Supplementary Information

Mechanisms of Cu/DMAP Cocatalyzed and DMAP-Catalyzed C-N Decarboxylative Cross-Coupling Reactions

Ruisheng Zhao, †,* Chaomin Hao, † Dan Liu, Zizhong Liu,* Yongsheng Bao*

Inner Mongolia Key Laboratory of Green Catalysis, College of Chemistry and Environmental Science, Inner Mongolia Normal University, Hohhot 010022, China. E-mail: zhaoruisheng@imnu.edu.cn

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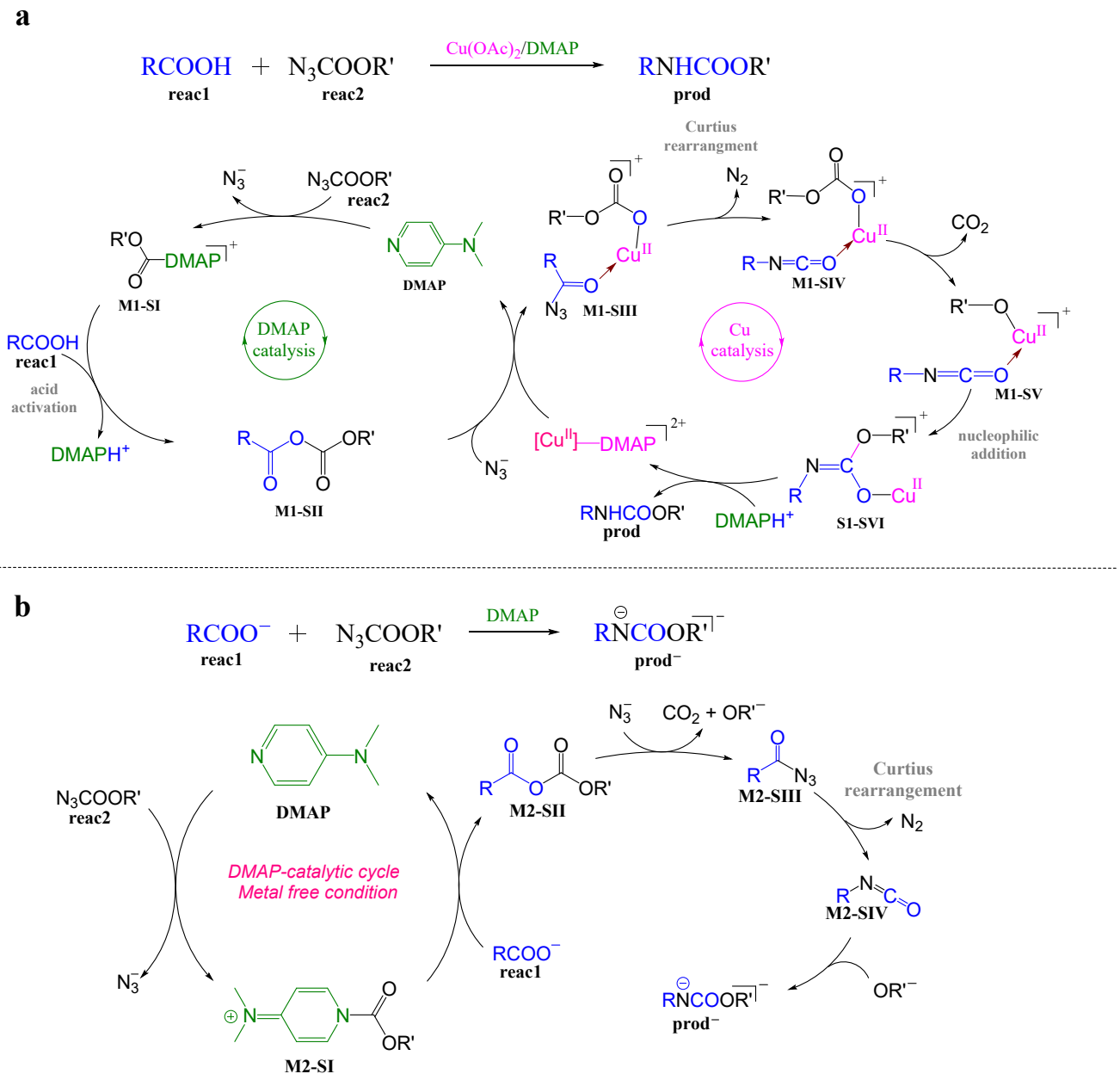
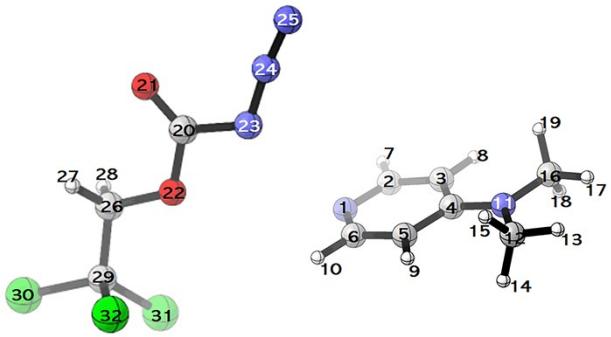
S1 Original Envisioned Mechanism of Cu/DMAP Cocatalyzed and DMAP-Catalyzed C-N DCC Reactions



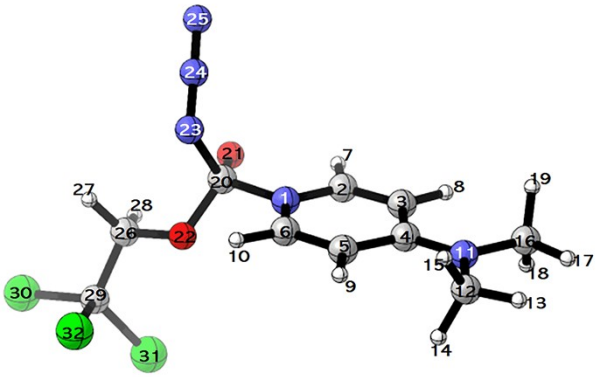
Scheme S1 Original Envisioned Mechanisms of C-N DCC Reactions (a) Cocatalyzed by Cu/DMAP and (b) Catalyzed by DMAP (Refs. 8 and 9)

S2 Cu/DMAP Cocatalyzed C-N DCC Reactions

S2.1 Cu/DMAP Cocatalyzed C(aryl)-N DCC Reactions



$M1_{RA}$-1



$M1_{RA}$-2

Fig. S1 Optimized structures of **$M1_{RA}$-1** and **$M1_{RA}$-2.**

Table S1 Natural Charges (q, in *e*) of **$M1_{RA}$-2** and **$M1_{RA}$-1** and Natural Charge Variation (Δq) between **$M1_{RA}$-1** and **$M1_{RA}$-2**

atoms	q(**$M1_{RA}$-2**)	q(**$M1_{RA}$-1**)	Δq[a]
N1	-0.388	-0.549	0.161
C2	0.064	0.008	0.056
C3	-0.324	-0.353	0.029
C4	0.251	0.208	0.043
C5	-0.319	-0.353	0.034
C6	0.062	0.008	0.054
H7	0.283	0.233	0.050
H8	0.282	0.260	0.022
H9	0.283	0.260	0.023
H10	0.281	0.233	0.048
N11	-0.380	-0.420	0.040
C12	-0.495	-0.490	-0.005
H13	0.260	0.253	0.007
H14	0.247	0.235	0.012
H15	0.246	0.235	0.011
C16	-0.495	-0.490	-0.005

H17	0.260	0.253	0.007
H18	0.245	0.234	0.011
H19	0.245	0.235	0.010
C20	0.897	0.923	-0.026
O21	-0.773	-0.618	-0.155
O22	-0.618	-0.540	-0.078
N23	-0.430	-0.395	-0.035
N24	0.225	0.259	-0.034
N25	-0.182	0.036	-0.218
C26	-0.162	-0.174	0.012
H27	0.258	0.285	-0.027
H28	0.267	0.285	-0.018
C29	-0.137	-0.154	0.017
Cl30	0.018	0.035	-0.017
Cl31	0.016	0.029	-0.013
Cl32	0.013	0.029	-0.016

[a]Δq=q(**M1$_{RA}$-2**)-q(**M1$_{RA}$-1**)

The natural charge variations Δq between **M1$_{RA}$-2** and **M1$_{RA}$-1** are collected in Table S1. The Δq(N1) is the most positive one and the Δq(O21) and Δq(N25) are the two negative ones, indicating that the negative charge of the ylide intermediate **M1$_{RA}$-2** mainly locates on the N1, namely N(pyridine), and the positive charge of **M1$_{RA}$-2** mainly accumulates on the O21 and N25, i.e., O(carbonyl) and N(azide). The positive and negative charges of **M1$_{RA}$-2** are labelled on the N(pyridine) and O(carbonyl) of the structural formula (see Fig. 1).

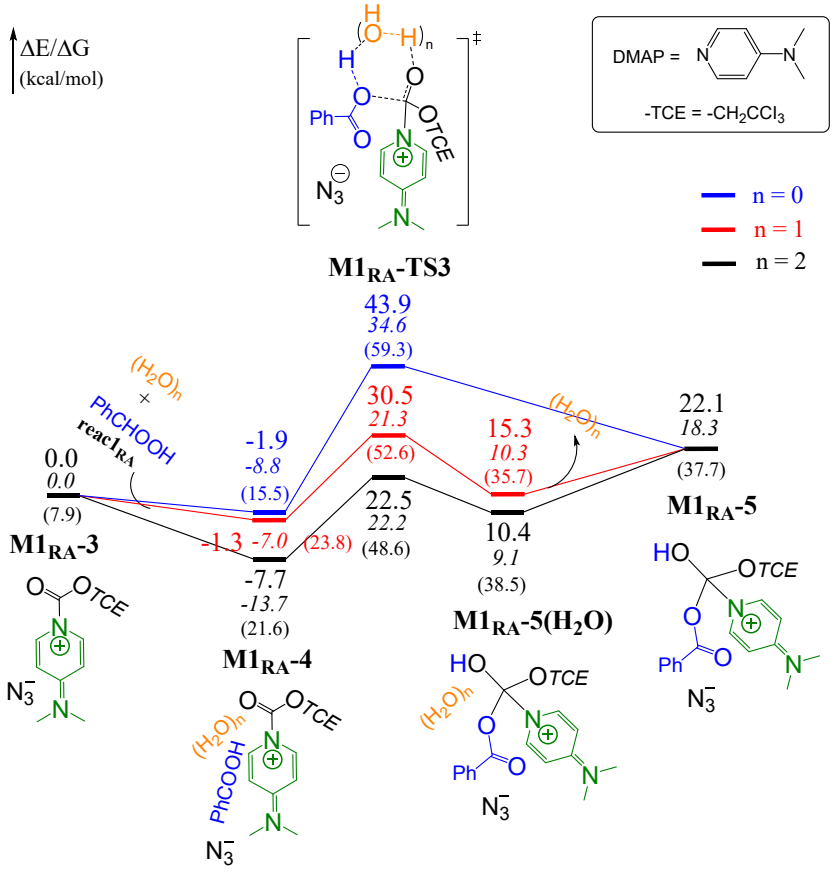


Fig. S2 (Free, in parentheses) Energy profile of the carbonyl addition step **(M1$_{RA}$-3** to **M1$_{RA}$-5)** facilitated by extra $(H_2O)_n$ (n=0, 1, 2) molecule(s), and energies with counterpoise corrections are given in italics.

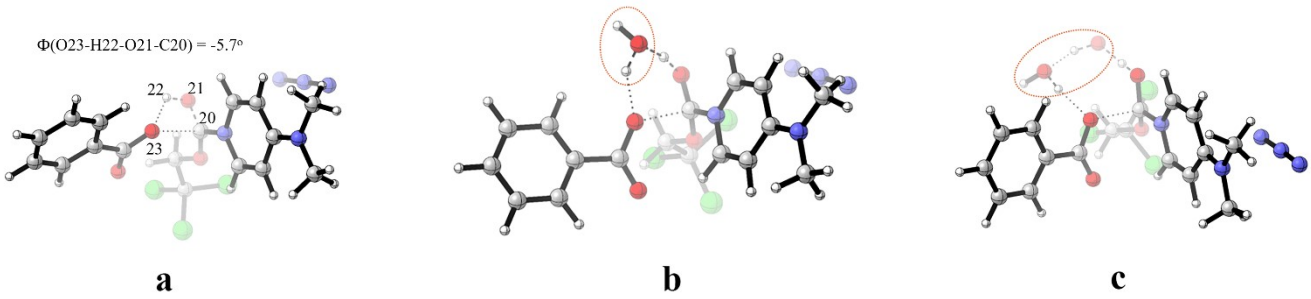


Fig. S3 Optimized structures of **$M1_{RA}$-TS3** (a) without and with (b) one and (c) two extra H_2O molecule(s). (Extra H_2O molecules are labelled with a dashed cycle)

As shown in Figs. S2 and S3, extra H_2O molecule(s) can act as a "water bridge" and reduce the barrier of the carbonyl addition step **$M1_{RA}$-4** to **$M1_{RA}$-5(H_2O)**. When one and two extra H_2O molecule(s) is (are) introduced as the "water bridge" which can facilitate hydrogen transfer, the energy barrier reduces from 45.8 kcal/mol to 31.8 and 30.2 kcal/mol, respectively, and the Gibbs free energy barrier reduces from 43.8 kcal/mol to 28.8 and 27.0 kcal/mol, respectively; if the BSSE is considered, the energy barrier reduces from 43.4 kcal/mol to 28.3 kcal/mol when one H_2O molecule is introduced, but the energy barrier is increased to 35.9 kcal/mol, though, when two H_2O molecule is introduced. Introduction of more extra H_2O molecules will damage the structure of "water bridge", as shown in Fig. S4, though. The distortion/interaction analysis indicate that introduction of extra H_2O molecules as "water bridge" can decrease the distortion energy of PhCOOH moiety and increase the interaction energy, shown in Table S1.

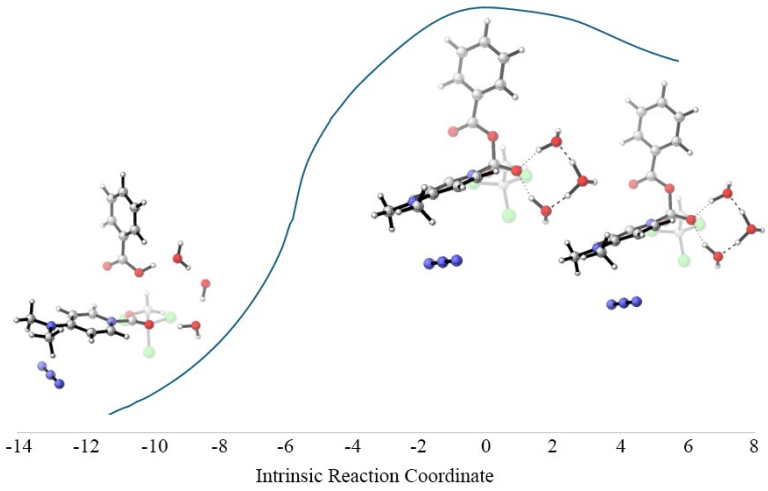


Fig. S4 Reaction path of the carbonyl addition with three extra H_2O molecules as "water bridge"

Table S2 Distortion (ΔE_{dist}) and Interaction (ΔE_{int}) Energy (in kcal/mol) Analysis of the Carbonyl Addition Step

	ΔE_{dist}						ΔE_{int}	$E^{\ddagger}$
	PhCOOH	DMAP-Troc	N_3	H_2O-1	H_2O-2	Sum		
$0H_2O$	95.3	14.3	0.0	—	—	109.6	-63.8	45.8
$1H_2O$	94.9	14.9	0.0	39.7	—	149.5	-117.7	31.8
$2H_2O$	85.5	21.8	0.0	45.6	4.4	157.2	-127.0	30.2

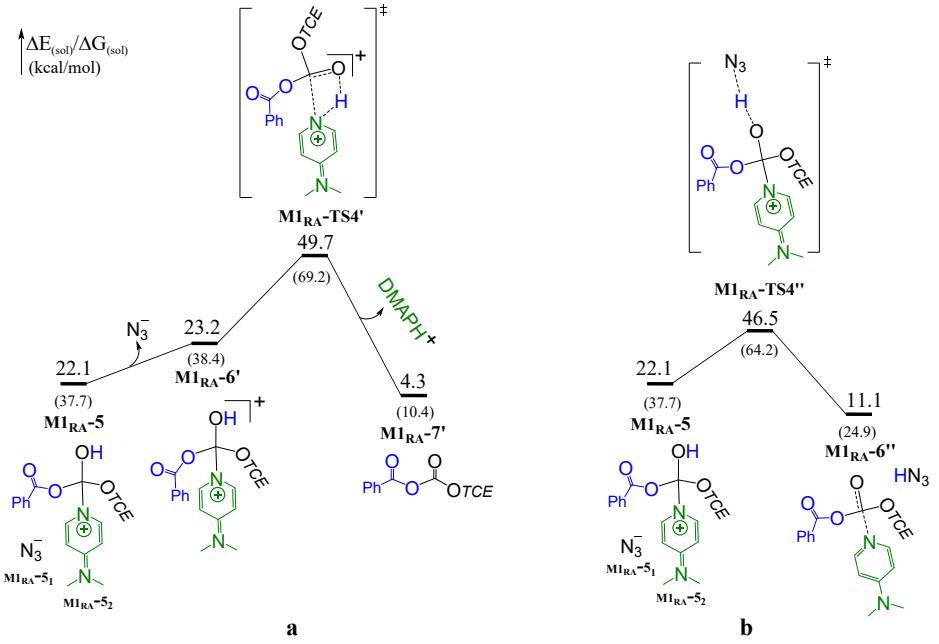


Fig. S5 (Free, parentheses) Energy profiles of (a) the reaction path followed the original envisioned mechanism and (b) the reaction path without release of N_3^-.

