

Supporting information

Substituent Effects and Chemoselectivity in the Intramolecular Buchner Reaction of Diazoacetamide Derivatives Catalyzed by Di-Rh(II)-Complex

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Table of contents:

Table S1. Energies calculated at ω B97X-D /BSI level including potential energy (E), Gibbs free energy (G), and correct Gibbs free-energy (G_{FEC}). (unit: a.u., Z=H)	S2
Table S2. Energies calculated at ω B97X-D /BSI level including potential energy (E), Gibbs free energy (G), and correct Gibbs free-energy (G_{FEC}). (unit: a.u., Z=Me)	S3
Table S3. Energies calculated at ω B97X-D /BSI level including potential energy (E), Gibbs free energy (G), and correct Gibbs free-energy (G_{FEC}). (unit: a.u., Z=OMe)	S4
Table S4. Energies calculated at ω B97X-D /BSI level including potential energy (E), Gibbs free energy (G), and correct Gibbs free-energy (G_{FEC}). (unit: a.u., Z=CN)	S5
Table S5. Energies calculated at ω B97X-D /BSI level including potential energy (E), Gibbs free energy (G), and correct Gibbs free-energy (G_{FEC}). (unit: a.u., Z=C(O)Me)	S6
Table S6. APT charge of molecular architectures 3 . (Z=H/Me/OMe/CN/C(O)Me)	S7
Figure S1. The free energy diagram of PhCH ₂ N(CH(CH ₃) ₂)COcMeN ₂ catalysed by Rh ₂ (OAc) ₄	S8
Figure S2. The free energy diagram of PhCH ₂ N(CH(CH ₃) ₂)COcOMeN ₂ catalysed by Rh ₂ (OAc) ₄	S8
Figure S3. The free energy diagram of PhCH ₂ N(CH(CH ₃) ₂)COCCNN ₂ catalysed by Rh ₂ (OAc) ₄	S9
Figure S4. The free energy diagram of PhCH ₂ N(CH(CH ₃) ₂)COCC(O)MeN ₂ catalysed by Rh ₂ (OAc) ₄	S9
Figure S5. The intrinsic reaction coordinates (IRC) for the transition states in the reactions of PhCH ₂ N(CH(CH ₃) ₂)COCCNN ₂ catalyzed by Rh ₂ (OAc) ₄	S10
Figure S6. The diagram of activation energy in the process of C-H activation / C-C aromatic cycloaddition and APT charge	S12
Cartesian coordinates of all stationary points optimized at ωB97X-D/BSI level (Z=H/Me/OMe/CN/C(O)Me)	S13

Table S1. Energies calculated at ω B97X-D /BSI level including potential energy (E), Gibbs free energy (G), and correct Gibbs free-energy (G_{FEC}). (unit: a.u., Z=H)

Complex	E	G	G_{FEC}
N₂	-109.4850486	-109.497784	-109.460787
Sub	-705.5209286	-705.304636	-705.267639
1	-1132.791953	-1132.626891	-1132.589894
2	-1838.345944	-1837.940431	-1837.903434
TS 2-3	-1838.314883	-1837.912814	-1837.875817
3	-1728.83908	-1728.443642	-1728.406645
4-1	-1728.842867	-1728.446861	-1728.409864
4-2	-1728.838555	-1728.444624	-1728.407627
4-3	-1728.843088	-1728.44511	-1728.408113
4-4	-1728.842329	-1728.444867	-1728.40787
TS 4-1	-1728.83274	-1728.43375	-1728.396753
TS 4-2	-1728.820144	-1728.427233	-1728.390236
TS 4-3	-1728.82682	-1728.43085	-1728.393853
TS 4-4	-1728.840051	-1728.440798	-1728.403801
A	-596.1316912	-595.918957	-595.88196
B	-596.1047605	-595.894933	-595.857936
C	-596.1068385	-595.897383	-595.860386
D	-596.0744768	-595.862024	-595.825027
TS D-D_{RE}	-596.0629018	-595.852016	-595.815019
D_{RE}	-596.0787133	-595.867073	-595.830076

Table S2. Energies calculated at ω B97X-D /BSI level including potential energy (E), Gibbs free energy (G), and correct Gibbs free-energy (G_{FEC}). (unit: a.u., Z=Me)

Complex	E	G	G_{FEC}
N₂	-109.4850486	-109.497784	-109.460787
Sub	-744.8212544	-744.576472	-744.539475
1	-1132.791953	-1132.626891	-1132.589894
2	-1877.647559	-1877.211444	-1877.174447
TS 2-3	-1877.6298	-1877.198764	-1877.161767
3	-1768.163439	-1767.740716	-1767.703719
4-1	-1768.165949	-1767.741213	-1767.704216
4-2	-1768.160258	-1767.739648	-1767.702651
4-3	-1768.165028	-1767.740713	-1767.703716
4-4	-1768.165877	-1767.74128	-1767.704283
TS 4-1	-1768.146881	-1767.72069	-1767.683693
TS 4-2	-1768.137746	-1767.719181	-1767.682184
TS 4-3	-1768.135588	-1767.715717	-1767.67872
TS 4-4	-1768.148058	-1767.72103	-1767.684033
A	-635.437418	-635.198383	-635.161386
B	-635.4105727	-635.172286	-635.135289
C	-635.4119702	-635.175531	-635.138534
D	-635.3847172	-635.146259	-635.109262
TS D-D_{RE}	-635.3719333	-635.134182	-635.097185
D_{RE}	-635.3858922	-635.147328	-635.110331

Table S3. Energies calculated at ω B97X-D /BSI level including potential energy (E), Gibbs free energy (G), and correct Gibbs free-energy (G_{FEC}). (unit: a.u., Z=OMe)

Complex	E	G	G_{FEC}
N₂	-109.4850486	-109.497784	-109.460787
Sub	-819.990272	-819.745142	-819.708145
1	-1132.791953	-1132.626891	-1132.589894
2	-1952.812975	-1952.374324	-1952.337327
TS 2-3	-1952.812652	-1952.375846	-1952.338849
3	-1843.371342	-1842.944129	-1842.907132
4-1	-1843.367239	-1842.938253	-1842.901256
4-2	-1843.370482	-1842.942911	-1842.905914
4-3	-1843.368259	-1842.939047	-1842.90205
4-4	-1843.369538	-1842.941208	-1842.904211
TS 4-1	-1843.320224	-1842.89096	-1842.853963
TS 4-2	-1843.319881	-1842.894978	-1842.857981
TS 4-3	-1843.31698	-1842.890191	-1842.853194
TS 4-4	-1843.332257	-1842.903413	-1842.866416
A	-710.60828	-710.365001	-710.328004
B	-710.584896	-710.343775	-710.306778
C	-710.5873163	-710.347338	-710.310341
D	-710.5604228	-710.319568	-710.282571
TS D-D_{RE}	-710.5468156	-710.306182	-710.269185
D_{RE}	-710.5604229	-710.319569	-710.282572

Table S4. Energies calculated at ω B97X-D /BSI level including potential energy (E), Gibbs free energy (G), and correct Gibbs free-energy(G_{FEC}). (unit: a.u., $Z=\text{CN}$)

Complex	E	G	G_{FEC}
N₂	-109.4850486	-109.497784	-109.460787
Sub	-797.720678	-797.508438	-797.498454
1	-1132.791953	-1132.626891	-1132.589894
2	-1930.534202	-1930.131668	-1930.094671
TS 2-3	-1930.512191	-1930.113512	-1930.076515
3	-1821.045867	-1820.651677	-1820.61468
4-1	-1821.050265	-1820.65568	-1820.618683
4-2	-1821.050928	-1820.658222	-1820.621225
4-3	-1821.050262	-1820.655461	-1820.618464
4-4	-1821.050893	-1820.658353	-1820.621356
TS 4-1	-1821.032959	-1820.637803	-1820.600806
TS 4-2	-1821.030593	-1820.638096	-1820.601099
TS 4-3	-1821.032846	-1820.644418	-1820.607421
TS 4-4	-1821.049176	-1820.654421	-1820.617424
A	-688.3311306	-688.122469	-688.085472
B	-1821.078577	-1820.684656	-1820.647659
C	-688.3094835	-688.103935	-688.067064
D	-688.2773819	-688.068545	-688.031548
TS D-D_{RE}	-688.2608289	-688.053994	-688.016997
D_{RE}	-688.2755032	-688.068085	-688.031088

Table S5. Energies calculated at ω B97X-D /BSI level including potential energy (E), Gibbs free energy (G), and correct Gibbs free-energy (G_{FEC}). (unit: a.u., Z=C(O)Me)

Complex	E	G	G_{FEC}
N₂	-109.4850486	-109.497784	-109.460787
Sub	-858.1173966	-857.866051	-857.829054
1	-1132.791953	-1132.626891	-1132.589894
2	-1990.934898	-1990.493824	-1990.456827
TS 2-3	-1990.909501	-1990.469509	-1990.432512
3	-1881.44704	-1881.019593	-1880.982596
4-1	-1881.445733	-1881.012867	-1880.97587
4-2	-1881.443804	-1881.012393	-1880.975396
4-3	-1881.451743	-1881.021515	-1880.984518
4-4	-1881.443809	-1881.015313	-1880.978316
TS 4-1	-1881.429369	-1880.994734	-1880.957737
TS 4-2	-1881.425017	-1880.997881	-1880.960884
TS 4-3	-1881.435457	-1881.008634	-1880.971637
TS 4-4	-1881.431172	-1880.998632	-1880.961635
A	-748.7255185	-748.479177	-748.44218
B	-748.6976982	-748.456662	-748.419665
C	-748.7020836	-748.461619	-748.424622
D	-748.6686773	-748.422819	-748.385822
TS D-D_{RE}	-748.6556792	-748.412756	-748.375759
D_{RE}	-748.6718674	-748.426256	-748.389259

Table S6. APT charge of molecular architectures **3**. (Z=H/Me/OMe/CN/C(O)Me)

	Rh	carbene-C	1°C	2°C	3°C	4°C
Z=H	1.058	0.343	-0.028	0.288	0.436	0.048
Z=Me	1.029	0.432	-0.018	0.317	0.415	-0.023
Z=OMe	1.055	0.738	-0.018	0.323	0.412	0.023
Z=CN	0.919	0.520	-0.023	0.315	0.428	0.026
Z=COMe	0.995	0.142	-0.024	0.341	0.417	0.008

Figure S1. The free energy diagram of $\text{PhCH}_2\text{N}(\text{CH}(\text{CH}_3)_2)\text{COCMeN}_2$ catalysed by $\text{Rh}_2(\text{OAc})_4$ ($Z=\text{Me}$) (unit: kcal/mol, R-E means ring expansion)

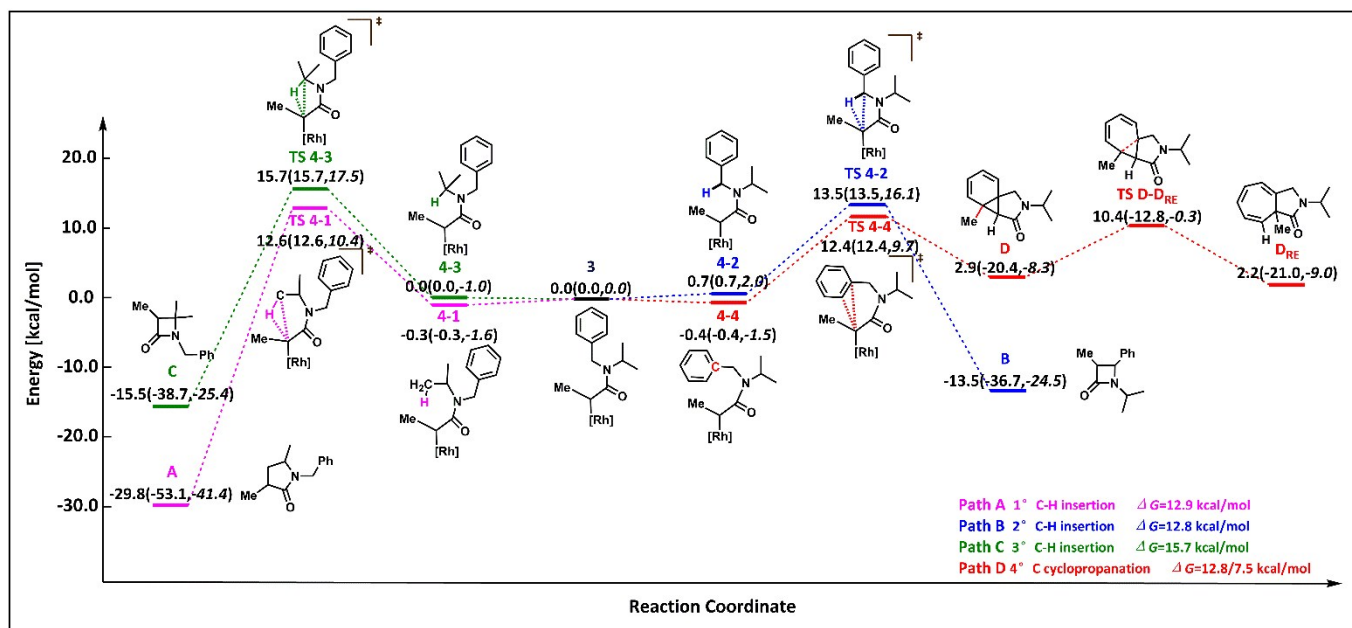


Figure S2. The free energy diagram of $\text{PhCH}_2\text{N}(\text{CH}(\text{CH}_3)_2)\text{COCOMeN}_2$ catalysed by $\text{Rh}_2(\text{OAc})_4$ ($Z=\text{OMe}$) (unit: kcal/mol, R-E means ring expansion)

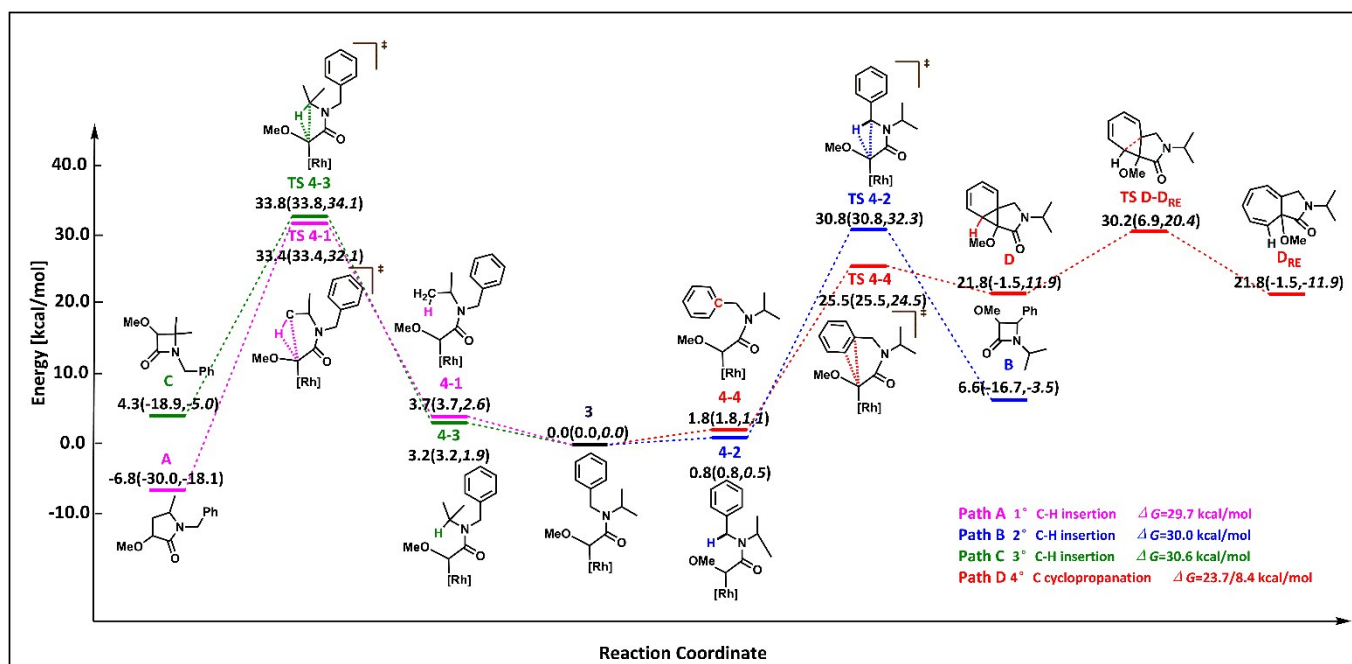


Figure S3. The free energy diagram of $\text{PhCH}_2\text{N}(\text{CH}(\text{CH}_3)_2)\text{COCCNN}_2$ catalysed by $\text{Rh}_2(\text{OAc})_4$ ($\text{Z}=\text{CN}$) (unit: kcal/mol, R-E means ring expansion)

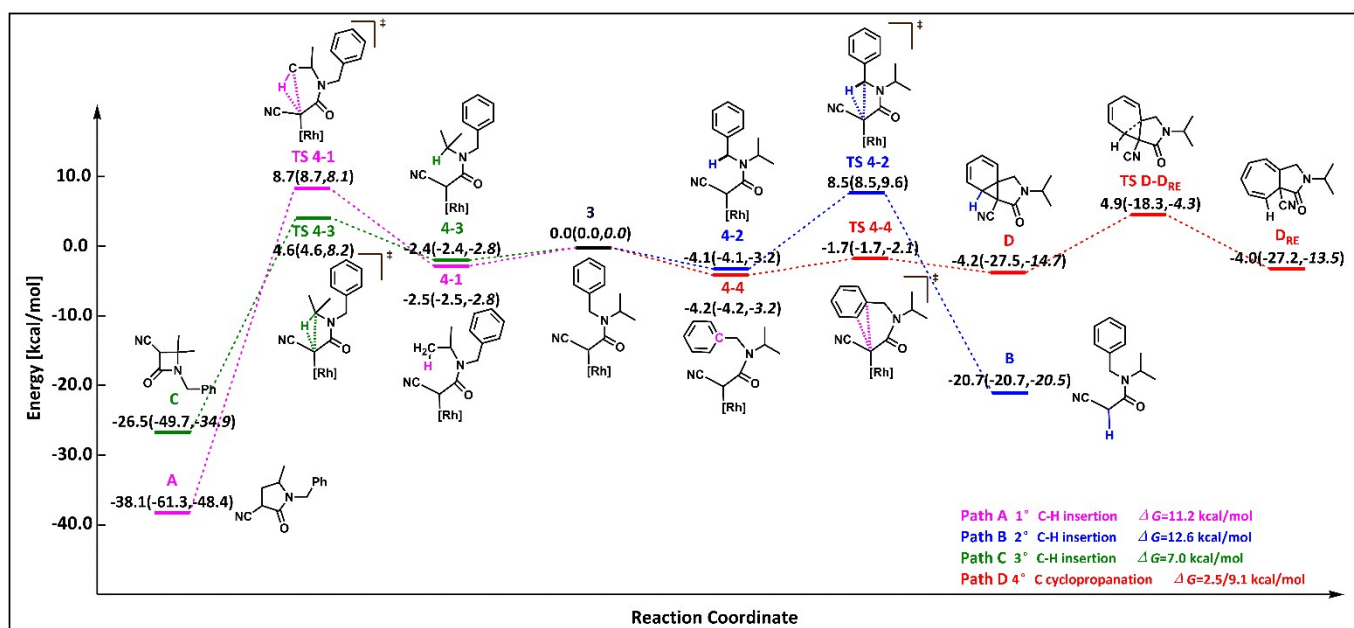


Figure S4. The free energy diagram of $\text{PhCH}_2\text{N}(\text{CH}(\text{CH}_3)_2)\text{COCC}(\text{O})\text{MeN}_2$ catalysed by $\text{Rh}_2(\text{OAc})_4$ ($\text{Z}=\text{C}(\text{O})\text{Me}$) (unit: kcal/mol, R-E means ring expansion)

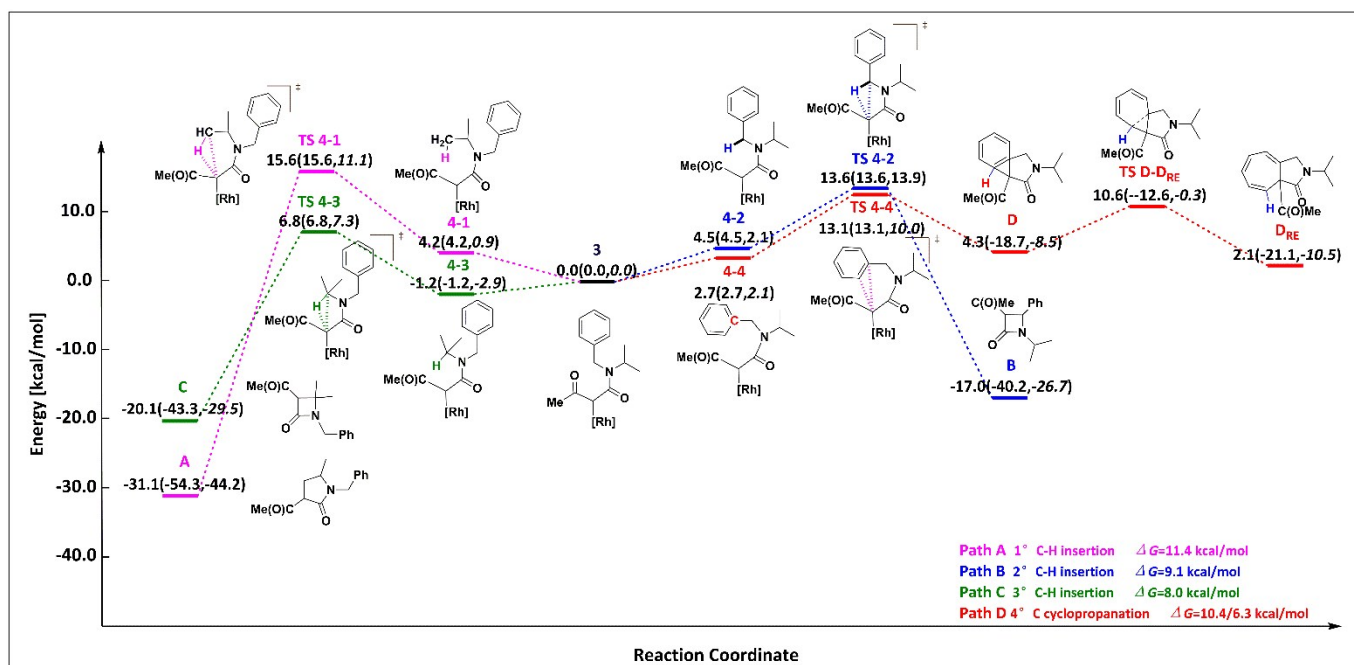
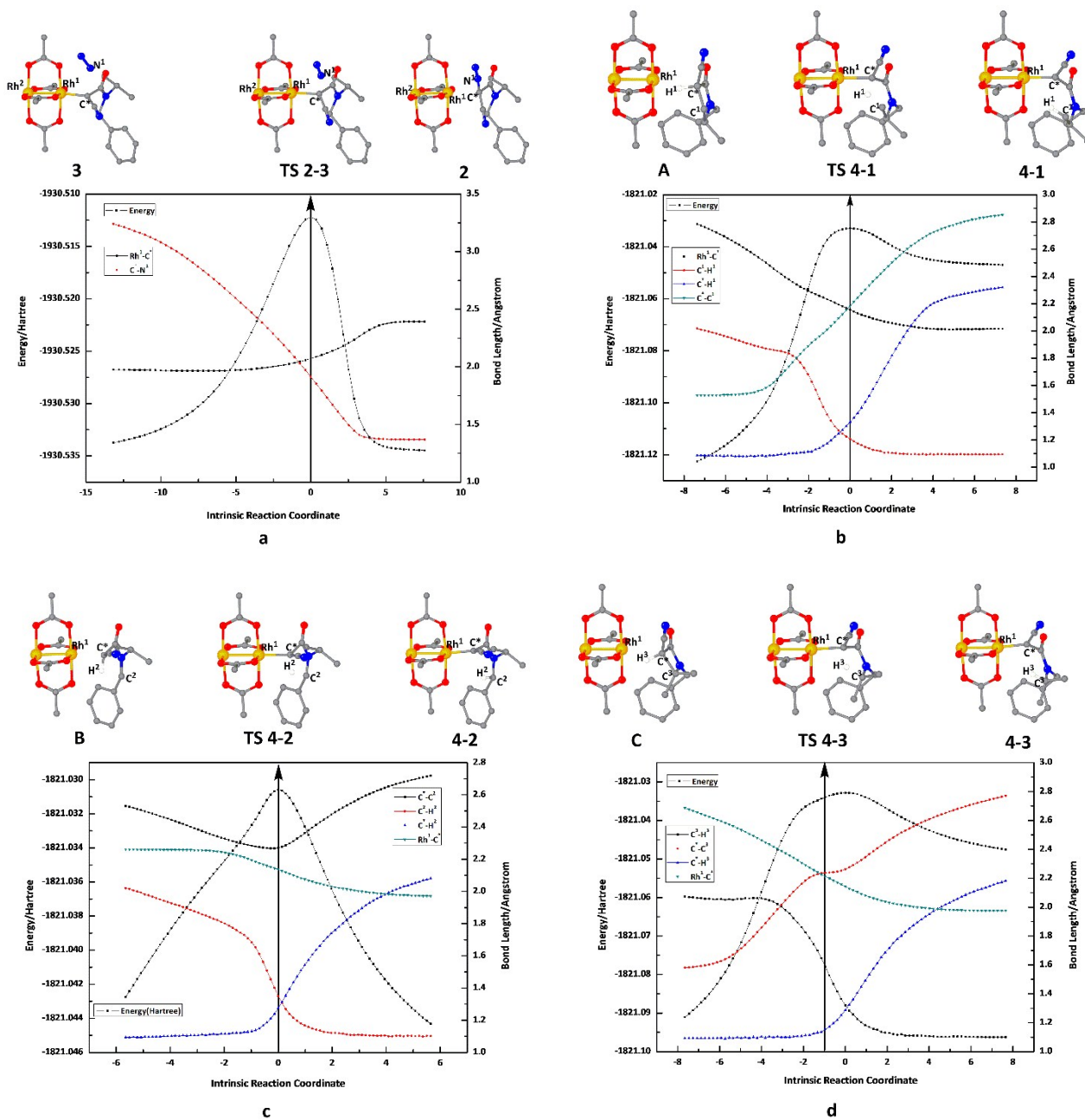
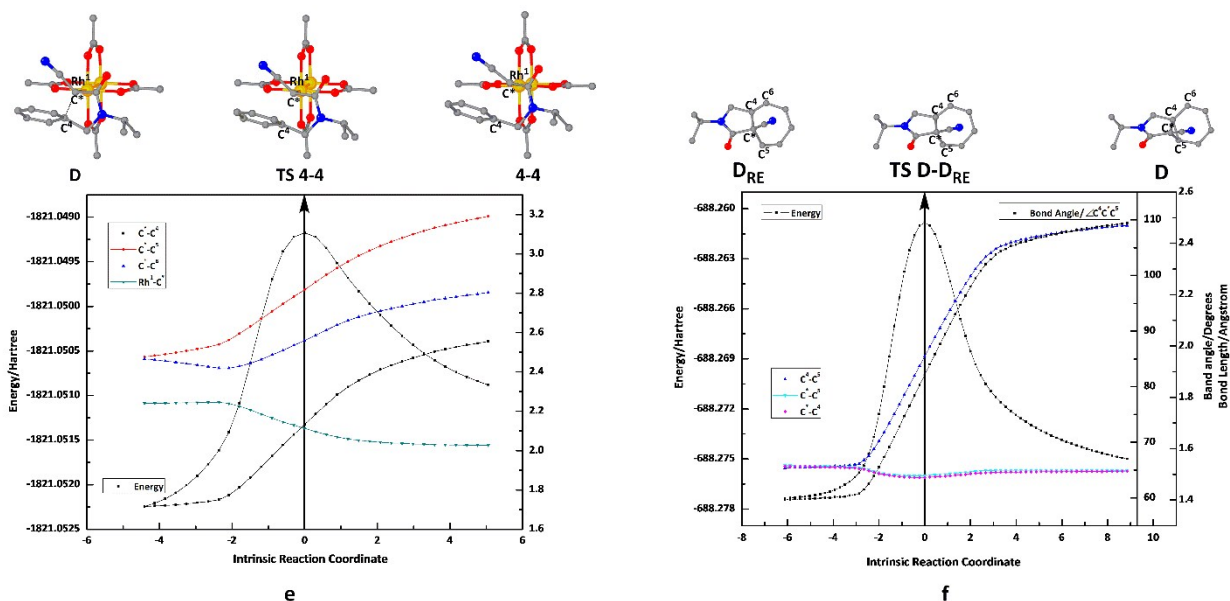


Figure S5. The intrinsic reaction coordinate (IRC) for the transition states of N₂ extrusion (a), 1° C-H insertion (b), 2° C-H insertion (c), 3° C-H insertion (d), 4° C- aromatic cycloaddition(e) and ring-expansion (f).





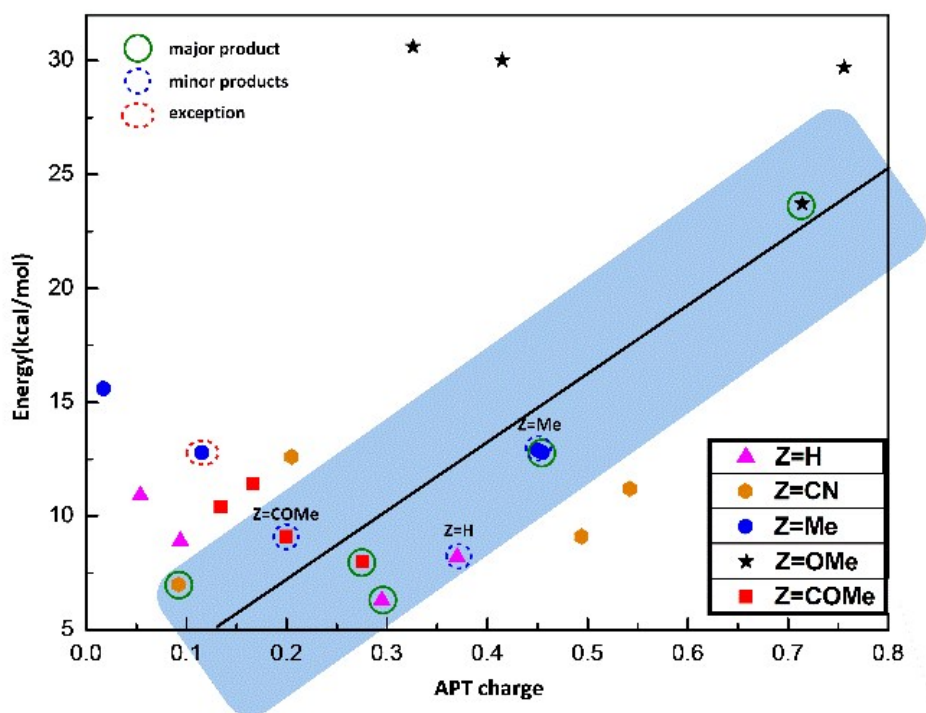
To confirm our assignment of the pathways, the IRC profiles are shown in Figure S5., in which key bond lengths are evaluated along the respective IRCs. All the transition states in the reactions of $\text{PhCH}_2\text{N}(\text{CH}(\text{CH}_3)_2)\text{COCCNN}_2$ catalyzed by $\text{Rh}_2(\text{OAc})_4$ are discussed. The IRC for N_2 extrusion is shown in Figure S5a. Among the IRC and the major structure displayed, it is notable that the $\text{Rh}^1\text{-C}^*$ distance decrease along the IRC, from 2.392 Å to 1.976 Å, and 2.073 Å in **TS 2-3**, consistent with the strengthening of the bond $\text{Rh}^1\text{-C}^*$, and generate metal-carbene **3**. The $\text{C}^*\text{-N}^1$ distance increase along the IRC, from 1.369 Å to 3.240 Å, consistent with the weakening of the bond $\text{C}^*\text{-N}$, accompanied with $\text{C}^*\text{-N}$ bond broken and the N_2 extrusion.

The IRC for 1° C-H insertion is shown in Figure S5.b. Among the IRC and the major structure displayed, it is notable that the $\text{Rh}^1\text{-C}^*$ distance along the IRC, from 2.017 Å in **4-1** increase to 2.786 Å in **A**, and the $\text{Rh}^1\text{-C}^*$ bond break with the $\text{C}^*\text{-C}^1$ formation in **TS 4-1**. The bond of $\text{C}^*\text{-C}^1$ generated, the bond length decrease from 2.852 Å in **4-1** to 1.527 Å in **A**, and 2.184 Å in **TS 4-1**. The H^1 transferred from C^1 to C^* , the bond length of $\text{C}^1\text{-H}^1$ increased from 1.094 Å in **4-1** to 2.017 Å in **A**, and 1.207 Å in **TS 4-1**. At the same time, the bond length of $\text{C}^*\text{-H}^1$, accompanied with the $\text{C}^*\text{-H}^1$ bond formation.

The IRC for 2° C-H insertion is shown in Figure S5.c. An interesting results was found in this step. The β -lactams did not produced When $\text{Z}=\text{CN}$. The reaction mechanism are different with the other substituent group. Among the IRC and the major structure displayed, it is notable that the $\text{C}^*\text{-H}^2$ distance along the IRC, decrease from 2.018 Å in **4-2** to 1.095 Å in **B**, and 1.276 Å in **TS 4-2**. The $\text{C}^2\text{-H}^2$ distance increase from 1.102 Å in **4-2** to 2.020 Å in **B**, and 1.305 Å in **TS 4-2**. There is noteworthy exception that the $\text{C}^*\text{-C}^2$ bond does not formation. The bond length decreased from 2.720 Å in **4-2** at the initial to 2.270 Å in **TS 4-2**, and then increased to 2.532 Å unexpected. Whereas among the IRC, the $\text{C}^*\text{-C}^2$ formation in other systems with different substituent group and generate β -lactams.

