3.7794320000 -0.6138150000 0.5551620000
C 4.3239330000 -0.8481990000 1.9592190000
C 3.7824790000 -1.8925770000 -0.2773750000
C 4.4756720000 0.5553880000 -0.1352800000
H 5.3749390000 -1.1443340000 1.8947140000
H 4.2615470000 0.0614830000 2.5636580000
H 3.7743650000 -1.6463400000 2.4668190000
H 5.5415450000 0.3235600000 -0.2264230000
H 4.0780060000 0.7323220000 -1.1357930000
H 4.3833570000 1.4699320000 0.4592610000

H 4.8148390000 -2.2347920000 -0.3993410000
H 3.2247520000 -2.6877030000 0.2280530000
H 3.3615230000 -1.7297150000 -1.2718850000

Equilibrium geometry of **r04-exo-3s-ts**.

C 0.2323673254 0.7333540484 0.3394629009
N -0.4832979845 1.3824483567 -0.5936664332
C -1.3407269135 2.5291487098 -0.3046690676
C 1.5513427532 0.1726456307 -0.1818388842
H 0.2484341150 1.1559958104 1.3380780567
H -0.1451654254 1.2548288615 -1.5455660955
C -0.6500763244 -1.0423285738 0.7515766360
C -1.0587071091 -1.4605211542 -0.6490433159
C -2.3840498071 -0.7973366442 -0.7973468877
C -2.8462837744 -0.3867783381 0.4315528249
C -1.8216612724 -0.5938232286 1.3879930372
H 0.1493400151 -1.5299809482 1.3002456483
H -2.9297022135 -0.7353815421 -1.7327321889
H -1.2121984209 -2.5526694671 -0.6438534200
H -0.3415967240 -1.2566544505 -1.4481297645
H -3.8194223962 0.0427727918 0.6375360340
H -1.9095859434 -0.3833545854 2.4494236531
H -2.0398683070 2.6762442651 -1.1287421306
H -1.9060474135 2.3408780574 0.6109665240
H -0.7434993623 3.4386011620 -0.1720871857
O 2.3596268176 -0.1151534349 0.8141316957
O 1.7252184433 0.0499127818 -1.3790220638
C 3.7535684141 -0.6631699174 0.5912263656
C 4.2692334571 -0.8165370624 2.0177695425
C 3.6408681550 -2.0110270943 -0.1172984921
C 4.5629649117 0.3630092946 -0.1965468966
H 5.2846302005 -1.2230212181 1.9945987791
H 4.2991788299 0.1484115389 2.5323223949
H 3.6394558616 -1.5020197101 2.5929370202
H 5.5988579517 0.0163070712 -0.2682185224
H 4.1763612243 0.4936032232 -1.2088025372
H 4.5680354284 1.3294229635 0.3177106328
H 4.6351351650 -2.4647278789 -0.1781546721
H 2.9991545737 -2.6953893409 0.4480340652
H 3.2533112081 -1.9042415031 -1.1319653444

Equilibrium geometry of **r05-endo-3r-mc**.

C 0.4854050000 1.0043800000 -0.3776240000
N -0.2775440000 1.6592360000 0.4355100000
H -0.1329540000 1.4258470000 1.4237210000
H 0.4750150000 1.2174420000 -1.4402920000
C 1.5428800000 0.1395750000 0.2517050000
C -1.1656000000 2.7933740000 0.1136430000
C -1.0146000000 -1.1280390000 -1.2374800000
C -2.3070840000 -0.3557950000 -1.2133570000
C -2.7069920000 -0.4111180000 0.2339210000
C -1.8392730000 -1.2043880000 0.9129560000
C -0.8075390000 -1.6654400000 -0.0001240000
H -0.4510480000 -1.3503960000 -2.1362170000
H -3.5983710000 0.0589200000 0.6335180000
H -3.0565770000 -0.8770830000 -1.8306420000
H -2.2533290000 0.6573950000 -1.6326330000
H -1.9010780000 -1.4779960000 1.9598010000
H -0.0090210000 -2.3459050000 0.2740410000
H -2.1179880000 2.6096590000 0.6148330000
C -0.5440050000 4.1141840000 0.5706340000
H -1.3338300000 2.7810950000 -0.9655930000
O 2.3610450000 -0.3507720000 -0.6620620000

O 1.5960430000 0.0016990000 1.4547950000
C 3.4735650000 -1.1461000000 -0.1680110000
H 4.0545170000 -1.3992030000 -1.0519050000
H 4.0615590000 -0.5571870000 0.5377560000
H 3.0929200000 -2.0432860000 0.3237770000
H -1.2404730000 4.9276530000 0.3480460000
H -0.3571710000 4.1187710000 1.6490290000
H 0.3962360000 4.3114800000 0.0483560000

Equilibrium geometry of **r05-endo-3r-prod**.

C 0.0513980000 0.4711870000 -0.5853990000
N -0.9209030000 1.0843470000 0.4113450000
H -0.4737030000 0.9376510000 1.3320240000
H 0.2361670000 1.1817790000 -1.3928220000
C 1.3453540000 0.1645780000 0.1625910000
C -1.1874430000 2.5627220000 0.2522410000
C -0.7406290000 -0.7728110000 -1.1188870000
C -2.1526510000 -0.1424150000 -1.2080110000
C -2.1982600000 0.1740790000 0.2929030000
C -1.7984650000 -1.1514380000 0.9038070000
C -0.9317230000 -1.7218900000 0.0560290000
H -0.3030030000 -1.1817410000 -2.0285410000
H -3.0488700000 0.7090790000 0.7116210000
H -2.9193860000 -0.8646350000 -1.4915760000
H -2.2173700000 0.7339230000 -1.8608840000
H -2.1164130000 -1.5025910000 1.8780830000
H -0.3915710000 -2.6511820000 0.1956510000
H -1.9575720000 2.8041090000 0.9897230000
C 0.0592560000 3.4094590000 0.4704430000
H -1.6128430000 2.7079300000 -0.7436910000
O 2.2717100000 -0.2994690000 -0.6536880000
O 1.4469710000 0.3285670000 1.3627430000
C 3.5513710000 -0.6480900000 -0.0533530000
H 4.1860020000 -0.9362590000 -0.8882940000
H 3.9580680000 0.2163060000 0.4731490000
H 3.4145860000 -1.4771400000 0.6426530000
H -0.2244790000 4.4645270000 0.4228620000
H 0.5078740000 3.2241590000 1.4509360000
H 0.8182200000 3.2392230000 -0.2989560000

Equilibrium geometry of **r05-endo-3r-ts**.

C 0.2363434732 0.7490712504 -0.4109072204
N -0.5353112120 1.4520112221 0.4343769509
H -0.3426773409 1.2631199528 1.4179248295
H 0.3654280856 1.1593846128 -1.4083445311
C 1.4471138053 0.1033123195 0.2222805465
C -1.1488313662 2.7552693431 0.1185679755
C -0.7935129777 -0.8837382611 -1.0557983877
C -2.1598571202 -0.2361140362 -1.1921575406
C -2.6882279261 -0.3386417354 0.1988683427
C -1.9506867093 -1.2567476938 0.9115482838
C -0.8432002144 -1.6497200414 0.1238359106
H -0.1945162177 -1.1760873580 -1.9126102994
H -3.5830410339 0.1650936981 0.5479775518
H -2.7704712578 -0.8823267232 -1.8444988201
H -2.1982039671 0.7619380064 -1.6340322243
H -2.1610960753 -1.6066188841 1.9150386920
H -0.0974584205 -2.3757822143 0.4290603819
H -2.0951812972 2.8209929362 0.6620205822
C -0.2318622600 3.9236120733 0.4844628109
H -1.3785175713 2.7625477493 -0.9507244836
O 2.3258119712 -0.2682693366 -0.6983642763
O 1.5404458609 -0.0393399444 1.4219094862

C 3.5516324364 -0.8770960549 -0.2101204078
H 4.0818564455 -1.2026050468 -1.1027053184
H 4.1331843354 -0.1351722066 0.3397987357
H 3.3162660855 -1.7198507100 0.4417220143
H -0.7300914449 4.8678686835 0.2448572477
H -0.0002893193 3.9270173262 1.5544344790
H 0.7084824747 3.8798361437 -0.0737518945

H 4.1922900000 -0.9234540000 0.8898660000
H 3.4197170000 -1.4770390000 -0.6357900000
H 3.9565700000 0.2195990000 -0.4784440000
H -0.2149390000 4.4643740000 -0.4010280000
H 0.8261330000 3.2326560000 0.3125320000
H 0.5127050000 3.2276710000 -1.4370800000

Equilibrium geometry of r05-endo-3s-mc.

C 0.4853860000 0.9979040000 0.3821250000
N -0.2766950000 1.6567600000 -0.4286450000
C -1.1618250000 2.7920270000 -0.1025800000
C 1.5436860000 0.1361110000 -0.2497520000
H 0.4747270000 1.2069550000 1.4456020000
H -0.1321580000 1.4271860000 -1.4178070000
C -2.7108040000 -0.4015470000 -0.2321480000
C -2.3051670000 -0.3608710000 1.2139780000
C -1.0159160000 -1.1388480000 1.2261820000
C -0.8161660000 -1.6665080000 -0.0165540000
C -1.8491740000 -1.1926960000 -0.9214400000
H -3.6015280000 0.0760560000 -0.6241570000
H -0.4500250000 -1.3717190000 2.1207700000
H -3.0545920000 -0.8844230000 1.8293850000
H -2.2455730000 0.6483520000 1.6421380000
H -0.0216290000 -2.3478220000 -0.3001130000
H -1.9163300000 -1.4568580000 -1.9703740000
H -2.1136980000 2.6141650000 -0.6067240000
H -1.3324770000 2.7744900000 0.9761920000
C -0.5347070000 4.1131570000 -0.5510310000
O 2.3646890000 -0.3522000000 0.6626130000
O 1.5958190000 -0.0004610000 -1.4530130000
C 3.4807900000 -1.1412200000 0.1665050000
H 4.0645870000 -1.3911560000 1.0493840000
H 3.1044190000 -2.0404060000 -0.3247520000
H 4.0642350000 -0.5488190000 -0.5400560000
H -1.2288290000 4.9278270000 -0.3253410000
H 0.4051240000 4.3043000000 -0.0258050000
H -0.3456600000 4.1230550000 -1.6289580000

Equilibrium geometry of r05-endo-3s-ts.

C 0.2367680571 0.7430672912 0.4147048719
N -0.5325021932 1.4518133580 -0.4277018574
C -1.1425057097 2.7552037412 -0.1056143306
C 1.4459940737 0.0966287187 -0.2201123976
H 0.3652559582 1.1478487293 1.4144182633
H -0.3421524387 1.2653750368 -1.4121033381
C -2.6906569244 -0.3311057519 -0.2045662867
C -2.1632764580 -0.2410435757 1.1877036519
C -0.7996020232 -0.8933279238 1.0478366279
C -0.8508564133 -1.6499638735 -0.1374906516
C -1.9560307730 -1.2466149580 -0.9233426054
H -3.5831932318 0.1786679211 -0.5505834730
H -0.2024740218 -1.1938836810 1.9030833696
H -2.7774360112 -0.8891656355 1.8347368846
H -2.1975895078 0.7539450339 1.6365894556
H -0.1078756382 -2.3765578372 -0.4478136059
H -2.1666255655 -1.5879593942 -1.9296830871
H -2.0844455868 2.8292569422 -0.6555290026
H -1.3802686426 2.7544237258 0.9618692754
C -0.2180499641 3.9227948359 -0.4543311362
O 2.3348062638 -0.2566571330 0.6978325898
O 1.5317818201 -0.0592296878 -1.4186941320
C 3.5582636363 -0.8667860614 0.2053160293
H 4.1593454359 -1.0537045035 1.0925773743
H 3.3242929441 -1.7972485871 -0.3152767390
H 4.0638152497 -0.1797962203 -0.4749388844
H -0.7143470347 4.8669198739 -0.2102667258
H 0.7176770652 3.8704026068 0.1108659056
H 0.0218212339 3.9346424677 -1.5223377451

Equilibrium geometry of r05-endo-3s-prod.

C 0.0514680000 0.4652230000 0.5871770000
N -0.9194100000 1.0857740000 -0.4061210000
C -1.1821510000 2.5637490000 -0.2389910000
C 1.3455290000 0.1614200000 -0.1614860000
H 0.2366420000 1.1702390000 1.3994390000
H -0.4729950000 0.9422070000 -1.3276970000
C -2.1991560000 0.1778510000 -0.2924850000
C -2.1533160000 -0.1484600000 1.2062910000
C -0.7426250000 -0.7812560000 1.1121970000
C -0.9365260000 -1.7219670000 -0.0690140000
C -1.8029380000 -1.1444020000 -0.9123000000
H -3.0486190000 0.7179080000 -0.7069730000
H -0.3054150000 -1.1971180000 2.0188230000
H -2.9213620000 -0.8709240000 1.4855520000
H -2.2158540000 0.7236600000 1.8649820000
H -0.3983190000 -2.6513670000 -0.2154490000
H -2.1221670000 -1.4887240000 -1.8885950000
H -1.9528170000 2.8110260000 -0.9741190000
H -1.6057100000 2.7049890000 0.7583840000
C 0.0661870000 3.4087210000 -0.4546450000
O 2.2748270000 -0.2960010000 0.6552720000
O 1.4447060000 0.3216590000 -1.3622950000
C 3.5546730000 -0.6430770000 0.0545470000

Equilibrium geometry of r05-exo-3r-mc.

C 0.4095370000 1.0073800000 -0.3816030000
N -0.3014230000 1.6312390000 0.5016740000
H -0.0394980000 1.4385120000 1.4733690000
H 0.2849180000 1.2137180000 -1.4368720000
C 1.5773870000 0.2148330000 0.1405580000
C -1.3143170000 2.6727980000 0.2419330000
C -2.4522100000 -0.8524580000 0.7839610000
C -1.1636940000 -1.6208130000 0.7126340000
C -0.7439430000 -1.4449920000 -0.7200390000
C -1.7286880000 -0.7698650000 -1.3861780000
C -2.7763250000 -0.3935430000 -0.4520560000
H -3.0432420000 -0.7482900000 1.6865440000
H 0.1155850000 -1.9256310000 -1.1718570000
H -1.3460870000 -2.6879460000 0.9178730000
H -0.4136670000 -1.3101470000 1.4517290000
H -1.7509510000 -0.5694920000 -2.4526400000
H -3.6762490000 0.1478860000 -0.7210630000
H -2.1792630000 2.4412620000 0.8661230000
C -0.7610730000 4.0647670000 0.5490190000
H -1.6142080000 2.5771730000 -0.8040470000
O 2.3603380000 -0.1886520000 -0.8429680000
O 1.7348020000 0.0528410000 1.3327650000
C 3.5645080000 -0.9061370000 -0.4526970000
H 4.0972070000 -1.0900500000 -1.3828690000

H 4.1544030000 -0.2899320000 0.2274820000
H 3.2896520000 -1.8423020000 0.0365030000
H -1.5453190000 4.8041710000 0.3622830000
H -0.4579990000 4.1559350000 1.5968470000
H 0.0958270000 4.3035650000 -0.0875040000

Equilibrium geometry of **r05-exo-3r-prod.**

C 0.0516480000 0.3342020000 -0.4755070000
N -0.8403260000 0.9204880000 0.6071650000
H -0.2427750000 0.9023690000 1.4531950000
H 0.0715930000 0.9894650000 -1.3463990000
C 1.4502740000 0.1948180000 0.1245700000
C -1.3172360000 2.3348320000 0.3989990000
C -1.9729970000 -0.1492890000 0.7902010000
C -1.1253000000 -1.4197840000 0.6488200000
C -0.6460870000 -1.0410330000 -0.7761480000
C -1.9725370000 -0.6956010000 -1.4353130000
C -2.7663270000 -0.1554190000 -0.5002280000
H -2.4901860000 0.0557120000 1.7265520000
H 0.0069600000 -1.7355960000 -1.3031370000
H -1.7421620000 -2.3187380000 0.6550970000
H -0.3279810000 -1.5126790000 1.3933530000
H -2.1814300000 -0.8098510000 -2.4930100000
H -3.7610370000 0.2557520000 -0.6202260000
H -2.0268570000 2.5301940000 1.2081710000
C -0.1754590000 3.3415090000 0.4164670000
H -1.8646800000 2.3454680000 -0.5458100000
O 2.3276020000 -0.1748400000 -0.7860480000
O 1.6659960000 0.3894550000 1.3067950000
C 3.6955640000 -0.3795450000 -0.3305670000
H 4.2713070000 -0.5540980000 -1.2368020000
H 4.0453760000 0.5084780000 0.1969140000
H 3.7328920000 -1.2467170000 0.3308420000
H -0.5956560000 4.3469030000 0.3233640000
H 0.3897790000 3.3010530000 1.3529650000
H 0.5181520000 3.1984070000 -0.4177000000

Equilibrium geometry of **r05-exo-3r-ts.**

C 0.2170472268 0.6967045743 -0.3425083338
N -0.5004809818 1.3563322215 0.5852171900
H -0.1586926569 1.2428989059 1.5382062589
H 0.2330304816 1.1120162496 -1.3442522294
C 1.5330036760 0.1481932294 0.1737510293
C -1.3217670303 2.5416343703 0.2917881942
C -2.4005608893 -0.7527320033 0.7974300283
C -1.0913735098 -1.4522689724 0.6827757193
C -0.6601214147 -1.0796060250 -0.7245490360
C -1.8221674035 -0.6417148950 -1.3893673183
C -2.8484927248 -0.3822226315 -0.4514996719
H -2.9517122593 -0.6449125953 1.7254587013
H 0.1360168387 -1.5978352702 -1.2501460210
H -1.2741904390 -2.5397331806 0.7004863382
H -0.3774938315 -1.2488581949 1.4847425811
H -1.8968155271 -0.4679937723 -2.4583675110
H -3.8125925853 0.0559255587 -0.6802039410
H -2.1332982261 2.5696398243 1.0234047229
C -0.5128338589 3.8391917434 0.3279215027
H -1.7743621959 2.3875930086 -0.6923583311
O 2.3517516132 -0.1577373548 -0.8207733303
O 1.7490361493 0.0260469297 1.3604447686
C 3.6610526395 -0.6651086433 -0.4434648066
H 4.1928144997 -0.8005268154 -1.3828416799
H 4.1669058128 0.0606265146 0.1947866905

H 3.5511436242 -1.6128414020 0.0866432360
H -1.1741419453 4.6862260075 0.1208924830
H -0.0616785641 3.9980023691 1.3125298828
H 0.2845492579 3.8372555194 -0.4220210513

Equilibrium geometry of **r05-exo-3s-mc.**

C 0.4088370000 1.0065880000 0.3799590000
N -0.3029070000 1.6293290000 -0.5035520000
C -1.3162880000 2.6704000000 -0.2436910000
C 1.5774530000 0.2149630000 -0.1418120000
H 0.2845680000 1.2138840000 1.4351160000
H -0.0411620000 1.4363240000 -1.4752200000
C -0.7439950000 -1.4443910000 0.7210580000
C -1.1637050000 -1.6214260000 -0.7114890000
C -2.4524050000 -0.8535280000 -0.7833720000
C -2.7767550000 -0.3939590000 0.4523750000
C -1.7290900000 -0.7693010000 1.3867560000
H 0.1156630000 -1.9245140000 1.1731960000
H -3.0434510000 -0.7501460000 -1.6860460000
H -1.3458700000 -0.26887970000 -0.9158280000
H -0.4137500000 -1.3112310000 -1.4508770000
H -3.6768780000 0.1473410000 0.7209600000
H -1.7514420000 -0.5682840000 2.4530950000
H -2.1795120000 2.4406350000 -0.8709600000
H -1.6192040000 2.5717320000 0.8011170000
C -0.7620480000 4.0632460000 -0.5446900000
O 2.3615060000 -0.1859320000 0.8418990000
O 1.7345380000 0.0514980000 -1.3338650000
C 3.5667850000 -0.9018670000 0.4521240000
H 4.1002990000 -1.0833970000 1.3823050000
H 3.2934170000 -1.8393560000 -0.0355810000
H 4.1553210000 -0.2857050000 -0.2292480000
H -1.5468360000 4.8021430000 -0.3582730000
H 0.0926730000 4.2999370000 0.0954520000
H -0.4553230000 4.1577630000 -1.5910260000

Equilibrium geometry of **r05-exo-3s-prod.**

C 0.0513850000 0.3337290000 0.4751980000
N -0.8411370000 0.9196790000 -0.6071170000
C -1.3179290000 2.3339970000 -0.3990040000
C 1.4499600000 0.1952900000 -0.1251600000
H 0.0712030000 0.9889060000 1.3461970000
H -0.2439370000 0.9014190000 -1.4533860000
C -0.6456730000 -1.0418150000 0.7760010000
C -1.1255730000 -1.4205620000 -0.6487140000
C -1.9736920000 -0.1502900000 -0.7895410000
C -2.7663050000 -0.1567170000 0.5013030000
C -1.9719170000 -0.6968460000 1.4359050000
H 0.0078280000 -1.7362820000 1.3025690000
H -2.4914610000 0.0546490000 -1.7255860000
H -1.7422280000 -2.3196820000 -0.6547130000
H -0.3286180000 -1.5132270000 -1.3936740000
H -3.7610530000 0.2542280000 0.6219240000
H -2.1802210000 -0.8112660000 2.4936930000
H -2.0276930000 2.5293290000 -1.2080920000
H -1.8652050000 2.3447460000 0.5459060000
C -0.1760590000 3.3405520000 -0.4167180000
O 2.3278920000 -0.1729740000 0.7854220000
O 1.6652160000 0.3896130000 -1.3075300000
C 3.6960540000 -0.3760150000 0.3297840000
H 4.2720440000 -0.5503180000 1.2358780000
H 3.7342850000 -1.2428150000 -0.3320570000
H 4.0449320000 0.5126440000 -0.1972860000

H -0.5961130000 4.3460140000 -0.3238990000
H 0.5175350000 3.1976130000 0.4174900000
H 0.3891800000 3.2997890000 -1.3531940000

Equilibrium geometry of r05-exo-3s-ts.

C 0.2167543730 0.6968166430 0.3422469332
N -0.5013406041 1.3559724751 -0.5853601504
C -1.3231863366 2.5408605532 -0.2918376953
C 1.5328339893 0.1488687009 -0.1742921897
H 0.2327878201 1.1122471302 1.3439397702
H -0.1597946363 1.2425651961 -1.5384382638
C -0.6594217414 -1.0799548157 0.7247813599
C -1.0908867149 -1.4530507863 -0.6823602848
C -2.4005037146 -0.7542649915 -0.7967314460
C -2.8482388773 -0.3837559498 0.4522621499
C -1.8214798787 -0.6425328360 1.3898657643
H 0.1371522075 -1.5976706919 1.2502230215
H -2.9519995046 -0.6469111748 -1.7246092161
H -1.2730902144 -2.5406211150 -0.6998795099
H -0.3773588212 -1.2493414144 -1.4845649721
H -3.8124988458 0.0539251778 0.6811849176
H -1.8958951321 -0.4686589564 2.4588575876
H -2.1348592188 2.5684302743 -1.0233139041
H -1.7755339989 2.3866287914 0.6923941685
C -0.5149218621 3.8388321633 -0.3281580107
O 2.3520209276 -0.1564613116 0.8200537323
O 1.7485847214 0.0266206335 -1.3610260464
C 3.6614827919 -0.6632068880 0.4424674477
H 4.1935059990 -0.7983824034 1.3817318397
H 3.5519195273 -1.6109811956 -0.0876378358
H 4.1668606635 0.0627829769 -0.1958736908
H -1.1766105019 4.6855288121 -0.1209656680
H 0.2826349379 3.8372916876 0.4216000854
H -0.0640786318 3.9978758056 -1.3128709474

Equilibrium geometry of r06-endo-3r-mc.

C 0.4700170000 0.9872780000 -0.3864570000
N -0.2800580000 1.6491740000 0.4322060000
H -0.1251200000 1.4160030000 1.4191920000
H 0.4481900000 1.1956720000 -1.4499690000
C 1.5317000000 0.1196060000 0.2362360000
C -1.1662530000 2.7863760000 0.1177180000
C -1.0612900000 -1.1423070000 -1.2266300000
C -2.3478880000 -0.3607350000 -1.1909500000
C -2.7317170000 -0.4074450000 0.2611440000
C -1.8601830000 -1.2013740000 0.9337700000
C -0.8414790000 -1.6731510000 0.0106780000
H -0.5091850000 -1.3710340000 -2.1309090000
H -3.6158270000 0.0695680000 0.6684810000
H -3.1084580000 -0.8770710000 -1.7986300000
H -2.2898540000 0.6510760000 -1.6134370000
H -1.9104520000 -1.4688800000 1.9828170000
H -0.0425340000 -2.3551490000 0.2794700000
H -2.1158180000 2.6058390000 0.6253420000
C -0.5363130000 4.1042590000 0.5718700000
H -1.3421920000 2.7758670000 -0.9603200000
O 2.3467370000 -0.3632470000 -0.6801490000
O 1.5843080000 -0.0170380000 1.4405260000
C 3.4932870000 -1.1505860000 -0.1990380000
C 4.3852800000 -1.4261780000 -1.3874510000
H 3.9898050000 -0.5661750000 0.5793780000
H 3.0944030000 -2.0617560000 0.2550350000
H 5.2543220000 -2.0021590000 -1.0541030000

H 3.8636130000 -2.0083640000 -2.1521070000
H 4.7450410000 -0.4952040000 -1.8346300000
H -1.2304360000 4.9212130000 0.3548840000
H -0.3422860000 4.1065300000 1.6489790000
H 0.4014010000 4.2979640000 0.0439120000

Equilibrium geometry of r06-endo-3r-prod.

C 0.0221480000 0.4335490000 -0.5981340000
N -0.9159090000 1.0749010000 0.4133660000
H -0.4501530000 0.9239670000 1.3246650000
H 0.2046060000 1.1338070000 -1.4150980000
C 1.3258950000 0.1054510000 0.1259100000
C -1.1531200000 2.5568450000 0.2486060000
C -0.8067350000 -0.7976300000 -1.1039800000
C -2.2068180000 -0.1386100000 -1.1697120000
C -2.2143270000 0.1917730000 0.3289090000
C -1.8302830000 -1.1366570000 0.9433710000
C -0.9933820000 -1.7323340000 0.0830850000
H -0.3966200000 -1.2236470000 -2.0185410000
H -3.0446590000 0.7484420000 0.7599620000
H -2.9946080000 -0.8465600000 -1.4307580000
H -2.2664520000 0.7332890000 -1.8289360000
H -2.1342920000 -1.4724440000 1.9274640000
H -0.4690860000 -2.6709080000 0.2209100000
H -1.9059340000 2.8200180000 0.9964860000
C 0.1145250000 3.3781870000 0.4425690000
H -1.5909440000 2.7057410000 -0.7414410000
O 2.2261410000 -0.3776810000 -0.7042220000
O 1.4478140000 0.2751500000 1.3246500000
C 3.5310320000 -0.7511390000 -0.1322990000
C 4.4335320000 -1.1433340000 -1.2791460000
H 3.9025180000 0.1098910000 0.4280510000
H 3.3564730000 -1.5705390000 0.5694560000
H 5.4124300000 -1.4281940000 -0.8809850000
H 4.0291360000 -1.9967380000 -1.8311340000
H 4.5773600000 -0.3106610000 -1.9734700000
H -0.1482740000 4.4389090000 0.3978960000
H 0.5762380000 3.1853120000 1.4155830000
H 0.8568330000 3.1916760000 -0.3393540000

Equilibrium geometry of r06-endo-3r-ts.

C 0.2210931638 0.7076864972 -0.4155106998
N -0.5327158727 1.4318762758 0.4278289191
H -0.3393554500 1.2443026700 1.4115414395
H 0.3469208006 1.1051516726 -1.4185373056
C 1.4283553726 0.0490561120 0.2142035109
C -1.1204676680 2.7450468331 0.1059912190
C -0.8417490048 -0.9182504372 -1.0260463351
C -2.1935599029 -0.2433748271 -1.1743620469
C -2.7225406212 -0.3079370543 0.2187409126
C -2.0051480909 -1.2285664747 0.9479725617
C -0.9066177246 -1.6602012018 0.1676110969
H -0.2499772341 -1.2394408171 -1.8774685700
H -3.6053205602 0.2225887806 0.5584692459
H -2.8196347042 -0.8868879965 -1.8144220104
H -2.2086546208 0.7472630210 -1.6337890722
H -2.2220816788 -1.5541504903 1.9581583471
H -0.1765018884 -2.3955882360 0.4872669208
H -2.0591603468 2.8370046342 0.6589326402
C -0.1743741232 3.8965521090 0.4497092785
H -1.3621400672 2.7468948161 -0.9606274595
O 2.3116708168 -0.3051399488 -0.7047929948
O 1.5098950306 -0.1091766270 1.4137717922

C 3.5520411703 -0.9275391550 -0.2218407676
C 4.4106682060 -1.2278817266 -1.4294934111
H 4.0241807099 -0.2255365599 0.4697118962
H 3.2762350182 -1.8257149293 0.3371922234
H 5.3428831415 -1.6953368338 -1.0977086883
H 3.9077236640 -1.9179738448 -2.1132767780
H 4.6628690612 -0.3136237118 -1.9743708596
H -0.6558541697 4.8492725701 0.2094428610
H 0.0720308930 3.9032350207 1.5162867308
H 0.7571285738 3.8287869715 -0.1208711036

Equilibrium geometry of **r06-endo-3s-mc**.

C 0.4805150000 1.0249370000 0.3848840000
N -0.2852810000 1.6705250000 -0.4321030000
C -1.1866210000 2.7956010000 -0.1170860000
C 1.5497170000 0.1689890000 -0.2412930000
H 0.4631120000 1.2386970000 1.4473600000
H -0.1336980000 1.4340100000 -1.4188270000
C -2.6977000000 -0.4311770000 -0.2508970000
C -2.3235900000 -0.3593460000 1.2027830000
C -1.0234140000 -1.1168680000 1.2559210000
C -0.7862880000 -1.6588330000 0.0266550000
C -1.8082810000 -1.2178760000 -0.9083210000
H -3.5882270000 0.0238700000 -0.6692850000
H -0.4724750000 -1.3236130000 2.1661160000
H -3.0782840000 -0.8821230000 1.8123050000
H -2.2868450000 0.6584090000 1.6133290000
H 0.0266370000 -2.3297220000 -0.2281390000
H -1.8473860000 -1.4996550000 -1.9540590000
H -2.1358870000 2.5990250000 -0.6193060000
H -1.3568250000 2.7863340000 0.9618480000
C -0.5787570000 4.1212410000 -0.5786660000
O 2.3788760000 -0.2979070000 0.6706720000
O 1.5949380000 0.0271820000 -1.4453430000
C 3.5324040000 -1.0705360000 0.1823470000
C 4.4248890000 -1.3526980000 1.3687820000
H 3.1420110000 -1.9793380000 -0.2836510000
H 4.0251240000 -0.4724750000 -0.5880240000
H 5.2993500000 -1.9168930000 1.0299730000
H 4.7757200000 -0.4243000000 1.8280330000
H 3.9070930000 -1.9486510000 2.1255860000
H -1.2840540000 4.9282880000 -0.3607280000
H 0.3586480000 4.3307850000 -0.0560170000
H -0.3901180000 4.1230600000 -1.6567600000

Equilibrium geometry of **r06-endo-3s-prod**.

C 0.0419470000 0.4673310000 0.6007920000
N -0.9120790000 1.0851950000 -0.4106060000
C -1.1744890000 2.5642160000 -0.2560420000
C 1.3464210000 0.1534580000 -0.1284480000
H 0.2175990000 1.1773520000 1.4106960000
H -0.4483590000 0.9356190000 -1.3231270000
C -2.1947210000 0.1813250000 -0.3124150000
C -2.1745040000 -0.1363500000 1.1887940000
C -0.7640890000 -0.7725910000 1.1214970000
C -0.9412660000 -1.7207210000 -0.0566430000
C -1.7919570000 -1.1460070000 -0.9175780000
H -3.0364870000 0.7199030000 -0.7442060000
H -0.3424700000 -1.1839230000 2.0376140000
H -2.9490770000 -0.8551250000 1.4595300000
H -2.2455210000 0.7399490000 1.8410650000
H -0.4025490000 -2.6518510000 -0.1887820000
H -2.0956860000 -1.4947790000 -1.8971720000

H -1.9313130000 2.8090920000 -1.0060120000
H -1.6151370000 2.7122210000 0.7328850000
C 0.0792760000 3.4057170000 -0.4544220000
O 2.2567900000 -0.3153590000 0.6987060000
O 1.4601540000 0.3196200000 -1.3284910000
C 3.5620630000 -0.6775340000 0.1204610000
C 4.4709030000 -1.0698680000 1.2622670000
H 3.3903770000 -1.4943700000 -0.5849880000
H 3.9262510000 0.1888440000 -0.4365290000
H 5.4501260000 -1.3466990000 0.8591530000
H 4.6121390000 -0.2398520000 1.9604050000
H 4.0737430000 -1.9287260000 1.8111920000
H -0.2012330000 4.4620780000 -0.4158670000
H 0.8236000000 3.2353900000 0.3290570000
H 0.5447660000 3.2148860000 -1.4258950000

Equilibrium geometry of **r06-endo-3s-ts**.

C 0.2350492670 0.7476705726 0.4172993529
N -0.5352757877 1.4535332465 -0.4273923518
C -1.1469654908 2.7566242196 -0.1091811524
C 1.4471101864 0.1026040265 -0.2175532735
H 0.3628718023 1.1563059962 1.4156332802
H -0.3408742653 1.2654072486 -1.4108047077
C -2.6862851614 -0.3351405973 -0.2069151874
C -2.1625839159 -0.2391933264 1.1862946200
C -0.7952135898 -0.8851226150 1.0505619770
C -0.8420796477 -1.6470409048 -0.1319286706
C -1.9472031237 -1.2507542945 -0.9209681213
H -3.5795860188 0.1706244989 -0.5567294536
H -0.1992803730 -1.1818437323 1.9079449940
H -2.7749943479 -0.8887081499 1.8335043984
H -2.2023954127 0.7568437767 1.6323057242
H -0.0952965629 -2.3711659198 -0.4386621314
H -2.1542888375 -1.5959146569 -1.9266982249
H -2.0880108380 2.8289773891 -0.6609283000
H -1.3868793065 2.7579505900 0.9578509259
C -0.2233425665 3.9248015469 -0.4582742000
O 2.3367478862 -0.2474040707 0.6969818427
O 1.5249323952 -0.0534617873 -1.4177142175
C 3.5748835571 -0.8692872715 0.2075730745
C 4.4456628999 -1.1570590223 1.4094221943
H 3.2964370591 -1.7732060816 -0.3408622973
H 4.0384501384 -0.1722055540 -0.4945584331
H 5.3738970948 -1.6293108548 1.0732731685
H 4.7043228919 -0.2370405837 1.9411608003
H 3.9491334039 -1.8388105239 2.1060609779
H -0.7207380528 4.8689361034 -0.2164544963
H 0.7117077707 3.8740026457 0.1082141010
H 0.0181682508 3.9349977876 -1.5259256619

Equilibrium geometry of **r06-exo-3r-mc**.

C 0.4014840000 1.0160460000 -0.4015550000
N -0.3048420000 1.6353670000 0.4878870000
H -0.0318240000 1.4405710000 1.4564300000
H 0.2652890000 1.2204060000 -1.4558750000
C 1.5791040000 0.2300440000 0.1132720000
C -1.3260660000 2.6713560000 0.2414530000
C -2.4479010000 -0.8583510000 0.7893420000
C -1.1572400000 -1.6226380000 0.7110790000
C -0.7486550000 -1.4506740000 -0.7251980000
C -1.7383570000 -0.7786490000 -1.3859090000
C -2.7811820000 -0.4029560000 -0.4451730000
H -3.0334090000 -0.7543380000 1.6955340000

H 0.1114810000 -1.9272650000 -1.1801110000
H -1.3334330000 -2.6894750000 0.9229060000
H -0.4019170000 -1.3052530000 1.4420170000
H -1.7679920000 -0.5794680000 -2.4523930000
H -3.6842160000 0.1356470000 -0.7094790000
H -2.1852860000 2.4304360000 0.8699770000
C -0.7792550000 4.0645770000 0.5542640000
H -1.6325090000 2.5807160000 -0.8030300000
O 2.3655640000 -0.1570660000 -0.8703150000
O 1.7337320000 0.0668170000 1.3068950000
C 3.6034350000 -0.8568970000 -0.4868400000
C 4.4191840000 -1.0631630000 -1.7425050000
H 4.1128230000 -0.2371400000 0.2548940000
H 3.3104550000 -1.7961470000 -0.0100960000
H 5.3453100000 -1.5841540000 -1.4805410000
H 3.8800790000 -1.6727310000 -2.4731740000
H 4.6840830000 -0.1079040000 -2.2041790000
H -1.5695100000 4.8006040000 0.3800890000
H -0.4676710000 4.1496570000 1.6000380000
H 0.0706230000 4.3134470000 -0.0875470000

Equilibrium geometry of r06-exo-3r-prod.

C 0.0354790000 0.3137130000 -0.4992620000
N -0.8297300000 0.9206490000 0.5939110000
H -0.2142650000 0.9026310000 1.4275270000
H 0.0478760000 0.9613430000 -1.3760200000
C 1.4435640000 0.1608180000 0.0786070000
C -1.2931250000 2.3382710000 0.3814810000
C -1.9707030000 -0.1329140000 0.8086600000
C -1.1413440000 -1.4149950000 0.6628220000
C -0.6850660000 -1.0545300000 -0.7743850000
C -2.0199400000 -0.6994330000 -1.4109770000
C -2.7891100000 -0.1412640000 -0.4660010000
H -2.4680530000 0.0856820000 1.7527970000
H -0.0505880000 -1.7616750000 -1.3071750000
H -1.7688770000 -2.3061450000 0.6893960000
H -0.3312510000 -1.5105660000 1.3931560000
H -2.2511450000 -0.8210780000 -2.4631630000
H -3.7810610000 0.2807310000 -0.5704840000
H -1.9915840000 2.5473350000 1.1970620000
C -0.1404390000 3.3324370000 0.3803140000
H -1.8511420000 2.3491590000 -0.5570800000
O 2.2983040000 -0.2367980000 -0.8379770000
O 1.6763450000 0.3719070000 1.2561460000
C 3.6893560000 -0.4610880000 -0.4054940000
C 4.5088530000 -0.7428130000 -1.6437240000
H 4.0161770000 0.4342120000 0.1278410000
H 3.6795990000 -1.2989180000 0.2962950000
H 5.5495500000 -0.9130810000 -1.3510690000
H 4.1507430000 -1.6354850000 -2.1644870000
H 4.4824130000 0.1040490000 -2.3350990000
H -0.5508760000 4.3418910000 0.2870430000
H 0.4352210000 3.2901870000 1.3102890000
H 0.5426380000 3.1783720000 -0.4606790000

Equilibrium geometry of r06-exo-3r-ts.