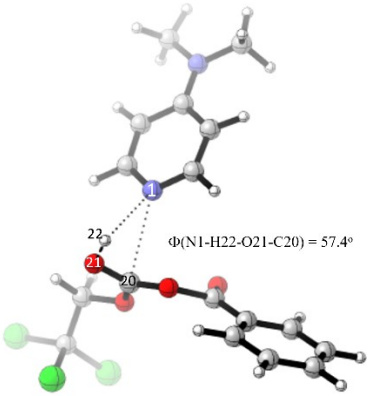


Fig. S6 Optimized structure of **M1$_{RA}$-TS4′**

The original envisioned mechanism for Cu/DMAP cocatalyzed C-N DCC reaction assumed that an anhydride intermediate (**M1-SII** of Scheme S1a) is formed during the reaction, and this reaction path was also investigated. As illustrated in Fig. S5a, the N_3^- releases from the **M1$_{RA}$-5**, forming the intermediate **M1$_{RA}$-6′** with an increase of energy by 1.1 kcal/mol. Then, the H(hydroxyl) of **M1$_{RA}$-6′** migrates to N(pyridine), accompanied with the cleavage of C(ester)-N(pyridine) bond, and the anhydride intermediate **M1$_{RA}$-7′** (corresponding to **M1-SII** of Scheme S1a) is formed via **M1$_{RA}$-TS4′**. The overall energy barrier (**M1$_{RA}$-TS4′** relative to **M1$_{RA}$-5**) is as large as 27.6 kcal/mol, which is 10.2 kcal/mol higher than that of the competing step (**M1$_{RA}$-5** to **M1$_{RA}$-6**) of the main path with an energy barrier of only 17.4 kcal/mol, as showing in Fig. 1. Different from the carbonyl addition step (**M1$_{RA}$-3** to **M1$_{RA}$-5**), it is impossible to introduce extra H_2O molecules to the $DMAPH^+$ elimination step (**M1$_{RA}$-6′** to **M1$_{RA}$-7′**), because the four relating atoms, i.e., N1, H22, O21, C20, of **M1$_{RA}$-TS4′** are not in a plane, as shown in Fig. S6. The dihedral angle of N1-H22-O21-C20 is as large as 57.4°, while that of O23-H22-O21-C20 of **M1$_{RA}$-TS3** without extra H_2O molecule is only -5.7° (see Fig. S3a). Noteworthy, before the $DMAPH^+$ elimination step (**M1$_{RA}$-6′** to **M1$_{RA}$-7′**), N_3^- must departure from the intermediate sphere (**M1$_{RA}$-5** to **M1$_{RA}$-6′**). Otherwise, the N_3^- tends to abstract the H(hydroxyl) of **M1$_{RA}$-5$_2$** depicted in Fig. S5b, which will impede the formation of the following intermediate **M1$_{RA}$-8** (corresponding to **M1-SIII** of Scheme S1a). Meanwhile, the release of N_3^- from **M1$_{RA}$-3** is also not favorable due to the attractive electrostatic interaction between the anionic N_3^- and cationic DMAP-Troc$^+$ (-Troc, 2,2,2-trichloroethoxycarbonyl, -$COOCH_2CCl_3$). Moreover, even if the anionic N_3^- can be released from **M1$_{RA}$-3** obeying the original envisioned mechanism, the following formation of anhydride intermediate step still need to overcome a barrier of 26.5

kcal/mol (**M1$_{RA}$-TS4′** relative to **M1$_{RA}$-5′**), which is still 9.1 kcal/mol higher than the competing step (**M1$_{RA}$-5** to **M1$_{RA}$-6**) of the main path. Therefore, the original envisioned anhydride intermediate **M1-SII** can be safely ruled out.

Table S3 Natural and Mulliken (in parentheses) Charges of Cu (q(Cu) in e) of $Cu(DMAP)^{2+}$ and $Cu(OAc)^{+}$, and Energy Levels (in Atomic Unit) of Several Most High-Lying Occupied and Low-Lying Unoccupied Molecules Orbitals of of $Cu(DMAP)^{2+}$ and $Cu(OAc)^{+}$ (o, Occupied Orbitals; v, Virtual Orbitals).

	$Cu(DMAP)^{2+}$				$Cu(OAc)^{+}$			
q(Cu)	1.633 (1.459)				1.469 (1.229)			
	Alpha		Beta		Alpha		Beta	
E(MO)	MO47 (*v*)	0.019	MO46 (*v*)	0.018	MO30 (*v*)	0.028	MO29 (*v*)	0.022
	MO46 (*v*)	0.017	MO45 (*v*)	-0.028	MO29 (*v*)	0.022	MO28 (*v*)	0.022
	MO45 (*v*)	-0.030	MO44 (*v*)	-0.039	MO28 (*v*)	0.021	MO27 (*v*)	-0.022
	MO44 (*v*)	-0.043	MO43 (*v*)	-0.057	MO27 (*v*)	-0.022	MO26 (*v*)	-0.052
	MO43 (*v*)	-0.062	MO42 (*v*)	-0.189	MO26 (*v*)	-0.057	MO25 (*v*)	-0.174
	MO42 (*o*)	-0.239	MO41 (*o*)	-0.230	MO25 (o)	-0.316	MO24 (*o*)	-0.322
	MO41 (*o*)	-0.290	MO40 (*o*)	-0.289	MO24 (o)	-0.329	MO23 (*o*)	-0.333
	MO40 (*o*)	-0.339	MO39 (*o*)	-0.338	MO23 (o)	-0.354	MO22 (*o*)	-0.334
	MO39 (*o*)	-0.344	MO38 (*o*)	-0.360	MO22 (o)	-0.380	MO21 (*o*)	-0.365
	MO38 (*o*)	-0.370	MO37 (*o*)	-0.361	MO21 (o)	-0.398	MO20 (*o*)	-0.378

S2.2 Cu/DMAP Cocatalyzed C(sp^3)-N DCC Reactions

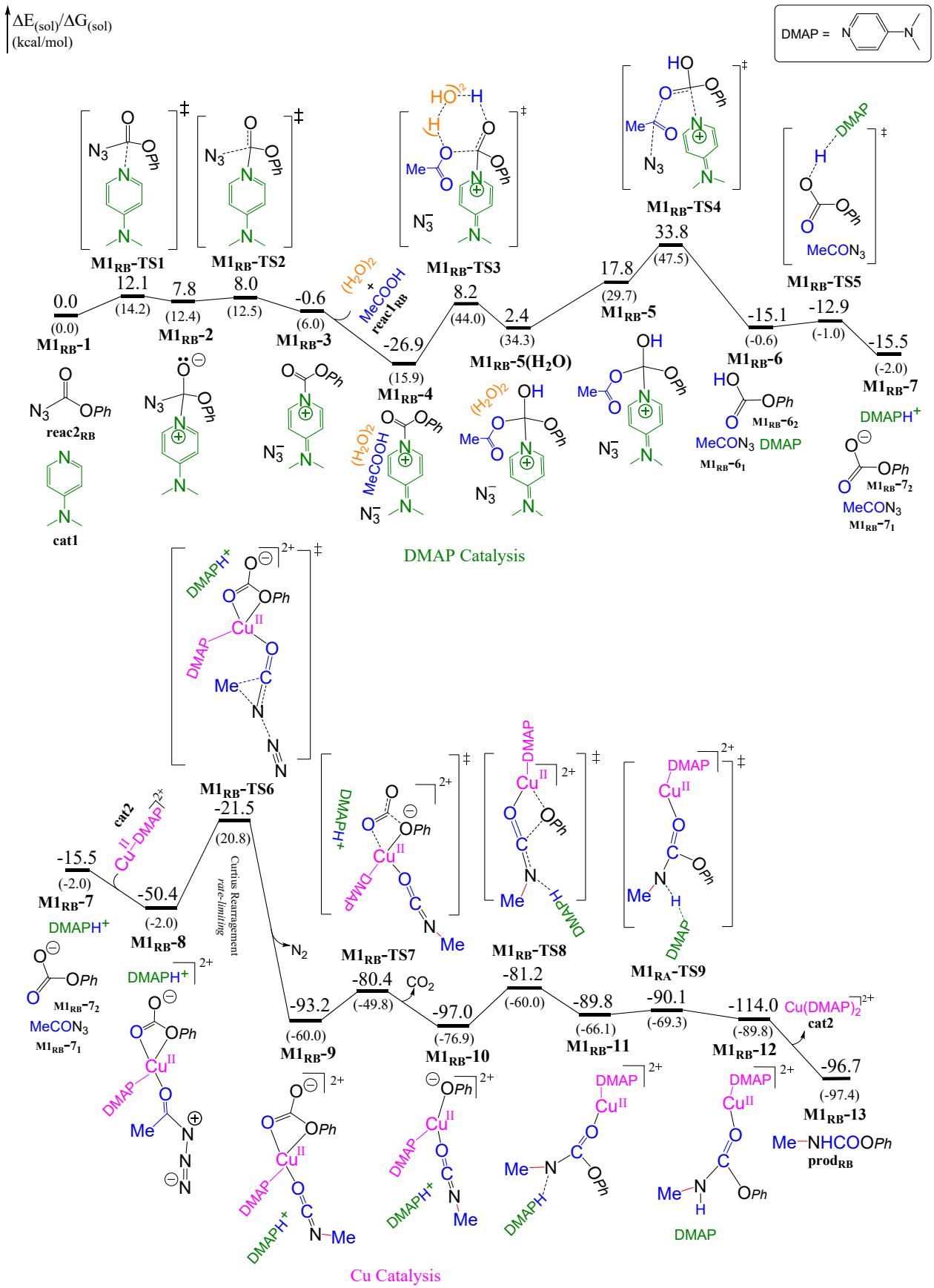


Fig. S7 (Free, in parentheses) Energy profile for the Cu/DMAP cocatalyzed C(sp^3)-N DCC reactions. (Up, DMAP catalysis cycle; down, Cu catalysis cycle)

The Cu/DMAP cocatalyzed C(sp^3)-N DCC reaction was also investigated utilizing the model reaction B, and the energy profile is portrayed in Fig. S7. In general, the energy profile is on par with that of the C(aryl)-N one shown in Fig. 1. Same with the case of C(aryl)-N DCC reaction, extra H_2O molecules also can act as a "water bridge" to assist the hydrogen transfer and to facilitate the carbonyl addition step, and the energy profile of the carbonyl addition step (**$M1_{RB}$-3** to **$M1_{RB}$-5**) of the C(sp^3)-N DCC reaction with 0 – 3 extra H_2O molecule(s) is depicted in Fig. S8.

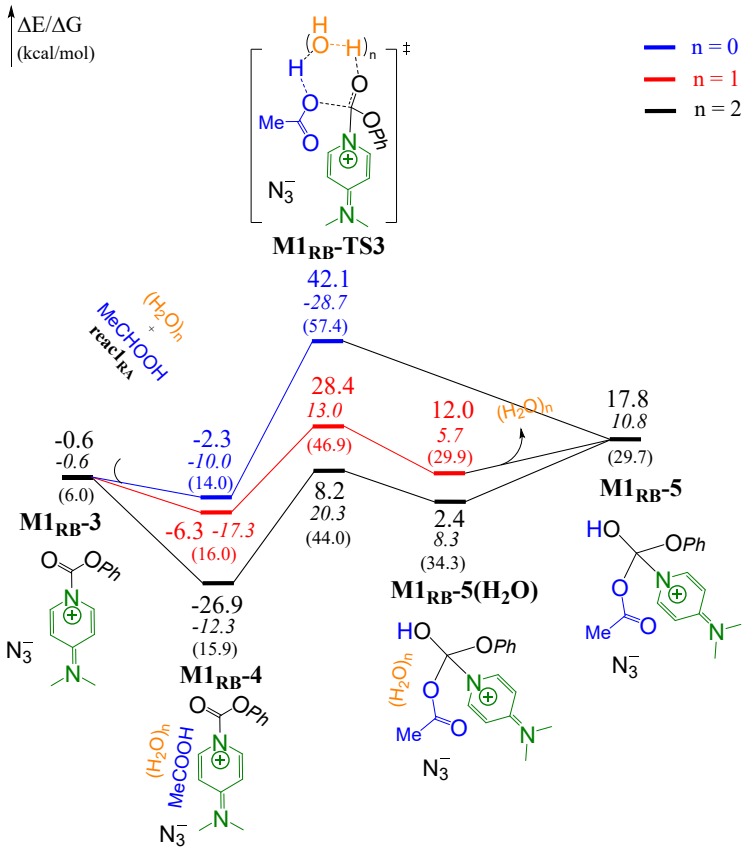


Fig. S8 (Free, in parentheses) Energy profile of the carbonyl addition step (**$M1_{RB}$-3** to **$M1_{RB}$-5**) facilitated by extra $(H_2O)_n$ (n=0, 1, 2) molecule(s), and energies with counterpoise corrections are given in italics.

S2.3 Supposing $Cu(OAc)^+$ instead of $Cu(DMAP)^{2+}$ as the Active Catalyst Species

Table S4 Energy Levels (in Atomic Unit) of Molecular Orbitals of $Cu(DMAP)^{2+}$ and $Cu(OAc)^+$. (Twenty Most High-Lying Occupied and Low-Lying Unoccupied Molecular Orbitals are listed. *o*, Occupied Orbitals; *v*, Virtual Orbitals)

$Cu(DMAP)^{2+}$				$Cu(OAc)^+$			
Alpha		Beta		Alpha		Beta	
MO62(*v*)	0.18825	MO61(*v*)	0.18165	MO45(*v*)	0.61756	MO44(*v*)	0.61108
MO61(*v*)	0.18126	MO60(*v*)	0.17563	MO44(*v*)	0.61069	MO43(*v*)	0.57302
MO60(*v*)	0.17510	MO59(*v*)	0.17344	MO43(*v*)	0.57086	MO42(*v*)	0.56373
MO59(*v*)	0.17252	MO58(*v*)	0.16764	MO42(*v*)	0.56054	MO41(*v*)	0.52949
MO58(*v*)	0.16594	MO57(*v*)	0.16224	MO41(*v*)	0.52984	MO40(*v*)	0.42722
MO57(*v*)	0.16049	MO56(*v*)	0.15712	MO40(*v*)	0.42358	MO39(*v*)	0.34955
MO56(*v*)	0.15666	MO55(*v*)	0.13614	MO39(*v*)	0.34566	MO38(*v*)	0.33984
MO55(*v*)	0,13564	MO54(*v*)	0.13322	MO38(*v*)	0.33531	MO37(*v*)	0.22885
MO54(*v*)	0.13090	MO53(*v*)	0.12522	MO37(*v*)	0.22782	MO36(*v*)	0.18194
MO53(*v*)	0.12484	MO52(*v*)	0.11910	MO36(*v*)	0.18150	MO35(*v*)	0.17147
MO52(*v*)	0.11668	MO51(*v*)	0.10810	MO35(*v*)	0.16956	MO34(*v*)	0.16937

MO51(*v*)	0.10589	MO50(*v*)	0.10544	MO34(*v*)	0.16742	MO33(*v*)	0.15238
MO50(*v*)	0.10467	MO49(*v*)	0.10102	MO33(*v*)	0.15169	MO32(*v*)	0.12933
MO49(*v*)	0.10047	MO48(*v*)	0.03475	MO32(*v*)	0.12687	MO31(*v*)	0.11689
MO48(*v*)	0.03411	MO47(*v*)	0.01953	MO31(*v*)	0.11740	MO30(*v*)	0.02864
MO47(*v*)	0.01876	MO46(*v*)	0.01761	MO30(*v*)	0.02822	MO29(*v*)	0.02224
MO46(*v*)	0.01710	MO45(*v*)	-0.02819	MO29(*v*)	0.02186	MO28(*v*)	0.02198
MO45(*v*)	-0.02983	MO44(*v*)	-0.03903	MO28(*v*)	0.02124	MO27(*v*)	-0.02166
MO44(*v*)	-0.04305	MO43(*v*)	-0.05651	MO27(*v*)	-0.02232	MO26(*v*)	-0.05248
MO43(*v*)	-0.06169	MO42(*v*)	-0.18863	MO26(*v*)	-0.05695	MO25(*v*)	-0.17359
MO42(*o*)	-0.23906	MO41(*o*)	-0.23028	MO25(*o*)	-0.31584	MO24(*o*)	-0.32156
MO41(*o*)	-0.28973	MO40(*o*)	-0.28875	MO24(*o*)	-0.32922	MO23(*o*)	-0.33282
MO40(*o*)	-0.38879	MO39(*o*)	-0.33755	MO23(*o*)	-0.35409	MO22(*o*)	-0.33391
MO39(*o*)	-0.34418	MO38(*o*)	-0.36027	MO22(*o*)	-0.37988	MO21(*o*)	-0.36483
MO38(*o*)	-0.36996	MO37(*o*)	-0.36109	MO21(*o*)	-0.39817	MO20(*o*)	-0.37846
MO37(*o*)	-0.38516	MO36(*o*)	-0.36760	MO20(*o*)	-0.40094	MO19(*o*)	-0.38210
MO36(*o*)	-0.38523	MO35(*o*)	-0.36922	MO19(*o*)	-0.41101	MO18(*o*)	-0.40256
MO35(*o*)	-0.39186	MO34(*o*)	-0.39138	MO18(*o*)	-0.41114	MO17(*o*)	-0.40520
MO34(*o*)	-0.40533	MO33(*o*)	-0.39574	MO17(*o*)	-0.41184	MO16(*o*)	-0.41004
MO33(*o*)	-0.41051	MO32(*o*)	-0.39641	MO16(*o*)	-0.44092	MO15(*o*)	-0.48589
MO32(*o*)	-0.41066	MO31(*o*)	-0.41115	MO15(*o*)	-0.48837	MO14(*o*)	-0.49568
MO31(*o*)	-0.41310	MO30(*o*)	-0.41218	MO14(*o*)	-0.50840	MO13(*o*)	-0.50337
MO30(*o*)	-0.43685	MO29(*o*)	-0.43353	MO13(*o*)	-0.52298	MO12(*o*)	-0.56377
MO29(*o*)	-0.45084	MO28(*o*)	-0.45011	MO12(*o*)	-0.56802	MO11(*o*)	-0.76098
MO28(*o*)	-0.45126	MO27(*o*)	-0.45769	MO11(*o*)	-0.76254	MO10(*o*)	-1.00352
MO27(*o*)	-0.45863	MO26(*o*)	-0.47767	MO10(*o*)	-1.01670	MO9(*o*)	-1.11837
MO26(*o*)	-0.48136	MO25(*o*)	-0.48327	MO9(*o*)	-1.12857	MO8(*o*)	-2.90366
MO25(*o*)	-0.48465	MO24(*o*)	-0.49327	MO8(*o*)	-2.91674	MO7(*o*)	-2.91255
MO24(*o*)	-0.50676	MO23(*o*)	-0.52608	MO7(*o*)	-2.97359	MO6(*o*)	-2.91330