The IRC for 3° C-H insertion is shown in Figure S5.d. Among the IRC and the major structure displayed, it is notable that the $\text{Rh}^1\text{-C}^*$ distance along the IRC, from 1.976 Å in **4-3** increased to 2.686 Å in **C** with the bond broken. The H^3 transferred from C^3 to C^* , the bond length of $\text{C}^3\text{-H}^3$ increased from 1.101 Å in **4-3** to 2.072 Å in **C**, and 1.320 Å in **TS 4-3**. At the same time, the bond length of $\text{C}^*\text{-H}^3$ decreased from 2.182 Å in **4-3** to 1.093 Å in **C**, and 1.288 Å in **TS 4-3**, accompanied with the bonds $\text{C}^*\text{-H}^3$ and $\text{C}^*\text{-C}^3$ formation. Meanwhile, the bond of $\text{C}^*\text{-C}^3$ decreased from 2.770 Å in **4-3** to 1.581 Å in **C**, and 2.262 Å in **TS 4-3**

Figure S6. The diagram of activation energy in the process of C-H activation / C-C aromatic cycloaddition and APT charge.



For well explained the main driving force of the chemoselectivity, scatter diagram was drawn using the activation energy in the process of C-H activation / C-C aromatic cycloaddition reaction and APT charge (APT charge adopted by the absolute value of C-atom in carbene and 1°/2°/3°/4° C-atom). Apparently, major products and the APT charge have a very nice linear relation, which is indicated in Fig.5 respectively. Minor products scatter across on both sides of the slope. If intersection point of activation energy and APT charge in the shadow area, reaction maybe feasible and product maybe generated. The electronegativity of CN is higher than H, Fig. 5 and Table 1 shows the results of the substituent group and Me/OMe is lower than H.

Cartesian coordinates of all stationary points optimized at ω B97X-D/BSI level (Z=H)

Sub

C	-1.53026200	-1.59883800	-0.36720000
C	-1.85318000	-0.24254100	0.10758200
C	-1.14761300	2.06456100	0.42235400
N	-2.46938500	-2.49063300	-0.21312100
N	-3.28632100	-3.26212000	-0.08869800
O	-2.90776800	-0.01380900	0.68945600
N	-0.89569700	0.71852000	-0.11321600
C	0.19519700	0.52692200	-1.04911600
H	0.40055500	1.48896900	-1.53054600
H	-0.13904700	-0.13049600	-1.86037200
C	1.48855200	-0.01392900	-0.45935200
C	2.65269800	0.02989600	-1.23027300
C	1.54594200	-0.57517200	0.81440900
C	3.84976000	-0.47717500	-0.73859400
H	2.62137700	0.47113000	-2.22450900
C	2.74477500	-1.08348200	1.31015700
H	0.64840000	-0.60529700	1.42509500
C	3.89931300	-1.03728700	0.53636300
H	4.74714500	-0.43177300	-1.34875300
H	2.77366700	-1.51625500	2.30581900
H	4.83336600	-1.43248700	0.92408200
H	-1.86516400	1.91202600	1.23038900
C	0.12329600	2.68150000	1.00471800
H	-0.12011100	3.64017700	1.47348000
H	0.56723000	2.02924500	1.76181300
H	0.88177100	2.87391600	0.23713300
C	-1.80621100	2.96516800	-0.62508300
H	-1.14435400	3.14246400	-1.48155400
H	-2.73179600	2.50808800	-0.98565400
H	-2.04889100	3.93931300	-0.18796900
H	-0.57578600	-1.97665100	-0.70464600

1

Rh	0.00026900	1.18725200	-0.00741800
Rh	-0.00026900	-1.18725200	-0.00741800
O	-1.45127700	1.12726300	-1.46116400
O	-1.45447200	-1.12879100	-1.45886000
O	1.45238800	1.12915600	1.44777100
O	1.45447200	-1.12688100	1.44453900
O	1.45127700	-1.12726300	-1.46116400
O	1.45447200	1.12879100	-1.45886000
O	-1.45447200	1.12688100	1.44453900
O	-1.45238800	-1.12915600	1.44777100
C	-1.86481500	-0.00100400	-1.86514300
C	-1.85866300	-0.00130400	1.85792800
C	1.86481500	0.00100400	-1.86514300
C	1.85866300	0.00130400	1.85792800
C	2.96008300	-0.00638200	-2.89873900
H	3.90866700	-0.23305600	-2.40109800
H	2.77211900	-0.79027200	-3.63531400
H	3.03693200	0.96775400	-3.38256800
C	-2.96008300	0.00638200	-2.89873900
H	-3.90866700	0.23305600	-2.40109800
H	-2.77211900	0.79027200	-3.63531400
H	-3.03693200	-0.96775400	-3.38256800
C	2.89311700	-0.00683000	2.95260500
H	3.37311100	0.96881000	3.03401300
H	2.39756600	-0.24106200	3.90043400
H	3.63272700	-0.78679700	2.76012800
C	-2.89311700	0.00683000	2.95260500
H	-3.37311100	-0.96881000	3.03401300

H	-2.39756600	0.24106200	3.90043400
H	-3.63272700	0.78679700	2.76012800

2

Rh	0.65423700	0.03041600	0.31211100
Rh	2.76022600	0.21658400	-0.85067700
O	1.53791000	-1.33408300	1.56394000
O	3.49428000	-1.21284300	0.44419700
O	-0.10829600	1.43407600	-1.00920500
O	1.87540200	1.63929800	-2.06805400
O	2.10575500	-1.27165100	-2.12218200
O	0.14656200	-1.47460700	-1.01642100
O	1.28594300	1.54495000	1.56163000
O	3.27225000	1.69699600	0.50009000
C	2.74803100	-1.66187600	1.35768300
C	2.44283300	2.04323300	1.38379700
C	0.97158500	-1.78908500	-1.93115800
C	0.66091900	1.92561100	-1.89430500
C	0.54915000	-2.89876500	-2.86167500
H	1.23470500	-2.96865200	-3.70652300
H	0.55345400	-3.84544300	-2.31208000
H	-0.47158100	-2.72366200	-3.21001200
C	3.33851200	-2.66185100	2.31878900
H	3.59910900	-2.14397900	3.24775800
H	2.59937300	-3.42888300	2.55839700
H	4.23954600	-3.10905300	1.89756900
C	0.03888800	2.93121100	-2.83260500
H	-0.58451900	3.62899000	-2.26801700
H	0.81006900	3.46812700	-3.38560000
H	-0.60534900	2.40084800	-3.54214900
C	2.83297500	3.17633100	2.29903800
H	3.91881900	3.26085800	2.35783400
H	2.43140600	4.10871800	1.88786100
H	2.40173900	3.02899800	3.29097800
C	-1.32101400	-0.05624800	1.47522000
C	-2.04776900	-1.36296900	1.28005400
C	-3.48143600	-2.73145500	-0.11011100
N	-0.85271300	0.01616600	2.74428900
N	-0.38442100	0.04215500	3.75468200
O	-1.89197700	-2.27304800	2.08273200
N	-2.86248700	-1.43070500	0.18950600
C	-2.91747300	-0.36461700	-0.80114900
H	-3.38780200	-0.78405900	-1.69548200
H	-1.90646800	-0.07879800	-1.10688200
C	-3.69066500	0.87235200	-0.37817600
C	-3.42668100	2.08180500	-1.02588700
C	-4.65448200	0.84403800	0.62937500
C	-4.12606200	3.23531800	-0.68700800
H	-2.65098300	2.11696800	-1.78516600
C	-5.35254600	1.99910700	0.97384400
H	-4.84611800	-0.08424200	1.15826400
C	-5.09375000	3.19719200	0.31459000
H	-3.90806400	4.16887000	-1.19778900
H	-6.09940000	1.96145600	1.76147000
H	-5.63574100	4.09853200	0.58490300
H	-3.34281900	-3.31483000	0.80113800
C	-4.97982200	-2.59815900	-0.37754200
H	-5.40451300	-3.58624800	-0.58217600
H	-5.49906100	-2.18075300	0.48991400
H	-5.19472400	-1.96135700	-1.24352500
C	-2.74146000	-3.44085600	-1.24520300
H	-2.86298700	-2.91475800	-2.20010000
H	-1.67436800	-3.49465200	-1.01638400
H	-3.13264000	-4.45565500	-1.37395300
H	-1.77560000	0.88976700	1.18659400

TS 2-3

Rh	0.59623700	0.01794900	0.28977400
Rh	2.74402800	0.22798200	-0.86478000
O	1.47477400	-1.40476500	1.48158700
O	3.44573400	-1.26564600	0.38513700
O	-0.11887400	1.47985100	-0.99546100
O	1.87893500	1.71561700	-2.02518000
O	2.05984400	-1.20928800	-2.19385300
O	0.09303200	-1.43297300	-1.10077200
O	1.23797200	1.47842500	1.59160700
O	3.24164800	1.65246300	0.55860300
C	2.68694100	-1.73625600	1.27083100
C	2.40395600	1.97259100	1.43953700
C	0.92384300	-1.71906000	-2.02556000
C	0.67022000	2.00529900	-1.84799900
C	0.48480700	-2.79257000	-2.99148600
H	1.13359000	-2.80323100	-3.86780900
H	0.54209500	-3.76440300	-2.49039900
H	-0.55513300	-2.63027200	-3.28417300
C	3.24813800	-2.77713800	2.20718900
H	3.46043900	-2.30384100	3.17144800
H	2.50876000	-3.56292300	2.37644900
H	4.17096900	-3.19433000	1.80286200
C	0.06181400	3.06541800	-2.73505000
H	-0.54497900	3.74844000	-2.13520700
H	0.84222000	3.61216600	-3.26504000
H	-0.59586400	2.58322700	-3.46632800
C	2.78315700	3.07182600	2.40089400
H	3.86835800	3.15496200	2.47207900
H	2.38352100	4.01812300	2.02075300
H	2.34346100	2.88868900	3.38312500
C	-1.18783400	-0.09929200	1.20303600
C	-2.02963700	-1.34670200	1.17393000
C	-3.52621700	-2.70877900	-0.16540300
N	-0.64954200	-0.22692700	3.15527600
N	0.01119900	-0.37020100	4.02317400
O	-1.90112300	-2.22310300	2.01788700
N	-2.88279800	-1.41506500	0.11245400
C	-2.96350400	-0.33772200	-0.86845300
H	-3.53295000	-0.72344200	-1.71903400
H	-1.96868700	-0.10169800	-1.26259900
C	-3.63619600	0.92772700	-0.36444400
C	-3.32455500	2.14561200	-0.97213900
C	-4.56933800	0.90940800	0.67245700
C	-3.94438600	3.32121900	-0.56190800
H	-2.57333500	2.16969000	-1.75501200
C	-5.18564500	2.08662300	1.08948100
H	-4.80142400	-0.02863100	1.16710600
C	-4.87791200	3.29542900	0.47161600
H	-3.68979100	4.26140200	-1.04262200
H	-5.90851400	2.05767500	1.89949600
H	-5.35695800	4.21341900	0.79852300
H	-3.33549200	-3.30417400	0.72883600
C	-5.03738900	-2.56243200	-0.33527100
H	-5.48145400	-3.54460700	-0.52658200
H	-5.49651800	-2.15407700	0.56967500
H	-5.30180400	-1.91181600	-1.17693200
C	-2.85909000	-3.40185500	-1.35437700
H	-3.03055900	-2.85801000	-2.29141200
H	-1.78098500	-3.46929100	-1.18844100
H	-3.26570700	-4.41105400	-1.47844900
H	-1.71976500	0.83576700	1.40089900

3

Rh	0.83465600	0.06563300	-0.56308200
Rh	2.65095000	-0.50341200	0.98360700

O	0.06223600	1.30294300	0.90665300
O	1.74469000	0.79926700	2.33150200
O	1.69222900	-1.19985000	-1.93615600
O	3.36498600	-1.75056000	-0.51354700
O	1.46084600	-2.05079900	1.69840800
O	-0.19862900	-1.54140700	0.25437600
O	2.01156900	1.60439600	-1.24002100
O	3.70032100	1.08207800	0.17013100
C	0.68973300	1.40067300	2.01362500
C	3.17097100	1.77043600	-0.74084200
C	0.32782300	-2.22975400	1.19264600
C	2.75716500	-1.82211100	-1.61287100
C	-0.51346000	-3.37498600	1.70090300
H	-0.51020900	-4.17227600	0.95083500
H	-0.10780500	-3.76072200	2.63665900
H	-1.54897800	-3.05085500	1.83244600
C	0.09138500	2.35576300	3.01884300
H	0.19299700	3.37855000	2.64251100
H	-0.97621400	2.15181700	3.13662800
H	0.60064500	2.26793900	3.97865900
C	3.34593600	-2.70917700	-2.68278500
H	2.55060400	-3.22874200	-3.22139500
H	3.88433200	-2.08151200	-3.40062800
H	4.04410400	-3.42230300	-2.24309900
C	3.98607000	2.89094700	-1.33813700
H	4.74670000	3.22302700	-0.63031000
H	4.48378400	2.51699800	-2.23908100
H	3.33614500	3.71824000	-1.62877400
C	-0.70890700	0.39130700	-1.74780700
C	-1.74998300	1.34358000	-1.46135600
C	-3.43854800	2.65574500	-0.37082800
O	-1.38215600	2.22085700	-2.26533100
N	-2.72444700	1.37921700	-0.56389200
C	-2.87811000	0.28327100	0.38608500
H	-2.97834000	0.71422900	1.38738300
H	-1.94824600	-0.29317600	0.39808200
C	-4.03550200	-0.64867200	0.09512200
C	-4.70196300	-1.26456800	1.15472100
C	-4.41050200	-0.96182400	-1.21126400
C	-5.72138700	-2.18215600	0.91602300
H	-4.42193500	-1.02443300	2.17827200
C	-5.43368400	-1.87371600	-1.45331200
H	-3.90774700	-0.48221600	-2.04693700
C	-6.09106800	-2.48847500	-0.39059400
H	-6.23045300	-2.65229400	1.75220800
H	-5.71620300	-2.10507500	-2.47606800
H	-6.88772000	-3.20134900	-0.58022200
H	-3.30530800	3.19792100	-1.31116800
C	-4.92983800	2.43464400	-0.13650600
H	-5.42940100	3.40642000	-0.07559200
H	-5.38142000	1.86068400	-0.95007600
H	-5.11985600	1.90242800	0.80159800
C	-2.77667800	3.46102700	0.74896300
H	-2.91051500	2.97350600	1.72126200
H	-1.70511700	3.56788500	0.56157800
H	-3.22980200	4.45559400	0.81051400
H	-0.83065600	-0.14187600	-2.69354200

4-1

Rh	-0.91778600	0.24129200	-0.56735300
Rh	-2.51774300	-0.64028400	1.07284600
O	0.52776100	-0.94613000	0.31264600
O	-0.94260800	-1.76523300	1.82519100
O	-2.44891900	1.36898600	-1.35632300
O	-3.93145000	0.57669900	0.15859200
O	-1.98629100	0.92117800	2.32994700

O	-0.52965200	1.74737500	0.81377700
O	-1.45596900	-1.32263300	-1.78358300
O	-2.93873000	-2.14035700	-0.28579400
C	0.19602400	-1.68219600	1.30254100
C	-2.33486200	-2.15578100	-1.38911500
C	-1.13945800	1.75747900	1.93473700
C	-3.60776000	1.28158800	-0.83089100
C	-0.80252100	2.91239600	2.84669500
H	-1.17294900	3.83956300	2.39840300
H	-1.26340800	2.77134200	3.82449900
H	0.28184700	3.00331500	2.94981800
C	1.29723500	-2.54096900	1.87327000
H	1.54973600	-3.31798000	1.14436900
H	2.19561300	-1.94046700	2.03829600
H	0.97173000	-3.00822800	2.80284800
C	-4.69613800	2.08687700	-1.49830000
H	-4.28549400	2.99931300	-1.93410800
H	-5.12785000	1.48562800	-2.30552300
H	-5.48415500	2.32015700	-0.78087900
C	-2.68919000	-3.24400900	-2.37198300
H	-3.16157700	-4.08071600	-1.85578600
H	-3.39319300	-2.83836800	-3.10621900
H	-1.79629700	-3.57240200	-2.90746500
C	0.32385300	1.05452200	-1.84899200
C	1.74524900	0.81809800	-1.96507700
C	2.50041700	2.19270800	-0.11554700
O	1.75677300	0.01117100	-2.90942600
N	2.76037600	1.27835700	-1.24277000
C	4.10863100	0.84043300	-1.59669600
H	4.75395900	1.72142500	-1.66338700
H	4.03447800	0.41168400	-2.60068000
C	4.70456600	-0.17678800	-0.64860000
C	5.95163600	0.04969000	-0.06882600
C	4.02277100	-1.36278900	-0.36589400
C	6.51843100	-0.89407100	0.78547300
H	6.48404000	0.97417500	-0.28193000
C	4.59188600	-2.30704300	0.48145600
H	3.04084500	-1.53785500	-0.79806200
C	5.83889700	-2.07599000	1.06062900
H	7.48841400	-0.70408400	1.23516700
H	4.06161700	-3.23118700	0.69073800
H	6.27644300	-2.81545400	1.72459400
H	1.43716000	2.44666900	-0.18712600
C	2.70277800	1.51170500	1.23686000
H	2.35737500	2.18509900	2.02798200
H	2.11707700	0.59089500	1.27891300
H	3.75531300	1.27770400	1.42098900
C	3.31371000	3.47884100	-0.24927000
H	4.38103300	3.30447700	-0.07340700
H	3.18892100	3.92910300	-1.23949400
H	2.97341100	4.19945100	0.50032300
H	-0.07218000	1.71624200	-2.62571900

TS 4-1

Rh	0.76288200	0.54454100	0.34357400
Rh	2.20230600	-1.11079600	-0.71523500
O	-0.65930700	0.10221100	-1.08921900
O	0.63470400	-1.48769300	-2.03354900
O	2.28673400	0.92210600	1.67711100
O	3.63573400	-0.59917800	0.68610500
O	2.85537200	0.43148300	-1.94816900
O	1.52676100	1.96515100	-0.95410300
O	0.07954900	-0.98491600	1.54541300
O	1.43802200	-2.51833700	0.59098700
C	-0.41465400	-0.79955000	-1.95575700
C	0.55432100	-2.15766200	1.41240100

C	2.40336600	1.59478100	-1.80315900
C	3.37003200	0.26571200	1.56422000
C	2.96713300	2.67727400	-2.69167600
H	3.78125800	3.17814600	-2.15681900
H	3.36968600	2.24260300	-3.60749900
H	2.20322000	3.42281700	-2.92117300
C	-1.48342200	-1.01289500	-2.99923900
H	-2.47394700	-0.88580400	-2.55763600
H	-1.35260900	-0.26366600	-3.78816000
H	-1.38797600	-2.00468600	-3.44316300
C	4.42723200	0.52789600	2.60875700
H	4.33069300	-0.22826400	3.39513100
H	5.42049400	0.43175100	2.16642400
H	4.29412700	1.51395700	3.05590600
C	-0.01985600	-3.19901300	2.34159500
H	0.46299900	-4.16360700	2.18326800
H	0.11529800	-2.87305000	3.37635900
H	-1.09695100	-3.28874500	2.16782800
C	-0.45236500	1.99425000	1.25057900
C	-1.74835700	1.57018400	1.83868000
C	-2.73716500	2.25973000	-0.26153100
O	-1.70384200	1.08016600	2.95705000
N	-2.87407800	1.68968300	1.07447400
C	-4.01945100	0.84773900	1.39755800
H	-4.94185500	1.42847200	1.29890400
H	-3.90324300	0.58334400	2.45147000
C	-4.07382000	-0.39758100	0.53424100
C	-5.14410500	-0.63710200	-0.32553900
C	-3.02075000	-1.31616700	0.58491800
C	-5.17451200	-1.78408500	-1.11922800
H	-5.96754300	0.07308400	-0.37103500
C	-3.04874100	-2.45823900	-0.20611400
H	-2.16989000	-1.12742100	1.23426300
C	-4.12733100	-2.69770300	-1.05835700
H	-6.01544000	-1.96030300	-1.78364900
H	-2.22010100	-3.16058200	-0.16935000
H	-4.14538400	-3.59010700	-1.67716100
H	-2.53467400	1.45965200	-0.98219800
C	-3.98401300	3.03350600	-0.68404600
H	-3.80477100	3.53790900	-1.63900500
H	-4.83175200	2.35756700	-0.82586200
H	-4.25239600	3.78403400	0.06706800
C	-1.53787500	3.18741800	-0.22262200
H	-1.65956400	4.05594700	0.42427300
H	-0.55277700	2.57586200	0.03060200
H	-1.18859400	3.48047400	-1.21728200
H	0.04296600	2.79542000	1.80482500

A

C	2.86393900	-0.81723100	-0.87636400
C	2.78477300	0.69940900	-1.05784800
H	2.47946000	-1.35685600	-1.75011300
C	1.92229800	-1.10175900	0.28591700
C	1.40520500	1.07390200	-0.48856300
O	1.79648000	-2.15588100	0.88352800
N	1.20217200	0.03925000	0.52320500
C	0.04670500	0.02371700	1.39859500
H	0.05640800	0.91731400	2.03247400
H	0.17367300	-0.84928400	2.04480300
C	-1.25808800	-0.06402800	0.63445300
C	-1.53707000	-1.19990400	-0.13209100
C	-2.18169500	0.97865500	0.65943400
C	-2.71927100	-1.28621000	-0.85732900
H	-0.82167900	-2.01856700	-0.14422300
C	-3.36926300	0.89364700	-0.06517900
H	-1.97447000	1.86533500	1.25486700

C	-3.63921300	-0.23865900	-0.82563000
H	-2.92898600	-2.17636700	-1.44336400
H	-4.08216300	1.71247300	-0.03492200
H	-4.56467500	-0.30892000	-1.38954100
H	0.63372500	0.97114800	-1.26810600
C	1.33851200	2.48340300	0.08093500
H	1.61141900	3.20791200	-0.69319400
H	0.33009200	2.73149600	0.42689400
H	2.03513600	2.59170200	0.91946800
H	3.56214900	1.19192400	-0.46249400
H	2.89781800	1.02509200	-2.09474000
H	3.86407400	-1.20175700	-0.66645800

4-2

Rh	0.92882400	0.11750600	-0.56437900
Rh	2.72399100	-0.52065900	0.97901000
O	-0.00704200	1.05849900	1.02865900
O	1.64284300	0.46634200	2.45814200
O	1.94770500	-0.85981200	-2.05570900
O	3.62259800	-1.44153400	-0.64873700
O	1.65952100	-2.26010100	1.37897800
O	0.00213000	-1.66984500	-0.03736000
O	1.99099200	1.82908100	-0.94969100
O	3.64863900	1.26124500	0.48017900
C	0.55384000	1.02228400	2.17376700
C	3.10066100	2.02497500	-0.35677500
C	0.55777800	-2.44712100	0.80978100
C	3.06141300	-1.41288700	-1.77431400
C	-0.19935600	-3.71501000	1.12217400
H	-0.13913100	-4.38699100	0.26008400
H	0.23062800	-4.20840500	1.99414200
H	-1.25510400	-3.48870300	1.29212900
C	-0.18707200	1.72974900	3.28443100
H	-0.28038200	2.79216100	3.03984900
H	-1.19773500	1.31885900	3.37173100
H	0.34127800	1.61443900	4.23090700
C	3.77753800	-2.06898200	-2.92971800
H	3.05902900	-2.54258500	-3.60165700
H	4.30968500	-1.29628600	-3.49467900
H	4.50170300	-2.79703800	-2.56220100
C	3.82497900	3.29475400	-0.73066600
H	4.58377900	3.53214900	0.01565100
H	4.31097400	3.14873200	-1.70089800
H	3.11179400	4.11517300	-0.83401700
C	-0.58795600	0.47511900	-1.77911000
C	-1.69984800	1.32004200	-1.43877600
C	-3.51402300	2.39816300	-0.28915200
O	-1.35593400	2.29121900	-2.14005200
N	-2.69333800	1.20364700	-0.57183100
C	-2.80392200	-0.01753400	0.22600400
H	-2.61842700	0.23054200	1.27496700
H	-1.98780300	-0.68458800	-0.06930500
C	-4.13299800	-0.71693300	0.06547400
C	-4.95854900	-0.93509600	1.16649300
C	-4.54900700	-1.15952900	-1.19240200
C	-6.18797000	-1.57455200	1.01631200
H	-4.64089800	-0.59694800	2.15038800
C	-5.77505700	-1.79443700	-1.34739300
H	-3.91099400	-0.99064300	-2.05685600
C	-6.59966000	-2.00172600	-0.24172100
H	-6.82325600	-1.73479100	1.88225900
H	-6.08969300	-2.13084700	-2.33082900
H	-7.55876800	-2.49582500	-0.36333900
H	-2.98920100	3.21237300	-0.79680700
C	-4.91960000	2.29102600	-0.88241800
H	-5.42764500	3.25553400	-0.77763900

H	-4.87214600	2.04233400	-1.94669000
H	-5.51930700	1.53081100	-0.37480900
C	-3.52986800	2.70168400	1.20745300
H	-4.12350200	1.96746500	1.76324200
H	-2.51199500	2.71660300	1.60844300
H	-3.98393500	3.68360000	1.37133200
H	-0.64182000	0.02453400	-2.77291500

TS 4-2

Rh	0.62915700	-0.07573000	-0.35006700
Rh	2.84804800	-0.25645300	0.61893500
O	0.48521600	1.80250800	0.51058600
O	2.55670600	1.64299100	1.39878200
O	0.88801200	-1.96877700	-1.12315400
O	2.96346800	-2.13567300	-0.24126000
O	1.92035700	-1.08347600	2.29454400
O	-0.14342900	-0.89014000	1.40124700
O	1.52182600	0.71892700	-2.02070100
O	3.58873100	0.57647400	-1.11357400
C	1.47253200	2.24405700	1.18218700
C	2.78083300	0.87664300	-2.03724400
C	0.67312800	-1.21824000	2.32552300
C	1.98852300	-2.57005900	-0.91168400
C	0.06285000	-1.85189200	3.55290400
H	-0.16864100	-2.89902100	3.33044300
H	0.76421100	-1.81612300	4.38704500
H	-0.87005000	-1.34746200	3.81602900
C	1.29816900	3.61757500	1.78449300
H	0.92508000	4.30853600	1.02411400
H	0.55131600	3.56623000	2.58367500
H	2.24137900	3.97817700	2.19559400
C	2.13481800	-3.92825400	-1.55406200
H	1.20600800	-4.49351700	-1.44940100
H	2.32434800	-3.79128300	-2.62367400
H	2.96932500	-4.47173700	-1.10998400
C	3.36195100	1.50980800	-3.27717400
H	4.31637200	1.03925900	-3.52183900
H	2.66320400	1.43039300	-4.11061900
H	3.54911300	2.56923000	-3.07349500
C	-1.34916800	0.04810600	-1.18478200
C	-1.94003100	1.39224300	-1.44800800
C	-3.38858900	2.74243900	0.11544200
O	-1.64337300	2.20364500	-2.29118500
N	-2.90827800	1.49180500	-0.46934500
C	-2.85844700	0.23832200	0.20386900
H	-2.53286800	0.30211200	1.25122200
H	-1.64236200	-0.25830600	-0.04977300
C	-3.91041300	-0.78336100	-0.01814800
C	-3.94436900	-1.90228000	0.81945200
C	-4.84897000	-0.65276200	-1.04378800
C	-4.91140800	-2.88247400	0.63372700
H	-3.19997800	-2.00473500	1.60576800
C	-5.81962700	-1.63178500	-1.22177800
H	-4.81539300	0.21932700	-1.68950100
C	-5.85217200	-2.74607600	-0.38538200
H	-4.93367300	-3.75074500	1.28487100
H	-6.55374600	-1.52545600	-2.01434200
H	-6.61193800	-3.50864000	-0.52712200
H	-3.14533000	3.48779300	-0.64821700
C	-4.90055000	2.70251700	0.32384000
H	-5.25037400	3.65476100	0.73509100
H	-5.42166000	2.52054700	-0.62053400
H	-5.18067400	1.91034800	1.02853300
C	-2.62563400	3.08134200	1.39872000
H	-2.91178100	2.41583600	2.22276500
H	-1.54906600	2.98740300	1.23061500

H	-2.85430100	4.10505800	1.71151000
H	-1.62547200	-0.76944200	-1.85332700

B

C	-1.01926900	-2.03113100	-0.61176900
C	-2.11563100	-1.23630900	0.11556600
C	-1.86837700	1.32095600	0.11843600
O	-3.15393700	-1.48631000	0.67946000
N	-1.47324500	-0.05406800	-0.13293300
C	-0.37664700	-0.64296200	-0.90923700
H	-0.43445100	-0.37622900	-1.97195700
C	1.01756900	-0.38136600	-0.39631900
C	2.02579500	0.01664000	-1.27189500
C	1.32127000	-0.53728900	0.95891500
C	3.31896200	0.24964400	-0.80825000
H	1.79880100	0.14791600	-2.32749200
C	2.60891700	-0.30448900	1.42528700
H	0.53667800	-0.82902800	1.65276000
C	3.61275900	0.08909900	0.54115600
H	4.09350900	0.56054500	-1.50299600
H	2.83072800	-0.42868800	2.48105400
H	4.61879800	0.27202400	0.90657200
H	-2.95123900	1.27692500	0.28270000
C	-1.20414000	1.88047900	1.37896000
H	-1.58286800	2.88582200	1.59267400
H	-1.41977300	1.24029700	2.23950800
H	-0.11809300	1.93990100	1.25323500
C	-1.57701200	2.18205400	-1.10949000
H	-0.49858700	2.23034400	-1.30140700
H	-2.07240600	1.78184100	-1.99966000
H	-1.93380600	3.20348700	-0.94677900
H	-1.36377300	-2.58763800	-1.48583000
H	-0.42448400	-2.68050700	0.03431800

4-3

Rh	0.85648900	0.24354200	0.60734000
Rh	2.31970400	-0.67524100	-1.13449800
O	-0.74927900	-0.50484500	-0.45180400
O	0.59004500	-1.35707200	-2.06199800
O	2.53915300	0.95005300	1.56143700
O	3.90179100	0.10449500	-0.03605100
O	2.12388300	1.12481800	-2.14708300
O	0.77864100	1.97321300	-0.54401900
O	1.05754400	-1.55115400	1.58082900
O	2.40506700	-2.41331300	-0.01674900
C	-0.53278200	-1.12338700	-1.54693900
C	1.77362100	-2.47201600	1.06938300
C	1.40937800	2.02814500	-1.65257800
C	3.67934000	0.71589000	1.04028200
C	1.26378900	3.32276200	-2.41508500
H	1.67525900	4.14272500	-1.81918600
H	1.78434100	3.26249900	-3.37092400
H	0.20263100	3.53129900	-2.57910300
C	-1.75045000	-1.63163800	-2.27870900
H	-1.89410400	-2.68780100	-2.02959400
H	-2.64886100	-1.09016900	-1.97804200
H	-1.58899200	-1.55632300	-3.35589800
C	4.87206400	1.20118000	1.82800000
H	4.65368700	2.16290100	2.29650400
H	5.08158600	0.47769000	2.62299300
H	5.74714600	1.27597600	1.18137700
C	1.88022000	-3.73961100	1.88085700
H	2.18380200	-4.57121500	1.24367000
H	2.63799200	-3.59537400	2.65824300
H	0.92919800	-3.95258200	2.37261200

C	-0.29456200	1.07467400	1.96103800
C	-1.73311800	0.92936300	1.99449600
C	-2.30250700	2.50582400	0.24508400
O	-1.85556700	0.07721300	2.89246200
N	-2.66361500	1.45158300	1.20743100
C	-4.04000400	0.97085000	1.34797400
H	-4.70916700	1.79431700	1.08500900
H	-4.19456600	0.74979100	2.40880800
C	-4.37009700	-0.25500900	0.51783600
C	-5.31381800	-0.18142000	-0.50623800
C	-3.77049500	-1.48653400	0.80048300
C	-5.65798500	-1.31420100	-1.24146600
H	-5.79452600	0.76894000	-0.72847900
C	-4.11892200	-2.61867300	0.07267200
H	-3.03309700	-1.55374500	1.59363300
C	-5.06251800	-2.53721400	-0.94986100
H	-6.39609300	-1.24026400	-2.03453900
H	-3.64878900	-3.56983800	0.30446300
H	-5.33201000	-3.42404100	-1.51590500
H	-1.21039900	2.57822900	0.27937500
C	-2.67640600	2.12463200	-1.18272400
H	-2.30557800	2.89185700	-1.87009800
H	-2.21920200	1.16836000	-1.43954400
H	-3.76045600	2.04929400	-1.31648800
C	-2.88864700	3.85306300	0.67021900
H	-3.98255600	3.86183600	0.60362200
H	-2.60272900	4.09915500	1.69767300
H	-2.51362500	4.64051900	0.00907800
H	0.12891400	1.62402400	2.80632500

TS 4-3

Rh	-0.70985100	0.55366000	-0.10323300
Rh	-2.31635000	-1.23511800	0.27709800
O	0.54152600	-0.39426100	1.24612500
O	-0.94382900	-2.05465300	1.60773900
O	-2.07003800	1.38728800	-1.40665400
O	-3.55506600	-0.28484500	-1.07510200
O	-3.08344800	-0.05516100	1.80110900
O	-1.57847300	1.59588500	1.45693900
O	0.06896500	-0.61423300	-1.61614100
O	-1.42695000	-2.27246000	-1.27834800
C	0.15176300	-1.47086700	1.80466300
C	-0.44474300	-1.74973500	-1.86853500
C	-2.56806200	1.06524500	2.05511600
C	-3.17098400	0.78763700	-1.61553200
C	-3.15439100	1.84923100	3.20487800
H	-2.63386000	1.56370900	4.12541700
H	-3.01521000	2.92021200	3.04789200
H	-4.21261500	1.61096400	3.32233400
C	1.11329800	-2.07299800	2.80029900
H	0.72772600	-3.01774000	3.18447500
H	2.08525900	-2.22494600	2.32149000
H	1.25688100	-1.37064600	3.62752200
C	-4.08862300	1.42748600	-2.62837800
H	-5.06330800	0.93909800	-2.62352300
H	-4.19451800	2.49365200	-2.41314000
H	-3.63660800	1.33327000	-3.62073600
C	0.20730000	-2.52213800	-2.98907800
H	-0.28015100	-3.48757000	-3.12688700
H	0.14738600	-1.93561300	-3.91020300
H	1.26901000	-2.66610800	-2.76553300
C	0.61741300	2.18712800	-0.50335300
C	1.71055400	1.96225300	-1.48658900
C	2.44103700	2.42381600	0.57453300
O	1.63610000	1.79665600	-2.68189900
N	2.84669000	1.93598300	-0.69922300