C 0.2119608475 0.6839438208 -0.3542285002
N -0.4979086512 1.3523383657 0.5737822414
H -0.1489198289 1.2431735908 1.5247461182
H 0.2250267773 1.0948380301 -1.3578981079
C 1.5309038174 0.1336766669 0.1585310753
C -1.3142307216 2.5400110758 0.2777323832
C -2.4047101874 -0.7428135372 0.8076132431

C -1.0993337615 -1.4490042140 0.6907430180
C -0.6730924475 -1.0853236963 -0.7205686545
C -1.8372306131 -0.6481205960 -1.3826231225
C -2.8577504896 -0.3788720621 -0.4414380474
H -2.9507195799 -0.6266966196 1.7376421114
H 0.1184963963 -1.6099160040 -1.2466749633
H -1.2871186628 -2.5354567992 0.7149428140
H -0.3803579873 -1.2441828228 1.4877335988
H -1.9162791100 -0.4801800325 -2.4522100916
H -3.8211319534 0.0619181867 -0.6680565929
H -2.1158691281 2.5820044475 1.0195068144
C -0.4967074273 3.8326232079 0.2880753794
H -1.7809929054 2.3780990336 -0.6985001083
O 2.3420985222 -0.1781469782 -0.8367566993
O 1.7464808895 0.0186412691 1.3470138281
C 3.6711854409 -0.6929147529 -0.4744877935
C 4.4492998265 -0.8710139457 -1.7587664786
H 4.1311486851 0.0294001101 0.2038146140
H 3.5248684639 -1.6310350877 0.0674116514
H 5.4487247750 -1.2499970529 -1.5241188495
H 3.9599118045 -1.5884544408 -2.4239473493
H 4.5597217541 0.0804042925 -2.2866250885
H -1.1551176826 4.6816938528 0.0799727681
H -0.0312003187 3.9996680972 1.2645420526
H 0.2905786937 3.8167947460 -0.4722758463

Equilibrium geometry of r06-exo-3s-prod.

C 0.4010060000 1.0176490000 0.4017480000
N -0.3059390000 1.6361050000 -0.4877730000
C -1.3282780000 2.6710760000 -0.2419140000
C 1.5790880000 0.2324150000 -0.1132250000
H 0.2646450000 1.2219750000 1.4561110000
H -0.0326370000 1.4413010000 -1.4562630000
C -0.7462240000 -1.4509810000 0.7257080000
C -1.1553150000 -1.6234640000 -0.7103590000
C -2.4468530000 -0.8605880000 -0.7880140000
C -2.7799880000 -0.4054040000 0.4466100000
C -1.7362240000 -0.7798500000 1.3868430000
H 0.1147240000 -1.9265240000 1.1802190000
H -3.0329870000 -0.7573380000 -1.6939130000
H -1.3304080000 -2.6905220000 -0.9221430000
H -0.4006830000 -1.3052200000 -1.4416480000
H -3.6834660000 0.1322530000 0.7113200000
H -1.7655150000 -0.5805590000 2.4533280000
H -2.1875850000 2.4283850000 -0.8696950000
H -1.6339660000 2.5813870000 0.8028330000
C -0.7833560000 4.0645390000 -0.5568850000
O 2.3656920000 -0.1549040000 0.8701510000
O 1.7337190000 0.0696300000 -1.3069180000
C 3.6031560000 -0.8551570000 0.4860750000
C 4.4177660000 -1.0651730000 1.7418130000
H 3.3095430000 -1.7930050000 0.0070020000
H 4.1136820000 -0.2342570000 -0.2539200000
H 5.3432600000 -1.5870100000 1.4793650000
H 4.6838400000 -0.1113070000 2.2056490000
H 3.8772870000 -1.6754710000 2.4708930000
H -1.5744030000 4.7998080000 -0.3832600000
H 0.0666180000 4.3153310000 0.0841560000
H -0.4724030000 4.1486560000 -1.6029330000

Equilibrium geometry of r06-exo-3s-prod.

C 0.0345910000 0.3087720000 0.4981700000
N -0.8303770000 0.9194550000 -0.5930990000

C -1.2886780000 2.3383290000 -0.3778670000
C 1.4424370000 0.1565050000 -0.0804280000
H 0.0479660000 0.9541990000 1.3764860000
H -0.2160890000 0.9005100000 -1.4275840000
C -0.6880580000 -1.0589970000 0.7706070000
C -1.1477690000 -1.4149120000 -0.6666570000
C -1.9744530000 -0.1306040000 -0.8078770000
C -2.7904860000 -0.1400040000 0.4683350000
C -2.0209930000 -0.7023750000 1.4105370000
H -0.0542440000 -1.7689670000 1.3005020000
H -2.4731480000 0.0912230000 -1.7505510000
H -1.7774240000 -2.3045290000 -0.6941990000
H -0.3391340000 -1.5105150000 -1.3985620000
H -3.7812160000 0.2841330000 0.5756820000
H -2.2504830000 -0.8259980000 2.4629180000
H -1.9871710000 2.5513480000 -1.1923780000
H -1.8459000000 2.3495170000 0.5612330000
C -0.1324680000 3.3284250000 -0.3759920000
O 2.2986130000 -0.2366430000 0.8366790000
O 1.6740650000 0.3655440000 -1.2585500000
C 3.6907570000 -0.4555950000 0.4054000000
C 4.5120570000 -0.7230330000 1.6458320000
H 3.6862690000 -1.2989520000 -0.2897860000
H 4.0122110000 0.4376430000 -0.1345230000
H 5.5538330000 -0.8889450000 1.3543990000
H 4.4801940000 0.1288320000 2.3307700000
H 4.1595260000 -1.6140440000 2.1731650000
H -0.5393370000 4.3391900000 -0.2815200000
H 0.5505290000 3.1712650000 0.4645930000
H 0.4426880000 3.2851610000 -1.3062620000

Equilibrium geometry of **r06-exo-3s-ts**.

C 0.2116225525 0.6841256246 0.3541328708
N -0.4987703930 1.3520379662 -0.5738092487
C -1.3156836171 2.5392973470 -0.2777245011
C 1.5307682175 0.1345078535 -0.1587944871
H 0.2246307390 1.0951182333 1.3577617617
H -0.1499388185 1.2429322250 -1.5248368727
C -0.6723880541 -1.0856675756 0.7208254387
C -1.0987579232 -1.4497119112 -0.6903501966
C -2.4045768791 -0.7442898749 -0.8069750442
C -2.8575001092 -0.3804391587 0.4421386688
C -1.8365886264 -0.6490062582 1.3831058815
H 0.1196281363 -1.6097536768 1.2467930052
H -2.9508873182 -0.6285940236 -1.7368796204
H -1.2859138129 -2.5362757737 -0.7144207640
H -0.3800868155 -1.2445384364 -1.4875254042
H -3.8210681412 0.0598463498 0.6689458983
H -1.9154659609 -0.4809803892 2.4526919068
H -2.1174490221 2.5808375747 -1.0193762514
H -1.7822176541 2.3772050543 0.6985764458
C -0.4988453985 3.8323306282 -0.2882660253
O 2.3423512961 -0.1766222625 0.8363925407
O 1.7461636637 0.0193586271 -1.3472976409
C 3.6716850960 -0.6906402955 0.4739736573
C 4.4500427927 -0.8683116292 1.7581664116
H 3.5258475946 -1.6288351374 -0.0679255257
H 4.1311737425 0.0319474794 -0.2043637572
H 5.4496400184 -1.2467730158 1.5234074145
H 4.5600325868 0.0831687843 2.2860037932
H 3.9611051645 -1.5860006491 2.4234113290
H -1.1576523932 4.6810642453 -0.0800300079
H 0.2886067351 3.8169028251 0.4719097172
H -0.0336381288 3.9996121349 -1.2648243220

Equilibrium geometry of **r07-endo-3r-mc**.

C 0.4899910000 1.1022900000 -0.3653430000
N -0.3113760000 1.7054610000 0.4483780000
H -0.1791230000 1.4438780000 1.4318010000
H 0.4888180000 1.3407850000 -1.4228380000
C 1.5671470000 0.2547480000 0.2636100000
C -1.2474260000 2.8034040000 0.1400770000
C -0.9682800000 -1.0684660000 -1.3169090000
C -2.2904310000 -0.3529010000 -1.2378350000
C -2.6579280000 -0.4800300000 0.2140860000
C -1.7407360000 -1.2544190000 0.8462080000
C -0.7075900000 -1.6348660000 -0.1044520000
H -0.4137230000 -1.2291450000 -2.2341520000
H -3.5617350000 -0.0669740000 0.6475060000
H -3.0315850000 -0.8776330000 -1.8621320000
H -2.2835090000 0.6782940000 -1.6159020000
H -1.7656440000 -1.5664060000 1.8838180000
H 0.1290320000 -2.2840260000 0.1287070000
H -2.2243740000 2.5155260000 0.5343090000
C -0.7653160000 4.1154110000 0.7589410000
H -1.3205160000 2.8739280000 -0.9477040000
O 2.4252090000 -0.1625460000 -0.6421030000
O 1.5767110000 0.0810710000 1.4655520000
C 3.6060290000 -0.9434600000 -0.1745680000
C 4.0240450000 -1.7964980000 -1.3570140000
C 4.6699750000 0.0319390000 0.3036620000
H 3.2506610000 -1.5593490000 0.6554490000
H 4.8645420000 -2.4316780000 -1.0613600000
H 3.2078380000 -2.4440120000 -1.6900860000
H 4.3461750000 -1.1738050000 -2.1974540000
H 5.5448950000 -0.5295510000 0.6459750000
H 4.9857360000 0.6930480000 -0.5096110000
H 4.3093750000 0.6342600000 1.1418010000
H -1.4980320000 4.8980450000 0.5422920000
H -0.6731690000 4.0356200000 1.8466870000
H 0.1994810000 4.4219260000 0.3451790000

Equilibrium geometry of **r07-endo-3r-prod**.

C 0.0705000000 0.5231770000 -0.5806260000
N -0.9099010000 1.0758970000 0.4433890000
H -0.4577680000 0.8837890000 1.3544060000
H 0.2522130000 1.2762830000 -1.3489130000
C 1.3636820000 0.1790480000 0.1583590000
C -1.1901370000 2.5573560000 0.3618970000
C -0.7117820000 -0.6961920000 -1.1794730000
C -2.1291060000 -0.0749260000 -1.2381640000
C -2.1782500000 0.1635450000 0.2770640000
C -1.7690200000 -1.1896950000 0.8185440000
C -0.8959760000 -1.7071950000 -0.0560940000
H -0.2705800000 -1.0547570000 -2.1085390000
H -3.0339840000 0.6680600000 0.7225390000
H -2.8893900000 -0.7883210000 -1.5590770000
H -2.2011710000 0.8330030000 -1.8459090000
H -2.0850180000 -1.5922450000 1.7732780000
H -0.3467680000 -2.6370280000 0.0355340000
H -1.9482570000 2.7559890000 1.1241480000
C 0.0538530000 3.4031740000 0.5982600000
H -1.6353330000 2.7470960000 -0.6178370000
O 2.2880170000 -0.2447610000 -0.6739880000
O 1.4407480000 0.2785840000 1.3701890000
C 3.5916720000 -0.6964860000 -0.1078850000
C 4.1724710000 -1.6405880000 -1.1434590000
C 4.4555820000 0.5193230000 0.1833060000
H 3.3494540000 -1.2239610000 0.8182780000

H 5.1116070000 -2.0560650000 -0.7657200000
H 3.4917250000 -2.4708370000 -1.3525780000
H 4.3841630000 -1.1140830000 -2.0793710000
H 5.4151710000 0.1877570000 0.5923640000
H 4.6540400000 1.0862860000 -0.7320080000
H 3.9849900000 1.1743250000 0.9211080000
H -0.2382980000 4.4570050000 0.6072900000
H 0.5222140000 3.1741950000 1.5602270000
H 0.7990810000 3.2755020000 -0.1922260000

Equilibrium geometry of r07-endo-3r-ts.

C 0.2456650725 0.7974479427 -0.3905285077
N -0.5498411984 1.4660365599 0.4623032342
H -0.3669948458 1.2532476019 1.4428587784
H 0.3905917112 1.2440170865 -1.3702537464
C 1.4557161971 0.1495840630 0.2513542043
C -1.1871750142 2.7626371143 0.1715678008
C -0.7401190634 -0.8151625365 -1.1039494835
C -2.1248068361 -0.2031367613 -1.2242087843
C -2.6599372606 -0.3818384985 0.1560743504
C -1.9019018317 -1.3089281469 0.8342939010
C -0.7777984940 -1.6349771817 0.0400119689
H -0.1315878748 -1.0593191980 -1.9690928936
H -3.5706246439 0.0809693319 0.5203762057
H -2.7104825496 -0.8379936136 -1.9096134815
H -2.1894882964 0.8117864041 -1.6222666701
H -2.1087394282 -1.7075759820 1.8200291398
H -0.0129744663 -2.3513749595 0.3191928785
H -2.1538088550 2.7850462045 0.6819708763
C -0.3166754315 3.9410273816 0.6109422969
H -1.3789417651 2.8035881417 -0.9044456364
O 2.3579319381 -0.1756828448 -0.6566610586
O 1.5042029380 -0.0297325412 1.4511234532
C 3.6215076331 -0.8074256758 -0.1906119278
C 4.1034191129 -1.6552442180 -1.3531602872
C 4.5870445911 0.2919051778 0.2220102892
H 3.3548322730 -1.4247389796 0.6705945983
H 5.0301613401 -2.1647045649 -1.0721216532
H 3.3668874990 -2.4174155294 -1.6252354393
H 4.3070013748 -1.0344575188 -2.2312211065
H 5.5321387141 -0.1563753334 0.5442818329
H 4.7948862863 0.9602012546 -0.6196853193
H 4.1902953971 0.8758771461 1.0571631039
H -0.8334167764 4.8799168980 0.3899771180
H -0.1203392816 3.9100092871 1.6874292562
H 0.6424834844 3.9442542361 0.0837711100

Equilibrium geometry of r07-endo-3s-mc.

C 0.4862660000 1.1234540000 0.3645640000
N -0.3271500000 1.7149060000 -0.4456110000
C -1.2719480000 2.8043050000 -0.1331890000
C 1.5662120000 0.2820460000 -0.2674740000
H 0.4884330000 1.3645340000 1.4215350000
H -0.1998560000 1.4510410000 -1.4290410000
C -2.6344990000 -0.4929660000 -0.2365790000
C -2.2858340000 -0.3658170000 1.2200720000
C -0.9589610000 -1.0703890000 1.3139050000
C -0.6791020000 -1.6330040000 0.1041120000
C -1.7037790000 -1.2595680000 -0.8585050000
H -3.5367890000 -0.0872350000 -0.6800240000
H -0.4135910000 -1.2267820000 2.2373990000
H -3.0300180000 -0.8987100000 1.8336360000
H -2.2925690000 0.6641840000 1.6013530000

H 0.1655090000 -2.2749700000 -0.1198940000
H -1.7135220000 -1.5704900000 -1.8966500000
H -2.2472050000 2.5090650000 -0.5260510000
H -1.3432470000 2.8718920000 0.9548900000
C -0.8023020000 4.1217650000 -0.7501750000
O 2.4386730000 -0.1143820000 0.6337930000
O 1.5646150000 0.0939820000 -1.4672830000
C 3.6125690000 -0.9059410000 0.1671200000
C 4.0673180000 -1.7038170000 1.3744310000
H 3.2379260000 -1.5597310000 -0.6249480000
C 4.6593580000 0.0494800000 -0.3827750000
H 4.9047380000 -2.3460660000 1.0855300000
H 4.4063990000 -1.0420690000 2.1775330000
H 3.2647750000 -2.3408300000 1.7571030000
H 5.5243500000 -0.5261430000 -0.7268570000
H 4.2743960000 0.6171360000 -1.2340980000
H 4.9993240000 0.7435550000 0.3924900000
H -1.5406620000 4.8978920000 -0.5292360000
H 0.1611810000 4.4348210000 -0.3383810000
H -0.7128290000 4.0454540000 -1.8383730000

Equilibrium geometry of r07-endo-3s-prod.

C 0.0672900000 0.5201910000 0.5714500000
N -0.9150230000 1.0681100000 -0.4528180000
C -1.1935070000 2.5499600000 -0.3760980000
C 1.3641880000 0.1869570000 -0.1655110000
H 0.2423160000 1.2728800000 1.3415530000
H -0.4648000000 0.8710780000 -1.3637820000
C -2.1833010000 0.1558590000 -0.2815870000
C -2.1280600000 -0.0842270000 1.2330670000
C -0.7099800000 -0.7036630000 1.1683070000
C -0.8967010000 -1.7128660000 0.0437790000
C -1.7751550000 -1.1963510000 -0.8260200000
H -3.0407480000 0.6608790000 -0.7230990000
H -0.2654200000 -1.0634520000 2.0953620000
H -2.8862170000 -0.7989720000 1.5560460000
H -2.1986900000 0.8229250000 1.8421480000
H -0.3460060000 -2.6414080000 -0.0518380000
H -2.0945530000 -1.5984460000 -1.7798290000
H -1.9495620000 2.7478640000 -1.1405890000
H -1.6406240000 2.7426060000 0.6022500000
C 0.0524550000 3.3933000000 -0.6114140000
O 2.3024370000 -0.1946790000 0.6716010000
O 1.4337560000 0.2605130000 -1.3796610000
C 3.6138840000 -0.6273320000 0.1082930000
C 4.2248400000 -1.5291090000 1.1640430000
H 3.3791360000 -1.1848150000 -0.8020660000
C 4.4445640000 0.6019250000 -0.2208140000
H 5.1732510000 -1.9284470000 0.7920620000
H 4.4260740000 -0.9738090000 2.0854840000
H 3.5672520000 -2.3714570000 1.3969070000
H 5.4081070000 0.2839300000 -0.6314000000
H 3.9511840000 1.2269330000 -0.9697640000
H 4.6378210000 1.1963020000 0.6780150000
H -0.2378820000 4.4476250000 -0.6231610000
H 0.7956720000 3.2660490000 0.1809980000
H 0.5224560000 3.1616720000 -1.5720330000

Equilibrium geometry of r07-endo-3s-ts.

C 0.2395068182 0.7902545958 0.3877683096
N -0.5498399830 1.4649441767 -0.4642710267
C -1.1876762345 2.7592878723 -0.1638323878
C 1.4552056333 0.1455760597 -0.2450809597

H 0.3717726349 1.2256533624 1.3741184188
H -0.3693630617 1.2553159240 -1.4457179977
C -2.6709108887 -0.3770761882 -0.1858065666
C -2.1376141094 -0.2270597194 1.1989718846
C -0.7563221835 -0.8445897804 1.0711701445
C -0.7924660520 -1.6388170565 -0.0897528769
C -1.9137302836 -1.2918646467 -0.8805829709
H -3.5800179524 0.0950858087 -0.5420328670
H -0.1495900585 -1.1049624806 1.9329066862
H -2.7289761297 -0.8705551797 1.8712802614
H -2.1976358449 0.7808062540 1.6156900699
H -0.0305337164 -2.3525449357 -0.3827364162
H -2.1189292081 -1.6698697678 -1.8748759919
H -2.1320551369 2.8033260329 -0.7128454618
H -1.4235916607 2.7718203245 0.9040787646
C -0.2901013074 3.9420005736 -0.5326585873
O 2.3756114643 -0.1173244398 0.6642409095
O 1.4936089086 -0.0822243521 -1.4369800374
C 3.6389774239 -0.7620676895 0.2158654700
C 4.2151561417 -1.4144976345 1.4589761485
H 3.3487311244 -1.5093777698 -0.5279839099
C 4.5407530802 0.2880676003 -0.4132910739
H 5.1278635926 -1.9573985093 1.1957010364
H 4.4690805370 -0.6613345714 2.2114876971
H 3.5097666697 -2.1258754295 1.8983277717
H 5.4828057682 -0.1805277584 -0.7149119599
H 4.0809367240 0.7227555670 -1.3042463292
H 4.7701995788 1.0839527151 0.3026867086
H -0.8044399244 4.8788733106 -0.2980506700
H 0.6494466738 3.9161074540 0.0283222764
H -0.0556740141 3.9446677721 -1.6018912320

Equilibrium geometry of **r07-exo-3r-mc**.

C 0.4019770000 1.0275860000 -0.3771790000
N -0.3194400000 1.6351190000 0.5080550000
H -0.0532240000 1.4378190000 1.4779930000
H 0.2733490000 1.2360820000 -1.4316370000
C 1.5881500000 0.2546390000 0.1443120000
C -1.3492840000 2.6607870000 0.2551360000
C -2.4490910000 -0.8695470000 0.7748630000
C -1.1503440000 -1.6209130000 0.7054770000
C -0.7313310000 -1.4409250000 -0.7268030000
C -1.7215130000 -0.7767170000 -1.3940750000
C -2.7762400000 -0.4141340000 -0.4612300000
H -3.0434780000 -0.7738410000 1.6761790000
H 0.1387880000 -1.9058800000 -1.1746400000
H -1.3177430000 -2.6899240000 0.9135080000
H -0.4036940000 -1.2976040000 1.4426910000
H -1.7435510000 -0.5737970000 -2.4600430000
H -3.6821100000 0.1166000000 -0.7317690000
H -2.2048080000 2.4193150000 0.8885170000
C -0.8124820000 4.0613920000 0.5519570000
H -1.6585220000 2.5577830000 -0.7873240000
O 2.3862480000 -0.1059270000 -0.8365500000
O 1.7222610000 0.0824020000 1.3403920000
C 3.6632790000 -0.7932290000 -0.4841090000
C 4.0416190000 -1.5955940000 -1.7142460000
C 4.6828140000 0.2630370000 -0.0866860000
H 3.4319720000 -1.4430270000 0.3633440000
H 4.9687680000 -2.1416780000 -1.5161960000
H 3.2664470000 -2.3237970000 -1.9706540000
H 4.2069960000 -0.9390510000 -2.5739300000
H 5.6314120000 -0.2260710000 0.1553880000
H 4.8585930000 0.9609840000 -0.9112540000
H 4.3569460000 0.8189500000 0.7964380000

H -1.6087070000 4.7897920000 0.3728730000
H -0.4976920000 4.1594880000 1.5956100000
H 0.0333640000 4.3101280000 -0.0954030000

Equilibrium geometry of **r07-exo-3r-prod**.

C 0.0524220000 0.3174300000 -0.4840500000
N -0.8182500000 0.9053850000 0.6154460000
H -0.2111390000 0.8536650000 1.4543670000
H 0.0860820000 0.9903650000 -1.3409970000
C 1.4521600000 0.1267490000 0.1076600000
C -1.2593300000 2.3345370000 0.4380610000
C -1.9750030000 -0.1374560000 0.7874610000
C -1.1619210000 -1.4265340000 0.6138430000
C -0.6842680000 -1.0311480000 -0.8071500000
C -2.0068090000 -0.6391010000 -1.4481860000
C -2.7795220000 -0.0984270000 -0.4958960000
H -2.4797800000 0.0611390000 1.7320120000
H -0.0534800000 -1.7312260000 -1.3534520000
H -1.8018520000 -2.3093560000 0.6081950000
H -0.3607520000 -1.5528060000 1.3488570000
H -2.2270640000 -0.7264270000 -2.5061550000
H -3.7643450000 0.3402300000 -0.5990910000
H -1.9591010000 2.5331900000 1.2551370000
C -0.0918260000 3.3106920000 0.4679090000
H -1.8119020000 2.3778410000 -0.5028190000
O 2.3100230000 -0.2496470000 -0.8112750000
O 1.6612970000 0.2916870000 1.2985540000
C 3.7138030000 -0.5404830000 -0.3935010000
C 4.2580770000 -1.4793960000 -1.4531610000
C 4.4720480000 0.7698470000 -0.2673990000
H 3.6396470000 -1.0360720000 0.5776680000
H 5.2784660000 -1.7718590000 -1.1871350000
H 3.6531840000 -2.3874810000 -1.5292770000
H 4.2862840000 -0.9907170000 -2.4320290000
H 5.5051510000 0.5598690000 0.0275200000
H 4.4937500000 1.3024130000 -1.2235850000
H 4.0304950000 1.4136050000 0.4976950000
H -0.4861010000 4.3285260000 0.4001350000
H 0.4793310000 3.2347480000 1.3985940000
H 0.5921700000 3.1675720000 -0.3741840000

Equilibrium geometry of **r07-exo-3r-ts**.

C 0.2162713695 0.6900201658 -0.3404771354
N -0.5009577943 1.3511293052 0.5878761746
H -0.1579018841 1.2348017510 1.5400687889
H 0.2361468799 1.1097732483 -1.3404528299
C 1.5353595689 0.1391180157 0.1774471228
C -1.3181431190 2.5385601205 0.2952215100
C -2.4036906029 -0.7502643736 0.7956019902
C -1.0950190818 -1.4505934486 0.6818274172
C -0.6606679595 -1.0736277178 -0.7237213531
C -1.8225623339 -0.6360984602 -1.3900589868
C -2.8501381368 -0.3783053185 -0.4535248035
H -2.9559755697 -0.6429122382 1.7230029196
H 0.1355594553 -1.5922019699 -1.2486865208
H -1.2783505686 -2.5379588251 0.6966475214
H -0.3815146124 -1.2484518317 1.4843510081
H -1.8952491416 -0.4597241361 -2.4587337670
H -3.8136616109 0.0608513255 -0.6827188691
H -2.1257310769 2.5727857915 1.0310499305
C -0.5047905750 3.8336713617 0.3217551613
H -1.7771866596 2.3833146161 -0.6858263335
O 2.3528520916 -0.1562025037 -0.8148122632

O 1.7305351887 0.0088701538 1.3692826027
C 3.6976211131 -0.6961153924 -0.4732334050
C 4.1375203869 -1.4837585378 -1.6934523590
C 4.6158864764 0.4603919300 -0.1150682339
H 3.5501138214 -1.3503261749 0.3900436391
H 5.1048385831 -1.9534954986 -1.4909358648
H 3.4220626057 -2.2741997243 -1.9392248966
H 4.2511711318 -0.8286504919 -2.5628857758
H 5.6096920178 0.0700137426 0.1259017477
H 4.7175919329 1.1527002590 -0.9571537358
H 4.2485664331 1.0053112201 0.7585830817
H -1.1639206902 4.6824014199 0.1145013189
H -0.0478637949 3.9947383518 1.3033496024
H 0.2888883880 3.8257246129 -0.4321300100

Equilibrium geometry of r07-exo-3s-mc.

C 0.4019010000 1.0279540000 0.3787510000
N -0.3198060000 1.6363080000 -0.5056270000
C -1.3502940000 2.6610970000 -0.2517330000
C 1.5877450000 0.2553330000 -0.1440400000
H 0.2733150000 1.2349560000 1.4335220000
H -0.0536890000 1.4400530000 -1.4758200000
C -0.7298220000 -1.4427680000 0.7255570000
C -1.1493400000 -1.6214380000 -0.7067220000
C -2.4486190000 -0.8708340000 -0.7747150000
C -2.7754020000 -0.4168090000 0.4619520000
C -1.7199940000 -0.7797200000 1.3939480000
H 0.1407660000 -1.9076110000 1.1725400000
H -3.0434770000 -0.7745930000 -1.6756620000
H -1.3160760000 -2.6902780000 -0.9159460000
H -0.4032500000 -1.2967180000 -1.4438770000
H -3.6814320000 0.1131380000 0.7334720000
H -1.7416500000 -0.5779120000 2.4600970000
H -2.2067790000 2.4181190000 -0.8832360000
H -1.6573960000 2.5588660000 0.7914490000
C -0.8155820000 4.0619510000 -0.5511850000
O 2.3854470000 -0.1078960000 0.8361180000
O 1.7217490000 0.0853200000 -1.3404640000
C 3.6612030000 -0.7969960000 0.4823650000
C 4.0383510000 -1.6017390000 1.7113100000
H 3.4284050000 -1.4452080000 -0.3659140000
C 4.6825390000 0.2579090000 0.0859690000
H 4.9646130000 -2.1489960000 1.5124430000
H 4.2048100000 -0.9466710000 2.5719080000
H 3.2620330000 -2.3290540000 1.9667160000
H 5.6302520000 -0.2325840000 -0.1567140000
H 4.3574900000 0.8152570000 -0.7965510000
H 4.8596090000 0.9547130000 0.9112240000
H -1.6122680000 4.7896470000 -0.3713910000
H 0.0312330000 4.3123330000 0.0942910000
H -0.5028840000 4.1592470000 -1.5955620000

Equilibrium geometry of r07-exo-3s-prod.

C 0.0519850000 0.3157230000 0.4843270000
N -0.8187790000 0.9048950000 -0.6144260000
C -1.2594850000 2.3339700000 -0.4356030000
C 1.4515950000 0.1253990000 -0.1078060000
H 0.0858550000 0.9877830000 1.3419520000
H -0.2118460000 0.8538230000 -1.4535340000
C -0.6848810000 -1.0330560000 0.8062120000
C -1.1629390000 -1.4269170000 -0.6150820000
C -1.9758060000 -0.1375130000 -0.7872000000
C -2.7799970000 -0.0995720000 0.4964070000

C -2.0071770000 -0.6414010000 1.4479430000
H -0.0541400000 -1.7338890000 1.3516530000
H -2.4807900000 0.0621200000 -1.7314190000
H -1.8029830000 -2.3096250000 -0.6101910000
H -0.3619500000 -1.5526070000 -1.3504190000
H -3.7646930000 0.3392080000 0.6002850000
H -2.2272260000 -0.7297330000 2.5058880000
H -1.9593700000 2.5335360000 -1.2523810000
H -1.8118620000 2.3765470000 0.5054550000
C -0.0917750000 3.3099240000 -0.4648220000
O 2.3095890000 -0.2520100000 0.8105890000
O 1.6605330000 0.2913790000 -1.2986040000
C 3.7132520000 -0.5424350000 0.3922360000
C 4.2577570000 -1.4825060000 1.4507700000
H 3.6389390000 -1.0369760000 -0.5794680000
C 4.4715320000 0.7679920000 0.2672760000
H 5.2780640000 -1.7746840000 1.1841920000
H 4.2861710000 -0.9948910000 2.4301810000
H 3.6528960000 -2.3906780000 1.5260140000
H 5.5045600000 0.5581420000 -0.0279860000
H 4.0299050000 1.4124780000 -0.4972170000
H 4.4934450000 1.2997870000 1.2239250000
H -0.4858520000 4.3277670000 -0.3960550000
H 0.5924160000 3.1660080000 0.3770040000
H 0.4791670000 3.2347180000 -1.3957590000

Equilibrium geometry of r07-exo-3s-ts.

C 0.2159205377 0.6884998672 0.3410069191
N -0.5013295254 1.3505885989 -0.5866379375
C -1.3184135041 2.5377703679 -0.2927131676
C 1.5348050752 0.1378056604 -0.1776756477
H 0.2360928211 1.1073708682 1.3413470656
H -0.1584672202 1.2350651041 -1.5389969118
C -0.6613226766 -1.0751983563 0.7228985612
C -1.0958565936 -1.4510141206 -0.6828960711
C -2.4044349280 -0.7504214224 -0.7960138931
C -2.8507187403 -0.3793516521 0.4534343282
C -1.8231077463 -0.6380232528 1.3896780014
H 0.1348415308 -1.5943361009 1.2474012161
H -2.9567830260 -0.6422899168 -1.7232834790
H -1.2793473703 -2.5383383691 -0.6985320297
H -0.3824122344 -1.2483513733 -1.4853401939
H -3.8141564158 0.0597708636 0.6830464299
H -1.8956831024 -0.4624739063 2.4584939352
H -2.1256006658 2.5731456116 -1.0289217348
H -1.7780110833 2.3812181215 0.6878695289
C -0.5048654527 3.8328027289 -0.3169681561
O 2.3524934414 -0.1584520544 0.8141380101
O 1.7296693340 0.0084917788 -1.3696651617
C 3.6970805853 -0.6983382730 0.4717720238
C 4.1372819944 -1.4867678163 1.6913686012
H 3.5491825430 -1.3519978367 -0.3918546039
C 4.6153902251 0.4582514108 0.1139784619
H 5.1044705907 -1.9565123957 1.4882516472
H 4.2512996359 -0.8321818523 2.5611445341
H 3.4218033581 -2.2772600639 1.9369176038
H 5.6090823768 0.0678768456 -0.1274652212
H 4.2479003313 1.0036726163 -0.7592854608
H 4.7174073194 1.1500964555 0.9564060834
H -1.1640120404 4.6813167340 -0.1088670662
H 0.2883868558 3.8237123967 0.4373499740
H -0.0473766113 3.9952106980 -1.2980750739

Equilibrium geometry of r08-endo-3r-mc.

C 0.4734680000 1.0365250000 -0.3631140000
 N -0.2963930000 1.6720490000 0.4561060000
 H -0.1383910000 1.4325260000 1.4414570000
 H 0.4463450000 1.2494980000 -1.4256210000
 C 1.5635610000 0.1919200000 0.2583190000
 C -1.2169070000 2.7819940000 0.1445800000
 C -1.0255570000 -1.1287620000 -1.2503420000
 C -2.3323590000 -0.3808830000 -1.2212340000
 C -2.7278920000 -0.4466610000 0.2272720000
 C -1.8385270000 -1.2159600000 0.9034820000
 C -0.7977370000 -1.6545000000 -0.0136320000
 H -0.4594210000 -1.3351040000 -2.1512410000
 H -3.6289920000 0.0025990000 0.6290180000
 H -3.0748800000 -0.9092410000 -1.8408100000
 H -2.2937120000 0.6360180000 -1.6345360000
 H -1.8887720000 -1.4883680000 1.9513230000
 H 0.0205920000 -2.3109740000 0.2596010000
 H -2.1567040000 2.5762890000 0.6608600000
 C -0.6218400000 4.1202360000 0.5857260000
 H -1.4016320000 2.7610930000 -0.9317740000
 O 2.3980330000 -0.2181420000 -0.6674580000
 O 1.5818720000 0.0384440000 1.4637060000
 C 3.6692600000 -0.9767920000 -0.3389160000
 C 4.2900060000 -1.1638530000 -1.7184560000
 C 4.5377330000 -0.1023370000 0.5617220000
 C 3.2913260000 -2.3073990000 0.3047040000
 H 5.2351980000 -1.7058370000 -1.6225740000
 H 3.6288690000 -1.7400400000 -2.3724850000
 H 4.4948870000 -0.1976410000 -2.1888100000
 H 5.5076520000 -0.5910300000 0.6966010000
 H 4.7166620000 0.8736950000 0.0996800000
 H 4.0882580000 0.0398110000 1.5462270000
 H 4.2002920000 -2.9001880000 0.4482610000
 H 2.8213770000 -2.1659000000 1.2802660000
 H 2.6208890000 -2.8787980000 -0.3458790000
 H -1.3400940000 4.9158220000 0.3674690000
 H -0.4207790000 4.1359550000 1.6614500000
 H 0.3067190000 4.3365330000 0.0499820000

Equilibrium geometry of **r08-endo-3r-prod.**

C 0.0507080000 0.4675440000 -0.5911870000
 N -0.9002030000 1.0633940000 0.4352570000
 H -0.4417310000 0.8665600000 1.3426280000
 H 0.2405040000 1.2013490000 -1.3756740000
 C 1.3492690000 0.1021500000 0.1349110000
 C -1.1334840000 2.5509500000 0.3349560000
 C -0.7724150000 -0.7402220000 -1.1585430000
 C -2.1713870000 -0.0778830000 -1.2150750000
 C -2.1980230000 0.1886090000 0.2961930000
 C -1.8246390000 -1.1662140000 0.8576550000
 C -0.9760070000 -1.7250330000 -0.0155030000
 H -0.3506500000 -1.1275280000 -2.0849570000
 H -3.0337340000 0.7271890000 0.7397930000
 H -2.9561760000 -0.7732770000 -1.5159610000
 H -2.2212960000 0.8211080000 -1.8379900000
 H -2.1424810000 -1.5425110000 1.8224460000
 H -0.4529350000 -2.6683920000 0.0895150000
 H -1.8793940000 2.7854540000 1.0991100000
 C 0.1383780000 3.3600840000 0.5508400000
 H -1.5792040000 2.7412530000 -0.6444510000
 O 2.2524480000 -0.3070640000 -0.7222920000
 O 1.4247240000 0.1926690000 1.3486790000
 C 3.6247810000 -0.7918450000 -0.2991110000
 C 4.2813610000 -1.0887850000 -1.6428180000
 C 4.3440390000 0.3295220000 0.4458560000

C 3.4493310000 -2.0522240000 0.5426260000
 H 5.2984530000 -1.4566280000 -1.4790430000
 H 3.7244710000 -1.8532870000 -2.1926020000
 H 4.3376690000 -0.1854650000 -2.2569580000
 H 5.3795240000 0.0234780000 0.6252620000
 H 4.3660320000 1.2438540000 -0.1556340000
 H 3.8780170000 0.5413410000 1.4094870000
 H 4.4358040000 -2.4743560000 0.7585510000
 H 2.9558520000 -1.8379020000 1.4930350000
 H 2.8751910000 -2.8080560000 -0.0033160000
 H -0.1204310000 4.4227010000 0.5494350000
 H 0.6071760000 3.1283080000 1.5119400000
 H 0.8734550000 3.2005800000 -0.2435350000

Equilibrium geometry of **r08-endo-3r-ts.**

C 0.2312557575 0.7471099532 -0.4027554549
 N -0.5431435181 1.4470668470 0.4434684855
 H -0.3513306766 1.2496193040 1.4257181669
 H 0.3633832466 1.1652376835 -1.3966095436
 C 1.4469179462 0.0964517890 0.2339240033
 C -1.1497813018 2.7538856615 0.1338715876
 C -0.7898634119 -0.8762143269 -1.0509818618
 C -2.1573512537 -0.2323971938 -1.1974138461
 C -2.6962513522 -0.3394859178 0.1891490614
 C -1.9637008588 -1.2591330358 0.9041555433
 C -0.8487497229 -1.6474297584 0.1248410472
 H -0.1848056034 -1.1669284032 -1.9038994470
 H -3.5937812557 0.1628159241 0.5329087793
 H -2.7612831581 -0.8780719314 -1.8562322506
 H -2.1937983255 0.7669857623 -1.6362062118
 H -2.1811321476 -1.6115965280 1.9051175274
 H -0.1030210552 -2.3714685296 0.4338871375
 H -2.0914022885 2.8260121319 0.6848182195
 C -0.2232926081 3.9172439116 0.4917051263
 H -1.3886671236 2.7638796355 -0.9333781739
 O 2.3260632138 -0.2316228213 -0.6907795997
 O 1.4963248948 -0.0625946897 1.4374029905
 C 3.6506058377 -0.8750680784 -0.3550660486
 C 4.2850638258 -1.0362430721 -1.7325156595
 C 4.4518050063 0.0782155425 0.5281897568
 C 3.3893557034 -2.2252420168 0.3084527523
 H 5.2720281498 -1.4961764971 -1.6284626197
 H 3.6741274839 -1.6782921745 -2.3742171450
 H 4.4082876332 -0.0661734491 -2.2227729001
 H 5.4513954986 -0.3398284736 0.6831076987
 H 4.5681717629 1.0518034874 0.0416505734
 H 3.9837440511 0.2165735504 1.5045891977
 H 4.3435661543 -2.7446577940 0.4409592463
 H 2.9245805405 -2.1114888718 1.2897944030
 H 2.7563357263 -2.8545744907 -0.3268240916
 H -0.7168752127 4.8647835731 0.2552837711
 H 0.0168296402 3.9194592637 1.5597141902
 H 0.7125728343 3.8666965881 -0.0735597980

Equilibrium geometry of **r08-endo-3s-mc.**

C 0.4735150000 1.0320330000 0.3691610000
 N -0.2938630000 1.6720450000 -0.4489690000
 C -1.2132730000 2.7821040000 -0.1345540000
 C 1.5658710000 0.1910410000 -0.2530180000
 H 0.4437850000 1.2402460000 1.4325210000
 H -0.1335850000 1.4371620000 -1.4350850000
 C -2.7313850000 -0.4387380000 -0.2258890000
 C -2.3291370000 -0.3874270000 1.2213270000