Table S5 Energy Levels (in Atomic Unit) of Molecular Orbitals of $PhCON_3$ ($\mathbf{M1_{RA}\text{-}7_1}$) and Troc-$COO^-$ ($\mathbf{M1_{RA}\text{-}7_2}$). (Twenty Most High-Lying Occupied and Most Low-Lying Unoccupied Molecular Orbitals are listed. *o*, Occupied Orbitals; *v*, Virtual Orbitals)

$PhCON_3$ ($\mathbf{M1_{RA}\text{-}7_1}$)				Troc-COO^- ($\mathbf{M1_{RA}\text{-}7_2}$)			
MO58(*v*)	0.44965	MO38(*o*)	-0.25963	MO68(*v*)	0.48366	MO48(*o*)	-0.20209
MO57(*v*)	0.37767	MO37(*o*)	-0.26157	MO67(*v*)	0.46115	MO47(*o*)	-0.22061
MO56(*v*)	0.36385	MO36(*o*)	-0.27804	MO66(*v*)	0.44434	MO46(*o*)	-0.23761
MO55(*v*)	0.30675	MO35(*o*)	-0.29132	MO65(*v*)	0.43550	MO45(*o*)	-0.25313
MO54(*v*)	0.30334	MO34(*o*)	-0.34179	MO64(*v*)	0.42323	MO44(*o*)	-0.30047
MO53(*v*)	0.28775	MO33(*o*)	-0.35595	MO63(*v*)	0.41394	MO43(*o*)	-0.30748
MO52(*v*)	0.27730	MO32(*o*)	-0.36065	MO62(*v*)	0.40677	MO42(*o*)	-0.31336
MO51(*v*)	0.24709	MO31(*o*)	-0.36632	MO61(*v*)	0.37698	MO41(*o*)	-0.31645
MO50(*v*)	0.20599	MO30(*o*)	-0.42410	MO60(*v*)	0.36872	MO40(*o*)	-0.32588
MO49(*v*)	0.19379	MO29(*o*)	-0.42416	MO59(*v*)	0.34658	MO39(*o*)	-0.34506
MO48(*v*)	0.17223	MO28(*o*)	-0.43446	MO58(*v*)	0.30469	MO38(*o*)	-0.34740
MO47(*v*)	0.16886	MO27(*o*)	-0.44562	MO57(*v*)	0.27275	MO37(*o*)	-0.36945

MO46(*v*)	0.15908	MO26(*o*)	-0.45802	MO56(*v*)	0.19997	MO36(*o*)	-0.37924
MO45(*v*)	0.15304	MO25(*o*)	-0.47802	MO55(*v*)	0.18988	MO35(*o*)	-0.41813
MO44(*v*)	0.10392	MO24(*o*)	-0.49486	MO54(*v*)	0.17224	MO34(*o*)	-0.42465
MO43(*v*)	0.06763	MO23(*o*)	-0.51974	MO53(*v*)	0.15593	MO33(*o*)	-0.44933
MO42(*v*)	-0.00216	MO22(*o*)	-0.53392	MO52(*v*)	0.12291	MO32(*o*)	-0.47104
MO41(*v*)	-0.01100	MO21(*o*)	-0.54770	MO51(*v*)	0.01430	MO31(*o*)	-0.48582
MO40(*v*)	-0.04637	MO20(*o*)	-0.60111	MO50(*v*)	0.00804	MO30(*o*)	-0.52624
MO39(*v*)	-0.07117	MO19(*o*)	-0.61951	MO49(*v*)	-0.03588	MO29(*o*)	-0.58837

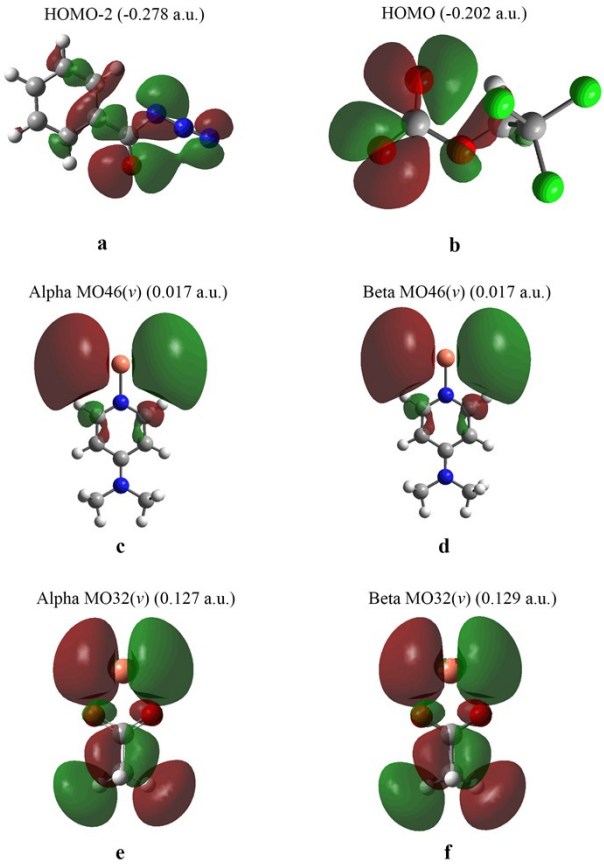


Fig. S9 (a) HOMO-2 of PhCON3 $\mathbf{M_{1RA}\text{-}7_1}$, (b) HOMO of OTroc$^-$ $\mathbf{M_{1RA}\text{-}7_2}$, (c) Alpha MO46(*v*) and (d) Beta MO46(*v*) of Cu(DMAP)$^{2+}$ and (e) Alpha MO32(*v*) and (f) Beta MO32(*v*) of Cu(OAc)$^+$ (*v*, Virtual Orbital).

For instance, as shown in Fig. S9, the portions populated on O atoms of HOMO-2 of $\mathbf{M1_{RA}\text{-}7_1}$ and HOMO of $\mathbf{M1_{RA}\text{-}7_2}$ possess significant lone-pair electron characteristics, and the alpha MO46(*v*) and beta MO46(*v*) of Cu(DMAP)$^{2+}$ and alpha MO32(*v*) and beta MO32(*v*) of Cu(OAc)$^+$ can symmetrically match with the HOMO-2 and HOMO, and the alpha MO46(*v*) and beta MO46(*v*) of Cu(DMAP)$^{2+}$ are much lower in energy level than alpha MO32(*v*) and beta MO32(*v*) of Cu(OAc)$^+$. Therefore, when alpha MO46(*v*) and beta MO46(*v*) of Cu(DMAP)$^{2+}$ combine with HOMO-2 of $\mathbf{M1_{RA}\text{-}7_1}$ and HOMO of $\mathbf{M1_{RA}\text{-}7_2}$, lower-energy bonding orbital of $\mathbf{M1_{RA}\text{-}8}$ will be formed.

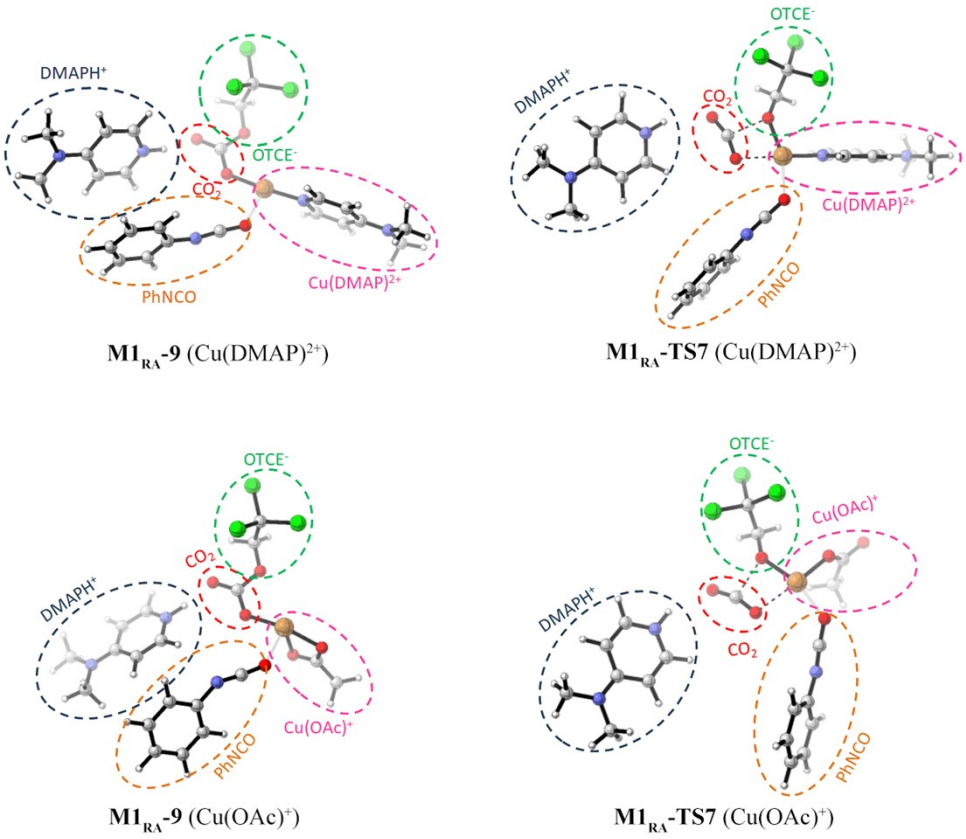


Fig. S10 Divided fragments of **M1$_{RA}$-9** and **M1$_{RA}$-TS7** during the distortion-interaction analysis.

S2.4 C-H Activation Ortho-Coupling Pattern

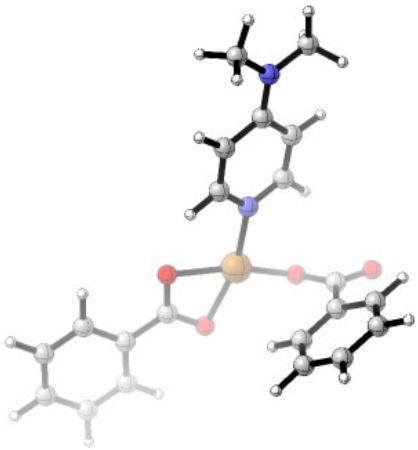


Fig. S11 Optimized structure of **M1'$_{RA}$-1**

S3 DMAP-Catalyzed C-N DCC Reactions

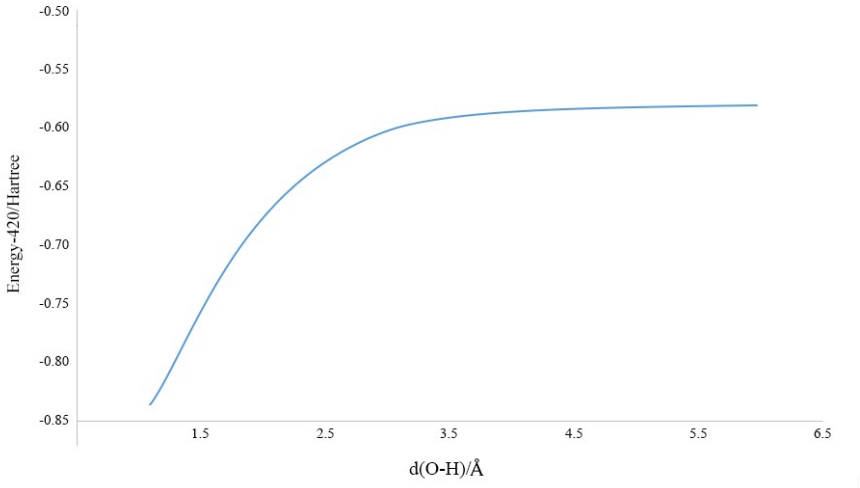


Fig. S12 Potential energy surface scan of elongation of O-H bond of PhCOOH

The potential energy surface scan of elongation of O-H bond of PhCOOH is illustrated in Fig. S12, indicating that the O-H bond energy of PhCOOH is over 166.8 kcal/mol (0.2659 Hartree).

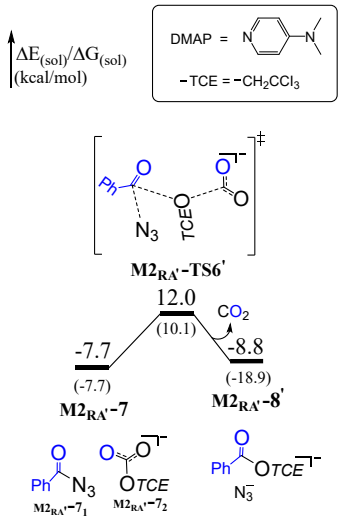


Fig. S13 (Free, in parentheses) Energy profile of the original envisioned mechanism of DMAP-catalyzed C-N DCC reaction.

The calculated results indicates that after the attack of N_3^- to the anhydride intermediate (**M2$_{RA'}$-6$_1$**), the alkoxy anion (plus CO_2) intermediate is not formed, as proposed by the original envisioned mechanism (**M2-SII** to **M2-SIII** of Scheme S1b), and instead a carbonate intermediate **M2$_{RA'}$-7$_2$** (corresponding to **M2-III$_2$** of Scheme 1b) is formed, as shown in Fig. 4 (**M2$_{RA'}$-6** to **M2$_{RA'}$-7**). Therefore, can the CO_2 be extruded from **M2$_{RA'}$-7$_2$**? This step was calculated, and the energy profile is shown in Fig. S13. If **M2$_{RA'}$-7$_2$** undergoes the decarboxylation, the —O*TCE* group **M2$_{RA'}$-7$_2$** will simultaneously transfer to **M2$_{RA'}$-7$_1$**, and at the same time, the N_3^- will be detached from **M2$_{RA'}$-7$_1$**, resulting in **M2$_{RA'}$-8'**. This way, it is impossible to generate the final product, so the original envisioned mechanism can be excluded.

S4 Influences of Neutral and Alkaline Conditions on Cu/DMAP Cocatalyzed and DMAP-Catalyzed (Metal-Free) C-N DCC Reactions.