C	4.09009300	1.27436400	-1.04456300
H	4.93803800	1.88220400	-0.70867500
H	4.10382400	1.27358400	-2.14009800
C	4.20287100	-0.14108000	-0.51099400
C	5.34619600	-0.55133600	0.17214600
C	3.15281900	-1.04423400	-0.69370400
C	5.44789500	-1.84932900	0.66900400
H	6.16474000	0.14975900	0.32274100
C	3.25258300	-2.33827500	-0.19430300
H	2.24518600	-0.73784300	-1.20781600
C	4.39916500	-2.74599500	0.48772600
H	6.34371900	-2.15640900	1.20062000
H	2.42556700	-3.03013500	-0.33174600
H	4.47268400	-3.75690600	0.87796000
H	1.13053000	2.05321700	0.59057100
C	2.84875100	1.60947800	1.78497200
H	2.39204200	2.01878200	2.68960900
H	2.56493300	0.56388200	1.67160800
H	3.93919900	1.68226400	1.88660800
C	2.53408500	3.92353000	0.76468000
H	3.57524400	4.16881900	1.01073500
H	2.26037000	4.46114300	-0.14519400
H	1.90322100	4.25694000	1.59359700
H	0.09851600	3.14732700	-0.53704900

C

C	2.73643300	0.41347800	0.89011200
C	1.91053800	1.28108900	-0.07007700
C	1.87926700	-0.78003400	0.37198100
O	1.81264100	2.45891300	-0.32986500
N	1.24716400	0.18793400	-0.54760500
C	0.11977600	0.08859300	-1.44301100
H	0.23599600	-0.80659800	-2.06506200
H	0.17843000	0.95889400	-2.10561500
C	-1.21451100	0.06506300	-0.72443500
C	-2.08399200	-1.01606800	-0.84587100
C	-1.57227100	1.13954000	0.09488500
C	-3.29555500	-1.03147100	-0.15692600
H	-1.81164900	-1.85628700	-1.48112400
C	-2.77835200	1.12480500	0.78468100
H	-0.89484800	1.98538500	0.18711000
C	-3.64323100	0.03781600	0.66124300
H	-3.96500100	-1.88073700	-0.25837300
H	-3.04818500	1.96427500	1.41881200
H	-4.58594800	0.02719600	1.20022000
H	2.60352400	0.66201100	1.94576300
C	0.91481800	-1.35671700	1.40456000
H	1.46681400	-1.92815500	2.15864900
H	0.35614300	-0.55950300	1.90465700
H	0.18842800	-2.02631900	0.93201200
C	2.64746900	-1.87180900	-0.36243600
H	1.95997000	-2.54095300	-0.89289300
H	3.33589200	-1.43682100	-1.09400900
H	3.22526900	-2.47805700	0.34320600
H	3.80156000	0.36311700	0.65056800

4-4

Rh	-0.39398000	0.11659500	-0.31514600
Rh	-2.65970000	-0.30044800	0.54171100
O	-0.18923400	-1.92890100	-0.48880700
O	-2.29884200	-2.31856100	0.22689100
O	-0.74393600	2.13396600	-0.04851200
O	-2.81719300	1.75810400	0.77735100
O	-1.83232800	-0.47203000	2.43746200
O	0.24745800	-0.06881300	1.65588000

O	-1.23684600	0.26017500	-2.18392400
O	-3.32652600	-0.11783500	-1.40746300
C	-1.17087500	-2.68472900	-0.19145200
C	-2.49496000	0.11667300	-2.32133300
C	-0.59506400	-0.33248400	2.57878800
C	-1.86678700	2.50337300	0.42644900
C	-0.00967500	-0.48328200	3.96242300
H	0.49415700	0.44507000	4.24795800
H	-0.79058200	-0.71822200	4.68567700
H	0.74186100	-1.27828400	3.95375000
C	-0.92130300	-4.16658300	-0.33282300
H	-0.19931100	-4.35439500	-1.12941400
H	-0.50526800	-4.54416600	0.60789100
H	-1.85962400	-4.68834600	-0.52679500
C	-2.07777600	3.99289900	0.56046100
H	-1.13684500	4.53233100	0.44582800
H	-2.77495200	4.31921700	-0.21778900
H	-2.53386200	4.21422700	1.52801200
C	-3.02198100	0.28119200	-3.72546600
H	-3.98429700	-0.22191300	-3.82812500
H	-3.16154700	1.34931300	-3.92320200
H	-2.30153000	-0.10697000	-4.44779200
C	1.38821200	0.42625900	-1.12754900
C	2.33569300	-0.68362000	-1.26597000
C	3.70256800	-2.42600400	-0.29063800
O	2.10515600	-1.26079400	-2.32871300
N	3.20311400	-1.04739800	-0.30461100
C	3.33031500	-0.18896400	0.87526400
H	4.28112100	-0.43359400	1.35854700
H	2.51995700	-0.38163400	1.58487100
C	3.32637300	1.26635000	0.45771500
C	4.31321400	1.74354200	-0.41804000
C	2.33005900	2.13962900	0.90057600
C	4.29270500	3.06080700	-0.84887600
H	5.08273300	1.06254900	-0.77299100
C	2.31032100	3.46569900	0.46339800
H	1.55463200	1.77075900	1.56275200
C	3.28521500	3.92625300	-0.40970200
H	5.05655500	3.41890200	-1.53251300
H	1.51686100	4.12486400	0.79918300
H	3.26562400	4.95484900	-0.75730300
H	3.39666300	-2.83701200	-1.25618300
C	5.22616400	-2.47762300	-0.20187100
H	5.56725200	-3.51345000	-0.29616100
H	5.68064600	-1.89190500	-1.00684200
H	5.59668800	-2.09826600	0.75747900
C	3.00868700	-3.21825500	0.82005100
H	3.30564500	-2.85837000	1.81248300
H	1.92342100	-3.11730100	0.72076100
H	3.27541600	-4.27803100	0.75425200
H	1.57406400	1.28566400	-1.77721100

TS 4-4

Rh	-0.32051900	0.16138500	-0.21458100
Rh	-2.61010100	-0.50319300	0.37348300
O	0.07867200	-1.84786500	-0.46639200
O	-2.05913900	-2.45730400	-0.05574400
O	-0.87948400	2.12655000	0.12490400
O	-2.96736100	1.50986700	0.74128900
O	-1.93871700	-0.75925200	2.32677600
O	0.14702100	-0.06744000	1.80548600
O	-0.97497800	0.34627100	-2.15541900
O	-3.09589700	-0.22210700	-1.61591200
C	-0.86299000	-2.69781400	-0.36352100
C	-2.19761200	0.12379000	-2.42705000
C	-0.74486000	-0.50274000	2.60916500

C	-2.06510800	2.35918700	0.52536200
C	-0.28456600	-0.72973500	4.02990600
H	0.16828900	0.18499200	4.42295900
H	-1.12077100	-1.03314200	4.66003100
H	0.48400200	-1.50890100	4.03716200
C	-0.47417100	-4.13572600	-0.60989600
H	0.30007700	-4.18593100	-1.37788500
H	-0.06665800	-4.55574400	0.31648200
H	-1.34866100	-4.71981200	-0.90013600
C	-2.42837800	3.80870300	0.75121500
H	-1.54797400	4.44961300	0.68773400
H	-3.15215800	4.11351000	-0.01083500
H	-2.91058400	3.91875400	1.72570000
C	-2.59465000	0.32943300	-3.86861400
H	-3.54613000	-0.16293600	-4.07282300
H	-2.70292200	1.40323400	-4.05411100
H	-1.81285700	-0.04960800	-4.52999600
C	1.54841600	0.67044100	-0.92863800
C	2.41290200	-0.50495400	-1.25570600
C	3.74760300	-2.26296100	-0.18379100
O	2.26667400	-1.06683500	-2.32798200
N	3.24135600	-0.89582800	-0.24600000
C	3.20738700	-0.03656600	0.92442500
H	4.17286600	-0.08580700	1.43976600
H	2.41433300	-0.32250600	1.62332000
C	2.96500800	1.37630600	0.41702100
C	3.91564700	1.95027700	-0.47353500
C	1.99263600	2.22264500	0.98889400
C	3.83795400	3.27854200	-0.82864200
H	4.68525600	1.30868900	-0.89317000
C	1.91329100	3.56402100	0.61751100
H	1.28051300	1.80035500	1.68842900
C	2.82636700	4.08684900	-0.28475300
H	4.55331500	3.69910300	-1.52776900
H	1.12568100	4.18369400	1.02987000
H	2.75964800	5.13086700	-0.57638700
H	3.46764000	-2.69793000	-1.14717300
C	5.27011100	-2.28698100	-0.05436800
H	5.63519600	-3.31904700	-0.07235000
H	5.73646600	-1.74214500	-0.88101700
H	5.60227600	-1.83799400	0.88957400
C	3.04781000	-3.04280900	0.93233800
H	3.34607900	-2.67771900	1.92294300
H	1.96400500	-2.93627000	0.83015000
H	3.31051000	-4.10419600	0.87571900
H	1.57985100	1.48450900	-1.65475300

D

C	-0.77814400	0.89352400	-0.59579200
C	0.69775800	1.15341200	-0.59078400
C	2.75209000	-0.00649500	0.15191900
O	1.26290000	2.15359100	-0.99313000
N	1.31036300	0.05681200	-0.03337300
C	0.42949100	-1.08091400	0.15254900
H	0.51889900	-1.49602100	1.16354500
H	0.65992100	-1.88389400	-0.56318300
C	-0.96351100	-0.52427700	-0.10967400
C	-1.38339200	0.66730200	0.77407900
C	-2.03216400	-1.39655900	-0.60851600
C	-2.83108200	0.84934600	0.95877800
H	-0.74560900	0.92212100	1.61927400
C	-3.32944400	-1.06859400	-0.46938200
H	-1.74100300	-2.32770300	-1.08856200
C	-3.73441000	0.08623300	0.31544900
H	-3.15440500	1.61532500	1.65786900
H	-4.10019900	-1.71697900	-0.87512300

H	-4.79569800	0.26807900	0.45693100
H	3.09781400	1.00256200	-0.09032100
C	3.11024900	-0.32003600	1.60539000
H	4.19192800	-0.24001200	1.75292900
H	2.61713600	0.38160800	2.28501700
H	2.81370200	-1.33865500	1.88243300
C	3.40116600	-0.99087000	-0.82365300
H	3.09319900	-2.02308400	-0.61835800
H	3.13214500	-0.74539100	-1.85537100
H	4.49130200	-0.94774300	-0.73265900
H	-1.38651300	1.33093700	-1.37795400

TS D-D_{RE}

C	-0.83381100	0.73781000	-0.56491700
C	0.63922000	1.09110900	-0.58413300
C	2.76884400	0.05313600	0.12130300
O	1.13172200	2.12766600	-0.98631700
N	1.32262900	0.03370400	-0.04367000
C	0.49768000	-1.12129000	0.25821200
H	0.56807300	-1.39730800	1.31727000
H	0.79814300	-1.99794400	-0.33395900
C	-0.89746600	-0.67452000	-0.13041300
C	-1.48730000	0.93116400	0.75609600
C	-1.97108100	-1.52691600	-0.40711900
C	-2.88083500	0.90933600	0.89522000
H	-0.86769400	1.30334200	1.56932900
C	-3.28110000	-1.08386200	-0.47331900
H	-1.76833700	-2.59165100	-0.50197100
C	-3.71991800	0.10319500	0.14233300
H	-3.31260400	1.49632700	1.70241800
H	-4.04050600	-1.77539100	-0.82857000
H	-4.79257500	0.25827800	0.22322200
H	3.05189400	1.08384700	-0.11081500
C	3.16502900	-0.26050200	1.56456800
H	4.24091100	-0.11223600	1.69934200
H	2.63702400	0.39530800	2.26363500
H	2.94026200	-1.30132800	1.82627300
C	3.45593400	-0.87965300	-0.87843700
H	3.20120100	-1.92926500	-0.68906300
H	3.16325900	-0.62938300	-1.90230500
H	4.54349400	-0.78377800	-0.79742700
H	-1.40588500	1.04989300	-1.43751300

D_{RE}

C	-0.86459700	0.54109400	-0.56968900
C	0.59561400	0.98448700	-0.58333500
C	2.81239300	0.07036400	-0.03434400
O	1.00070600	2.10342900	-0.84270700
N	1.37627400	-0.08036200	-0.23249300
C	0.63519500	-1.25184300	0.19699700
H	0.81222600	-1.46442200	1.26117400
H	0.93245200	-2.14346700	-0.37054700
C	-0.80479300	-0.87786800	-0.07561300
C	-1.70600300	1.38869000	0.34805500
C	-1.86701900	-1.68665200	0.04376900
C	-3.00377800	1.12866900	0.57242500
H	-1.23194800	2.25442500	0.80375900
C	-3.24346400	-1.26758800	-0.13463100
H	-1.70502100	-2.73133300	0.30759900
C	-3.74070100	-0.02689700	0.09184800
H	-3.57123500	1.83737900	1.17286200
H	-3.95513900	-2.05305800	-0.38086300
H	-4.81839600	0.09842400	0.00739400
H	3.08475100	0.93954600	-0.63998100
C	3.13599700	0.38384100	1.42883800

H	4.21047900	0.55198000	1.55528600
H	2.60666700	1.28637700	1.74743500
H	2.84734300	-0.44312500	2.08833800
C	3.56899800	-1.15355100	-0.54596900
H	3.35030900	-2.04433600	0.05488900
H	3.31147400	-1.36605500	-1.58828200
H	4.64694400	-0.97468600	-0.48798000
H	-1.26752700	0.59097900	-1.59209200

(Z=Me)

Sub

C	1.94451600	-1.34760500	0.07656300
C	1.87220400	0.10208500	-0.22739100
C	0.72171800	2.22274400	-0.34194600
N	3.18104800	-1.77739000	0.03183200
N	4.24910500	-2.15266400	0.00541900
O	2.85788100	0.66437400	-0.69598100
N	0.69336300	0.78509000	0.00070700
C	-0.28781900	0.35031300	0.97858900
H	-0.47826900	1.17842400	1.67270800
H	0.14946100	-0.43829900	1.59692200
C	-1.61785600	-0.12630600	0.41839600
C	-2.69295800	-0.30032600	1.29169900
C	-1.79454500	-0.41991200	-0.93204400
C	-3.91857800	-0.76343500	0.82597400
H	-2.56868500	-0.07100600	2.34817800
C	-3.02172000	-0.88110000	-1.40286700
H	-0.96331400	-0.27741000	-1.61708900
C	-4.08726300	-1.05511400	-0.52561900
H	-4.74458000	-0.89281500	1.51925300
H	-3.14438400	-1.10088200	-2.45936500
H	-5.04414200	-1.41422000	-0.89232100
H	1.36688600	2.28960900	-1.21930900
C	-0.65988200	2.75652900	-0.71390700
H	-0.56110200	3.80415000	-1.01562100
H	-1.09788600	2.20049700	-1.54649900
H	-1.36475400	2.72165800	0.12420600
C	1.37100500	3.04452700	0.77527200
H	0.78093300	3.01155400	1.69929900
H	2.37589700	2.66791200	0.98033000
H	1.45192200	4.09408900	0.47377800
C	0.88546700	-2.41259900	0.24590300
H	0.61455800	-2.59405800	1.29310800
H	-0.02294500	-2.13805400	-0.29302800
H	1.23701600	-3.36018600	-0.17415700

2

Rh	-0.82784700	0.06668600	0.35719400
Rh	-2.66656500	-0.68239400	-1.02145100
O	-1.93200300	1.73694800	0.80629700
O	-3.64405800	1.06095800	-0.50055100
O	0.15851400	-1.67965600	-0.17183700
O	-1.55383300	-2.37330900	-1.46579200
O	-1.78638000	0.29440200	-2.61092300
O	-0.07792000	1.01622300	-1.32167600
O	-1.69720400	-0.91181700	1.95204300
O	-3.42093500	-1.60776800	0.67040500
C	-3.08457800	1.87206500	0.28694700
C	-2.79164400	-1.53130100	1.75969600
C	-0.70912800	0.92150700	-2.42094400

C	-0.40372000	-2.49730100	-0.96747600
C	-0.09049700	1.61986600	-3.60628600
H	-0.74668800	1.55323300	-4.47424600
H	0.10371400	2.66622600	-3.35717500
H	0.87159800	1.15120000	-3.83589000
C	-3.85281800	3.10720300	0.68276300
H	-4.32557900	2.92909900	1.65448400
H	-3.17169700	3.95375200	0.78876400
H	-4.62939100	3.32306200	-0.05185000
C	0.37848900	-3.73886900	-1.31809100
H	1.44255400	-3.58726800	-1.12819900
H	0.02365300	-4.56598800	-0.69443100
H	0.20380700	-4.00604900	-2.36219900
C	-3.37696800	-2.26253600	2.94209500
H	-4.45425200	-2.08852200	2.98712200
H	-3.21884200	-3.33686900	2.80302600
H	-2.89949600	-1.94668500	3.87025300
C	0.91888900	0.68530800	1.72884700
C	1.73304600	1.79779000	1.08307200
C	3.38435800	2.63662400	-0.44335300
N	0.15225100	1.30111900	2.68636200
N	-0.54088400	1.75599200	3.42981800
O	1.51403200	2.95397200	1.42851500
N	2.69359000	1.47943600	0.16597300
C	2.75184100	0.21130000	-0.54162200
H	2.80555200	0.42500800	-1.61538900
H	1.80969300	-0.32154800	-0.41962400
C	3.89458900	-0.70839400	-0.15645800
C	4.17555000	-1.80445200	-0.97600400
C	4.64176300	-0.53199000	1.00574800
C	5.17875400	-2.70702100	-0.63871000
H	3.60356000	-1.94837000	-1.89078400
C	5.64897500	-1.43166100	1.34623900
H	4.43164400	0.32175000	1.64360200
C	5.92033900	-2.52288600	0.52668900
H	5.38647100	-3.55175000	-1.28924800
H	6.22219500	-1.27776100	2.25593300
H	6.70519300	-3.22495300	0.79132300
H	3.41363100	3.39381300	0.34124200
C	4.81735900	2.30546200	-0.85342600
H	5.28722100	3.21271200	-1.24671000
H	5.41018500	1.95242100	-0.00582600
H	4.86247400	1.54400500	-1.63944900
C	2.56909300	3.19959700	-1.60946300
H	2.52066600	2.48725800	-2.44072100
H	1.55007700	3.42165500	-1.28364100
H	3.03162900	4.11963000	-1.98240700
C	1.52869500	-0.58954800	2.31201500
H	1.87204600	-1.24396200	1.51335200
H	2.36933500	-0.37149300	2.98020100
H	0.75689500	-1.13676300	2.85940900

TS 2-3

Rh	-0.66494600	-0.01973600	0.25561900
Rh	-2.80003500	-0.30223100	-0.93303700
O	-1.51143600	1.56996900	1.23022900
O	-3.47569300	1.34039800	0.13160300
O	0.03417200	-1.63127800	-0.84813700
O	-1.93754800	-1.92679800	-1.91060500
O	-2.05645700	0.94648500	-2.39615600
O	-0.09133400	1.22537500	-1.31159500
O	-1.43496400	-1.27221800	1.70037400
O	-3.39934700	-1.54226700	0.61737900
C	-2.71243500	1.90034400	0.96026200
C	-2.61150300	-1.75038700	1.57228600
C	-0.89538400	1.41261400	-2.28411700
C	-0.73935200	-2.21448200	-1.68130400

C	-0.39228000	2.28302200	-3.41124200
H	-1.14708700	2.35328400	-4.19460100
H	-0.16044200	3.28182900	-3.03388900
H	0.53088900	1.86037600	-3.81762900
C	-3.25355200	3.06468700	1.75176800
H	-3.48402300	2.72004700	2.76517800
H	-2.49581300	3.84700800	1.83050400
H	-4.16261400	3.45087800	1.28958900
C	-0.11315400	-3.33785900	-2.47201000
H	0.47401800	-3.97931000	-1.81020000
H	-0.88112800	-3.91575800	-2.98654500
H	0.56947300	-2.91034900	-3.21422800
C	-3.06308700	-2.67578800	2.67485200
H	-4.15242300	-2.71931000	2.70848900
H	-2.67862000	-3.68040700	2.46824100
H	-2.65966600	-2.34754600	3.63463500
C	1.09557400	0.04618100	1.17974000
C	1.96300800	1.27250300	1.14324700
C	3.27100300	2.80923300	-0.22749800
N	0.31225400	0.38773100	3.59621400
N	-0.42276700	0.60197700	4.38761100
O	1.90598700	2.04580700	2.09321300
N	2.65811900	1.49327900	-0.00417000
C	2.88974500	0.39690600	-0.92905000
H	3.27020500	0.82016000	-1.86416300
H	1.92326100	-0.05033800	-1.19280400
C	3.82676300	-0.69903400	-0.44927400
C	3.79219500	-1.91472100	-1.13860800
C	4.65481100	-0.58484000	0.66451600
C	4.57951400	-2.98718300	-0.73585900
H	3.12541300	-2.02484600	-1.98982600
C	5.44753400	-1.65665100	1.06960900
H	4.66074100	0.33394900	1.24262600
C	5.41536900	-2.85986100	0.37163200
H	4.53420700	-3.92549400	-1.28107800
H	6.08398700	-1.55028000	1.94328100
H	6.02999900	-3.69542100	0.69259000
H	3.05298300	3.36984000	0.68418200
C	4.78861300	2.74492000	-0.39906600
H	5.17583900	3.75479900	-0.56879300
H	5.27828600	2.34261200	0.49133000
H	5.08005800	2.13109300	-1.25932500
C	2.58346200	3.50477100	-1.40109800
H	2.76492000	2.97765800	-2.34536200
H	1.50530200	3.53352400	-1.22973400
H	2.96072400	4.52679200	-1.51212000
C	1.68023800	-1.21327300	1.66622500
H	1.84829400	-1.78881900	0.73957300
H	2.62461900	-1.13779400	2.21493700
H	0.91000100	-1.76098400	2.22085100

3

Rh	0.56814500	-0.04271600	-0.38765100
Rh	2.75214900	-0.06478800	0.74940000
O	-0.05530400	1.32972700	1.03738700
O	1.93530400	1.27813700	2.10914400
O	1.35139400	-1.39940600	-1.72569100
O	3.36961100	-1.40914400	-0.70549500
O	2.04392200	-1.65285600	1.88872800
O	0.03140800	-1.60669300	0.86089900
O	1.29456400	1.50434100	-1.52717500
O	3.29476300	1.51506000	-0.47157300
C	0.75534800	1.67714300	1.96050100
C	2.47322100	1.94002200	-1.32512600
C	0.87447700	-2.06581100	1.70047200
C	2.56366600	-1.77581100	-1.59618500
C	0.37984700	-3.20331000	2.56325900

H	1.22159700	-3.73965100	3.00254500
H	-0.23548600	-2.79348300	3.37184400
H	-0.24246500	-3.87943800	1.97243300
C	0.22914100	2.69161200	2.94803700
H	0.32749200	3.69095000	2.51050000
H	-0.82969700	2.51498600	3.14906900
H	0.80828200	2.65617100	3.87157500
C	3.05993200	-2.74417500	-2.64231400
H	2.31786600	-3.52955700	-2.80529100
H	3.19165700	-2.20888600	-3.58812500
H	4.01317500	-3.17669300	-2.33751100
C	2.92223800	3.05838100	-2.23328900
H	3.69198700	3.65546600	-1.74190300
H	3.35008800	2.61896000	-3.14063000
H	2.07173300	3.67786200	-2.52269800
C	-1.19131600	-0.07684800	-1.31563200
C	-2.05816900	1.10653400	-1.25779300
C	-3.44747700	2.77834300	-0.20227300
O	-1.81564100	1.77582300	-2.26576300
N	-2.89616800	1.41692800	-0.25582700
C	-3.04126900	0.50088200	0.87413600
H	-3.72649500	0.97481600	1.58313800
H	-2.07767400	0.39181000	1.38278400
C	-3.58458800	-0.85504200	0.47298000
C	-3.07028200	-2.00785200	1.06543700
C	-4.59222500	-0.97786000	-0.48657800
C	-3.54479900	-3.26422400	0.69752600
H	-2.26210700	-1.92189300	1.78334800
C	-5.06592500	-2.23166700	-0.85761000
H	-4.99077800	-0.08642100	-0.96218400
C	-4.54025000	-3.38027400	-0.26872900
H	-3.12457700	-4.15397400	1.15731200
H	-5.84311300	-2.31312300	-1.61172900
H	-4.90429000	-4.35983800	-0.56393600
H	-3.15747100	3.23015000	-1.15371600
C	-4.97239700	2.76674100	-0.11794500
H	-5.34971200	3.79419900	-0.10035200
H	-5.40727000	2.26034400	-0.98502800
H	-5.33203700	2.26902800	0.79004700
C	-2.79187200	3.57378500	0.92747200
H	-3.07216500	3.18141300	1.91230000
H	-1.70411000	3.52237700	0.83394300
H	-3.10696500	4.62136000	0.88344300
C	-1.58321200	-1.19529200	-2.18987600
H	-1.84512400	-2.01006400	-1.49375100
H	-2.44611600	-0.98594100	-2.82731700
H	-0.72099200	-1.55330300	-2.76049300

4-1

Rh	-0.81254400	0.45784700	-0.31976300
Rh	-2.22890700	-1.23963700	0.75314200
O	0.65846100	-0.05260400	1.04536800
O	-0.62724300	-1.64593400	2.00467400
O	-2.38636800	0.84360000	-1.59592600
O	-3.70521100	-0.70031700	-0.60311100
O	-2.85533300	0.26981400	2.03838000
O	-1.58130200	1.83484000	1.01708500
O	-0.13051000	-1.04255800	-1.55033200
O	-1.46709700	-2.60504100	-0.60906000
C	0.43718200	-0.99001500	1.88338100
C	-0.59047400	-2.22507800	-1.42558900
C	-2.42363700	1.43907300	1.89166800
C	-3.47033900	0.18348800	-1.46387600
C	-2.96425000	2.50695400	2.81178000
H	-3.76656300	3.04265600	2.29306200
H	-3.37396600	2.05380400	3.71519100
H	-2.18294600	3.22757600	3.06181200

C	1.57668400	-1.32388400	2.81478600
H	2.46907800	-1.56591600	2.22956700
H	1.80648400	-0.45277900	3.43595200
H	1.30688200	-2.16617300	3.45237300
C	-4.55574300	0.47888400	-2.46996300
H	-4.43029500	1.47402700	-2.89902400
H	-4.48989000	-0.25996000	-3.27559600
H	-5.53558200	0.37976900	-1.99942700
C	-0.02521400	-3.24262000	-2.38617100
H	-0.20695200	-4.25337300	-2.01872100
H	-0.51864800	-3.12158800	-3.35600600
H	1.04307800	-3.06856300	-2.53499400
C	0.25914000	1.86089000	-1.20889100
C	1.65542500	1.59020100	-1.56246600
C	2.48206100	2.42460900	0.56331300
O	1.68862100	1.16870700	-2.72157100
N	2.67603500	1.70209200	-0.70256600
C	3.96553800	1.14479100	-1.09397200
H	4.76214100	1.81487200	-0.75592000
H	3.98523000	1.13415600	-2.18780800
C	4.17795000	-0.25832100	-0.55555100
C	5.35786500	-0.59387400	0.10509400
C	3.18564100	-1.23053100	-0.71477900
C	5.55171500	-1.87953900	0.60689300
H	6.13143200	0.15927000	0.24020500
C	3.37805700	-2.51307800	-0.21253100
H	2.25369900	-0.98932400	-1.21785100
C	4.55977300	-2.84262200	0.45116100
H	6.47495800	-2.12376900	1.12411300
H	2.59594800	-3.25813400	-0.33205400
H	4.70345700	-3.84347900	0.84743100
H	1.41870600	2.31761200	0.81015200
C	3.27162400	1.80528200	1.71072900
H	2.98536800	2.29768100	2.64530000
H	3.05683300	0.74062900	1.79334500
H	4.35100900	1.93990500	1.58082800
C	2.80871200	3.90887700	0.38069400
H	3.86170300	4.04689000	0.10929200
H	2.19274500	4.35411300	-0.40779500
H	2.62537600	4.45594700	1.31130100
C	-0.37292600	3.10841400	-1.66748700
H	-1.31437200	2.87110500	-2.17788700
H	-0.67639900	3.63000200	-0.74485500
H	0.26371000	3.75346300	-2.27947500

TS 4-1

Rh	-0.79423200	0.51008800	-0.13831700
Rh	-2.21035100	-1.39883100	0.38699100
O	0.55670900	-0.20168300	1.25707300
O	-0.71658900	-2.01213500	1.70138100
O	-2.24863400	1.12344900	-1.46436200
O	-3.57618500	-0.63819200	-0.96596000
O	-3.02838300	-0.20740300	1.88339600
O	-1.71944700	1.56469600	1.38353600
O	0.05506200	-0.65988700	-1.60704300
O	-1.27703200	-2.42639400	-1.14579300
C	0.30299400	-1.29576400	1.86237800
C	-0.36111200	-1.84876000	-1.78910200
C	-2.62879700	0.97263500	2.05183600
C	-3.30166200	0.42227400	-1.59033800
C	-3.29940300	1.77145400	3.14373300
H	-4.34766200	1.93041700	2.87347700
H	-3.28379700	1.20007200	4.07540200
H	-2.80926300	2.73567900	3.28337300
C	1.33995400	-1.74315800	2.86271800

H	1.05381500	-2.69390800	3.31292800
H	2.30794700	-1.83891600	2.36184300
H	1.44094000	-0.98150200	3.64225300
C	-4.30320400	0.89941700	-2.61334800
H	-4.10484400	0.38608400	-3.56020800
H	-5.31591500	0.64633100	-2.29454300
H	-4.20453400	1.97383700	-2.77496000
C	0.33902100	-2.62233900	-2.87898100
H	-0.13507400	-3.59299300	-3.02664800
H	0.32002000	-2.04317200	-3.80578500
H	1.38994300	-2.76226000	-2.60457200
C	0.42043400	2.25983600	-0.56394200
C	1.67101100	1.96871700	-1.32402500
C	2.73745200	1.98295100	0.85133900
O	1.60553000	1.86028600	-2.53799000
N	2.82034700	1.82119900	-0.59297500
C	3.96427400	1.14863600	-1.18804100
H	4.86549200	1.75751200	-1.05431000
H	3.75298800	1.09926300	-2.25958200
C	4.17346700	-0.23752900	-0.61142100
C	5.38474500	-0.60285900	-0.02745400
C	3.12679100	-1.16296400	-0.64685900
C	5.55705300	-1.87764000	0.51123200
H	6.20345300	0.11334200	0.00556000
C	3.29689300	-2.43455000	-0.11122900
H	2.17415300	-0.87892400	-1.08596400
C	4.51301000	-2.79613700	0.47051200
H	6.50592900	-2.14904600	0.96455800
H	2.47421800	-3.14483600	-0.13923800
H	4.64300100	-3.78843500	0.89239600
H	2.59122300	1.00566400	1.32520500
C	3.98001300	2.65433100	1.43255400
H	3.83425700	2.84907600	2.50006500
H	4.85366600	2.00395400	1.33325300
H	4.18489100	3.60311100	0.92501300
C	1.50679000	2.82701500	1.10494100
H	1.58322100	3.86583000	0.78775400
H	0.52310300	2.20845200	0.70053300
H	1.13002400	2.75713400	2.13060300
C	-0.35991700	3.46933800	-0.98378300
H	-0.80757700	3.19853300	-1.94522100
H	-1.17749900	3.66414800	-0.28614600
H	0.25057900	4.36926400	-1.12677000

A

C	2.74951800	-0.60263100	-0.37165300
C	2.55961400	0.79800700	-0.96587800
C	1.78475200	-0.61549200	0.81066600
C	1.13410100	1.20218900	-0.55336000
O	1.71036300	-1.47554500	1.67172200
N	0.96132200	0.47269900	0.70044800
C	-0.25802900	0.56150900	1.48120100
H	-0.38680200	1.58617700	1.84647100
H	-0.10826400	-0.08999900	2.34637500
C	-1.47165800	0.12728000	0.68588700
C	-1.57387000	-1.19820700	0.25159800
C	-2.47293500	1.03193300	0.34002100
C	-2.66022200	-1.60557900	-0.51328500
H	-0.79755100	-1.90746100	0.52828700
C	-3.56438500	0.62542000	-0.42558200
H	-2.40147700	2.06464600	0.67480500
C	-3.65851900	-0.69369700	-0.85485700
H	-2.73352800	-2.63877500	-0.84024500
H	-4.33760300	1.34153900	-0.68793500
H	-4.50737300	-1.01364300	-1.45196100

H	0.40505700	0.83008400	-1.28996100
C	0.94292600	2.70391000	-0.39706500
H	1.19170300	3.20777800	-1.33677700
H	-0.09407100	2.95445200	-0.15143000
H	1.59565100	3.09405100	0.39139900
H	3.27332100	1.50055400	-0.52028400
H	2.69124800	0.82788300	-2.05144000
H	3.76659100	-0.76960100	-0.00624100
C	2.36219300	-1.73811800	-1.32621500
H	3.04481600	-1.77202800	-2.18136400
H	2.40171300	-2.69947500	-0.80672600
H	1.34350700	-1.59985400	-1.70875600