C -1.0242220000 -1.1391880000 1.2375820000
 C -0.8036020000 -1.6543190000 -0.0049330000
 C -1.8472310000 -1.2043390000 -0.9131760000
 H -3.6328620000 0.0169060000 -0.6194410000
 H -0.4548020000 -1.3556520000 2.1340020000
 H -3.0702690000 -0.9192760000 1.8393330000
 H -2.2857200000 0.6255100000 1.6437350000
 H 0.0117000000 -2.3102240000 -0.2881960000
 H -1.9031350000 -1.4670030000 -1.9632120000
 H -2.1514440000 2.5814480000 -0.6554420000
 H -1.4020730000 2.7554170000 0.9409900000
 C -0.6134150000 4.1214660000 -0.5658000000
 O 2.3994250000 -0.2198130000 0.6732540000
 O 1.5868400000 0.0410730000 -1.4587670000
 C 3.6750310000 -0.9712110000 0.3449120000
 C 4.2937100000 -1.1598490000 1.7251790000
 C 3.3049840000 -2.3014520000 -0.3041020000
 C 4.5412000000 -0.0895020000 -0.5508750000
 H 5.2421820000 -1.6960080000 1.6294150000
 H 4.4919660000 -0.1942800000 2.1995520000
 H 3.6344380000 -1.7422690000 2.3754900000
 H 5.5134550000 -0.5735670000 -0.6859000000
 H 4.0928830000 0.0542620000 -1.5356730000
 H 4.7151900000 0.8855750000 -0.0849100000
 H 4.2170320000 -2.8898580000 -0.4459940000
 H 2.6344730000 -2.8776360000 0.3421370000
 H 2.8379560000 -2.1589140000 -1.2809340000
 H -1.3303280000 4.9175760000 -0.3452530000
 H 0.3138420000 4.3321820000 -0.0256870000
 H -0.4087610000 4.1430550000 -1.6407140000

Equilibrium geometry of **r08-endo-3s-prod.**

C 0.0515640000 0.4649680000 0.5943280000
 N -0.8975140000 1.0650180000 -0.4313830000
 C -1.1289230000 2.5525400000 -0.3266440000
 C 1.3514010000 0.1024420000 -0.1309620000
 H 0.2406150000 1.1961090000 1.3815530000
 H -0.4382870000 0.8707200000 -1.3388490000
 C -2.1964090000 0.1911530000 -0.2964240000
 C -2.1715250000 -0.0802910000 1.2140730000
 C -0.7731620000 -0.7439340000 1.1567230000
 C -0.9765800000 -1.7246770000 0.0101990000
 C -1.8237730000 -1.1621440000 -0.8619950000
 H -3.0311310000 0.7320700000 -0.7389910000
 H -0.3527450000 -1.1347110000 2.0821880000
 H -2.9574290000 -0.7757030000 1.5119730000
 H -2.2210000000 0.8168320000 1.8397470000
 H -0.4543880000 -2.6682710000 -0.0973870000
 H -2.1409480000 -1.5350570000 -1.8283170000
 H -1.8747580000 2.7903230000 -1.0898950000
 H -1.5741630000 2.7406050000 0.6534150000
 C 0.1439370000 3.3605890000 -0.5405910000
 O 2.2525970000 -0.3114000000 0.7260790000
 O 1.4296970000 0.1997810000 -1.3440240000
 C 3.6281700000 -0.7878800000 0.3042280000
 C 4.2788120000 -1.0984690000 1.6477440000
 C 3.4617000000 -2.0389830000 -0.5532910000
 C 4.3472750000 0.3444910000 -0.4238940000
 H 5.2984240000 -1.4598240000 1.4850050000
 H 4.3276570000 -0.2025210000 2.2733090000
 H 3.7222640000 -1.8721070000 2.1849870000
 H 5.3843420000 0.0435850000 -0.6030750000
 H 3.8845220000 0.5667340000 -1.3867890000
 H 4.3644720000 1.2516160000 0.1886410000
 H 4.4509300000 -2.4545380000 -0.7689900000

H 2.8878730000 -2.8035130000 -0.0191590000
 H 2.9722240000 -1.8155300000 -1.5037000000
 H -0.1135320000 4.4234900000 -0.5363170000
 H 0.8790640000 3.1981940000 0.2532140000
 H 0.6123420000 3.1306410000 -1.5023500000

Equilibrium geometry of **r08-endo-3s-ts.**

C 0.2326226035 0.7460478646 0.4071928625
 N -0.5406697977 1.4494507985 -0.4371307553
 C -1.1482774720 2.7546961702 -0.1226946976
 C 1.4500311487 0.0990176948 -0.2297064037
 H 0.3622000553 1.1593521076 1.4033771677
 H -0.3474210277 1.2561363075 -1.4199137692
 C -2.6945224833 -0.3366393216 -0.1927444925
 C -2.1560850970 -0.2385808156 1.1947980378
 C -0.7887063408 -0.8820113631 1.0447516439
 C -0.8473888560 -1.6457566059 -0.1360296899
 C -1.9620334568 -1.2521131756 -0.9133106510
 H -3.5917416390 0.1683249567 -0.5336200032
 H -0.1838135534 -1.1781804772 1.8960056748
 H -2.7605885455 -0.8880896578 1.8493146464
 H -2.1922468871 0.7580892350 1.6397859517
 H -0.1017948283 -2.3681065485 -0.4495212429
 H -2.1792583583 -1.5981489858 -1.9166441158
 H -2.0878154929 2.8299075260 -0.6769436683
 H -1.3913787532 2.7586457284 0.9437107775
 C -0.2202829379 3.9200527953 -0.4704517574
 O 2.3278496042 -0.2311859092 0.6955185622
 O 1.5017811078 -0.0557662097 -1.4336435471
 C 3.6537604622 -0.8720500820 0.3602755186
 C 4.2859047941 -1.0364970660 1.7384160803
 C 3.3951720136 -2.2205803110 -0.3076457512
 C 4.4554191364 0.0847243914 -0.5187889872
 H 5.2735548431 -1.4950837322 1.6348255718
 H 4.4071799796 -0.0676905621 2.2316712687
 H 3.6744839716 -1.6810420307 2.3771658503
 H 5.4558711420 -0.3315627052 -0.6729497017
 H 3.9889976084 0.2250698048 -1.4956832446
 H 4.5695285999 1.0571452469 -0.0293680762
 H 4.3501585438 -2.7387093191 -0.4397042866
 H 2.7614376571 -2.8523411092 0.3245016128
 H 2.9322715193 -2.1044788057 -1.2896180349
 H -0.7148959272 4.8662196256 -0.2306503618
 H 0.7134328113 3.8663060731 0.0982608847
 H 0.0240464544 3.9284155287 -1.5375717792

Equilibrium geometry of **r08-exo-3r-mc.**

C 0.4092080000 1.0318980000 -0.3815780000
 N -0.3097930000 1.6431660000 0.5016730000
 H -0.0356380000 1.4517330000 1.4710660000
 H 0.2719150000 1.2275730000 -1.4373930000
 C 1.6025210000 0.2639080000 0.1444230000
 C -1.3495700000 2.6586280000 0.2499360000
 C -2.4497400000 -0.8734770000 0.7867140000
 C -1.1488050000 -1.6214510000 0.7179130000
 C -0.7348010000 -1.4500430000 -0.7168940000
 C -1.7262950000 -0.7899350000 -1.3845290000
 C -2.7801780000 -0.4245550000 -0.4503620000
 H -3.0422310000 -0.7750260000 1.6889740000
 H 0.1368700000 -1.9135090000 -1.1630100000
 H -1.3109550000 -2.6892260000 0.9357940000
 H -0.4005850000 -1.2882690000 1.4492970000
 H -1.7512120000 -0.5912390000 -2.4512390000

H -3.6876370000 0.1031840000 -0.7215400000
H -2.2013580000 2.4095040000 0.8854380000
C -0.8254690000 4.0643960000 0.5449270000
H -1.6602610000 2.5520030000 -0.7917360000
O 2.3899780000 -0.0912270000 -0.8418930000
O 1.7248040000 0.1098860000 1.3453860000
C 3.7264110000 -0.7721300000 -0.6077650000
C 4.2475150000 -0.9498860000 -2.0286950000
C 4.6079410000 0.1681070000 0.2098500000
C 3.4804720000 -2.1128210000 0.0795630000
H 5.2247750000 -1.4400930000 -1.9952390000
H 3.5718270000 -1.5739420000 -2.6210730000
H 4.3652820000 0.0153550000 -2.5294980000
H 5.6032710000 -0.2770510000 0.3049140000
H 4.7193040000 1.1336910000 -0.2932590000
H 4.2102430000 0.3256010000 1.2141800000
H 4.4322270000 -2.6485630000 0.1499700000
H 3.0848340000 -1.9882050000 1.0892650000
H 2.7945660000 -2.7329220000 -0.5070000000
H -1.6292930000 4.7850880000 0.3688970000
H -0.5076490000 4.1655080000 1.5874070000
H 0.0155870000 4.3213620000 -0.1055000000

Equilibrium geometry of **r08-exo-3r-prod.**

C 0.0476520000 0.3263860000 -0.4944990000
N -0.8200280000 0.9030950000 0.6130910000
H -0.2058530000 0.8457760000 1.4472650000
H 0.0780640000 1.0062590000 -1.3458470000
C 1.4521980000 0.1263760000 0.0928680000
C -1.2683010000 2.3310920000 0.4496310000
C -1.9716610000 -0.1447880000 0.7845740000
C -1.1560430000 -1.4300520000 0.5956100000
C -0.6876640000 -1.0209300000 -0.8247120000
C -2.0155150000 -0.6287950000 -1.4545690000
C -2.7846150000 -0.0989350000 -0.4933260000
H -2.4712990000 0.0446160000 1.7337530000
H -0.0581410000 -1.7145040000 -1.3805820000
H -1.7937090000 -2.3144570000 0.5861830000
H -0.3503700000 -1.5600670000 1.3247840000
H -2.2420780000 -0.7084990000 -2.5118060000
H -3.7718320000 0.3365600000 -0.5866680000
H -1.9631690000 2.5209340000 1.2730040000
C -0.1048690000 3.3121580000 0.4783310000
H -1.8277760000 2.3793720000 -0.4869460000
O 2.2959050000 -0.2289350000 -0.8425660000
O 1.6473650000 0.2731640000 1.2898260000
C 3.7363470000 -0.6047000000 -0.5494190000
C 4.2774510000 -0.8992070000 -1.9437930000
C 4.4447660000 0.5849760000 0.0920410000
C 3.7317870000 -1.8490030000 0.3339170000
H 5.3258340000 -1.2022970000 -1.8685370000
H 3.7196070000 -1.7110520000 -2.4197730000
H 4.2223150000 -0.0124330000 -2.5819610000
H 5.5088950000 0.3478020000 0.1899480000
H 4.3587970000 1.4759020000 -0.5381110000
H 4.0513710000 0.8059400000 1.0855220000
H 4.7619230000 -2.1929040000 0.4693990000
H 3.3121410000 -1.6432660000 1.3211170000
H 3.1687230000 -2.6598860000 -0.1393740000
H -0.5035570000 4.3288650000 0.4205230000
H 0.4733270000 3.2316140000 1.4042740000
H 0.5737660000 3.1771690000 -0.3693450000

Equilibrium geometry of **r08-exo-3r-ts.**

C 0.2133629786 0.6911468561 -0.3429286019
N -0.5057245984 1.3489836274 0.5866137546
H -0.1572347205 1.2315600865 1.5370137477
H 0.2334184868 1.1135552552 -1.3417683892
C 1.5382009247 0.1436151298 0.1789409128
C -1.3214667836 2.5385044027 0.3003412370
C -2.4051188729 -0.7516177286 0.7867278642
C -1.0953142951 -1.4501652210 0.6738219947
C -0.6585005995 -1.0684479473 -0.7297942675
C -1.8203336788 -0.6328912471 -1.3975090935
C -2.8501725787 -0.3788240511 -0.4625190664
H -2.9590487107 -0.6465720865 1.7133437676
H 0.1399699365 -1.5841414021 -1.2538580694
H -1.2772231828 -2.5377494010 0.6853751080
H -0.3838407866 -1.2482013195 1.4780947189
H -1.8911600470 -0.4537705877 -2.4658193546
H -3.8139305247 0.0593313712 -0.6925930970
H -2.1341621796 2.5655268453 1.0309164244
C -0.5086031354 3.8334271285 0.3466072688
H -1.7737839805 2.3937241735 -0.6853841630
O 2.3411153019 -0.1594764780 -0.8181115588
O 1.7216764105 0.0387413896 1.3762686464
C 3.7372774371 -0.6982255842 -0.5956095949
C 4.2381150804 -0.8911829376 -2.0228450032
C 4.5516856283 0.3524352710 0.1539612072
C 3.6397016486 -2.0264673569 0.1515981652
H 5.2558986018 -1.2915948916 -1.9990484616
H 3.6057431160 -1.5970966508 -2.5699714178
H 4.2569368914 0.0577510736 -2.5670287037
H 5.5887292958 0.0101759731 0.2281579704
H 4.5503272872 1.3029807459 -0.3888564130
H 4.1724762752 0.5117960421 1.1649220116
H 4.6364911437 -2.4749392994 0.2099550953
H 3.2661799750 -1.8936270901 1.1683992803
H 2.9925198742 -2.7282778618 -0.3855580965
H -1.1662324443 4.6847825973 0.1455327625
H -0.0574992925 3.9826793777 1.3328076427
H 0.2897660751 3.8338368136 -0.4023022196

Equilibrium geometry of **r08-exo-3s-mc.**

C 0.4093320000 1.0363050000 0.3824090000
N -0.3106740000 1.6465340000 -0.5006650000
C -1.3532010000 2.6592130000 -0.2493320000
C 1.6030420000 0.2692130000 -0.1440020000
H 0.2714470000 1.2310390000 1.4383570000
H -0.0360870000 1.4556100000 -1.4700940000
C -0.7285880000 -1.4506920000 0.7159890000
C -1.1432760000 -1.6221190000 -0.7186140000
C -2.4461100000 -0.8772820000 -0.7858960000
C -2.7764480000 -0.4296320000 0.4516240000
C -1.7208480000 -0.7929820000 1.3847350000
H 0.1445470000 -1.9121830000 1.1611270000
H -3.0396080000 -0.7798020000 -1.6876360000
H -1.3027500000 -2.6900670000 -0.9374750000
H -0.3964280000 -1.2862580000 -1.4501950000
H -3.6848850000 0.0959570000 0.7238760000
H -1.7452560000 -0.5948410000 2.4515620000
H -2.2053180000 2.4059170000 -0.8829430000
H -1.6617060000 2.5540580000 0.7931370000
C -0.8342490000 4.0659230000 -0.5489000000
O 2.3902310000 -0.0871370000 0.8420680000
O 1.7254140000 0.1162760000 -1.3451020000
C 3.7246940000 -0.7717640000 0.6076340000
C 4.2468240000 -0.9486990000 2.0282760000
C 3.4740080000 -2.1128260000 -0.0773180000

C 4.6081990000 0.1642650000 -0.2125150000
H 5.2226660000 -1.4416380000 1.9945830000
H 4.3678070000 0.0170450000 2.5273090000
H 3.5700600000 -1.5698530000 2.6224380000
H 5.6021270000 -0.2839600000 -0.3071090000
H 4.2103920000 0.3208000000 -1.2169390000
H 4.7227100000 1.1305560000 0.2884010000
H 4.4242480000 -2.6512600000 -0.1484540000
H 2.7872420000 -2.7303070000 0.5111330000
H 3.0772510000 -1.9885500000 -1.0866080000
H -1.6400430000 4.7845610000 -0.3731370000
H 0.0072110000 4.3272820000 0.0992310000
H -0.5188560000 4.1653250000 -1.5922940000

Equilibrium geometry of r08-exo-3s-prod.

C 0.0475120000 0.3259360000 0.4943560000
N -0.8205270000 0.9022710000 -0.6131440000
C -1.2688820000 2.3302500000 -0.4498220000
C 1.4520270000 0.1263450000 -0.0932610000
H 0.0779930000 1.0060170000 1.3455240000
H -0.2065520000 0.8448040000 -1.4474440000
C -0.6875290000 -1.0214060000 0.8250580000
C -1.1562890000 -1.4308770000 -0.5950320000
C -1.9721120000 -0.1457280000 -0.7840130000
C -2.7846540000 -0.0996630000 0.4941600000
C -2.0151880000 -0.6292490000 1.4552630000
H -0.0577640000 -1.7147860000 1.3808880000
H -2.4720530000 0.0434460000 -1.7330750000
H -1.7938170000 -2.3153810000 -0.5853010000
H -0.3507920000 -1.5608690000 -1.3244110000
H -3.7717750000 0.3357230000 0.5876920000
H -2.2413940000 -0.7086960000 2.5126000000
H -1.9639420000 2.5199160000 -1.2730990000
H -1.8281340000 2.3786210000 0.4868330000
C -0.1055670000 3.3114370000 -0.4789220000
O 2.2961530000 -0.2282110000 0.8420820000
O 1.6468870000 0.2730120000 -1.2902720000
C 3.7372910000 -0.6012680000 0.5489130000
C 4.2787140000 -0.8957920000 1.9431860000
C 3.7351790000 -1.8450150000 -0.3352400000
C 4.4434410000 0.5902990000 -0.0914860000
H 5.3274900000 -1.1972340000 1.8678320000
H 4.2221810000 -0.0096090000 2.5818870000
H 3.7221200000 -1.7087670000 2.4185380000
H 5.5080980000 0.3555690000 -0.1890150000
H 4.0500400000 0.8111050000 -1.0850160000
H 4.3552140000 1.4805730000 0.5391910000
H 4.7658920000 -2.1869530000 -0.4707870000
H 3.1734920000 -2.6571560000 0.1375360000
H 3.3152220000 -1.6394620000 -1.3223150000
H -0.5043680000 4.3279950000 -0.4205940000
H 0.5734600000 3.1762200000 0.3683690000
H 0.4722080000 3.2312300000 -1.4052700000

Equilibrium geometry of r08-exo-3s-ts.

C 0.2130777772 0.6914313856 0.3427839621
N -0.5065421841 1.3486871731 -0.5867305242
C -1.3229457368 2.5377624305 -0.3005013749
C 1.5381609626 0.1446148106 -0.1791997316
H 0.2330011598 1.1139669882 1.3415701781
H -0.1581737257 1.2312931466 -1.5371795574
C -0.6576634601 -1.0687761012 0.7300757671
C -1.0945250903 -1.4509351371 -0.6733989655

C -2.4048077637 -0.7532415290 -0.7861296405
C -2.8497976629 -0.3804869489 0.4631442120
C -1.8195866980 -0.6337695505 1.3979584404
H 0.1412628786 -1.5838658818 1.2540393247
H -2.9590131447 -0.6487041340 -1.7126394913
H -1.2757352029 -2.5386379001 -0.6847919701
H -0.3833427120 -1.2486141130 -1.4778405118
H -3.8137665519 0.0571304231 0.6933609000
H -1.8902873490 -0.4545014989 2.4662535130
H -2.1357554054 2.5642443183 -1.0309688421
H -1.7750442092 2.3928453847 0.6853029394
C -0.5108174697 3.8331378353 -0.3470372501
O 2.3414367435 -0.1577492940 0.8177814478
O 1.7215091553 0.0396428170 -1.3765377885
C 3.7380619613 -0.6952467686 0.5951681250
C 4.2391471048 -0.8878157329 2.0223683541
C 3.6416758281 -2.0235269582 -0.1521196772
C 4.5514711526 0.3561906550 -0.1543919983
H 5.2574141181 -1.2869923507 1.9985295181
H 4.2568307314 0.0610665491 2.5666843972
H 3.6076285123 -1.5945576070 2.5694080733
H 5.5887940469 0.0148155702 -0.2287465011
H 4.1720157411 0.5153251996 -1.1652988387
H 4.5493715301 1.3066825193 0.3885180313
H 4.6388629769 -2.4711168790 -0.2104685026
H 2.9950885135 -2.7259436342 0.3849587344
H 3.2680648589 -1.8909274703 -1.1689156141
H -1.1688714359 4.6841414579 -0.1458720353
H 0.2877146747 3.8340272525 0.4016978560
H -0.0600149931 3.9825756858 -1.3333460205

Equilibrium geometry of r09-endo-3r-mc.

C 0.5089460000 1.0775940000 -0.3425670000
N -0.1533300000 1.8238920000 0.4750760000
H 0.0645780000 1.6589250000 1.4650500000
H 0.4123320000 1.2065180000 -1.4140370000
C 1.5723930000 0.2029780000 0.2668880000
C -1.0787960000 2.9389650000 0.1451530000
C -0.9995270000 -1.1210290000 -1.1989970000
C -2.3733630000 -0.5049670000 -1.2509960000
C -2.8736030000 -0.6688430000 0.1564580000
C -1.9526880000 -1.3397920000 0.8895970000
C -0.8043620000 -1.6409890000 0.0460890000
H -0.3573450000 -1.2589870000 -2.0610690000
H -3.8476610000 -0.3341060000 0.4936410000
H -3.0083310000 -1.0619840000 -1.9577270000
H -2.3963000000 0.5349820000 -1.6076340000
H -2.0479330000 -1.6381110000 1.9270600000
H 0.0526970000 -2.2218190000 0.3688910000
C -2.2513280000 2.9290030000 1.1242470000
C -0.2903970000 4.2547950000 0.1769050000
H -1.4294820000 2.7419870000 -0.8726870000
O 2.3069860000 -0.3750590000 -0.6666060000
O 1.7011530000 0.1327090000 1.4696010000
C 3.4112300000 -1.1963390000 -0.1963150000
H 3.9106620000 -1.5414550000 -1.0987610000
H 4.0798830000 -0.5945420000 0.4211390000
H 3.0228370000 -2.0348640000 0.3846410000
H -0.9631840000 5.0780640000 -0.0806660000
H 0.1132750000 4.4497710000 1.1758430000
H 0.5348570000 4.2480700000 -0.5410450000
H -2.9536040000 3.7220970000 0.8537150000
H -2.7791750000 1.9724130000 1.1064870000
H -1.9102870000 3.1241900000 2.1475400000

Equilibrium geometry of **r09-endo-3r-prod.**

C 0.0371800000 0.4451670000 -0.6120760000
 N -0.9419880000 1.0890040000 0.3611770000
 H -0.5033820000 0.9684700000 1.2894120000
 H 0.2100300000 1.1213240000 -1.4501230000
 C 1.3389210000 0.1831660000 0.1375010000
 C -1.1788830000 2.5894680000 0.1644930000
 C -0.7315240000 -0.8292350000 -1.0998400000
 C -2.1492570000 -0.2202910000 -1.2210660000
 C -2.2083950000 0.1540880000 0.2645950000
 C -1.7930230000 -1.1404500000 0.9300120000
 C -0.9164050000 -1.7344360000 0.1096000000
 H -0.2817840000 -1.2655160000 -1.9906900000
 H -3.0761590000 0.6762410000 0.6546580000
 H -2.9061470000 -0.9622830000 -1.4790600000
 H -2.2207440000 0.6288940000 -1.9087360000
 H -2.1104370000 -1.4562650000 1.9165720000
 H -0.3666040000 -2.6514070000 0.2878730000
 C -2.1517150000 3.1080000000 1.2236980000
 C 0.1540540000 3.3391850000 0.2317840000
 H -1.6172930000 2.6844410000 -0.8339840000
 O 2.2749620000 -0.2656090000 -0.6782320000
 O 1.4418900000 0.3629620000 1.3348610000
 C 3.5651320000 -0.5747500000 -0.0809030000
 H 4.2010760000 -0.8628280000 -0.9149100000
 H 3.9558540000 0.3077790000 0.4275510000
 H 3.4527280000 -1.3941880000 0.6306000000
 H -0.0413180000 4.4062060000 0.0956460000
 H 0.6339710000 3.2057830000 1.2065050000
 H 0.8579370000 3.0380610000 -0.5485210000
 H -2.2568500000 4.1891370000 1.0985630000
 H -3.1527490000 2.6784470000 1.1453790000
 H -1.7678160000 2.9319700000 2.2352950000

Equilibrium geometry of **r09-endo-3r-ts.**

C 0.2247721688 0.7624968906 -0.4066738979
 N -0.5357059728 1.4745992502 0.4390256485
 H -0.3382054271 1.2922936071 1.4233623779
 H 0.3427235757 1.1635559632 -1.4091886486
 C 1.4441148019 0.1231817314 0.2170640269
 C -1.1312819196 2.7969768242 0.1212807581
 C -0.7911365415 -0.8868716424 -1.0407142919
 C -2.1748562667 -0.2783917095 -1.1767980043
 C -2.7172515348 -0.4243908602 0.2043154914
 C -1.9449076278 -1.3090395771 0.9199027870
 C -0.8180021079 -1.6560665246 0.1365272279
 H -0.1859688359 -1.1620681187 -1.8987693796
 H -3.6408531906 0.0294062836 0.5453208785
 H -2.7593438172 -0.9246441737 -1.8526228688
 H -2.2376151571 0.7289837567 -1.5951336266
 H -2.1486512478 -1.6740492906 1.9192174799
 H -0.0492887862 -2.3574797383 0.4421523930
 C -2.2421265008 3.1142649582 1.1185526310
 C -0.0392105205 3.8769689489 0.1139489685
 H -1.5525904388 2.7115826538 -0.8870685307
 O 2.3244676532 -0.2319269747 -0.7090721414
 O 1.5456731723 -0.0264794444 1.4150755275
 C 3.5544575198 -0.8351781932 -0.2251704138
 H 4.1505242060 -1.0192740632 -1.1163911481
 H 4.0611067013 -0.1458345013 0.4518444169
 H 3.3293340413 -1.7668884402 0.2971429986
 H -0.4765104595 4.8441459521 -0.1513047731
 H 0.4227305614 3.9722285036 1.1025400268
 H 0.7457246677 3.6484024784 -0.6140951360

H -2.6872162469 4.0839427812 0.8805072616
 H -3.0354280695 2.3615519074 1.1004681303
 H -1.8460598595 3.1752084688 2.1391290432

Equilibrium geometry of **r09-endo-3s-mc.**

C 0.5097300000 1.0692480000 0.3516260000
 N -0.1472180000 1.8240020000 -0.4625640000
 C -1.0701870000 2.9395930000 -0.1275390000
 C 1.5728290000 0.1961150000 -0.2604630000
 H 0.4095760000 1.1903910000 1.4236600000
 H 0.0737800000 1.6660970000 -1.4529770000
 C -2.8794440000 -0.6592290000 -0.1637160000
 C -2.3773110000 -0.5133830000 1.2449710000
 C -1.0056370000 -1.1335470000 1.1844920000
 C -0.8135170000 -1.6398090000 -0.0666790000
 C -1.9616310000 -1.3248720000 -0.9054990000
 H -3.8527290000 -0.3172220000 -0.4960550000
 H -0.3632320000 -1.2838780000 2.0443400000
 H -3.0135370000 -1.0764270000 1.9457740000
 H -2.3964250000 0.5224240000 1.6137500000
 H 0.0412000000 -2.2196710000 -0.3972220000
 H -2.0589710000 -1.6108930000 -1.9462410000
 C -2.2409170000 2.9391170000 -1.1089290000
 H -1.4233330000 2.7373280000 0.8884280000
 C -0.2781550000 4.2534290000 -0.1498410000
 O 2.3026000000 -0.3905930000 0.6714600000
 O 1.7058210000 0.1342110000 -1.4631600000
 C 3.4065200000 -1.2111290000 0.1991590000
 H 3.9034960000 -1.5618310000 1.1007950000
 H 3.0179450000 -2.0460450000 -0.3869800000
 H 4.0773400000 -0.6072030000 -0.4137550000
 H -0.9491670000 5.0768580000 0.1115680000
 H 0.5459540000 4.2401900000 0.5694610000
 H 0.1277420000 4.4534560000 -1.1469490000
 H -2.9409870000 3.7330040000 -0.8350560000
 H -1.8972940000 3.1391930000 -2.1304350000
 H -2.7718950000 1.9842520000 -1.0976950000

Equilibrium geometry of **r09-endo-3s-prod.**

C 0.0351900000 0.4359030000 0.6154060000
 N -0.9392400000 1.0912960000 -0.3549990000
 C -1.1710360000 2.5910720000 -0.1475980000
 C 1.3380690000 0.1758300000 -0.1328040000
 H 0.2084510000 1.1041730000 1.4596560000
 H -0.4988890000 0.9762210000 -1.2830780000
 C -2.2093860000 0.1602880000 -0.2687280000
 C -2.1548460000 -0.2273530000 1.2135570000
 C -0.7389820000 -0.8401410000 1.0902250000
 C -0.9243040000 -1.7339090000 -0.1276310000
 C -1.7972970000 -1.1298470000 -0.9446000000
 H -3.0744960000 0.6890320000 -0.6557240000
 H -0.2926940000 -1.2857730000 1.9781520000
 H -2.9148050000 -0.9691170000 1.4630540000
 H -2.2252860000 0.6157780000 1.9088260000
 H -0.3771480000 -2.6510810000 -0.3128660000
 H -2.1136390000 -1.4360070000 -1.9344590000
 C -2.1393810000 3.1208610000 -1.2054270000
 H -1.6116080000 2.6801100000 0.8503970000
 C 0.1648990000 3.3359720000 -0.2056810000
 O 2.2712110000 -0.2798150000 0.6824500000
 O 1.4441410000 0.3629550000 -1.3287640000
 C 3.5624970000 -0.5874940000 0.0868310000
 H 4.1971700000 -0.8763380000 0.9216290000

H 3.4515220000 -1.4063130000 -0.6256890000
H 3.9535270000 0.2958590000 -0.4200000000
H -0.0267520000 4.4026590000 -0.0620840000
H 0.8652790000 3.0260280000 0.5743350000
H 0.6470010000 3.2081330000 -1.1800420000
H -2.2399970000 4.2016760000 -1.0736990000
H -1.7545090000 2.9494970000 -2.2174710000
H -3.1424650000 2.6953920000 -1.1315380000

Equilibrium geometry of **r09-endo-3s-ts**.

C 0.2246058318 0.7532416771 0.4128129861
N -0.5317263826 1.4741660416 -0.4293095365
C -1.1231759603 2.7965868462 -0.1041513360
C 1.4448118727 0.1160735051 -0.2113882628
H 0.3401173930 1.1458246274 1.4189770855
H -0.3328100850 1.2978858718 -1.4144542134
C -2.7218065997 -0.4120849720 -0.2093714829
C -2.1769437243 -0.2860769868 1.1728019975
C -0.7964158674 -0.8996132460 1.0270664775
C -0.8290958954 -1.6545491080 -0.1594197801
C -1.9552170630 -1.2922024373 -0.9367598255
H -3.6433938517 0.0509293094 -0.5433094977
H -0.1912733124 -1.1883146502 1.8806980763
H -2.7639666854 -0.9378038174 1.8411229526
H -2.2341138503 0.7163543006 1.6036141990
H -0.0644620926 -2.3560095269 -0.4749708273
H -2.1623893388 -1.6438762830 -1.9401559423
C -2.2318136992 3.1234491518 -1.1008334536
H -1.5459027974 2.7064038580 0.9031655726
C -0.0278542072 3.8731011370 -0.0894727474
O 2.3215138057 -0.2461088123 0.7154981287
O 1.5499366656 -0.0264392057 -1.4099488907
C 3.5521417924 -0.8486567072 0.2324323086
H 4.1463463529 -1.0354077445 1.1243501656
H 3.3274878744 -1.7789691810 -0.2925851435
H 4.0604503956 -0.1579075666 -0.4418768412
H -0.4626821947 4.8401371487 0.1803147866
H 0.7555547996 3.6384450995 0.6382912804
H 0.4356237271 3.9723395676 -1.0769453287
H -2.6739752091 4.0932750726 -0.8579636733
H -1.8343163440 3.1887683239 -2.1205885202
H -3.0275265857 2.3732581192 -1.0879180002

Equilibrium geometry of **r09-exo-3r-mc**.

C 0.4057630000 1.0349970000 -0.3374980000
N -0.2788500000 1.6731200000 0.5543790000
H -0.0058840000 1.4796190000 1.5234590000
H 0.2644400000 1.2354450000 -1.3917760000
C 1.5729120000 0.2300300000 0.1680540000
C -1.3047350000 2.7241060000 0.3069020000
C -2.5021400000 -0.9752450000 0.7597210000
C -1.1752340000 -1.6741890000 0.6852000000
C -0.7389330000 -1.4230250000 -0.7317880000
C -1.7376450000 -0.7590440000 -1.3871120000
C -2.8202170000 -0.4716150000 -0.4596240000
H -3.1160970000 -0.9409500000 1.6521840000
H 0.1448570000 -1.8529150000 -1.1876130000
H -1.3010900000 -2.7556900000 0.8526290000
H -0.4556570000 -1.3459070000 1.4473630000
H -1.7495540000 -0.5132120000 -2.4442610000
H -3.7376430000 0.0421320000 -0.7236690000
C -2.2571160000 2.7859140000 1.4977120000
C -0.5988550000 4.0603260000 0.0392460000

H -1.8434240000 2.4027440000 -0.5900120000
O 2.3547740000 -0.1541180000 -0.8248830000
O 1.7337690000 0.0459260000 1.3562660000
C 3.5632450000 -0.8723810000 -0.4504770000
H 4.0932580000 -1.0393290000 -1.3854760000
H 4.1533030000 -0.2641520000 0.2368130000
H 3.2948460000 -1.8174570000 0.0252090000
H -1.3505640000 4.8208630000 -0.1898390000
H -0.0351080000 4.3931740000 0.9165780000
H 0.0858240000 3.9903640000 -0.8117930000
H -3.0264970000 3.5372050000 1.3027100000
H -2.7483640000 1.8242890000 1.6652670000
H -1.7299020000 3.0834070000 2.4115680000

Equilibrium geometry of **r09-exo-3r-prod**.

C 0.0440020000 0.3201860000 -0.4863610000
N -0.8491670000 0.9294020000 0.5845190000
H -0.2551630000 0.9319030000 1.4327660000
H 0.0565650000 0.9527190000 -1.3732060000
C 1.4464200000 0.2020900000 0.1076170000
C -1.3057370000 2.3634470000 0.3348310000
C -1.9723160000 -0.1499710000 0.7916920000
C -1.1144570000 -1.4160380000 0.6736560000
C -0.6424760000 -1.0650730000 -0.7582830000
C -1.9725750000 -0.7422940000 -1.4219330000
C -2.7676820000 -0.1879380000 -0.4965500000
H -2.4879880000 0.0540740000 1.7265390000
H 0.0149770000 -1.7647350000 -1.2729550000
H -1.7259830000 -2.3183730000 0.7031150000
H -0.3144430000 -1.4875490000 1.4177970000
H -2.1830310000 -0.8800620000 -2.4765170000
H -3.7648450000 0.2149610000 -0.6245850000
C -2.2686790000 2.8024240000 1.4365900000
C -0.0867160000 3.2822990000 0.2494780000
H -1.8252290000 2.3273010000 -0.6273150000
O 2.3224110000 -0.1666620000 -0.8061720000
O 1.6699040000 0.4108930000 1.2857160000
C 3.6953030000 -0.3497220000 -0.3586350000
H 4.2672350000 -0.5258060000 -1.2669720000
H 4.0378980000 0.5476020000 0.1577830000
H 3.7486680000 -1.2096700000 0.3109900000
H -0.4296780000 4.3014820000 0.0521300000
H 0.4721780000 3.2934820000 1.1914300000
H 0.5986020000 3.0101950000 -0.5583470000
H -2.5521050000 3.8431990000 1.2578320000
H -3.1895690000 2.2143210000 1.4557560000
H -1.7965610000 2.7571370000 2.4249990000

Equilibrium geometry of **r09-exo-3r-ts**.

C 0.2193041910 0.7071048523 -0.3408648421
N -0.4898658048 1.3782320871 0.5841028025
H -0.1521991950 1.2668455883 1.5392276190
H 0.2392706031 1.1180653298 -1.3443531371
C 1.5350035031 0.1576680287 0.1772662600
C -1.3234015580 2.5651817531 0.2890241170
C -2.4023679363 -0.8115606665 0.8001604680
C -1.0717904517 -1.4670864975 0.6720098397
C -0.6524604121 -1.0598531237 -0.7296417110
C -1.8256477453 -0.6328000553 -1.3826866031
C -2.8579455409 -0.4204686810 -0.4388813436
H -2.9570468834 -0.7444493969 1.7297599654
H 0.1454290250 -1.5612913211 -1.2688643664
H -1.2189567797 -2.5600856591 0.6763224640

H -0.3650220643 -1.2507815503 1.4770775025
H -1.9069195503 -0.4394576194 -2.4478566586
H -3.8329876401 -0.0020482068 -0.6581823679
C -2.2762879681 2.8206992414 1.4535808632
C -0.4388497527 3.7855364012 -0.0066671972
H -1.8973508598 2.3117110752 -0.6108525915
O 2.3531110027 -0.1553731638 -0.8161794412
O 1.7519773401 0.0386504014 1.3639962501
C 3.6586628347 -0.6692679895 -0.4356071165
H 4.1915330989 -0.8097908319 -1.3736376379
H 4.1676407448 0.0545414639 0.2023216385
H 3.5424538466 -1.6153780989 0.0961602180
H -1.0676704711 4.6397609920 -0.2754744133
H 0.1514300074 4.0617780116 0.8734066697
H 0.2476053884 3.5988163313 -0.8390680108
H -2.8944755585 3.6976161613 1.2443105994
H -2.9382637220 1.9678922389 1.6278969212
H -1.7200737598 3.0243104229 2.3764512870

Equilibrium geometry of **r09-exo-3s-mc**.

C 0.4056920000 1.0269220000 0.3388620000
N -0.2762270000 1.6682510000 -0.5527880000
C -1.2985920000 2.7224270000 -0.3045380000
C 1.5705890000 0.2186770000 -0.1664990000
H 0.2640260000 1.2264580000 1.3932380000
H -0.0031950000 1.4750540000 -1.5219120000
C -0.7477270000 -1.4276520000 0.7292860000
C -1.1829060000 -1.6764350000 -0.6884590000
C -2.5076220000 -0.9734320000 -0.7642720000
C -2.8256110000 -0.4695410000 0.4549800000
C -1.7452010000 -0.7609970000 1.3837550000
H 0.1342390000 -1.8605340000 1.1857670000
H -3.1200290000 -0.9363360000 -1.6577550000
H -1.3117530000 -2.7573920000 -0.8569660000
H -0.4614200000 -1.3495910000 -1.4493100000
H -3.7416970000 0.0470200000 0.7182450000
H -1.7578620000 -0.5160220000 2.4410300000
C -2.2505360000 2.7888230000 -1.4953830000
H -1.8385190000 2.4019870000 0.5919310000
C -0.5882350000 4.0558790000 -0.0353560000
O 2.3502870000 -0.1689140000 0.8267730000
O 1.7318670000 0.0351430000 -1.3547280000
C 3.5565880000 -0.8910110000 0.4529600000
H 4.0857320000 -1.0600360000 1.3881240000
H 3.2854000000 -1.8350540000 -0.0229980000
H 4.1489750000 -0.2846950000 -0.2338880000
H -1.3374610000 4.8185450000 0.1949780000
H 0.0963350000 3.9826500000 0.8153030000
H -0.0236220000 4.3879710000 -0.9124340000
H -3.0171680000 3.5427730000 -1.2996930000
H -1.7221040000 3.0852610000 -2.4088820000
H -2.7451900000 1.8291190000 -1.6638710000

Equilibrium geometry of **r09-exo-3s-prod**.