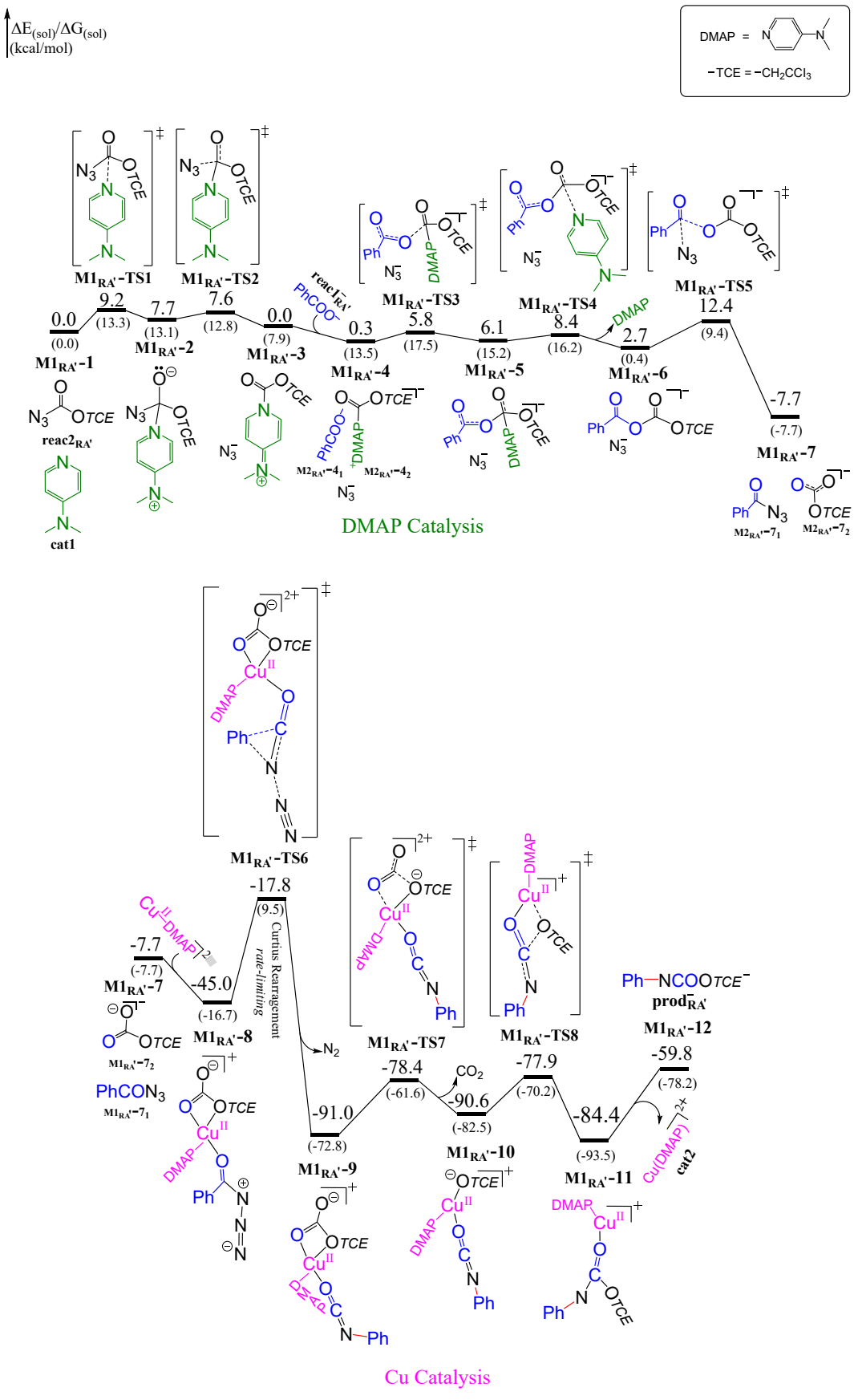


Fig. S14 (Free, in parentheses) Energy profile of Cu/DMAP cocatalyzed C-N DCC reaction, assuming carboxylate as the carbon source (under alkaline condition)

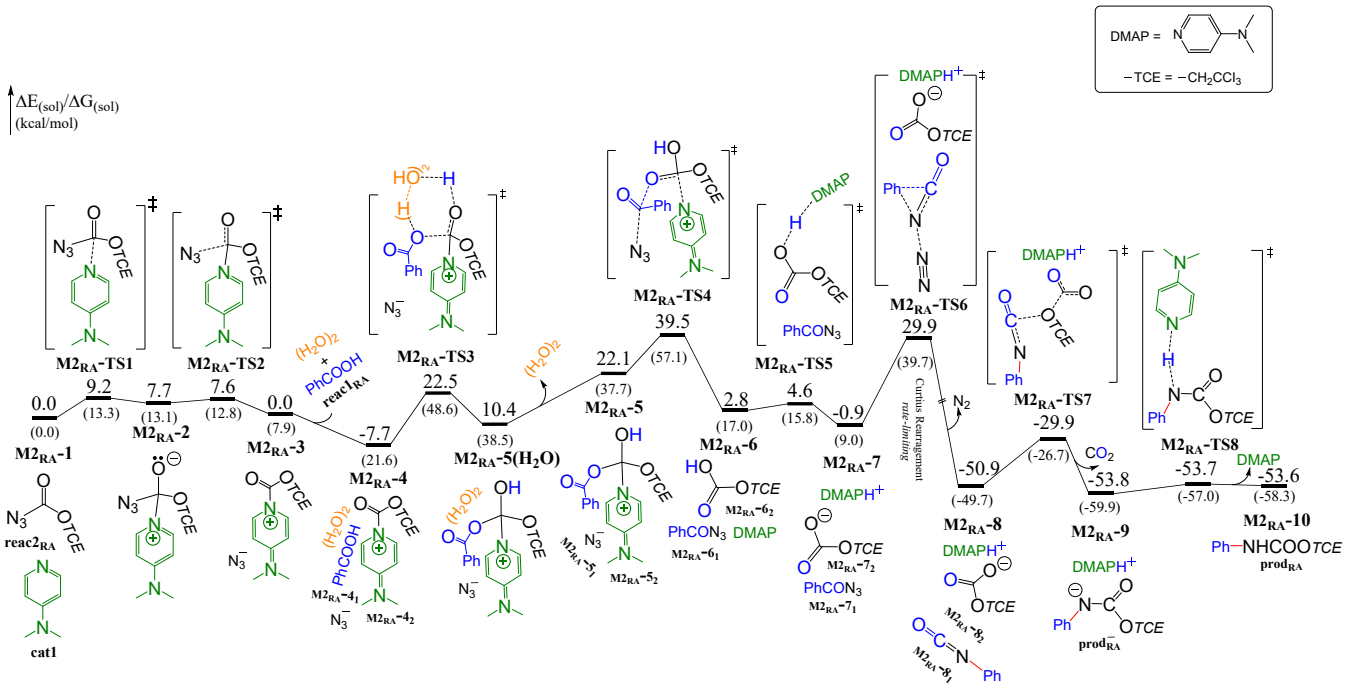


Fig. S15 (Free, in parentheses) Energy profile of DMAP-catalyzed C-N DCC reaction, assuming carboxylic acid as the carbon source (under neutral condition)

S5 Curtius Rearrangement

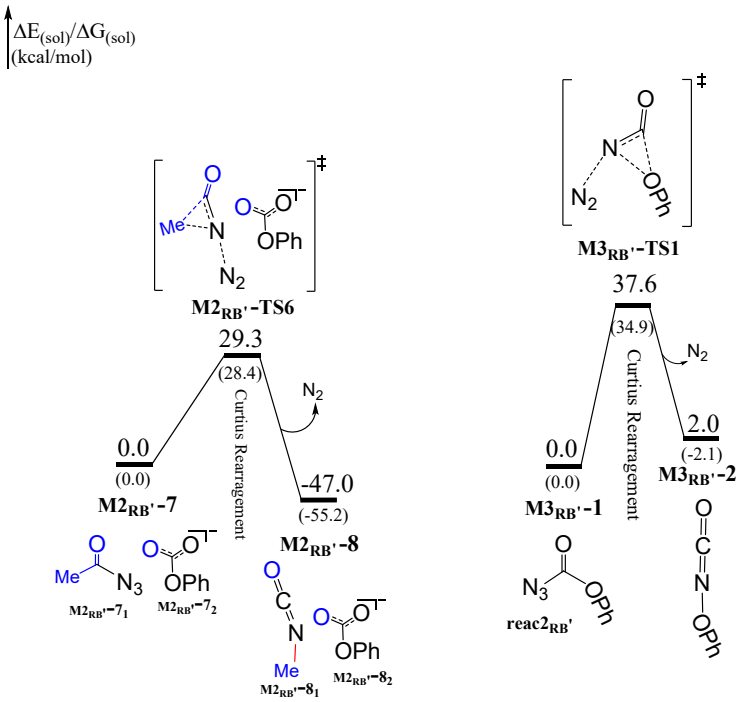


Fig. S16 (Free, in parentheses) Energy profiles of the Curtius Rearrangement of DMAP-catalyzed (left) and catalyst-free (right) C(sp^3)-N DCC reaction, assuming carboxylic acid as the carbon source

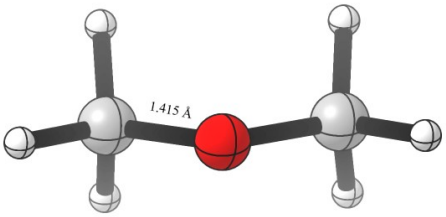


Fig. S17 Optimized Structures of methoxymethane, aiming to provide a benchmark for C-O sing bond

S6 Coordinates

DMAP

C	1.956204	-1.135775	-0.004552
C	0.570510	-1.200907	-0.004709
C	-0.185148	0.000019	-0.000071
C	0.570532	1.200930	0.004648
C	1.956239	1.135760	0.004558
N	2.677849	-0.000011	0.000046
H	2.524957	-2.065024	-0.008691
H	0.087685	-2.169933	-0.009891
H	0.087728	2.169963	0.009895
H	2.525006	2.065001	0.008843
N	-1.550583	0.000001	-0.000116
C	-2.283486	1.260338	-0.008067
H	-2.038640	1.865723	-0.889827
H	-3.352292	1.049287	-0.029634
H	-2.071448	1.860078	0.886322
C	-2.283450	-1.260351	0.008173
H	-2.038616	-1.865563	0.890056
H	-3.352253	-1.049292	0.029642
H	-2.071398	-1.860256	-0.886094

$DMAPH^+$

C	1.887373	1.181611	0.006962
C	0.520159	1.216722	0.006377
C	-0.232607	0.000012	-0.000382
C	0.520171	-1.216704	-0.006995
C	1.887381	-1.181612	-0.006871
N	2.552558	0.000001	0.000195
H	2.496711	2.076369	0.013434
H	0.032070	2.180595	0.014135
H	0.032069	-2.180568	-0.015073
H	2.496739	-2.076359	-0.013100
N	-1.576196	-0.000001	-0.000241
C	-2.319425	1.263209	-0.012019
H	-2.062583	1.862554	-0.891566
H	-3.384574	1.042636	-0.045967
H	-2.113533	1.850959	0.888996
C	-2.319380	-1.263235	0.012509
H	-2.062759	-1.861774	0.892684
H	-3.384550	-1.042673	0.045839
H	-2.113197	-1.851790	-0.887904
H	3.567041	0.000039	0.001363

PhCOOH

C	0.449519	1.203958	-0.000141
C	-0.221977	-0.028236	0.000051
C	0.512644	-1.223076	0.000203
C	1.904874	-1.187243	0.000057
C	2.571392	0.041855	-0.000054
C	1.843258	1.234867	-0.000063
H	-0.116659	2.128507	-0.000442
H	-0.019705	-2.168240	0.000422
H	2.470384	-2.114180	0.000167
H	3.657277	0.069879	-0.000028
H	2.361467	2.189062	-0.000274
O	-2.337800	-1.160513	-0.000385
C	-1.706055	-0.117984	0.000076
O	-2.312339	1.088889	0.000334
H	-3.273589	0.923122	-0.000227

H_2O

O	0.000000	0.000000	0.120415
H	0.000000	-0.757293	-0.481659
H	0.000000	0.757293	-0.481659

N_2

N	0.000000	0.000000	0.552500
N	0.000000	0.000000	-0.552500

CO_2

C	0.000000	0.000000	-0.000018
O	0.000000	0.000000	1.169012
O	0.000000	0.000000	-1.168998

$Cu(DMAP)^{2+}$

Cu	3.202951	-0.000017	-0.000041
C	0.536365	1.166063	0.011522
C	-0.837239	1.216706	0.010932
C	-1.583160	0.000059	0.000062
C	-0.837271	-1.216604	-0.010878
C	0.536329	-1.166000	-0.011346
N	1.235383	0.000025	0.000038
H	1.121248	2.078511	0.021940
H	-1.325512	2.181190	0.023767
H	-1.325591	-2.181067	-0.024065
H	1.121176	-2.078471	-0.021762
N	-2.934659	0.000002	0.000134
C	-3.684564	-1.260373	0.020496
H	-3.405519	-1.852471	0.896892
H	-4.747314	-1.036462	0.064604
H	-3.474743	-1.838822	-0.884912
C	-3.684788	1.260253	-0.020639
H	-3.406975	1.851378	-0.898109
H	-4.747553	1.036103	-0.063058
H	-3.473908	1.839795	0.883800

$Cu(DMAP)_2^{2+}$

Cu	-0.000001	-0.000597	-0.341979
C	2.710253	-0.952421	-0.813724
C	4.082747	-0.962319	-0.721662
C	4.749864	-0.006326	0.100454
C	3.913197	0.922010	0.787241
C	2.547999	0.857392	0.635676
N	1.934553	-0.068815	-0.140826
H	2.191203	-1.672318	-1.438625
H	4.633079	-1.705919	-1.282009
H	4.326102	1.687867	1.429643
H	1.900392	1.561338	1.149128
N	6.095473	0.022598	0.215783
C	6.746061	1.032797	1.051197
H	6.388749	0.978893	2.085127
H	7.819817	0.851573	1.051218
H	6.564350	2.044851	0.670684
C	6.922849	-0.916310	-0.542481
H	6.775952	-0.794685	-1.621727
H	7.970406	-0.725850	-0.314898
H	6.694109	-1.953391	-0.273425
C	-2.548390	-0.857497	0.636410
C	-3.913620	-0.921391	0.787961
C	-4.749874	0.006678	0.100329
C	-4.082321	0.961790	-0.722462
C	-2.709823	0.951217	-0.814454
N	-1.934531	0.067770	-0.140861
H	-1.901106	-1.561268	1.150508
H	-4.326892	-1.686454	1.431070
H	-4.632304	1.705213	-1.283387
H	-2.190437	1.670421	-1.439872
N	-6.095513	-0.021750	0.215523
C	-6.922498	0.917092	-0.543230
H	-6.775450	0.794986	-1.622405
H	-7.970155	0.727010	-0.315766
H	-6.693526	1.954217	-0.274549
C	-6.746421	-1.030879	1.051959
H	-6.389574	-0.975704	2.086000
H	-7.820182	-0.849702	1.051268
H	-6.564514	-2.043397	0.672797

Cu(DMAP)(OAc)$^+$

Cu	1.825417	-0.110547	-0.535708
C	-0.788395	1.152452	-0.250439
C	-2.156298	1.216174	-0.110412
C	-2.914096	0.018505	0.055254
C	-2.166497	-1.193582	0.089720
C	-0.799481	-1.162575	-0.061513
N	-0.098698	-0.014900	-0.244590
H	-0.204599	2.057693	-0.382813
H	-2.632628	2.186533	-0.130489
H	-2.650134	-2.151279	0.229339
H	-0.222097	-2.081348	-0.041413
N	-4.260577	0.026523	0.175491
C	-4.987488	-1.226511	0.380105
H	-4.692288	-1.711295	1.318095
H	-6.054369	-1.013118	0.425163
H	-4.811634	-1.926081	-0.444173
C	-5.002840	1.286922	0.142448
H	-4.798118	1.841316	-0.779749
H	-6.069323	1.069804	0.178480
H	-4.749854	1.926125	0.996546
C	3.989040	0.067555	0.392309
O	2.988815	0.261800	1.147515
O	3.740431	-0.205741	-0.825449
C	5.391532	0.161724	0.881829
H	5.914491	-0.776361	0.662719
H	5.904612	0.966066	0.341141
H	5.416919	0.363977	1.954020

methoxymethane

C	1.171829	0.197145	-0.000011
O	0.000080	-0.595880	-0.000020
C	-1.172002	0.197174	-0.000010
H	-1.232893	0.839819	-0.892610
H	-1.230988	0.842575	0.890747
H	-2.029350	-0.482015	0.002016
H	2.029548	-0.481677	0.000839
H	1.232446	0.840646	-0.892061
H	1.231629	0.841776	0.891357

$M1_{RA}$-1/$M2_{RA'}$-1/ $M1_{RA'}$-1/ $M2_{RA}$-1

C	-1.634309	2.110507	-0.187616
O	-1.098871	2.282228	-1.260732
N	-1.854042	3.084405	0.812939
N	-1.445726	4.224193	0.508221
N	-1.123638	5.297064	0.359153
O	-2.133633	0.957909	0.275975
C	-1.975436	-0.170811	-0.597547
C	-2.853359	-1.295083	-0.053262
H	-0.922344	-0.486591	-0.600501
H	-2.300528	0.080217	-1.609303
Cl	-2.346996	-1.760804	1.612860
Cl	-4.590546	-0.809353	-0.024779
Cl	-2.649814	-2.708594	-1.153065
C	2.029954	-1.558239	0.218901
C	3.405043	-1.540104	0.393102
C	4.150674	-0.414672	-0.045446
C	3.396397	0.629351	-0.642139
C	2.021570	0.497374	-0.760632
N	1.313409	-0.569925	-0.347198
H	1.465843	-2.425478	0.558391
H	3.887254	-2.387035	0.864400
H	3.872762	1.530319	-1.007593
H	1.447047	1.302493	-1.215212
N	5.505561	-0.340302	0.097787
C	6.225050	0.847800	-0.346850
H	5.874356	1.750399	0.169072
H	7.285438	0.723672	-0.128769
H	6.114674	1.008058	-1.426732
C	6.238514	-1.435531	0.722204
H	6.096030	-2.377649	0.178917
H	7.302441	-1.200485	0.716094
H	5.928577	-1.591848	1.763429

$M1_{RA}$-TS1/ $M2_{RA'}$-TS1/ $M1_{RA'}$-TS1/ $M2_{RA}$-TS1

C	0.445442	1.591359	0.226466
O	0.531808	2.018915	1.374723
N	0.243415	2.507527	-0.938825
N	-0.327045	3.554677	-0.633104
N	-0.844936	4.552251	-0.440397
O	1.328587	0.641936	-0.303524
C	-1.485301	-0.118903	-0.948921
C	-2.691523	-0.780043	-1.029580
C	-3.632066	-0.670794	0.035694
C	-3.237610	0.133325	1.142672
C	-2.005010	0.751317	1.133998
N	-1.143033	0.633548	0.112932
H	-0.753369	-0.181815	-1.747668
H	-2.902606	-1.370988	-1.910794
H	-3.884952	0.271585	1.998263
H	-1.661598	1.369673	1.958079
N	-4.833722	-1.297075	-0.002854
C	-5.781026	-1.139349	1.098478
H	-6.060873	-0.088738	1.238811
H	-6.683169	-1.706233	0.873230
H	-5.365473	-1.515477	2.040647
C	-5.203789	-2.115330	-1.155482
H	-4.503780	-2.946780	-1.296810
H	-6.196697	-2.531061	-0.989818
H	-5.229058	-1.522728	-2.077614
C	1.846189	-0.249853	0.661065
H	1.132987	-1.051695	0.886404
H	2.097742	0.276671	1.585317
C	3.118338	-0.887549	0.099764
Cl	2.774816	-1.796404	-1.421266
Cl	3.748426	-2.038244	1.341579
Cl	4.372233	0.362248	-0.237773