4-2

Rh	0.90055200	0.06073100	-0.49177200
Rh	2.78076700	-0.39068400	1.02683900
O	-0.00697000	1.07385000	1.06873100
O	1.71356200	0.65088500	2.47406000
O	1.93454200	-0.96805600	-1.94777600
O	3.67312200	-1.38497300	-0.56194000
O	1.80026200	-2.14223300	1.57420200
O	0.08051500	-1.72886400	0.16913300
O	1.86750000	1.78781800	-1.02463100
O	3.60621700	1.38741700	0.36631700
C	0.59479100	1.14404400	2.19111600
C	2.98923700	2.07061700	-0.49159700
C	0.69753900	-2.42165800	1.04830800
C	3.08104900	-1.45426600	-1.66747500
C	0.01602700	-3.70520200	1.45574300
H	0.11161600	-4.43226600	0.64280400
H	0.47855500	-4.11180300	2.35546400
H	-1.04977500	-3.52767600	1.61917400
C	-0.13536900	1.90453500	3.27295500
H	-0.27819200	2.94109200	2.95305400
H	-1.12554800	1.46443300	3.42635100
H	0.42920500	1.88060200	4.20515700
C	3.77961400	-2.16523900	-2.80121300
H	3.09844400	-2.88405200	-3.26392500
H	4.05696700	-1.43157900	-3.56443200
H	4.67525800	-2.66995800	-2.43860100
C	3.63427700	3.34566400	-0.97588800
H	4.39815500	3.67495400	-0.27057500
H	4.10384200	3.15527700	-1.94654500
H	2.87612200	4.11871800	-1.11652600
C	-0.68105900	0.27928600	-1.65400800
C	-1.68920400	1.31289400	-1.39119000
C	-3.47470400	2.42525100	-0.21137300
O	-1.46556500	2.24985500	-2.16220800
N	-2.64232000	1.23370600	-0.45308400
C	-2.75005200	0.04491700	0.38223800
H	-2.59256800	0.32280800	1.42817500
H	-1.91748600	-0.62274200	0.13684700
C	-4.05937900	-0.69441600	0.22071300
C	-4.85135200	-0.98085400	1.33066700
C	-4.48550800	-1.11640100	-1.04100000
C	-6.05353700	-1.67164800	1.18738100
H	-4.52799300	-0.65617400	2.31729000
C	-5.68456300	-1.80238000	-1.18946600
H	-3.88216000	-0.88362800	-1.91552400
C	-6.47327800	-2.08182600	-0.07351600
H	-6.66189100	-1.88414300	2.06147900
H	-6.00764400	-2.11981800	-2.17656000
H	-7.41248900	-2.61395100	-0.19006000
H	-2.92822400	3.23892700	-0.69572500
C	-4.84905300	2.31539600	-0.87522100

H	-5.37258400	3.27364600	-0.78899700
H	-4.74199400	2.07884400	-1.93804800
H	-5.46594000	1.54347600	-0.40628600
C	-3.57388000	2.73282500	1.28083300
H	-4.18538700	1.99266300	1.80926700
H	-2.57982700	2.76590800	1.73679500
H	-4.04938900	3.70897000	1.41645500
C	-0.91804100	-0.61939100	-2.79954500
H	-1.22732900	-1.57105000	-2.33250300
H	-1.70535200	-0.28030800	-3.47938700
H	0.01371800	-0.83770100	-3.32887100

TS 4-2

Rh	0.62885400	-0.19359200	-0.25869700
Rh	2.90577000	-0.07632300	0.57809900
O	0.71984700	1.85170000	-0.52290700
O	2.85327800	1.96032300	0.21024200
O	0.67142000	-2.22965900	0.09732500
O	2.78720700	-2.12178200	0.88247200
O	2.07773100	0.25725100	2.45946600
O	-0.03745900	0.13683300	1.67989000
O	1.41685100	-0.52030500	-2.12852000
O	3.53973000	-0.40083700	-1.35900200
C	1.79280300	2.47126200	-0.23953000
C	2.67934800	-0.54002700	-2.27125400
C	0.83083800	0.29988900	2.60008400
C	1.73371200	-2.74029500	0.57494800
C	0.27905500	0.58507600	3.97610300
H	-0.45687400	-0.17766700	4.24487300
H	1.08037100	0.60936800	4.71459200
H	-0.23394500	1.55211200	3.96033400
C	1.75951500	3.96734500	-0.43179500
H	1.31524900	4.42431100	0.45955100
H	2.76996300	4.35919100	-0.55568800
H	1.13591600	4.22030700	-1.29137800
C	1.73586500	-4.23888600	0.75557500
H	0.72187000	-4.60974000	0.91414000
H	2.13346500	-4.69723100	-0.15627800
H	2.38487900	-4.51730100	1.58752500
C	3.18020500	-0.73521600	-3.68095300
H	2.92061700	0.14788100	-4.27299400
H	4.26128200	-0.87637700	-3.68727700
H	2.68129200	-1.59530400	-4.13474600
C	-1.42509300	-0.32374900	-1.06971100
C	-1.90295600	1.01470000	-1.51147400
C	-2.88049700	2.80285600	-0.01096600
O	-1.65721700	1.60961000	-2.53551500
N	-2.69409200	1.42377900	-0.45232500
C	-2.82319200	0.27250600	0.35907800
H	-2.46153600	0.38931900	1.38779100
H	-1.61058200	-0.39257900	0.10791700
C	-3.99404500	-0.61847600	0.23030500
C	-4.16679000	-1.64101400	1.16969300
C	-4.91033000	-0.48241500	-0.81687100
C	-5.23988000	-2.51637400	1.06408600
H	-3.45071800	-1.74969000	1.98111300
C	-5.98736000	-1.35685500	-0.91631800
H	-4.77611000	0.31405700	-1.54239400
C	-6.15372000	-2.37393000	0.02105700
H	-5.36694700	-3.30694800	1.79709200
H	-6.70020600	-1.24289300	-1.72713200
H	-6.99517600	-3.05526800	-0.05953600
H	-2.56965700	3.39361000	-0.87853000
C	-4.35173200	3.07822800	0.29193800
H	-4.49371700	4.12543100	0.57751300
H	-4.97532700	2.86910400	-0.58232500
H	-4.70390100	2.45223600	1.12100800

C	-1.96500800	3.13595800	1.17024400
H	-2.27365900	2.60469400	2.07898300
H	-0.93417200	2.85800600	0.93513200
H	-2.01134200	4.20861000	1.38527400
C	-1.72840300	-1.55015600	-1.85964900
H	-2.80044500	-1.68272900	-2.05986300
H	-1.22078500	-1.41067000	-2.82160100
H	-1.31437600	-2.44170600	-1.38504300

B

C	-0.90845900	1.84413900	0.55821600
C	-2.03708900	1.09008000	-0.16142800
C	-1.99466100	-1.46540100	-0.04350100
O	-3.07242000	1.38661400	-0.70960600
N	-1.44520600	-0.12350400	0.07338700
C	-0.32543500	0.41300300	0.85033600
H	-0.40435300	0.16079800	1.91578900
C	1.06464200	0.08725300	0.36739400
C	2.11203300	0.02160100	1.28673300
C	1.34450300	-0.11320300	-0.98601900
C	3.41415600	-0.23424000	0.86649100
H	1.90639300	0.17118200	2.34436900
C	2.64325700	-0.37427800	-1.40921000
H	0.53438100	-0.07307200	-1.70824500
C	3.68268300	-0.43455600	-0.48402600
H	4.21692200	-0.28316800	1.59621800
H	2.84355000	-0.53248500	-2.46480000
H	4.69655600	-0.63943700	-0.81450600
H	-3.05515000	-1.30879300	-0.27201000
C	-1.35727800	-2.25057400	-1.19139200
H	-1.84949900	-3.22253600	-1.30461000
H	-1.45810400	-1.70357700	-2.13355100
H	-0.29290300	-2.42482000	-1.00276700
C	-1.87005600	-2.20789300	1.28669600
H	-0.81643100	-2.36420600	1.54650700
H	-2.35042400	-1.65142000	2.09775900
H	-2.34602900	-3.19058800	1.21523000
H	-1.27719500	2.31725100	1.47429500
C	-0.09679200	2.83227700	-0.26058900
H	-0.71483000	3.70127900	-0.50504200
H	0.78016400	3.17445900	0.29813300
H	0.25372900	2.39148700	-1.19784500

4-3

Rh	-0.86163200	0.31286600	-0.46886400
Rh	-2.26572000	-1.03042200	1.03279800
O	0.78275000	-0.49502600	0.48212900
O	-0.50267100	-1.76283600	1.84378100
O	-2.59853500	1.03428000	-1.32121900
O	-3.90139300	-0.17164300	0.08077500
O	-2.20604100	0.55794800	2.37413000
O	-0.95947300	1.81075600	0.96693700
O	-0.89094400	-1.28055600	-1.76270200
O	-2.20811300	-2.51843400	-0.40378800
C	0.60411700	-1.35260600	1.40953300
C	-1.54810500	-2.32815400	-1.45739500
C	-1.58170800	1.59883300	2.06265300
C	-3.72182300	0.63739700	-0.86294300
C	-1.54337900	2.73612800	3.05484200
H	-2.00507100	3.62227600	2.60956000
H	-2.07027700	2.46360900	3.96932900
H	-0.50236300	2.98387200	3.28222300
C	1.84637700	-1.94393500	2.02843500
H	1.99616700	-2.94594900	1.61446500
H	2.73193000	-1.34926500	1.80081300
H	1.70654900	-2.04354700	3.10703100
C	-4.94102600	1.19457300	-1.55735600

H	-4.81953900	2.26741800	-1.72421000
H	-5.04076700	0.71352000	-2.53586700
H	-5.83769200	0.99745800	-0.96917800
C	-1.54328800	-3.42608100	-2.49227800
H	-1.79370600	-4.38128300	-2.02905500
H	-2.29620300	-3.19396700	-3.25271700
H	-0.57053700	-3.47616400	-2.98507600
C	0.26278100	1.46743000	-1.61256700
C	1.70368300	1.21174800	-1.74482700
C	2.22236100	2.43653400	0.29110600
O	1.89831600	0.58649500	-2.79245000
N	2.61420200	1.58049000	-0.83711500
C	4.00597600	1.19212400	-1.05954000
H	4.64773800	1.97324400	-0.64169000
H	4.16510000	1.17861800	-2.14210500
C	4.37537000	-0.15848400	-0.47627200
C	5.30835900	-0.25853200	0.55502600
C	3.81056400	-1.32855500	-0.99478100
C	5.67483300	-1.50174700	1.06782700
H	5.76014100	0.64324800	0.96245700
C	4.18139600	-2.56953900	-0.48942700
H	3.08252300	-1.25935000	-1.79676800
C	5.11324500	-2.66131600	0.54330700
H	6.40324200	-1.56115800	1.87115100
H	3.73892300	-3.47054000	-0.90431800
H	5.39880200	-3.63207100	0.93774200
H	1.13278300	2.35940300	0.37031000
C	2.78625900	1.94016800	1.61798900
H	2.35026500	2.52604100	2.43354200
H	2.53313400	0.88998900	1.76639900
H	3.87398800	2.05573000	1.67164300
C	2.58744600	3.89617700	0.01206400
H	3.67188800	4.02851900	-0.07732600
H	2.12518100	4.24415200	-0.91784200
H	2.23933000	4.53564400	0.82966500
C	-0.29305400	2.59372300	-2.38536800
H	-1.28240500	2.35336700	-2.78367800
H	-0.46018300	3.37977900	-1.62782400
H	0.37900700	2.98084600	-3.15680100

TS 4-3

Rh	-0.86928600	0.42659700	-0.02011900
Rh	-2.54130700	-1.33033900	0.06812500
O	0.55036200	-1.04622300	-0.38038100
O	-1.01708300	-2.67345300	-0.32609400
O	-2.39736200	1.76470700	0.36640500
O	-3.95034600	0.12712000	0.46510300
O	-2.12096400	-1.47885000	2.10089700
O	-0.58595500	0.17612800	2.02034800
O	-1.26009300	0.58303300	-2.02864300
O	-2.82098600	-1.05143300	-1.95755100
C	0.16407800	-2.25830100	-0.44479000
C	-2.13429300	-0.17344400	-2.55214900
C	-1.26439600	-0.71941400	2.62099400
C	-3.58252300	1.33160700	0.51377000
C	-1.00446600	-0.85807600	4.10188400
H	-1.31403000	0.06113700	4.60858200
H	-1.55522600	-1.70524100	4.51076000
H	0.06758800	-0.98780300	4.27533800
C	1.24115300	-3.29052400	-0.67552600
H	1.74837300	-3.08798300	-1.62379800
H	1.98412500	-3.21790100	0.12422500
H	0.81009000	-4.29150600	-0.69416000
C	-4.65598100	2.36918000	0.73651200
H	-4.22422900	3.29634400	1.11598500
H	-5.14536400	2.57393700	-0.22150300
H	-5.41080200	1.98453700	1.42512300

C	-2.39120900	0.02953700	-4.02458900
H	-2.76434000	-0.89190000	-4.47431700
H	-3.15489600	0.80602300	-4.14130100
H	-1.48072100	0.36758700	-4.52192100
C	0.61112700	2.08931500	-0.12251500
C	1.65197600	1.93157700	-1.17603700
C	2.35495400	1.78882500	0.91354100
O	1.58704500	2.15164700	-2.36462800
N	2.74205700	1.52808700	-0.44300600
C	4.09357600	1.39747600	-0.94053200
H	4.69793100	2.26137100	-0.62842400
H	3.99227700	1.45518900	-2.03013300
C	4.77886400	0.11340200	-0.53012100
C	6.06878600	0.13919100	-0.00395200
C	4.12910800	-1.11303000	-0.68939900
C	6.71328700	-1.04481800	0.35095600
H	6.57662300	1.09193800	0.12939700
C	4.77338300	-2.29424500	-0.34068100
H	3.10788300	-1.12504200	-1.06212900
C	6.06728200	-2.26413100	0.17960700
H	7.71748400	-1.01113300	0.76310200
H	4.26921200	-3.24640900	-0.47797600
H	6.56639500	-3.18925200	0.45199300
H	0.95753700	1.52280900	0.84544800
C	2.53142800	0.62031900	1.86790800
H	2.07931100	0.83430300	2.83915300
H	2.08835700	-0.28528900	1.44871600
H	3.60755200	0.45459600	2.00022800
C	2.74382100	3.13061000	1.48460400
H	3.76938900	3.05949700	1.86936900
H	2.71691200	3.91817400	0.72915900
H	2.09426100	3.40703400	2.32057300
C	-0.01721800	3.43851700	0.05921200
H	-0.58932100	3.49054400	0.98712100
H	0.69019800	4.27371900	-0.00211300
H	-0.73365400	3.54961600	-0.76153300

C			
C	2.46324900	0.32627300	0.74858800
C	1.63016200	1.19626900	-0.20504100
C	1.54404300	-0.85535700	0.27587700
O	1.57994200	2.36971700	-0.50082200
N	0.90437400	0.12126200	-0.62684800
C	-0.25889500	0.04748700	-1.47748000
H	-0.19517800	-0.85714200	-2.09368400
H	-0.19863400	0.90885200	-2.15160100
C	-1.56495500	0.07323600	-0.70908700
C	-2.47191900	-0.98061100	-0.78914200
C	-1.85967400	1.16603200	0.111103200
C	-3.65899300	-0.95021400	-0.05941400
H	-2.24824900	-1.83529000	-1.42401600
C	-3.04141600	1.19716000	0.84139900
H	-1.15292000	1.99057300	0.17051800
C	-3.94457200	0.13775500	0.75820800
H	-4.35879800	-1.77794000	-0.12898200
H	-3.26269500	2.05142400	1.47457100
H	-4.86874300	0.16330400	1.32799400
H	2.27021000	0.58789800	1.79477600
C	0.61023000	-1.37931100	1.36451700
H	1.17794300	-1.95909700	2.10068000
H	0.10720300	-0.55393900	1.87802000
H	-0.16364300	-2.02875900	0.94156800
C	2.21707100	-2.00004600	-0.47225300
H	1.46243300	-2.67530300	-0.89195000
H	2.83750000	-1.63257400	-1.29413600
H	2.84657800	-2.58741900	0.20467000
C	3.95967900	0.28138600	0.48412900

H	4.40732400	1.24598600	0.74056600
H	4.44566200	-0.49284400	1.08705900
H	4.17978600	0.08533600	-0.56954000

4-4

Rh	-0.44032000	0.07939800	-0.30508000
Rh	-2.71587800	-0.20623000	0.59859500
O	-0.35194100	-1.97325800	-0.47750800
O	-2.46381300	-2.24282300	0.28723900
O	-0.66741800	2.11449300	-0.03619100
O	-2.74188100	1.86243500	0.83129700
O	-1.87055600	-0.41676000	2.48011800
O	0.21428700	-0.13856900	1.65765400
O	-1.31160900	0.27043500	-2.15834200
O	-3.40330500	0.00702900	-1.34423600
C	-1.36655400	-2.67208300	-0.15160600
C	-2.57971400	0.19609300	-2.27321800
C	-0.62481300	-0.34842200	2.59676500
C	-1.75474600	2.54962200	0.46664100
C	-0.02326900	-0.51968400	3.97134900
H	0.49912000	0.39909600	4.25572300
H	-0.79851400	-0.74358800	4.70420000
H	0.71531800	-1.32628000	3.94908400
C	-1.19828800	-4.16641800	-0.28265200
H	-0.50841300	-4.40010800	-1.09539500
H	-0.77627400	-4.55467400	0.65103600
H	-2.16679000	-4.64179800	-0.44506600
C	-1.86678300	4.04856900	0.61586200
H	-0.89409200	4.52684900	0.49364600
H	-2.55178500	4.42691000	-0.14970700
H	-2.29513400	4.28968500	1.59131200
C	-3.12381900	0.39057600	-3.66711500
H	-4.09254500	-0.10151500	-3.76374400
H	-3.26000700	1.46304600	-3.84322500
H	-2.41923700	0.00788800	-4.40762700
C	1.33088200	0.30655900	-1.20100200
C	2.23664100	-0.85501200	-1.27138300
C	3.53813000	-2.62220100	-0.27119800
O	2.01404700	-1.46572000	-2.31751900
N	3.07758500	-1.22763600	-0.28761200
C	3.21218600	-0.40425900	0.91605200
H	4.11918700	-0.73783300	1.42945900
H	2.36168500	-0.56165200	1.58432900
C	3.34062600	1.06551200	0.58101100
C	4.35444800	1.50611600	-0.27891400
C	2.45663200	1.99838600	1.12475600
C	4.47040700	2.85149000	-0.59970900
H	5.04126300	0.78042300	-0.70794200
C	2.57439600	3.34965600	0.80464600
H	1.64993300	1.65443500	1.76266900
C	3.57576300	3.77803800	-0.05925800
H	5.25555100	3.18250300	-1.27298500
H	1.86831600	4.06198500	1.22013500
H	3.66512700	4.83008600	-0.31344600
H	3.23489900	-3.02170400	-1.24154900
C	5.05826400	-2.71900700	-0.16302300
H	5.36806800	-3.76464200	-0.25823500
H	5.53975100	-2.14476800	-0.96063800
H	5.43080600	-2.35532300	0.80155200
C	2.80576400	-3.40051000	0.82459700
H	3.09916600	-3.05935800	1.82462000
H	1.72554000	-3.26551800	0.71122900
H	3.04022800	-4.46752700	0.75251000
C	1.53410300	1.42236700	-2.13968000
H	1.39383800	2.35991100	-1.58690700
H	2.49423600	1.41466100	-2.65998500
H	0.70256800	1.37927600	-2.85757500

TS 4-4

Rh	-0.31366000	0.13855800	-0.18092000
Rh	-2.63562000	-0.40364500	0.36169100
O	0.02519500	-1.89372800	-0.28930900
O	-2.14934200	-2.39542000	0.07077700
O	-0.80877200	2.13744800	-0.00420800
O	-2.93122700	1.63848400	0.59738700
O	-2.08818200	-0.55913800	2.35369100
O	0.02988500	0.05561400	1.88408600
O	-0.92158000	0.12582800	-2.15464700
O	-3.08505700	-0.25017100	-1.63992900
C	-0.95033700	-2.69896000	-0.17934300
C	-2.14161100	-0.05586500	-2.45263300
C	-0.90451600	-0.29382900	2.67568900
C	-1.99138600	2.44051800	0.35008300
C	-0.53780000	-0.36707600	4.13904600
H	-1.32325400	-0.86865600	4.70495500
H	0.41330900	-0.89189100	4.26037700
H	-0.41045700	0.64907300	4.52721900
C	-0.62686400	-4.16544200	-0.33173400
H	0.29428700	-4.29305300	-0.90229800
H	-0.49086200	-4.60318400	0.66335600
H	-1.45764100	-4.68197800	-0.81626500
C	-2.30090300	3.91522500	0.45451200
H	-1.39107600	4.48424400	0.65379000
H	-2.71944900	4.25284700	-0.49955700
H	-3.04622100	4.08990400	1.23252700
C	-2.46903300	-0.04682700	-3.92510000
H	-2.07013900	0.86082700	-4.38557200
H	-1.97789200	-0.90094100	-4.40105800
H	-3.54657900	-0.10902600	-4.07909800
C	1.80336000	0.69759800	-0.93430400
C	2.41148500	-0.63269100	-1.24264400
C	3.42896500	-2.52699500	-0.02245700
O	2.31963800	-1.21343800	-2.31162300
N	3.04280500	-1.12757300	-0.12521100
C	2.91892300	-0.27128900	1.03698900
H	3.84422300	-0.28058000	1.62538100
H	2.07986000	-0.55626000	1.67730800
C	2.68104400	1.12938900	0.46469500
C	3.72933600	1.60456300	-0.39732700
C	1.99788800	2.14402900	1.25116100
C	3.92773000	2.96930300	-0.63529100
H	4.36610500	0.87045200	-0.87917300
C	2.20612700	3.46839600	1.01553000
H	1.27069300	1.80704200	1.97979700
C	3.16566000	3.88595000	0.05472700
H	4.67961600	3.29194000	-1.34691000
H	1.64491500	4.21381500	1.56862500
H	3.31221200	4.94831700	-0.11878100
H	3.06417300	-2.97756400	-0.95022400
C	4.95143400	-2.66794400	0.03356300
H	5.24090300	-3.72366800	0.07553100
H	5.40987900	-2.21881000	-0.85276000
H	5.36062200	-2.17458700	0.92421600
C	2.74494600	-3.20870700	1.16426500
H	3.13604500	-2.83783900	2.12008300
H	1.66788500	-3.02699900	1.12948400
H	2.92558500	-4.28804600	1.13026300
C	1.56026600	1.66729400	-2.06606100
H	1.17076800	2.61282500	-1.67732300
H	2.43451600	1.85932600	-2.69720900
H	0.78316900	1.23072000	-2.69491100
D			
C	-0.71207500	0.88851200	-0.06409100

C	0.76150200	1.15723400	0.09710100
C	2.87731400	-0.10556500	0.19845600
O	1.28213300	2.25493700	0.19030000
N	1.42541000	-0.04218900	0.11288400
C	0.59616500	-1.17185700	-0.26150600
H	0.70570800	-1.99913500	0.44960500
H	0.85784200	-1.54856400	-1.26192000
C	-0.81790000	-0.61044300	-0.25460200
C	-1.26606400	0.03924500	1.07387900
C	-1.86374800	-1.22693400	-1.07732300
C	-2.70746300	-0.00227700	1.35553900
H	-0.60839600	-0.07310200	1.93472300
C	-3.16938600	-1.10046500	-0.77534100
H	-1.54822300	-1.80794800	-1.94078600
C	-3.59967600	-0.47248100	0.46275000
H	-3.03596900	0.33448000	2.33491300
H	-3.92100100	-1.54371900	-1.42173100
H	-4.65941800	-0.47115400	0.70089900
H	3.16847400	0.86557300	0.60859700
C	3.32765200	-1.20792100	1.15597800
H	4.40981000	-1.15021700	1.30884000
H	2.83598800	-1.10406900	2.12819300
H	3.10343100	-2.20434700	0.75736400
C	3.51163100	-0.25210500	-1.18730800
H	3.23949600	-1.20643300	-1.65344800
H	3.18695100	0.56202000	-1.84184800
H	4.60341400	-0.21842400	-1.11118900
C	-1.51306700	1.93269200	-0.78852500
H	-1.24934700	1.95520700	-1.85089900
H	-2.58556900	1.74654700	-0.70386100
H	-1.28743000	2.91330500	-0.36008400

TS D-DRE

C	-0.75948800	0.73690000	-0.29258300
C	0.71789800	1.11198500	-0.23043900
C	2.89255800	-0.01311600	0.08510500
O	1.16502100	2.24355700	-0.26387800
N	1.45177300	-0.03515500	-0.12236800
C	0.65990200	-1.24884700	-0.12345200
H	0.80773400	-1.82463700	0.79894800
H	0.92469800	-1.90165100	-0.96753200
C	-0.76236000	-0.74850900	-0.26631200
C	-1.30923500	0.55297300	1.08584900
C	-1.83841600	-1.55831700	-0.63766800
C	-2.66890800	0.38121400	1.36421000
H	-0.62871300	0.74889200	1.91312600
C	-3.16668000	-1.23011000	-0.41230200
H	-1.61046900	-2.54534200	-1.03634300
C	-3.56944300	-0.28838800	0.54708600
H	-3.01564600	0.71201500	2.34089600
H	-3.93228000	-1.87030800	-0.84278800
H	-4.62488100	-0.25095500	0.80397000
H	3.17746700	1.02387400	-0.11400800
C	3.24739300	-0.34866000	1.53593000
H	4.32387500	-0.23534100	1.69976300
H	2.72274900	0.32189100	2.22304500
H	2.97986300	-1.38245000	1.78460600
C	3.60857700	-0.92767800	-0.90800100
H	3.37560700	-1.98330500	-0.72387900
H	3.32649900	-0.68396900	-1.93683600
H	4.69199500	-0.80806300	-0.81051700
C	-1.53012400	1.53773300	-1.31957700
H	-1.17088300	1.30085400	-2.32602600
H	-2.60015500	1.33195800	-1.27497300
H	-1.36008000	2.60108600	-1.13093200

DRE

C	0.78697600	0.57627800	0.34675900
C	-0.66638800	1.04091900	0.19071800
C	-2.91145600	0.07152300	-0.11042500
O	-1.03558500	2.20225000	0.16825600
N	-1.47491400	-0.05225200	0.09619200
C	-0.76759900	-1.31565100	0.03959100
H	-0.98621700	-1.85227900	-0.89351800
H	-1.05746700	-1.97148400	0.87245800
C	0.68970400	-0.91467100	0.13171800
C	1.63999900	1.21031100	-0.72498000
C	1.71579200	-1.77725400	0.07363900
C	2.90683400	0.85374600	-0.99764300
H	1.19457400	2.04809900	-1.25692100
C	3.12002700	-1.42654700	0.02562700
H	1.48791600	-2.84197700	0.01955900
C	3.64126500	-0.26893900	-0.44652400
H	3.45270800	1.46202300	-1.71681600
H	3.81835800	-2.21218700	0.30640500
H	4.72543200	-0.20172100	-0.51122700
H	-3.13094100	1.11537800	0.13116200
C	-3.28258500	-0.17580400	-1.57484200
H	-4.35016500	0.00875800	-1.73216300
H	-2.71637400	0.49295800	-2.22946500
H	-3.07720400	-1.21112400	-1.87130200
C	-3.68575000	-0.83864900	0.84158800
H	-3.50562200	-1.89771700	0.62168500
H	-3.40320000	-0.64790500	1.88148800
H	-4.76027100	-0.65911200	0.73807600
C	1.27214900	0.95762500	1.75775500
H	2.30745100	0.63863100	1.90050100
H	1.20819400	2.04228500	1.88283800
H	0.64808600	0.47782400	2.51996300

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Sub

C	-1.92994600	-1.02042800	0.04003200
C	-1.83086800	0.44079400	0.22245900
C	-0.54570800	2.48364800	0.29242600
N	-3.13597600	-1.51299100	0.21686200
N	-4.16437700	-1.98865000	0.29307500
O	-2.81601500	1.05434000	0.62228800
N	-0.62354100	1.04568200	-0.02595600
C	0.34548100	0.50189600	-0.96394900
H	0.61064100	1.29428900	-1.67451400
H	-0.14471900	-0.26578100	-1.56813500
C	1.62140900	-0.05920200	-0.36345500
C	2.76286800	-0.13929600	-1.16211700
C	1.68419600	-0.51811100	0.95073100
C	3.94565100	-0.67553500	-0.66232500
H	2.72835100	0.22746300	-2.18634800
C	2.86696800	-1.04964200	1.45547500
H	0.80063900	-0.45669200	1.57677900
C	4.00075000	-1.13222200	0.65144300
H	4.82602600	-0.72762500	-1.29638800
H	2.90238300	-1.40157000	2.48248400
H	4.92280500	-1.54647600	1.04831200
H	-1.21539800	2.61874900	1.14407200
C	0.86560500	2.88963000	0.71187000
H	0.85559700	3.93756500	1.02825100
H	1.22387600	2.27932000	1.54514200
H	1.58741900	2.79874900	-0.10731500
C	-1.07926600	3.34179100	-0.85744100
H	-0.47137400	3.23091700	-1.76340700
H	-2.11116500	3.06287400	-1.08532200
H	-1.06181700	4.40030600	-0.57744200
O	-0.89034200	-1.90497300	0.11234000

C	-0.74785500	-2.79248300	-0.98850800
H	-0.76974500	-2.25300700	-1.94306800
H	0.22045000	-3.27782800	-0.85968000
H	-1.54155200	-3.54951800	-0.98816400

2

C	1.08531400	0.15842300	1.50256700
C	1.80887200	1.46948600	1.23704400
C	3.16400900	2.89809100	-0.12601200
N	0.44518600	0.36227200	2.78226800
N	-0.18823900	0.36001000	3.69363600
O	1.52236200	2.42549000	1.95145400
N	2.69946300	1.53181600	0.20706700
C	2.77823200	0.48680500	-0.82007100
H	3.02570300	0.99139200	-1.75966100
H	1.79007100	0.05205600	-0.97797700
C	3.77623000	-0.63059400	-0.58036100
C	5.03888800	-0.42066300	-0.02749000
C	3.41170300	-1.93010000	-0.94136000
C	5.92223300	-1.48173600	0.15634200
H	5.32888200	0.57361800	0.29111000
C	4.29319900	-2.99171700	-0.76537200
H	2.40803300	-2.10709400	-1.31560500
C	5.55458300	-2.77174700	-0.21553500
H	6.89864200	-1.29907400	0.59599700
H	3.98832800	-3.99682700	-1.04322100
H	6.24270300	-3.59963800	-0.07169800
H	3.08559800	3.45020600	0.81083100
C	4.61937000	2.93803000	-0.58281300
H	4.87148500	3.96459600	-0.86759900
H	5.29947700	2.64231000	0.22102200
H	4.80932100	2.29936100	-1.45263700
C	2.22406100	3.55958600	-1.13546500
H	2.28224300	3.07635200	-2.11729300
H	1.19269900	3.49481900	-0.78221800
H	2.49427100	4.61316300	-1.26364300
O	1.72475000	-1.04288200	1.51373300
C	2.84731800	-1.15876500	2.38664700
H	2.50451300	-1.29893700	3.42005300
H	3.40124000	-2.03754700	2.05574000
H	3.49317600	-0.27725300	2.32343900
Rh	-0.78796100	-0.02313400	0.27828700
Rh	-2.85013900	-0.33196400	-0.95981900
O	-1.48256800	-1.41037600	1.63416700
O	-3.41892500	-1.68087500	0.50378800
O	-0.23844800	1.36066000	-1.16393000
O	-2.14002700	1.02931500	-2.33843400
O	-3.63880300	1.22270200	0.15590800
O	-1.73726800	1.45175700	1.35152200
O	0.02282600	-1.52867200	-0.89818400
O	-1.92508300	-1.86430800	-1.99214000
C	-2.63274800	-1.92566600	1.45651000
C	-0.71370200	-2.11466200	-1.75240100
C	-2.93527600	1.75823100	1.05387400
C	-1.01664900	1.56725000	-2.14883400
C	-3.56911400	2.84617500	1.88378500
H	-4.38962300	3.31124400	1.33573900
H	-3.97111700	2.39847400	2.79899900
H	-2.82095200	3.58831700	2.16782800
C	-3.08238000	-2.91457800	2.50319200
H	-2.31780300	-3.68582800	2.62932900
H	-3.19355700	-2.39849200	3.46174400
H	-4.03202200	-3.36768000	2.21832700
C	-0.53347600	2.55072000	-3.18660800
H	0.41753200	2.20293900	-3.60058200
H	-1.26983500	2.65376000	-3.98376300
H	-0.35356400	3.52136200	-2.71646200

C	-0.05021300	-3.20533300	-2.55836400
H	-0.79007500	-3.76311000	-3.13301700
H	0.67316600	-2.75246200	-3.24463800
H	0.49784100	-3.87518300	-1.89072200

TS 2-3

C	1.06216500	0.15909900	1.44956900
C	1.83012000	1.45840500	1.22796000
C	3.17707400	2.89226700	-0.13972500
N	0.41116200	0.44704100	2.83117700
N	-0.26623500	0.42725300	3.70479100
O	1.57228900	2.40489900	1.96664600
N	2.70840600	1.52629400	0.18888900
C	2.78644900	0.48002000	-0.84001400
H	3.05883800	0.98283000	-1.77315000
H	1.79275600	0.06395000	-1.01467500
C	3.76086000	-0.65629800	-0.58463300
C	5.06319900	-0.45381000	-0.12668300
C	3.33466900	-1.96348800	-0.83228900
C	5.92184700	-1.53051700	0.07907400
H	5.40892800	0.54899500	0.09413100
C	4.19259800	-3.04148400	-0.63539800
H	2.30323000	-2.13057900	-1.12672100
C	5.49095500	-2.82942800	-0.17787200
H	6.92973100	-1.35295500	0.44331500
H	3.83903900	-4.05116600	-0.82449000
H	6.16049600	-3.66936400	-0.01695900
H	3.09233000	3.44289800	0.79724300
C	4.63594000	2.93365200	-0.58330500
H	4.89645500	3.96497000	-0.84223000
H	5.30586000	2.61512700	0.22060000
H	4.82867900	2.31493700	-1.46689600
C	2.24451400	3.55379200	-1.15571200
H	2.30784500	3.06967000	-2.13679300
H	1.21069400	3.49006900	-0.80945500
H	2.51659400	4.60697200	-1.28310600
O	1.69145400	-1.02465600	1.56047000
C	2.85172000	-1.08343700	2.39230300
H	2.54519600	-1.10400700	3.44572900
H	3.36602100	-2.00866400	2.13346700
H	3.51561200	-0.23416800	2.20920300
Rh	-0.77419100	-0.02420100	0.27253700
Rh	-2.84986800	-0.32926300	-0.96207000
O	-1.47081000	-1.40381600	1.63526100
O	-3.40593800	-1.68492500	0.50333300
O	-0.22626500	1.35518200	-1.17635500
O	-2.14024100	1.04025600	-2.33664700
O	-3.63223900	1.22141700	0.16639200
O	-1.71805900	1.46057800	1.34085200
O	0.02334000	-1.53755600	-0.90334600
O	-1.92249700	-1.85533400	-2.00678900
C	-2.61940800	-1.92397100	1.45606300
C	-0.71459700	-2.11301100	-1.76560600
C	-2.92119200	1.76094300	1.05427500
C	-1.01284700	1.56961600	-2.15406400
C	-3.54935600	2.84816100	1.89028600
H	-4.37707800	3.31019300	1.35058200
H	-3.94065800	2.40003700	2.80998000
H	-2.80092500	3.59320800	2.16599600
C	-3.06397600	-2.91398100	2.50453900
H	-2.29812500	-3.68454500	2.62748600
H	-3.17228100	-2.39886200	3.46393700
H	-4.01407000	-3.36814200	2.22282200
C	-0.53124000	2.55551000	-3.19093700
H	0.42189400	2.21227700	-3.60367900
H	-1.26708500	2.65638000	-3.98885400
H	-0.35651400	3.52697800	-2.72024300