C 0.0424100000 0.3167050000 0.4877640000
N -0.8484150000 0.9279170000 -0.5840890000
C -1.3059620000 2.3617680000 -0.3346120000
C 1.4446230000 0.1930490000 -0.1059610000
H 0.0564390000 0.9494370000 1.3745100000
H -0.2527540000 0.9311370000 -1.4311060000
C -0.6475070000 -1.0667190000 0.7595350000
C -1.1164620000 -1.4177950000 -0.6733530000
C -1.9720630000 -0.1504430000 -0.7941750000

C -2.7708530000 -0.1867480000 0.4919490000
C -1.9786980000 -0.7415690000 1.4196360000
H 0.0076680000 -1.7670540000 1.2762890000
H -2.4850410000 0.0538540000 -1.7304980000
H -1.7294020000 -2.3191240000 -0.7039080000
H -0.3148280000 -1.4909330000 -1.4155550000
H -3.7678890000 0.2174950000 0.6172580000
H -2.1920020000 -0.8784750000 2.4737400000
C -2.2608340000 2.8031480000 -1.4424910000
H -1.8320790000 2.3240920000 0.6238790000
C -0.0874330000 3.2803020000 -0.2391000000
O 2.3175090000 -0.1871790000 0.8060710000
O 1.6700810000 0.4064390000 -1.2828160000
C 3.6886740000 -0.3806810000 0.3573210000
H 4.2601590000 -0.5605040000 1.2651650000
H 3.7347220000 -1.2417400000 -0.3116300000
H 4.0374950000 0.5135670000 -0.1602830000
H -0.4317480000 4.2992990000 -0.0428370000
H 0.5921060000 3.0068340000 0.5731490000
H 0.4780470000 3.2924300000 -1.1769760000
H -2.5469800000 3.8430430000 -1.2627310000
H -1.7806960000 2.7614950000 -2.4272160000
H -3.1809390000 2.2142180000 -1.4710090000

Equilibrium geometry of **r09-exo-3s-ts**.

C 0.2176558580 0.6989507161 0.3418358221
N -0.4886585123 1.3733443878 -0.5830309458
C -1.3180525979 2.5631695388 -0.2874407877
C 1.5323697775 0.1464689039 -0.1755261557
H 0.2376896527 1.1084900427 1.3458993796
H -0.1499746670 1.2623258509 -1.5378552617
C -0.6597799165 -1.0659798494 0.7266466032
C -1.0797986577 -1.4686550072 -0.6761105244
C -2.4075890132 -0.8074587803 -0.8036475516
C -2.8626049623 -0.4176966525 0.4360658682
C -1.8318230363 -0.6361724048 1.3800235678
H 0.1360746311 -1.5713680078 1.2651864582
H -2.9614229666 -0.7360797932 -1.7334239429
H -1.2314938509 -2.5610081623 -0.6826149665
H -0.3715725003 -1.2536968796 -1.4802579866
H -3.8362096238 0.0038803358 0.6556943468
H -1.9130196446 -0.4449581686 2.4455827914
C -2.2693487026 2.8232452703 -1.4523073560
H -1.8934025143 2.3111098606 0.6119428711
C -0.4290120967 3.7799488528 0.0096468260
O 2.3484150044 -0.1702048942 0.8184752360
O 1.7503982835 0.0284113849 -1.3621619303
C 3.6529387578 -0.6873549704 0.4387951522
H 4.1847372731 -0.8293853931 1.3772067233
H 3.5346833937 -1.6331096004 -0.0931539150
H 4.1642321378 0.0352169128 -0.1986722474
H -1.0546723800 4.6366152987 0.2780502058
H 0.2558188762 3.5902353422 0.8427200472
H 0.1633414759 4.0541128665 -0.8697066411
H -2.8842567730 3.7022874168 -1.2424237997
H -1.7118879238 3.0256985309 -2.3746692648
H -2.9344192969 1.9731204930 -1.6277782189

Equilibrium geometry of **r10-endo-3r-mc**.

C 0.5241340000 1.0705390000 -0.3524680000
N -0.2618350000 1.6895350000 0.4592860000
H -0.1718780000 1.3758540000 1.4328550000
H 0.5618790000 1.3239660000 -1.4042370000

C 1.5245720000 0.1328360000 0.2734590000
 C -1.1636530000 2.8526560000 0.2100670000
 C -1.0697780000 -1.1274430000 -1.3194300000
 C -2.3689030000 -0.3752060000 -1.2071290000
 C -2.7035810000 -0.4900290000 0.2544780000
 C -1.7875920000 -1.2804710000 0.8655750000
 C -0.7876880000 -1.6899080000 -0.1123680000
 H -0.5420900000 -1.3006420000 -2.2501560000
 H -3.5869200000 -0.0554200000 0.7086240000
 H -3.1408760000 -0.8751310000 -1.8138000000
 H -2.3375880000 0.6562750000 -1.5836060000
 H -1.7916780000 -1.5883280000 1.9047720000
 H 0.0380730000 -2.3590320000 0.1024540000
 H -2.1783640000 2.4631090000 0.3369640000
 C -0.8847090000 3.8852910000 1.3077060000
 C -0.9925800000 3.4158520000 -1.1956100000
 O 2.3575390000 -0.3374700000 -0.6332180000
 O 1.5227700000 -0.0608950000 1.4708130000
 C 3.4388720000 -1.2128860000 -0.1563870000
 C 4.3337410000 -1.5069310000 -1.3384470000
 H 3.9558080000 -0.6889520000 0.6514420000
 H 2.9723330000 -2.1110870000 0.2580730000
 H 5.1500680000 -2.1611120000 -1.0171140000
 H 3.7829920000 -2.0142050000 -2.1357220000
 H 4.7704430000 -0.5880430000 -1.7397540000
 H -1.5922110000 4.7130980000 1.2089260000
 H -1.0137980000 3.4582900000 2.3081020000
 H 0.1296360000 4.2877700000 1.2245640000
 H -1.6852550000 4.2524060000 -1.3193560000
 H 0.0215150000 3.7989850000 -1.3533260000
 H -1.2253670000 2.6858160000 -1.9771990000

Equilibrium geometry of **r10-endo-3r-prod.**

C 0.0174980000 0.3514610000 -0.7046760000
 N -0.8523200000 1.1400040000 0.2655500000
 H -0.3376900000 1.0942240000 1.1616000000
 H 0.1435750000 0.9217500000 -1.6252070000
 C 1.3666900000 0.1147930000 -0.0319760000
 C -1.0557990000 2.6241500000 -0.0543290000
 C -0.8372360000 -0.9300460000 -0.9836120000
 C -2.2332520000 -0.2680640000 -1.0702100000
 C -2.1611660000 0.2685680000 0.3649340000
 C -1.7536080000 -0.9664560000 1.1395840000
 C -0.9647670000 -1.6864430000 0.3308150000
 H -0.4787100000 -1.4859120000 -1.8491010000
 H -2.9728750000 0.8771520000 0.7512450000
 H -3.0381560000 -0.9948330000 -1.1865510000
 H -2.3215840000 0.5042270000 -1.8418400000
 H -2.0091760000 -1.1568710000 2.1749370000
 H -0.4404390000 -2.6044310000 0.5699070000
 H -1.6561140000 2.6405860000 -0.9694520000
 C -1.8131720000 3.2926800000 1.0940260000
 C 0.2912690000 3.3115710000 -0.2864720000
 O 2.2054390000 -0.4912110000 -0.8473410000
 O 1.5763900000 0.4472850000 1.1193670000
 C 3.5438390000 -0.8028950000 -0.3207350000
 C 4.3399980000 -1.4186680000 -1.4486720000
 H 3.9795100000 0.1291140000 0.0467690000
 H 3.4136310000 -1.4810810000 0.5264040000
 H 5.3419970000 -1.6670610000 -1.0854210000
 H 3.8706180000 -2.3377850000 -1.8109080000
 H 4.4429440000 -0.7221600000 -2.2855690000
 H -1.9498330000 4.3502590000 0.8530310000
 H -2.8064150000 2.8720360000 1.2666100000
 H -1.2405750000 3.2402270000 2.0273250000

H 0.1089000000 4.3737000000 -0.4712800000
 H 0.9352680000 3.2300900000 0.5950010000
 H 0.8334750000 2.9243370000 -1.1531790000

Equilibrium geometry of **r10-endo-3r-ts.**

C 0.2179456557 0.6977600077 -0.4558408112
 N -0.5246377705 1.4515658565 0.3848392340
 H -0.3299275643 1.2590710204 1.3663345755
 H 0.3859038454 1.1017879552 -1.4480785026
 C 1.4278234796 0.0616723669 0.2014895406
 C -1.1585819725 2.7749388075 0.1034246470
 C -0.8044710403 -0.8600154707 -1.0478979132
 C -2.1804221521 -0.2185346337 -1.1603895119
 C -2.6772283529 -0.3265272569 0.2404514845
 C -1.9421380937 -1.2673819895 0.9285407227
 C -0.8539159076 -1.6571733091 0.1204488566
 H -0.2445778923 -1.1781080187 -1.9226102051
 H -3.5520528187 0.1919743022 0.6177423084
 H -2.8004753401 -0.8671413541 -1.8007310290
 H -2.2285051049 0.7817003834 -1.5959591803
 H -2.1405566273 -1.6267447865 1.9309792124
 H -0.1098254336 -2.3940099080 0.4029148044
 H -2.2356684250 2.6113547231 -0.0174395596
 C -0.9415674555 3.6589533975 1.3341412980
 C -0.6209384815 3.4261623203 -1.1703479596
 O 2.3096111475 -0.3323049595 -0.7036572794
 O 1.5078641431 -0.0606616262 1.4052658195
 C 3.5433008119 -0.9527669421 -0.2041230954
 C 4.3255844692 -1.4323168896 -1.4068385139
 H 4.0806854426 -0.1956979298 0.3727375019
 H 3.2621342600 -1.7641320491 0.4721709375
 H 5.2601445874 -1.8905546867 -1.0690486262
 H 3.7630371238 -2.1813288405 -1.9721194849
 H 4.5733270917 -0.6010715338 -2.0729289149
 H -1.4817545662 4.6016988768 1.2123422111
 H -1.3178876650 3.1785439377 2.2444477621
 H 0.1205586553 3.8868351018 1.4723595312
 H -1.1157435731 4.3921121680 -1.3036355013
 H 0.4573079668 3.6063464322 -1.1027838971
 H -0.8256638798 2.8374841216 -2.0711621389

Equilibrium geometry of **r10-endo-3s-mc.**

C 0.5257120000 1.0691850000 0.3651240000
 N -0.2616890000 1.6909730000 -0.4430210000
 C -1.1636140000 2.8524920000 -0.1867050000
 C 1.5286300000 0.1371270000 -0.2650180000
 H 0.5627720000 1.3169480000 1.4183420000
 H -0.1723080000 1.3824510000 -1.4182430000
 C -2.6990880000 -0.4808490000 -0.2664400000
 C -2.3700730000 -0.3850180000 1.1978230000
 C -1.0735190000 -1.1423760000 1.3060040000
 C -0.7883670000 -1.6913140000 0.0935350000
 C -1.7831760000 -1.2670490000 -0.8832870000
 H -3.5794920000 -0.0385740000 -0.7188090000
 H -0.5501440000 -1.3282110000 2.2366820000
 H -3.1459230000 -0.8905590000 1.7949230000
 H -2.3377290000 0.6413550000 1.5877370000
 H 0.0363330000 -2.3600900000 -0.1264510000
 H -1.7842270000 -1.5625700000 -1.9260960000
 H -2.1783100000 2.4638300000 -0.3157550000
 C -0.9921570000 3.4070060000 1.2224060000
 C -0.8847280000 3.8917770000 -1.2780760000
 O 2.3681510000 -0.3265040000 0.6391390000

O 1.5237780000 -0.0566180000 -1.4623400000
C 3.4547950000 -1.1947100000 0.1613000000
C 4.3919380000 -1.4247320000 1.3248020000
H 2.9952030000 -2.1182000000 -0.2026140000
H 3.9347270000 -0.6922440000 -0.6819250000
H 5.2076070000 -2.0801710000 1.0044240000
H 4.8269650000 -0.4832760000 1.6719730000
H 3.8757810000 -1.9053310000 2.1607510000
H -1.5903770000 4.7202750000 -1.1722040000
H 0.1305880000 4.2917610000 -1.1942370000
H -1.0167400000 3.4717730000 -2.2810300000
H -1.6849410000 4.2425030000 1.3517060000
H -1.2244000000 2.6719700000 1.9994800000
H 0.0219170000 3.7895350000 1.3820360000

Equilibrium geometry of r10-endo-3s-prod.

C 0.0210730000 0.3426900000 0.7030360000
N -0.8501920000 1.1391300000 -0.2590380000
C -1.0459040000 2.6211530000 0.0746590000
C 1.3709720000 0.1151460000 0.0289760000
H 0.1460080000 0.9047690000 1.6287010000
H -0.3394540000 1.0972280000 -1.1575110000
C -2.1615380000 0.2711370000 -0.3601350000
C -2.2282570000 -0.2784790000 1.0702430000
C -0.8332910000 -0.9414260000 0.9716390000
C -0.9672230000 -1.6852400000 -0.3493810000
C -1.7591880000 -0.9572090000 -1.1478020000
H -2.9737620000 0.8845550000 -0.7375750000
H -0.4721120000 -1.5057990000 1.8305590000
H -3.0335580000 -1.0052990000 1.1834240000
H -2.3121870000 0.4868560000 1.8492030000
H -0.4446140000 -2.6013200000 -0.5992440000
H -2.0197680000 -1.1379260000 -2.1836310000
H -1.6324730000 2.6316060000 0.9987570000
C 0.3067310000 3.3024280000 0.2927720000
C -1.8187080000 3.3017660000 -1.0559080000
O 2.2196660000 -0.4700870000 0.8492740000
O 1.5736170000 0.4388670000 -1.1260780000
C 3.5642700000 -0.7615590000 0.3273040000
C 4.3736790000 -1.3396230000 1.4660370000
H 3.4493180000 -1.4573100000 -0.5076730000
H 3.9799630000 0.1732940000 -0.0557530000
H 5.3815460000 -1.5705780000 1.1074720000
H 4.4596900000 -0.6268580000 2.2910990000
H 3.9251740000 -2.2632140000 1.8428610000
H -1.9432420000 4.3588330000 -0.8060910000
H -1.2633430000 3.2509530000 -1.9996820000
H -2.8179190000 2.8893400000 -1.2129100000
H 0.1304330000 4.3629710000 0.4918660000
H 0.8614080000 2.9042830000 1.1465250000
H 0.9370200000 3.2289080000 -0.5992930000

Equilibrium geometry of r10-endo-3s-ts.

C 0.2160525831 0.6856596269 0.4707486875
N -0.5159352993 1.4533824224 -0.3666187024
C -1.1468419811 2.7758714300 -0.0762128141
C 1.4243585307 0.0489094193 -0.1884026338
H 0.3804235023 1.0779801875 1.4682970071
H -0.3206066182 1.2664522068 -1.3489821616
C -2.6793744889 -0.3150271745 -0.2626862624
C -2.1941548039 -0.2261017001 1.1437060891
C -0.8208797979 -0.8742111420 1.0355767677
C -0.8644960739 -1.6573318396 -0.1424360563

C -1.9433738871 -1.2515976611 -0.9554868780
H -3.5480494592 0.2129066122 -0.6414221786
H -0.2717868753 -1.2070554284 1.9118889462
H -2.8234437396 -0.8784241692 1.7711423068
H -2.2401692069 0.7693433675 1.5902142356
H -0.1226969007 -2.3955615065 -0.4272313554
H -2.1347547546 -1.5979473929 -1.9638657536
H -2.2251918192 2.6150214985 0.0364478012
C -0.6150699171 3.4122069809 1.2074506612
C -0.9188211738 3.6709073147 -1.2968793478
O 2.3169553081 -0.3305836742 0.7120197858
O 1.4954241324 -0.0849125647 -1.3917706237
C 3.5433322380 -0.9574903916 0.2010711907
C 4.4214270706 -1.2737962041 1.3903431354
H 3.2507620945 -1.8497684067 -0.3591280509
H 4.0082950525 -0.2547787934 -0.4944167399
H 5.3423968726 -1.7494674685 1.0393305524
H 4.6930437408 -0.3650571213 1.9349272808
H 3.9236694805 -1.9617256377 2.0800156125
H -1.4572926119 4.6139911866 -1.1703481911
H 0.1448148768 3.8970727985 -1.4255833123
H -1.2899245616 3.1999322099 -2.2142700425
H -1.1058540140 4.3794096316 1.3461957406
H -0.8294991521 2.8159322329 2.1009532075
H 0.4645546832 3.5872425906 1.1496804163

Equilibrium geometry of r10-exo-3r-mc.

C 0.4083460000 1.0592160000 -0.3419220000
N -0.2754090000 1.6920130000 0.5532970000
H 0.0050600000 1.4953600000 1.5200320000
H 0.2585210000 1.2563040000 -1.3957900000
C 1.5805480000 0.2569760000 0.1615730000
C -1.3116590000 2.7347620000 0.3177350000
C -2.4973770000 -0.9942040000 0.7472850000
C -1.1636940000 -1.6811800000 0.6783050000
C -0.7229140000 -1.4249850000 -0.7363470000
C -1.7209550000 -0.7644210000 -1.3944290000
C -2.8115750000 -0.4879820000 -0.4715280000
H -3.1168460000 -0.9681370000 1.6362900000
H 0.1688250000 -1.8440070000 -1.1868520000
H -1.2787600000 -2.7637230000 0.8465350000
H -0.4498560000 -1.3443540000 1.4423010000
H -1.7287250000 -0.5140850000 -2.4506330000
H -3.7310420000 0.0202840000 -0.7392700000
C -2.2689800000 2.7675940000 1.5059150000
C -0.6192180000 4.0825180000 0.0742020000
H -1.8435690000 2.4214040000 -0.5861220000
O 2.3664560000 -0.1178630000 -0.8279060000
O 1.7336440000 0.0734660000 1.3520960000
C 3.6008800000 -0.8290050000 -0.4557070000
C 4.4166590000 -1.0155670000 -1.7145640000
H 4.1125220000 -0.2246030000 0.2972300000
H 3.3042850000 -1.7756450000 0.0040430000
H 5.3417610000 -1.5431060000 -1.4622530000
H 3.8759220000 -1.6106230000 -2.4559030000
H 4.6834150000 -0.0527700000 -2.1592810000
H -1.3785410000 4.8390060000 -0.1429920000
H -0.0603170000 4.4059340000 0.9581140000
H 0.0672450000 4.0341590000 -0.7767490000
H -3.0478130000 3.5113390000 1.3183890000
H -2.7477520000 1.7971860000 1.6579900000
H -1.7486190000 3.0591170000 2.4256590000

Equilibrium geometry of r10-exo-3r-prod.

C 0.0347640000 0.3108100000 -0.4993590000
N -0.8437100000 0.9276350000 0.5798380000
H -0.2378910000 0.9266030000 1.4202790000
H 0.0442790000 0.9427710000 -1.3866900000
C 1.4422630000 0.1808240000 0.0838790000
C -1.2932990000 2.3641930000 0.3347850000
C -1.9710510000 -0.1433430000 0.8006710000
C -1.1236390000 -1.4157260000 0.6738890000
C -0.6650170000 -1.0685600000 -0.7633340000
C -2.0002720000 -0.7372760000 -1.4122490000
C -2.7813150000 -0.1769330000 -0.4785330000
H -2.4752710000 0.0641280000 1.7410690000
H -0.0179900000 -1.7729020000 -1.2846550000
H -1.7413340000 -2.3135290000 0.7108330000
H -0.3160400000 -1.4919910000 1.4092960000
H -2.2237810000 -0.8741340000 -2.4642370000
H -3.7771510000 0.2325380000 -0.5957350000
C -2.2374350000 2.8121040000 1.4491060000
C -0.0684400000 3.2737470000 0.2315650000
H -1.8262920000 2.3314430000 -0.6200700000
O 2.3055530000 -0.2092210000 -0.8294290000
O 1.6715020000 0.4005430000 1.2602510000
C 3.6972930000 -0.4118420000 -0.3908280000
C 4.5201260000 -0.7186660000 -1.6209350000
H 4.0169220000 0.4992940000 0.1199590000
H 3.6944040000 -1.2309850000 0.3328660000
H 5.5622660000 -0.8709420000 -1.3238910000
H 4.1708270000 -1.6283210000 -2.1178410000
H 4.4858020000 0.1087640000 -2.3350790000
H -0.4057620000 4.2956200000 0.0385010000
H 0.5040580000 3.2800260000 1.1653150000
H 0.6027750000 2.9946330000 -0.5855510000
H -2.5182710000 3.8537940000 1.2710430000
H -3.1609970000 2.2289520000 1.4844420000
H -1.7505470000 2.7676570000 2.4303610000

Equilibrium geometry of r10-exo-3r-ts.

C 0.2197787501 0.7062457889 -0.3404832662
N -0.4902230719 1.3770758430 0.5847674369
H -0.1502688530 1.2657400158 1.5391910650
H 0.2409967817 1.1194280758 -1.3431207317
C 1.5378500590 0.1575157593 0.1785803443
C -1.3220947162 2.5647310408 0.2899966082
C -2.4006022969 -0.8107884154 0.7980084568
C -1.0694019275 -1.4651351290 0.6705995251
C -0.6489009950 -1.0552815256 -0.7301019993
C -1.8225299762 -0.6303223155 -1.3841996104
C -2.8558566278 -0.4199866937 -0.4413041543
H -2.9560149709 -0.7443352779 1.7272064699
H 0.1500172692 -1.5556216728 -1.2687771876
H -1.2155808250 -2.5582444880 0.6734475555
H -0.3632911590 -1.2486274151 1.4761447092
H -1.9029170678 -0.4358586805 -2.4492271507
H -3.8311216617 -0.0023461303 -0.6611101925
C -2.2767386316 2.8202801094 1.4531562792
C -0.4365750262 3.7850080559 -0.0033933679
H -1.8951286890 2.3128440024 -0.6109640339
O 2.3548576299 -0.1543693956 -0.8125638590
O 1.7482948877 0.0407144861 1.3677126922
C 3.6787818492 -0.6749842893 -0.4414275104
C 4.4616933853 -0.8663430904 -1.7209235409
H 4.1404711471 0.0484994863 0.2344324846
H 3.5244976028 -1.6087539887 0.1057771582
H 5.4576714661 -1.2498392254 -1.4791887256
H 3.9709400020 -1.5852264890 -2.3835394281

H 4.5801099241 0.0808417161 -2.2545916003
H -1.0643129837 4.6399881374 -0.2724045844
H 0.1526631114 4.0599812579 0.8777963480
H 0.2510921363 3.5984169645 -0.8348287619
H -2.8940526293 3.6977370499 1.2434740022
H -2.9394557839 1.9677206029 1.6258297309
H -1.7218773714 3.0227969550 2.3770704076

Equilibrium geometry of r10-exo-3s-mc.

C 0.4086160000 1.0642970000 0.3424160000
N -0.2756010000 1.6959810000 -0.5531130000
C -1.3143550000 2.7364780000 -0.3188570000
C 1.5812720000 0.2624630000 -0.1609390000
H 0.2578120000 1.2607440000 1.3962520000
H 0.0057000000 1.4994420000 -1.5196670000
C -0.7178370000 -1.4250390000 0.7371830000
C -1.1594690000 -1.6827710000 -0.6769120000
C -2.4947130000 -0.9987330000 -0.7449040000
C -2.8085340000 -0.4921810000 0.4737700000
C -1.7163120000 -0.7657610000 1.3957570000
H 0.1754160000 -1.8415710000 1.1868110000
H -3.1150950000 -0.9744480000 -1.6333760000
H -1.2720500000 -2.7655110000 -0.8449800000
H -0.4471480000 -1.3442840000 -1.4415880000
H -3.7286940000 0.0145810000 0.7421450000
H -1.7233970000 -0.5146420000 2.4516110000
C -2.2738030000 2.7630170000 -1.5054880000
H -1.8436810000 2.4243680000 0.5868680000
C -0.6251920000 4.0869790000 -0.0810530000
O 2.3664350000 -0.1139170000 0.8285110000
O 1.7348390000 0.0800070000 -1.3515710000
C 3.5991360000 -0.8276100000 0.4558330000
C 4.4102760000 -1.0256860000 1.7158920000
H 3.3002960000 -1.7700770000 -0.0107120000
H 4.1151670000 -0.2205950000 -0.2916830000
H 5.3330170000 -1.5568760000 1.4629060000
H 4.6812650000 -0.0671070000 2.1669650000
H 3.8643830000 -1.6222620000 2.4522780000
H -1.3863310000 4.8422690000 0.1342650000
H 0.0624060000 4.0434800000 0.7692370000
H -0.0683020000 4.4087710000 -0.9668080000
H -3.0549460000 3.5044440000 -1.3185810000
H -1.7559690000 3.0539620000 -2.4266860000
H -2.7493830000 1.7905710000 -1.6541510000

Equilibrium geometry of r10-exo-3s-prod.

C 0.0331200000 0.3038130000 0.4974450000
N -0.8449670000 0.9253180000 -0.5793180000
C -1.2878770000 2.3632990000 -0.3311610000
C 1.4402450000 0.1738620000 -0.0866980000
H 0.0440990000 0.9330670000 1.3865750000
H -0.2407500000 0.9229650000 -1.4208290000
C -0.6697050000 -1.0747250000 0.7583550000
C -1.1325380000 -1.4164360000 -0.6788370000
C -1.9764340000 -0.1411120000 -0.8001210000
C -2.7838390000 -0.1756270000 0.4808620000
C -2.0025350000 -0.7412720000 1.4111820000
H -0.0236320000 -1.7825990000 1.2761920000
H -2.4823340000 0.0704450000 -1.7387680000
H -1.7529330000 -2.3123340000 -0.7169770000
H -0.3266580000 -1.4929010000 -1.4160450000
H -3.7781460000 0.2365860000 0.6015050000
H -2.2240970000 -0.8805720000 2.4632750000

C -2.2300290000 2.8180410000 -1.4442620000
H -1.8208510000 2.3310070000 0.6237650000
C -0.0585500000 3.2666410000 -0.2259580000
O 2.3052420000 -0.2092850000 0.8278140000
O 1.6679870000 0.3893120000 -1.2641260000
C 3.6980670000 -0.4067150000 0.3914810000
C 4.5247170000 -0.6832940000 1.6263970000
H 3.7024870000 -1.2393240000 -0.3165410000
H 4.0092190000 0.4977870000 -0.1357920000
H 5.5678170000 -0.8332930000 1.3311100000
H 4.4846500000 0.1579220000 2.3240050000
H 4.1827020000 -1.5857060000 2.1412970000
H -0.3909290000 4.2899050000 -0.0324540000
H 0.6101240000 2.9833950000 0.5918060000
H 0.5149730000 3.2706350000 -1.1590480000
H -2.5069680000 3.8602210000 -1.2631010000
H -1.7433130000 2.7743940000 -2.4256300000
H -3.1558040000 2.2385100000 -1.4814830000

Equilibrium geometry of **r10-exo-3s-ts**.

C 0.2195100426 0.7070252121 0.3406202842
N -0.4908921174 1.3771656412 -0.5848042567
C -1.3237366819 2.5641852823 -0.2902993990
C 1.5378914526 0.1589209171 -0.1783272566
H 0.2405092945 1.1205175775 1.3431358456
H -0.1509469843 1.2657646505 -1.5392201025
C -0.6480693733 -1.0548927582 0.7309340037
C -1.0680581650 -1.4657849719 -0.6696171958
C -2.3998450824 -0.8127082104 -0.7975068813
C -2.8555393712 -0.4215828895 0.4415336454
C -1.8221189704 -0.6305341988 1.3846540501
H 0.1511456118 -1.5543626482 1.2699768659
H -2.9552061416 -0.7472276101 -1.7268062156
H -1.2132298042 -2.5590319330 -0.6719977079
H -0.3620805325 -1.2489937276 -1.4752024379
H -3.8311781510 -0.0046453361 0.6610202851
H -1.9027963589 -0.4355811734 2.4495715745
C -2.2784321914 2.8187903783 -1.4536238789
H -1.8966970901 2.3119476698 0.6106138938
C -0.4392634133 3.7852272476 0.0030644102
O 2.3550916095 -0.1522605871 0.8128777303
O 1.7483861265 0.0419458562 -1.3674335892
C 3.6792967769 -0.6722419117 0.4418524611
C 4.4622324783 -0.8631095744 1.7214029485
H 3.5255187233 -1.6061281752 -0.1052912973
H 4.1406631784 0.0514223414 -0.2340316119
H 5.4584005393 -1.2461706855 1.4797584812
H 4.5801867760 0.0841782497 2.2549833169
H 3.9717779246 -1.5821532606 2.3840606763
H -1.0677521517 4.6396887150 0.2719733643
H 0.2484991931 3.5992786314 0.8345622297
H 0.1498009903 4.0606373050 -0.8781025839
H -2.8965504142 3.6957408332 -1.2441731242
H -1.7236086664 3.0216463840 -2.3774882975
H -2.9403957935 1.9656362416 -1.6262828687

Equilibrium geometry of **r11-endo-3r-mc**.

C 0.5192260000 1.1454260000 -0.4010820000
N -0.2708520000 1.7454680000 0.4201550000
H -0.1447550000 1.4468160000 1.3947750000
H 0.5231890000 1.3837180000 -1.4571970000
C 1.5700440000 0.2568140000 0.2191730000
C -1.2241970000 2.8675090000 0.1805710000

C -1.0319030000 -1.1292350000 -1.3138900000
C -2.3585300000 -0.4327810000 -1.1698810000
C -2.6421610000 -0.5406010000 0.3030700000
C -1.6732590000 -1.2804570000 0.8947890000
C -0.6865720000 -1.6599000000 -0.1093540000
H -0.5262780000 -1.2914520000 -2.2587170000
H -3.5292540000 -0.1382610000 0.7789810000
H -3.1265220000 -0.9740440000 -1.7454000000
H -2.3844420000 0.5935620000 -1.5605390000
H -1.6304600000 -1.5724490000 1.9377330000
H 0.1746690000 -2.2882840000 0.0880980000
H -2.2160000000 2.4446160000 0.3681380000
C -0.9318370000 3.9438600000 1.2322460000
C -1.1412700000 3.3930870000 -1.2473180000
O 2.4146650000 -0.1756460000 -0.6919090000
O 1.5774420000 0.0721350000 1.4194210000
C 3.5668300000 -1.0023600000 -0.2342830000
C 3.9665100000 -1.8413200000 -1.4332630000
C 4.6589670000 -0.0745410000 0.2743910000
H 3.1857120000 -1.6255840000 0.5788880000
H 4.7797600000 -2.5149190000 -1.1459710000
H 3.1308360000 -2.4500820000 -1.7905490000
H 4.3196980000 -1.2103730000 -2.2548780000
H 5.5106810000 -0.6736030000 0.6111170000
H 5.0051980000 0.5928510000 -0.5210740000
H 4.3117360000 0.5213130000 1.1226610000
H -1.6817300000 4.7355960000 1.1532770000
H -0.9818200000 3.5415360000 2.2498430000
H 0.0559180000 4.3890780000 1.0774720000
H -1.8758250000 4.1942680000 -1.3633270000
H -0.1538260000 3.8158870000 -1.4622590000
H -1.3748120000 2.6287920000 -1.9951300000

Equilibrium geometry of **r11-endo-3r-prod**.

C 0.0523650000 0.3884070000 -0.7117860000
N -0.8367670000 1.1532660000 0.2604640000
H -0.3278600000 1.0990820000 1.1597190000
H 0.1790100000 0.9699580000 -1.6250120000
C 1.3991230000 0.1604970000 -0.0276840000
C -1.0575090000 2.6385240000 -0.0378150000
C -0.7831010000 -0.9012030000 -1.0114970000
C -2.1868910000 -0.2568350000 -1.1043090000
C -2.1354050000 0.2648900000 0.3370610000
C -1.7199700000 -0.9735630000 1.1020280000
C -0.9130730000 -1.6733570000 0.2933390000
H -0.4097120000 -1.4435870000 -1.8792850000
H -2.9588400000 0.8589010000 0.7215450000
H -2.9811050000 -0.9926600000 -1.2362010000
H -2.2778670000 0.5226940000 -1.8683410000
H -1.9821570000 -1.1785740000 2.1329280000
H -0.3778890000 -2.5861290000 0.5283450000
H -1.6609210000 2.6616820000 -0.9507850000
C -1.8188180000 3.2811210000 1.1228890000
C 0.2802830000 3.3454670000 -0.2638990000
O 2.2542090000 -0.4138110000 -0.8453630000
O 1.5773640000 0.4697820000 1.1370010000
C 3.6078870000 -0.7549300000 -0.3228340000
C 4.0982710000 -1.8974430000 -1.1921130000
C 4.4802380000 0.4887800000 -0.3731720000
H 3.4596250000 -1.0772850000 0.7105860000
H 5.0779480000 -2.2282490000 -0.8344750000
H 3.4138440000 -2.7497150000 -1.1513820000
H 4.2035930000 -1.5794000000 -2.2340200000
H 5.4793290000 0.2454060000 0.0020900000
H 4.5816590000 0.8522540000 -1.4008460000

H 4.0717910000 1.2853670000 0.2543770000
H -1.9735600000 4.3394030000 0.8962390000
H -2.8041020000 2.8423390000 1.2957290000
H -1.2401100000 3.2256380000 2.0522580000
H 0.0850720000 4.4082190000 -0.4311730000
H 0.9278650000 3.2575030000 0.6143250000
H 0.8238610000 2.9779280000 -1.1382690000

Equilibrium geometry of **r11-endo-3r-ts**.

C 0.2255186222 0.7183566852 -0.4901548943
N -0.5080680414 1.4810099438 0.3502522895
H -0.3001512667 1.3027071745 1.3315786563
H 0.3719193353 1.1064766740 -1.4921621472
C 1.4536384688 0.1056454349 0.1593003495
C -1.1688959366 2.7872811675 0.0557047521
C -0.7919674559 -0.8611497298 -1.0309485146
C -2.1791021796 -0.2406215084 -1.1232641723
C -2.6447978291 -0.3341410448 0.2893919830
C -1.8802857518 -1.2512539088 0.9766103865
C -0.8036749087 -1.6386252656 0.1512953037
H -0.2491821905 -1.1882815255 -1.9132302123
H -3.5191632254 0.1773424139 0.6773228237
H -2.8033196829 -0.9069617351 -1.7408741119
H -2.2505677024 0.7525893326 -1.5716386815
H -2.0510161003 -1.5964568300 1.9890595996
H -0.0427417446 -2.3595194382 0.4294617773
H -2.2428291147 2.6023116474 -0.0598401925
C -0.9643396621 3.6894061998 1.2752419307
C -0.6473470753 3.4334703394 -1.2275944551
O 2.3421238260 -0.2521691924 -0.7504864365
O 1.5266518693 -0.0270378245 1.3640166377
C 3.6153549398 -0.8605731160 -0.2819015690
C 4.1014079487 -1.7193057426 -1.4346789649
C 4.5715349069 0.2541378561 0.1107038614
H 3.3606050481 -1.4689254149 0.5895179350
H 5.0320187557 -2.2191997718 -1.1491342213
H 3.3695186278 -2.4893237412 -1.6968082317
H 4.2994895583 -1.1075945674 -2.3203917580
H 5.5229041505 -0.1801256457 0.4339133277
H 4.7687229655 0.9131038700 -0.7409367683
H 4.1729402529 0.8448721466 0.9399401088
H -1.5213977566 4.6211547203 1.1452991770
H -1.3287279242 3.2124450329 2.1922133206
H 0.0940454555 3.9376170662 1.4069227257
H -1.1577483652 4.3901555674 -1.3686726479
H 0.4283562724 3.6306514150 -1.1675893538
H -0.8474437169 2.8318169191 -2.1207952479

Equilibrium geometry of **r11-endo-3s-mc**.

C 0.5212010000 1.1322740000 0.3727780000
N -0.2772740000 1.7273950000 -0.4440900000
C -1.2180110000 2.8602140000 -0.2047530000
C 1.5576230000 0.2303690000 -0.2522790000
H 0.5431980000 1.3843540000 1.4254630000
H -0.1678700000 1.4157380000 -1.4166130000
C -2.6599350000 -0.5355990000 -0.2634240000
C -2.3525400000 -0.4108170000 1.2034680000
C -1.0298130000 -1.1168660000 1.3361430000
C -0.7075160000 -1.6659050000 0.1334090000
C -1.7063420000 -1.2911640000 -0.8602800000
H -3.5509360000 -0.1320930000 -0.7309310000
H -0.5110000000 -1.2711770000 2.2751310000
H -3.1162010000 -0.9375460000 1.7979280000

H -2.3633940000 0.6208770000 1.5806640000
H 0.1456420000 -2.3037130000 -0.0689340000
H -1.6820800000 -1.5969670000 -1.8998210000
H -2.2168700000 2.4415560000 -0.3616790000
C -1.0988020000 3.4124680000 1.2103660000
C -0.9423960000 3.9132990000 -1.2840240000
O 2.4139300000 -0.1956870000 0.6510380000
O 1.5465010000 0.0317800000 -1.4502950000
C 3.5562610000 -1.0312550000 0.1850880000
C 3.9665310000 -1.8648760000 1.3842930000
H 3.1627040000 -1.6575850000 -0.6196310000
C 4.6467030000 -0.1117050000 -0.3420300000
H 4.7756080000 -2.5411320000 1.0919270000
H 4.3291750000 -1.2305200000 2.1990320000
H 3.1337180000 -2.4705910000 1.7531380000
H 5.4908360000 -0.7169320000 -0.6869410000
H 4.2918400000 0.4822030000 -1.1885550000
H 5.0066250000 0.5576560000 0.4457540000
H -1.6822580000 4.7141350000 -1.2014970000
H 0.0534830000 4.3512810000 -1.1641580000
H -1.0228530000 3.4917060000 -2.2918560000
H -1.8222300000 4.2236830000 1.3263890000
H -1.3241590000 2.6655030000 1.9778670000
H -0.1023410000 3.8281270000 1.3957770000

Equilibrium geometry of **r11-endo-3s-prod**.

C 0.0575500000 0.3896250000 0.6984770000
N -0.8423820000 1.1453460000 -0.2713650000
C -1.0558160000 2.6350020000 0.0093660000
C 1.3919870000 0.1434350000 -0.0035070000
H 0.2034300000 0.9844030000 1.6003630000
H -0.3469250000 1.0768080000 -1.1770880000
C -2.1458440000 0.2614890000 -0.3162010000
C -2.1791350000 -0.2379680000 1.1334360000
C -0.7799720000 -0.8905120000 1.0306770000
C -0.9324840000 -1.6819420000 -0.2600680000
C -1.7472220000 -0.9903450000 -1.0679890000
H -2.9721250000 0.8534680000 -0.6977560000
H -0.3967160000 -1.4214240000 1.9012510000
H -2.9749750000 -0.9676550000 1.2878960000
H -2.2560770000 0.5530580000 1.8872630000
H -0.4051180000 -2.6008710000 -0.4886050000
H -2.0248410000 -1.2097250000 -2.0918620000
H -1.6530110000 2.6710510000 0.9260040000
C 0.2848690000 3.3415530000 0.2174890000
C -1.8239900000 3.2645060000 -1.1540260000
O 2.2550330000 -0.4278310000 0.8079140000
O 1.5543000000 0.4375840000 -1.1744180000
C 3.5969780000 -0.7881250000 0.2686440000
C 4.0865620000 -1.9307540000 1.1383500000
H 3.4301860000 -1.1153450000 -0.7603650000
C 4.4839450000 0.4459610000 0.2989620000
H 5.0584250000 -2.2732590000 0.7706620000
H 4.2078110000 -1.6080980000 2.1770890000
H 3.3931480000 -2.7762020000 1.1107630000
H 5.4754950000 0.1888420000 -0.0868740000
H 4.0763560000 1.2427330000 -0.3289720000
H 4.6021020000 0.8155320000 1.3226660000
H -1.9784460000 4.3250680000 -0.9381690000
H -1.2500640000 3.1993320000 -2.0857320000
H -2.8096830000 2.8228970000 -1.3170600000
H 0.0929290000 4.4067690000 0.3725020000
H 0.8328800000 2.9841330000 1.0931560000
H 0.9270520000 3.2413100000 -0.6634540000

Equilibrium geometry of **r11-endo-3s-ts**.