$M1_{RA}$-2/ $M2_{RA'}$-2/ $M1_{RA'}$-2/ $M2_{RA}$-2

C	-0.191553	1.293240	-0.313225
O	-0.375047	1.918337	-1.366292
N	-0.219220	2.211860	1.064264
N	-0.078569	3.394983	0.806720
N	0.041780	4.515731	0.581901
O	-1.064213	0.218594	0.056033
C	1.529849	-0.147272	0.895088
C	2.763948	-0.729939	1.006093
C	3.743610	-0.545463	-0.017462
C	3.352328	0.268647	-1.122057
C	2.096412	0.816230	-1.165606
N	1.195412	0.611996	-0.178515
H	0.767665	-0.266476	1.652777
H	2.970160	-1.326087	1.884195
H	4.026689	0.467671	-1.943385
H	1.744861	1.437617	-1.979556
N	4.965525	-1.107246	0.057655
C	5.944696	-0.892012	-1.009245
H	6.183419	0.171472	-1.118611
H	6.859967	-1.426077	-0.760346
H	5.573530	-1.269050	-1.968413
C	5.331443	-1.939462	1.205474
H	4.665100	-2.803931	1.295786
H	6.348334	-2.302407	1.066891
H	5.292486	-1.366975	2.138656
C	-2.422375	0.527036	-0.140347
H	-2.586377	0.974127	-1.126055
H	-2.799025	1.211788	0.630034
C	-3.231343	-0.768104	-0.057179
Cl	-2.713323	-1.936994	-1.329424
Cl	-4.972305	-0.356155	-0.308378
Cl	-3.041978	-1.547191	1.561139

$M1_{RA}$-TS2/ $M2_{RA'}$-TS2/ $M1_{RA'}$-TS2/ $M2_{RA}$-TS2

C	-0.145542	1.159724	-0.459447
O	-0.300260	1.942251	-1.394268
N	-0.220548	2.005430	1.157016
N	-0.105353	3.196218	0.976777
N	0.000396	4.333473	0.788594

O	-1.044879	0.113955	-0.199802
C	1.482972	-0.389343	0.671676
C	2.729999	-0.928472	0.825809
C	3.800242	-0.537075	-0.037362
C	3.477049	0.423414	-1.043387
C	2.204558	0.917235	-1.144158
N	1.216410	0.518340	-0.305291
H	0.655677	-0.656606	1.313534
H	2.878755	-1.647219	1.619249
H	4.219209	0.776988	-1.745269
H	1.908021	1.645557	-1.887410
N	5.039762	-1.042211	0.093231
C	6.118315	-0.597683	-0.792633
H	6.272576	0.483626	-0.714200
H	7.039898	-1.099364	-0.503396
H	5.899821	-0.847178	-1.836602
C	5.332718	-2.034859	1.129898
H	4.698215	-2.919921	1.017267
H	6.372415	-2.342977	1.037320
H	5.181584	-1.617676	2.131532
C	-2.393999	0.508546	-0.334036
H	-2.601093	0.876687	-1.343299
H	-2.646424	1.288318	0.393296
C	-3.282014	-0.706925	-0.067314
Cl	-2.930982	-2.033724	-1.238466
Cl	-4.999463	-0.185233	-0.263840
Cl	-3.044731	-1.331396	1.608423

$M1_{RA}$-3/ $M2_{RA'}$-3/ $M1_{RA'}$-3/ $M2_{RA}$-3

C	-0.178648	0.831967	-0.901005
O	-0.338113	1.800772	-1.600188
N	-0.114131	2.177613	1.578451
N	0.734199	2.909179	1.181331
N	1.584045	3.629558	0.781012
O	-1.133891	0.046379	-0.395919
C	-2.456737	0.590818	-0.481281
C	-3.435424	-0.480320	-0.000151
H	-2.693938	0.860190	-1.512091
H	-2.524433	1.470232	0.163928
Cl	-3.347120	-1.943894	-1.048335
Cl	-3.096029	-0.953922	1.702825
Cl	-5.088106	0.229965	-0.104818
C	1.311607	-0.781879	0.218979
C	2.556866	-1.261559	0.477302
C	3.716109	-0.643101	-0.098384
C	3.475360	0.492295	-0.936464
C	2.207438	0.933761	-1.159509
N	1.120439	0.303759	-0.603329
H	0.424315	-1.224730	0.645366
H	2.642045	-2.118231	1.130603
H	4.288078	1.029648	-1.404218
H	1.981979	1.788016	-1.781056
N	4.949256	-1.099372	0.139321
C	6.115745	-0.448466	-0.468996
H	6.214915	0.582955	-0.116151
H	7.010532	-1.000513	-0.188957
H	6.034021	-0.445797	-1.559946
C	5.161198	-2.258170	1.015188
H	4.676990	-3.149993	0.605257
H	6.229699	-2.446763	1.093207
H	4.765440	-2.065996	2.016900

$M1_{RA}$-4 (oH2O)/ $M2_{RA}$-4 (oH2O)

C	0.693473	-0.086355	-0.379116
O	-2.604595	1.880688	-0.776010
O	-0.075217	0.663164	-0.944533
H	-1.792236	1.337020	-0.851328
O	0.485480	-1.374430	-0.126806
C	-0.779896	-1.906311	-0.570233
C	2.339286	1.642218	-0.167530
C	3.535841	2.124301	0.261480
C	4.457771	1.282809	0.962149
C	4.029074	-0.067786	1.203798
C	2.819318	-0.501303	0.769895
N	1.957363	0.338400	0.092631
H	1.615102	2.245756	-0.691448
H	3.770262	3.156363	0.046129
H	4.659407	-0.773286	1.726015
H	2.478176	-1.512219	0.934796
N	5.645330	1.727520	1.377012
C	6.559838	0.853255	2.122827
H	6.899561	0.019687	1.499774
H	7.425814	1.435540	2.430530
H	6.071438	0.457285	3.017223
C	6.083379	3.088650	1.044342
H	5.435105	3.833245	1.516667
H	7.099430	3.228483	1.406897
H	6.070476	3.235002	-0.039900
C	-3.524862	1.185109	-0.093047
O	-3.327491	0.047984	0.315311
C	-4.796539	1.928254	0.116361
N	3.007208	1.110543	-2.966268
N	4.133642	1.398657	-2.730575
N	5.256410	1.688645	-2.483480
H	-1.604694	-1.321648	-0.151751
H	-0.822081	-1.890200	-1.661613
C	-0.861399	-3.351271	-0.078211
Cl	-2.442108	-4.005630	-0.638109
Cl	-0.785333	-3.420672	1.719816
Cl	0.475483	-4.345052	-0.764037
C	-4.971754	3.241045	-0.346987
C	-5.838794	1.285219	0.800355
H	-5.689970	0.270405	1.153501
H	-4.166951	3.739742	-0.875017
C	-7.044330	1.947594	1.019045
C	-6.179927	3.900417	-0.125228
H	-7.849141	1.446716	1.548569
C	-7.215883	3.255825	0.556393
H	-8.155827	3.772731	0.727373
H	-6.313275	4.916770	-0.483479

$M1_{RA}$-TS3 (oH2O)/ $M2_{RA}$-TS3 (oH2O)

C	-0.060935	0.535579	-0.845333
O	0.934323	-1.435897	-0.684750
O	0.190140	0.361332	-2.120955
H	0.591297	-0.557259	-2.137641
O	0.583391	1.414512	-0.142826
C	1.901797	1.841314	-0.585540
C	-2.185518	-0.530138	-1.118390
C	-3.361550	-0.977512	-0.609343
C	-3.713173	-0.743273	0.759205
C	-2.725363	-0.069594	1.565724
C	-1.557687	0.348122	1.029752
N	-1.264225	0.135918	-0.312841
H	-1.893146	-0.693899	-2.141983
H	-4.027674	-1.503827	-1.276658
H	-2.898672	0.136870	2.612336
H	-0.803780	0.858173	1.610802
N	-4.881340	-1.134103	1.261828
C	-5.207016	-0.950865	2.683303
H	-5.415657	0.101529	2.902052
H	-6.091529	-1.542163	2.912861
H	-4.387325	-1.298371	3.314632
C	-5.922945	-1.673838	0.376876
H	-5.640379	-2.661569	-0.000175
H	-6.848607	-1.763781	0.941218
H	-6.080902	-0.991035	-0.463175
C	2.103110	-1.720680	-0.202831
O	2.930396	-0.889670	0.212832
C	2.447715	-3.192264	-0.153321
N	-3.065746	1.839843	-2.350867
N	-4.133533	1.669705	-1.863153
N	-5.191373	1.478689	-1.365043
H	2.574485	0.985995	-0.432009
H	1.855450	2.153844	-1.628486
C	2.309787	3.020529	0.293760
Cl	3.939402	3.532938	-0.274525
Cl	2.401391	2.539212	2.024807
Cl	1.153255	4.391587	0.123306
C	1.534836	-4.167349	-0.578759

C	3.702081	-3.591630	0.329038
H	4.400982	-2.829225	0.656558
H	0.565149	-3.853540	-0.949540
C	4.038857	-4.943573	0.386343
C	1.871264	-5.520387	-0.522252
H	5.012965	-5.244406	0.761841
C	3.123523	-5.910938	-0.039628
H	3.385219	-6.964484	0.004681
H	1.158126	-6.269972	-0.853797

$M1_{RA}$-5 (oH2O)/ $M1_{RA}$-5 /$M2_{RA}$-5 (oH2O)/ $M2_{RA}$-5

C	-0.60973	-0.01299	-0.98428
O	-1.7934	0.673442	-0.6527
O	-0.49838	-0.33875	-2.30403
H	-0.86317	0.377033	-2.85518
O	-0.53345	-1.13237	-0.18543
C	0.403488	-2.14118	-0.57667
C	1.446861	1.357342	-1.4549
C	2.433382	2.222842	-1.07284
C	2.481916	2.733199	0.25974
C	1.439846	2.29588	1.139176
C	0.482891	1.430328	0.699047
N	0.472248	0.963774	-0.5855
H	1.403941	0.945716	-2.45149
H	3.175052	2.49556	-1.80914
H	1.393181	2.622701	2.168359
H	-0.30672	1.073168	1.345917
N	3.448992	3.569415	0.664528
C	3.46155	4.095094	2.032795
H	3.631136	3.296349	2.763273
H	4.265728	4.823491	2.119329
H	2.517671	4.596217	2.266401
C	4.553478	3.911703	-0.23737
H	4.194585	4.479841	-1.10198
H	5.273429	4.521352	0.305159
H	5.055488	3.004647	-0.58904
C	-3.02881	0.055338	-0.84048
O	-3.15683	-1.00706	-1.39855
C	-4.12616	0.884711	-0.28903
N	3.376354	-1.16751	-1.82216
N	4.213521	-0.57495	-1.22266
N	5.054003	0.015059	-0.63285
H	0.008428	-2.71352	-1.42002
H	1.384799	-1.72134	-0.84212
C	0.583605	-3.09009	0.608789
Cl	1.712476	-4.39505	0.084453
Cl	-0.98662	-3.83083	1.099099
Cl	1.289719	-2.22855	2.026066
C	-3.90103	2.099371	0.378276
C	-5.43698	0.407279	-0.45192
H	-5.59737	-0.5324	-0.96941
H	-2.89203	2.47323	0.50569
C	-6.51111	1.137063	0.048351
C	-4.98149	2.824445	0.877119
H	-7.52337	0.765932	-0.07858
C	-6.28423	2.345891	0.713592
H	-7.12284	2.914569	1.104628
H	-4.80693	3.762805	1.394401

$M1_{RA}$-TS3 (1H2O)/ $M2_{RA}$-TS3 (1H2O)

C	0.113273	0.373463	0.781287
O	-1.360131	-1.081304	0.695438
O	-0.050261	0.628660	2.020083
H	-0.208662	-0.281517	2.633551
O	-0.272779	1.226280	-0.144933
C	-1.501654	1.945742	0.057069
C	2.225233	-0.707932	1.239491
C	3.310129	-1.425264	0.840742
C	3.444354	-1.862483	-0.514996
C	2.350650	-1.555242	-1.395215
C	1.281258	-0.845867	-0.953815
N	1.209050	-0.408765	0.353164
H	2.114689	-0.341079	2.246723
H	4.071653	-1.634965	1.576747
H	2.350399	-1.879031	-2.426525
H	0.411761	-0.630057	-1.563320
N	4.521437	-2.529781	-0.935536
C	4.622287	-3.002176	-2.321783
H	4.670121	-2.160434	-3.020040
H	5.529635	-3.593929	-2.422583
H	3.766632	-3.632697	-2.578392
C	5.648897	-2.766957	-0.025970
H	5.361883	-3.441562	0.786882
H	6.462314	-3.221066	-0.587839
H	5.998536	-1.820398	0.396805
C	-2.031244	-1.383150	-0.380573
O	-1.765232	-0.961845	-1.515407
N	3.379970	1.960522	1.499819
N	4.369224	1.561902	0.979271
N	5.353097	1.154330	0.458622
H	-1.068068	-1.730665	2.310148
O	-0.537385	-1.481760	3.111629
H	-1.149787	-1.431098	3.866316
C	-3.210146	-2.305237	-0.179714
C	-3.764240	-2.539154	1.086399
C	-3.779786	-2.924207	-1.301704
C	-4.865225	-3.384471	1.228872
H	-3.345082	-2.045772	1.956561
C	-4.873256	-3.776954	-1.158590
H	-3.351613	-2.727917	-2.278907
C	-5.418788	-4.008197	0.107734
H	-5.292501	-3.553979	2.213041
H	-5.302544	-4.258601	-2.032510
H	-6.273403	-4.669338	0.219749
H	-2.267739	1.453193	-0.544085
H	-1.777672	1.956733	1.110875
C	-1.307316	3.382809	-0.434533
Cl	-0.019709	4.211231	0.508501
Cl	-2.877499	4.232998	-0.193752
Cl	-0.873982	3.411544	-2.181411

$M1_{RA}$-5 (1H2O)/ $M2_{RA}$-5 (1H2O)

C	-0.378150	-0.072395	0.849090
O	-0.578443	0.267501	2.140195
N	2.208485	2.276200	-2.356993
N	3.351923	1.952934	-2.367606
N	4.493186	1.635539	-2.390087
O	-0.549871	0.956641	-0.072821
C	0.009438	2.232733	0.244636
C	-1.063556	3.318745	0.089390
H	0.820482	2.449058	-0.462018
H	0.380332	2.263989	1.270416
Cl	-0.259271	4.906597	0.389178
Cl	-2.404755	3.105005	1.277316
Cl	-1.756511	3.307887	-1.572953
C	1.827180	-0.369994	-0.304643
C	3.096555	-0.871493	-0.370800
C	3.613703	-1.689985	0.679150
C	2.717463	-1.965937	1.759712
C	1.464378	-1.427352	1.774447
N	1.017136	-0.622030	0.764815
H	1.425831	0.255888	-1.087788
H	3.693850	-0.604575	-1.231230
H	3.011106	-2.589594	2.592120
H	0.773329	-1.601417	2.586832
N	4.866163	-2.168634	0.656054
C	5.760059	-1.859037	-0.464939
H	5.835416	-0.778212	-0.617696
H	6.751971	-2.246802	-0.240376
H	5.403516	-2.321651	-1.391658
C	5.357025	-3.021715	1.742729
H	4.747104	-3.925317	1.840941
H	6.379909	-3.318697	1.520067
H	5.350252	-2.483764	2.696456
C	-3.457766	-2.781135	0.235105
C	-2.528817	-2.615700	-0.805001
C	-2.675998	-3.341909	-1.997369
C	-3.739539	-4.227215	-2.147461
C	-4.662559	-4.391612	-1.110135

C	-4.520184	-3.669215	0.077719
H	-3.350587	-2.220590	1.156520
H	-1.952140	-3.204149	-2.793281
H	-3.850588	-4.787759	-3.070545
H	-5.492339	-5.082440	-1.227706
H	-5.238434	-3.796677	0.881839
O	-0.557623	-1.493752	-1.579881
C	-1.375270	-1.687297	-0.707857
O	-1.332344	-1.073874	0.524331
H	-3.720559	0.309683	2.094045
H	-1.557228	0.222916	2.362835
O	-3.118459	0.041713	2.806649
H	-3.390211	0.567978	3.576313

$M1_{RA}$-4 (2H2O)/ $M2_{RA}$-4 (2H2O)

C	0.379822	0.888871	0.980141
O	-2.135575	-0.833018	0.548278
O	0.101265	1.016300	2.152186
H	-2.208682	-1.543645	1.261639
O	-0.171307	1.533712	-0.041982
C	-1.329001	2.347357	0.215774
C	2.205069	-0.596745	1.471786
C	3.187354	-1.462919	1.119073
C	3.409833	-1.799795	-0.259429
C	2.577356	-1.123109	-1.214571
C	1.610822	-0.259929	-0.810764
N	1.401623	0.008380	0.527595
H	2.010014	-0.326398	2.499294
H	3.790787	-1.887356	1.908099
H	2.691312	-1.287705	-2.276262
H	0.964903	0.249280	-1.509908
N	4.335297	-2.682076	-0.629835
C	4.586425	-2.952110	-2.052747
H	4.996903	-2.059000	-2.534816
H	5.306519	-3.764035	-2.130271
H	3.665255	-3.256506	-2.555810
C	5.226983	-3.297776	0.363735
H	4.648248	-3.773378	1.159339
H	5.823245	-4.061101	-0.131677
H	5.891168	-2.538751	0.790250
C	-3.042969	-0.878881	-0.430036
O	-3.195824	0.089510	-1.163769
C	-3.838372	-2.134342	-0.613128
O	-2.067877	-2.463809	2.576043
H	-1.555053	-1.924861	3.233160
H	-2.936053	-2.610653	2.981333
O	-0.625036	-0.866591	4.209949
H	-0.356040	-0.152291	3.605601
H	-1.179983	-0.432015	4.875955
N	6.453449	0.008950	0.465776
N	6.182960	0.154545	-0.680715
N	5.915305	0.313894	-1.825881
C	-5.062652	-2.044840	-1.293691
C	-3.379659	-3.386665	-0.177783
H	-5.402089	-1.074341	-1.639643
H	-2.428525	-3.476277	0.334768
C	-5.828096	-3.186866	-1.515517
C	-4.142748	-4.530685	-0.414650
H	-6.779783	-3.108019	-2.032566
C	-5.368217	-4.432623	-1.077150
H	-5.961673	-5.324589	-1.255865
H	-3.778084	-5.498360	-0.083343
H	-2.151884	1.902559	-0.349690
H	-1.556529	2.359919	1.281258
C	-1.056501	3.775080	-0.264835
Cl	-0.674813	3.800390	-2.024657
Cl	-2.556163	4.725907	0.035988
Cl	0.314959	4.509508	0.645592