C	-0.05509700	-3.21289400	-2.56306800
H	-0.75782700	-3.64523400	-3.27562000
H	0.81124200	-2.80746200	-3.09457000
H	0.30783700	-3.98580900	-1.87914400

3

Rh	-0.79831300	-0.06107400	0.41375600
Rh	-2.82603700	-0.15151600	-0.96555900
O	-0.06232900	1.32218000	-0.93795900
O	-1.91928400	1.22692200	-2.22131700
O	-1.71440600	-1.43386700	1.66569700
O	-3.57865600	-1.52262700	0.39068300
O	-1.90910900	-1.69754200	-2.01954000
O	-0.04004600	-1.60532700	-0.75278600
O	-1.68876100	1.46183400	1.46169100
O	-3.56175600	1.39419900	0.19418300
C	-0.77294400	1.65588600	-1.94300600
C	-2.85502400	1.84938100	1.13242900
C	-0.75562100	-2.07349100	-1.70229700
C	-2.88540300	-1.85137300	1.38504400
C	-0.13837300	-3.20860100	-2.48327100
H	-0.28307800	-4.14020300	-1.92587500
H	-0.62150200	-3.30594500	-3.45622100
H	0.93581800	-3.04876200	-2.59859500
C	-0.15879700	2.67859100	-2.86761000
H	-0.13263300	3.64841000	-2.36102500
H	0.87266500	2.39962900	-3.09785300
H	-0.74324700	2.76330800	-3.78395500
C	-3.48399400	-2.82612400	2.37072000
H	-2.75266600	-3.59769600	2.62430500
H	-3.73545300	-2.29047600	3.29167600
H	-4.38626700	-3.27843600	1.95842700
C	-3.44316500	2.94549000	1.98608000
H	-4.25283100	3.44722800	1.45450400
H	-3.84561800	2.49731100	2.90061200
H	-2.66615000	3.65605200	2.27397200
C	0.95793100	0.03660400	1.42146100
C	1.76365300	1.31829500	1.42083900
C	3.39276000	2.75560300	0.35553700
O	1.49020700	2.12373200	2.29719700
N	2.71108000	1.45635600	0.46397600
C	2.85714300	0.46148400	-0.58679100
H	3.01424900	0.98616000	-1.53542400
H	1.90556200	-0.06494800	-0.71871400
C	3.95924100	-0.55997100	-0.37656800
C	4.35100400	-1.34904800	-1.46075800
C	4.55662700	-0.77559900	0.86363500
C	5.31931600	-2.33543500	-1.30947000
H	3.89099300	-1.18816800	-2.43381400
C	5.53019900	-1.76077500	1.01736200
H	4.26338700	-0.16586700	1.71229000
C	5.91391700	-2.54401200	-0.06655200
H	5.61452300	-2.93846600	-2.16329300
H	5.99152700	-1.91237500	1.98899600
H	6.67411700	-3.31011700	0.05333800
H	3.29414300	3.20535200	1.34618200
C	4.87640900	2.59440300	0.03356800
H	5.35009400	3.58100200	0.01645300
H	5.38381600	1.98095500	0.78273500
H	5.03639600	2.13252400	-0.94711600
C	2.67006600	3.65360100	-0.65047200
H	2.74760900	3.25461000	-1.66851700
H	1.61133800	3.73574500	-0.39085900
H	3.11438600	4.65434500	-0.64933700
O	1.59934000	-0.86287200	2.07319800
C	1.03715800	-2.18580600	2.25861600
H	1.86578400	-2.78532500	2.63095800

H	0.22526800	-2.11909400	2.97962000
H	0.67172600	-2.55240700	1.30044700
4-1			
Rh	-0.94501200	0.38923300	-0.20395200
Rh	-2.52610400	-1.35038200	0.48868400
O	0.53646000	-1.05832000	-0.18589400
O	-0.92311100	-2.66771200	0.44545300
O	-2.51954100	1.71846200	-0.17095200
O	-3.98676400	0.12022700	0.47339900
O	-2.06471300	-0.87009700	2.45522100
O	-0.62148000	0.74629100	1.81496100
O	-1.40779600	-0.09459800	-2.14972200
O	-2.86438600	-1.70634700	-1.52246000
C	0.21915100	-2.25544900	0.12490600
C	-2.25132900	-1.02004100	-2.38016700
C	-1.23755300	0.04553900	2.68447100
C	-3.67654800	1.29665600	0.15027900
C	-0.91530500	0.36581500	4.12469200
H	-1.06645900	1.43344400	4.30593900
H	-1.54214700	-0.22235000	4.79507100
H	0.13861700	0.14140300	4.31631300
C	1.33818600	-3.26581900	0.07834000
H	1.58985600	-3.45993400	-0.96967400
H	2.23158900	-2.86524400	0.56291400
H	1.02719700	-4.19738700	0.55178900
C	-4.78936800	2.31629800	0.10160500
H	-4.39415200	3.32279700	0.24687600
H	-5.26353400	2.26643800	-0.88435100
H	-5.54417600	2.08306400	0.85453700
C	-2.54856500	-1.28466300	-3.83601600
H	-3.02163900	-2.26012700	-3.95486800
H	-3.23203600	-0.51113100	-4.20152800
H	-1.62925200	-1.22572400	-4.42237100
C	0.34012400	1.80421900	-0.82507300
C	1.79149900	1.53879600	-1.16730900
C	2.33682600	1.70445300	1.22673600
O	2.00497500	1.36193500	-2.36278100
N	2.71353400	1.53133200	-0.18548500
C	4.11220000	1.37670000	-0.57525500
H	4.70836400	2.09358600	-0.00260100
H	4.16816400	1.66644200	-1.62861800
C	4.68840000	-0.01339200	-0.41080500
C	5.90871400	-0.18642600	0.24155900
C	4.04046600	-1.12524600	-0.95308000
C	6.48366000	-1.45010600	0.35269700
H	6.41538300	0.67568300	0.67032100
C	4.61790300	-2.38652700	-0.84632400
H	3.08238100	-1.00132800	-1.44997100
C	5.83853300	-2.55415900	-0.19490100
H	7.43332200	-1.57000600	0.86563800
H	4.11332100	-3.24646200	-1.27673900
H	6.28296900	-3.54158900	-0.11374600
H	1.25013600	1.83122000	1.24269200
C	2.63708600	0.45522600	2.05139800
H	2.22616800	0.58569200	3.05756600
H	2.16285200	-0.41281000	1.58871600
H	3.71255000	0.27232100	2.13900200
C	2.96265400	2.96404700	1.82760700
H	4.04500100	2.86132000	1.96136700
H	2.77097600	3.84273000	1.20210800
H	2.52691100	3.14720300	2.81439200
O	-0.10313700	2.96899300	-1.13576900
C	0.74123200	3.99722200	-1.70353400
H	0.17629300	4.92097200	-1.59881200
H	1.68570600	4.05703700	-1.15814400
H	0.91926000	3.75560400	-2.75099000

TS 4-1

Rh	-0.78104000	0.45572600	-0.03443200
Rh	-2.15942600	-1.51967200	0.21933100
O	0.66049100	-0.50359100	1.09568400
O	-0.57551600	-2.38241900	1.25471100
O	-2.32369900	1.30137500	-1.10092000
O	-3.62752700	-0.52626000	-0.83154200
O	-2.85451600	-0.66426700	1.98017100
O	-1.56878000	1.17660000	1.73644600
O	-0.06887900	-0.39475800	-1.77321300
O	-1.37104800	-2.22775600	-1.55093100
C	0.45234200	-1.69552800	1.49032400
C	-0.51133800	-1.52518600	-2.14929800
C	-2.43206400	0.46373000	2.34387700
C	-3.39132700	0.63788900	-1.26473500
C	-3.01770700	1.05747200	3.60153300
H	-3.47485200	0.27890800	4.21315500
H	-2.24726300	1.58828500	4.16500600
H	-3.78687000	1.78337600	3.31792800
C	1.52730000	-2.31039200	2.35106800
H	1.56863700	-3.38837500	2.18771400
H	2.49744200	-1.85965100	2.13487400
H	1.27481100	-2.13238900	3.40236400
C	-4.48255400	1.29468800	-2.07386600
H	-4.27908500	2.35767400	-2.20592000
H	-4.53100900	0.81184600	-3.05513900
H	-5.44668900	1.14499900	-1.58241200
C	0.07660500	-2.06627800	-3.42907000
H	-0.43749500	-2.97804400	-3.73390200
H	0.00635000	-1.30596100	-4.21086300
H	1.14021900	-2.27692600	-3.27481100
C	0.50075100	2.32506700	-0.22383900
C	1.74900600	2.02581400	-1.00319000
C	2.71169600	1.77746300	1.20181700
O	1.73392800	2.06197700	-2.22311900
N	2.84504700	1.71494700	-0.24835200
C	3.97481100	1.04058000	-0.86679700
H	4.90545100	1.52310700	-0.54994000
H	3.86350000	1.20604700	-1.94136900
C	4.01186800	-0.44217200	-0.55741000
C	5.07680300	-1.01528100	0.13427800
C	2.95480100	-1.25488000	-0.97628000
C	5.09841500	-2.38635600	0.39302600
H	5.90434600	-0.39024500	0.46426800
C	2.97363700	-2.62031100	-0.71971700
H	2.10885600	-0.80575100	-1.48904500
C	4.04880400	-3.19114100	-0.03753800
H	5.93722500	-2.82260600	0.92751900
H	2.14135500	-3.24139300	-1.04106400
H	4.06310500	-4.25867200	0.16193000
H	2.51089200	0.77431200	1.59260700
C	3.95697300	2.35231600	1.87456900
H	3.76537000	2.50469400	2.94171600
H	4.80470700	1.66603300	1.78775600
H	4.23210600	3.31317600	1.42631500
C	1.49593000	2.64759100	1.45038400
H	1.64550600	3.71713300	1.30480300
H	0.42353800	2.01741000	0.92553500
H	1.00486200	2.46177800	2.41117200
O	-0.23789500	3.40157100	-0.51892400
C	0.39923000	4.52050100	-1.13299600
H	0.66731900	4.28271100	-2.16345600
H	-0.33180600	5.32816900	-1.10266600
H	1.29871900	4.82001500	-0.57980700

A

C	-2.81633800	0.21008800	-0.16442600
C	-1.56166500	-0.21695900	-0.94331700
C	-0.99808200	1.77718400	0.21720400
O	-1.44825700	-1.18791100	-1.67185500
N	-0.59244200	0.70523500	-0.69055600
C	0.66251100	0.70505600	-1.41671900
H	0.90271700	1.73545300	-1.70552300
H	0.48848000	0.13007000	-2.33220800
C	1.80976700	0.09374900	-0.63789100
C	3.00885700	0.77969800	-0.45899500
C	1.66868700	-1.18354200	-0.08934400
C	4.05407800	0.20559100	0.26172900
H	3.12831000	1.77424200	-0.88392000
C	2.70803100	-1.75585300	0.63416900
H	0.74100200	-1.72756700	-0.24568000
C	3.90360400	-1.06192800	0.81388300
H	4.98345200	0.75155500	0.39516600
H	2.58745200	-2.74887300	1.05741400
H	4.71532200	-1.51025700	1.37907200
H	-1.25647600	2.66828300	-0.37699400
C	-2.26400500	1.19789600	0.87042100
H	-2.98234500	1.97227800	1.14721200
H	-3.45883700	0.73973000	-0.87875900
H	-1.98070100	0.65998200	1.78195100
C	0.08109000	2.15558700	1.22370300
H	0.40316700	1.27617800	1.79026800
H	0.96185300	2.58494300	0.73701100
H	-0.31639500	2.89992600	1.92186700
O	-3.60665900	-0.83400400	0.32390900
C	-2.92687100	-1.84111300	1.04258500
H	-2.42191800	-1.44911700	1.93731500
H	-3.69076400	-2.55176200	1.36327000
H	-2.19587300	-2.35911300	0.41197700

4-2

Rh	0.90597400	0.10314300	0.39829800
Rh	2.89831200	-0.03353500	-1.02833700
O	-0.04992200	-1.07353900	-1.01114700
O	1.77719000	-1.18475300	-2.33575800
O	2.04542400	1.24274400	1.69961500
O	3.88221600	1.11459800	0.38857200
O	2.20863200	1.69265900	-1.96401000
O	0.36929300	1.81241400	-0.65613800
O	1.57206800	-1.59720600	1.33238700
O	3.40662500	-1.74502400	0.01628000
C	0.58517500	-1.45401000	-2.04817500
C	2.65366200	-2.14350200	0.94455900
C	1.13631800	2.22563000	-1.59058100
C	3.26661200	1.47876300	1.42110900
C	0.70297200	3.49787300	-2.27824700
H	0.96941700	4.34939100	-1.64282400
H	1.21110900	3.60289700	-3.23731100
H	-0.38078500	3.50546100	-2.41375500
C	-0.19206000	-2.33103700	-3.00041500
H	-0.33160400	-3.31510400	-2.54119400
H	-1.18159500	-1.90191600	-3.17940500
H	0.34599300	-2.44591700	-3.94169500
C	4.03943000	2.24961300	2.46428800
H	3.41136200	3.02590600	2.90688700
H	4.33401700	1.55887800	3.26126500
H	4.93761600	2.68590600	2.02591600
C	3.07423500	-3.37431500	1.70928000
H	3.71638800	-4.00225700	1.08987600
H	3.64019000	-3.05983400	2.59261100
H	2.19591600	-3.92645800	2.04779300
C	-0.82235400	0.19227600	1.45864700
C	-1.74881600	-0.99951700	1.49213200

C	-3.47924700	-2.37213600	0.52346700
O	-1.54646100	-1.76696500	2.42324300
N	-2.67168500	-1.14065900	0.51886200
C	-2.83736700	-0.13520600	-0.52192400
H	-2.72338600	-0.61047800	-1.49992200
H	-2.00644800	0.57419200	-0.45539300
C	-4.15593400	0.60492000	-0.44540400
C	-5.01629600	0.63334000	-1.54100700
C	-4.52739400	1.26994400	0.72605100
C	-6.23356400	1.30884600	-1.47069000
H	-4.73601300	0.11768200	-2.45691000
C	-5.74032800	1.94380400	0.80004400
H	-3.86592300	1.24206600	1.58809700
C	-6.59875500	1.96309000	-0.29896500
H	-6.89784700	1.31744800	-2.32985700
H	-6.02043400	2.45240900	1.71788100
H	-7.54945400	2.48424500	-0.23860800
H	-2.89271000	-3.07460200	1.12098200
C	-4.82931600	-2.17345400	1.21716700
H	-5.32667800	-3.14211200	1.33725700
H	-4.68616300	-1.73658400	2.20975700
H	-5.48718300	-1.51810100	0.63871600
C	-3.63321500	-2.94492800	-0.88325700
H	-4.28369400	-2.32319400	-1.50881500
H	-2.65972600	-3.04806300	-1.37276200
H	-4.09217500	-3.93614700	-0.81709100
O	-1.32997300	1.15159400	2.14767100
C	-0.57374800	2.37051400	2.36326400
H	-0.26009100	2.76369000	1.39680300
H	-1.26525700	3.04074600	2.87048000
H	0.29325200	2.13690400	2.97720000

TS 4-2

C	-1.55105400	-0.49329300	-0.87970500
C	-2.84462600	0.41579400	0.50721800
H	-1.50126200	-0.48368300	0.27001400
Rh	0.66827600	-0.24164600	-0.15773300
Rh	2.97920200	0.10375800	0.46021400
O	0.11822500	0.72229300	1.58876300
O	2.27508100	1.08859100	2.14544000
O	1.34543700	-1.20155300	-1.84701500
O	3.50672700	-0.89008500	-1.26736500
O	2.89169700	-1.69436900	1.47577300
O	0.73789600	-2.03111500	0.88814600
O	0.75454700	1.58989200	-1.09052400
O	2.93462600	1.87908400	-0.58707900
C	1.03492200	1.19203000	2.33671500
C	1.84467600	2.23831600	-1.11374900
C	1.81942200	-2.35677500	1.47060000
C	2.59724300	-1.31740500	-2.03114000
C	1.81635700	-3.67982300	2.19649300
H	2.61945300	-3.71163200	2.93352200
H	0.84836400	-3.84618800	2.67361400
H	1.97656200	-4.48014700	1.46613200
C	0.57872100	1.97621400	3.54170700
H	0.38311600	3.00817400	3.23020500
H	-0.34881800	1.55953000	3.93990600
H	1.35589400	1.98492900	4.30672600
C	3.01901500	-2.06178700	-3.27289700
H	4.07926000	-1.90256400	-3.47126700
H	2.83835400	-3.13112300	-3.12190500
H	2.41423200	-1.73684900	-4.12239600
C	1.80875200	3.57598100	-1.80759400
H	1.01296200	3.58989400	-2.55351400
H	1.60626700	4.35158300	-1.06074400
H	2.77667300	3.78850800	-2.26480300
C	-1.94708000	0.81698600	-1.47937900

C	-2.71594500	2.87548100	-0.22561700
O	-1.78655200	1.21926600	-2.61004500
N	-2.54849600	1.43984400	-0.41352100
H	-2.49178300	0.59243000	1.52811100
C	-4.06081300	-0.40148200	0.40326800
C	-4.44780100	-1.17398500	1.50664500
C	-4.80865700	-0.48290000	-0.77841600
C	-5.55933600	-2.00377700	1.43533300
H	-3.87064900	-1.11800100	2.42709200
C	-5.92302100	-1.31046500	-0.84491500
H	-4.51705200	0.10369200	-1.64405200
C	-6.30150400	-2.07328400	0.25762200
H	-5.85052300	-2.59305500	2.29973300
H	-6.49573100	-1.36327900	-1.76584400
H	-7.17240700	-2.71928700	0.20043100
H	-2.50335500	3.29816400	-1.21276100
C	-4.15611700	3.19978900	0.16611200
H	-4.29257800	4.28199800	0.25707200
H	-4.85939800	2.82032700	-0.58119000
H	-4.40802300	2.74569500	1.13196900
C	-1.69481000	3.41207600	0.77917600
H	-1.85747700	2.97886100	1.77291900
H	-0.68328100	3.15406900	0.45550400
H	-1.78443200	4.50022100	0.86526200
O	-1.99065200	-1.57820300	-1.49714500
C	-1.47383700	-2.83587800	-1.06344700
H	-1.61833500	-2.95438500	0.01458100
H	-2.04499500	-3.59042200	-1.60398100
H	-0.41133400	-2.90271300	-1.30311200

B

C	0.83200800	1.71704200	-0.48002000
C	1.97754000	1.05090000	0.30995800
C	2.15392700	-1.50039300	0.12934400
O	2.92247600	1.42578100	0.95935200
N	1.54071500	-0.19578100	-0.04265400
C	0.38442100	0.24102900	-0.82728800
H	0.49426900	0.01152600	-1.89511600
H	1.18866500	2.25736000	-1.37018300
C	-0.96594800	-0.21494400	-0.34297400
C	-1.89649500	-0.72315700	-1.24918100
C	-1.31549300	-0.12346700	1.00748200
C	-3.15787100	-1.13013200	-0.82112400
H	-1.63177100	-0.80453700	-2.30128800
C	-2.57278300	-0.53004400	1.43660900
H	-0.59781100	0.26934800	1.72010900
C	-3.49813200	-1.03371300	0.52400800
H	-3.87089700	-1.52560500	-1.53851300
H	-2.83233300	-0.45237500	2.48823900
H	-4.47943600	-1.35264100	0.86280500
H	3.12181500	-1.28831200	0.59683000
C	1.33294000	-2.39057100	1.06486700
H	1.85317100	-3.33900800	1.23557400
H	1.18001300	-1.89947700	2.03000200
H	0.35113100	-2.61051900	0.63341200
C	2.38314900	-2.16412400	-1.22910600
H	1.42780900	-2.36855900	-1.72691000
H	2.98687900	-1.52557700	-1.88143200
H	2.90269000	-3.11880400	-1.10175800
O	-0.00529400	2.50139200	0.29358500
C	-1.03707100	3.11114600	-0.45155600
H	-0.62379600	3.75584300	-1.24149800
H	-1.70144100	2.36514200	-0.90728700
H	-1.61256400	3.72185300	0.24596500

4-3

Rh	-0.88371500	0.38429400	-0.26962400
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Rh	-2.32199900	-1.37042800	0.65865400
O	0.73599200	-0.80420400	0.21954800
O	-0.58467400	-2.41610200	1.09467200
O	-2.59457100	1.45704800	-0.68723500
O	-3.93095800	-0.16694200	0.14791900
O	-2.16599600	-0.40518200	2.49153000
O	-0.83499900	1.20729900	1.63534100
O	-1.05435600	-0.56829200	-2.08692200
O	-2.35348600	-2.21122400	-1.23329800
C	0.53319400	-1.91987800	0.80313300
C	-1.73670100	-1.63965900	-2.16931400
C	-1.47145100	0.63579100	2.58174900
C	-3.72473700	0.94660900	-0.40102200
C	-1.36999600	1.30709900	3.93063800
H	-1.87169700	2.27862600	3.88606200
H	-1.83471100	0.69010900	4.69991000
H	-0.31929200	1.48692700	4.17392000
C	1.76018000	-2.72041700	1.16248800
H	1.94324600	-3.45666900	0.37356200
H	2.64131100	-2.08084900	1.23445600
H	1.58828600	-3.25770400	2.09720800
C	-4.93182600	1.76441400	-0.79496300
H	-4.74418700	2.82500100	-0.61510200
H	-5.10968200	1.63061600	-1.86719600
H	-5.81304700	1.42963000	-0.24642500
C	-1.83011200	-2.25362400	-3.54528700
H	-2.05625100	-3.31799400	-3.46773000
H	-2.64121600	-1.76184900	-4.09279000
H	-0.90100800	-2.09252600	-4.09503600
C	0.30883900	1.81011400	-1.04517100
C	1.78941200	1.58361500	-1.26247700
C	2.17884400	2.10719100	1.10279200
O	2.08876000	1.30556700	-2.42259500
N	2.63013300	1.64041100	-0.21693700
C	4.03615400	1.30919300	-0.45716200
H	4.64013900	1.88387900	0.25012800
H	4.27837600	1.66316900	-1.46376300
C	4.37657000	-0.16479200	-0.34787700
C	5.22648900	-0.62192200	0.65908900
C	3.89348400	-1.07711800	-1.29176200
C	5.59126300	-1.96522700	0.73033900
H	5.61704600	0.07940300	1.39347900
C	4.26237400	-2.41588700	-1.22571200
H	3.23330100	-0.72820700	-2.07858000
C	5.11181700	-2.86504000	-0.21612800
H	6.25511400	-2.30379300	1.52033100
H	3.88439300	-3.11318500	-1.96778500
H	5.39652900	-3.91191300	-0.16666400
H	1.08640100	2.15596200	1.05782800
C	2.51905700	1.11571600	2.20960100
H	2.07459200	1.46092800	3.14840300
H	2.10823300	0.13591400	1.96483100
H	3.59959700	1.02578400	2.36206800
C	2.70402200	3.51408300	1.39983700
H	3.79457400	3.53035800	1.50587500
H	2.42623800	4.21728800	0.60761800
H	2.27538900	3.87659900	2.33943100
O	-0.19291100	2.88078700	-1.54292700
C	0.61132000	3.87792600	-2.21434100
H	0.83018300	3.51679200	-3.21862000
H	-0.00505300	4.77425500	-2.23748600
H	1.53780300	4.05742400	-1.66470800

TS 4-3

Rh	-0.83442400	0.44801100	-0.11848300
Rh	-2.27735600	-1.46566000	0.39589400
O	0.58130600	-0.41760700	1.12911500

O	-0.75004200	-2.18384300	1.59538100
O	-2.34730200	1.15155500	-1.32519500
O	-3.68852900	-0.60841100	-0.85644800
O	-3.00435100	-0.33800400	1.97939600
O	-1.66474500	1.42063500	1.49978100
O	-0.08277000	-0.67317600	-1.68051500
O	-1.41815800	-2.43895800	-1.22444200
C	0.32102300	-1.53333800	1.68987100
C	-0.52244700	-1.85217300	-1.88231400
C	-2.55763700	0.81943800	2.18191900
C	-3.42239400	0.47751700	-1.43270700
C	-3.11329300	1.59493900	3.35259100
H	-3.46286000	2.57284400	3.01071600
H	-3.93011600	1.04570100	3.82130400
H	-2.31668900	1.76468200	4.08346100
C	1.41909700	-2.11724200	2.54552300
H	1.09141400	-3.05730700	2.98982700
H	2.30751400	-2.28574100	1.92826900
H	1.68811800	-1.40787600	3.33336200
C	-4.45791900	1.04789200	-2.37164700
H	-5.41309300	0.53898200	-2.23895700
H	-4.56868500	2.12090400	-2.19854600
H	-4.11430300	0.90910500	-3.40176900
C	0.09818500	-2.58312600	-3.04820200
H	-0.33439600	-2.19441300	-3.97580200
H	1.17407800	-2.39458300	-3.08231500
H	-0.10598400	-3.65231500	-2.97965100
C	0.29242700	2.02759100	-0.66128100
C	1.71912200	1.84037600	-1.11893600
C	2.45060500	2.02529600	1.21823900
O	1.84827600	1.74086300	-2.33593500
N	2.68627700	1.68334200	-0.19491700
C	3.99239000	1.22735700	-0.65764100
H	4.77357700	1.77493000	-0.12059500
H	4.06402400	1.49907100	-1.71453000
C	4.18262600	-0.26958800	-0.49289000
C	5.38067400	-0.77631900	0.00712600
C	3.15924600	-1.15575900	-0.83968800
C	5.56132000	-2.14885400	0.16426400
H	6.17796700	-0.09203700	0.28981100
C	3.33778700	-2.52595800	-0.67844900
H	2.21347100	-0.78215100	-1.22058900
C	4.53763300	-3.02800900	-0.17554700
H	6.49790600	-2.52904200	0.56159400
H	2.53100600	-3.20529300	-0.94079800
H	4.67157300	-4.09783000	-0.04633900
H	1.37934500	1.87810500	1.39451900
C	3.19186400	1.09225400	2.17012500
H	2.85809900	1.29590400	3.19233500
H	2.97704900	0.05165400	1.93324100
H	4.27564700	1.24912400	2.13545500
C	2.80847400	3.48985500	1.48605100
H	2.63763400	3.73300400	2.53962900
H	3.86349500	3.68333800	1.26014400
H	2.19703200	4.16842600	0.88288200
O	-0.26701400	3.15814800	-0.88948600
C	0.41430700	4.24887000	-1.55066200
H	0.38491000	4.05726000	-2.62285300
H	-0.15160500	5.14115600	-1.29061400
H	1.44814900	4.32945400	-1.20996500
C			
C	-2.41775100	-0.14311500	-0.04728000
C	-1.50243300	0.47904400	1.03327700
C	-1.25314000	-1.15635600	-0.28320900
O	-1.50863700	1.46812400	1.73469100
N	-0.60088800	-0.53021900	0.88672000

C	0.69314200	-0.72861200	1.49578900
H	0.84103700	-1.80005700	1.67353400
H	0.64909200	-0.23511800	2.47259700
C	1.83377900	-0.16529800	0.67320600
C	2.84593300	-0.98781300	0.18495300
C	1.86247900	1.20092100	0.38091900
C	3.87625700	-0.45773900	-0.58937300
H	2.82788400	-2.05292300	0.40573200
C	2.88812600	1.73084400	-0.39246700
H	1.07158000	1.84272900	0.76217100
C	3.89786400	0.90188400	-0.88017300
H	4.65879500	-1.10962200	-0.96657400
H	2.90299800	2.79406000	-0.61341400
H	4.69869700	1.31689300	-1.48494900
H	-3.31471800	-0.61461200	0.38661200
C	-0.50374600	-0.93761700	-1.59213900
H	-1.12534100	-1.25418600	-2.43515100
H	-0.25165000	0.11614200	-1.72773700
H	0.42428300	-1.51861700	-1.60109700
C	-1.59950800	-2.62193700	-0.05627200
H	-0.69171000	-3.23600300	-0.03479700
H	-2.12840700	-2.75687200	0.89280700
H	-2.23451200	-2.99286200	-0.86729100
O	-2.73782700	0.64311500	-1.14761100
C	-3.68084700	1.64954800	-0.83633700
H	-3.29695200	2.33412300	-0.07142900
H	-3.87006200	2.19710700	-1.76143400
H	-4.62402200	1.20892500	-0.47862900

4-4

Rh	-0.61314700	-0.11614100	0.26797800
Rh	-2.89821200	0.06519200	-0.61415400
O	-0.41994500	1.92283100	-0.04719900
O	-2.54500400	2.10401700	-0.80106400
O	-0.94198600	-2.13781500	0.49148800
O	-3.04386700	-1.98575800	-0.33610000
O	-2.11278800	-0.24998600	-2.50988900
O	-0.01697900	-0.45579700	-1.69662400
O	-1.41218200	0.21371300	2.13356700
O	-3.52089700	0.37291200	1.33447200
C	-1.42410800	2.57560600	-0.48401900
C	-2.66787100	0.38008300	2.25884900
C	-0.88065300	-0.43933900	-2.63707900
C	-2.06909600	-2.61885200	0.14724600
C	-0.32981000	-0.67242900	-4.02346400
H	0.18160400	-1.63897700	-4.05425500
H	-1.13051100	-0.65187700	-4.76277500
H	0.41027400	0.09934300	-4.25524700
C	-1.22014600	4.06176000	-0.66182500
H	-0.57466700	4.45240500	0.12759700
H	-0.73048500	4.23916100	-1.62571000
H	-2.18224200	4.57561300	-0.66217800
C	-2.25370100	-4.09984700	0.37861800
H	-1.29547100	-4.61903000	0.32368200
H	-2.66927200	-4.24630600	1.38133200
H	-2.95911100	-4.50769700	-0.34729800
C	-3.16483600	0.57424200	3.67054700
H	-4.15076100	1.04049400	3.66233000
H	-3.24087500	-0.40551400	4.15375500
H	-2.45588500	1.17826200	4.24020000
C	1.20793600	-0.21325200	1.13428200
C	2.08320200	1.02341500	1.22721500
C	3.32529200	2.80058700	0.15845300
O	1.95603800	1.62336500	2.29091100
N	2.81030900	1.42365600	0.16699100
C	2.89941200	0.59437100	-1.04073900
H	3.51797000	1.14628100	-1.75274800

H	1.91007400	0.47306900	-1.49170000
C	3.52530800	-0.75984300	-0.77562200
C	4.84478000	-0.85453700	-0.31802500
C	2.78570400	-1.92822400	-0.96156000
C	5.41129900	-2.09389100	-0.04337100
H	5.42584000	0.05196900	-0.16958800
C	3.35130300	-3.17088400	-0.67817000
H	1.75859800	-1.85677800	-1.30925300
C	4.66112200	-3.25729600	-0.21836100
H	6.43697800	-2.15486300	0.30891700
H	2.76106600	-4.07198800	-0.81484000
H	5.10134300	-4.22579800	-0.00032800
H	3.03810300	3.20371200	1.13147300
C	4.84806400	2.83783700	0.04921600
H	5.19869300	3.87400300	0.09486800
H	5.30949300	2.28378900	0.87270700
H	5.20097400	2.41358200	-0.89849300
C	2.63048100	3.62228300	-0.92896600
H	2.94772300	3.32413000	-1.93515300
H	1.54863800	3.49045600	-0.85092400
H	2.87102800	4.68338700	-0.80685400
O	1.49254600	-1.21264700	1.87835500
C	2.71343800	-1.27429200	2.65429500
H	2.64791000	-0.53934300	3.45585400
H	2.75183500	-2.28977000	3.04189700
H	3.56792000	-1.07828400	2.00325600

TS 4-4

Rh	-0.35424900	-0.12489000	0.05312400
Rh	-2.72165100	0.34621800	-0.13202100
O	-0.07916800	1.89788500	0.36907300
O	-2.29237200	2.32966700	0.25766500
O	-0.79786700	-2.10522600	-0.31197300
O	-3.00658700	-1.66528200	-0.49963100
O	-2.44203400	0.67398500	-2.15467200
O	-0.24414800	0.18735700	-2.00551900
O	-0.67148400	-0.38376800	2.06956900
O	-2.88748500	0.00981500	1.89061900
C	-1.08705700	2.66631400	0.42526100
C	-1.83983700	-0.26374700	2.54354700
C	-1.29224500	0.52411200	-2.64330800
C	-2.00589800	-2.43752900	-0.50196400
C	-1.11842600	0.76019100	-4.12390800
H	-0.73985600	-0.15190200	-4.59485700
H	-2.06463500	1.04774800	-4.58231900
H	-0.37353700	1.54606600	-4.28054200
C	-0.80528000	4.12627900	0.68095400
H	0.12516700	4.23884100	1.23998100
H	-0.69740100	4.63716300	-0.28221300
H	-1.63877300	4.58287800	1.21726500
C	-2.27211200	-3.90705500	-0.71936100
H	-1.42089900	-4.37618300	-1.21619600
H	-2.40261000	-4.38445600	0.25764700
H	-3.18676100	-4.04750500	-1.29727100
C	-1.97843800	-0.48439600	4.02924600
H	-1.73060600	-1.52510400	4.25957900
H	-1.26452600	0.15183000	4.55886900
H	-2.99540400	-0.26799700	4.35732600
C	1.93627800	-0.71359900	0.59192400
C	2.42580100	0.61838800	1.07284900
C	3.13889900	2.74088600	0.04158600
O	2.37480700	1.05236100	2.21337600
N	2.86797000	1.31153700	-0.02566000
C	2.71708600	0.60078500	-1.28784700
H	3.58743000	0.77533800	-1.93064100
H	1.80798600	0.89799400	-1.81838300
C	2.64622400	-0.87424000	-0.89732500