C 0.2280094571 0.7192664336 0.4624263144
 N -0.5229829651 1.4661305501 -0.3777238898
 C -1.1687176178 2.7830574067 -0.0962958159
 C 1.4427966856 0.0923635807 -0.1983451529
 H 0.3952405906 1.1274082410 1.4530685911
 H -0.3308371381 1.2719251965 -1.3593195189
 C -2.6547478911 -0.3376918271 -0.2392115094
 C -2.1623704082 -0.2210509233 1.1626018959
 C -0.7777577343 -0.8449268756 1.0539350118
 C -0.8154517997 -1.6457017203 -0.1127789369
 C -1.9068288010 -1.2709563129 -0.9236990344
 H -3.5348235707 0.1695674636 -0.6198071851
 H -0.2172902580 -1.1561177745 1.9308321589
 H -2.7753325329 -0.8764343560 1.8027956286
 H -2.2240363826 0.7793746921 1.5959523973
 H -0.0616586020 -2.3736434077 -0.3922540580
 H -2.0982495245 -1.6344620649 -1.9259953509
 H -2.2458988978 2.6113024362 0.0121543022
 C -0.6501230458 3.4313777093 1.1867750045
 C -0.9450087844 3.6760085891 -1.3194208406
 O 2.3398667144 -0.2654323286 0.7033478924
 O 1.4986849460 -0.0522266793 -1.4025050890
 C 3.5999150636 -0.8932273223 0.2255976063
 C 4.0791806032 -1.7630788388 1.3729323477
 H 3.3306743043 -1.4949700730 -0.6459527454
 C 4.5706978129 0.2080660507 -0.1694502423
 H 5.0013666598 -2.2749093825 1.0812665402
 H 4.2898753872 -1.1580044565 2.2603034815
 H 3.3376608566 -2.5238389371 1.6353078755
 H 5.5133930909 -0.2392175063 -0.5001751925
 H 4.1754940520 0.8075196620 -0.9941207258
 H 4.7826917681 0.8611903963 0.6830997517
 H -1.4918930321 4.6149119684 -1.1975570396
 H 0.1170955287 3.9108053270 -1.4457203278
 H -1.3091628015 3.1987861190 -2.2363383325
 H -1.1554396838 4.3917573622 1.3208004075
 H -0.8583166350 2.8352116633 2.0818271588
 H 0.4270227521 3.6222548599 1.1317239081

Equilibrium geometry of **r11-exo-3r-mc**.

C 0.4045460000 1.0466270000 -0.3397190000
 N -0.2834150000 1.6816170000 0.5507440000
 H -0.0061770000 1.4878600000 1.5189720000
 H 0.2584300000 1.2412190000 -1.3945000000
 C 1.5836450000 0.2541020000 0.1695050000
 C -1.3183970000 2.7233510000 0.3062360000
 C -2.5057030000 -0.9886090000 0.7563380000
 C -1.1718140000 -1.6752880000 0.6890920000
 C -0.7339550000 -1.4280250000 -0.7280080000
 C -1.7337370000 -0.7729670000 -1.3885900000
 C -2.8228080000 -0.4912150000 -0.4653470000
 H -3.1235790000 -0.9571410000 1.6463310000
 H 0.1587150000 -1.8473060000 -1.1762350000
 H -1.2860860000 -2.7567020000 0.8649350000
 H -0.4560470000 -1.3330220000 1.4487810000
 H -1.7433020000 -0.5286960000 -2.4461000000
 H -3.7431210000 0.0147360000 -0.7345830000
 C -2.2715560000 2.7731990000 1.4969460000
 C -0.6241230000 4.0665570000 0.0432610000
 H -1.8544330000 2.4004490000 -0.5917210000
 O 2.3743300000 -0.1050180000 -0.8186750000
 O 1.7225070000 0.0701230000 1.3629220000
 C 3.6504840000 -0.7985020000 -0.4771950000

C 4.0207970000 -1.5941500000 -1.7141850000
 C 4.6752040000 0.2523750000 -0.0784620000
 H 3.4219510000 -1.4531960000 0.3672380000
 H 4.9476350000 -2.1436670000 -1.5242870000
 H 3.2426270000 -2.3190090000 -1.9711080000
 H 4.1833970000 -0.9328120000 -2.5707570000
 H 5.6234530000 -0.2407580000 0.1567070000
 H 4.8493190000 0.9543930000 -0.8999650000
 H 4.3549890000 0.8043480000 0.8091810000
 H -1.3821740000 4.8220300000 -0.1819860000
 H -0.0620080000 4.4001650000 0.9213550000
 H 0.0601870000 4.0054470000 -0.8086520000
 H -3.0493990000 3.5161860000 1.3029140000
 H -2.7519090000 1.8057580000 1.6624850000
 H -1.7474410000 3.0747830000 2.4112820000

Equilibrium geometry of **r11-exo-3r-prod**.

C 0.0422540000 0.2945490000 -0.4940720000
 N -0.8322430000 0.9125110000 0.5875580000
 H -0.2327090000 0.8829380000 1.4322690000
 H 0.0735540000 0.9412930000 -1.3701800000
 C 1.4428950000 0.1212080000 0.0987950000
 C -1.2475830000 2.3617700000 0.3614030000
 C -1.9842560000 -0.1357730000 0.7818350000
 C -1.1645220000 -1.4246910000 0.6404190000
 C -0.6866440000 -1.0636740000 -0.7871250000
 C -2.0088240000 -0.6918030000 -1.4408890000
 C -2.7853090000 -0.1304730000 -0.5039620000
 H -2.4914540000 0.0676280000 1.7215880000
 H -0.0511630000 -1.7732760000 -1.3154750000
 H -1.8021480000 -2.3090980000 0.6578090000
 H -0.3641460000 -1.5293220000 1.3798440000
 H -2.2263170000 -0.8055240000 -2.4969110000
 H -3.7707330000 0.3032680000 -0.6222520000
 C -2.2021460000 2.8088700000 1.4672050000
 C -0.0026890000 3.2467200000 0.2933940000
 H -1.7653950000 2.3562160000 -0.6023270000
 O 2.3009810000 -0.2642280000 -0.8178900000
 O 1.6563370000 0.3048210000 1.2857960000
 C 3.7063370000 -0.5403530000 -0.4002220000
 C 4.2514980000 -1.4983780000 -1.4425140000
 C 4.4596540000 0.7754240000 -0.3034730000
 H 3.6392040000 -1.0165850000 0.5811550000
 H 5.2733900000 -1.7825590000 -1.1733650000
 H 3.6489990000 -2.4094370000 -1.4990060000
 H 4.2757790000 -1.0292850000 -2.4310410000
 H 5.4943410000 0.5760460000 -0.0068140000
 H 4.4767930000 1.2883240000 -1.2705170000
 H 4.0170030000 1.4330150000 0.4492090000
 H -0.3145950000 4.2773370000 0.1037570000
 H 0.5503720000 3.2325070000 1.2387910000
 H 0.6800640000 2.9612460000 -0.5118730000
 H -2.4436940000 3.8644620000 1.3161320000
 H -3.1451790000 2.2562590000 1.4608610000
 H -1.7426630000 2.7161620000 2.4581770000

Equilibrium geometry of **r11-exo-3r-ts**.

C 0.2179289876 0.6945438424 -0.3405484160
 N -0.4889067187 1.3705353766 0.5842552145
 H -0.1492885595 1.2576634984 1.5385406250
 H 0.2423184442 1.1080405042 -1.3430518002
 C 1.5357707531 0.1405101089 0.1795714216
 C -1.3158153220 2.5608692779 0.2882554276

C -2.4080187532 -0.8048239549 0.8021927381
 C -1.0800932517 -1.4654518300 0.6749312165
 C -0.6580887505 -1.0580990880 -0.7262355011
 C -1.8307562352 -0.6297383612 -1.3805574862
 C -2.8625238677 -0.4139571521 -0.4374671502
 H -2.9626163029 -0.7344780837 1.7315999159
 H 0.1379398663 -1.5632577414 -1.2645899833
 H -1.2311694159 -2.5578530651 0.6786994232
 H -0.3721136534 -1.2510376430 1.4793438899
 H -1.9107775441 -0.4359588422 -2.4457204391
 H -3.8361177033 0.0076547732 -0.6570965622
 C -2.2656434297 2.8248147469 1.4535698247
 C -0.4263525251 3.7765354510 -0.0123951850
 H -1.8931131458 2.3088574477 -0.6099977678
 O 2.3508321076 -0.1670527580 -0.8115895576
 O 1.7326454003 0.0162309565 1.3716517877
 C 3.6901980270 -0.7172659406 -0.4667209885
 C 4.1235764316 -1.5155218174 -1.6823505741
 C 4.6189985554 0.4324530024 -0.1136701362
 H 3.5365817951 -1.3654271477 0.4000555334
 H 5.0866307870 -1.9927294072 -1.4769991591
 H 3.4011798310 -2.3009797643 -1.9239192404
 H 4.2429519156 -0.8662879482 -2.5553836196
 H 5.6092727459 0.0343641295 0.1292665910
 H 4.7268595147 1.1201446162 -0.9587575756
 H 4.2560178625 0.9842265899 0.7574215741
 H -1.0513214555 4.6330681110 -0.2829747927
 H 0.1665677176 4.0524859984 0.8660335288
 H 0.2581965091 3.5839429941 -0.8450499104
 H -2.8793549823 3.7045570197 1.2429948682
 H -2.9317536257 1.9759219301 1.6310519152
 H -1.7068888372 3.0275440795 2.3750833337

Equilibrium geometry of **r11-exo-3s-mc**.

C 0.4042660000 1.0471900000 0.3394420000
 N -0.2844010000 1.6814580000 -0.5509540000
 C -1.3200730000 2.7225420000 -0.3062690000
 C 1.5837530000 0.2553270000 -0.1699390000
 H 0.2583360000 1.2418210000 1.3942530000
 H -0.0073760000 1.4876280000 -1.5192130000
 C -0.7328890000 -1.4281820000 0.7281150000
 C -1.1708650000 -1.6756400000 -0.6888830000
 C -2.5050570000 -0.9895500000 -0.7559190000
 C -2.8222140000 -0.4923240000 0.4657970000
 C -1.7328770000 -0.7735900000 1.3888760000
 H 0.1600960000 -1.8469930000 1.1761340000
 H -3.1230170000 -0.9583210000 -1.6457940000
 H -1.2847170000 -2.7570990000 -0.8646550000
 H -0.4553980000 -1.3330970000 -1.4486870000
 H -3.7426900000 0.0132520000 0.7351790000
 H -1.7424400000 -0.5293270000 2.4463630000
 C -2.2729790000 2.7723210000 -1.4972540000
 H -1.8562420000 2.3989980000 0.5913430000
 C -0.6265750000 4.0660160000 -0.0424510000
 O 2.3751380000 -0.1026560000 0.8180920000
 O 1.7223020000 0.0709450000 -1.3633230000
 C 3.6519130000 -0.7948770000 0.4763820000
 C 4.0234580000 -1.5899130000 1.7133850000
 H 3.4238450000 -1.4499630000 -0.3678650000
 C 4.6753780000 0.2570640000 0.0772230000
 H 4.9506650000 -2.1386830000 1.5231600000
 H 4.1859170000 -0.9282640000 2.5697460000
 H 3.2460260000 -2.3153700000 1.9708310000
 H 5.6241500000 -0.2349870000 -0.1580080000
 H 4.3544100000 0.8085620000 -0.8104770000

H 4.8488000000 0.9594120000 0.8985560000
 H -1.3850790000 4.8210220000 0.1827360000
 H 0.0573520000 4.0048500000 0.8097250000
 H -0.0641720000 4.4002360000 -0.9201640000
 H -3.0516330000 3.5143980000 -1.3029290000
 H -1.7489200000 3.0750910000 -2.4111950000
 H -2.7524060000 1.8045370000 -1.6636490000

Equilibrium geometry of **r11-exo-3s-prod**.

C 0.0425600000 0.2949850000 0.4939190000
 N -0.8326050000 0.9122880000 -0.5875930000
 C -1.2487260000 2.3613130000 -0.3615470000
 C 1.4431200000 0.1225570000 -0.0992700000
 H 0.0735900000 0.9418790000 1.3699500000
 H -0.2333170000 0.8828100000 -1.4325270000
 C -0.6854760000 -1.0636270000 0.7873090000
 C -1.1635330000 -1.4251130000 -0.6400440000
 C -1.9841170000 -0.1366740000 -0.7813920000
 C -2.7847960000 -0.1315990000 0.5046200000
 C -2.0077040000 -0.6923630000 1.4414160000
 H -0.0494960000 -1.7728930000 1.3155590000
 H -2.4916470000 0.0663590000 -1.7210200000
 H -1.8006130000 -2.3099210000 -0.6570650000
 H -0.3632930000 -1.5294040000 -1.3796470000
 H -3.7703900000 0.3014510000 0.6231860000
 H -2.2248280000 -0.8060670000 2.4975580000
 C -2.2045230000 2.8075510000 -1.4666280000
 H -1.7657020000 2.3557380000 0.6026630000
 C -0.0043960000 3.2470720000 -0.2946320000
 O 2.3018130000 -0.2619950000 0.8172250000
 O 1.6561020000 0.3061300000 -1.2863760000
 C 3.7074350000 -0.5365420000 0.3993260000
 C 4.2533990000 -1.4954600000 1.4404530000
 H 3.6407910000 -1.0116980000 -0.5824820000
 C 4.4595680000 0.7800220000 0.3041780000
 H 5.2753980000 -1.7785600000 1.1709760000
 H 4.2773440000 -1.0276680000 2.4296210000
 H 3.6516220000 -2.4070590000 1.4957590000
 H 5.4944840000 0.5818760000 0.0074700000
 H 4.0163900000 1.4379660000 -0.4478330000
 H 4.4761550000 1.2919610000 1.2717340000
 H -0.3169390000 4.2773390000 -0.1042200000
 H 0.6795730000 2.9618560000 0.5097420000
 H 0.5476040000 3.2335990000 -1.2406250000
 H -2.4462920000 3.8632960000 -1.3157810000
 H -1.7458470000 2.7147480000 -2.4578940000
 H -3.1473900000 2.2545790000 -1.4590830000

Equilibrium geometry of **r11-exo-3s-ts**.

C 0.2179649709 0.6955333983 0.3403677980
 N -0.4895298703 1.3709266874 -0.5843578659
 C -1.3175674367 2.5604251495 -0.2882577219
 C 1.5360742577 0.1423652351 -0.1800192117
 H 0.2423139354 1.1091845984 1.3428110153
 H -0.1500780804 1.2582055518 -1.5387168944
 C -0.6566632995 -1.0576075941 0.7266324052
 C -1.0783930833 -1.4658752231 -0.6743564728
 C -2.4070215723 -0.8066764268 -0.8017423077
 C -2.8617730319 -0.4157193769 0.4377906231
 C -1.8296902761 -0.6301044087 1.3808697862
 H 0.1398203225 -1.5618935651 1.2651328800
 H -2.9617645622 -0.7372396911 -1.7311322631
 H -1.2283128929 -2.5584387208 -0.6777686642

H -0.3707435959 -1.2509675714 -1.4789265281
H -3.8357565111 0.0050311005 0.6573454751
H -1.9098150700 -0.4359942555 2.4459655915
C -2.2676610884 2.8235041126 -1.4535523469
H -1.8946261275 2.3077673497 0.6099722223
C -0.4293350068 3.7769591143 0.0125039817
O 2.3515311612 -0.1647297579 0.8109597206
O 1.7327833525 0.0182321800 -1.3721428003
C 3.6911092106 -0.7142262201 0.4657646957
C 4.1251249791 -1.5124199490 1.6812105032
H 3.5376382444 -1.3623606205 -0.4010578647
C 4.6192778284 0.4359865220 0.1126786869
H 5.0883629591 -1.9891455034 1.4755981652
H 4.2443843630 -0.8632320742 2.5542940291
H 3.4031610669 -2.2982556275 1.9228455473
H 5.6096954137 0.0383999182 -0.1304971946
H 4.2558748141 0.9877026832 -0.7582757355
H 4.7269744579 1.1236245725 0.9578302494
H -1.0551822908 4.6327684248 0.2833435240
H 0.2555292322 3.5849314166 0.8450289069
H 0.1631665447 4.0537157102 -0.8659499793
H -2.8822948581 3.7026001900 -1.2429586619
H -1.7091082087 3.0268431430 -2.3750524741
H -2.9329022323 1.9739398311 -1.6310931063

Equilibrium geometry of **r12-endo-3r-mc**.

C 0.5199830000 1.1071070000 -0.3534070000
N -0.2712260000 1.7108970000 0.4635170000
H -0.1584760000 1.4029750000 1.4370000000
H 0.5370680000 1.3542310000 -1.4071980000
C 1.5668810000 0.2084350000 0.2704920000
C -1.2082360000 2.8464550000 0.2208400000
C -1.0468070000 -1.1232530000 -1.3274390000
C -2.3654750000 -0.4041080000 -1.2247170000
C -2.7047160000 -0.5214420000 0.2358240000
C -1.7687940000 -1.2801060000 0.8554440000
C -0.7525380000 -1.6677650000 -0.1159740000
H -0.5105390000 -1.2859500000 -2.2551530000
H -3.6018130000 -0.1086510000 0.6831830000
H -3.1220220000 -0.9230630000 -1.8347330000
H -2.3566930000 0.6273810000 -1.6029970000
H -1.7681790000 -1.5806750000 1.8968270000
H 0.0920260000 -2.3096330000 0.1071460000
H -2.2101150000 2.4284500000 0.3587260000
C -0.9477970000 3.8899330000 1.3126050000
C -1.0667240000 3.4111200000 -1.1875890000
O 2.4173760000 -0.1902340000 -0.6458020000
O 1.5485350000 0.0156060000 1.4700490000
C 3.6641600000 -0.9841130000 -0.3098920000
C 4.3034200000 -1.1626930000 -1.6822610000
C 4.5349140000 -0.1408190000 0.6181900000
C 3.2505310000 -2.3170920000 0.3058200000
H 5.2339140000 -1.7285880000 -1.5805730000
H 3.6398070000 -1.7121940000 -2.3564340000
H 4.5387940000 -0.1941070000 -2.1328800000
H 5.4940750000 -0.6484980000 0.7598770000
H 4.7375860000 0.8391230000 0.1745600000
H 4.0727290000 -0.0058660000 1.5980600000
H 4.1463600000 -2.9273250000 0.4587460000
H 2.7630060000 -2.1822920000 1.2734520000
H 2.5848610000 -2.8674840000 -0.3671580000
H -1.6823010000 4.6949070000 1.2229010000
H -1.0488740000 3.4607890000 2.3153400000
H 0.0520650000 4.3244160000 1.2148680000
H -1.7826000000 4.2286710000 -1.3057620000

H -0.0646430000 3.8204230000 -1.3561090000
H -1.2873250000 2.6731370000 -1.9650790000

Equilibrium geometry of **r12-endo-3r-prod**.

C 0.0536230000 0.3897130000 -0.7006460000
N -0.8460720000 1.1314570000 0.2795860000
H -0.3573840000 1.0321550000 1.1866100000
H 0.2143790000 1.0041560000 -1.5864280000
C 1.3830020000 0.1101420000 0.0064670000
C -1.0425280000 2.6291360000 0.0358490000
C -0.7948550000 -0.8721680000 -1.0705460000
C -2.1859350000 -0.2019950000 -1.1697320000
C -2.1600760000 0.2623040000 0.2917000000
C -1.7829520000 -1.0118050000 1.0162250000
C -0.9684210000 -1.6927330000 0.1991270000
H -0.4093670000 -1.3863180000 -1.9500490000
H -2.9829780000 0.8546770000 0.6800150000
H -2.9890500000 -0.9181080000 -1.3490540000
H -2.2474430000 0.6074580000 -1.9052120000
H -2.0717220000 -1.2526640000 2.0321440000
H -0.4523590000 -2.6220080000 0.4111740000
H -1.6419730000 2.6940970000 -0.8777990000
C -1.8007130000 3.2383420000 1.2165450000
C 0.3042770000 3.3272440000 -0.1601450000
O 2.2397680000 -0.4253490000 -0.8302550000
O 1.5207640000 0.3636530000 1.1912100000
C 3.6310480000 -0.8518740000 -0.4143790000
C 4.2160450000 -1.3580050000 -1.7281020000
C 4.3883160000 0.3668280000 0.1080940000
C 3.5067490000 -1.9676620000 0.6192840000
H 5.2392710000 -1.7069400000 -1.5609600000
H 3.6303170000 -2.1930640000 -2.1239930000
H 4.2438560000 -0.5621550000 -2.4781450000
H 5.4308100000 0.0840580000 0.2847390000
H 4.3826650000 1.1735350000 -0.6320550000
H 3.9690840000 0.7328730000 1.0465130000
H 4.5058010000 -2.3510060000 0.8495100000
H 3.0565640000 -1.6114130000 1.5478080000
H 2.9145260000 -2.7991880000 0.2233140000
H -1.9481860000 4.3047660000 1.0256950000
H -2.7888390000 2.8000180000 1.3743970000
H -1.2228770000 3.1473710000 2.1437490000
H 0.1218690000 4.3973720000 -0.2908690000
H 0.9484390000 3.2016100000 0.7161230000
H 0.8461360000 2.9841600000 -1.0453510000

Equilibrium geometry of **r12-endo-3r-ts**.

C 0.2239737978 0.7230855633 -0.4569995372
N -0.5305825075 1.4621054834 0.3875227132
H -0.3349686636 1.2622956973 1.3675271178
H 0.3934465077 1.1407595645 -1.4431882740
C 1.4418799123 0.0928211886 0.2044260077
C -1.1741170374 2.7815924935 0.1151178687
C -0.7756479225 -0.8322254960 -1.0637812942
C -2.1627240280 -0.2123789964 -1.1663883539
C -2.6537684376 -0.3442522442 0.2344978347
C -1.9041942056 -1.2842882892 0.9080683499
C -0.8121392476 -1.6474911855 0.0931757842
H -0.2144831498 -1.1325701381 -1.9439269454
H -3.5345684076 0.1570881006 0.6211536215
H -2.7734567635 -0.8640586628 -1.8124136112
H -2.2278395560 0.7918531954 -1.5902309625
H -2.0947886350 -1.6590987322 1.9063329307

H -0.0558793489 -2.3763612576 0.3633328630
H -2.2519613147 2.6125589065 0.0081267068
C -0.9463708810 3.6682866250 1.3421089585
C -0.6578059899 3.4366616775 -1.1655761646
O 2.3303085047 -0.2524674830 -0.7058504686
O 1.4836578648 -0.0479770950 1.4105437125
C 3.6480620431 -0.8946207717 -0.3459646696
C 4.2959765326 -1.0793782743 -1.7144678928
C 4.4446763555 0.0689175620 0.5304397314
C 3.3764719210 -2.2336999797 0.3355721999
H 5.2823175842 -1.5368648211 -1.5943679062
H 3.6909628660 -1.7322097180 -2.3509893045
H 4.4226384269 -0.1173292244 -2.2193828845
H 5.4440265855 -0.3463913923 0.6942015336
H 4.5622144233 1.0371089036 0.0335194557
H 3.9718883749 0.2178952171 1.5029524670
H 4.3278191599 -2.7536308470 0.4860729121
H 2.9017611570 -2.1035920356 1.3101568600
H 2.7486888134 -2.8714523128 -0.2967124819
H -1.4913815073 4.6089663690 1.2254099918
H -1.3098779912 3.1875359110 2.2574037739
H 0.1165137322 3.9000493275 1.4676112683
H -1.1626659247 4.3981177625 -1.2936622337
H 0.4196063807 3.6265039636 -1.1117168737
H -0.8678864261 2.8452669555 -2.0633315176

Equilibrium geometry of **r12-endo-3s-mc**.

C 0.5217400000 1.1106610000 0.3642030000
N -0.2697040000 1.7181600000 -0.4497960000
C -1.2100960000 2.8494570000 -0.1999440000
C 1.5738360000 0.2209200000 -0.2636230000
H 0.5358560000 1.3499820000 1.4197760000
H -0.1542400000 1.4181430000 -1.4253680000
C -2.6961200000 -0.5175600000 -0.2453880000
C -2.3584920000 -0.4141680000 1.2165270000
C -1.0387450000 -1.1322060000 1.3133400000
C -0.7428150000 -1.6648110000 0.0969820000
C -1.7587670000 -1.2691840000 -0.8714620000
H -3.5933710000 -0.1016930000 -0.6895850000
H -0.5031320000 -1.3031740000 2.2399570000
H -3.1147290000 -0.9407140000 1.8204330000
H -2.3520970000 0.6132990000 1.6054860000
H 0.1028180000 -2.3032720000 -0.1316700000
H -1.7569660000 -1.5597080000 -1.9156980000
H -2.2109380000 2.4290040000 -0.3375090000
C -1.0670630000 3.4078800000 1.2108970000
C -0.9556170000 3.8989120000 -1.2873240000
O 2.4241870000 -0.1793970000 0.6521380000
O 1.5592290000 0.0359320000 -1.4644210000
C 3.6782190000 -0.9608670000 0.3142790000
C 4.3145080000 -1.1442700000 1.6874020000
C 3.2772120000 -2.2925570000 -0.3125310000
C 4.5450310000 -0.1041280000 -0.6050160000
H 5.2503220000 -1.7011460000 1.5847230000
H 4.5396760000 -0.1770210000 2.1460910000
H 3.6533720000 -1.7045450000 2.3551110000
H 5.5082390000 -0.6037950000 -0.7478840000
H 4.0845010000 0.0343970000 -1.5851580000
H 4.7394660000 0.8740210000 -0.1537010000
H 4.1782210000 -2.8952220000 -0.4650650000
H 2.6120920000 -2.8522420000 0.3533290000
H 2.7933640000 -2.1546290000 -1.2815820000
H -1.6914760000 4.7018190000 -1.1907580000
H 0.0435710000 4.3351490000 -1.1909120000
H -1.0594610000 3.4747030000 -2.2919330000

H -1.7843750000 4.2233810000 1.3344620000
H -1.2846570000 2.6657430000 1.9852380000
H -0.0653980000 3.8183400000 1.3793140000

Equilibrium geometry of **r12-endo-3s-prod**.

C 0.0581160000 0.3916930000 0.7041200000
N -0.8419520000 1.1377610000 -0.2725000000
C -1.0438210000 2.6326650000 -0.0162500000
C 1.3909300000 0.1238660000 -0.0009860000
H 0.2125740000 0.9988830000 1.5959590000
H -0.3503670000 1.0479590000 -1.1789550000
C -2.1523830000 0.2635410000 -0.2957060000
C -2.1801320000 -0.2140930000 1.1613680000
C -0.7859220000 -0.8773990000 1.0598090000
C -0.9523930000 -1.6870460000 -0.2178110000
C -1.7680010000 -1.0024170000 -1.0307390000
H -2.9767360000 0.8559810000 -0.6808220000
H -0.4007360000 -1.3979710000 1.9356680000
H -2.9804390000 -0.9354290000 1.3317620000
H -2.2470200000 0.5884240000 1.9039750000
H -0.4315930000 -2.6120240000 -0.4368420000
H -2.0531330000 -1.2351590000 -2.0495830000
H -1.6423490000 2.6880340000 0.8986030000
C 0.3012170000 3.3332630000 0.1837310000
C -1.8055470000 3.2492940000 -1.1907160000
O 2.2486470000 -0.4112090000 0.8350540000
O 1.5299650000 0.3840320000 -1.1841270000
C 3.6420890000 -0.8310030000 0.4196470000
C 4.2278400000 -1.3376820000 1.7328710000
C 3.5226650000 -1.9449880000 -0.6165370000
C 4.3954100000 0.3916290000 -0.0995530000
H 5.2521010000 -1.6835300000 1.5655930000
H 4.2530990000 -0.5429490000 2.4841540000
H 3.6441830000 -2.1749760000 2.1272270000
H 5.4395140000 0.1135570000 -0.2741980000
H 3.9768220000 0.7572450000 -1.0384130000
H 4.3846150000 1.1973600000 0.6416420000
H 4.5231950000 -2.3242160000 -0.8470870000
H 2.9332160000 -2.7796270000 -0.2228220000
H 3.0717340000 -1.5882830000 -1.5445900000
H -1.9548740000 4.3138500000 -0.9913070000
H -1.2295480000 3.1669150000 -2.1197990000
H -2.7930550000 2.8101510000 -1.3499100000
H 0.1160130000 4.4019890000 0.3221890000
H 0.8446390000 2.9852920000 1.0660100000
H 0.9449540000 3.2153990000 -0.6939340000

Equilibrium geometry of **r12-endo-3s-ts**.

C 0.2281813062 0.7254004253 0.4648551425
N -0.5252794257 1.4702182285 -0.3752724725
C -1.1754011045 2.7844212317 -0.0930674570
C 1.4504042416 0.1050363959 -0.1977861132
H 0.3925309740 1.1339437488 1.4557449259
H -0.3273884325 1.2786291847 -1.3564438898
C -2.6463144434 -0.3418535047 -0.2443903237
C -2.1579368839 -0.2236434539 1.1587238445
C -0.7695090299 -0.8399340345 1.0522930234
C -0.8018412425 -1.6423104257 -0.1137103124
C -1.8932435324 -1.2725829089 -0.9267756693
H -3.5275677446 0.1617524421 -0.6271259353
H -0.2095891695 -1.1488744865 1.9303004080
H -2.7687465547 -0.8828198667 1.7969719306
H -2.2256331663 0.7762360073 1.5924287207

H -0.0436782575 -2.3667294298 -0.3904796172
H -2.0811238711 -1.6369468471 -1.9294459644
H -2.2518309691 2.6089250225 0.0173508805
C -0.6574550845 3.4354173477 1.1890262521
C -0.9572538873 3.6783250812 -1.3164451223
O 2.3393305102 -0.2396419682 0.7121722423
O 1.4948654276 -0.0292060879 -1.4045738557
C 3.6615305281 -0.8719232682 0.3511140806
C 4.3093172201 -1.0579188284 1.7195109480
C 3.3987370199 -2.2099813870 -0.3358199572
C 4.4530194996 0.0999268486 -0.5207368598
H 5.2983917706 -1.5091813541 1.5984094096
H 4.4300061785 -0.0970393910 2.2280939914
H 3.7077229585 -1.7166636249 2.3531577027
H 5.4551315814 -0.3084589836 -0.6849349018
H 3.9803814526 0.2496371007 -1.4931912189
H 4.5639067203 1.0669062165 -0.0199734853
H 4.3532683792 -2.7238208938 -0.4870417243
H 2.7738734687 -2.8537103359 0.2932386051
H 2.9245472590 -2.0789859655 -1.3105583839
H -1.5068080549 4.6155591138 -1.1936021146
H 0.1038920050 3.9163960365 -1.4447644191
H -1.3215055037 3.1998202464 -2.2326313796
H -1.1660584495 4.3940141774 1.3235010998
H -0.8619921768 2.8386813097 2.0845007514
H 0.4189278231 3.6299936187 1.1322749563

Equilibrium geometry of **r12-exo-3r-mc**.

C 0.4178530000 1.0935270000 -0.3437040000
N -0.2778760000 1.7206580000 0.5446070000
H 0.0122590000 1.5369890000 1.5116510000
H 0.2587360000 1.2704560000 -1.3997030000
C 1.6141310000 0.3218920000 0.1719550000
C -1.3428650000 2.7322530000 0.3056930000
C -2.4737640000 -1.0115590000 0.7560270000
C -1.1253020000 -1.6700320000 0.6954520000
C -0.6890340000 -1.4213800000 -0.7219650000
C -1.6976730000 -0.7869510000 -1.3871400000
C -2.7960910000 -0.5240180000 -0.4676410000
H -3.0952450000 -0.9903600000 1.6437610000
H 0.2153590000 -1.8213130000 -1.1639820000
H -1.2150740000 -2.7523120000 0.8795290000
H -0.4186370000 -1.3055190000 1.4536160000
H -1.7086390000 -0.5450730000 -2.4451870000
H -3.7252580000 -0.0370540000 -0.7415010000
C -2.2928800000 2.7498850000 1.5001490000
C -0.6895390000 4.0961540000 0.0455300000
H -1.8724930000 2.3970050000 -0.5914910000
O 2.3972940000 -0.0285310000 -0.8200550000
O 1.7428040000 0.1621310000 1.3711820000
C 3.7336720000 -0.7113000000 -0.5942660000
C 4.2480010000 -0.8866330000 -2.0179900000
C 4.6203500000 0.2261690000 0.2210310000
C 3.4902930000 -2.0535850000 0.0911790000
H 5.2250580000 -1.3776650000 -1.9901010000
H 3.5691130000 -1.5090170000 -2.6085460000
H 4.3642620000 0.0794850000 -2.5175290000
H 5.6153340000 -0.2206790000 0.3115000000
H 4.7311410000 1.1922850000 -0.2812040000
H 4.2269370000 0.3829640000 1.2271600000
H 4.4420270000 -2.5901150000 0.1558090000
H 3.0994220000 -1.9311130000 1.1029590000
H 2.8012150000 -2.6720920000 -0.4934790000
H -1.4710280000 4.8307750000 -0.1681580000
H -0.1295820000 4.4403720000 0.9209300000

H -0.0115190000 4.0602610000 -0.8129020000
H -3.0976020000 3.4643920000 1.3086370000
H -2.7381440000 1.7662930000 1.6682780000
H -1.7761290000 3.0707760000 2.4121040000

Equilibrium geometry of **r12-exo-3r-prod**.

C 0.0508600000 0.3272190000 -0.5058860000
N -0.8305990000 0.9218640000 0.5826510000
H -0.2271880000 0.8891300000 1.4251740000
H 0.0752780000 0.9849280000 -1.3738490000
C 1.4563870000 0.1581980000 0.0865420000
C -1.2652720000 2.3674240000 0.3740520000
C -1.9686280000 -0.1426940000 0.7673410000
C -1.1332740000 -1.4196730000 0.6100170000
C -0.6618060000 -1.0358570000 -0.8138380000
C -1.9899200000 -0.6742880000 -1.4612560000
C -2.7721600000 -0.1336790000 -0.5169440000
H -2.4765130000 0.0439630000 1.7102110000
H -0.0181930000 -1.7310910000 -1.3511900000
H -1.7600660000 -2.3119710000 0.6180100000
H -0.3307280000 -1.5227790000 1.3470630000
H -2.2079030000 -0.7788150000 -2.5181080000
H -3.7633820000 0.2883490000 -0.6286940000
C -2.2299730000 2.7863040000 1.4825440000
C -0.0333350000 3.2710600000 0.3222270000
H -1.7801350000 2.3678320000 -0.5912310000
O 2.3052290000 -0.2007770000 -0.8445720000
O 1.6522680000 0.3286890000 1.2798310000
C 3.7532490000 -0.5382150000 -0.5488430000
C 4.2926680000 -0.8671760000 -1.9364400000
C 4.4389000000 0.6879030000 0.0470400000
C 3.7820080000 -1.7531130000 0.3742720000
H 5.3471190000 -1.1476400000 -1.8579810000
H 3.7478630000 -1.7044320000 -2.3826420000
H 4.2168210000 -0.0026410000 -2.6023600000
H 5.5083370000 0.4781210000 0.1495170000
H 4.3310770000 1.5529640000 -0.6151220000
H 4.0435630000 0.9370220000 1.0332500000
H 4.8200540000 -2.0717190000 0.5110560000
H 3.3657420000 -1.5243390000 1.3575890000
H 3.2319410000 -2.5897600000 -0.0684680000
H -0.3595990000 4.2987600000 0.1410890000
H 0.5144200000 3.2554920000 1.2707290000
H 0.6588900000 3.0041790000 -0.4814960000
H -2.4794830000 3.8425760000 1.3502050000
H -3.1682930000 2.2260860000 1.4601440000
H -1.7755320000 2.6783300000 2.4742960000

Equilibrium geometry of **r12-exo-3r-ts**.

C 0.2258676153 0.7328232819 -0.3428177231
N -0.4928592741 1.3924160348 0.5844594607
H -0.1479867031 1.2804958493 1.5372372521
H 0.2470560295 1.1530029081 -1.3426432561
C 1.5552202526 0.1970502823 0.1828228808
C -1.3410326474 2.5684568877 0.2965718301
C -2.3750800477 -0.8307203839 0.7879575514
C -1.0320850276 -1.4589929713 0.6512548777
C -0.6204622714 -1.0249953915 -0.7451599472
C -1.8031426951 -0.6143117369 -1.3925030379
C -2.8389691430 -0.4336590895 -0.4459495218
H -2.9296930420 -0.7842363027 1.7188747599
H 0.1846119060 -1.5074957497 -1.2905324153
H -1.1573792996 -2.5546678608 0.6428649670

H -0.3294751637 -1.2362236747 1.4579849291
H -1.8887049343 -0.4082800712 -2.4549667538
H -3.8217437676 -0.0305078676 -0.6595194327
C -2.2952106177 2.8064477898 1.4640799779
C -0.4748869618 3.8028751148 0.0045281786
H -1.9142608789 2.3125009124 -0.6031668425
O 2.3597944585 -0.1126046887 -0.8114154807
O 1.7405328430 0.1025560999 1.3806128476
C 3.7542963370 -0.6519877097 -0.5820551880
C 4.2573300243 -0.8582992717 -2.0065653011
C 4.5702317811 0.4027452725 0.1599900944
C 3.6533410472 -1.9739310226 0.1759344865
H 5.2744826213 -1.2602609662 -1.9773411467
H 3.6247193460 -1.5680515683 -2.5484789186
H 4.2784410347 0.0857399843 -2.5590002360
H 5.6064494998 0.0587355159 0.2382388874
H 4.5714121565 1.3489146177 -0.3901875730
H 4.1900282619 0.5708922433 1.1690629076
H 4.6490761426 -2.4242368680 0.2386223512
H 3.2795267988 -1.8321761146 1.1913495006
H 3.0049916654 -2.6786694401 -0.3558871727
H -1.1158370498 4.6493352831 -0.2602403313
H 0.1124618325 4.0835932833 0.8850911058
H 0.2134326567 3.6286498901 -0.8289584778
H -2.9268706652 3.6752743647 1.2609011331
H -2.9441834190 1.9431926114 1.6362253362
H -1.7396530290 3.0131149865 2.3866838799

Equilibrium geometry of **r12-exo-3s-mc**.