$M1_{RA}$-TS3 (2H2O)/ $M2_{RA}$-TS3 (2H2O)

C	0.465398	-0.398459	0.757486
O	1.283945	1.203251	0.497307
O	0.664313	-0.624588	1.970963
H	2.756489	1.541390	1.365920
O	0.974783	-1.190315	-0.228775
C	2.325552	-1.600199	-0.095618
C	-1.722423	0.469400	1.353250
C	-3.010638	0.827242	1.093592
C	-3.564942	0.659179	-0.216644
C	-2.694809	0.078945	-1.192322
C	-1.408435	-0.248836	-0.876852
N	-0.915042	-0.062729	0.385815
H	-1.273874	0.574709	2.330697
H	-3.596178	1.232342	1.906327
H	-3.028461	-0.116086	-2.201458
H	-0.725385	-0.665369	-1.598815
N	-4.822029	1.021148	-0.505048
C	-5.395585	0.745669	-1.826894
H	-5.548364	-0.330687	-1.963475
H	-6.356696	1.251683	-1.901844
H	-4.747135	1.127763	-2.619032
C	-5.711593	1.527669	0.547096
H	-5.270064	2.396679	1.042564
H	-6.650097	1.835743	0.089681
H	-5.914059	0.744990	1.287068
C	1.221787	1.849671	-0.666144
O	0.895083	1.334613	-1.729735
C	1.588538	3.305007	-0.579626
O	3.492628	1.570241	2.033085
H	3.073164	0.625216	2.938607
H	4.308017	1.327640	1.562235
O	2.510850	-0.100156	3.517106
H	1.723930	-0.383508	2.875791
H	3.059143	-0.877046	3.734926
N	-5.867710	-2.605711	-0.432649
N	-5.770066	-2.193145	0.675596
N	-5.672779	-1.793743	1.789535
C	1.906624	3.986320	-1.763997
C	1.583353	4.001921	0.637610
H	1.895587	3.441172	-2.701966
H	1.317269	3.485264	1.553006
C	2.232429	5.340521	-1.729478
C	1.899212	5.360632	0.668263
H	2.485653	5.860412	-2.648855
C	2.228382	6.030124	-0.512828
H	2.477710	7.087058	-0.486782
H	1.885221	5.896509	1.612773
H	2.962089	-0.967923	-0.720504
H	2.656749	-1.552056	0.942247
C	2.452662	-3.053070	-0.569903
Cl	1.924790	-3.219730	-2.283773
Cl	4.192851	-3.509529	-0.437908
Cl	1.464522	-4.149058	0.460893

$M1_{RA}$-5 (2H2O)/ $M2_{RA}$-5 (2H2O)

C	-0.256794	0.094593	0.626550
O	-1.157997	-1.021202	0.508134
O	-0.266575	0.449310	1.922752
H	-4.854156	-1.016453	1.361048
O	-0.593365	1.110175	-0.262596
C	-1.813604	1.785198	0.000871
C	1.779562	-1.164452	1.106718
C	3.034401	-1.624996	0.837732
C	3.711997	-1.232619	-0.360800
C	3.003166	-0.324621	-1.208396
C	1.741842	0.090092	-0.891894
N	1.126537	-0.317610	0.256054
H	1.249830	-1.434555	2.009560
H	3.497155	-2.281079	1.560735
H	3.439336	0.049047	-2.123562
H	1.182645	0.758992	-1.526279
N	4.936337	-1.682951	-0.667623
C	5.644565	-1.163323	-1.843183
H	5.830090	-0.089447	-1.733299
H	6.598924	-1.678998	-1.931872
H	5.070297	-1.344688	-2.756443
C	5.659526	-2.568264	0.251969
H	5.052517	-3.440629	0.508540
H	6.565038	-2.917865	-0.241217
H	5.934804	-2.030068	1.165897

C	-1.360215	-1.669365	-0.687718
O	-0.761447	-1.396448	-1.705297
C	-2.389527	-2.731665	-0.556295
O	-4.712370	-0.144941	1.764571
H	-3.245935	-0.150776	2.668059
H	-4.669139	0.464260	1.010728
O	-2.406091	-0.198230	3.190346
H	-1.122025	0.161936	2.396965
H	-2.549448	0.350089	3.976925
N	5.748282	1.795403	0.203211
N	5.773437	1.127515	1.183928
N	5.796634	0.471248	2.172668
C	-2.730717	-3.453246	-1.710263
C	-3.016693	-3.027841	0.665640
H	-2.235759	-3.218547	-2.646448
H	-2.742016	-2.487648	1.564065
C	-3.694955	-4.455970	-1.645953
C	-3.982051	-4.032149	0.722444
H	-3.956756	-5.012056	-2.540860
C	-4.323218	-4.744503	-0.431074
H	-5.075683	-5.526141	-0.382091
H	-4.464120	-4.262228	1.667616
H	-2.644720	1.299472	-0.520878
H	-2.021761	1.824280	1.072312
C	-1.693363	3.225663	-0.510866
Cl	-1.380262	3.252945	-2.285561
Cl	-3.263837	4.047983	-0.174262
Cl	-0.368164	4.100446	0.334331

$M1_{RA}$-TS3 (3H2O)/ $M2_{RA}$-TS3 (3H2O)

C	0.253803	-0.242392	0.614767
O	1.156845	1.200489	0.356110
O	0.538114	-0.534464	1.790578
H	3.326719	-0.001226	3.055138
O	0.559764	-1.078185	-0.444226
C	1.897765	-1.531955	-0.506769
C	-1.894082	0.568564	1.448051
C	-3.177288	1.014231	1.316920
C	-3.773155	1.141510	0.022905
C	-2.951652	0.761595	-1.084236
C	-1.670815	0.328663	-0.887758
N	-1.139937	0.226215	0.365961
H	-1.408620	0.450241	2.406733
H	-3.724708	1.256696	2.216419
H	-3.319063	0.808454	-2.099629
H	-1.014268	0.061339	-1.701360
N	-5.028776	1.585590	-0.140527
C	-5.642730	1.601033	-1.472034
H	-5.738299	0.581508	-1.861684
H	-6.634330	2.043952	-1.394705
H	-5.051233	2.204231	-2.166727
C	-5.868264	1.883313	1.024337
H	-5.386747	2.619874	1.673774
H	-6.811483	2.301411	0.677375
H	-6.071653	0.970319	1.595027
C	1.348278	1.810487	-0.813709
O	1.012996	1.357296	-1.902153
C	2.035377	3.140931	-0.692317
O	3.557824	-0.921515	3.545590
H	2.686243	-1.570949	3.535647
H	4.300145	-1.355420	3.087313
O	1.497697	-2.252487	3.486831
H	0.993230	-1.768485	2.778116
H	1.586432	-3.176918	3.203234
N	-5.509812	-1.956989	-0.971427
N	-5.605847	-1.824087	0.204016
N	-5.699701	-1.705810	1.381398
C	2.595217	3.705454	-1.848012
C	2.107136	3.839986	0.521834
H	2.523843	3.162538	-2.784505
H	1.660163	3.419385	1.415309
C	3.234554	4.941938	-1.787365
C	2.739541	5.082581	0.577813
H	3.673622	5.368778	-2.684321
C	3.307661	5.632740	-0.573892
H	3.803276	6.598125	-0.527171
H	2.785756	5.621759	1.519376
H	2.472481	-0.904501	-1.194844
H	2.367525	-1.529078	0.479007
C	1.910915	-2.967397	-1.045010
Cl	1.161914	-3.046178	-2.681048
Cl	3.633657	-3.491636	-1.156159
Cl	1.020531	-4.082647	0.057817
O	2.962283	1.225835	2.468971
H	2.287042	1.154921	1.751588
H	3.710968	1.713017	2.087857

$M1_{RA}$-TS4/ $M2_{RA}$-TS4

C	0.187583	-0.286393	0.896085
O	0.355805	-0.862390	2.152906
N	-1.177294	2.760243	0.468548
N	-2.177553	2.713454	-0.219576
N	-3.126995	2.668427	-0.871752
O	0.965337	-0.943957	-0.091736
C	1.126873	-2.346990	0.000155
C	2.616082	-2.698518	-0.144276
H	0.591952	-2.849100	-0.812874
H	0.781416	-2.737390	0.959060
Cl	2.765080	-4.497982	-0.077294
Cl	3.260059	-2.114687	-1.724499
Cl	3.591112	-1.973047	1.185569
C	-2.220578	-0.304356	1.523558
C	-3.558607	-0.443753	1.281204
C	-4.021143	-0.860757	-0.005004
C	-3.013120	-1.081394	-0.990150
C	-1.690075	-0.908596	-0.683323
N	-1.286363	-0.551436	0.564547
H	-1.840242	-0.002901	2.489196
H	-4.246268	-0.239219	2.089594
H	-3.264500	-1.373887	-1.999959
H	-0.908912	-1.036500	-1.415962
N	-5.328667	-1.028673	-0.270037
C	-5.765092	-1.471731	-1.596350
H	-5.302264	-2.427694	-1.861743
H	-6.845266	-1.605152	-1.585393
H	-5.511792	-0.732944	-2.364562
C	-6.336218	-0.758089	0.758904
H	-6.276588	0.279044	1.104878
H	-7.324733	-0.921985	0.334050
H	-6.211749	-1.425105	1.618730
C	1.551915	3.697628	1.009991
C	1.241058	3.043539	-0.189250
C	1.982993	3.329007	-1.339025
C	3.028255	4.255116	-1.294323
C	3.336747	4.903847	-0.097441
C	2.595733	4.621172	1.055257
H	0.976477	3.482332	1.903819
H	1.730416	2.817302	-2.261973
H	3.598454	4.469606	-2.194080
H	4.147734	5.625896	-0.060347
H	2.830823	5.124000	1.989372
O	-0.164862	1.491894	-1.380102
C	0.111144	2.035268	-0.311357
O	0.493266	1.009079	0.943875
H	1.039199	-0.330256	2.594409

$M1_{RA}$-6/ $M2_{RA}$-6

C	-0.876702	-1.591199	1.639540
O	-1.372739	-0.738277	2.548008
N	3.247718	-0.532115	1.635194
N	2.310275	0.131744	2.103849
N	1.491287	0.711146	2.630168
O	-1.768188	-1.913605	0.689423
C	-3.043928	-1.254990	0.664044
C	-3.867675	-1.906598	-0.446209
H	-2.909207	-0.189293	0.438059
H	-3.570939	-1.386791	1.611188
Cl	-5.464939	-1.069293	-0.485545
Cl	-3.061106	-1.720147	-2.046597
Cl	-4.124737	-3.662607	-0.120107

C	-2.425464	3.045593	-0.069357
C	-1.705453	4.226838	-0.165063
C	-0.290439	4.177031	-0.264785
C	0.280988	2.878161	-0.258805
C	-0.544141	1.768557	-0.160755
N	-1.886304	1.812687	-0.065078
H	-3.510667	3.094819	0.006923
H	-2.238685	5.169211	-0.164027
H	1.350085	2.727509	-0.332543
H	-0.089506	0.780237	-0.162781
N	0.472703	5.304556	-0.360226
C	1.920052	5.197297	-0.501153
H	2.202063	4.655272	-1.413051
H	2.346964	6.198291	-0.555082
H	2.370877	4.681087	0.355161
C	-0.160859	6.617198	-0.402644
H	-0.760046	6.802779	0.496863
H	0.611426	7.384105	-0.457118
H	-0.815202	6.727170	-1.277273
C	5.334441	-2.035413	0.562777
C	4.468547	-1.341294	-0.297564
C	4.657865	-1.413763	-1.687616
C	5.701331	-2.171657	-2.209892
C	6.562835	-2.860732	-1.349931
C	6.378274	-2.791758	0.033632
H	5.190750	-1.982107	1.636167
H	3.981799	-0.873464	-2.341470
H	5.845283	-2.226281	-3.284554
H	7.377435	-3.451538	-1.758589
H	7.047446	-3.327089	0.700094
O	2.579651	0.118581	-0.498523
C	3.346231	-0.517350	0.205288
O	0.239802	-2.055986	1.642615
H	-0.659977	-0.536486	3.181685

$M1_{RA}$-TS5/ $M2_{RA}$-TS5

C	-1.462090	-1.711849	-0.783492
O	-1.429277	-2.980362	-0.560950
O	-2.565260	-1.064149	-0.261077
C	1.589275	3.000287	-0.154153
O	2.009738	1.863955	-0.293745
O	-0.652333	-1.018803	-1.391292
C	3.692807	-3.695647	-0.393920
C	4.852090	-3.113297	0.074882
C	4.908351	-1.702698	0.256353
C	3.724414	-0.980905	-0.062147
C	2.614035	-1.656900	-0.523174
N	2.581458	-2.994968	-0.694290
H	3.635935	-4.770533	-0.541419
H	5.703022	-3.744513	0.293751
H	3.665410	0.093199	0.048129
H	1.697666	-1.126721	-0.769332
N	6.027190	-1.080128	0.706967
C	6.043229	0.371487	0.871275
H	5.316084	0.700805	1.623012
H	7.035784	0.680194	1.196783
H	5.818754	0.881757	-0.072221
C	7.214455	-1.857373	1.052342
H	7.604372	-2.402277	0.184447
H	7.990239	-1.180295	1.407708
H	7.001653	-2.581410	1.847776
H	-0.463877	-3.502957	-1.070952
H	1.449695	-3.583812	-1.167553
O	0.485341	-4.059892	-1.553119
H	0.456072	-3.897257	-2.509274
N	2.420858	4.073094	0.309312
N	3.594094	3.751357	0.565243
N	4.679965	3.562819	0.826913
C	-3.506347	-1.852515	0.447900
H	-3.792134	-2.744348	-0.114344
H	-3.118104	-2.156651	1.425115
C	-4.761052	-1.004205	0.672881
Cl	-4.383894	0.478251	1.627015
Cl	-5.948177	-2.008860	1.592231
Cl	-5.496390	-0.517938	-0.900989
C	0.201775	3.432017	-0.432506
C	-0.207841	4.766435	-0.274716
C	-0.718506	2.461723	-0.865196
C	-1.525316	5.125655	-0.550420
H	0.501205	5.515198	0.060688
C	-2.033360	2.829818	-1.137130
H	-0.406078	1.428153	-0.980905
C	-2.438303	4.159296	-0.981704
H	-1.839544	6.157735	-0.428949
H	-2.743436	2.078221	-1.467566
H	-3.465193	4.441624	-1.195269

$M1_{RA}$-7/ $M2_{RA}$-7

C	-4.094556	-2.650494	0.964656
C	-2.616779	-0.729076	1.055399
O	-3.639991	-0.043144	0.774606
O	-2.818063	-2.128839	1.217808
C	5.619480	-0.044457	-0.434480
O	4.413752	0.062685	-0.572200
O	-1.446189	-0.381818	1.234483
C	-1.566053	2.761404	0.746274
C	-1.072168	4.034193	0.609070
C	-1.926346	5.090331	0.169141
C	-3.284433	4.739262	-0.100206
C	-3.703911	3.443374	0.063520
N	-2.859717	2.473153	0.478179
H	-0.969075	1.914741	1.066067
H	-0.030128	4.210701	0.836078
H	-4.000954	5.476271	-0.434780
H	-4.726153	3.140168	-0.131034
N	-1.475024	6.352469	0.013469
C	-2.375923	7.407713	-0.452710
H	-3.203399	7.563048	0.248536
H	-1.816915	8.338062	-0.536450
H	-2.791728	7.166391	-1.436974
C	-0.079635	6.681138	0.310030
H	0.606041	6.117156	-0.332131
H	0.078864	7.743464	0.132833
H	0.164516	6.466030	1.356141
H	-3.197542	1.465235	0.595720
N	6.520450	1.046714	-0.676578
N	5.969942	2.101566	-1.037831
N	5.565316	3.105504	-1.371320
C	6.320775	-1.277680	-0.008844
C	5.541124	-2.413606	0.264550
C	7.716860	-1.338978	0.127013
C	6.152011	-3.596654	0.669132
H	4.463576	-2.352953	0.155722
C	8.322838	-2.526609	0.532314
H	8.320817	-0.463379	-0.083511
C	7.543103	-3.654294	0.803507
H	5.547308	-4.473308	0.880207
H	9.402436	-2.572474	0.636959
H	8.018818	-4.578109	1.119560
H	-4.406986	-3.276415	1.807812
H	-4.822697	-1.852278	0.804936
C	-4.087032	-3.549895	-0.284382
Cl	-3.622779	-2.616959	-1.756783
Cl	-5.754399	-4.218851	-0.509049
Cl	-2.929631	-4.923796	-0.085262