C	3.80571100	-1.31056200	-0.14128600
C	2.02270300	-1.87201400	-1.76090300
C	4.05740100	-2.68317900	0.03738700
H	4.48143000	-0.56264100	0.25659800
C	2.28340000	-3.18535800	-1.55801200
H	1.28177200	-1.53622000	-2.47692200
C	3.26990400	-3.60175400	-0.60806200
H	4.87252800	-3.00248500	0.67892900
H	1.75509000	-3.93872800	-2.13335100
H	3.43916700	-4.66366700	-0.45691700
H	2.71978200	3.05893200	1.00069700
C	4.64668200	3.00244900	0.04761900
H	4.85491500	4.07503800	0.12812800
H	5.11673800	2.49555000	0.89592500
H	5.11064500	2.63693600	-0.87704600
C	2.43126800	3.49655900	-1.08338100
H	2.86835100	3.26562100	-2.06252000
H	1.36886000	3.24206300	-1.10084600
H	2.53422200	4.57481400	-0.92411700
O	1.62324900	-1.76604200	1.34545300
C	2.22064900	-1.87270400	2.63452300
H	1.85590800	-1.07439400	3.28045500
H	1.92998200	-2.85236700	3.01487200
H	3.31319400	-1.80862700	2.54892200

D

C	-0.72176100	0.41212800	-0.02297500
C	0.71167500	0.90576700	0.25923700
C	3.02207000	0.05850000	0.13205600
O	1.01289600	2.01669900	0.66662300
N	1.58336700	-0.09495200	-0.03793600
C	0.95378000	-1.34837000	-0.40208300
H	1.25856500	-2.15539800	0.27723800
H	1.22912400	-1.64842300	-1.42239200
C	-0.52422500	-1.04922600	-0.30085400
C	-1.49905000	-1.94748800	-0.52174400
C	-1.59899400	0.63590200	1.17341100
C	-2.91425600	-1.73836900	-0.34954000
H	-1.20260100	-2.94504500	-0.84674700
C	-2.84374900	0.13744600	1.30645500
H	-1.21180600	1.30948200	1.93423400
C	-3.50624500	-0.81772900	0.45133600
H	-3.56252900	-2.45988000	-0.84179900
H	-3.42385100	0.47812500	2.16287500
H	-4.58882200	-0.86698300	0.54592400
H	3.16646700	1.13415900	0.26574300
C	3.50842100	-0.65848900	1.39388700
H	4.57570900	-0.47060600	1.54918600
H	2.96401300	-0.29926700	2.27198100
H	3.36973000	-1.74324900	1.31658300
C	3.77507700	-0.39667700	-1.11730200
H	3.67978900	-1.47791000	-1.27249100
H	3.39816700	0.11558100	-2.00763900
H	4.84090900	-0.17157300	-1.01308300
O	-1.20230300	1.01013100	-1.22384200
C	-1.54872800	2.38051400	-1.13443700
H	-1.85499900	2.67191000	-2.14136900
H	-2.38870500	2.53961300	-0.44633100
H	-0.70156400	2.99604400	-0.81328800

TS D-D_{RE}

C	-0.68117000	0.49902900	-0.04674200
C	0.75715100	1.00088200	0.11035600
C	3.03253600	0.04849600	0.17624500
O	1.10228100	2.16054000	0.24873900
N	1.58519500	-0.08263900	0.07400400
C	0.91479200	-1.33275300	-0.23026500

H	1.09470600	-2.08123900	0.55017700
H	1.26319800	-1.75456000	-1.18428600
C	-0.54522700	-0.94694400	-0.32086900
C	-1.25459500	-0.00515600	1.23400700
C	-1.53564800	-1.72840700	-0.92344300
C	-2.61251600	-0.31827700	1.37911900
H	-0.63188600	0.08338700	2.12216700
C	-2.89092600	-1.53644900	-0.72547200
H	-1.20921800	-2.57800400	-1.51987300
C	-3.41323000	-0.84552400	0.37892100
H	-3.03736800	-0.21033900	2.37460500
H	-3.58302500	-2.11187900	-1.33445800
H	-4.48121800	-0.92592600	0.56353200
H	3.18807100	1.06371500	0.55234300
C	3.60693900	-0.95099800	1.17969600
H	4.67340100	-0.75785300	1.33060000
H	3.10206200	-0.86738700	2.14711800
H	3.50615500	-1.98272800	0.82275200
C	3.69537900	-0.06734300	-1.19815000
H	3.54857600	-1.06380500	-1.63134000
H	3.28125500	0.67554500	-1.88585200
H	4.77359500	0.10271300	-1.11366100
O	-1.46306100	1.23362700	-0.91783900
C	-1.96808100	2.44443100	-0.37731500
H	-1.15554700	3.10501800	-0.06190400
H	-2.53645100	2.91381600	-1.18228000
H	-2.63885500	2.24874000	0.46860100

D_{RE}

C	-0.72177700	0.41213100	-0.02302500
C	0.71167100	0.90573100	0.25923600
C	3.02203800	0.05846600	0.13201700
O	1.01290600	2.01660500	0.66679000
N	1.58334800	-0.09491400	-0.03819500
C	0.95373700	-1.34835200	-0.40226300
H	1.25862700	-2.15539600	0.27698700
H	1.22891700	-1.64836800	-1.42263000
C	-0.52426000	-1.04923600	-0.30084800
C	-1.59904100	0.63603200	1.17329800
C	-1.49908400	-1.94753400	-0.52157200
C	-2.84379500	0.13760500	1.30640000
H	-1.21183100	1.30967600	1.93405500
C	-2.91427900	-1.73843300	-0.34934100
H	-1.20264100	-2.94512600	-0.84647600
C	-3.50628400	-0.81769400	0.45140100
H	-3.42389200	0.47838400	2.16278300
H	-3.56253700	-2.46004300	-0.84147000
H	-4.58885600	-0.86698600	0.54601100
H	3.16647400	1.13414900	0.26547900
C	3.50816600	-0.65820700	1.39411200
H	4.57540900	-0.47023100	1.54960000
H	2.96354300	-0.29882900	2.27200800
H	3.36957400	-1.74299900	1.31703100
C	3.77521200	-0.39705700	-1.11712500
H	3.67976700	-1.47830600	-1.27213100
H	3.39854500	0.11509700	-2.00761900
H	4.84106400	-0.17213100	-1.01272500
O	-1.20216700	1.01012000	-1.22396200
C	-1.54848800	2.38054500	-1.13467600
H	-0.70133700	2.99600800	-0.81336400
H	-1.85446200	2.67196200	-2.14169500
H	-2.38861400	2.53975500	-0.44679000

Z=CN

Sub

C	-1.98806900	-1.16363900	-0.12767300
C	-1.84129500	0.29004500	0.21107700

C	-0.61181500	2.35589800	0.33513900
N	-3.22036200	-1.59999200	0.08669200
N	-4.27473300	-1.94276900	0.26784100
O	-2.79373400	0.82755200	0.76334200
N	-0.67875600	0.93708500	-0.07889200
C	0.32041000	0.45145200	-1.02087100
H	0.56464700	1.27361600	-1.70335200
H	-0.12559700	-0.31994600	-1.65408000
C	1.59900500	-0.07484200	-0.39618700
C	2.78676000	-0.01411700	-1.12420100
C	1.61445300	-0.64320400	0.87576300
C	3.96995300	-0.51875200	-0.59450400
H	2.78823700	0.43490300	-2.11517500
C	2.79652800	-1.14498800	1.41039400
H	0.69725000	-0.68424400	1.45649200
C	3.97766300	-1.08575100	0.67658000
H	4.88770400	-0.46332700	-1.17241700
H	2.79299000	-1.58701400	2.40216400
H	4.89968000	-1.47851700	1.09427400
C	-1.05821000	-2.16862000	-0.49124500
N	-0.30744100	-3.00500100	-0.78667300
H	-1.25558000	2.42378000	1.21343100
C	0.80188800	2.76857100	0.73836200
H	0.76862100	3.78997700	1.13026600
H	1.20388200	2.11310100	1.51485100
H	1.49958300	2.76056300	-0.10582200
C	-1.19586500	3.26368000	-0.74896700
H	-0.61587300	3.20804000	-1.67781800
H	-2.23102600	2.98336700	-0.96117300
H	-1.18402700	4.30562300	-0.41316400

2

Rh	-0.88224100	0.03094500	0.32181100
Rh	-2.74531600	-0.56940900	-1.06621400
O	-1.93105500	1.69854500	0.90497200
O	-3.67376800	1.15784700	-0.42195800
O	0.05731100	-1.67834200	-0.34189100
O	-1.70086700	-2.25816000	-1.62841800
O	-1.86244500	0.47718000	-2.60356900
O	-0.11467200	1.05999300	-1.29910500
O	-1.76253300	-1.01452600	1.86016300
O	-3.51350300	-1.58641300	0.55771900
C	-3.08549700	1.90015800	0.41240800
C	-2.87015000	-1.59975600	1.64368200
C	-0.75913300	1.05319500	-2.39433200
C	-0.54224500	-2.44194600	-1.16044300
C	-0.13379500	1.79603800	-3.54751300
H	-0.78888100	1.76967700	-4.41837100
H	0.06312200	2.83061800	-3.25464900
H	0.82676000	1.33347500	-3.79396500
C	-3.81863100	3.12269200	0.90001400
H	-4.32139200	2.87630900	1.84134100
H	-3.11178900	3.93146200	1.09402400
H	-4.57091900	3.42968900	0.17259200
C	0.19315900	-3.68803800	-1.57979400
H	1.26671100	-3.56274100	-1.43155500
H	-0.14915000	-4.52073000	-0.95662300
H	-0.03390100	-3.92600500	-2.62072400
C	-3.45259300	-2.40149400	2.77851700
H	-4.53277400	-2.24861300	2.82557900
H	-3.27178700	-3.46346200	2.58318700
H	-2.98284500	-2.13111600	3.72468700
C	0.92541400	0.54459300	1.79474000
C	1.70974900	1.71259000	1.19481600
C	3.31294500	2.65015300	-0.31150000
N	0.14309100	1.03228300	2.80668300
N	-0.55892000	1.43764800	3.56765700

O	1.44462700	2.82917600	1.61569700
N	2.65328900	1.45177400	0.25717600
C	2.74375300	0.19693200	-0.47992400
H	2.65181700	0.42744100	-1.54745900
H	1.87335800	-0.42267800	-0.25988700
C	3.99879300	-0.61557000	-0.23661200
C	4.44690500	-1.47501400	-1.24049800
C	4.69334400	-0.57045400	0.97037000
C	5.56602000	-2.27782900	-1.04242300
H	3.91617800	-1.51368300	-2.18983500
C	5.81641400	-1.36725800	1.17035600
H	4.35820700	0.10052700	1.75568900
C	6.25615600	-2.22457100	0.16565800
H	5.90275800	-2.94053100	-1.83436600
H	6.34620500	-1.32009200	2.11706200
H	7.13289200	-2.84572500	0.32215800
C	1.49411000	-0.72180400	2.15640900
N	1.95339100	-1.74742700	2.44262200
H	3.33345400	3.37408400	0.50459900
C	4.74832900	2.37233100	-0.74944600
H	5.19589500	3.31358200	-1.08461200
H	5.35263100	1.97475800	0.06940500
H	4.80063100	1.66475700	-1.58342700
C	2.47343600	3.23963500	-1.44605700
H	2.43901300	2.56085700	-2.30507000
H	1.45103100	3.42462700	-1.10804400
H	2.91321100	4.18454900	-1.78202400

TS 2-3

Rh	-0.84222500	0.02266900	0.31340500
Rh	-2.74942500	-0.59565900	-1.06014200
O	-1.89637200	1.69291300	0.88203600
O	-3.67193100	1.13048400	-0.39458100
O	0.07385000	-1.70367500	-0.35506000
O	-1.69406200	-2.28342900	-1.63150700
O	-1.87844200	0.46449500	-2.60844100
O	-0.10562500	1.04124800	-1.33187400
O	-1.70524100	-1.01424600	1.86370800
O	-3.47159900	-1.61436400	0.59011500
C	-3.06374300	1.88389600	0.41014000
C	-2.81239300	-1.61333100	1.66215900
C	-0.77400500	1.03534000	-2.41670500
C	-0.53947600	-2.46916700	-1.16889900
C	-0.15941500	1.78260100	-3.57426400
H	-0.82245900	1.75601000	-4.43908500
H	0.03715300	2.81753600	-3.28188700
H	0.80030500	1.32344600	-3.83032100
C	-3.76221300	3.14802400	0.84219700
H	-3.32282800	3.53727200	1.76142900
H	-3.64734600	3.89781900	0.05251000
H	-4.82895300	2.95686100	0.97343600
C	0.19987000	-3.71799200	-1.57558400
H	-0.23290300	-4.13801100	-2.48421200
H	1.26074500	-3.49880700	-1.71472200
H	0.11588700	-4.45252200	-0.76801900
C	-3.35022600	-2.41371900	2.82061900
H	-3.17710900	-1.88476600	3.75998500
H	-4.41273900	-2.61487400	2.68050800
H	-2.81032600	-3.36524100	2.86707800
C	0.81898400	0.47612100	1.46679700
C	1.69531200	1.67821900	1.10091800
C	3.32394600	2.65164100	-0.37238500
N	-0.01332300	1.28958900	2.98498800
N	-0.82018500	1.65613600	3.63768100
O	1.47928800	2.76246400	1.61906100
N	2.64461500	1.45046400	0.16091500
C	2.76199100	0.19184100	-0.56551000

H	2.72467300	0.41199100	-1.63837100
H	1.87422400	-0.42179000	-0.38731500
C	3.99510700	-0.62726800	-0.24490300
C	4.47438400	-1.52635900	-1.19913100
C	4.63665900	-0.54880300	0.98959200
C	5.57269600	-2.33484000	-0.92413200
H	3.98451400	-1.59214500	-2.16865500
C	5.73883500	-1.35224900	1.26610900
H	4.27923700	0.15313000	1.73698400
C	6.20989500	-2.24837100	0.31117800
H	5.93458000	-3.02861100	-1.67733800
H	6.22774100	-1.27832100	2.23273400
H	7.06976500	-2.87521000	0.52725900
C	1.42164100	-0.62921500	2.13814300
N	1.88833000	-1.56851900	2.63859600
H	3.33004200	3.36269000	0.45528200
C	4.76700300	2.36976300	-0.78183400
H	5.22554500	3.30919900	-1.10656900
H	5.35228100	1.96849100	0.04890200
H	4.83281600	1.66263400	-1.61547900
C	2.50774300	3.25552900	-1.51638100
H	2.47364300	2.57886200	-2.37733500
H	1.48303200	3.45194300	-1.19096700
H	2.96216200	4.19618300	-1.84433600

3

Rh	-0.85441300	-0.01608700	0.45135300
Rh	-2.74347700	-0.26286200	-1.07240700
O	-0.10456000	1.42372300	-0.83573500
O	-1.84813000	1.19024900	-2.25405000
O	-1.70583900	-1.44962700	1.63810100
O	-3.46393900	-1.69288800	0.23836600
O	-1.67572500	-1.72593300	-2.07505200
O	0.07327300	-1.49627300	-0.66837200
O	-1.94387900	1.42529400	1.41349800
O	-3.69724500	1.21622600	0.00528400
C	-0.76207000	1.70691000	-1.89155300
C	-3.10860400	1.72540600	0.99482100
C	-0.52478500	-2.01831500	-1.66792600
C	-2.81174600	-1.97016200	1.27988800
C	0.23469100	-3.10167800	-2.39031200
H	0.17070000	-4.02436000	-1.80438200
H	-0.19940300	-3.27482700	-3.37548800
H	1.29030100	-2.83291300	-2.47277600
C	-0.16420900	2.78040400	-2.76723800
H	-0.23420700	3.74249100	-2.25002300
H	0.89550800	2.57395500	-2.93765000
H	-0.69666800	2.83904400	-3.71660400
C	-3.39708900	-2.99561600	2.21691100
H	-2.64142800	-3.35461500	2.91607900
H	-4.21227400	-2.52831200	2.77896100
H	-3.81858600	-3.82315700	1.64240300
C	-3.84189500	2.77320100	1.79215600
H	-4.64642200	3.20666900	1.19705600
H	-4.27300400	2.29809700	2.67949500
H	-3.14618100	3.54409900	2.12872800
C	0.76271400	0.09285800	1.60033200
C	1.72974400	1.19538000	1.50424900
C	3.40471300	2.61577100	0.53353800
O	1.43676800	1.95466100	2.43220600
N	2.67113600	1.33718300	0.57445900
C	2.80312400	0.36090600	-0.50100400
H	2.83659200	0.90242700	-1.45196100
H	1.88819200	-0.23939000	-0.53724000
C	3.99717200	-0.56193900	-0.37784600
C	4.72452200	-0.90377900	-1.51747800
C	4.35114600	-1.12998400	0.84661800

C	5.78682700	-1.80058200	-1.43993400
H	4.46069300	-0.46135100	-2.47575100
C	5.41450000	-2.02316200	0.92796300
H	3.79939000	-0.87408400	1.74727700
C	6.13515600	-2.36202200	-0.21520800
H	6.34469500	-2.05496100	-2.33633900
H	5.67649800	-2.45939000	1.88703700
H	6.96348400	-3.06098800	-0.15080900
C	1.03597800	-0.87824300	2.58594700
N	1.24871100	-1.72893600	3.35242200
H	3.27609100	3.04323900	1.53159300
C	4.89477300	2.40923200	0.27793600
H	5.40595700	3.37313400	0.36387300
H	5.33109700	1.71692800	1.00283500
H	5.08676200	2.01591700	-0.72568700
C	2.75854200	3.56154500	-0.48038300
H	2.88789300	3.19517200	-1.50514300
H	1.68843600	3.66306400	-0.28107200
H	3.22698600	4.54881500	-0.41797000

4-1

Rh	0.85654500	0.31899300	0.37865400
Rh	2.23379600	-1.23845700	-0.89594700
O	-0.80101200	-0.61087200	-0.43470900
O	0.47275300	-2.04722000	-1.62620500
O	2.58565700	1.14598500	1.10638100
O	3.87774500	-0.29514700	-0.06188300
O	2.23766600	0.12718600	-2.45036800
O	0.95108900	1.56306800	-1.27865200
O	0.88194400	-1.06302600	1.89013800
O	2.14999200	-2.51953500	0.72008400
C	-0.63252200	-1.57810100	-1.24800800
C	1.50788600	-2.16256800	1.74141000
C	1.60480000	1.20196400	-2.31367200
C	3.70569500	0.66258400	0.73722400
C	1.60440000	2.18265900	-3.45902900
H	2.12902200	3.09263500	-3.15294500
H	2.09497900	1.74940600	-4.33062200
H	0.57519800	2.45965600	-3.70331700
C	-1.87822100	-2.22742000	-1.79549100
H	-2.00846600	-3.19904000	-1.30903400
H	-2.76464700	-1.62406100	-1.59759000
H	-1.75575900	-2.40361400	-2.86665200
C	4.92673200	1.29479000	1.35462500
H	4.77001900	2.36667900	1.48798200
H	5.08509100	0.85062700	2.34304000
H	5.80559200	1.10203200	0.73820400
C	1.46060200	-3.09899000	2.92155100
H	1.97115200	-4.03342200	2.68810900
H	1.93701100	-2.61775400	3.78055700
H	0.41851100	-3.29216100	3.18974100
C	-0.26981100	1.64629000	1.32587400
C	-1.71808000	1.44855900	1.51238000
C	-2.23241000	2.35852900	-0.67862100
O	-1.88520500	0.99300600	2.64702700
N	-2.62453800	1.67715600	0.56628400
C	-4.01748100	1.32423000	0.84748100
H	-4.65710800	2.02672800	0.30653200
H	-4.17991400	1.48702900	1.91741400
C	-4.37695500	-0.10407100	0.48537400
C	-3.79671000	-1.17445400	1.17426000
C	-5.31654600	-0.36970600	-0.51009900
C	-4.15715200	-2.48213500	0.87001800
H	-3.06478800	-0.97708900	1.95092200
C	-5.67586400	-1.68084800	-0.81843100
H	-5.78029900	0.45459800	-1.04735200
C	-5.09758500	-2.73996000	-0.12631200

H	-3.70224400	-3.30448100	1.41437800
H	-6.41095500	-1.87115500	-1.59475600
H	-5.37739900	-3.76285400	-0.36026700
C	0.27602900	2.80815000	1.90768100
N	0.76104100	3.78352200	2.32054800
H	-1.14127900	2.27667700	-0.74029200
C	-2.79337000	1.66234300	-1.91325000
H	-2.36298100	2.12303600	-2.80782300
H	-2.53161000	0.60371300	-1.90296500
H	-3.88205500	1.76049300	-1.98064000
C	-2.60236900	3.84140500	-0.61821700
H	-3.68702400	3.98211000	-0.54759400
H	-2.13499200	4.32581900	0.24498300
H	-2.25734100	4.34847200	-1.52465100

TS 4-1

C	0.38411400	2.21368000	-0.47812700
C	1.50188400	2.77627500	1.31201100
H	0.52555000	2.24273500	0.84468300
Rh	-0.79709400	0.44998000	-0.10912800
Rh	-2.14253900	-1.51040200	0.35155900
O	0.62169000	-0.30891300	1.19511500
O	-0.59917000	-2.16611700	1.58110200
O	-2.30325100	1.09921500	-1.33879200
O	-3.57253800	-0.71960300	-0.90597600
O	-2.94928300	-0.44034300	1.93546300
O	-1.68118000	1.37880500	1.50977000
O	0.02361400	-0.60973400	-1.67475100
O	-1.24114900	-2.43443500	-1.26029300
C	0.41272400	-1.43916800	1.74761800
C	-0.36727500	-1.79831700	-1.90770200
C	-2.56823700	0.73737800	2.16215400
C	-3.34663400	0.38605900	-1.47205700
C	-3.24140900	1.48178200	3.28799500
H	-4.11030600	2.00978500	2.88121300
H	-3.58838200	0.78118900	4.04888800
H	-2.56423500	2.22097800	3.71957500
C	1.48057000	-1.91420500	2.70107200
H	1.32599400	-2.96397600	2.95197500
H	2.46729500	-1.77182200	2.25306900
H	1.42982700	-1.31613200	3.61723700
C	-4.39055400	0.91820800	-2.41997400
H	-4.51628200	1.99241400	-2.26838000
H	-4.04163700	0.76497100	-3.44624200
H	-5.33679900	0.39471600	-2.27986500
C	0.30746900	-2.49373400	-3.06299500
H	-0.15827000	-3.46094400	-3.25294300
H	0.25085800	-1.86035300	-3.95190800
H	1.36833000	-2.63419200	-2.83016100
C	1.67141700	2.00092500	-1.21765900
C	2.72035000	1.94161000	0.98201400
O	1.60233400	1.92756500	-2.43095000
N	2.80154400	1.85000300	-0.47241600
C	3.96267900	1.22239400	-1.09256100
H	4.85580400	1.82264600	-0.89095300
H	3.77863400	1.25465900	-2.16930600
C	4.15898800	-0.20343100	-0.61853300
C	3.12336700	-1.13000500	-0.77000600
C	5.35122700	-0.60688900	-0.02086000
C	3.28584700	-2.43962900	-0.33336800
H	2.18421000	-0.81949100	-1.22017400
C	5.51633700	-1.92082400	0.41636600
H	6.16215500	0.10874000	0.09977100
C	4.48342400	-2.83961800	0.26118400
H	2.47114800	-3.15034000	-0.44752000
H	6.45104900	-2.22316000	0.87917100
H	4.60774100	-3.86274900	0.60334500

C	-0.33639300	3.40481900	-0.79702000
N	-0.95582400	4.35751600	-1.03477600
H	2.57860600	0.93989300	1.40066300
C	3.96809500	2.58404500	1.58678900
H	3.82243700	2.74183100	2.66018900
H	4.83680400	1.93112400	1.46662700
H	4.17880900	3.54887100	1.11375500
H	1.56841900	3.82850700	1.03828800
H	1.13919400	2.64682700	2.33638500

A

C	2.86065000	0.13850000	0.11833000
C	1.61453400	-0.37591300	0.86898900
C	1.03807600	1.72543300	-0.08257000
O	1.53231800	-1.40367100	1.50864200
N	0.64335300	0.56252500	0.70799400
C	-0.60594300	0.48347600	1.44455800
H	-0.83041000	1.47344000	1.85934900
H	-0.42501500	-0.19878900	2.28107700
C	-1.76773600	-0.02035100	0.61323500
C	-2.95195400	0.70619300	0.51368700
C	-1.65849900	-1.24172300	-0.05622100
C	-4.01521000	0.22650700	-0.24831400
H	-3.04610000	1.65785300	1.03260300
C	-2.71634000	-1.71965400	-0.82033000
H	-0.74256600	-1.81949600	0.03513300
C	-3.89758300	-0.98603000	-0.91906800
H	-4.93327000	0.80233100	-0.31911500
H	-2.62143300	-2.67102200	-1.33519500
H	-4.72363800	-1.36108100	-1.51582700
C	3.59174900	-0.92254800	-0.56686900
N	4.17335600	-1.74075100	-1.14186800
H	1.30409900	2.54660600	0.60169700
C	2.29476800	1.22140500	-0.81326500
H	3.00696700	2.02232300	-1.02020500
H	2.00254700	0.76702900	-1.76531300
C	-0.04474000	2.21006600	-1.03767700
H	-0.37741700	1.39575700	-1.68850200
H	-0.91738700	2.59327100	-0.50146700
H	0.35327800	3.01983900	-1.65809200
H	3.52421200	0.57672600	0.87492400

4-2

Rh	-0.44597500	-0.10742700	0.22600000
Rh	-2.75223100	0.28809500	-0.48393600
O	-0.28720500	1.93237300	0.50605200
O	-2.43566200	2.29704700	-0.09190000
O	-0.74702600	-2.10841600	-0.14383200
O	-2.87806600	-1.75548500	-0.81170400
O	-2.05147700	0.56440000	-2.41396000
O	0.07707100	0.19399600	-1.76554800
O	-1.19016700	-0.36686000	2.11984100
O	-3.32306000	-0.00203400	1.47557500
C	-1.30036500	2.67515000	0.29699700
C	-2.44084200	-0.26396400	2.33385800
C	-0.82086200	0.46024300	-2.63227800
C	-1.88648100	-2.49094100	-0.56285900
C	-0.33420600	0.63105600	-4.05037700
H	-0.16010600	-0.35903300	-4.48507500
H	-1.08317700	1.15103100	-4.64846800
H	0.61274100	1.17556300	-4.06365300
C	-1.08657400	4.15300100	0.51136100
H	-0.35432000	4.31677000	1.30408400
H	-0.69589000	4.58901100	-0.41485300
H	-2.03307600	4.64055800	0.74883200
C	-2.06174600	-3.97563300	-0.76543500
H	-1.10659600	-4.49450700	-0.68011400

H	-2.74841700	-4.35419900	-0.00198600
H	-2.51695300	-4.16158100	-1.74124100
C	-2.87418500	-0.49626500	3.75845100
H	-3.93649600	-0.28103600	3.87518100
H	-2.67649400	-1.53936300	4.02325000
H	-2.28010100	0.13190500	4.42685600
C	1.40228400	-0.39684000	0.99194200
C	2.25698300	0.80006200	1.21978500
C	3.46495600	2.69203200	0.32040600
O	2.05942600	1.28922300	2.32652600
N	3.02170100	1.29638400	0.23151100
C	3.12735300	0.56259700	-1.03097400
H	4.01159100	0.94140700	-1.55243600
H	2.25018000	0.74684800	-1.65812000
C	3.28518600	-0.91982800	-0.77107700
C	4.36099800	-1.38045700	0.00430000
C	2.37619800	-1.84613700	-1.29788500
C	4.49846200	-2.73033500	0.27695100
H	5.06726000	-0.66294100	0.41418800
C	2.52231500	-3.20506600	-1.02769200
H	1.53715200	-1.48934500	-1.88462600
C	3.57093100	-3.64660500	-0.23308900
H	5.31812700	-3.07804200	0.89758300
H	1.79335100	-3.90896500	-1.41506800
H	3.67375300	-4.70212000	-0.00225000
C	1.66411500	-1.54117600	1.76838400
N	1.83713000	-2.52399200	2.36957300
H	3.16402800	3.01123800	1.32120900
C	4.98364800	2.80998600	0.20983800
H	5.28596300	3.84955600	0.37120200
H	5.47584800	2.18797400	0.96361900
H	5.34936100	2.51359200	-0.78025100
C	2.72007900	3.54362400	-0.70945100
H	3.01692200	3.28867400	-1.73383600
H	1.64248100	3.38484300	-0.60748900
H	2.94020400	4.60438500	-0.55239300

TS 4-2

Rh	0.71845500	-0.34031200	0.33340000
Rh	2.40339200	0.95630000	-0.83234400
O	-0.30085300	-0.48160400	-1.47783300
O	1.31472600	0.65306900	-2.57524700
O	1.83107800	-0.11691600	2.04189800
O	3.36660300	1.15729300	0.98195200
O	1.24993800	2.63796200	-0.40543000
O	-0.24666900	1.42967000	0.77257100
O	1.80061200	-2.01673500	-0.15333500
O	3.41453300	-0.80701100	-1.17354500
C	0.23069000	0.01992800	-2.52235800
C	2.89983500	-1.88943900	-0.77643500
C	0.21452600	2.51726900	0.29988400
C	2.89485600	0.57592000	1.99834600
C	-0.55404900	3.77309900	0.63010900
H	0.05860000	4.40275400	1.28258500
H	-0.74396600	4.33421600	-0.28850700
H	-1.49576200	3.53270200	1.12532600
C	-0.53936900	-0.17454300	-3.80662400
H	-0.65146300	-1.24517600	-4.00124500
H	-1.54440600	0.24683500	-3.70001200
H	-0.02501100	0.30279000	-4.64077900
C	3.67091500	0.70534200	3.28468100
H	3.12944100	0.24580500	4.11163700
H	4.64189200	0.21625500	3.16160700
H	3.85801700	1.76253700	3.49062600
C	3.64272300	-3.16989800	-1.06338100
H	4.58185700	-2.96292400	-1.57691200
H	3.83373100	-3.69381000	-0.12289600

H	3.01303500	-3.81912600	-1.67840700
C	-0.77471800	-1.47212900	1.35989600
C	-1.60335100	-2.39833000	0.52102100
C	-3.83652300	-2.27432900	-0.57037300
O	-1.29243500	-3.49114600	0.11255600
N	-2.77999700	-1.72117600	0.28595000
C	-2.87193900	-0.62383500	1.17195800
H	-1.55129900	-0.46067400	1.40120900
C	-0.49058900	-1.89237400	2.69043100
N	-0.26688600	-2.20488400	3.78759000
H	-3.61254000	-3.34748500	-0.56806600
C	-5.21970400	-2.05311500	0.03574500
H	-5.96917100	-2.56570100	-0.57434000
H	-5.27855400	-2.45554400	1.05239300
H	-5.48079400	-0.98944900	0.06047600
C	-3.73432800	-1.77684000	-2.01191300
H	-4.06566400	-0.73700500	-2.09818000
H	-2.70032900	-1.84848900	-2.36029800
H	-4.36808100	-2.39190000	-2.65930500
H	-3.19280600	-0.85772000	2.19304000
C	-3.31673600	0.68353800	0.67306600
C	-4.10875500	1.49891100	1.48989800
C	-2.93128600	1.12780300	-0.59870900
C	-4.55304900	2.72912400	1.02052100
H	-4.38722700	1.16049300	2.48462400
C	-3.37396400	2.35862500	-1.06045800
H	-2.25057800	0.51672600	-1.18277100
C	-4.18991000	3.15521100	-0.25628300
H	-5.18016500	3.35456900	1.64751900
H	-3.07068200	2.70831200	-2.04245200
H	-4.53489600	4.11770200	-0.62202700

B

C	2.00026800	1.04963200	-0.14317300
C	0.36537300	0.15897200	0.85881500
C	0.89577300	1.63904400	0.78394500
O	2.98683800	1.48108300	-0.67795800
N	1.44581900	-0.19377200	-0.06913700
C	2.02852700	-1.48301600	-0.41171900
H	2.81079400	-1.24147500	-1.13889600
C	2.67403600	-2.12718700	0.81760600
H	3.41763700	-1.45822000	1.26137300
H	1.91921900	-2.36583800	1.57593500
H	0.52746500	-0.25510900	1.86155400
C	-1.03804700	-0.13991500	0.40344900
C	-1.96711200	-0.64325900	1.31200900
C	-1.43026600	0.09062800	-0.91706400
C	-3.27338500	-0.91204300	0.91211800
H	-1.66915600	-0.82762100	2.34169600
C	-2.73260600	-0.17791500	-1.31806400
H	-0.71175300	0.47965700	-1.63288700
C	-3.65707400	-0.67982000	-0.40440600
H	-3.98862300	-1.30335200	1.62912500
H	-3.02761800	0.00836400	-2.34598500
H	-4.67510800	-0.88786600	-0.71932300
H	1.31207900	1.99565100	1.73003600
C	0.02511200	2.65140300	0.21411800
N	-0.66489200	3.45545700	-0.25183400
H	3.17277500	-3.06090800	0.53997700
C	0.99776500	-2.40147400	-1.06525000
H	0.18868800	-2.64488500	-0.36845900
H	0.55518600	-1.93226300	-1.94776700
H	1.47704300	-3.33689100	-1.37021500