C 0.4170790000 1.0931070000 0.3427940000
N -0.2794500000 1.7185970000 -0.5460770000
C -1.3445640000 2.7302890000 -0.3080030000
C 1.6138560000 0.3219460000 -0.1724500000
H 0.2585370000 1.2715910000 1.3985980000
H 0.0103600000 1.5337630000 -1.5129890000
C -0.6893440000 -1.4204520000 0.7253390000
C -1.1258180000 -1.6708950000 -0.6917500000
C -2.4742330000 -1.0124220000 -0.7530010000
C -2.7964810000 -0.5234640000 0.4701400000
C -1.6980070000 -0.7853140000 1.3898610000
H 0.2150940000 -1.8198940000 1.1677440000
H -3.0958000000 -0.9922470000 -1.6407080000
H -1.2157240000 -2.7534020000 -0.8743190000
H -0.4192640000 -1.3075110000 -1.4504790000
H -3.7256090000 -0.0362010000 0.7434480000
H -1.7088870000 -0.5421780000 2.4476210000
C -2.2939470000 2.7475170000 -1.5029360000
H -1.8746320000 2.3952760000 0.5890500000
C -0.6913780000 4.0942810000 -0.0479670000
O 2.3979070000 -0.0263430000 0.8196060000
O 1.7421530000 0.1608610000 -1.3715420000
C 3.7357040000 -0.7063490000 0.5937300000
C 4.2502410000 -0.8811880000 2.0174420000
C 3.4954950000 -2.0489040000 -0.0923200000
C 4.6203010000 0.2336070000 -0.2210510000
H 5.2281420000 -1.3704580000 1.9894400000
H 4.3647800000 0.0849480000 2.5173290000
H 3.5724260000 -1.5049690000 2.6077420000
H 5.6162160000 -0.2110470000 -0.3121060000
H 4.2263610000 0.3902950000 -1.2270030000
H 4.7291180000 1.1995890000 0.2818850000
H 4.4484420000 -2.5832600000 -0.1568770000
H 2.8076580000 -2.6691650000 0.4919090000
H 3.1046190000 -1.9269780000 -1.1041560000
H -1.4729760000 4.8289150000 0.1652190000

H -0.0137180000 4.0586630000 0.8107270000
H -0.1311020000 4.4382550000 -0.9232430000
H -3.0988500000 3.4619840000 -1.3120940000
H -1.7767540000 3.0681230000 -2.4146750000
H -2.7391070000 1.7639140000 -1.6709960000

Equilibrium geometry of **r12-exo-3s-prod**.

C 0.0529160000 0.3345290000 0.5062980000
N -0.8309260000 0.9246940000 -0.5826740000
C -1.2749130000 2.3673890000 -0.3734560000
C 1.4590270000 0.1693140000 -0.0858460000
H 0.0744640000 0.9925650000 1.3740900000
H -0.2268380000 0.8958140000 -1.4248370000
C -0.6531340000 -1.0319960000 0.8143220000
C -1.1208590000 -1.4188760000 -0.6099610000
C -1.9628770000 -0.1464890000 -0.7687170000
C -2.7680360000 -0.1415530000 0.5144900000
C -1.9839810000 -0.6774860000 1.4599860000
H -0.0064060000 -1.7235170000 1.3527040000
H -2.4704110000 0.0370990000 -1.7123230000
H -1.7429700000 -2.3144140000 -0.6183340000
H -0.3170950000 -1.5181900000 -1.3462090000
H -3.7617410000 0.2750230000 0.6247740000
H -2.2027740000 -0.7830410000 2.5165990000
C -2.2410350000 2.7812790000 -1.4826240000
H -1.7908980000 2.3637050000 0.5912370000
C -0.0489990000 3.2789880000 -0.3196450000
O 2.3079340000 -0.1892070000 0.8454440000
O 1.6546810000 0.3397320000 -1.2791280000
C 3.7524160000 -0.5401190000 0.5489490000
C 4.2932580000 -0.8594910000 1.9382140000
C 3.7674820000 -1.7644420000 -0.3619890000
C 4.4475810000 0.6731790000 -0.0620440000
H 5.3450930000 -1.1495170000 1.8596620000
H 4.2264550000 0.0124810000 2.5953750000
H 3.7427900000 -1.6875110000 2.3945800000
H 5.5150770000 0.4529110000 -0.1627790000
H 4.0533750000 0.9136320000 -1.0507590000
H 4.3479360000 1.5471980000 0.5894700000
H 4.8023370000 -2.0925190000 -0.5006170000
H 3.2128730000 -2.5923760000 0.0913080000
H 3.3486580000 -1.5420640000 -1.3457890000
H -0.3823460000 4.3045150000 -0.1390410000
H 0.6438630000 3.0168370000 0.4851030000
H 0.5002110000 3.2670460000 -1.2673310000
H -2.4999990000 3.8348890000 -1.3471550000
H -1.7834220000 2.6809470000 -2.4736600000
H -3.1744070000 2.2129150000 -1.4643710000

Equilibrium geometry of **r12-exo-3s-ts**.

C 0.2257943385 0.7342651783 0.3425314936
N -0.4937418386 1.3923425335 -0.5851576901
C -1.3430463454 2.5677365686 -0.2981153513
C 1.5552568168 0.1987718417 -0.1831375299
H 0.2471513492 1.1555848740 1.3418751668
H -0.1493060745 1.2796045510 -1.5379899009
C -0.6191101489 -1.0236497397 0.7475701738
C -1.0303655825 -1.4602706777 -0.6481356999
C -2.3741956619 -0.8339009520 -0.7856964749
C -2.8383504892 -0.4352611351 0.4475876197
C -1.8021778122 -0.6131835346 1.3943345058
H 0.1864743725 -1.5044949864 1.2936618897
H -2.9289506332 -0.7895825990 -1.7166436695

H -1.1542340694 -2.5561080523 -0.6381559831
H -0.3281583485 -1.2377773086 -1.4552942275
H -3.8215659349 -0.0328784001 0.6606259251
H -1.8878809699 -0.4055444330 2.4564783174
C -2.2976031505 2.8037975554 -1.4657059016
H -1.9159275710 2.3119295911 0.6018919060
C -0.4781388048 3.8032773118 -0.0071240352
O 2.3604681574 -0.1093822925 0.8110536864
O 1.7400973821 0.1031548296 -1.3809181575
C 3.7551749189 -0.6482212642 0.5815970697
C 4.2589892574 -0.8527607504 2.0060680948
C 3.6545842057 -1.9709955572 -0.1749791949
C 4.5701978156 0.4061613852 -0.1619350889
H 5.2763711542 -1.2541675541 1.9768069649
H 4.2798132348 0.0918754253 2.5574750714
H 3.6270290982 -1.5622925513 2.5490232559
H 5.6066612894 0.0628430298 -0.2399162093
H 4.1897176248 0.5727592269 -1.1711386225
H 4.5707625981 1.3530018648 0.3870331405
H 4.6505391368 -2.4208114984 -0.2377594672
H 3.0069077337 -2.6755531324 0.3578772028
H 3.2801515335 -1.8304464484 -1.1903182807
H -1.1199328424 4.6492751706 0.2570556507
O 2.2104407328 3.6303970220 0.8264195393
H 0.1088251905 4.0839006094 -0.8879667478
H -2.9303191738 3.6719936490 -1.2630979759
H -1.7423619956 3.0104908101 -2.3884976297
H -2.9455527728 1.9396330155 -1.6372131458

Equilibrium geometry of **r13-endo-3r-mc**.

C 0.5352740000 1.1760860000 -0.2871500000
N -0.0747760000 1.9593820000 0.5296080000
O 0.1742970000 1.7959220000 1.5136450000
H 0.3938710000 1.2529540000 -1.3570020000
C 1.5741240000 0.2675460000 0.3205390000
C -1.0590150000 3.0587690000 0.2717260000
C -0.9144280000 -1.2867560000 -1.1822330000
C -2.3016670000 -0.8949100000 -1.6181570000
C -3.0923030000 -0.9522600000 -0.3402850000
C -2.2888100000 -1.3627560000 0.6679800000
C -0.9434370000 -1.5873250000 0.1439330000
H -0.0795470000 -1.4279020000 -1.8584410000
H -4.1506760000 -0.7287530000 -0.2747690000
H -2.6886750000 -1.6177830000 -2.3531080000
H -2.3566730000 0.0814890000 -2.1215890000
H -2.5820570000 -1.5314150000 1.6978080000
H -0.1208980000 -1.9769980000 0.7342000000
C -2.3651120000 2.6560660000 0.9800420000
C -0.4554260000 4.3205900000 0.9139760000
C -1.2636920000 3.2430990000 -1.2308910000
O 2.2583200000 -0.3665690000 -0.6138120000
O 1.7272910000 0.2188400000 1.5214590000
C 3.3313920000 -1.2321910000 -0.1491000000
H 3.8033170000 -1.6072190000 -1.0543290000
H 4.0329110000 -0.6547130000 0.4545710000
H 2.9122640000 -2.0474130000 0.4435710000
H -1.1608880000 5.1478460000 0.7976280000
H -0.2797160000 4.1819910000 1.9862300000
H 0.4874190000 4.6038220000 0.4364270000
H -3.0987280000 3.4571660000 0.8521150000
H -2.7722300000 1.7311150000 0.5630070000
H -2.2099340000 2.5146560000 2.0551640000
H -1.9761380000 4.0568660000 -1.3872300000
H -0.3343850000 3.5191310000 -1.7409450000
H -1.6834560000 2.3485790000 -1.7023540000

Equilibrium geometry of **r13-endo-3r-prod**.

C 0.0786790000 0.4264280000 -0.6191180000
N -1.0120130000 1.0631510000 0.2264820000
H -0.7016610000 0.8800880000 1.1942820000
H 0.3428000000 1.0864750000 -1.4449940000
C 1.2878200000 0.1694810000 0.2716140000
C -1.1927810000 2.6084980000 0.1539620000
C -0.6162430000 -0.8704390000 -1.1673650000
C -2.0019020000 -0.2734160000 -1.5035450000
C -2.2672050000 0.1465640000 -0.0518800000
C -1.9636240000 -1.1366400000 0.6946410000
C -0.9728070000 -1.7438910000 0.0278910000
H -0.0481770000 -1.3323020000 -1.9741570000
H -3.1754860000 0.6872360000 0.1966540000
H -2.7142770000 -1.0305900000 -1.8345580000
H -1.9765390000 0.5475800000 -2.2234330000
H -2.4239360000 -1.4303390000 1.6303530000
H -0.4542120000 -2.6542150000 0.3054860000
C -2.1777360000 2.9840160000 1.2708360000
C 0.1749700000 3.2464420000 0.4398300000
C -1.7237730000 3.0361280000 -1.2143230000
O 2.3328030000 -0.2004510000 -0.4470010000
O 1.2379330000 0.2734460000 1.4812210000
C 3.5476480000 -0.5188860000 0.2857800000
H 4.2744880000 -0.7892260000 -0.4773570000
H 3.8769410000 0.3548790000 0.8501630000
H 3.3614670000 -1.3524500000 0.9645950000
H 0.0473010000 4.3314740000 0.4839730000
H 0.5873090000 2.9182730000 1.3984160000
H 0.9077190000 3.0416770000 -0.3469600000
H -2.2287700000 4.0737360000 1.3424950000
H -3.1934240000 2.6266220000 1.0799240000
H -1.8485700000 2.6082700000 2.2462800000
H -1.8327830000 4.1244890000 -1.2123790000
H -1.0386320000 2.7857730000 -2.0304970000
H -2.7080550000 2.6125600000 -1.4328220000

Equilibrium geometry of **r13-endo-3r-ts**.

C 0.1749701065 0.7290712572 -0.4374691372
N -0.6363290211 1.4430968478 0.3647106293
H -0.5139633796 1.2050231889 1.3495646068
H 0.3427587310 1.1235569997 -1.4334277121
C 1.3834218683 0.1254735901 0.2466077960
C -1.1315275680 2.8489675652 0.1591689282
C -0.7390070313 -0.9566733511 -1.0480828452
C -2.1269613671 -0.4203890408 -1.3446247914
C -2.7946064181 -0.5259028183 -0.0157461517
C -2.0634442036 -1.3456988983 0.8122274383
C -0.8552758405 -1.6800617699 0.1567148315
H -0.0583069356 -1.2648770349 -1.8360569719
H -3.7592414905 -0.0891776472 0.2158143085
H -2.6152049115 -1.1263586255 -2.0369660612
H -2.1879943597 0.5621060850 -1.8142902208
H -2.3512048339 -1.6749508474 1.8033740521
H -0.0975127153 -2.3395571766 0.5652995865
C -2.5490215740 2.9434330224 0.7392847823
C -0.1755525978 3.7634744253 0.9523523815
C -1.1210665868 3.2420948066 -1.3201503714
O 2.3214820134 -0.1887127389 -0.6379923808
O 1.4326185211 -0.0357094785 1.4462776592
C 3.5473485889 -0.7538490745 -0.1018009364
H 4.1734014208 -0.9494413620 -0.9697726151
H 4.0208471478 -0.0355393074 0.5693329451
H 3.3255936344 -1.6746733952 0.4405423299

H -0.5109073787 4.8024133532 0.8788868222
H -0.1540291281 3.4942685204 2.0141519345
H 0.8445381058 3.7035022568 0.5600742298
H -2.8901981796 3.9822459504 0.7195147477
H -3.2574331940 2.3436994731 0.1600675621
H -2.5766314387 2.6048624061 1.7809735634
H -1.5113267103 4.2594155987 -1.4093181659
H -0.1114739687 3.2485991882 -1.7435765648
H -1.7603971842 2.5990035995 -1.9329783823

Equilibrium geometry of **r13-endo-3s-mc**.

C 0.5323470000 1.1622900000 0.2971610000
N -0.0749700000 1.9540340000 -0.5135540000
C -1.0500170000 3.0597950000 -0.2474370000
C 1.5688030000 0.2557610000 -0.3175110000
H 0.3915810000 1.2317340000 1.3676040000
H 0.1735980000 1.7970760000 -1.4987280000
C -3.0961430000 -0.9415470000 0.3276290000
C -2.3076160000 -0.9028600000 1.6074870000
C -0.9227080000 -1.3015690000 1.1705060000
C -0.9516410000 -1.5898070000 -0.1584280000
C -2.2940860000 -1.3494800000 -0.6828680000
H -4.1526100000 -0.7090940000 0.2622760000
H -0.0901940000 -1.4551560000 1.8469480000
H -2.7018540000 -1.6300470000 2.3343450000
H -2.3555920000 0.0687040000 2.1208250000
H -0.1310990000 -1.9806120000 -0.7507420000
H -2.5867350000 -1.5066770000 -1.7146490000
C -2.3545900000 2.6817100000 -0.9711120000
C -1.2641930000 3.2257050000 1.2559010000
C -0.4265540000 4.3236750000 -0.8671000000
O 2.2523520000 -0.3862450000 0.6119020000
O 1.7217340000 0.2158040000 -1.5187940000
C 3.3248380000 -1.2488540000 0.1403480000
H 3.7986850000 -1.6287670000 1.0426040000
H 2.9048960000 -2.0609500000 -0.4559930000
H 4.0250590000 -0.6677990000 -0.4615400000
H -1.1223660000 5.1580470000 -0.7437760000
H 0.5162490000 4.5873250000 -0.3783220000
H -0.2442980000 4.1983600000 -1.9398900000
H -3.0798370000 3.4896260000 -0.8388900000
H -2.1924140000 2.5522010000 -2.0467250000
H -2.7760430000 1.7563250000 -0.5693310000
H -1.9664430000 4.0471240000 1.4182700000
H -1.7000260000 2.3302970000 1.7109380000
H -0.3354620000 3.4813520000 1.7774620000

Equilibrium geometry of **r13-endo-3s-prod**.

C 0.0795810000 0.4172420000 0.6237580000
N -1.0080550000 1.0652300000 -0.2171530000
C -1.1852130000 2.6107480000 -0.1342650000
C 1.2853590000 0.1602810000 -0.2720030000
H 0.3482040000 1.0705330000 1.4535020000
H -0.6971350000 0.8881320000 -1.1859360000
C -2.2670480000 0.1525920000 0.0544070000
C -2.0043950000 -0.2779320000 1.5037280000
C -0.6215490000 -0.8794810000 1.1641410000
C -0.9824760000 -1.7443340000 -0.0362040000
C -1.9696950000 -1.1276980000 -0.6996380000
H -3.1729620000 0.6988020000 -0.1911400000
H -0.0556410000 -1.3486180000 1.9682460000
H -2.7204300000 -1.0339170000 1.8296410000
H -1.9754280000 0.5379130000 2.2293160000

H -0.4691040000 -2.6561450000 -0.3185080000
H -2.4318950000 -1.4135240000 -1.6368060000
C -2.1416580000 2.9972810000 -1.2719120000
C -1.7511470000 3.0247580000 1.2244940000
C 0.1891890000 3.2503410000 -0.3787760000
O 2.3289180000 -0.2273390000 0.4389070000
O 1.2336780000 0.2791620000 -1.4802910000
C 3.5382830000 -0.5477990000 -0.3023220000
H 4.2692400000 -0.8213200000 0.4555950000
H 3.3451530000 -1.3801360000 -0.9807520000
H 3.8661900000 0.3255980000 -0.8679770000
H 0.0623750000 4.3357730000 -0.4159550000
H 0.9010910000 3.0388350000 0.4251080000
H 0.6268650000 2.9321910000 -1.3295530000
H -2.1966020000 4.0876470000 -1.3304460000
H -1.7841380000 2.6360610000 -2.2429590000
H -3.1602440000 2.6319630000 -1.1137160000
H -1.8580180000 4.1133480000 1.2320590000
H -2.7414970000 2.6002010000 1.4106700000
H -1.0884790000 2.7632320000 2.0556610000

Equilibrium geometry of **r13-endo-3s-ts**.

C 0.1746111769 0.7215847011 0.4445289757
N -0.6352837453 1.4439471433 -0.3520756303
C -1.1241349871 2.8506811018 -0.1368412508
C 1.3796476474 0.1184178873 -0.2458951149
H 0.3450743579 1.1085766853 1.4430156486
H -0.5118422032 1.2136527389 -1.3386823362
C -2.7945897556 -0.5191440935 0.0063747913
C -2.1321239661 -0.4255946033 1.3386919985
C -0.7446266469 -0.9637010782 1.0433740332
C -0.8595685297 -1.6801581345 -0.1659969675
C -2.0637571679 -1.3372577817 -0.8238570919
H -3.7564068691 -0.0768825756 -0.2263539804
H -0.0673501039 -1.2787400006 1.8315498266
H -2.6250635114 -1.1356229675 2.0235055580
H -2.1919060270 0.5533704641 1.8154896780
H -0.1026788329 -2.3399544690 -0.5757225841
H -2.3489441052 -1.6590966905 -1.8181740250
C -2.5335184266 2.9590341271 -0.7336768550
C -1.1298054706 3.2281928286 1.3466138459
C -0.1534579915 3.7685204748 -0.9080914495
O 2.3139810108 -0.2166578599 0.6350321610
O 1.4286387598 -0.0271115155 -1.4476298035
C 3.5336299142 -0.7886341561 0.0918865897
H 4.1569284511 -1.0032665269 0.9573503555
H 3.3014922138 -1.6995120667 -0.4629459210
H 4.0156184850 -0.0670637080 -0.5696767296
H -0.4853636853 4.8081837313 -0.8291728373
H 0.8608821025 3.7004782986 -0.5025119500
H -0.1184431230 3.5093949457 -1.9719907411
H -2.8702591917 3.9990860842 -0.7055465595
H -2.5490442967 2.6338330821 -1.7799615987
H -3.2523762841 2.3552014140 -0.1717889197
H -1.5159450051 4.2465990440 1.4414900263
H -1.7799903768 2.5821438047 1.9446749132
H -0.1253675916 3.2253103037 1.7821193419

Equilibrium geometry of **r13-exo-3r-mc**.

C 0.3815400000 1.1096570000 -0.3869520000
N -0.2435330000 1.8079620000 0.4958090000
H 0.0635580000 1.6213010000 1.4582670000
H 0.1948530000 1.2350960000 -1.4445800000

C 1.5171890000 0.2645870000 0.1321830000
 C -1.2595440000 2.8996310000 0.3307800000
 C -2.6194730000 -1.2316020000 0.6871020000
 C -1.2291680000 -1.8011780000 0.7248970000
 C -0.7299150000 -1.5748520000 -0.6757190000
 C -1.7278400000 -1.0132970000 -1.4130440000
 C -2.8950520000 -0.7932260000 -0.5650020000
 H -3.2899310000 -1.2211570000 1.5384480000
 H 0.2142530000 -1.9427810000 -1.0580490000
 H -1.2536150000 -2.8778460000 0.9548630000
 H -0.5937620000 -1.3546800000 1.5031330000
 H -1.6920720000 -0.8030920000 -2.4773740000
 H -3.8339810000 -0.3720920000 -0.9066100000
 C -2.4020470000 2.5941770000 1.3116590000
 C -0.5368350000 4.2018880000 0.7254290000
 C -1.7527790000 2.9507830000 -1.1143550000
 O 2.2777320000 -0.1714710000 -0.8549180000
 O 1.6795380000 0.1072660000 1.3238640000
 C 3.4544360000 -0.9354380000 -0.4692340000
 H 3.9697070000 -1.1500370000 -1.4026180000
 H 4.0765780000 -0.3389360000 0.1996950000
 H 3.1446760000 -1.8547060000 0.0313130000
 H -1.2482550000 5.0309320000 0.6722470000
 H -0.1533930000 4.1561030000 1.7501370000
 H 0.2950270000 4.4187450000 0.0482820000
 H -3.1348220000 3.4046940000 1.2695830000
 H -2.8991090000 1.6549710000 1.0572810000
 H -2.0372120000 2.5326960000 2.3433490000
 H -2.5106330000 3.7345540000 -1.1942410000
 H -0.9521880000 3.2048870000 -1.8172680000
 H -2.2175720000 2.0074430000 -1.4163080000

Equilibrium geometry of **r13-exo-3r-prod.**

C 0.0153200000 0.2888350000 -0.5166690000
 N -0.9361120000 0.9026530000 0.4975740000
 H -0.3844130000 0.8742710000 1.3723770000
 H 0.0568640000 0.8875850000 -1.4237010000
 C 1.3930740000 0.2034660000 0.1376810000
 C -1.3235970000 2.4015740000 0.3403920000
 C -2.0553390000 -0.1932070000 0.6699180000
 C -1.1544530000 -1.4373300000 0.6543560000
 C -0.6169230000 -1.1301050000 -0.7655030000
 C -1.9211280000 -0.8950560000 -1.5093100000
 C -2.7813030000 -0.3311270000 -0.6511230000
 H -2.6282790000 0.0322110000 1.5654310000
 H 0.0899780000 -1.8284840000 -1.2125040000
 H -1.7419690000 -2.3553470000 0.6862520000
 H -0.3944010000 -1.4584380000 1.4419210000
 H -2.0744110000 -1.0976520000 -2.5630570000
 H -3.7915440000 0.0085810000 -0.8406500000
 C -2.2645980000 2.7357200000 1.5050440000
 C -0.0170120000 3.2010490000 0.4740200000
 C -1.9945830000 2.6937420000 -1.0030950000
 O 2.3218110000 -0.1069430000 -0.7459730000
 O 1.5566340000 0.3734480000 1.3318010000
 C 3.6759870000 -0.2707690000 -0.2395720000
 H 4.2873410000 -0.4470020000 -1.1219220000
 H 3.9868080000 0.6354140000 0.2818970000
 H 3.7127750000 -1.1238570000 0.4399080000
 H -0.2569210000 4.2675670000 0.4609010000
 H 0.5013930000 2.9856190000 1.4132370000
 H 0.6711010000 3.0157200000 -0.3571500000
 H -2.4580270000 3.8117620000 1.5037910000
 H -3.2313710000 2.2321690000 1.4163020000
 H -1.8201570000 2.4858070000 2.4754460000

H -2.1566200000 3.7740820000 -1.0629170000
 H -1.3746190000 2.4137120000 -1.8595180000
 H -2.9668190000 2.2098350000 -1.1058860000

Equilibrium geometry of **r13-exo-3r-ts.**

C 0.1275442699 0.6476886243 -0.3933020479
 N -0.6131935722 1.3244041070 0.5115250481
 H -0.2767137764 1.1863886655 1.4646972440
 H 0.1559932914 1.0378279889 -1.4034264678
 C 1.4617555915 0.1664152217 0.1547834173
 C -1.2941752423 2.6492659791 0.3154133016
 C -2.4655326526 -0.8871000518 0.7247544856
 C -1.1069130460 -1.4930981384 0.6996346810
 C -0.6393974532 -1.1509351132 -0.7066401406
 C -1.8066761942 -0.8489091833 -1.4404887005
 C -2.8863412263 -0.6195038590 -0.5610137537
 H -3.0621268417 -0.7711755387 1.6230100733
 H 0.1975464633 -1.6590193969 -1.1764118240
 H -1.2155543289 -2.5887826148 0.7595511090
 H -0.4464138126 -1.2052592297 1.5205852222
 H -1.8484483378 -0.7403790203 -2.5196541329
 H -3.8717998453 -0.2739857433 -0.8495217601
 C -2.4255831248 2.7317921967 1.3483291893
 C -0.2444199484 3.7437679145 0.5909342914
 C -1.8481223716 2.7880197882 -1.1052726755
 O 2.3078962701 -0.1291298930 -0.8210615568
 O 1.6701011317 0.0793687760 1.3459753970
 C 3.6290411655 -0.5753405426 -0.4111047679
 H 4.1810067599 -0.7147504425 -1.3382370798
 H 4.0973033314 0.1853055911 0.2151921444
 H 3.5479080100 -1.5124601556 0.1427242837
 H -0.7099734089 4.7317806535 0.5182166280
 H 0.1795707731 3.6472033444 1.5964645752
 H 0.5741884429 3.7001451251 -0.1354553061
 H -2.8818326384 3.7252098677 1.3238230151
 H -3.2043227966 1.9920147974 1.1423647216
 H -2.0488507682 2.5677322368 2.3645815545
 H -2.3694367069 3.7461077390 -1.1839348224
 H -1.0605564226 2.7943529116 -1.8661353501
 H -2.5683970340 2.0008662441 -1.3422161508

Equilibrium geometry of **r13-exo-3s-mc.**

C 0.3802710000 1.1081100000 0.3856680000
 N -0.2480460000 1.8035430000 -0.4972170000
 C -1.2629490000 2.8962120000 -0.3318570000
 C 1.5169990000 0.2650270000 -0.1341030000
 H 0.1959920000 1.2357240000 1.4434620000
 H 0.0575330000 1.6157050000 -1.4599530000
 C -0.7274710000 -1.5731040000 0.6790960000
 C -1.2263680000 -1.7986100000 -0.7217200000
 C -2.6157960000 -1.2270820000 -0.6845010000
 C -2.8917850000 -0.7893770000 0.5678020000
 C -1.7253810000 -1.0111800000 1.4163570000
 H 0.2162260000 -1.9419520000 1.0616350000
 H -3.2856790000 -1.2153310000 -1.5362850000
 H -1.2526590000 -2.8752860000 -0.9513580000
 H -0.5898830000 -1.3537820000 -1.4999960000
 H -3.8304620000 -0.3674690000 0.9090680000
 H -1.6897820000 -0.8013470000 2.4807790000
 C -2.4039370000 2.5946430000 -1.3156550000
 C -1.7592400000 2.9450980000 1.1123510000
 C -0.5374320000 4.1983890000 -0.7221030000
 O 2.2817340000 -0.1652320000 0.8523010000

O 1.6770490000 0.1048600000 -1.3257440000
C 3.4615220000 -0.9238990000 0.4656070000
H 3.9842640000 -1.1271940000 1.3974520000
H 3.1554590000 -1.8495350000 -0.0254380000
H 4.0750050000 -0.3284130000 -0.2121800000
H -1.2480930000 5.0281540000 -0.6701460000
H 0.2924610000 4.4131400000 -0.0417490000
H -0.1505110000 4.1540050000 -1.7455740000
H -3.1361330000 3.4057060000 -1.2728630000
H -2.0373400000 2.5354400000 -2.3468690000
H -2.9024270000 1.6553090000 -1.0644710000
H -2.5165680000 3.7293470000 1.1921450000
H -2.2252630000 2.0015400000 1.4115970000
H -0.9600970000 3.1972150000 1.8173810000

Equilibrium geometry of **r13-exo-3s-prod.**

C 0.0164590000 0.2906910000 0.5165330000
N -0.9363950000 0.9026440000 -0.4974850000
C -1.3256510000 2.4012740000 -0.3412110000
C 1.3938310000 0.2061550000 -0.1388410000
H 0.0581060000 0.8902880000 1.4229790000
H -0.3852320000 0.8743970000 -1.3726540000
C -0.6140630000 -1.1286840000 0.7670630000
C -1.1520180000 -1.4377380000 -0.6522400000
C -2.0543610000 -0.1946210000 -0.6683260000
C -2.7794610000 -0.3323200000 0.6531840000
C -1.9181570000 -0.8945490000 1.5113580000
H 0.0938530000 -1.8258720000 1.2142200000
H -2.6280210000 0.0293730000 -1.5637060000
H -1.7385100000 -2.3565060000 -0.6830170000
H -0.3923490000 -1.4586300000 -1.4402310000
H -3.7899600000 0.0064460000 0.8431150000
H -2.0706070000 -1.0963650000 2.5653770000
C -2.2678900000 2.7332090000 -1.5054620000
C -1.9959560000 2.6937550000 1.0025150000
C -0.0201430000 3.2022150000 -0.4763400000
O 2.3234560000 -0.1033650000 0.7441720000
O 1.5563550000 0.3759330000 -1.3331140000
C 3.6773530000 -0.2663730000 0.2369680000
H 4.2893800000 -0.4417310000 1.1190660000
H 3.7143410000 -1.1197540000 -0.4421680000
H 3.9871210000 0.6398590000 -0.2850250000
H -0.2613280000 4.2685430000 -0.4646270000
H 0.6683080000 3.0187400000 0.3549830000
H 0.4983890000 2.9862050000 -1.4154570000
H -2.4628630000 3.8090490000 -1.5048910000
H -1.8237050000 2.4832100000 -2.4759570000
H -3.2338790000 2.2284430000 -1.4157700000
H -2.1597780000 3.7738900000 1.0613670000
H -2.9670850000 2.2082520000 1.1067850000
H -1.3747120000 2.4157760000 1.8586640000

Equilibrium geometry of **r13-exo-3s-ts.**

C 0.1290111187 0.6506480308 0.3928523915
N -0.6133554823 1.3255601157 -0.5119363130
C -1.2968342657 2.6490722130 -0.3163269318
C 1.4627449281 0.1695709075 -0.1564468242
H 0.1582865746 1.0419801520 1.4025142869
H -0.2779467430 1.1866703112 -1.4653675840
C -0.6362057861 -1.1479505779 0.7098981482
C -1.1029846443 -1.4936001654 -0.6958247562
C -2.4627876436 -0.8902245408 -0.7221330702
C -2.8842398713 -0.6211292897 0.5630877382

C -1.8041589537 -0.8468482796 1.4430675108
H 0.2014194246 -1.6538653953 1.1807675813
H -3.0593653974 -0.7768448881 -1.6207096948
H -1.2094365432 -2.5896889939 -0.7536972215
H -0.4430803907 -1.2058946693 -1.5173874285
H -3.8704674587 -0.2770523728 0.8509018613
H -1.8463823760 -0.7365427997 2.5220510548
C -2.4272082790 2.7296670466 -1.3505723222
C -1.8528316733 2.7865861721 1.1037001615
C -0.2490506379 3.7456655478 -0.5903153220
O 2.3100268460 -0.1261835460 0.8183899255
O 1.6696632442 0.0823860735 -1.3478377007
C 3.6302137234 -0.5736714565 0.4067571482
H 4.1833051493 -0.7136545023 1.3331439277
H 3.5473866131 -1.5107032376 -0.1469052004
H 4.0984063840 0.1864404532 -0.2201873185
H -0.7169015608 4.7324189284 -0.5179410702
H 0.5687455807 3.7038208165 0.1370381403
H 0.1762429213 3.6501436143 -1.5952776185
H -2.8861684941 3.7218567872 -1.3255912653
H -2.0488385953 2.5676680548 -2.3665894134
H -3.2041753965 1.9875435855 -1.1462518930
H -2.3746783320 3.7443991273 1.1821983812
H -2.5731321388 1.9989887475 1.3390927720
H -1.0663764154 2.7928179842 1.8657508381

Equilibrium geometry of **r14-endo-3r-mc.**

C 0.5440810000 1.2025810000 -0.2713360000
N -0.0766400000 1.9749200000 0.5470090000
H 0.1760310000 1.8128160000 1.5304530000
H 0.3979580000 1.2783480000 -1.3406640000
C 1.6002510000 0.3075860000 0.3308670000
C -1.0813490000 3.0556560000 0.2902680000
C -0.8714650000 -1.2924770000 -1.1750850000
C -2.2508900000 -0.9261520000 -1.6557970000
C -3.0766550000 -0.9740140000 -0.3996580000
C -2.2958020000 -1.3562430000 0.6369780000
C -0.9323370000 -1.5694830000 0.1544300000
H -0.0154210000 -1.4286210000 -1.8252320000
H -4.1393410000 -0.7645450000 -0.3674950000
H -2.6086160000 -1.6636020000 -2.3910670000
H -2.3026070000 0.0427780000 -2.1743160000
H -2.6148090000 -1.5122240000 1.6611840000
H -0.1201020000 -1.9332750000 0.7748140000
C -2.3792860000 2.6284470000 0.9991080000
C -0.5023600000 4.3295150000 0.9308750000
C -1.2913210000 3.2350660000 -1.2124370000
O 2.3015870000 -0.2932560000 -0.6086820000
O 1.7435420000 0.2493170000 1.5334420000
C 3.4206540000 -1.1434780000 -0.1683030000
C 4.1832780000 -1.5569950000 -1.4059400000
H 4.0227900000 -0.5585100000 0.5308370000
H 2.9897990000 -1.9917940000 0.3704380000
H 5.0188640000 -2.2003010000 -1.1141620000
H 3.5449080000 -2.1171290000 -2.0950910000
H 4.5884130000 -0.6855070000 -1.9278460000
H -1.2237770000 5.1426650000 0.8129680000
H -0.3246540000 4.1957590000 2.0034040000
H 0.4351290000 4.6305920000 0.4534630000
H -2.0203760000 4.0342730000 -1.3682620000
H -0.3684590000 3.5298850000 -1.7236530000
H -1.6934700000 2.3319670000 -1.6830450000
H -3.1275140000 3.4159770000 0.8718380000
H -2.7695310000 1.6965430000 0.5813730000
H -2.2210210000 2.4894710000 2.0741380000

Equilibrium geometry of **r14-endo-3r-prod.**

C 0.0426380000 0.4014000000 -0.6686720000
N -1.0064390000 1.0542350000 0.2161940000
H -0.6601960000 0.8621790000 1.1705250000
H 0.2925470000 1.0588850000 -1.5011190000
C 1.2759750000 0.1200080000 0.1838100000
C -1.1709410000 2.6021930000 0.1584510000
C -0.6928420000 -0.8804050000 -1.1972080000
C -2.0785180000 -0.2577480000 -1.4825540000
C -2.2854550000 0.1603870000 -0.0203120000
C -1.9795930000 -1.1314640000 0.7095030000
C -1.0239580000 -1.7533540000 0.0057810000
H -0.1600130000 -1.3475120000 -2.0246260000
H -3.1755480000 0.7154640000 0.2608790000
H -2.8159880000 -0.9999160000 -1.7921470000
H -2.0633460000 0.5665140000 -2.1989650000
H -2.4125110000 -1.4218990000 1.6591370000
H -0.5130410000 -2.6743510000 0.2615070000
C -2.0502310000 2.9844380000 1.3580890000
C 0.2212010000 3.2278340000 0.3229370000
C -1.8169760000 3.0339870000 -1.1586240000
O 2.2861800000 -0.2801740000 -0.5625780000
O 1.2628890000 0.2373200000 1.3945840000
C 3.5362750000 -0.6252600000 0.1310280000
C 4.5486040000 -1.0017270000 -0.9275240000
H 3.8401950000 0.2453880000 0.7169450000
H 3.3167840000 -1.4461580000 0.8180880000
H 5.4937630000 -1.2640830000 -0.4424400000
H 4.2110850000 -1.8646480000 -1.5085320000
H 4.7342610000 -0.1678160000 -1.6102760000
H 0.1059700000 4.3133390000 0.3876720000
H 0.7175130000 2.8892120000 1.2369380000
H 0.8756860000 3.0255950000 -0.5303390000
H -1.9084730000 4.1240060000 -1.1529110000
H -1.2118310000 2.7693920000 -2.0315560000
H -2.8227220000 2.6240730000 -1.2840170000
H -2.1195220000 4.0742140000 1.4118730000
H -3.0708860000 2.6002410000 1.2777960000
H -1.6162470000 2.6380000000 2.3030650000

Equilibrium geometry of **r14-endo-3r-ts.**

C 0.1656142532 0.7072359447 -0.4466461429
N -0.6348624104 1.4309461544 0.3586263726
H -0.5070226321 1.1934972878 1.3430545018
H 0.3308647968 1.0990213587 -1.4441651449
C 1.3753166134 0.0952777282 0.2317429046
C -1.1164905415 2.8409542608 0.1532736801
C -0.7630527884 -0.9681543835 -1.0423461444
C -2.1481886848 -0.4233773550 -1.3379969015
C -2.8123696578 -0.5169177720 -0.0065652666
C -2.0859536983 -1.3397201561 0.8226928858
C -0.8824153300 -1.6865791739 0.1656088403
H -0.0877015905 -1.2866846555 -1.8307942032
H -3.7722338344 -0.0704546235 0.2262204890
H -2.6437919197 -1.1292972194 -2.0250257287
H -2.2030391850 0.5572250253 -1.8123054250
H -2.3735778804 -1.6619752128 1.8161790087
H -0.1286455594 -2.3497943368 0.5753932151
C -2.5286048206 2.9515738756 0.7435890901
C -0.1456147791 3.7484306196 0.9364657842
C -1.1134102562 3.2304281905 -1.3271219057
O 2.3053894376 -0.2236526760 -0.6556828874
O 1.4224556273 -0.0662831285 1.4324389073
C 3.5448670415 -0.8127551870 -0.1333915087

C 4.4387239606 -1.1102667580 -1.3160549598
H 3.9862205793 -0.0925164463 0.5598635588
H 3.2746532761 -1.7092576948 0.4309471839
H 5.3702388377 -1.5594476899 -0.9581407462
H 3.9631270936 -1.8142114416 -2.0052224064
H 4.6887252915 -0.1970239990 -1.8634866865
H -0.4723113701 4.7902519974 0.8642561190
H -0.1171202047 3.4806576698 1.9984679444
H 0.8705111040 3.6787906451 0.5356500623
H -1.4949831103 4.2511012728 -1.4159852498
H -0.1068566739 3.2264322961 -1.7575320268
H -1.7629184598 2.5915316440 -1.9335346333
H -2.8593861552 3.9937564521 0.7241303877
H -3.2471991453 2.3572884225 0.1711959242
H -2.5518145085 2.6154531480 1.7862561379

Equilibrium geometry of **r14-endo-3s-mc.**

C 0.5473840000 1.2036070000 0.2803000000
N -0.0713820000 1.9815530000 -0.5342330000
C -1.0769630000 3.0603200000 -0.2725690000
C 1.6049550000 0.3126210000 -0.3254270000
H 0.3985530000 1.2719690000 1.3496850000
H 0.1839080000 1.8264290000 -1.5182160000
C -3.0739120000 -0.9735090000 0.3927140000
C -2.2485930000 -0.9350970000 1.6494500000
C -0.8690400000 -1.2978350000 1.1665050000
C -0.9293270000 -1.5645610000 -0.1651480000
C -2.2927060000 -1.3478120000 -0.6465180000
H -4.1366530000 -0.7639230000 0.3618260000
H -0.0131070000 -1.4385260000 1.8159820000
H -2.6065800000 -1.6778850000 2.3791600000
H -2.3002620000 0.0299730000 2.1750410000
H -0.1167630000 -1.9234360000 -0.7881150000
H -2.6114230000 -1.4959360000 -1.6719530000
C -2.3736230000 2.6368950000 -0.9859870000
C -1.2895240000 3.2306290000 1.2308410000
C -0.4974100000 4.3382000000 -0.9045680000
O 2.3025030000 -0.2964350000 0.6116310000
O 1.7522040000 0.2637190000 -1.5279730000
C 3.4214240000 -1.1452690000 0.1683320000
C 4.1759200000 -1.5739630000 1.4058980000
H 2.9910090000 -1.9867140000 -0.3816030000
H 4.0291130000 -0.5548720000 -0.5213510000
H 5.0108750000 -2.2172340000 1.1121090000
H 4.5812770000 -0.7091530000 1.9388000000
H 3.5318420000 -2.1387760000 2.0859390000
H -1.2192120000 5.1504290000 -0.7826950000
H 0.4393710000 4.6365650000 -0.4240400000
H -0.3181720000 4.2109980000 -1.9776530000
H -2.0183500000 4.0292020000 1.3902550000
H -1.6929840000 2.3249500000 1.6951700000
H -0.3673890000 3.5218140000 1.7455350000
H -3.1220840000 3.4238280000 -0.8559660000
H -2.2133850000 2.5036350000 -2.0614900000
H -2.7645590000 1.7027700000 -0.5738340000

Equilibrium geometry of **r14-endo-3s-prod.**

C 0.0445420000 0.3992490000 0.6720300000
N -1.0024430000 1.0586530000 -0.2104140000
C -1.1656240000 2.6064730000 -0.1428980000
C 1.2787180000 0.1210810000 -0.1802670000
H 0.2943200000 1.0518050000 1.5083930000
H -0.6549350000 0.8723670000 -1.1654190000

C -2.2825930000 0.1645550000 0.0188480000
C -2.0785670000 -0.2623240000 1.4790100000
C -0.6930250000 -0.8845600000 1.1924000000
C -1.0230690000 -1.7504600000 -0.0160480000
C -1.9767480000 -1.1234260000 -0.7178580000
H -3.1717950000 0.7218770000 -0.2607120000
H -0.1618110000 -1.3566570000 2.0180060000
H -2.8172070000 -1.0057460000 1.7827490000
H -2.0641230000 0.5573760000 2.2006950000
H -0.5127280000 -2.6705560000 -0.2760730000
H -2.4084020000 -1.4078070000 -1.6699050000
C -2.0431590000 2.9972510000 -1.3410050000
C -1.8127150000 3.0301440000 1.1762000000
C 0.2273140000 3.2318350000 -0.3016140000
O 2.2867510000 -0.2861560000 0.5652730000
O 1.2680990000 0.2467520000 -1.3902170000
C 3.5375830000 -0.6290290000 -0.1280580000
C 4.5494740000 -1.0065020000 0.9305950000
H 3.3191010000 -1.4490820000 -0.8164790000
H 3.8412460000 0.2426830000 -0.7124660000
H 5.4950090000 -1.2679840000 0.4457110000
H 4.7345080000 -0.1733540000 1.6144650000
H 4.2119180000 -1.8702130000 1.5104140000
H 0.1132320000 4.3179340000 -0.3581910000
H 0.8808220000 3.0224320000 0.5507300000
H 0.7240690000 2.8994750000 -1.2177500000
H -1.9029110000 4.1202670000 1.1776590000
H -2.8191870000 2.6206010000 1.2976210000
H -1.2089910000 2.7587990000 2.0479960000
H -2.1124330000 4.0874300000 -1.3871380000
H -1.6077820000 2.6576170000 -2.2878520000
H -3.0638640000 2.6124780000 -1.2650640000

Equilibrium geometry of **r14-endo-3s-ts**.