$M1_{RA}$-8

C	0.478017	-1.665035	-0.947535
O	1.611533	-2.085518	-1.183480
N	0.540813	2.507006	-2.061429
N	-0.077748	1.658934	-2.737361
N	-0.544304	0.928770	-3.462131
O	-0.604039	-2.515316	-0.929859
C	-0.370562	-3.906941	-1.091278
C	-0.716907	-4.659812	0.203144
H	0.674532	-4.093347	-1.342219
H	-1.020185	-4.274017	-1.889274
Cl	-0.415329	-6.412327	-0.085578
Cl	0.313009	-4.091289	1.568639
Cl	-2.449404	-4.421624	0.643023

C	1.849213	4.542598	-0.715619
C	0.831846	3.816310	-0.068653
C	0.496900	4.109705	1.266554
C	1.174493	5.117130	1.944284
C	2.186568	5.836006	1.298287
C	2.522431	5.548014	-0.028513
H	2.106905	4.319504	-1.744929
H	-0.289001	3.545850	1.756747
H	0.916874	5.343886	2.974030
H	2.714033	6.622563	1.829980
H	3.307652	6.108154	-0.526277
O	-0.836924	2.130091	-0.214224
C	0.099530	2.746038	-0.757100
O	0.157443	-0.444163	-0.715847
H	3.086879	-1.226940	-0.807798
Cu	-1.605371	0.192149	-0.347509
C	4.433954	-1.151545	0.757450
C	5.648201	-0.711483	1.212723
C	6.496235	0.063189	0.360737
C	6.001884	0.335868	-0.953178
C	4.775187	-0.136615	-1.338931
N	4.006474	-0.866800	-0.495844
H	3.763081	-1.743214	1.368607
H	5.942071	-0.965764	2.221514
H	6.577796	0.912850	-1.663141
H	4.365158	0.046302	-2.324898
N	7.696399	0.511267	0.773941
C	8.547399	1.291663	-0.127623
H	8.040700	2.206120	-0.453719
H	9.456904	1.572660	0.400781
H	8.825888	0.709026	-1.012759
C	8.177083	0.205636	2.123529
H	8.273317	-0.875088	2.274998
H	9.156453	0.660788	2.259971
H	7.499213	0.608790	2.883570
C	-4.289189	0.948713	-1.033017
C	-5.598864	1.322239	-0.847692
C	-6.133611	1.411863	0.472101
C	-5.230639	1.117316	1.537199
C	-3.935292	0.751381	1.257469
N	-3.458342	0.639186	-0.006924
H	-3.869952	0.876712	-2.031359
H	-6.202280	1.539479	-1.718490
H	-5.541610	1.168134	2.571892
H	-3.238828	0.523001	2.057707
N	-7.417098	1.762808	0.699809
C	-7.917336	1.897933	2.069149
H	-7.391120	2.692862	2.609947
H	-8.976962	2.145857	2.034370
H	-7.800456	0.960368	2.622691
C	-8.303862	2.096300	-0.416454
H	-8.355599	1.271159	-1.134042
H	-9.305142	2.275797	-0.028530
H	-7.964804	2.997468	-0.940421

$M1_{RA}$-8 (OAc^-)

C	0.600610	1.277037	0.243020
O	1.788179	1.566415	0.330593
N	-1.926378	-2.972803	1.383960
N	-1.333429	-2.082279	2.026751
N	-0.767665	-1.387178	2.713630
O	-0.391698	2.237052	0.479831
C	-0.010807	3.580038	0.758207
C	-0.371660	4.507045	-0.413709
H	1.065394	3.626325	0.930440
H	-0.551360	3.911009	1.646995
Cl	0.158545	6.170315	0.033939
Cl	0.470004	3.992715	-1.920753
Cl	-2.147974	4.508047	-0.709374
C	-3.559861	-3.593710	-1.867478
C	-3.027176	-3.797170	-0.581264
C	-3.118244	-5.063463	0.025308
C	-3.737057	-6.110634	-0.651118
C	-4.265688	-5.903977	-1.929190
C	-4.176871	-4.646028	-2.535602
H	-3.485861	-2.614793	-2.328271
H	-2.707743	-5.222093	1.016282
H	-3.807386	-7.087356	-0.182826
H	-4.747990	-6.723986	-2.453188
H	-4.588855	-4.488916	-3.527546
O	-2.249070	-1.557453	-0.448318
C	-2.379478	-2.666101	0.100364
O	0.048866	0.159988	-0.034434
H	3.153045	0.456775	0.130746
Cu	-1.876412	0.385434	0.115193
C	4.798916	-0.065292	-1.015879
C	5.975433	-0.763480	-1.081507
C	6.414695	-1.537312	0.037921
C	5.566237	-1.532957	1.189059
C	4.402804	-0.810509	1.182799
N	4.028343	-0.090991	0.097904
H	4.431220	0.535259	-1.839162
H	6.555465	-0.709857	-1.992182
H	5.819261	-2.091482	2.079418
H	3.732715	-0.777562	2.033544
N	7.567887	-2.230878	0.010481
C	7.994375	-3.007689	1.176761
H	7.275929	-3.801735	1.407918
H	8.957556	-3.466977	0.960931
H	8.106971	-2.366485	2.057373
C	8.407123	-2.227325	-1.190220
H	8.751994	-1.215159	-1.428168
H	9.278165	-2.855272	-1.012260
H	7.862916	-2.625190	-2.053586
C	-5.754020	0.806233	1.387468
H	-5.809811	1.898231	1.415664
H	-6.207745	0.385975	2.286427
H	-6.316029	0.471433	0.508536
C	-4.318299	0.352967	1.261439
O	-3.825677	-0.528684	1.970427
O	-3.639250	0.965039	0.318168

$M1_{RA}$-TS6

C	0.476480	-1.795085	-0.898748
O	1.607038	-2.220741	-1.142681
N	0.684813	2.427504	-1.968994
N	-0.032104	1.128229	-2.851478
N	-0.045036	0.536008	-3.788242
O	-0.614071	-2.631837	-0.903689
C	-0.395818	-4.023497	-1.086819
C	-0.740686	-4.792160	0.198777
H	0.645487	-4.217191	-1.347839
H	-1.054912	-4.371627	-1.885456
Cl	-0.458192	-6.542972	-0.118937
Cl	0.303974	-4.254044	1.564995
Cl	-2.467533	-4.543778	0.654703
C	0.497303	5.057550	-0.779172
C	0.871284	3.780953	-0.327894
C	1.896358	3.610664	0.619837
C	2.509942	4.738100	1.154379
C	2.123028	6.016507	0.729410
C	1.121356	6.176747	-0.232841
H	-0.274761	5.160741	-1.534718
H	2.189978	2.613908	0.933219
H	3.293748	4.625255	1.896720
H	2.613078	6.891189	1.146540
H	0.834524	7.170023	-0.562959
O	-0.784200	1.988606	-0.139346
C	0.105019	2.559417	-0.810814
O	0.168793	-0.577259	-0.640534
H	3.018989	-1.299201	-0.715786
Cu	-1.584247	0.100738	-0.267883
C	4.783610	-1.646554	0.305953
C	5.978761	-1.142544	0.745355
C	6.333665	0.213369	0.462483
C	5.382376	0.979266	-0.281671
C	4.205865	0.406888	-0.689217
N	3.914731	-0.883812	-0.399455
H	4.477818	-2.668030	0.497562

H	6.637010	-1.793182	1.303762
H	5.567302	2.012967	-0.538403
H	3.458299	0.951361	-1.253734
N	7.501837	0.738842	0.876078
C	7.842368	2.129442	0.566878
H	7.108147	2.820545	0.994644
H	8.817136	2.355968	0.995262
H	7.892175	2.294095	-0.515064
C	8.453312	-0.076761	1.634652
H	8.787085	-0.941432	1.050603
H	9.322664	0.531547	1.877808
H	8.008380	-0.434396	2.569420
C	-4.441442	0.149570	-0.480837
C	-5.745154	0.532401	-0.264296
C	-6.031539	1.606980	0.627864
C	-4.904085	2.231863	1.236865
C	-3.633480	1.783417	0.959924
N	-3.386290	0.749136	0.121969
H	-4.210126	-0.668190	-1.156581
H	-6.533027	0.003571	-0.783512
H	-5.020648	3.060606	1.922076
H	-2.768480	2.256304	1.410871
N	-7.295449	2.013638	0.878261
C	-7.541719	3.154092	1.760597
H	-7.098377	4.073172	1.359574
H	-8.616358	3.302613	1.853756
H	-7.130582	2.976487	2.760263
C	-8.427039	1.368530	0.212327
H	-8.447412	0.293566	0.421036
H	-9.351729	1.806259	0.585626
H	-8.389067	1.513287	-0.873944

$M1_{RA}$-TS6 (OAc^-)

C	-1.108812	1.318348	0.587740
O	-0.717718	2.453831	0.834540
N	1.543540	-2.519140	1.206962
N	0.404323	-1.857810	2.331781
N	0.239002	-1.531043	3.377860
O	-2.468010	1.011487	0.533504
C	-3.426449	2.054084	0.680587
C	-4.156510	2.310256	-0.647455
H	-2.928045	2.971173	0.998121
H	-4.158070	1.741531	1.428118
Cl	-5.337588	3.640767	-0.364571
Cl	-2.994061	2.798666	-1.933466
Cl	-5.039406	0.836590	-1.188287
C	2.471617	-4.702662	-0.392674
C	2.156216	-3.359672	-0.656149
C	2.870909	-2.615340	-1.612406
C	3.871433	-3.245956	-2.343006
C	4.174038	-4.593838	-2.103561
C	3.477793	-5.319876	-1.133212
H	1.927620	-5.247139	0.372088
H	2.629126	-1.571190	-1.784543
H	4.421404	-2.690287	-3.096028
H	4.963248	-5.075598	-2.673090
H	3.723999	-6.360431	-0.947511
O	-0.120841	-2.470501	-0.500699
C	0.976983	-2.705274	0.048077
O	-0.422995	0.261962	0.359428
H	1.057332	2.671878	0.751912
Cu	-1.627524	-1.243769	0.113579
C	2.711201	3.923976	0.671327
C	4.067462	4.018910	0.504766
C	4.848877	2.840977	0.287275
C	4.140652	1.598755	0.275625
C	2.782733	1.579300	0.452989
N	2.083712	2.723874	0.643218
H	2.082256	4.791493	0.830538
H	4.521894	4.999243	0.535812
H	4.653459	0.658824	0.128243
H	2.203312	0.664128	0.451882
N	6.180720	2.898669	0.101791
C	6.948560	1.675977	-0.145178
H	6.596071	1.165637	-1.048071
H	7.995347	1.939769	-0.285175
H	6.876159	0.983817	0.700775
C	6.877901	4.186715	0.127167
H	6.758243	4.680728	1.097428
H	7.939185	4.016112	-0.044672
H	6.503223	4.854957	-0.655877
C	-4.130492	-4.342376	0.904315
H	-4.143389	-4.908822	1.836610
H	-3.936506	-5.021077	0.067064
H	-5.109921	-3.884630	0.734670
C	-3.061776	-3.277855	0.948932
O	-2.260409	-3.166530	1.886498
O	-3.032893	-2.474221	-0.086620

$M1_{RA}$-9

C	-0.029496	1.308413	-1.069291
O	-1.167201	1.734386	-1.266444
N	-1.056804	-3.214953	-0.265788
O	1.053737	2.158431	-1.065957
C	0.817138	3.551089	-1.210067
C	1.176687	4.293347	0.087038
H	-0.230769	3.739078	-1.447724
H	1.457992	3.926214	-2.011467
Cl	0.872187	6.048324	-0.184345
Cl	0.160650	3.714771	1.458800
Cl	2.913412	4.051566	0.507130
C	-3.178006	-4.155007	-0.887479
C	-2.381632	-3.497538	0.058250
C	-2.895097	-3.131657	1.311153
C	-4.221490	-3.433988	1.611298
C	-5.026578	-4.093096	0.676291
C	-4.503002	-4.450594	-0.569441
H	-2.755030	-4.427887	-1.848547
H	-2.256893	-2.624647	2.027691
H	-4.625256	-3.155848	2.580082
H	-6.057832	-4.329931	0.920124
H	-5.125169	-4.963219	-1.296634
O	1.187035	-2.488835	0.062687
C	0.038506	-2.819744	-0.058409
O	0.300281	0.083770	-0.872145
H	-2.733058	1.028707	-0.932854
Cu	2.059210	-0.546160	-0.519389
C	-4.285136	1.505274	0.343633
C	-5.581277	1.270849	0.718755
C	-6.358775	0.284393	0.035234
C	-5.707070	-0.418372	-1.025920
C	-4.406956	-0.129321	-1.346480
N	-3.710893	0.816130	-0.671391
H	-3.662332	2.245273	0.831852
H	-5.993335	1.847390	1.535143
H	-6.217338	-1.184736	-1.592088
H	-3.878192	-0.636594	-2.144211
N	-7.637021	0.032657	0.372836
C	-8.408162	-0.984717	-0.345546
H	-7.968340	-1.979721	-0.214542
H	-9.423047	-0.999532	0.047892
H	-8.455977	-0.759087	-1.415973
C	-8.270777	0.763279	1.472735
H	-8.303275	1.838419	1.265576
H	-9.291487	0.403960	1.591077
H	-7.736225	0.602209	2.415104
C	4.700861	-1.371623	-1.221371
C	6.003194	-1.778987	-1.059190
C	6.561486	-1.867195	0.250952
C	5.689035	-1.538145	1.331664
C	4.398682	-1.139956	1.074590
N	3.901607	-1.024081	-0.181830
H	4.262372	-1.297874	-2.211377
H	6.582624	-2.022675	-1.939225
H	6.021466	-1.585375	2.359790
H	3.724997	-0.884188	1.885817
N	7.839722	-2.248757	0.456512
C	8.363992	-2.387321	1.816808
H	7.812978	-3.149698	2.378643

H	9.409563	-2.685802	1.762404
H	8.302018	-1.437722	2.358764
C	8.702148	-2.595257	-0.674891
H	8.751279	-1.770977	-1.393495
H	9.707330	-2.788232	-0.304448
H	8.340851	-3.491854	-1.191446

$M1_{RA}$-9 (OAc^-)

C	-1.738036	-0.719599	-0.529860
O	-1.186058	-1.821843	-0.577074
N	2.027213	2.191897	1.573807
O	-3.109978	-0.614697	-0.579530
C	-3.874725	-1.809208	-0.623005
C	-4.666658	-1.989095	0.682173
H	-3.226418	-2.674755	-0.766047
H	-4.586829	-1.730572	-1.448016
Cl	-5.621149	-3.511737	0.537378
Cl	-3.557100	-2.111458	2.096230
Cl	-5.793946	-0.605986	0.944859
C	4.053977	3.177954	0.640733
C	3.423516	2.285624	1.519757
C	4.176354	1.464059	2.367166
C	5.569653	1.539001	2.332349
C	6.207705	2.424454	1.459765
C	5.446226	3.241144	0.617709
H	3.453515	3.807653	-0.008953
H	3.667517	0.784676	3.043220
H	6.154854	0.905218	2.992025
H	7.291851	2.480189	1.436641
H	5.936396	3.932333	-0.061642
O	-0.078546	3.037907	0.848613
C	1.000411	2.652692	1.164890
O	-1.157533	0.416734	-0.445326
H	0.527686	-1.998774	-0.649793
Cu	-2.013514	2.122129	-0.460083
C	1.932396	-3.309204	-1.427997
C	3.254095	-3.656167	-1.524532
C	4.251302	-2.874901	-0.861753
C	3.787036	-1.740814	-0.125249
C	2.447791	-1.455842	-0.073168
N	1.538668	-2.229036	-0.712480
H	1.145946	-3.875186	-1.912766
H	3.516083	-4.526732	-2.109153
H	4.471428	-1.092263	0.403479
H	2.053785	-0.608536	0.475203
N	5.558411	-3.191724	-0.927431
C	6.557642	-2.365795	-0.245750
H	6.392824	-2.358743	0.837361
H	7.546557	-2.776470	-0.441819
H	6.533098	-1.333872	-0.611862
C	5.998668	-4.372594	-1.673601
H	5.757897	-4.281769	-2.738606
H	7.077937	-4.471302	-1.570675
H	5.529799	-5.282601	-1.284289
C	-2.015597	5.314427	-2.634757
H	-1.988591	5.091176	-3.703074
H	-1.108360	5.872569	-2.374488
H	-2.882371	5.932934	-2.393088
C	-2.039441	4.053655	-1.837902
O	-1.497234	2.977873	-2.259058
O	-2.576814	4.004331	-0.675658