4-3

Rh	-0.85545700	0.31998000	-0.37685600
Rh	-2.23204800	-1.23841400	0.89720500

O	0.80221400	-0.61099700	0.43498300
O	-0.47120600	-2.04751700	1.62668900
O	-2.58491500	1.14805400	-1.10296600
O	-3.87646200	-0.29452800	0.06406500
O	-2.23527200	0.12654800	2.45229100
O	-0.94856600	1.56296600	1.28133200
O	-0.88152500	-1.06023800	-1.88995500
O	-2.14788500	-2.51836100	-0.71998900
C	0.63396000	-1.57872200	1.24773400
C	-1.51009600	-2.15820700	-1.74323800
C	-1.60147000	1.20091000	2.31651700
C	-3.70479100	0.66445300	-0.73359800
C	-1.59895400	2.17986400	3.46337800
H	-2.12503900	3.08990900	3.15997100
H	-2.08723400	1.74498500	4.33545700
H	-0.56939800	2.45730000	3.70559700
C	1.87964000	-2.22899000	1.79405000
H	2.00912600	-3.20029900	1.30677000
H	2.76632200	-1.62604000	1.59613800
H	1.75755500	-2.40590300	2.86513900
C	-4.92623500	1.29795800	-1.34894000
H	-4.76809100	2.36936400	-1.48427100
H	-5.08793900	0.85253200	-2.33626800
H	-5.80389700	1.10750400	-0.73008900
C	-1.49751200	-3.08108800	-2.93473800
H	-1.73778400	-4.09972800	-2.62797600
H	-2.25291600	-2.73790500	-3.64925600
H	-0.52540300	-3.04212800	-3.42977700
C	0.27079700	1.64760400	-1.32430400
C	1.71844900	1.44835100	-1.51259700
C	2.23707500	2.35664200	0.67790400
O	1.88296200	0.99291100	-2.64774400
N	2.62658300	1.67533100	-0.56785200
C	4.01859000	1.32020500	-0.85106200
H	4.66007700	2.02185300	-0.31121600
H	4.17962100	1.48262400	-1.92126100
C	4.37650300	-0.10858700	-0.48933800
C	5.31768300	-0.37539900	0.50433000
C	3.79331100	-1.17825700	-1.17683400
C	5.67568700	-1.68699600	0.81220700
H	5.78369700	0.44834900	1.04049200
C	4.15248500	-2.48642300	-0.87310900
H	3.06006200	-0.98014100	-1.95203900
C	5.09450900	-2.74539700	0.12140200
H	6.41198000	-1.87825700	1.58715400
H	3.69512100	-3.30814400	-1.41633800
H	5.37327600	-3.76865100	0.35504600
C	-0.27481200	2.81017700	-1.90482900
N	-0.75986300	3.78602100	-2.31653100
H	1.14591500	2.27597200	0.74118000
C	2.79923500	1.65937800	1.91135100
H	2.37126700	2.12058900	2.80680900
H	2.53573800	0.60117600	1.90133500
H	3.88821400	1.75567800	1.97657400
C	2.60864100	3.83911500	0.61733300
H	3.69333300	3.97857700	0.54483200
H	2.14032300	4.32430300	-0.24492600
H	2.26581500	4.34632700	1.52451700

TS 4-3

Rh	-0.72603600	0.41247200	-0.06253600
Rh	-2.22537100	-1.47156000	0.23852500
O	0.59888300	-0.55023000	1.20294800
O	-0.78464100	-2.31109700	1.47639500
O	-2.15325500	1.23615800	-1.29294900
O	-3.55621700	-0.51036700	-1.00795700
O	-3.01610900	-0.44566400	1.85316500

O	-1.60811300	1.29963000	1.57728200
O	0.07812300	-0.61652800	-1.66189700
O	-1.33145000	-2.36151800	-1.40209900
C	0.28147500	-1.68158000	1.69497500
C	-0.38866300	-1.75702100	-1.97841400
C	-2.56251100	0.69049200	2.15691600
C	-3.23739700	0.60686600	-1.49972500
C	-3.23158900	1.41826900	3.29621000
H	-4.09493800	1.96178300	2.89818400
H	-3.59059600	0.70393300	4.03910400
H	-2.54788900	2.13893900	3.74734800
C	1.28693600	-2.29149300	2.64026700
H	1.01910400	-3.32310400	2.87043400
H	2.28459700	-2.24831900	2.19485900
H	1.30318300	-1.70753800	3.56647500
C	-4.21183500	1.26115500	-2.44565400
H	-5.19350500	0.79355500	-2.36433700
H	-4.27364700	2.33119000	-2.23578100
H	-3.83874000	1.14249800	-3.46807400
C	0.27298100	-2.42829600	-3.15608700
H	0.20967000	-1.77018300	-4.02697700
H	1.33563100	-2.57903700	-2.94048000
H	-0.20264900	-3.38556300	-3.36997100
C	0.51588700	2.12701900	-0.39505100
C	1.67828800	1.95329300	-1.33524700
C	2.43506900	2.30087400	0.78933200
O	1.62664500	1.84787200	-2.53550800
N	2.78599700	1.87404000	-0.52155000
C	4.04446600	1.27314800	-0.92750400
H	4.87500300	1.87571400	-0.54343500
H	4.05411700	1.36170400	-2.01947400
C	4.19485100	-0.17663900	-0.50905400
C	5.35211100	-0.61087000	0.13419900
C	3.16988300	-1.08971000	-0.76749300
C	5.49297900	-1.94443300	0.51389400
H	6.15144300	0.09699800	0.34385000
C	3.30847500	-2.41910900	-0.38436000
H	2.25287300	-0.76414500	-1.25148500
C	4.47004000	-2.85172300	0.25562400
H	6.39973400	-2.27141800	1.01390700
H	2.50089300	-3.12004700	-0.57894600
H	4.57508100	-3.89111300	0.55212300
C	-0.18396000	3.36637600	-0.42884100
N	-0.75248400	4.38040800	-0.41902100
H	1.13923900	2.05661600	0.72991000
C	2.85678000	1.41278700	1.93543200
H	2.40041900	1.75764400	2.86647700
H	2.57959600	0.37672100	1.75011500
H	3.94725400	1.48825000	2.04087400
C	2.55907300	3.78684100	1.04696700
H	3.62094200	4.00643000	1.21597200
H	2.21697200	4.38246500	0.19823900
H	2.00398400	4.08033000	1.94219000

C

C	-2.26120000	-0.31447400	0.74755600
C	-1.44378600	-1.21233500	-0.22814200
C	-1.33852700	0.85490500	0.24191700
O	-1.41901300	-2.38586900	-0.49836100
N	-0.70726800	-0.14857000	-0.63811500
C	0.46040200	-0.09241300	-1.48853000
H	0.39238900	0.79747600	-2.12434000
H	0.40178200	-0.96859400	-2.14263300
C	1.75929500	-0.09509400	-0.70890500
C	2.65189000	0.97080500	-0.79146900
C	2.05859300	-1.17432400	0.12697300
C	3.82967000	0.96548800	-0.04635300

H	2.42521400	1.81390600	-1.44045100
C	3.23088100	-1.17985900	0.87312300
H	1.36522400	-2.01019400	0.18730200
C	4.11917700	-0.10818900	0.78865000
H	4.51900500	1.80158000	-0.11766400
H	3.45645800	-2.02324500	1.51895400
H	5.03591900	-0.11353300	1.37060100
C	-3.68687400	-0.20221900	0.49638400
N	-4.81935300	-0.08998200	0.28346700
H	-2.08485000	-0.58243600	1.79311100
C	-0.40876400	1.39616400	1.32293300
H	-0.97983400	1.98574400	2.04743900
H	0.10218500	0.58289700	1.84750600
H	0.35810600	2.04201600	0.88412800
C	-2.02980100	1.96889200	-0.53111500
H	-1.28201000	2.60626000	-1.01547700
H	-2.69457800	1.56535200	-1.29975800
H	-2.62229000	2.59549900	0.14257300

4-4

Rh	-0.44651600	-0.10713600	0.22743200
Rh	-2.75117500	0.29037400	-0.48644900
O	-0.28679400	1.93236400	0.50861000
O	-2.43246300	2.29949000	-0.09783100
O	-0.74849200	-2.10782200	-0.14320200
O	-2.87962400	-1.75386100	-0.81023300
O	-2.04862200	0.56229100	-2.41634100
O	0.07898800	0.19473600	-1.76342700
O	-1.19304700	-0.36608800	2.12119400
O	-3.32346800	0.00623900	1.47301600
C	-1.29835100	2.67626900	0.29576900
C	-2.44345400	-0.25989600	2.33281900
C	-0.81749800	0.45932300	-2.63216800
C	-1.88820000	-2.48976200	-0.56206200
C	-0.32825300	0.62938700	-4.04945400
H	-0.15462500	-0.36096200	-4.48375900
H	-1.07569600	1.15006500	-4.64885700
H	0.61929400	1.17285500	-4.06128200
C	-1.08397500	4.15385700	0.51131500
H	-0.35193400	4.31675000	1.30439400
H	-0.69313900	4.59053700	-0.41451800
H	-2.03039900	4.64149800	0.74897900
C	-2.06399800	-3.97436200	-0.76502000
H	-1.10893000	-4.49349000	-0.68034700
H	-2.75033900	-4.35310500	-0.00135600
H	-2.51975800	-4.15988100	-1.74064500
C	-2.89153300	-0.51097000	3.74962400
H	-3.86493000	-0.05073100	3.92382200
H	-2.97925300	-1.59188400	3.90134800
H	-2.14879100	-0.13013400	4.45289600
C	1.40163200	-0.39801800	0.99380900
C	2.25695600	0.79818000	1.22235300
C	3.46573500	2.69090800	0.32580900
O	2.05928900	1.28582500	2.32978600
N	3.02192100	1.29554300	0.23488400
C	3.12773400	0.56342300	-1.02858800
H	4.01169400	0.94344800	-1.54961700
H	2.25042400	0.74815600	-1.65536100
C	3.28639800	-0.91926800	-0.77078600
C	4.36282400	-1.38034600	0.00339600
C	2.37746000	-1.84530000	-1.29806600
C	4.50118600	-2.73052800	0.27418300
H	5.06904500	-0.66301800	0.41368900
C	2.52438600	-3.20451600	-1.02966400
H	1.53785600	-1.48817200	-1.88379100
C	3.57379900	-3.64660500	-0.23643000
H	5.32151600	-3.07863200	0.89371600

H	1.79551600	-3.90827900	-1.41748100
H	3.67736800	-4.70237600	-0.00709700
C	1.66410400	-1.54347500	1.76833600
N	1.83762700	-2.52707200	2.36811000
H	3.16585600	3.00847500	1.32744800
C	4.98436100	2.80867800	0.21399600
H	5.28707500	3.84776900	0.37767700
H	5.47722200	2.18464000	0.96566400
H	5.34897100	2.51479600	-0.77724400
C	2.72025200	3.54455000	-0.70191400
H	3.01590100	3.29100000	-1.72699500
H	1.64268900	3.38618600	-0.59913000
H	2.94109400	4.60495500	-0.54345300

TS 4-4

Rh	-0.38104100	0.13486100	-0.14155700
Rh	-2.71689700	-0.39620000	0.32821600
O	-0.00427400	-0.26868800	1.87280700
O	-2.16060900	-0.78462600	2.29094700
O	-0.96486600	0.48839300	-2.07596500
O	-3.12979800	0.01189200	-1.64770400
O	-2.96333500	1.61177300	0.78212900
O	-0.79812000	2.09508600	0.34679100
O	-0.11384400	-1.87444900	-0.54219100
O	-2.29059200	-2.35946500	-0.17960100
C	-0.95991500	-0.65029500	2.62743300
C	-1.11030100	-2.66369900	-0.49603700
C	-1.98744100	2.40037700	0.68359400
C	-2.18464000	0.35677700	-2.40685900
C	-2.23137200	3.86122900	0.97456700
H	-2.14932900	4.42485500	0.04010100
H	-3.22292300	4.00630000	1.40390900
H	-1.46467900	4.23730600	1.65719400
C	-0.58114700	-0.99264400	4.04830800
H	-0.08682700	-1.96994600	4.05455800
H	0.12686000	-0.25737500	4.43842300
H	-1.46915100	-1.04000700	4.67922100
C	-2.50093500	0.62388100	-3.85606100
H	-1.97220700	1.51899300	-4.19078000
H	-2.14065300	-0.21888000	-4.45457900
H	-3.57648700	0.73409300	-3.99789800
C	-0.82359300	-4.10920000	-0.82184200
H	-1.71310100	-4.58363700	-1.23926000
H	0.01529400	-4.17906100	-1.51651300
H	-0.55709300	-4.63329300	0.10267300
C	1.58057500	0.57889000	-0.78962600
C	2.33348000	-0.66198800	-1.19603900
C	3.41467600	-2.64788900	-0.26152600
O	2.19781100	-1.09602200	-2.32482500
N	3.02753600	-1.24170100	-0.18319700
C	3.02710000	-0.51942600	1.07723100
H	3.94164500	-0.76253400	1.62919000
H	2.16019100	-0.77435700	1.69482500
C	3.01603500	0.96150700	0.74177500
C	4.12154900	1.49304100	0.01933100
C	2.11689600	1.86538800	1.35820900
C	4.23959300	2.84683300	-0.18137800
H	4.84122500	0.80211000	-0.41038600
C	2.23968600	3.23245000	1.14529400
H	1.29985100	1.46528600	1.94692800
C	3.27804300	3.71805000	0.36177400
H	5.05754400	3.24491200	-0.77181400
H	1.50210600	3.90815500	1.56206900
H	3.35779400	4.78362000	0.17138600
C	1.67163700	1.71508300	-1.62570300
N	1.71260200	2.70325900	-2.24000800
H	3.08048600	-2.96617600	-1.25269300

C	4.93212400	-2.80878900	-0.17760000
H	5.20702300	-3.86241600	-0.29131000
H	5.42384000	-2.23733600	-0.97079100
H	5.32174300	-2.46884900	0.78988100
C	2.67386000	-3.46721500	0.79702400
H	3.01950600	-3.22413800	1.80926400
H	1.60050500	-3.26799100	0.73396600
H	2.84862300	-4.53561300	0.63489700

D

Rh	-0.44651600	-0.10713600	0.22743200
Rh	-2.75117500	0.29037400	-0.48644900
O	-0.28679400	1.93236400	0.50861000
O	-2.43246300	2.29949000	-0.09783100
O	-0.74849200	-2.10782200	-0.14320200
O	-2.87962400	-1.75386100	-0.81023300
O	-2.04862200	0.56229100	-2.41634100
O	0.07898800	0.19473600	-1.76342700
O	-1.19304700	-0.36608800	2.12119400
O	-3.32346800	0.00623900	1.47301600
C	-1.29835100	2.67626900	0.29576900
C	-2.44345400	-0.25989600	2.33281900
C	-0.81749800	0.45932300	-2.63216800
C	-1.88820000	-2.48976200	-0.56206200
C	-0.32825300	0.62938700	-4.04945400
H	-0.15462500	-0.36096200	-4.48375900
H	-1.07569600	1.15006500	-4.64885700
H	0.61929400	1.17285500	-4.06128200
C	-1.08397500	4.15385700	0.51131500
H	-0.35193400	4.31675000	1.30439400
H	-0.69313900	4.59053700	-0.41451800
H	-2.03039900	4.64149800	0.74897900
C	-2.06399800	-3.97436200	-0.76502000
H	-1.10893000	-4.49349000	-0.68034700
H	-2.75033900	-4.35310500	-0.00135600
H	-2.51975800	-4.15988100	-1.74064500
C	-2.89153300	-0.51097000	3.74962400
H	-3.86493000	-0.05073100	3.92382200
H	-2.97925300	-1.59188400	3.90134800
H	-2.14879100	-0.13013400	4.45289600
C	1.40163200	-0.39801800	0.99380900
C	2.25695600	0.79818000	1.22235300
C	3.46573500	2.69090800	0.32580900
O	2.05928900	1.28582500	2.32978600
N	3.02192100	1.29554300	0.23488400
C	3.12773400	0.56342300	-1.02858800
H	4.01169400	0.94344800	-1.54961700
H	2.25042400	0.74815600	-1.65536100
C	3.28639800	-0.91926800	-0.77078600
C	4.36282400	-1.38034600	0.00339600
C	2.37746000	-1.84530000	-1.29806600
C	4.50118600	-2.73052800	0.27418300
H	5.06904500	-0.66301800	0.41368900
C	2.52438600	-3.20451600	-1.02966400
H	1.53785600	-1.48817200	-1.88379100
C	3.57379900	-3.64660500	-0.23643000
H	5.32151600	-3.07863200	0.89371600
H	1.79551600	-3.90827900	-1.41748100
H	3.67736800	-4.70237600	-0.00709700
C	1.66410400	-1.54347500	1.76833600
N	1.83762700	-2.52707200	2.36811000
H	3.16585600	3.00847500	1.32744800
C	4.98436100	2.80867800	0.21399600
H	5.28707500	3.84776900	0.37767700
H	5.47722200	2.18464000	0.96566400
H	5.34897100	2.51479600	-0.77724400
C	2.72025200	3.54455000	-0.70191400

H	3.01590100	3.29100000	-1.72699500
H	1.64268900	3.38618600	-0.59913000
H	2.94109400	4.60495500	-0.54345300

TS D-D_{RE}

C	0.62142600	0.53488400	0.06850400
C	0.79069000	-0.86446000	-0.40921300
C	1.19622900	-0.04105500	1.32241700
H	0.49410500	-0.18625900	2.13961800
C	-0.89822200	0.74660500	0.16575500
C	-2.94038100	-0.66340300	-0.06585500
H	-3.07348100	-1.73371600	-0.26233500
O	-1.44374800	1.79414300	0.44459500
N	-1.48926600	-0.45267100	-0.08411400
C	-0.57893400	-1.49852600	-0.50892900
H	-0.78583400	-1.80747900	-1.54422500
H	-0.67483600	-2.38428900	0.13048000
C	1.95035600	-1.36248100	-1.00143000
C	3.22470900	-0.93717800	-0.65864500
H	1.84206100	-2.17606400	-1.71527800
C	2.57039800	-0.11792600	1.55492900
C	3.52315000	-0.32554100	0.56767000
H	4.05748800	-1.26760000	-1.27257700
H	2.89625900	-0.09189400	2.59165000
H	4.57068600	-0.21235800	0.83086900
C	1.32916500	1.62200100	-0.58789900
N	1.88909700	2.48027900	-1.12403700
C	-3.52776900	-0.35363500	1.31154200
H	-3.40101600	0.70507800	1.54881600
H	-4.59624000	-0.59082800	1.32234200
H	-3.03414200	-0.94963100	2.08594200
C	-3.62162800	0.12505300	-1.18598800
H	-3.19134100	-0.13228000	-2.15923700
H	-4.69191100	-0.10324900	-1.21094700
H	-3.49575700	1.19815100	-1.02197500

D_{RE}

C	3.58344700	-0.22888300	0.56319800
C	3.24135200	-1.12752300	-0.39083100
C	1.91086400	-1.63400900	-0.65020500
C	2.69222400	0.39949700	1.51788300
C	0.76610200	-0.97934300	-0.41158400
C	1.38961400	0.67248200	1.34591300
C	0.66836300	0.46338400	0.03229900
H	4.64306100	-0.02739800	0.70039500
H	4.04670200	-1.59123400	-0.95512500
H	1.84752900	-2.64027900	-1.06296000
H	3.13802400	0.67667100	2.47097600
H	0.80131000	1.11142200	2.14647800
C	-0.62638300	-1.53641300	-0.58975200
H	-0.80267400	-2.41653900	0.04360900
C	-0.85771500	0.67173700	0.22850700
O	-1.35618600	1.66851700	0.71312000
H	-0.81477200	-1.83039100	-1.63142400
N	-1.49698100	-0.44432000	-0.19874500
C	-2.95058400	-0.62706800	-0.11756400
H	-3.13881800	-1.59869400	-0.58908000
C	1.14845100	1.39346200	-1.00659300
N	1.51887200	2.11009500	-1.83659800
C	-3.41034800	-0.69387700	1.34020600
H	-3.22012800	0.26050400	1.83787700
H	-4.48330400	-0.90512000	1.38830300
H	-2.87990800	-1.48487700	1.88096500
C	-3.69017700	0.44512600	-0.91787500
H	-3.34290900	0.46173600	-1.95549000
H	-4.76406100	0.23290900	-0.91501900
H	-3.52505300	1.43130300	-0.47868100

Z=C(O)Me**Sub**

C	-2.23998000	-0.48703900	-0.04394000
C	-1.60130200	0.81774200	0.36108600
C	0.17042900	2.42321100	0.42876800
N	-3.52888200	-0.31975400	-0.27992900
N	-4.62339500	-0.17966500	-0.50445600
O	-2.32825000	1.65019500	0.89256100
N	-0.28052800	1.04839800	0.09851500
C	0.46726700	0.30477200	-0.91036100
H	0.66519200	0.97623300	-1.75682400
H	-0.17482800	-0.48892200	-1.29489600
C	1.78090600	-0.29879900	-0.45122600
C	2.84165300	-0.36583100	-1.35358500
C	1.95458000	-0.81012400	0.83398400
C	4.05599800	-0.93908000	-0.98539100
H	2.72128700	0.04178600	-2.35550600
C	3.16878800	-1.37434600	1.20777300
H	1.12984100	-0.76747400	1.53561600
C	4.22321500	-1.44379600	0.29974600
H	4.87162300	-0.98201900	-1.70135700
H	3.29087700	-1.76863000	2.21247600
H	5.16993700	-1.88704100	0.59418700
H	-0.37513000	2.68475600	1.33632800
C	1.66406300	2.51873100	0.72576300
H	1.87949300	3.53998600	1.05682900
H	1.96669300	1.82854600	1.51618300
H	2.28190900	2.31666800	-0.15448300
C	-0.24908400	3.40513000	-0.66958000
H	0.26133900	3.19286900	-1.61647000
H	-1.32951400	3.36295800	-0.82823900
H	0.01250900	4.42716000	-0.37701900
C	-1.79560200	-1.88003400	0.11427200
C	-2.81532000	-2.97433600	-0.14903600
H	-3.62598700	-2.93742600	0.58768400
H	-3.26298600	-2.88177200	-1.14462300
H	-2.30744400	-3.93563800	-0.06798300
O	-0.65910700	-2.14295700	0.45863400

2

Rh	-0.96020100	0.12088800	0.26738900
Rh	-2.65449800	-0.86174700	-1.12979700
O	-2.09263600	1.83590400	0.32408700
O	-3.70860800	0.90131000	-0.94266300
O	0.05595200	-1.66456400	0.13451600
O	-1.48194500	-2.55722900	-1.25122300
O	-1.68023100	-0.08438800	-2.76298500
O	-0.06819200	0.81082000	-1.46266900
O	-2.01632400	-0.59838200	1.89458400
O	-3.54999700	-1.59652500	0.57841300
C	-3.20818500	1.85525900	-0.28467200
C	-3.05304300	-1.31030100	1.69953800
C	-0.61420500	0.56752400	-2.58313100
C	-0.39582300	-2.59124300	-0.60735500
C	0.08747600	1.10005400	-3.80567900
H	-0.50683900	0.91103600	-4.69966800
H	0.26882500	2.17117400	-3.68797700
H	1.06086600	0.60888100	-3.90298400
C	-4.00377500	3.13078400	-0.18396000
H	-4.47227200	3.17788900	0.80450300
H	-3.33816600	3.99128900	-0.27965900
H	-4.78069000	3.15650700	-0.94840200
C	0.43596000	-3.84447200	-0.69034000
H	1.49233200	-3.60490400	-0.55386500
H	0.13081400	-4.52101700	0.11495300
H	0.26818100	-4.34715500	-1.64413200

C	-3.71972300	-1.86565900	2.93177900
H	-4.66907900	-2.33640100	2.67642400
H	-3.05589200	-2.60645800	3.38883600
H	-3.87646000	-1.06604600	3.66042100
C	0.76451800	1.08409900	1.71668100
C	1.69372800	2.00039600	0.91462500
C	3.39334600	2.53090200	-0.66521300
N	-0.12099000	1.90299300	2.35451800
N	-0.88515500	2.54502400	2.84902600
O	1.51085300	3.20560400	1.05781800
N	2.66833500	1.49303600	0.11069400
C	2.66001600	0.13146600	-0.41437400
H	2.42217200	0.18328900	-1.48328600
H	1.84252500	-0.41955400	0.04388300
C	3.92736200	-0.67502200	-0.22540500
C	4.24787600	-1.63309000	-1.18780500
C	4.75487000	-0.54127000	0.88872000
C	5.36893600	-2.44679800	-1.04332800
H	3.61430700	-1.74089500	-2.06645400
C	5.88198600	-1.34300100	1.03129200
H	4.50749200	0.19630200	1.64386600
C	6.19300900	-2.30092900	0.06807000
H	5.60270800	-3.18642400	-1.80378400
H	6.51875100	-1.22342000	1.90327800
H	7.07348100	-2.92629900	0.18297300
H	3.43912800	3.39508600	-0.00227900
C	4.82162200	2.13486500	-1.02917300
H	5.29897000	2.99573600	-1.50966500
H	5.40778700	1.86437300	-0.14799000
H	4.85967200	1.29717600	-1.73216800
C	2.59473200	2.93290000	-1.90781700
H	2.57403700	2.12080800	-2.64238300
H	1.56713300	3.18982600	-1.63958500
H	3.06200000	3.80144400	-2.38391500
C	1.21573900	-0.04015400	2.61446500
O	2.20619200	-0.67829500	2.33905400
C	0.40070800	-0.32886600	3.85570200
H	0.47623700	0.49905300	4.57123500
H	-0.65303000	-0.47936900	3.60248700
H	0.80781200	-1.22933200	4.31686400

TS 2-3

Rh	-0.90226100	0.10358200	0.24355100
Rh	-2.67982700	-0.97269000	-1.03136900
O	-1.97145400	1.85873700	0.05370200
O	-3.60857500	0.87002100	-1.14676900
O	0.01891000	-1.73964300	0.31580200
O	-1.62848900	-2.74747700	-0.85258900
O	-1.61835800	-0.52694700	-2.74392500
O	0.00349100	0.51648700	-1.56741500
O	-1.97549500	-0.35190600	1.95167600
O	-3.62575200	-1.34437400	0.77321200
C	-3.06436700	1.86422700	-0.59977600
C	-3.08692900	-0.96900700	1.84379600
C	-0.53700000	0.10902900	-2.64544900
C	-0.52558700	-2.74456900	-0.24654300
C	0.20879000	0.42629400	-3.91767900
H	-0.32923300	0.03780500	-4.78238100
H	0.33369000	1.50875700	-4.00833300
H	1.20751100	-0.01897400	-3.87230900
C	-3.74451100	3.20394400	-0.72829400
H	-3.12036300	3.86102000	-1.34164500
H	-4.72485400	3.09121700	-1.19156000
H	-3.84000700	3.66621800	0.25763200
C	0.23388300	-4.04232800	-0.13998200
H	-0.13353500	-4.76044900	-0.87383100
H	1.30235900	-3.85978300	-0.27506300

H	0.09169100	-4.45281800	0.86498400
C	-3.79890500	-1.26363000	3.14073500
H	-3.97541600	-0.32799000	3.67911800
H	-4.74623400	-1.76836500	2.95141300
H	-3.16122700	-1.89319400	3.76854900
C	0.66050800	0.95917600	1.36196600
C	1.63016900	1.92949400	0.69219900
C	3.31977800	2.45608400	-0.90947400
N	-0.37918200	2.35169500	2.26722400
N	-1.20335900	3.03268300	2.52846900
O	1.45412400	3.13168200	0.86256100
N	2.61860000	1.43075400	-0.09719900
C	2.71472900	0.03547800	-0.51666100
H	2.56214000	-0.00541400	-1.60096400
H	1.89254200	-0.53123600	-0.07997100
C	4.00863100	-0.66568800	-0.16059000
C	4.48689000	-1.66013000	-1.01398200
C	4.71619800	-0.38493700	1.00750000
C	5.64912000	-2.36442700	-0.70986300
H	3.94812900	-1.88153100	-1.93344700
C	5.88216500	-1.07964600	1.31091500
H	4.35188400	0.38710100	1.67681000
C	6.35303800	-2.07275100	0.45447600
H	6.00883700	-3.13216300	-1.38890000
H	6.42428100	-0.84667100	2.22298000
H	7.26515200	-2.61222600	0.69218600
H	3.32784200	3.35149700	-0.28742700
C	4.76526300	2.09044600	-1.23474800
H	5.21905300	2.93730900	-1.76033800
H	5.34849600	1.89197600	-0.33277800
H	4.84036700	1.21403100	-1.88595300
C	2.51987200	2.76485700	-2.17754500
H	2.52453800	1.91117900	-2.86381300
H	1.48279800	3.00730700	-1.93220700
H	2.96693800	3.61754800	-2.69931000
C	1.11234700	0.16022900	2.54070100
O	2.01365800	-0.61909700	2.30034600
C	0.42700500	0.23158400	3.87780100
H	0.82680600	-0.57135000	4.49953200
H	0.61617000	1.19360700	4.36556600
H	-0.65181900	0.10727300	3.74399800

3

Rh	-0.89346500	-0.05420300	0.34400000
Rh	-2.75529500	-0.07889500	-1.23918000
O	-0.12265200	1.55502200	-0.69811800
O	-1.85342900	1.55546700	-2.15216800
O	-1.77832500	-1.65509000	1.29522600
O	-3.48254200	-1.71101800	-0.18935300
O	-1.63392100	-1.34467500	-2.43633200
O	0.07090000	-1.33951000	-0.95746900
O	-2.02222800	1.21649700	1.50501500
O	-3.75199800	1.19320100	0.05024300
C	-0.76872100	2.00220100	-1.70315700
C	-3.18626500	1.55505200	1.11448300
C	-0.49009000	-1.68885400	-2.04856100
C	-2.86456000	-2.12837300	0.82300100
C	0.32083200	-2.60974600	-2.92472200
H	0.43225100	-3.57435900	-2.42040900
H	-0.17041200	-2.75253800	-3.88740200
H	1.32308100	-2.19579300	-3.06436000
C	-0.15370300	3.19388700	-2.39536800
H	-0.20196200	4.05973300	-1.72753300
H	0.90121900	2.99698600	-2.60327900
H	-0.68698100	3.41561600	-3.31991100
C	-3.46033600	-3.28443400	1.58725600
H	-2.67605700	-3.99019800	1.86975000

H	-3.91441400	-2.90120900	2.50711600
H	-4.22711200	-3.77966700	0.99099700
C	-3.94755700	2.46425400	2.04687400
H	-4.83794700	2.85624900	1.55484400
H	-4.24346700	1.89544900	2.93419500
H	-3.30010600	3.27977800	2.37764100
C	0.67909300	-0.06089500	1.57702500
C	1.67806300	0.99184000	1.56002300
C	3.40229000	2.47680500	0.83578100
O	1.31307900	1.70043100	2.51369200
N	2.67395800	1.19968200	0.70468100
C	2.80384400	0.37264300	-0.49721300
H	2.77048500	1.03688600	-1.36749700
H	1.91598000	-0.26252800	-0.56679400
C	4.04371300	-0.49336200	-0.54145900
C	4.93653400	-0.39541600	-1.60804600
C	4.28221700	-1.43487000	0.46114400
C	6.06289800	-1.21247500	-1.66877600
H	4.75379700	0.33203300	-2.39656200
C	5.40837500	-2.24901600	0.40465400
H	3.56902300	-1.54974100	1.27251400
C	6.30364400	-2.13790000	-0.65786400
H	6.75272900	-1.12290500	-2.50287000
H	5.58144700	-2.98121300	1.18776600
H	7.18185300	-2.77544000	-0.70005600
H	3.23734700	2.78233900	1.87235100
C	4.90250200	2.31311800	0.61114200
H	5.40417500	3.24651700	0.88582200
H	5.31160000	1.50286100	1.22058300
H	5.13797100	2.10260900	-0.43613600
C	2.78361900	3.53672700	-0.07703100
H	2.94493600	3.29607900	-1.13391500
H	1.70806700	3.61447300	0.10165500
H	3.24791100	4.50923200	0.11537000
C	0.83299900	-1.12248200	2.60425000
C	0.07966400	-0.98245800	3.88921300
H	0.26138800	0.00384100	4.32584300
H	-0.98859200	-1.05580700	3.65686700
H	0.37344000	-1.77962200	4.57512000
O	1.51367800	-2.07726600	2.27836200

4-1

Rh	-0.84714900	0.25289500	-0.29239500
Rh	-2.18149800	-1.48637300	0.78939500
O	0.83620200	-0.72339700	0.40598500
O	-0.39512600	-2.33699800	1.39950500
O	-2.61558800	1.12422900	-0.90153600
O	-3.85706200	-0.48868400	0.08177000
O	-2.18956900	-0.31773800	2.50447900
O	-0.95244200	1.28806800	1.50984100
O	-0.84274900	-0.92477300	-1.96605800
O	-2.07586100	-2.54100800	-0.98035200
C	0.69527200	-1.78961400	1.08977700
C	-1.44819200	-2.04391200	-1.95224500
C	-1.57896800	0.77781500	2.49798100
C	-3.71813700	0.56195200	-0.59542200
C	-1.56886200	1.59897500	3.76444600
H	-2.05543600	2.56082700	3.57742600
H	-2.08627600	1.07252800	4.56655800
H	-0.53457100	1.80256700	4.05671400
C	1.95735800	-2.46036300	1.57179100
H	2.06885600	-3.41747600	1.05382700
H	2.83792700	-1.84989900	1.37135300
H	1.86686200	-2.67046500	2.64072300
C	-4.96811000	1.21363300	-1.13244100
H	-4.80590400	2.27882200	-1.30402200
H	-5.21801100	0.74419400	-2.08965100

H	-5.79951300	1.05221000	-0.44423500
C	-1.42234200	-2.81989700	-3.24453700
H	-1.62468400	-3.87497100	-3.05605800
H	-2.19911700	-2.42300000	-3.90645400
H	-0.45930100	-2.69010400	-3.74176800
C	0.25730500	1.72138900	-1.10123500
C	1.69229300	1.55351100	-1.24011800
C	2.25632100	2.19417000	1.02400700
O	1.80851300	1.20749300	-2.42231300
N	2.62766200	1.68835500	-0.30603900
C	4.01221800	1.37228500	-0.66503300
H	4.66712700	2.00797200	-0.06261300
H	4.14508200	1.66320100	-1.71173900
C	4.38354300	-0.08784200	-0.48970300
C	3.80686100	-1.06524900	-1.30788000
C	5.33187800	-0.47287200	0.45720900
C	4.17743500	-2.39861800	-1.17575100
H	3.06857600	-0.77593300	-2.04867800
C	5.70095200	-1.81012700	0.59337500
H	5.79359800	0.27827000	1.09431100
C	5.12529200	-2.77593400	-0.22601200
H	3.72469300	-3.14645000	-1.82011200
H	6.44109900	-2.09345700	1.33565000
H	5.41201800	-3.81843200	-0.12450900
H	1.16903300	2.07939600	1.09532000
C	2.85474200	1.35455700	2.14696900
H	2.44318900	1.69373600	3.10287600
H	2.60105700	0.30304700	2.00826400
H	3.94383200	1.45506200	2.20013600
C	2.60689700	3.67777400	1.14950300
H	3.68952900	3.83871800	1.09317900
H	2.13482200	4.26054300	0.35153600
H	2.26061400	4.06701200	2.11244200
C	-0.34268500	2.99020500	-1.59984200
C	-0.98460900	3.82112000	-0.51172600
H	-1.97623700	3.39719700	-0.32208000
H	-0.42935000	3.78281900	0.43058100
H	-1.07699600	4.84943600	-0.86781600
O	-0.34953900	3.28567000	-2.77289300