C 0.1681333368 0.7089926180 0.4536440304
N -0.6319694754 1.4367340563 -0.3489749706
C -1.1143865089 2.8455048206 -0.1368805137
C 1.3790714158 0.1020161903 -0.2271049959
H 0.3325264307 1.0961076250 1.4531769464
H -0.5010823004 1.2053801440 -1.3344281999
C -2.8048454609 -0.5146855900 -0.0022402543
C -2.1460081800 -0.4271605611 1.3321202244
C -0.7588976081 -0.9678611934 1.0385445904
C -0.8737586156 -1.6818465776 -0.1728344969
C -2.0749316946 -1.3333445224 -0.8325827604
H -3.7639463821 -0.0677041608 -0.2366746096
H -0.0861016634 -1.2897059097 1.8277331600
H -2.6428182062 -1.1377776486 2.0132409166
H -2.2043121531 0.5507601022 1.8113768914
H -0.1178551999 -2.3424084108 -0.5827976226
H -2.3586198778 -1.6512033652 -1.8285613338
C -2.5276159440 2.9574306546 -0.7245486472
C -1.1088494251 3.2286212016 1.3452426148
C -0.1454594732 3.7573749031 -0.9175296442
O 2.3049269398 -0.2302694928 0.6598540517
O 1.4299276278 -0.0464711236 -1.4293494346
C 3.5434241311 -0.8193949076 0.1353456764
C 4.4311511790 -1.1352135627 1.3178480733
H 3.2711390285 -1.7080226418 -0.4403673741
H 3.9906416271 -0.0934084562 -0.5480815757
H 5.3622282863 -1.5841325179 0.9584959869
H 4.6826713129 -0.2298800228 1.8775068758
H 3.9496340395 -1.8454456186 1.9964091453
H -0.4735032051 4.7984610513 -0.8416861153
H 0.8711796658 3.6880114779 -0.5175783559

H -0.1171192620 3.4933449546 -1.9803839172
H -1.4948258846 4.2470897700 1.4397228833
H -1.7530036141 2.5839406470 1.9513342300
H -0.1007393430 3.2275756632 1.7721427684
H -2.8596392134 3.9991215560 -0.6997805571
H -2.5521283240 2.6261183609 -1.7687237501
H -3.2445983135 2.3597738128 -0.1535611973

Equilibrium geometry of **r14-exo-3r-mc**.

C 0.3932640000 1.1483040000 -0.3845620000
N -0.2386360000 1.8369240000 0.5000510000
H 0.0726850000 1.6478350000 1.4611110000
H 0.2027850000 1.2718950000 -1.4418840000
C 1.5370120000 0.3116630000 0.1359480000
C -1.2750150000 2.9092550000 0.3433220000
C -2.6027550000 -1.2736040000 0.6605720000
C -1.2003560000 -1.8123370000 0.7066720000
C -0.6939540000 -1.5648360000 -0.6879020000
C -1.6955840000 -1.0162980000 -1.4288450000
C -2.8756310000 -0.8288980000 -0.5895210000
H -3.2813330000 -1.2860750000 1.5053830000
H 0.2631400000 -1.9059850000 -1.0628750000
H -1.2015140000 -2.8903140000 0.9312940000
H -0.5814410000 -1.3544530000 1.4916950000
H -1.6544660000 -0.7941730000 -2.4905670000
H -3.8198300000 -0.4242960000 -0.9364430000
C -2.4165430000 2.5656610000 1.3127950000
C -0.5824460000 4.2208860000 0.7607990000
C -1.7600330000 2.9700040000 -1.1041180000
O 2.3089100000 -0.1089970000 -0.8451270000
O 1.6865010000 0.1528010000 1.3302780000
C 3.5094050000 -0.8686320000 -0.4564690000
C 4.3101510000 -1.1315410000 -1.7110130000
H 4.0519900000 -0.2694650000 0.2787490000
H 3.1672630000 -1.7858170000 0.0305520000
H 5.2018700000 -1.7081230000 -1.4466230000
H 3.7329020000 -1.7102790000 -2.4376840000
H 4.6336990000 -0.1976340000 -2.1788980000
H -1.3135490000 5.0336180000 0.7245320000
H -0.1962080000 4.1653220000 1.7840140000
H 0.2425350000 4.4692140000 0.0862990000
H -3.1671560000 3.3601390000 1.2775820000
H -2.8919370000 1.6190430000 1.0436680000
H -2.0563540000 2.4982050000 2.3457370000
H -2.5303250000 3.7418400000 -1.1797300000
H -0.9589330000 3.2454510000 -1.7982350000
H -2.2067580000 2.0226100000 -1.4207310000

Equilibrium geometry of **r14-exo-3r-prod**.

C -0.0006540000 0.2724540000 -0.5373250000
N -0.9289980000 0.8977470000 0.4913330000
H -0.3600400000 0.8655400000 1.3554870000
H 0.0330870000 0.8691290000 -1.4460640000
C 1.3874260000 0.1723940000 0.0959460000
C -1.3057450000 2.3992660000 0.3384680000
C -2.0548370000 -0.1864610000 0.6862430000
C -1.1664550000 -1.4393970000 0.6573190000
C -0.6515360000 -1.1399310000 -0.7725400000
C -1.9664860000 -0.8942870000 -1.4932910000
C -2.8057220000 -0.3202900000 -0.6212170000
H -2.6098200000 0.0455550000 1.5913820000
H 0.0410080000 -1.8457700000 -1.2300470000
H -1.7620740000 -2.3516590000 0.7021670000

H -0.3924560000 -1.4658100000 1.4310290000
H -2.1407930000 -1.0972270000 -2.5437000000
H -3.8157760000 0.0291950000 -0.7937670000
C -2.2299710000 2.7422610000 1.5140420000
C 0.0089350000 3.1880500000 0.4555820000
C -1.9904630000 2.6973370000 -0.9967600000
O 2.2962450000 -0.1625960000 -0.7955930000
O 1.5664340000 0.3537450000 1.2875520000
C 3.6729430000 -0.3508580000 -0.3090740000
C 4.5379130000 -0.6663210000 -1.5077440000
H 3.9699400000 0.5692170000 0.1997800000
H 3.6522360000 -1.1599210000 0.4254160000
H 5.5703340000 -0.8107190000 -1.1746860000
H 4.2087930000 -1.5826720000 -2.0061390000
H 4.5239480000 0.1530610000 -2.2320110000
H -0.2223270000 4.2565770000 0.4460540000
H 0.5382310000 2.9672610000 1.3874490000
H 0.6845020000 2.9970210000 -0.3845820000
H -2.4114360000 3.8204110000 1.5162600000
H -3.2030190000 2.2492750000 1.4353000000
H -1.7775810000 2.4862280000 2.4791390000
H -2.1471980000 3.7787050000 -1.0531530000
H -1.3814000000 2.4155200000 -1.8603630000
H -2.9663510000 2.2188700000 -1.0897380000

Equilibrium geometry of **r14-exo-3r-ts**.

C 0.1284736467 0.6393566639 -0.3968782559
N -0.6096316285 1.3195812242 0.5079857347
H -0.2703001736 1.1812888006 1.4602813520
H 0.1587705829 1.0296760006 -1.4069573386
C 1.4627892954 0.1538484846 0.1528620796
C -1.2864351175 2.6459151508 0.3114485910
C -2.4655773045 -0.8856840232 0.7281536475
C -1.1087138898 -1.4949644064 0.6977475976
C -0.6450632568 -1.1513479744 -0.7096082328
C -1.8145616555 -0.8475273846 -1.4392164263
C -2.8905771736 -0.6168751963 -0.5559038367
H -3.0583917927 -0.7686304606 1.6286575122
H 0.1890725185 -1.6608329958 -1.1825999695
H -1.2198270338 -2.5904781265 0.7564235609
H -0.4446354558 -1.2093594482 1.5164547477
H -1.8600858184 -0.7376454851 -2.5180521785
H -3.8762603140 -0.2690306597 -0.8405453690
C -2.4157496259 2.7338918358 1.3464706365
C -0.2334037616 3.7381137496 0.5830104241
C -1.8432761972 2.7844640391 -1.1082862770
O 2.3074098860 -0.1463492552 -0.8192631612
O 1.6634027002 0.0702115028 1.3465966576
C 3.6440614856 -0.6044483309 -0.4142530337
C 4.4556592062 -0.8004219565 -1.6751041909
H 4.0671687321 0.1545611095 0.2477422230
H 3.5181730620 -1.5281020563 0.1566442143
H 5.4607613985 -1.1395879355 -1.4061250637
H 4.0036324979 -1.5547396087 -2.3255668117
H 4.5483701976 0.1357521746 -2.2324586247
H -0.6965453415 4.7270093939 0.5093817697
H 0.1921646013 3.6419794213 1.5877583173
H 0.5838779595 3.6911388122 -0.1447223724
H -2.8696386444 3.7283223389 1.3206839749
H -3.1965833534 1.9955438354 1.1436655374
H -2.0374503274 2.5710424456 2.3622944514
H -2.3604180535 3.7447921187 -1.1876465092
H -1.0573739797 2.7855621062 -1.8710257665
H -2.5676044875 2.0000194138 -1.3420700948

Equilibrium geometry of **r14-exo-3s-mc**.

C 0.3922160000 1.1476300000 0.3846550000
N -0.2399680000 1.8359260000 -0.5000170000
C -1.2763150000 2.9083020000 -0.3433170000
C 1.5362940000 0.3114500000 -0.1357670000
H 0.2019370000 1.2715010000 1.4419710000
H 0.0712740000 1.6467320000 -1.4611000000
C -0.6941500000 -1.5654340000 0.6881340000
C -1.2005890000 -1.8128460000 -0.7064560000
C -2.6030260000 -1.2741390000 -0.6603160000
C -2.8758990000 -0.8296010000 0.5898270000
C -1.6958470000 -1.0170370000 1.4291270000
H 0.2628680000 -1.9064720000 1.0629940000
H -3.2815820000 -1.2864630000 -1.5051430000
H -1.2017550000 -2.8907720000 -0.9310680000
H -0.5816770000 -1.3549780000 -1.4914520000
H -3.8201350000 -0.4249400000 0.9367680000
H -1.6547090000 -0.7949840000 2.4909660000
C -2.4177190000 2.5647740000 -1.3129260000
C -1.7614040000 2.9690250000 1.1041000000
C -0.5836870000 4.2199220000 -0.7606630000
O 2.3087600000 -0.1081720000 0.8453160000
O 1.6855420000 0.1520880000 -1.3300490000
C 3.5104140000 -0.8660760000 0.4566550000
C 4.3136610000 -1.1243650000 1.7104860000
H 3.1695720000 -1.7851350000 -0.0277250000
H 4.0506510000 -0.2674520000 -0.2807600000
H 5.2065450000 -1.6991180000 1.4458120000
H 4.6356130000 -0.1887350000 2.1760920000
H 3.7390120000 -1.7031860000 2.4391390000
H -1.3147790000 5.0326660000 -0.7245080000
H 0.2411390000 4.4682340000 -0.0860520000
H -0.1973850000 4.1643380000 -1.7838330000
H -3.1684250000 3.3592660000 -1.2778810000
H -2.0573370000 2.4973310000 -2.3458210000
H -2.8931220000 1.6182210000 -1.0438640000
H -2.5317190000 3.7408860000 1.1796660000
H -2.2081160000 2.0216190000 1.4207020000
H -0.9603570000 3.2445330000 1.7982380000

Equilibrium geometry of **r14-exo-3s-prod**.

C -0.0005750000 0.2732240000 0.5374040000
N -0.9294500000 0.8975350000 -0.4913720000
C -1.3077360000 2.3987180000 -0.3387130000
C 1.3875150000 0.1736580000 -0.0959190000
H 0.0329120000 0.8702770000 1.4459050000
H -0.3604860000 0.8657250000 -1.3555300000
C -0.6504320000 -1.1395270000 0.7731980000
C -1.1649860000 -1.4399400000 -0.6565970000
C -2.0543560000 -0.1877320000 -0.6860700000
C -2.8052700000 -0.3216680000 0.6213560000
C -1.9656400000 -0.8946620000 1.4937280000
H 0.0426310000 -1.8446280000 1.2310430000
H -2.6093970000 0.0435320000 -1.5913590000
H -1.7598750000 -2.3526620000 -0.7011550000
H -0.3909190000 -1.4660490000 -1.4302300000
H -3.8155830000 0.0270190000 0.7936620000
H -2.1398890000 -1.0973670000 2.5441920000
C -2.2338250000 2.7401690000 -1.5132660000
C -1.9911400000 2.6966550000 0.9972300000
C 0.0059280000 3.1888940000 -0.4578060000
O 2.2962980000 -0.1615250000 0.7955960000
O 1.5665380000 0.3553440000 -1.2874590000
C 3.6730410000 -0.3498050000 0.3092400000

C 4.5378940000 -0.6647150000 1.5081660000
H 3.6524860000 -1.1591900000 -0.4248830000
H 3.9700110000 0.5700840000 -0.1999550000
H 5.5703460000 -0.8092110000 1.1753020000
H 4.5237740000 0.1550180000 2.2320830000
H 4.2087410000 -1.5808380000 2.0069520000
H -0.2264900000 4.2571700000 -0.4483040000
H 0.6828140000 2.9988380000 0.3815150000
H 0.5342250000 2.9683910000 -1.3902890000
H -2.4165520000 3.8180990000 -1.5156570000
H -1.7823140000 2.4843290000 -2.4787920000
H -3.2062090000 2.2460960000 -1.4332160000
H -2.1497140000 3.7777590000 1.0529480000
H -2.9659570000 2.2164850000 1.0919520000
H -1.3803910000 2.4167050000 1.8602290000

Equilibrium geometry of **r14-exo-3s-ts**.

C 0.1281001297 0.6396718378 0.3969115712
N -0.6104903541 1.3192998777 -0.5079999637
C -1.2880419630 2.6452759456 -0.3116851156
C 1.4625956405 0.1547487041 -0.1529137510
H 0.1583345951 1.0302418665 1.4068979723
H -0.2712526231 1.1809579365 -1.4603186884
C -0.6443620977 -1.1513939675 0.7101414010
C -1.1080872855 -1.4956009495 -0.6970502420
C -2.4653553477 -0.8872034891 -0.7273078539
C -2.8902504850 -0.6183339643 0.5567707901
C -1.8139006967 -0.8481138609 1.4399170618
H 0.1901588271 -1.6602955368 1.1830840797
H -3.0584293371 -0.7707225233 -1.6277170080
H -1.2184871228 -2.5912027482 -0.7554797234
H -0.4443592787 -1.2097314137 -1.5159579421
H -3.8760941650 -0.2710376252 0.8415445760
H -1.8592726170 -0.7380085838 2.5187395365
C -2.4173218404 2.7324667769 -1.3468138167
C -1.8450882459 2.7837027250 1.1079790570
C -0.2356262644 3.7380528640 -0.5832972795
O 2.3075079975 -0.1447792299 0.8191618783
O 1.6630789850 0.0709401001 -1.3466581455
C 3.6443385711 -0.6022856707 0.4140824908
C 4.4562690248 -0.7973888571 1.6748501510
H 3.5188522710 -1.5261975232 -0.1564688450
H 4.0669290798 0.1567205409 -0.2482288664
H 5.4614858243 -1.1361965211 1.4058193607
H 4.5486514615 0.1390421033 2.2318166420
H 4.0047133910 -1.5516606902 2.3256870861
H -0.6993822312 4.7266706078 -0.5098748829
H 0.5816021230 3.6916856902 0.1445299956
H 0.1901031722 3.6420178142 -1.5879838794
H -2.8718033546 3.7266251834 -1.3211878044
H -2.0388461348 2.5697183159 -2.3625842518
H -3.1977250274 1.9936776185 -1.1439848260
H -2.3626821598 3.7437982926 1.1871828751
H -2.5690833824 1.9989488145 1.3417574142
H -1.0592710771 2.7852398360 1.8708050752

Equilibrium geometry of **r15-endo-3r-mc**.

C 0.5396320000 1.2260190000 -0.2811000000
N -0.0924010000 1.9849560000 0.5409750000
H 0.1630270000 1.8170580000 1.5230420000
H 0.3951730000 1.3059940000 -1.3503130000
C 1.6086680000 0.3438490000 0.3226970000
C -1.1114300000 3.0533190000 0.2937530000

C -0.8608210000 -1.2724100000 -1.1996060000
C -2.2506970000 -0.9214730000 -1.6615710000
C -3.0623280000 -0.9973330000 -0.3975860000
C -2.2647800000 -1.3795300000 0.6260500000
C -0.9031370000 -1.5656360000 0.1269530000
H -0.0092800000 -1.3865120000 -1.8599900000
H -4.1276940000 -0.8042410000 -0.3515450000
H -2.6050750000 -1.6545180000 -2.4027820000
H -2.3226670000 0.0533240000 -2.1662940000
H -2.5706620000 -1.5516690000 1.6516520000
H -0.0782770000 -1.9225630000 0.7344080000
C -2.4022430000 2.6045700000 1.0021910000
C -0.5483960000 4.3303050000 0.9425390000
C -1.3265550000 3.2408110000 -1.2072860000
O 2.3186490000 -0.2472110000 -0.6131310000
O 1.7373040000 0.2910000000 1.5287450000
C 3.4735430000 -1.0877630000 -0.1826440000
C 3.6857440000 -2.0883910000 -1.3028850000
C 4.6620940000 -0.1761920000 0.0778010000
H 3.1589990000 -1.5829030000 0.7393670000
H 4.5049070000 -2.7627260000 -1.0349050000
H 2.7906650000 -2.6946150000 -1.4710200000
H 3.9512330000 -1.5827310000 -2.2365090000
H 5.5166110000 -0.7823760000 0.3941730000
H 4.9444770000 0.3636400000 -0.8315340000
H 4.4480440000 0.5418100000 0.8742020000
H -1.2806740000 5.1347220000 0.8318020000
H -0.3670890000 4.1909980000 2.0137970000
H 0.3842250000 4.6471290000 0.4658350000
H -2.0666060000 4.0310470000 -1.3563710000
H -0.4086060000 3.5518470000 -1.7177360000
H -1.7167550000 2.3355850000 -1.6836170000
H -3.1609940000 3.3829300000 0.8811390000
H -2.7809150000 1.6699060000 0.5799730000
H -2.2398920000 2.4612790000 2.0760540000

Equilibrium geometry of **r15-endo-3r-prod**.

C 0.0426120000 0.3890210000 -0.6900900000
N -0.9875180000 1.0454570000 0.2144010000
H -0.6286600000 0.8397760000 1.1614790000
H 0.2899410000 1.0504630000 -1.5200720000
C 1.2835060000 0.0806990000 0.1443650000
C -1.1363690000 2.5944660000 0.1727720000
C -0.7140330000 -0.8799200000 -1.2194070000
C -2.0967140000 -0.2404100000 -1.4805630000
C -2.2792790000 0.1673600000 -0.0121470000
C -1.9778050000 -1.1337810000 0.7024030000
C -1.0383930000 -1.7596330000 -0.0194560000
H -0.1968060000 -1.3452950000 -2.0575340000
H -3.1596270000 0.7292940000 0.2856040000
H -2.8466200000 -0.9716170000 -1.7864270000
H -2.0820520000 0.5902050000 -2.1895130000
H -2.4001390000 -1.4275140000 1.6558030000
H -0.5334060000 -2.6875830000 0.2224970000
C -1.9974570000 2.9759740000 1.3858370000
C 0.2646720000 3.2032600000 0.3264390000
C -1.7923940000 3.0459840000 -1.1327220000
O 2.2738930000 -0.3264800000 -0.6210260000
O 1.2761110000 0.1801120000 1.3582270000
C 3.5431360000 -0.7499530000 0.0324860000
C 4.1987650000 -1.7065800000 -0.9458010000
C 4.3724340000 0.4837630000 0.3490050000
H 3.2527440000 -1.2617040000 0.9534950000
H 5.1205270000 -2.0981710000 -0.5050020000
H 3.5438010000 -2.5519440000 -1.1753270000

H 4.4559480000 -1.1963500000 -1.8793200000
H 5.3110170000 0.1750360000 0.8201320000
H 4.6159520000 1.0363910000 -0.5642130000
H 3.8502480000 1.1458920000 1.0447820000
H 0.1634460000 4.2897320000 0.3986440000
H 0.7659740000 2.8527930000 1.2333540000
H 0.9079060000 2.9975520000 -0.5345300000
H -1.8708990000 4.1368970000 -1.1162450000
H -1.2003470000 2.7818670000 -2.0146650000
H -2.8043920000 2.6489460000 -1.2502960000
H -2.0514580000 4.0659560000 1.4517960000
H -3.0240400000 2.6066440000 1.3122550000
H -1.5587250000 2.6131800000 2.3224430000

Equilibrium geometry of **r15-endo-3r-ts**.

C 0.1640127395 0.6866566359 -0.4531658472
N -0.6254885617 1.4175333699 0.3566583950
H -0.4951540088 1.1760972817 1.3397847355
H 0.3287794917 1.0786638459 -1.4506934986
C 1.3736431291 0.0631655466 0.2190894900
C -1.0943618362 2.8320986167 0.1564502152
C -0.7821427264 -0.9762227399 -1.0453798290
C -2.1634287249 -0.4187633391 -1.3362491767
C -2.8243221651 -0.5078972473 -0.0028469972
C -2.1028717576 -1.3381572942 0.8230845452
C -0.9041331177 -1.6947324700 0.1622232472
H -0.1121083548 -1.3002217392 -1.8360409275
H -3.7790994088 -0.0526045678 0.2336733539
H -2.6674986875 -1.1191356734 -2.0227802017
H -2.2107119736 0.5631070446 -1.8089347038
H -2.3901782638 -1.6586052570 1.8172442699
H -0.1544655255 -2.3642454899 0.5691302324
C -2.5074258005 2.9527272295 0.7427672706
C -0.1182725851 3.7277348781 0.9467480293
C -1.0831280400 3.2285308699 -1.3220748162
O 2.2910728567 -0.2628152768 -0.6757012390
O 1.4164185414 -0.0966155304 1.4214652286
C 3.5651645143 -0.8526948250 -0.1891694762
C 4.0750935408 -1.7140945495 -1.3298799241
C 4.5017377418 0.2786065185 0.2030587152
H 3.3091921475 -1.4572248490 0.6843475662
H 5.0096689314 -2.1988182041 -1.0313406120
H 3.3566812906 -2.4965078187 -1.5926840670
H 4.2736882742 -1.1071001598 -2.2187882384
H 5.4550714202 -0.1386093390 0.5425339905
H 4.7003961068 0.9315452828 -0.6529235629
H 4.0854631957 0.8730312736 1.0211934651
H -0.4361826864 4.7725780122 0.8794701562
H -0.0947618707 3.4539608365 2.0073054282
H 0.8982854475 3.6519504089 0.5481769197
H -1.4547966517 4.2531588740 -1.4072171516
H -0.0753019239 3.2166843101 -1.7495496895
H -1.7367576218 2.5985394658 -1.9335731121
H -2.8280772596 3.9981700286 0.7294908193
H -3.2293321659 2.3691590339 0.1636359164
H -2.5372788070 2.6093436542 1.7828377123

Equilibrium geometry of **r15-endo-3s-mc**.

C 0.5413190000 1.2200720000 0.2931900000
N -0.0857430000 1.9871960000 -0.5250990000
C -1.1024300000 3.0567720000 -0.2732870000
C 1.6095990000 0.3393290000 -0.3140350000
H 0.3935600000 1.2922050000 1.3624320000

H 0.1725690000 1.8260260000 -1.5075560000
C -3.0672910000 -0.9938800000 0.3823230000
C -2.2584960000 -0.9312750000 1.6488150000
C -0.8685690000 -1.2824610000 1.1871900000
C -0.9085430000 -1.5640080000 -0.1419870000
C -2.2684150000 -1.3696060000 -0.6426830000
H -4.1319240000 -0.7971560000 0.3353430000
H -0.0189920000 -1.4047330000 1.8485890000
H -2.6169370000 -1.6693500000 2.3829260000
H -2.3285050000 0.0394980000 2.1614950000
H -0.0833430000 -1.9179040000 -0.7506650000
H -2.5723140000 -1.5320010000 -1.6704830000
C -2.3926000000 2.6164020000 -0.9881710000
C -1.3211830000 3.2346190000 1.2283800000
C -0.5339860000 4.3364350000 -0.9119600000
O 2.3143510000 -0.2619770000 0.6192500000
O 1.7422070000 0.2960330000 -1.5200780000
C 3.4676450000 -1.1030890000 0.1855530000
C 3.6741400000 -2.1121020000 1.2992510000
H 3.1536620000 -1.5908000000 -0.7406300000
C 4.6595750000 -0.1934990000 -0.0659890000
H 4.4916050000 -2.7873130000 1.0282140000
H 3.9393630000 -1.6137480000 2.2368740000
H 2.7766280000 -2.7163640000 1.4614120000
H 5.5131610000 -0.8002790000 -0.3836360000
H 4.4498600000 0.5299070000 -0.8586200000
H 4.9409590000 0.3400250000 0.8474130000
H -1.2638990000 5.1423840000 -0.7974190000
H 0.3985560000 4.6470830000 -0.4310550000
H -0.3505860000 4.2038420000 -1.9837120000
H -2.0590640000 4.0262500000 1.3808310000
H -1.7156320000 2.3274530000 1.6973470000
H -0.4036530000 3.5390410000 1.7435290000
H -3.1492340000 3.3963290000 -0.8646650000
H -2.2276980000 2.4789150000 -2.0623520000
H -2.7753810000 1.6804460000 -0.5724820000

Equilibrium geometry of **r15-endo-3s-prod**.

C 0.0409590000 0.3819000000 0.6936080000
N -0.9845060000 1.0481100000 -0.2090100000
C -1.1294550000 2.5972880000 -0.1560700000
C 1.2830390000 0.0751940000 -0.1397050000
H 0.2885710000 1.0370410000 1.5285390000
H -0.6234470000 0.8485780000 -1.1565530000
C -2.2793030000 0.1719440000 0.0076310000
C -2.1025150000 -0.2464690000 1.4737890000
C -0.7209310000 -0.8880820000 1.2125240000
C -1.0442480000 -1.7589460000 0.0057790000
C -1.9793640000 -1.1252450000 -0.7148230000
H -3.1572890000 0.7381110000 -0.2890710000
H -0.2073080000 -1.3602780000 2.0490190000
H -2.8554360000 -0.9777350000 1.7720140000
H -2.0879810000 0.5788040000 2.1889600000
H -0.5413570000 -2.6868340000 -0.2406860000
H -2.3996700000 -1.4110410000 -1.6715460000
C -1.9857870000 2.9900820000 -1.3689170000
C -1.7885300000 3.0401130000 1.1508450000
C 0.2735990000 3.2037130000 -0.3004940000
O 2.2695070000 -0.3419660000 0.6253820000
O 1.2797090000 0.1843770000 -1.3527310000
C 3.5391650000 -0.7651990000 -0.0274740000
C 4.1896980000 -1.7293650000 0.9467580000
H 3.2495950000 -1.2705520000 -0.9523030000
C 4.3730390000 0.4678880000 -0.3345390000
H 5.1109300000 -2.1215240000 0.5055250000

H 4.4468810000 -1.2250280000 1.8834800000
H 3.5316130000 -2.5738090000 1.1705700000
H 5.3118350000 0.1590720000 -0.8051170000
H 3.8546090000 1.1357870000 -1.0274940000
H 4.6159420000 1.0141780000 0.5826390000
H 0.1754640000 4.2909990000 -0.3630520000
H 0.9136670000 2.9882590000 0.5602920000
H 0.7765920000 2.8601800000 -1.2090500000
H -1.8648420000 4.1312630000 1.1425910000
H -2.8015840000 2.6442560000 1.2622240000
H -1.1996590000 2.7678890000 2.0324460000
H -2.0376520000 4.0806310000 -1.4264690000
H -1.5443560000 2.6340830000 -2.3069410000
H -3.0132110000 2.6219090000 -1.3018340000

Equilibrium geometry of **r15-endo-3s-ts**.

C 0.1633142984 0.6811720272 0.4609226987
N -0.6213529600 1.4207910237 -0.3463928975
C -1.0882167151 2.8345866749 -0.1366325082
C 1.3739238154 0.0603552433 -0.2123372540
H 0.3265343421 1.0662914950 1.4614231346
H -0.4874264317 1.1867745950 -1.3307812363
C -2.8238161842 -0.5021763386 -0.0139354435
C -2.1700097200 -0.4233348258 1.3235833007
C -0.7876006339 -0.9803819922 1.0358102030
C -0.9054549678 -1.6920153025 -0.1768369969
C -2.0999002117 -1.3289736817 -0.8414770562
H -3.7762250151 -0.0429852144 -0.2527314100
H -0.1229412637 -1.3121852003 1.8278287590
H -2.6784549564 -1.1280429572 2.0024290005
H -2.2187287940 0.5553915178 1.8025515827
H -0.1550631849 -2.3605729270 -0.5841038283
H -2.3827307326 -1.6424254628 -1.8391553366
C -2.5032791610 2.9599357604 -0.7173837998
C -1.0712734554 3.2224098305 1.3441066487
C -0.1141823075 3.7339563767 -0.9251332141
O 2.2870835770 -0.2767019932 0.6826962919
O 1.4201605182 -0.0898244791 -1.4158456345
C 3.5584787543 -0.8717662790 0.1955668421
C 4.0617648089 -1.7406463699 1.3334562772
H 3.3001458492 -1.4714804255 -0.6805998791
C 4.5022709051 0.2552850461 -0.1914888871
H 4.9931876875 -2.2306370265 1.0337525388
H 4.2638733347 -1.1383910395 2.2247834791
H 3.3378875451 -2.5191319689 1.5929070388
H 5.4533474078 -0.1664923326 -0.5315448310
H 4.0902274787 0.8550205819 -1.0078102288
H 4.7040393579 0.9038455421 0.6670794729
H -0.4316986187 4.7785239118 -0.8518072214
H 0.9035625605 3.6560302170 -0.5298230342
H -0.0937483140 3.4655783887 -1.9871550746
H -1.4459634991 4.2452681743 1.4370614889
H -1.7195937189 2.5865287004 1.9552775419
H -0.0612354314 3.2111705852 1.7664985991
H -2.8219234413 4.0059467474 -0.6999782178
H -2.5373640348 2.6194797517 -1.7582929010
H -3.2242072821 2.3762151672 -0.1370957151

Equilibrium geometry of **r15-exo-3r-mc**.

C 0.3906620000 1.1466880000 -0.3832420000
N -0.2500710000 1.8304380000 0.4989540000
H 0.0605400000 1.6434350000 1.4606140000
H 0.2036210000 1.2697580000 -1.4411040000

C 1.5492080000 0.3288550000 0.1408030000
C -1.2886650000 2.8998660000 0.3385240000
C -2.5983010000 -1.2624090000 0.6567120000
C -1.1929490000 -1.7927940000 0.7099910000
C -0.6858620000 -1.5560450000 -0.6861130000
C -1.6895880000 -1.0213560000 -1.4340710000
C -2.8719770000 -0.8323720000 -0.5983370000
H -3.2781650000 -1.2704460000 1.5005280000
H 0.2752240000 -1.8927410000 -1.0547880000
H -1.1887710000 -2.8685550000 0.9450200000
H -0.5770370000 -1.3241390000 1.4909030000
H -1.6478270000 -0.8082670000 -2.4976080000
H -3.8179750000 -0.4365000000 -0.9506530000
C -2.4281710000 2.5610220000 1.3117250000
C -0.5968360000 4.2146160000 0.7474510000
C -1.7764350000 2.9528230000 -1.1083430000
O 2.3306200000 -0.0659170000 -0.8401550000
O 1.6861800000 0.1694820000 1.3377960000
C 3.5917680000 -0.7811430000 -0.4842220000
C 3.9502050000 -1.5997410000 -1.7095570000
C 4.6359510000 0.2535890000 -0.0936500000
H 3.3454410000 -1.4199090000 0.3673710000
H 4.8671870000 -2.1624480000 -1.5105900000
H 3.1600220000 -2.3143770000 -1.9582810000
H 4.1253310000 -0.9527060000 -2.5744770000
H 5.5743090000 -0.2555430000 0.1469680000
H 4.8242860000 0.9447030000 -0.9212040000
H 4.3254330000 0.8190190000 0.7888530000
H -1.3282130000 5.0268140000 0.7071810000
H -0.2092720000 4.1651590000 1.7705230000
H 0.2273160000 4.4594780000 0.0706650000
H -3.1788430000 3.3553380000 1.2748210000
H -2.9040490000 1.6133430000 1.0474680000
H -2.0657080000 2.4979300000 2.3442430000
H -2.5482610000 3.7230120000 -1.1861510000
H -0.9770510000 3.2265160000 -1.8051750000
H -2.2214990000 2.0028420000 -1.4195930000

Equilibrium geometry of **r15-exo-3r-prod**.

C 0.0124620000 0.2711820000 -0.5435620000
N -0.9146680000 0.8884450000 0.4912060000
H -0.3486780000 0.8332220000 1.3564440000
H 0.0592220000 0.8839390000 -1.4408980000
C 1.3967780000 0.1381990000 0.0963710000
C -1.2734670000 2.3960850000 0.3645480000
C -2.0536660000 -0.1856120000 0.6607700000
C -1.1799040000 -1.4484000000 0.6128850000
C -0.6541950000 -1.1281460000 -0.8086490000
C -1.9622900000 -0.8539560000 -1.5311400000
C -2.7996500000 -0.2871450000 -0.6526120000
H -2.6105520000 0.0361310000 1.5672900000
H 0.0329220000 -1.8329150000 -1.2756760000
H -1.7864910000 -2.3541390000 0.6376150000
H -0.4098410000 -1.4972920000 1.3892230000
H -2.1334820000 -1.0347700000 -2.5861070000
H -3.8045910000 0.0772650000 -0.8239850000
C -2.1892140000 2.7310550000 1.5490930000
C 0.0505040000 3.1678000000 0.4897140000
C -1.9598970000 2.7241200000 -0.9630120000
O 2.2982400000 -0.2012140000 -0.7975280000
O 1.5626240000 0.2957390000 1.2946940000
C 3.6929640000 -0.4584550000 -0.3375370000
C 4.2871010000 -1.3966260000 -1.3714080000
C 4.4193710000 0.8692620000 -0.2055490000
H 3.6039820000 -0.9456140000 0.6366730000

H 5.3069800000 -1.6621550000 -1.0766040000
H 3.7053930000 -2.3193690000 -1.4522810000
H 4.3284830000 -0.9185820000 -2.3550580000
H 5.4475370000 0.6865280000 0.1226570000
H 4.4571410000 1.3910270000 -1.1672170000
H 3.9399760000 1.5119310000 0.5376470000
H -0.1688740000 4.2388140000 0.4973130000
H 0.5793240000 2.9266660000 1.4168490000
H 0.7218570000 2.9816930000 -0.3548860000
H -2.3600640000 3.8107360000 1.5681080000
H -3.1673880000 2.2487350000 1.4679260000
H -1.7348040000 2.4565860000 2.5082450000
H -2.0984600000 3.8087130000 -1.0045800000
H -1.3601460000 2.4430780000 -1.8333490000
H -2.9441960000 2.2635050000 -1.0565280000

Equilibrium geometry of **r15-exo-3r-ts**.

C 0.1358019893 0.6446752020 -0.3991502840
N -0.6042190599 1.3192996180 0.5091845827
H -0.2647014416 1.1752027062 1.4605389078
H 0.1674242641 1.0419991652 -1.4065301222
C 1.4726192779 0.1577870529 0.1494522243
C -1.2819887295 2.6455729180 0.3204716988
C -2.4574851675 -0.8885936809 0.7143026320
C -1.0989188337 -1.4940789501 0.6838152841
C -0.6327913069 -1.1411728495 -0.7206549450
C -1.8020560714 -0.8375056966 -1.4514665901
C -2.8806459654 -0.6146057608 -0.5694003091
H -3.0526530582 -0.7774537670 1.6140657762
H 0.2031924595 -1.6469270957 -1.1943339448
H -1.2068276449 -2.5902359564 0.7364906456
H -0.4369226148 -1.2106089259 1.5050263456
H -1.8453731103 -0.7220223481 -2.5298413427
H -3.8667907044 -0.2680370785 -0.8543591259
C -2.4091922946 2.7276480545 1.3583225538
C -0.2301106136 3.7381043882 0.5947570413
C -1.8424353833 2.7906816350 -1.0971772179
O 2.3149434469 -0.1338174300 -0.8243112482
O 1.6610904958 0.0638301956 1.3457510797
C 3.6689378252 -0.6229520081 -0.4475969989
C 4.1477709817 -1.4408912082 -1.6327330788
C 4.5504047192 0.5708988825 -0.1196356647
H 3.5284328817 -1.2495245402 0.4369451860
H 5.1256169410 -1.8743558297 -1.4016119687
H 3.4588317300 -2.2604408230 -1.8586119180
H 4.2538070491 -0.8144034551 -2.5240055022
H 5.5520733903 0.2178972134 0.1453598687
H 4.6417565364 1.2368670574 -0.9838866848
H 4.1573922197 1.1344239453 0.7308109803
H -0.6943520111 4.7267341706 0.5254566311
H 0.1966749273 3.6383990021 1.5986225921
H 0.5862518624 3.6947819500 -0.1340754848
H -2.8643717949 3.7217024885 1.3381267185
H -3.1896073303 1.9891783340 1.1539137791
H -2.0284151288 2.5604178566 2.3725754241
H -2.3618942267 3.7502110036 -1.1704297973
H -1.0582939447 2.7970572422 -1.8615550598
H -2.5654034322 2.0057886451 -1.3331769776

Equilibrium geometry of **r15-exo-3s-mc**.