TS 4-1

C	0.38411400	2.21368000	-0.47812700
C	1.50188400	2.77627500	1.31201100
H	0.52555000	2.24273500	0.84468300
Rh	-0.79709400	0.44998000	-0.10912800
Rh	-2.14253900	-1.51040200	0.35155900
O	0.62169000	-0.30891300	1.19511500
O	-0.59917000	-2.16611700	1.58110200
O	-2.30325100	1.09921500	-1.33879200
O	-3.57253800	-0.71960300	-0.90597600
O	-2.94928300	-0.44034300	1.93546300
O	-1.68118000	1.37880500	1.50977000
O	0.02361400	-0.60973400	-1.67475100
O	-1.24114900	-2.43443500	-1.26029300
C	0.41272400	-1.43916800	1.74761800
C	-0.36727500	-1.79831700	-1.90770200
C	-2.56823700	0.73737800	2.16215400
C	-3.34663400	0.38605900	-1.47205700
C	-3.24140900	1.48178200	3.28799500
H	-4.11030600	2.00978500	2.88121300
H	-3.58838200	0.78118900	4.04888800
H	-2.56423500	2.22097800	3.71957500
C	1.48057000	-1.91420500	2.70107200
H	1.32599400	-2.96397600	2.95197500
H	2.46729500	-1.77182200	2.25306900
H	1.42982700	-1.31613200	3.61723700
C	-4.39055400	0.91820800	-2.41997400

H	-4.51628200	1.99241400	-2.26838000
H	-4.04163700	0.76497100	-3.44624200
H	-5.33679900	0.39471600	-2.27986500
C	0.30746900	-2.49373400	-3.06299500
H	-0.15827000	-3.46094400	-3.25294300
H	0.25085800	-1.86035300	-3.95190800
H	1.36833000	-2.63419200	-2.83016100
C	1.67141700	2.00092500	-1.21765900
C	2.72035000	1.94161000	0.98201400
O	1.60233400	1.92756500	-2.43095000
N	2.80154400	1.85000300	-0.47241600
C	3.96267900	1.22239400	-1.09256100
H	4.85580400	1.82264600	-0.89095300
H	3.77863400	1.25465900	-2.16930600
C	4.15898800	-0.20343100	-0.61853300
C	3.12336700	-1.13000500	-0.77000600
C	5.35122700	-0.60688900	-0.02086000
C	3.28584700	-2.43962900	-0.33336800
H	2.18421000	-0.81949100	-1.22017400
C	5.51633700	-1.92082400	0.41636600
H	6.16215500	0.10874000	0.09977100
C	4.48342400	-2.83961800	0.26118400
H	2.47114800	-3.15034000	-0.44752000
H	6.45104900	-2.22316000	0.87917100
H	4.60774100	-3.86274900	0.60334500
C	-0.33639300	3.40481900	-0.79702000
N	-0.95582400	4.35751600	-1.03477600
H	2.57860600	0.93989300	1.40066300
C	3.96809500	2.58404500	1.58678900
H	3.82243700	2.74183100	2.66018900
H	4.83680400	1.93112400	1.46662700
H	4.17880900	3.54887100	1.11375500
H	1.56841900	3.82850700	1.03828800
H	1.13919400	2.64682700	2.33638500

A

C	2.56155600	0.42644300	0.23253100
C	1.33154500	0.00724900	1.03355400
C	0.65551300	1.85789900	-0.28886400
O	1.27188100	-0.89338500	1.85434900
N	0.30214700	0.82740300	0.68293200
C	-0.96453500	0.79223400	1.38642200
H	-1.26591800	1.82006100	1.62289600
H	-0.77725400	0.27062500	2.33056100
C	-2.06293300	0.08643000	0.61722900
C	-3.30022100	0.69315500	0.41435600
C	-1.84145600	-1.19409300	0.10440300
C	-4.30463000	0.03804800	-0.29481800
H	-3.48100300	1.69011900	0.81062000
C	-2.84032400	-1.84767300	-0.60781400
H	-0.88385100	-1.67809000	0.27832400
C	-4.07469000	-1.23240700	-0.81151500
H	-5.26368500	0.52412800	-0.44770400
H	-2.65839100	-2.84284600	-1.00306500
H	-4.85373000	-1.74433300	-1.36856300
H	0.83536900	2.80483900	0.24420000
C	1.97553800	1.32160100	-0.87216100
H	2.65462200	2.12105500	-1.17377700
H	1.74915200	0.72250000	-1.76325300
C	-0.41376900	2.08583800	-1.34984800
H	-0.65789000	1.14774000	-1.85805900
H	-1.33581700	2.48801800	-0.92021400
H	-0.04453300	2.80387100	-2.08977400
H	3.21822000	1.00271100	0.89339100
C	3.38582400	-0.72938600	-0.32656700
C	2.63395400	-1.96416400	-0.76630400
H	2.33348200	-2.51805800	0.12974600

H	1.71464000	-1.70544300	-1.30443600
H	3.27619700	-2.58746600	-1.38986600
O	4.58775900	-0.62640300	-0.42874400

4-2

Rh	0.64591000	-0.04369900	-0.25022200
Rh	2.86061000	-0.02719500	0.79262000
O	0.30551300	1.81124700	0.60855900
O	2.35001100	1.82492700	1.57619900
O	1.11733200	-1.88413900	-1.03657000
O	3.16446900	-1.88397900	-0.07792000
O	2.02233400	-0.94520100	2.44548400
O	-0.03009200	-0.91179200	1.50573400
O	1.53853300	0.83034400	-1.88897400
O	3.57635100	0.88780000	-0.91593000
C	1.22490800	2.32668200	1.32766600
C	2.78214800	1.10612900	-1.86579100
C	0.78804200	-1.17320600	2.44806800
C	2.25671500	-2.39489000	-0.78425600
C	0.18732500	-1.82320400	3.67044900
H	-0.23009500	-2.79604800	3.39344700
H	0.94426300	-1.95321100	4.44412600
H	-0.63292600	-1.20603100	4.04838800
C	0.91744100	3.67949400	1.92318200
H	0.84080200	4.41788000	1.11878900
H	-0.04662800	3.64768800	2.43767300
H	1.70483000	3.97685600	2.61583600
C	2.53937900	-3.73670200	-1.41282500
H	1.63523700	-4.15603100	-1.85469800
H	3.30240900	-3.61065300	-2.18749000
H	2.94442700	-4.41480300	-0.65776700
C	3.32425700	1.76234400	-3.11090000
H	4.40010500	1.91433100	-3.02318500
H	3.10017500	1.13805400	-3.98020900
H	2.82196300	2.72284300	-3.25810300
C	-1.12394400	-0.05829700	-1.18991000
C	-1.97735600	1.12416200	-1.20116700
C	-3.36924800	2.88587300	-0.34334200
O	-1.63707400	1.72400700	-2.23130000
N	-2.83335700	1.51660300	-0.25967200
C	-2.95810100	0.71878600	0.96515800
H	-3.53388500	1.32240300	1.67244500
H	-1.96529000	0.57435400	1.40524800
C	-3.63785700	-0.61824600	0.75484000
C	-4.78442200	-0.73293000	-0.03340000
C	-3.12902300	-1.75422600	1.38159200
C	-5.41253900	-1.96295400	-0.18802300
H	-5.18095200	0.14089100	-0.54138800
C	-3.76096400	-2.98505500	1.23269700
H	-2.20759400	-1.67683900	1.94819800
C	-4.90395000	-3.09284600	0.44860200
H	-6.30009600	-2.04101100	-0.80917600
H	-3.34470400	-3.86512900	1.71393100
H	-5.39102300	-4.05507600	0.32169500
H	-3.13797900	3.21156000	-1.36043300
C	-4.88417300	2.91561900	-0.15954400
H	-5.23731800	3.95017400	-0.21372900
H	-5.38643900	2.34537600	-0.94641100
H	-5.19178100	2.51089100	0.81102000
C	-2.62757600	3.80340100	0.62905600
H	-2.84166700	3.54445600	1.67278300
H	-1.55101900	3.71686300	0.46483300
H	-2.93238500	4.84311000	0.47270100
C	-1.43108800	-1.16697500	-2.13681000
C	-0.88854200	-1.04374900	-3.53061400
H	-1.33341500	-0.17397400	-4.02362200
H	0.19082800	-0.87063000	-3.47514500

H	-1.10796400	-1.96092000	-4.08122900
O	-2.04242400	-2.11554000	-1.69366900

TS 4-2

Rh	-0.74938600	-0.03997800	0.26352900
Rh	-2.94066800	-0.16900500	-0.75286300
O	-0.47277500	1.76455700	-0.71410700
O	-2.53430900	1.66258000	-1.63088500
O	-1.15077600	-1.85782600	1.14940900
O	-3.19261000	-1.98618800	0.19254800
O	-2.02408600	-1.13678200	-2.35579400
O	0.02326200	-0.99873100	-1.41835800
O	-1.63060500	0.91658200	1.84204700
O	-3.68488800	0.79268100	0.90665000
C	-1.42425300	2.21980400	-1.42796300
C	-2.88291900	1.12084400	1.82714600
C	-0.78503700	-1.33633400	-2.34640800
C	-2.26732500	-2.42253900	0.93108500
C	-0.16572200	-2.02207200	-3.54022700
H	0.50277800	-2.81883900	-3.20334800
H	-0.93858200	-2.42714100	-4.19364200
H	0.43299300	-1.29545500	-4.09958400
C	-1.19196500	3.56442600	-2.07299400
H	-1.18212800	4.33460000	-1.29523000
H	-0.21690400	3.58003400	-2.56642500
H	-1.98306100	3.78471700	-2.78996500
C	-2.51231800	-3.72484600	1.65092400
H	-1.56819800	-4.23526100	1.84811300
H	-2.99216300	-3.50683700	2.61079600
H	-3.18206400	-4.35801800	1.06685500
C	-3.44934100	1.82277500	3.03488600
H	-4.52322200	1.97301000	2.92243700
H	-3.24347300	1.22489200	3.92713900
H	-2.94401500	2.78391800	3.16314600
C	1.30782900	0.03775200	1.10708600
C	1.83110100	1.37393200	1.52856600
C	3.21540000	2.98920600	0.17725700
O	1.53319800	2.06156800	2.47059800
N	2.75735000	1.64770900	0.53787500
C	2.69662700	0.54421300	-0.35455400
H	2.26256600	0.77674900	-1.33762600
H	1.49204100	-0.04533000	-0.08135300
C	3.78839000	-0.44853200	-0.41212500
C	4.73992200	-0.54375400	0.60702900
C	3.82299700	-1.34252600	-1.48640500
C	5.71895700	-1.52781500	0.54641900
H	4.69674700	0.14818700	1.44234800
C	4.80010600	-2.32805100	-1.54092300
H	3.06305000	-1.27742200	-2.26118200
C	5.74876700	-2.42103000	-0.52405700
H	6.45774400	-1.60233200	1.33789900
H	4.82122600	-3.02620900	-2.37171400
H	6.51275900	-3.19119300	-0.56479100
H	3.17936600	3.53364900	1.12604400
C	4.65531300	2.94776200	-0.32902200
H	5.00944000	3.96358800	-0.52946200
H	5.32108400	2.48808900	0.40702800
H	4.73254400	2.37808800	-1.26311600
C	2.26417400	3.66279000	-0.81240900
H	2.26507900	3.14604900	-1.77998500
H	1.24443700	3.65296400	-0.42224000
H	2.57391000	4.69824900	-0.98716600
C	1.66060700	-1.19209600	1.86593500
O	1.77178900	-1.12462400	3.07342200
C	1.81086300	-2.49131600	1.10576300
H	1.42179400	-2.42678600	0.08706800
H	2.87057400	-2.76758200	1.07654600

H 1.26603400 -3.26417800 1.65203100

B

C 1.84138000 1.08222100 -0.12993800
C 0.37346100 -0.04719800 0.86336000
C 0.65968400 1.49607100 0.75549300
O 2.75055500 1.65313000 -0.68514000
N 1.51959700 -0.24639900 -0.03119800
C 2.37142100 -1.40617400 -0.25004100
H 3.15781500 -1.03863100 -0.91806800
C 3.01251500 -1.86284800 1.06344600
H 3.54722700 -1.03630700 1.54164200
H 2.25485000 -2.23853600 1.76095300
H 0.55934100 -0.41761800 1.87837600
C -0.96345900 -0.54377900 0.37305300
C -1.97080700 -0.82000300 1.29687400
C -1.23676900 -0.67858600 -0.98853000
C -3.23018800 -1.22693100 0.86932000
H -1.77085300 -0.70571800 2.35932100
C -2.49390900 -1.09013200 -1.41874300
H -0.45300000 -0.47235400 -1.71172000
C -3.49405200 -1.36515200 -0.49033200
H -4.00555800 -1.43708700 1.59971600
H -2.69101500 -1.19897500 -2.48107000
H -4.47550700 -1.68687700 -0.82549000
H 0.99913800 1.91186200 1.70875800
H 3.72550100 -2.67227700 0.87797400
C 1.61739700 -2.54249400 -0.93813300
H 0.77971200 -2.88799400 -0.32274000
H 1.21937900 -2.22392300 -1.90526400
H 2.29102000 -3.38924500 -1.10394900
C -0.45349700 2.39391100 0.22733600
C -0.34272700 2.87805900 -1.19478800
H 0.64183700 3.32459900 -1.36954900
H -0.42706500 2.02076400 -1.87408300
H -1.13893900 3.59211200 -1.40941400
O -1.37477500 2.68177000 0.95798100

4-3

Rh -0.90689300 0.29037900 -0.17368800
Rh -2.44579900 -1.48105500 0.51479300
O 0.59513900 -1.12380700 -0.19840600
O -0.82125400 -2.76542900 0.44605900
O -2.50274700 1.59519700 -0.10981500
O -3.93243700 -0.03456900 0.52948000
O -1.98677300 -1.02340700 2.48033600
O -0.55409900 0.60007600 1.83961600
O -1.41088400 -0.17067400 -2.11706900
O -2.80448000 -1.83481500 -1.48981800
C 0.30950400 -2.32823000 0.11490500
C -2.22850500 -1.11996300 -2.34921200
C -1.16150700 -0.10485900 2.71118300
C -3.65169000 1.15151500 0.22347400
C -0.85736700 0.23445400 4.14875700
H -1.32177900 1.19607100 4.38909900
H -1.25062600 -0.53437600 4.81415500
H 0.22113500 0.34328700 4.28570700
C 1.45163400 -3.30998700 0.05525900
H 1.68305400 -3.51177000 -0.99599800
H 2.34472700 -2.87892500 0.51329800
H 1.17587600 -4.24292100 0.54743100
C -4.76670400 2.16752000 0.22188800
H -4.44423700 3.07265600 0.74199100
H -4.99454800 2.44151100 -0.81334100
H -5.65964900 1.75329700 0.69036900
C -2.53611800 -1.37558100 -3.80344900
H -3.01468300 -2.34795200 -3.92388900

H	-3.21555600	-0.59596900	-4.16326000
H	-1.61895300	-1.31985500	-4.39368700
C	0.32967100	1.73089700	-0.73839800
C	1.73914700	1.53173400	-1.07838400
C	2.43405500	1.71228300	1.24546800
O	1.80271400	1.35676800	-2.30083700
N	2.73267000	1.55299100	-0.18969800
C	4.09970600	1.44021900	-0.68911400
H	4.71126000	2.19649800	-0.18865200
H	4.05841000	1.70104100	-1.75110400
C	4.72741100	0.07252200	-0.52956900
C	5.96744800	-0.06184500	0.09313900
C	4.09318200	-1.06198600	-1.04086700
C	6.57369700	-1.31094000	0.20741600
H	6.46391200	0.81789200	0.49690100
C	4.70177600	-2.30794600	-0.93234500
H	3.12118500	-0.96562300	-1.51722500
C	5.94135000	-2.43750100	-0.30797300
H	7.53800300	-1.40197000	0.69837800
H	4.20856000	-3.18511200	-1.34071000
H	6.41061800	-3.41311800	-0.22414700
H	1.35176900	1.86673200	1.30790700
C	2.75569400	0.44392000	2.03164100
H	2.40788300	0.56552500	3.06261000
H	2.23906600	-0.40958500	1.58600400
H	3.83045300	0.23900500	2.05391200
C	3.10328900	2.95902500	1.81868300
H	4.19217900	2.85127300	1.87924600
H	2.86027700	3.83980000	1.21709300
H	2.73356600	3.12811700	2.83432600
C	-0.17492000	3.10966600	-0.95396700
C	-0.86930000	3.42653600	-2.23920100
H	-0.25520400	3.09810300	-3.08377200
H	-1.80322400	2.85482600	-2.26372700
H	-1.07613300	4.49732600	-2.29418200
O	-0.01562700	3.86128100	-0.00986800

TS 4-3

Rh	-0.86758700	0.25223600	-0.02136800
Rh	-2.49559000	-1.53415400	0.08489100
O	0.57401600	-1.18498900	-0.44639100
O	-0.95882200	-2.84281800	-0.36062400
O	-2.40806000	1.54749800	0.42412800
O	-3.92769600	-0.11737600	0.53395500
O	-2.04051300	-1.69837700	2.10389100
O	-0.51300700	-0.03919700	1.99695200
O	-1.32622200	0.44226000	-2.01510300
O	-2.82807700	-1.24440800	-1.93008700
C	0.21067100	-2.40355400	-0.51198400
C	-2.18589700	-0.33735500	-2.53003800
C	-1.17616100	-0.93595400	2.61030100
C	-3.58216900	1.09332300	0.59686700
C	-0.89028300	-1.07339100	4.08542700
H	-1.20440200	-0.15779700	4.59573000
H	-1.42287300	-1.92815400	4.50253300
H	0.18602100	-1.18756900	4.24220200
C	1.29822900	-3.41504900	-0.78068600
H	1.82518500	-3.15729500	-1.70405100
H	2.02222900	-3.38447900	0.03934800
H	0.87425900	-4.41595200	-0.86163500
C	-4.65248300	2.11844900	0.87494000
H	-4.27609400	2.86917000	1.57322400
H	-4.90265500	2.62708300	-0.06199500
H	-5.54844300	1.63849800	1.26978600
C	-2.45868100	-0.13690700	-3.99959100
H	-3.12853700	-0.91083500	-4.37506500
H	-2.91321500	0.84744000	-4.14734700

H	-1.51362500	-0.14808600	-4.54844600
C	0.61680900	1.92886600	-0.11626300
C	1.64084300	1.76283400	-1.18293000
C	2.39936700	1.67970000	0.90847700
O	1.55963300	1.93534100	-2.37871500
N	2.74526000	1.39633900	-0.45402000
C	4.09174600	1.28172400	-0.97269800
H	4.68325200	2.16287000	-0.68682600
H	3.96951200	1.31665000	-2.06098400
C	4.80370800	0.01675000	-0.54988800
C	6.10129400	0.07135800	-0.04556300
C	4.16844700	-1.22089300	-0.67645800
C	6.76760800	-1.09733500	0.32013200
H	6.59792300	1.03311200	0.06228100
C	4.83401700	-2.38647700	-0.31603500
H	3.14199300	-1.25299600	-1.03317900
C	6.13573000	-2.32826300	0.18216700
H	7.77774400	-1.04236800	0.71495400
H	4.34084900	-3.34775300	-0.42743300
H	6.65201600	-3.24103900	0.46388100
H	1.00982500	1.44664100	0.88649300
C	2.58413100	0.52645600	1.87385100
H	2.14682100	0.75757500	2.84729200
H	2.13874000	-0.38548500	1.47169500
H	3.66358700	0.36831800	1.98903200
C	2.77145900	3.03846500	1.43914900
H	3.79983400	2.97844700	1.81856500
H	2.72438600	3.80133300	0.65979400
H	2.10851800	3.33132000	2.25525200
C	-0.06517800	3.22169000	0.12890300
C	-0.74899200	3.81569700	-1.07642300
H	-0.17398500	3.65188900	-1.99167100
H	-1.70874500	3.30091500	-1.19142000
H	-0.92683200	4.87829100	-0.89767400
O	-0.10655300	3.71974000	1.24016400

C

C	1.99963300	-0.13007200	-0.59255600
C	1.26849500	-1.09215000	0.36996600
C	0.90742700	0.91704000	-0.19587400
O	1.43346600	-2.22829500	0.75518300
N	0.32144600	-0.15863500	0.63614800
C	-0.85172000	-0.21271400	1.47380800
H	-0.83448900	0.62360300	2.18308400
H	-0.76344600	-1.13793700	2.05342200
C	-2.13912000	-0.20253500	0.67599400
C	-3.08399000	0.80636400	0.84492100
C	-2.37617300	-1.20715400	-0.26538800
C	-4.25178900	0.81672900	0.08386900
H	-2.90601200	1.59316000	1.57461700
C	-3.53807000	-1.19838500	-1.02688000
H	-1.63879200	-1.99551100	-0.39874800
C	-4.47926600	-0.18390500	-0.85446000
H	-4.98120800	1.60916500	0.22334400
H	-3.71298600	-1.98394200	-1.75609900
H	-5.38755100	-0.17642000	-1.44960400
H	1.86932900	-0.48245300	-1.62441000
C	0.01676600	1.34532400	-1.35844600
H	0.57833200	2.00039800	-2.03263700
H	-0.34051800	0.47771600	-1.92210600
H	-0.86029800	1.89246700	-0.99829200
C	1.33932800	2.11096900	0.64657300
H	0.44865400	2.61723500	1.03789000
H	1.96307500	1.79997100	1.48805000
H	1.91148300	2.82226600	0.04825100
C	3.48475400	0.09357900	-0.37668600
C	4.31579900	-1.16800000	-0.39188500

H	5.35717300	-0.92964600	-0.17032800
H	3.91656300	-1.89200800	0.32677900
H	4.25052500	-1.64110600	-1.37909500
O	3.96748400	1.19616500	-0.23704500

4-4

Rh	0.64518000	-0.04381700	-0.24867300
Rh	2.86010900	-0.01737600	0.79380400
O	0.29600200	1.80849700	0.61178900
O	2.33929900	1.82969000	1.58178800
O	1.12497200	-1.88176100	-1.03624200
O	3.17346100	-1.87110000	-0.08059700
O	2.02654500	-0.94305000	2.44488800
O	-0.02675700	-0.91588300	1.50680700
O	1.53305700	0.83529900	-1.88658900
O	3.57030900	0.90594100	-0.91320800
C	1.21221400	2.32672400	1.33303600
C	2.77549100	1.11577000	-1.86461000
C	0.79305000	-1.17552700	2.44812900
C	2.26719100	-2.38681100	-0.78530500
C	0.19534100	-1.82871400	3.67028700
H	-0.22450600	-2.79999100	3.39156000
H	0.95431800	-1.96195700	4.44140900
H	-0.62279700	-1.21137900	4.05259000
C	0.89790800	3.67696500	1.93071100
H	0.82735500	4.41788500	1.12807300
H	-0.07039700	3.64227100	2.43689200
H	1.67932400	3.97311600	2.63060300
C	2.55545800	-3.72762800	-1.41357000
H	1.65353200	-4.14980300	-1.85724200
H	3.31982400	-3.59932500	-2.18653100
H	2.96096200	-4.40451200	-0.65764700
C	3.32391600	1.73642700	-3.12509900
H	4.30216100	2.17969400	-2.93663100
H	3.42457200	0.95653200	-3.88708500
H	2.62604600	2.48600900	-3.50448100
C	-1.12416800	-0.06452200	-1.18894000
C	-1.97794500	1.11774900	-1.20527700
C	-3.37125400	2.88182500	-0.35449400
O	-1.63772700	1.71396800	-2.23750900
N	-2.83419000	1.51336300	-0.26533700
C	-2.95849500	0.71980900	0.96229900
H	-3.53519100	1.32526500	1.66727900
H	-1.96554100	0.57817900	1.40315400
C	-3.63681400	-0.61859300	0.75595600
C	-4.78355800	-0.73645900	-0.03162400
C	-3.12650800	-1.75251900	1.38520900
C	-5.41037900	-1.96750400	-0.18318100
H	-5.18125900	0.13571500	-0.54150500
C	-3.75716800	-2.98439200	1.23935700
H	-2.20489700	-1.67281600	1.95121200
C	-4.90029300	-3.09533400	0.45592100
H	-6.29808400	-2.04796700	-0.80381300
H	-3.33972400	-3.86290500	1.72240900
H	-5.38628200	-4.05841600	0.33135300
H	-3.14014400	3.20358600	-1.37287900
C	-4.88622900	2.91099200	-0.17101100
H	-5.24026800	3.94501000	-0.22940400
H	-5.38792100	2.33718100	-0.95563700
H	-5.19360900	2.50990200	0.80113700
C	-2.63064900	3.80398700	0.61426500
H	-2.84380300	3.54828300	1.65899400
H	-1.55403800	3.71876700	0.44985400
H	-2.93731900	4.84262800	0.45447400
C	-1.42917500	-1.17648900	-2.13257100
O	-2.03791200	-2.12545800	-1.68671700
C	-0.88794900	-1.05545100	-3.52715100

H	-1.34013700	-0.19159300	-4.02395000
H	0.19002100	-0.87347300	-3.47360000
H	-1.10078200	-1.97675000	-4.07343300

TS 4-4

Rh	-0.40276500	-0.09831300	0.13763200
Rh	-2.77440000	0.32113300	-0.35771400
O	-0.01029400	0.59562600	-1.79174600
O	-2.17927800	1.06829100	-2.20210900
O	-1.02110500	-0.73281900	1.99702700
O	-3.20694800	-0.42400200	1.51999400
O	-2.84753000	-1.60093600	-1.14240000
O	-0.67884000	-1.99963800	-0.64917500
O	-0.33021800	1.86015900	0.77386900
O	-2.54074000	2.20355800	0.46088600
C	-0.96323900	1.05240900	-2.50684400
C	-1.38795900	2.56284300	0.81980800
C	-1.82017700	-2.32286900	-1.11216000
C	-2.26176800	-0.75297100	2.28156500
C	-1.91893700	-3.71298000	-1.69637300
H	-1.48142900	-4.43745000	-1.00437200
H	-2.95889600	-3.96652500	-1.90302800
H	-1.34662600	-3.75162000	-2.62928400
C	-0.55574300	1.64275000	-3.83583500
H	-0.02336600	2.58256800	-3.65580600
H	0.12938500	0.96611400	-4.35344800
H	-1.43271800	1.83840700	-4.45325100
C	-2.60076900	-1.20632500	3.67972100
H	-2.08747200	-2.14592900	3.90047500
H	-2.23668300	-0.45850000	4.39080100
H	-3.67836800	-1.32664100	3.79308000
C	-1.21278300	3.97273700	1.32725400
H	-2.15164200	4.34856600	1.73672300
H	-0.41953600	4.00217600	2.07620300
H	-0.91928200	4.61385400	0.48839900
C	1.59744900	-0.43402200	0.78686400
C	2.25374100	0.86583500	1.15650200
C	3.29731500	2.85379400	0.19537500
O	2.02732600	1.37174600	2.23862900
N	3.00604200	1.42325900	0.16062300
C	2.96413800	0.70204100	-1.09097700
H	3.89098400	0.87698500	-1.64820200
H	2.11312800	1.00039700	-1.70973800
C	2.85568800	-0.78792400	-0.77741300
C	3.91937800	-1.39393000	-0.04622900
C	2.08923100	-1.62247300	-1.63768100
C	4.14701800	-2.75525500	-0.11123300
H	4.53024000	-0.76237600	0.59193500
C	2.33099700	-2.98096700	-1.71046700
H	1.29150700	-1.16663900	-2.21234500
C	3.35863600	-3.54545500	-0.95183100
H	4.93682900	-3.20419900	0.48104200
H	1.71472600	-3.60652100	-2.34684500
H	3.54391900	-4.61409100	-1.01083600
H	3.12569500	3.13284900	1.23838300
C	4.75715600	3.13171000	-0.15908100
H	4.98065500	4.19381400	-0.01641100
H	5.42800100	2.54825400	0.47880800
H	4.97336700	2.89016300	-1.20701000
C	2.31961500	3.63480200	-0.68797300
H	2.49098700	3.43099200	-1.75236200
H	1.29128700	3.35634500	-0.43875000
H	2.44698400	4.71104800	-0.53183100
C	1.84328200	-1.56573700	1.80279800
O	2.53579400	-1.36606700	2.77570600
C	1.14548900	-2.88362800	1.59572500
H	0.15901000	-2.79442900	2.06269100

H	0.97345000	-3.10985900	0.54474600
H	1.71412500	-3.67112900	2.09505200

D

C	-0.49943500	0.40830300	-0.30302500
C	0.99682700	0.57568900	-0.41589600
C	3.04670200	-0.74057600	0.13175000
H	3.18706600	-1.76768200	0.48937700
O	1.56493400	1.57638100	-0.82206800
N	1.59554500	-0.57114900	0.02624600
C	0.69059300	-1.46069600	0.72858500
H	0.88284000	-1.44186700	1.81262100
H	0.80997100	-2.49452400	0.38267600
C	-0.69583700	-0.91962500	0.41999800
C	-1.80303400	-1.16441000	1.35339900
C	-1.04651300	-0.77734300	-1.07014700
C	-3.08433600	-1.14973100	0.94196500
H	-1.55121200	-1.38031800	2.38885500
C	-2.47789800	-0.88014500	-1.40448200
H	-0.35700100	-1.20609600	-1.79628300
C	-3.42720700	-1.00942000	-0.46193700
H	-3.88288500	-1.31383500	1.65928800
H	-2.74089900	-0.87913100	-2.45756200
H	-4.47248100	-1.06918400	-0.74792900
C	3.72384900	-0.61752500	-1.23293300
H	3.59671700	0.38979800	-1.63470600
H	4.79431200	-0.82494700	-1.13457100
H	3.29635600	-1.33426800	-1.94116100
C	3.63737500	0.21981200	1.16742900
H	3.14675000	0.09419200	2.13888300
H	4.70716900	0.02779000	1.29864300
H	3.50354200	1.25341300	0.83842400
C	-1.30126400	1.65644000	-0.01334600
O	-2.22391700	2.00532400	-0.71138500
C	-0.85906100	2.43212300	1.20564300
H	-0.81621500	1.77143100	2.07906800
H	0.14731800	2.82911800	1.03453100
H	-1.55287400	3.25313600	1.39173500

TS D-D_{RE}

C	-0.54623200	0.29252300	-0.28065500
C	-0.64880800	-0.92434000	0.56247200
C	-1.09562700	-0.63333700	-1.30112100
C	0.95846000	0.52509700	-0.43500000
C	3.06789100	-0.65994400	0.17971400
H	3.24930300	-1.63374900	0.64985800
O	1.46867700	1.50044900	-0.95591700
N	1.60977900	-0.53446900	0.12040800
C	0.74132900	-1.47123600	0.80513300
H	0.96389200	-1.50354100	1.88247700
H	0.86803900	-2.48653500	0.40937900
C	-1.77821700	-1.29055500	1.30505400
C	-3.07557600	-1.05743900	0.88092900
H	-1.61806700	-1.86290100	2.21679900
C	-2.46988100	-0.83878300	-1.48099400
H	-0.40316500	-0.99121600	-2.06041800
C	-3.40917800	-0.83056500	-0.46498500
H	-3.88642700	-1.26008800	1.57534600
H	-2.79753300	-1.10139800	-2.48377800
H	-4.46101800	-0.86237500	-0.73410600
C	3.68331900	-0.68343600	-1.21972300
H	3.51443300	0.26968600	-1.72599900
H	4.76158700	-0.85825300	-1.14829000
H	3.24248400	-1.48438000	-1.82168100
C	3.67371500	0.42813400	1.06918900
H	3.21917700	0.41089500	2.06543100
H	4.75119100	0.27014400	1.18084100

H	3.50751500	1.41264000	0.62461300
C	-1.28564600	1.58787100	0.06282200
O	-2.01922600	2.12424200	-0.72885100
C	-0.98915000	2.15158800	1.43271300
H	-1.31575000	1.44473300	2.20265400
H	0.08975800	2.30387200	1.55071100
H	-1.50787700	3.10274000	1.55815800

D_{RE}

C	3.49046200	-0.71608700	0.49190500
C	3.11759300	-1.20103000	-0.71738900
C	1.76753700	-1.52785100	-1.12258000
C	2.62661200	-0.43178900	1.61957700
C	0.65102000	-0.96266100	-0.63712100
C	1.33427800	-0.07001200	1.57340300
C	0.60645900	0.22284200	0.29284600
H	4.55750300	-0.61338200	0.67664400
H	3.90566900	-1.46494100	-1.41902800
H	1.66286500	-2.31732800	-1.86681400
H	3.08998100	-0.51383100	2.60058200
H	0.78059600	0.08306800	2.49573400
C	-0.75763700	-1.38450900	-0.98779300
H	-0.96575000	-2.42261900	-0.69299800
C	-0.90386700	0.39660000	0.55740800
O	-1.38217300	1.18507300	1.35270000
H	-0.94991400	-1.30144500	-2.06701200
N	-1.59105700	-0.46109400	-0.24431200
C	-3.05086600	-0.58642300	-0.24362300
H	-3.27181600	-1.33178500	-1.01680800
C	-3.55924700	-1.11550500	1.09910200
H	-3.34447700	-0.39461500	1.89170500
H	-4.64078700	-1.27904200	1.05475400
H	-3.07698300	-2.06637500	1.34855900
C	-3.71785200	0.72983100	-0.64480200
H	-3.34398300	1.07211100	-1.61553000
H	-4.80079100	0.59062100	-0.72324300
H	-3.51361400	1.50146800	0.10064200
C	1.10295200	1.54242100	-0.36957200
O	1.80793700	2.31661600	0.22593500
C	0.63498500	1.79276800	-1.78791700
H	0.79973600	2.84100400	-2.04065700
H	1.21149800	1.16144900	-2.47236600
H	-0.42300700	1.53821300	-1.91373800