C 0.3913220000 1.1446780000 0.3801630000
N -0.2492300000 1.8293440000 -0.5014220000
C -1.2875220000 2.8989090000 -0.3401900000

C 1.5480140000 0.3249000000 -0.1450070000
H 0.2050250000 1.2675360000 1.4382290000
H 0.0605840000 1.6421860000 -1.4633810000
C -0.6874300000 -1.5582810000 0.6861070000
C -1.1964290000 -1.7967850000 -0.7090130000
C -2.6018100000 -1.2665600000 -0.6544130000
C -2.8737090000 -0.8348470000 0.6004240000
C -1.6901070000 -1.0226380000 1.4347300000
H 0.2741190000 -1.8944190000 1.0538940000
H -3.2828960000 -1.2757570000 -1.4973380000
H -1.1923360000 -2.8727930000 -0.9428690000
H -0.5817660000 -1.3287430000 -1.4913280000
H -3.8192410000 -0.4386140000 0.9536280000
H -1.6468310000 -0.8081260000 2.4979810000
C -2.4289000000 2.5587250000 -1.3107390000
C -1.7723750000 2.9534870000 1.1075860000
C -0.5967150000 4.2132800000 -0.7520800000
O 2.3283790000 -0.0734590000 0.8353170000
O 1.6843730000 0.1668130000 -1.3422370000
C 3.5866840000 -0.7932210000 0.4784010000
C 3.9415040000 -1.6151990000 1.7025380000
H 3.3377600000 -1.4296210000 -0.3741710000
C 4.6350770000 0.2378410000 0.0894340000
H 4.8564520000 -2.1810470000 1.5031910000
H 4.1185380000 -0.9702290000 2.5686680000
H 3.1485040000 -2.3272700000 1.9496420000
H 5.5716250000 -0.2746770000 -0.1512670000
H 4.3271080000 0.8053430000 -0.7926580000
H 4.8256580000 0.9274440000 0.9177960000
H -1.3281560000 5.0254240000 -0.7110660000
H 0.2289360000 4.4589830000 -0.0773160000
H -0.2113900000 4.1627320000 -1.7759470000
H -3.1796650000 3.3529430000 -1.2733140000
H -2.0684350000 2.4944520000 -2.3438200000
H -2.9042160000 1.6112720000 -1.0444910000
H -2.5440830000 3.7237590000 1.1861560000
H -2.2168310000 2.0039850000 1.4208700000
H -0.9715190000 3.2279750000 1.8025100000

Equilibrium geometry of **r15-exo-3s-prod**.

C 0.0099980000 0.2635760000 0.5419380000
N -0.9166810000 0.8836080000 -0.4916540000
C -1.2687700000 2.3928510000 -0.3658670000
C 1.3931490000 0.1280410000 -0.0999800000
H 0.0592230000 0.8759420000 1.4394600000
H -0.3521780000 0.8255410000 -1.3576910000
C -0.6604440000 -1.1338560000 0.8076160000
C -1.1902570000 -1.4520160000 -0.6128600000
C -2.0598170000 -0.1862270000 -0.6586560000
C -2.8033370000 -0.2855590000 0.6563330000
C -1.9661240000 -0.8554220000 1.5329810000
H 0.0253200000 -1.8410490000 1.2730020000
H -2.6180130000 0.0375370000 -1.5638970000
H -1.7998590000 -2.3557570000 -0.6364920000
H -0.4219130000 -1.5031000000 -1.3907530000
H -3.8066790000 0.0821850000 0.8299640000
H -2.1357550000 -1.0359420000 2.5882680000
C -2.1792410000 2.7320750000 -1.5532480000
C -1.9578210000 2.7235670000 0.9596200000
C 0.0589470000 3.1587320000 -0.4870390000
O 2.2963570000 -0.2096850000 0.7927180000
O 1.5568300000 0.2835320000 -1.2989040000
C 3.6909660000 -0.4632290000 0.3305050000
C 4.2883280000 -1.4034960000 1.3605910000
H 3.6019650000 -0.9473870000 -0.6451170000

C 4.4143500000 0.8665530000 0.2019860000
H 5.3083320000 -1.6659940000 1.0635620000
H 4.3300850000 -0.9286240000 2.3457810000
H 3.7086710000 -2.3276830000 1.4390850000
H 5.4423370000 0.6871360000 -0.1286370000
H 3.9323200000 1.5107600000 -0.5381320000
H 4.4526270000 1.3851860000 1.1653400000
H -0.1558410000 4.2306610000 -0.4948030000
H 0.7270890000 2.9694210000 0.3593760000
H 0.5891520000 2.9157380000 -1.4128720000
H -2.3448500000 3.8126140000 -1.5728100000
H -1.7231700000 2.4554090000 -2.5109850000
H -3.1599050000 2.2544330000 -1.4750670000
H -2.0901200000 3.8088970000 1.0020470000
H -2.9452900000 2.2688290000 1.0488610000
H -1.3630250000 2.4376430000 1.8317980000

Equilibrium geometry of r15-exo-3s-ts.

C 0.1348635581 0.6397469908 0.3969734787
N -0.6048636016 1.3156404120 -0.5106878165
C -1.2801647830 2.6431010519 -0.3213079795
C 1.4703529215 0.1505926447 -0.1527984456
H 0.1681022437 1.0370978703 1.4042882733
H -0.2665990685 1.1708156694 -1.4623872436
C -0.6365024800 -1.1445907310 0.7192172045
C -1.1046195798 -1.4967894747 -0.6847468439
C -2.4621428392 -0.8888532048 -0.7139408873
C -2.8835765750 -0.6140839932 0.5701632678
C -1.8045334998 -0.8388498986 1.4511808378
H 0.1990149022 -1.6518186161 1.1921370944
H -3.0579517575 -0.7766908188 -1.6131464000
H -1.2145214482 -2.5927838035 -0.7372887452
H -0.4429344300 -1.2145024632 -1.5066505922
H -3.8688558662 -0.2657793437 0.8560739676
H -1.8465810888 -0.7232196585 2.5295837925
C -2.4086241623 2.7269127737 -1.3576590609
C -1.8384415796 2.7893314651 1.0970929396
C -0.2268159363 3.7338073875 -0.5971804629
O 2.3132554178 -0.1416849086 0.8202573794
O 1.6574025864 0.0556720712 -1.3492315798
C 3.6661454843 -0.6330935343 0.4425278365
C 4.1455149124 -1.4495033391 1.6284942850
H 3.5236385692 -1.2610841241 -0.4406710677
C 4.5487349263 0.5589251882 0.1111867597
H 5.1225832129 -1.8845189328 1.3970013729
H 4.2533303512 -0.8215646758 2.5184926639
H 3.4558893419 -2.2678131570 1.8566281828
H 5.5495012695 0.2040293695 -0.1547195307
H 4.1552327968 1.1215253938 -0.7396345039
H 4.6424142344 1.2262510967 0.9741083897
H -0.6893087542 4.7231863007 -0.5274217279
H 0.5904522483 3.6893107815 0.1305713974
H 0.1984168168 3.6331982021 -1.6015764327
H -2.8622801714 3.7217038448 -1.3368466054
H -2.0293835542 2.5591473210 -2.3724299477
H -3.1899312951 1.9896098156 -1.1522282730
H -2.3562267166 3.7497239965 1.1709641990
H -2.5623831613 2.0056481899 1.3341885829
H -1.0532418855 2.7945250146 1.8604097421

Equilibrium geometry of r16-endo-3r-mc.

C 0.5575470000 1.2650770000 -0.2616430000
N -0.0755920000 2.0141250000 0.5674030000

H 0.2034950000 1.8563950000 1.5450910000
H 0.3890510000 1.3336700000 -1.3280340000
C 1.6568760000 0.4033710000 0.3291870000
C -1.1302740000 3.0505420000 0.3349460000
C -0.7998960000 -1.2724720000 -1.1885920000
C -2.1681770000 -0.9636670000 -1.7365510000
C -3.0497420000 -1.0304280000 -0.5196080000
C -2.3035470000 -1.3691680000 0.5564140000
C -0.9103340000 -1.5323440000 0.1402410000
H 0.0901210000 -1.3779210000 -1.7974610000
H -4.1199940000 -0.8620160000 -0.5399880000
H -2.4644160000 -1.7179760000 -2.4818680000
H -2.2299730000 -0.0002680000 -2.2645400000
H -2.6630800000 -1.5257720000 1.5670330000
H -0.1124120000 -1.8504710000 0.8028040000
C -2.3974420000 2.5606620000 1.0583480000
C -0.5991120000 4.3438100000 0.9780500000
C -1.3710090000 3.2320910000 -1.1630920000
O 2.3498030000 -0.1721270000 -0.6240430000
O 1.7963630000 0.3712140000 1.5357740000
C 3.5641680000 -1.0345020000 -0.3302440000
C 3.9888910000 -1.4758550000 -1.7257080000
C 4.6213770000 -0.1585290000 0.3367960000
C 3.1314710000 -2.2167820000 0.5322110000
H 4.8821230000 -2.1031900000 -1.6501350000
H 3.2025040000 -2.0621240000 -2.2107640000
H 4.2287480000 -0.6158990000 -2.3576120000
H 5.5314370000 -0.7503630000 0.4770270000
H 4.8722990000 0.6976680000 -0.2969050000
H 4.2950950000 0.1971280000 1.3160620000
H 3.9801410000 -2.8992450000 0.6432900000
H 2.8179910000 -1.9008720000 1.5289110000
H 2.3190520000 -2.7736190000 0.0536140000
H -1.3557820000 5.1263290000 0.8755970000
H -0.4024430000 4.2095370000 2.0472000000
H 0.3185040000 4.6881140000 0.4918160000
H -2.1326190000 4.0036690000 -1.3017270000
H -0.4685120000 3.5661420000 -1.6861220000
H -1.7451400000 2.3171010000 -1.6336820000
H -3.1793310000 3.3180640000 0.9520060000
H -2.7557570000 1.6183410000 0.6351650000
H -2.2167160000 2.4166710000 2.1291850000

Equilibrium geometry of r16-endo-3r-prod.

C 0.0428830000 0.3899450000 -0.7020610000
N -0.9834770000 1.0393290000 0.2113030000
H -0.6217520000 0.8199150000 1.1546440000
H 0.2861260000 1.0574980000 -1.5279550000
C 1.2907260000 0.0733270000 0.1252030000
C -1.1239680000 2.5882330000 0.1862410000
C -0.7175380000 -0.8734920000 -1.2379580000
C -2.0991350000 -0.2285720000 -1.4928200000
C -2.2789920000 0.1683590000 -0.0212140000
C -1.9809220000 -1.1391590000 0.6827810000
C -1.0427520000 -1.7610400000 -0.0441110000
H -0.2030530000 -1.3344830000 -2.0801870000
H -3.1571580000 0.7309970000 0.2816260000
H -2.8515930000 -0.9550800000 -1.8036500000
H -2.0825700000 0.6079680000 -2.1947920000
H -2.4024920000 -1.4388440000 1.6346670000
H -0.5380980000 -2.6906980000 0.1918080000
C -1.9928510000 2.9632640000 1.3957670000
C 0.2800110000 3.1862540000 0.3577460000
C -1.7660170000 3.0591560000 -1.1194270000
O 2.2769560000 -0.2853820000 -0.6636990000

O 1.2669110000 0.1407960000 1.3422580000
C 3.6286230000 -0.7197560000 -0.1413100000
C 4.4028150000 -0.9613150000 -1.4331690000
C 4.2382850000 0.4162960000 0.6761410000
C 3.4443920000 -2.0038040000 0.6619790000
H 5.4156540000 -1.3001150000 -1.1963700000
H 3.9178550000 -1.7290560000 -2.0433100000
H 4.4771090000 -0.0416910000 -2.0209000000
H 5.2727130000 0.1565240000 0.9224700000
H 4.2566500000 1.3444020000 0.0958870000
H 3.6961050000 0.5825670000 1.6082390000
H 4.4272710000 -2.3785510000 0.9645090000
H 2.8528520000 -1.8331330000 1.5639260000
H 2.9655010000 -2.7773180000 0.0527390000
H 0.1861640000 4.2725320000 0.4418580000
H 0.7723040000 2.8212090000 1.2638300000
H 0.9281390000 2.9853080000 -0.5006680000
H -1.8366530000 4.1503700000 -1.0914860000
H -1.1688520000 2.8001720000 -1.9994070000
H -2.7799050000 2.6707820000 -1.2494540000
H -2.0319440000 4.0527220000 1.4781400000
H -3.0237320000 2.6102300000 1.3045130000
H -1.5701960000 2.5793970000 2.3312790000

Equilibrium geometry of **r16-endo-3r-ts**.

C 0.1688090674 0.7057761269 -0.4573437947
N -0.6292354150 1.4256688656 0.3539942386
H -0.4931931021 1.1826766514 1.3361884697
H 0.3306325980 1.1030367892 -1.4532165296
C 1.3866965940 0.0914094425 0.2177276639
C -1.1072641059 2.8375319818 0.1595860431
C -0.7594078437 -0.9613191034 -1.0569005197
C -2.1468057929 -0.4172421436 -1.3444926422
C -2.8055312410 -0.5189566761 -0.0108061586
C -2.0756408765 -1.3469324069 0.8098549268
C -0.8739034484 -1.6882241418 0.1463201499
H -0.0862618408 -1.2740726323 -1.8493779072
H -3.7643744885 -0.0739089033 0.2287580307
H -2.6439276055 -1.1203811146 -2.0332524079
H -2.2049611720 0.5659424228 -1.8131020703
H -2.3590050263 -1.6753543133 1.8025428150
H -0.1170129888 -2.3527998758 0.5479081343
C -2.5194674467 2.9480659880 0.7499316209
C -0.1347349711 3.7373041801 0.9496594378
C -1.1027418319 3.2386141013 -1.3178206248
O 2.2965944057 -0.2218523120 -0.6842662666
O 1.4167098045 -0.0568925648 1.4229231009
C 3.6340107409 -0.8125723199 -0.3116632154
C 4.3015495533 -0.9757546931 -1.6734271179
C 4.3844355745 0.1844648458 0.5681834481
C 3.4090175117 -2.1593245775 0.3717246056
H 5.3033632436 -1.3947756095 -1.5416040979
H 3.7289797453 -1.6534281612 -2.3140102999
H 4.3969812587 -0.0111879135 -2.1805257207
H 5.3970106224 -0.1913314168 0.7453466939
H 4.4705107442 1.1537622462 0.0669044891
H 3.8957423237 0.3204525397 1.5347954599
H 4.3782047893 -2.6430249686 0.5291059827
H 2.9238235221 -2.0444428188 1.3428642352
H 2.8090264115 -2.8213750526 -0.2623006493
H -0.4570004304 4.7808774980 0.8829860896
H -0.1091791980 3.4629885363 2.0100996660
H 0.8818950313 3.6656355425 0.5504452537
H -1.4853366635 4.2595456827 -1.3998931109
H -0.0954393576 3.2382195116 -1.7466147372

H -1.7502723945 2.6031602911 -1.9300433189
H -2.8465070567 3.9915942103 0.7396264418
H -3.2394931136 2.3613136456 0.1717023810
H -2.5445544692 2.6023471313 1.7893333090

Equilibrium geometry of **r16-endo-3s-mc**.

C 0.5609340000 1.2675170000 0.2751530000
N -0.0731760000 2.0201950000 -0.5499350000
C -1.1259150000 3.0571970000 -0.3115500000
C 1.6598220000 0.4086940000 -0.3204310000
H 0.3941480000 1.3321110000 1.3421300000
H 0.2042080000 1.8661620000 -1.5286740000
C -3.0423470000 -1.0302520000 0.4858640000
C -2.1759590000 -0.9634580000 1.7136910000
C -0.8010200000 -1.2724680000 1.1825940000
C -0.8951240000 -1.5330530000 -0.1473650000
C -2.2829250000 -1.3693790000 -0.5807590000
H -4.1126960000 -0.8613670000 0.4926110000
H 0.0814690000 -1.3783730000 1.8020840000
H -2.4813340000 -1.7178960000 2.4553210000
H -2.2445230000 -0.0000660000 2.2407960000
H -0.0892600000 -1.8515820000 -0.8000340000
H -2.6298860000 -1.5256510000 -1.5957670000
C -2.3954970000 2.5720430000 -1.0338760000
C -1.3629520000 3.2342730000 1.1876200000
C -0.5942700000 4.3518660000 -0.9514200000
O 2.3563640000 -0.1672770000 0.6299440000
O 1.7965300000 0.3795080000 -1.5274200000
C 3.5730500000 -1.0246430000 0.3312540000
C 4.0053230000 -1.4643330000 1.7249450000
C 3.1412920000 -2.2083770000 -0.5295900000
C 4.6243400000 -0.1446100000 -0.3399060000
H 4.9006460000 -2.0882080000 1.6457760000
H 4.2446380000 -0.6032960000 2.3555790000
H 3.2232400000 -2.0534650000 2.2134890000
H 5.5359520000 -0.7332000000 -0.4842820000
H 4.2927410000 0.2104470000 -1.3175730000
H 4.8749550000 0.7121190000 0.2929840000
H 3.9920690000 -2.8874780000 -0.6449450000
H 2.3332550000 -2.7685770000 -0.0472610000
H 2.8219020000 -1.8933270000 -1.5247060000
H -1.3494590000 5.1351600000 -0.8446170000
H 0.3250030000 4.6932300000 -0.4659810000
H -0.4001840000 4.2209360000 -2.0215160000
H -2.1233480000 4.0062010000 1.3303880000
H -1.7369890000 2.3183600000 1.6563800000
H -0.4587990000 3.5656410000 1.7096380000
H -3.1759480000 3.3302400000 -0.9230610000
H -2.2173300000 2.4315190000 -2.1055610000
H -2.7542600000 1.6286270000 -0.6135550000

Equilibrium geometry of **r16-endo-3s-prod**.

C 0.0478040000 0.3916170000 0.7057950000
N -0.9770480000 1.0456760000 -0.2059180000
C -1.1205790000 2.5942550000 -0.1709540000
C 1.2975350000 0.0813080000 -0.1210780000
H 0.2889370000 1.0544240000 1.5361550000
H -0.6123070000 0.8330510000 -1.1496930000
C -2.2718210000 0.1714810000 0.0176510000
C -2.0955680000 -0.2341870000 1.4873510000
C -0.7124590000 -0.8757510000 1.2324350000
C -1.0334630000 -1.7567170000 0.0325710000
C -1.9702300000 -1.1314920000 -0.6932640000

H -3.1499940000 0.7346510000 -0.2842330000
H -0.1995490000 -1.3409030000 2.0733310000
H -2.8479040000 -0.9636640000 1.7914780000
H -2.0822850000 0.5977610000 2.1948570000
H -0.5271330000 -2.6844340000 -0.2073840000
H -2.3889020000 -1.4259140000 -1.6480740000
C -1.9813400000 2.9754990000 -1.3842940000
C -1.7733550000 3.0541010000 1.1333850000
C 0.2830170000 3.1968030000 -0.3279860000
O 2.2826400000 -0.2821910000 0.6669930000
O 1.2760100000 0.1571640000 -1.3377060000
C 3.6352230000 -0.7122430000 0.1433760000
C 4.4085910000 -0.9605540000 1.4344260000
C 3.4527150000 -1.9916980000 -0.6676090000
C 4.2448410000 0.4288880000 -0.6670850000
H 5.4218540000 -1.2972720000 1.1964150000
H 4.4818050000 -0.0441810000 2.0273360000
H 3.9237550000 -1.7320020000 2.0399660000
H 5.2800900000 0.1717390000 -0.9127460000
H 3.7041770000 0.5992220000 -1.5992930000
H 4.2610150000 1.3540860000 -0.0820500000
H 4.4361050000 -2.3635760000 -0.9720840000
H 2.9743080000 -2.7694190000 -0.0632860000
H 2.8613250000 -1.8161720000 -1.5687260000
H 0.1869150000 4.2834640000 -0.4042910000
H 0.9256430000 2.9908260000 0.5333300000
H 0.7825000000 2.8401970000 -1.2335320000
H -1.8471890000 4.1452600000 1.1127410000
H -2.7869120000 2.6617050000 1.2534230000
H -1.1816100000 2.7906000000 2.0156960000
H -2.0272500000 4.0654350000 -1.4564230000
H -1.5477030000 2.6037800000 -2.3196940000
H -3.0104890000 2.6144720000 -1.3059440000

Equilibrium geometry of **r16-endo-3s-ts**.

C 0.1743076623 0.7106022420 0.4609148903
N -0.6232197451 1.4352317468 -0.3473668805
C -1.1073485701 2.8435497361 -0.1426715415
C 1.3960149577 0.1042971499 -0.2149344471
H 0.3335732171 1.1021791727 1.4594693050
H -0.4839130475 1.2002573771 -1.3309926303
C -2.7957883097 -0.5188937838 -0.0002969825
C -2.1391556382 -0.4227243703 1.3347295567
C -0.7490514050 -0.9594325839 1.0454154873
C -0.8600271086 -1.6801921243 -0.1623310421
C -2.0619324608 -1.3391966396 -0.8252296391
H -3.7557586299 -0.0755489085 -0.2384564652
H -0.0769726456 -1.2765814566 1.8370557708
H -2.6342034298 -1.1318581321 2.0187594817
H -2.2018189255 0.5576435037 1.8086540739
H -0.1003630298 -2.3397658184 -0.5669151861
H -2.3430528073 -1.6624407442 -1.8202449105
C -2.5248899884 2.9497184967 -0.7214010914
C -1.0937587098 3.2373541894 1.3366116998
C -0.1460408167 3.7524389295 -0.9358019272
O 2.3022097338 -0.2164870094 0.6882392515
O 1.4311954444 -0.0338422640 -1.4211628521
C 3.6393160358 -0.8089692322 0.3175906772
C 4.3001568828 -0.9825816086 1.6813934634
C 3.4128002485 -2.1508707854 -0.3747893896
C 4.3968678653 0.1906041212 -0.5531498024
H 5.3009060276 -1.4048650983 1.5518970015
H 4.3968867941 -0.0212561182 2.1943410780
H 3.7218673569 -1.6615473779 2.3154804536
H 5.4092603527 -0.1871538471 -0.7272642067

H 3.9131673076 0.3329218388 -1.5213500639
H 4.4830932120 1.1570040398 -0.0463641504
H 4.3809746282 -2.6372018738 -0.5302706867
H 2.8072860492 -2.8145085888 0.2523303349
H 2.9328400820 -2.0286183551 -1.3476811068
H -0.4747281189 4.7936213403 -0.8633550743
H 0.8736836384 3.6859784113 -0.5436397625
H -0.1258098563 3.4821196730 -1.9973595696
H -1.4804419812 4.2560152304 1.4265951844
H -1.7338435267 2.5957971383 1.9504142636
H -0.0833859550 3.2392624419 1.7582083602
H -2.8580293258 3.9912378623 -0.7029213779
H -2.5559706113 2.6092765414 -1.7623286493
H -3.2371566026 2.3560974942 -0.1405191972

Equilibrium geometry of **r16-exo-3r-mc**.

C 0.4053820000 1.1597060000 -0.3840120000
N -0.2360080000 1.8432440000 0.4969190000
H 0.0845300000 1.6631990000 1.4571660000
H 0.2088760000 1.2711480000 -1.4415090000
C 1.5770460000 0.3533360000 0.1425220000
C -1.2906420000 2.8968410000 0.3396630000
C -2.5927330000 -1.2795610000 0.6542340000
C -1.1796850000 -1.7893260000 0.7076490000
C -0.6776980000 -1.5507130000 -0.6902360000
C -1.6887110000 -1.0317920000 -1.4381700000
C -2.8733290000 -0.8569350000 -0.6014930000
H -3.2716610000 -1.2950840000 1.4986540000
H 0.2889790000 -1.8717800000 -1.0575250000
H -1.1592350000 -2.8634690000 0.9485860000
H -0.5697460000 -1.3066810000 1.4848730000
H -1.6508530000 -0.8194980000 -2.5020410000
H -3.8249870000 -0.4750910000 -0.9540420000
C -2.4191710000 2.5428440000 1.3202660000
C -0.6167340000 4.2228720000 0.7415040000
C -1.7876430000 2.9389220000 -1.1043860000
O 2.3495660000 -0.0286030000 -0.8455270000
O 1.7041940000 0.2096210000 1.3436020000
C 3.6772550000 -0.7277020000 -0.6125270000
C 4.1889220000 -0.9218240000 -2.0347600000
C 4.5762380000 0.2050410000 0.1946190000
C 3.4162910000 -2.0596630000 0.0858950000
H 5.1603990000 -1.4235080000 -2.0028550000
H 3.5027520000 -1.5414970000 -2.6194000000
H 4.3155410000 0.0385850000 -2.5423310000
H 5.5673050000 -0.2509800000 0.2821010000
H 4.6941410000 1.1678680000 -0.3123460000
H 4.1893640000 0.3695800000 1.2020010000
H 4.3627440000 -2.6041470000 0.1614670000
H 3.0214480000 -1.9219490000 1.0942740000
H 2.7246330000 -2.6785180000 -0.4951210000
H -1.3617110000 5.0230420000 0.7082340000
H -0.2184930000 4.1800150000 1.7607520000
H 0.1967030000 4.4807780000 0.0567720000
H -3.1822540000 3.3255270000 1.2864550000
H -2.8823480000 1.5875870000 1.0606080000
H -2.0494460000 2.4873980000 2.3505890000
H -2.5691960000 3.6994240000 -1.1801770000
H -0.9953920000 3.2197670000 -1.8063960000
H -2.2225280000 1.9824100000 -1.4098910000

Equilibrium geometry of **r16-exo-3r-prod**.

C 0.0113000000 0.2778910000 -0.5614050000

N -0.9128820000 0.8845170000 0.4819760000
H -0.3404790000 0.8215360000 1.3430710000
H 0.0538020000 0.8975970000 -1.4540790000
C 1.4015960000 0.1384720000 0.0734150000
C -1.2747050000 2.3916240000 0.3710310000
C -2.0488640000 -0.1924350000 0.6484910000
C -1.1730330000 -1.4532200000 0.5872590000
C -0.6536050000 -1.1204590000 -0.8338630000
C -1.9655350000 -0.8444190000 -1.5485650000
C -2.8005030000 -0.2861950000 -0.6623160000
H -2.6023580000 0.0211060000 1.5590810000
H 0.0330170000 -1.8200980000 -1.3090790000
H -1.7779190000 -2.3602200000 0.6072700000
H -0.3998050000 -1.5061850000 1.3599360000
H -2.1411010000 -1.0176780000 -2.6040900000
H -3.8070330000 0.0769750000 -0.8268840000
C -2.1789760000 2.7164200000 1.5673070000
C 0.0491420000 3.1646710000 0.4889370000
C -1.9753400000 2.7290970000 -0.9466190000
O 2.2885530000 -0.1789790000 -0.8378000000
O 1.5553790000 0.2800490000 1.2766510000
C 3.7314010000 -0.4981550000 -0.5042920000
C 4.3205140000 -0.7806280000 -1.8820130000
C 4.3740160000 0.7234880000 0.1464230000
C 3.7550910000 -1.7365990000 0.3873660000
H 5.3765140000 -1.0460890000 -1.7773330000
H 3.8038140000 -1.6141590000 -2.3668890000
H 4.2503250000 0.0999400000 -2.5272620000
H 5.4435930000 0.5313790000 0.2777610000
H 4.2695710000 1.6048110000 -0.4945250000
H 3.9416330000 0.9360120000 1.1256530000
H 4.7938550000 -2.0455020000 0.5403810000
H 3.3127110000 -1.5401570000 1.3662760000
H 3.2269090000 -2.5686890000 -0.0895200000
H -0.1718950000 4.2352320000 0.5083670000
H 0.5883250000 2.9159400000 1.4080210000
H 0.7117770000 2.9867880000 -0.3642660000
H -2.3500330000 3.7958960000 1.5972700000
H -3.1576430000 2.2342720000 1.4914800000
H -1.7152290000 2.4338000000 2.5195740000
H -2.1127730000 3.8140830000 -0.9805200000
H -1.3861110000 2.4517950000 -1.8252450000
H -2.9614940000 2.2706690000 -1.0315440000

Equilibrium geometry of **r16-exo-3r-ts**.

C 0.1377052887 0.6501238044 -0.4060941981
N -0.6045836713 1.3156684342 0.5064580227
H -0.2599764476 1.1658148540 1.4554204042
H 0.1685973859 1.0539377640 -1.4108641082
C 1.4805497101 0.1651846846 0.1443867473
C -1.2842590299 2.6422372267 0.3314786557
C -2.4542311332 -0.8963029745 0.6918964007
C -1.0939852714 -1.4986516041 0.6596859990
C -0.6255974382 -1.1342831110 -0.7410490183
C -1.7935817094 -0.8275366555 -1.4719827028
C -2.8749709302 -0.6137092806 -0.5904721709
H -3.0516530335 -0.7934261141 1.5911612227
H 0.2138377613 -1.6328568406 -1.2159197631
H -1.1992993000 -2.5953836156 0.7042743786
H -0.4345419348 -1.2189057398 1.4842747211
H -1.8346179482 -0.7027542659 -2.5494633911
H -3.8610495193 -0.2665979220 -0.8750996980
C -2.4105598740 2.7126302607 1.3714125561
C -0.2336908002 3.7335776221 0.6161871359
C -1.8465158296 2.8010576118 -1.0838772197

O 2.3077840176 -0.1326110335 -0.8353442427
O 1.6577272576 0.0953090206 1.3451235628
C 3.7209917081 -0.6055716517 -0.5798119869
C 4.2460244583 -0.8273991991 -1.9940411168
C 4.4835681851 0.5032838382 0.1400221951
C 3.6734209368 -1.9097894959 0.2132006031
H 5.2844811084 -1.1682072207 -1.9470156419
H 3.6599128562 -1.5895415330 -2.5165942760
H 4.2159569872 0.0983523926 -2.5761971671
H 5.5306925848 0.2024171114 0.2449702803
H 4.4572742985 1.4314619786 -0.4394948595
H 4.0809228754 0.6878006995 1.1376852806
H 4.6885865416 -2.3105117508 0.2972504192
H 3.2827408564 -1.7579754548 1.2207192324
H 3.0641735480 -2.6587039521 -0.3043232516
H -0.6997277331 4.7222558920 0.5597123103
H 0.1956014073 3.6224108549 1.6178069317
H 0.5813493824 3.6998377334 -0.1146756744
H -2.8685657659 3.7055417771 1.3604083907
H -3.1890869790 1.9736786189 1.1615925287
H -2.0279947658 2.5374835864 2.3836580548
H -2.3669885902 3.7607324644 -1.1471145313
H -1.0630888642 2.8151470913 -1.8488592825
H -2.5689481368 2.0176619622 -1.3265798305

Equilibrium geometry of **r16-exo-3s-mc**.

C 0.4044490000 1.1587750000 0.3834200000
N -0.2378160000 1.8409290000 -0.4979810000
C -1.2918070000 2.8953050000 -0.3413060000
C 1.5762310000 0.3524690000 -0.1429000000
H 0.2088800000 1.2717290000 1.4408000000
H 0.0820510000 1.6596490000 -1.4581880000
C -0.6778290000 -1.5509070000 0.6934840000
C -1.1800100000 -1.7904710000 -0.7042000000
C -2.5927350000 -1.2797070000 -0.6512630000
C -2.8730310000 -0.8557670000 0.6040880000
C -1.6885350000 -1.0306400000 1.4409510000
H 0.2887030000 -1.8721610000 1.0610140000
H -3.2717960000 -1.2956300000 -1.4957320000
H -1.1601900000 -2.8649470000 -0.9441300000
H -0.5697520000 -1.3089710000 -1.4818720000
H -3.8244270000 -0.4730210000 0.9563000000
H -1.6505350000 -0.8173850000 2.5046170000
C -2.4205480000 2.5415700000 -1.3218660000
C -1.7889790000 2.9383350000 1.1026650000
C -0.6169520000 4.2207470000 -0.7436040000
O 2.3500100000 -0.0271730000 0.8450370000
O 1.7025560000 0.2071810000 -1.3438740000
C 3.6788970000 -0.7240360000 0.6116380000
C 4.1912880000 -0.9174710000 2.0336810000
C 3.4202830000 -2.0564820000 -0.0868490000
C 4.5758150000 0.2106670000 -0.1956250000
H 5.1633030000 -1.4180200000 2.0015690000
H 4.3167710000 0.0430650000 2.5413540000
H 3.5059570000 -1.5380910000 2.6184720000
H 5.5675930000 -0.2436090000 -0.2841970000
H 4.1878880000 0.3751240000 -1.2026300000
H 4.6924950000 1.1734570000 0.3117940000
H 4.3675960000 -2.5993500000 -0.1622490000
H 2.7295650000 -2.6764080000 0.4940520000
H 3.0253060000 -1.9195410000 -1.0952760000
H -1.3615450000 5.0213030000 -0.7111920000
H 0.1963660000 4.4786590000 -0.0585680000
H -0.2182470000 4.1770520000 -1.7626220000
H -3.1832810000 3.3245470000 -1.2882000000

H -2.0509740000 2.4855970000 -2.3522430000
H -2.8840620000 1.5865030000 -1.0619260000
H -2.5700390000 3.6993700000 1.1780860000
H -2.2244490000 1.9822660000 1.4084820000
H -0.9966290000 3.2188940000 1.8046560000

Equilibrium geometry of **r16-exo-3s-prod.**

C 0.0126190000 0.2814170000 0.5616300000
N -0.9130240000 0.8851950000 -0.4821170000
C -1.2789550000 2.3913970000 -0.3719160000
C 1.4028750000 0.1429050000 -0.0734310000
H 0.0544880000 0.9021740000 1.4535900000
H -0.3405490000 0.8231980000 -1.3432320000
C -0.6495030000 -1.1179140000 0.8358000000
C -1.1678310000 -1.4534630000 -0.5850850000
C -2.0464520000 -0.1946850000 -0.6479160000
C -2.7982810000 -0.2887250000 0.6627090000
C -1.9622430000 -0.8440100000 1.5498230000
H 0.0385590000 -1.8154660000 1.3120610000
H -2.6000910000 0.0166100000 -1.5589290000
H -1.7707850000 -2.3617740000 -0.6042360000
H -0.3943110000 -1.5057050000 -1.3575500000
H -3.8057050000 0.0722660000 0.8265430000
H -2.1377030000 -1.0165440000 2.6054930000
C -2.1869230000 2.7124040000 -1.5664150000
C -1.9776550000 2.7283580000 0.9468750000
C 0.0424350000 3.1680030000 -0.4934800000
O 2.2899220000 -0.1745030000 0.8377500000
O 1.5564560000 0.2843400000 -1.2766830000
C 3.7315410000 -0.4985740000 0.5040310000
C 4.3208780000 -0.7791220000 1.8820300000
C 3.7504990000 -1.7395070000 -0.3842930000
C 4.3776760000 0.7190980000 -0.1506590000
H 5.3761010000 -1.0476670000 1.7772850000
H 4.2535190000 0.1032820000 2.5250330000
H 3.8022990000 -1.6099770000 2.3694430000
H 5.4465360000 0.5230910000 -0.2821030000
H 3.9453150000 0.9301370000 -1.1302010000
H 4.2765940000 1.6026780000 0.4876940000
H 4.7881410000 -2.0517690000 -0.5379730000
H 3.2205560000 -2.5687950000 0.0954870000
H 3.3073650000 -1.5444180000 -1.3631510000
H -0.1814860000 4.2379530000 -0.5134590000
H 0.7073790000 2.9927260000 0.3583720000
H 0.5802780000 2.9198460000 -1.4134980000
H -2.3614790000 3.7912940000 -1.5968730000
H -1.7244720000 2.4304950000 -2.5195380000
H -3.1639090000 2.2272560000 -1.4879440000
H -2.1190490000 3.8129160000 0.9793710000
H -2.9618190000 2.2662500000 1.0350130000
H -1.3852270000 2.4547510000 1.8245360000

Equilibrium geometry of **r16-exo-3s-ts.**

C 0.1376186620 0.6511936712 0.4061341665
N -0.6055990369 1.3152393507 -0.5067745881
C -1.2858636802 2.6415937675 -0.3330867949
C 1.4806014508 0.1667567595 -0.1445745033
H 0.1686888756 1.0560586375 1.4104846119
H -0.2613157599 1.1645442434 -1.4557299086
C -0.6239257214 -1.1334662462 0.7432169312
C -1.0929501648 -1.4996661871 -0.6568220039
C -2.4539238986 -0.8990284253 -0.6886290553
C -2.8740417779 -0.6156680780 0.5937219527

C -1.7917402283 -0.8273577853 1.4746485674
H 0.2162586149 -1.6308575270 1.2179900204
H -3.0521062397 -0.7976939106 -1.5875476948
H -1.1969763948 -2.5965295927 -0.7003825764
H -0.4344743227 -1.2198807358 -1.4821244329
H -3.8603410478 -0.2695691865 0.8787427732
H -1.8321353299 -0.7016180746 2.5520028913
C -2.4121443694 2.7104056708 -1.3731884869
C -1.8482884372 2.8016619847 1.0821062599
C -0.2357700676 3.7330968084 -0.6188983004
O 2.3084421388 -0.1299537920 0.8349798238
O 1.6572675874 0.0961322010 -1.3453760873
C 3.7214012672 -0.6033080733 0.5789662134
C 4.2470490353 -0.8251004950 1.9930638705
C 3.6732008905 -1.9077741954 -0.2138065120
C 4.4838329104 0.5052946742 -0.1414911436
H 5.2846620079 -1.1681564472 1.9455334807
H 4.2194677995 0.1010957048 2.5745979247
H 3.6597953738 -1.5855838334 2.5166238094
H 5.5308411453 0.2042236218 -0.2469187294
H 4.0806588219 0.6896195276 -1.1390283651
H 4.4580004410 1.4336584060 0.4378509924
H 4.6881669823 -2.3089290622 -0.2978554306
H 3.0637085910 -2.6563123319 0.3040360541
H 3.2824740636 -1.7561082722 -1.2213831782
H -0.7023003676 4.7216232485 -0.5633920090
H 0.5792458452 3.7002820943 0.1120936922
H 0.1936679484 3.6212190297 -1.6204438039
H -2.8707091626 3.7029895108 -1.3631976985
H -2.0294678717 2.5345153932 -2.3852168043
H -3.1902211682 1.9712706815 -1.1627351423
H -2.3686354333 3.7614901588 1.1443941803
H -2.5709547492 2.0186025017 1.3254056464
H -1.0649429183 2.8162749292 1.8472306441