$M1_{RA}$-TS_7

C	-0.728288	-1.186025	0.270821
O	-1.148890	-2.209309	0.660024
O	1.280670	-1.463619	-0.057498
C	-0.203043	2.932644	-0.794154
O	0.875906	2.394062	-0.814783
O	-0.708517	-0.037890	-0.074792
C	-5.304464	-3.288487	0.485503
C	-6.622102	-2.963535	0.314301
C	-7.034432	-1.593078	0.327020
C	-6.006220	-0.617333	0.526313
C	-4.706568	-1.010178	0.692632
N	-4.368759	-2.323796	0.670940
H	-4.946887	-4.310393	0.481213
H	-7.333046	-3.764376	0.168010
H	-6.229125	0.440005	0.551295
H	-3.896474	-0.307663	0.845820
N	-8.320404	-1.241519	0.158360
C	-8.711727	0.170932	0.160126
H	-8.207028	0.719563	-0.642048
H	-9.786176	0.237936	-0.000106
H	-8.472780	0.645658	1.117738
C	-9.350625	-2.266247	-0.034362
H	-9.398286	-2.942834	0.825429
H	-10.317260	-1.777715	-0.142827
H	-9.155927	-2.855548	-0.936707
H	-3.396868	-2.590665	0.793803
N	-1.250694	3.463694	-0.867903
Cu	1.432818	0.429199	-0.253526
C	4.121620	1.202530	-1.012557
C	5.439478	1.568274	-0.857830
C	6.013332	1.633944	0.445333
C	5.147727	1.299173	1.527359
C	3.840879	0.944065	1.279205
N	3.316811	0.898647	0.032198
H	3.675407	1.150424	-2.000188
H	6.015598	1.804904	-1.742193
H	5.491333	1.319912	2.552851
H	3.173042	0.688701	2.095570
N	7.302131	1.990523	0.642810
C	7.843787	2.086070	1.998515
H	7.811322	1.117453	2.510087
H	8.882234	2.409376	1.941723
H	7.288228	2.815974	2.598454
C	8.159136	2.322342	-0.495500
H	7.790790	3.206143	-1.029656
H	9.163184	2.533593	-0.130966
H	8.219099	1.487129	-1.201740
C	-2.382815	4.190915	-0.508646
C	-3.383312	4.397011	-1.465431
C	-2.501396	4.700801	0.791576
C	-4.517443	5.126081	-1.109872
H	-3.263879	3.991854	-2.464719
C	-3.642288	5.426394	1.128656
H	-1.709414	4.527422	1.512848
C	-4.649715	5.640448	0.182759
H	-5.297988	5.291525	-1.846023
H	-3.742313	5.825418	2.133448
H	-5.535178	6.207845	0.452812
C	2.046467	-2.365644	0.662441
H	2.832407	-1.879500	1.254277
H	1.412958	-2.946331	1.347817
C	2.746576	-3.390242	-0.261691
Cl	3.923397	-2.576081	-1.357886
Cl	3.631406	-4.575304	0.777183
Cl	1.536195	-4.274292	-1.264435

$M1_{RA}$-TS_7 (OAc^-)

C	0.241243	-0.635191	0.450082
O	-0.069742	-1.644273	0.963547
O	2.259864	-0.827029	-0.024672
C	0.695733	3.565734	-0.496662
O	1.733466	3.000743	-0.737006
O	0.161716	0.470978	0.004286
C	-3.737873	-3.731720	0.469811
C	-5.083269	-3.758931	0.223484
C	-5.842421	-2.545716	0.228603
C	-5.119800	-1.340820	0.501797
C	-3.773270	-1.383446	0.738393
N	-3.100101	-2.561194	0.721704
H	-3.124822	-4.624201	0.476882
H	-5.550045	-4.714207	0.029325
H	-5.613224	-0.379564	0.525054
H	-3.187157	-0.496665	0.946496
N	-7.165012	-2.538419	-0.009688
C	-7.917569	-1.280812	0.017659
H	-7.539385	-0.578582	-0.732760
H	-8.962409	-1.490815	-0.202865

H	-7.858126	-0.808663	1.004105
C	-7.876031	-3.788460	-0.293013
H	-7.803496	-4.484234	0.549710
H	-8.927108	-3.563739	-0.465118
H	-7.474243	-4.275368	-1.187912
H	-2.100616	-2.566439	0.902179
N	-0.266647	4.176078	-0.199150
Cu	2.347992	1.061772	-0.236514
C	-1.558758	4.691548	-0.277954
C	-2.361509	4.399145	-1.388947
C	-2.025991	5.499022	0.765073
C	-3.649826	4.927371	-1.446019
H	-1.973363	3.772062	-2.185067
C	-3.317894	6.018506	0.690601
H	-1.381616	5.709278	1.612130
C	-4.130196	5.735315	-0.410663
H	-4.278292	4.706424	-2.303439
H	-3.688022	6.646051	1.495512
H	-5.135140	6.143088	-0.462914
C	3.152610	-1.652275	0.631768
H	4.029196	-1.108285	1.006239
H	2.673949	-2.163473	1.479886
C	3.692027	-2.767537	-0.296768
Cl	4.603717	-2.075449	-1.688143
Cl	4.801685	-3.821268	0.669817
Cl	2.338171	-3.775514	-0.937590
O	4.199521	1.450102	-0.118049
C	3.797360	2.436716	2.065294
H	3.286895	3.372220	1.807354
H	4.369837	2.601279	2.980366
H	3.028786	1.675900	2.246778
C	4.729888	2.050245	0.928148
O	5.929108	2.311610	0.961066

$M1_{RA}$-10

N	4.669610	-0.495477	-0.641972
O	-0.545967	-0.202233	1.200833
C	-1.158616	0.369065	2.306844
C	-0.610323	-0.173446	3.650523
H	-2.235132	0.148196	2.305929
H	-1.039953	1.460779	2.339207
Cl	-1.552474	0.583455	4.991619
Cl	-0.794697	-1.965320	3.737952
Cl	1.135834	0.236756	3.855746
C	5.487141	-1.782579	-2.514406
C	5.582011	-1.405250	-1.168007
C	6.578214	-1.924225	-0.332946
C	7.490803	-2.836961	-0.860063
C	7.408558	-3.223822	-2.200474
C	6.408242	-2.696184	-3.022844
H	4.705128	-1.362403	-3.138361
H	6.627356	-1.612830	0.705036
H	8.266825	-3.245645	-0.220288
H	8.122492	-3.935277	-2.604276
H	6.342937	-2.995243	-4.064475
O	2.884555	1.044006	-0.292963
C	3.768858	0.243589	-0.499442
H	-1.622804	-1.221875	0.276632
Cu	0.921028	0.588813	0.330138
C	-2.776414	-2.952219	0.218502
C	-3.715044	-3.682968	-0.460099
C	-4.241185	-3.203447	-1.700464
C	-3.720761	-1.958305	-2.173417
C	-2.780823	-1.283138	-1.441286
N	-2.320048	-1.770510	-0.263368
H	-2.360396	-3.277818	1.163904
H	-4.047265	-4.617854	-0.030731
H	-4.051428	-1.527367	-3.108109
H	-2.363373	-0.337113	-1.764191
N	-5.176514	-3.886584	-2.384612
C	-5.712389	-3.358329	-3.641379
H	-4.937006	-3.309439	-4.414289
H	-6.507003	-4.016543	-3.988619
H	-6.132299	-2.357327	-3.499040
C	-5.662967	-5.176516	-1.889558
H	-6.156108	-5.066041	-0.917583
H	-6.384804	-5.576158	-2.599678
H	-4.842473	-5.894926	-1.789551
C	-1.195712	2.379574	-0.612657
C	-1.785366	3.520444	-1.107820
C	-0.990271	4.664686	-1.406218
C	0.404636	4.534945	-1.147988
C	0.908749	3.354483	-0.651391
N	0.136355	2.273542	-0.385378
H	-1.796433	1.507554	-0.382107
H	-2.855643	3.518737	-1.265773
H	1.091236	5.351072	-1.328845
H	1.969900	3.256286	-0.455072
N	-1.524935	5.802812	-1.900774
C	-0.668543	6.950180	-2.201432
H	0.126664	6.674291	-2.902122
H	-1.272503	7.730223	-2.662686
H	-0.208047	7.357925	-1.293547
C	-2.970724	5.918201	-2.091345
H	-3.508879	5.778590	-1.146751
H	-3.198717	6.913250	-2.470771
H	-3.337782	5.180890	-2.814245

$M1_{RA}$-10 (OAc^-)

N	4.712519	0.498085	0.133347
O	-0.705053	-1.199763	0.026232
C	-1.359560	-2.377336	0.345310
C	-1.117455	-3.490930	-0.703624
H	-2.448564	-2.225860	0.379305
H	-1.049182	-2.786664	1.316794
Cl	-2.043879	-4.961462	-0.209208
Cl	-1.681150	-2.964300	-2.336316
Cl	0.635979	-3.908447	-0.810748
C	5.471172	2.751878	-0.321086
C	5.604828	1.367254	-0.493004
C	6.623725	0.828223	-1.286271
C	7.519219	1.692231	-1.915703
C	7.398190	3.074871	-1.753676
C	6.375540	3.599877	-0.957337
H	4.672630	3.143301	0.300933
H	6.703671	-0.247724	-1.400474
H	8.312349	1.281953	-2.533222
H	8.098842	3.742553	-2.245866
H	6.279569	4.673788	-0.829144
O	2.887800	-0.251825	1.469582
C	3.786959	0.172980	0.787776
H	-1.805305	0.087853	-0.204214
Cu	0.919994	-0.751822	0.877612
C	-3.345706	0.797104	-1.411775
C	-4.338239	1.725564	-1.585854
C	-4.547044	2.744710	-0.605297
C	-3.665069	2.735422	0.518821
C	-2.691115	1.777010	0.626039
N	-2.538825	0.821810	-0.323705
H	-3.161492	0.006087	-2.128187
H	-4.953271	1.660620	-2.472664
H	-3.744482	3.476374	1.302416
H	-1.991098	1.736526	1.453943
N	-5.522726	3.664162	-0.734118
C	-5.714322	4.689783	0.293637
H	-4.822905	5.317978	0.397573
H	-6.551290	5.324499	0.007119
H	-5.939950	4.237164	1.265425
C	-6.408302	3.647748	-1.900047
H	-6.959163	2.703218	-1.965621
H	-7.128424	4.458820	-1.806825
H	-5.844184	3.790595	-2.828112
C	-0.599284	0.289919	4.491116
H	0.113485	-0.126434	5.208445
H	-0.810469	1.331553	4.736839
H	-1.522111	-0.295261	4.567499
C	-0.054650	0.178700	3.083454
O	-0.037641	1.145444	2.297047
O	0.379301	-0.996979	2.742184

$M1_{RA}$-TS8

O	-0.881851	-0.467729	-0.138960
C	0.968509	-0.159440	0.070381
O	0.856266	0.982113	0.502186
C	4.868094	0.981915	-1.003704
C	6.001711	1.747631	-1.039150
C	6.865285	1.807908	0.100055
C	6.477036	1.032253	1.238070
C	5.329452	0.287190	1.205381
N	4.542269	0.267250	0.101538
H	4.184556	0.908096	-1.840606
H	6.221132	2.298867	-1.942793
H	7.073440	1.017184	2.139488
H	4.996932	-0.312492	2.043641
N	7.983341	2.554883	0.100681
C	8.849385	2.595013	1.282247
H	9.250977	1.602092	1.511871
H	9.682298	3.267292	1.084925
H	8.304272	2.965485	2.156947
C	8.361119	3.326167	-1.086613
H	7.582163	4.049148	-1.350366
H	9.279558	3.871240	-0.875360
H	8.537219	2.668373	-1.944558
H	3.682038	-0.285783	0.099566
N	1.746610	-1.055825	-0.245515
Cu	-1.185427	1.406741	0.361900
C	-3.593541	1.401229	-1.248659
C	-4.914322	1.607495	-1.573300
C	-5.794121	2.216304	-0.630853
C	-5.216608	2.575675	0.622663
C	-3.884088	2.329621	0.862083
N	-3.065319	1.758650	-0.053746
H	-2.915753	0.938469	-1.958403
H	-5.258630	1.301837	-2.552022
H	-5.802972	3.042267	1.402832
H	-3.435000	2.594504	1.813784
N	-7.097919	2.434118	-0.908856
C	-7.971340	3.059605	0.084511
H	-7.612770	4.059227	0.354816
H	-8.971793	3.155860	-0.334607
H	-8.035140	2.453679	0.995502
C	-7.652247	2.043221	-2.205529
H	-7.545591	0.965979	-2.375240
H	-8.712558	2.289734	-2.224339
H	-7.158524	2.576644	-3.025802
C	1.715798	-2.208110	-1.044658
C	1.028649	-2.228161	-2.269374
C	2.453489	-3.325661	-0.630490
C	1.065245	-3.377950	-3.057666
H	0.478401	-1.349770	-2.591409
C	2.482234	-4.468234	-1.429492
H	2.990575	-3.288952	0.311972
C	1.789425	-4.499766	-2.642958
H	0.529326	-3.393329	-4.002222
H	3.050099	-5.334454	-1.102930
H	1.816130	-5.390564	-3.263242
C	-1.666484	-1.616829	-0.139574
C	-1.951779	-2.224223	1.258044
Cl	-2.859666	-3.766431	1.002301
Cl	-2.963713	-1.122158	2.268014
Cl	-0.426445	-2.575771	2.147539
H	-2.641972	-1.418355	-0.600326
H	-1.167623	-2.399372	-0.722752

$M1_{RA}$-TS8 (OAc^-)

O	-0.881851	-0.467729	-0.138960
C	0.968509	-0.159440	0.070381
O	0.856266	0.982113	0.502186
C	4.868094	0.981915	-1.003704
C	6.001711	1.747631	-1.039150
C	6.865285	1.807908	0.100055
C	6.477036	1.032253	1.238070
C	5.329452	0.287190	1.205381
N	4.542269	0.267250	0.101538
H	4.184556	0.908096	-1.840606
H	6.221132	2.298867	-1.942793
H	7.073440	1.017184	2.139488
H	4.996932	-0.312492	2.043641
N	7.983341	2.554883	0.100681
C	8.849385	2.595013	1.282247
H	9.250977	1.602092	1.511871
H	9.682298	3.267292	1.084925
H	8.304272	2.965485	2.156947
C	8.361119	3.326167	-1.086613
H	7.582163	4.049148	-1.350366
H	9.279558	3.871240	-0.875360
H	8.537219	2.668373	-1.944558
H	3.682038	-0.285783	0.099566
N	1.746610	-1.055825	-0.245515
Cu	-1.185427	1.406741	0.361900
C	-3.593541	1.401229	-1.248659
C	-4.914322	1.607495	-1.573300
C	-5.794121	2.216304	-0.630853
C	-5.216608	2.575675	0.622663
C	-3.884088	2.329621	0.862083
N	-3.065319	1.758650	-0.053746
H	-2.915753	0.938469	-1.958403
H	-5.258630	1.301837	-2.552022
H	-5.802972	3.042267	1.402832
H	-3.435000	2.594504	1.813784
N	-7.097919	2.434118	-0.908856
C	-7.971340	3.059605	0.084511
H	-7.612770	4.059227	0.354816
H	-8.971793	3.155860	-0.334607
H	-8.035140	2.453679	0.995502
C	-7.652247	2.043221	-2.205529
H	-7.545591	0.965979	-2.375240
H	-8.712558	2.289734	-2.224339
H	-7.158524	2.576644	-3.025802
C	1.715798	-2.208110	-1.044658
C	1.028649	-2.228161	-2.269374
C	2.453489	-3.325661	-0.630490
C	1.065245	-3.377950	-3.057666
H	0.478401	-1.349770	-2.591409
C	2.482234	-4.468234	-1.429492
H	2.990575	-3.288952	0.311972
C	1.789425	-4.499766	-2.642958
H	0.529326	-3.393329	-4.002222
H	3.050099	-5.334454	-1.102930
H	1.816130	-5.390564	-3.263242
C	-1.666484	-1.616829	-0.139574
C	-1.951779	-2.224223	1.258044
Cl	-2.859666	-3.766431	1.002301
Cl	-2.963713	-1.122158	2.268014
Cl	-0.426445	-2.575771	2.147539
H	-2.641972	-1.418355	-0.600326
H	-1.167623	-2.399372	-0.722752

$M1_{RA}$-11

N	2.396230	1.169334	0.577374
O	0.621470	2.321499	-0.286064
C	-0.668090	2.320537	-0.915759
C	-0.921937	3.731840	-1.454172
H	-1.451277	2.065262	-0.196013
H	-0.680980	1.611349	-1.746851
Cl	-2.521777	3.696704	-2.281541
Cl	-0.969138	4.929533	-0.111895
Cl	0.350030	4.209892	-2.631676
C	4.435560	2.052529	1.379512
C	3.004737	2.133532	1.286621
C	2.326670	3.185634	1.992542
C	3.055140	4.106074	2.715841
C	4.460986	4.022367	2.772848
C	5.143128	2.989683	2.101806
H	4.935297	1.243012	0.857794
H	1.245286	3.243374	1.960871
H	2.542368	4.899206	3.250366
H	5.020134	4.756075	3.344866
H	6.225195	2.930596	2.157447

O	0.428986	0.111670	0.234252
C	1.084447	1.164981	0.209882
H	3.249023	-0.513085	0.115830
Cu	-1.419636	-0.468030	0.386917
C	4.380744	-1.723908	-1.130660
C	4.825287	-2.990989	-1.399126
C	4.448209	-4.080451	-0.551909
C	3.606454	-3.761939	0.560138
C	3.201611	-2.470851	0.768619
N	3.583939	-1.472158	-0.063678
H	4.638328	-0.872070	-1.748358
H	5.456451	-3.141656	-2.263802
H	3.276830	-4.521641	1.254920
H	2.566204	-2.185728	1.598240
N	4.863330	-5.337823	-0.788622
C	4.434776	-6.439022	0.077431
H	3.342698	-6.514262	0.105919
H	4.833276	-7.371668	-0.317885
H	4.805697	-6.307006	1.099882
C	5.744772	-5.627885	-1.922240
H	6.670933	-5.047302	-1.859010
H	6.000774	-6.685692	-1.905458
H	5.252133	-5.403886	-2.874941
C	-4.208426	-0.604891	1.109490
C	-5.496053	-1.093129	1.171160
C	-5.824309	-2.318844	0.527122
C	-4.753047	-2.967352	-0.149022
C	-3.496585	-2.399416	-0.155439
N	-3.195476	-1.228720	0.458744
H	-3.959278	0.329857	1.600842
H	-6.238631	-0.525401	1.716008
H	-4.898381	-3.905879	-0.667845
H	-2.680604	-2.892735	-0.673116
N	-7.077135	-2.835126	0.556880
C	-7.364742	-4.109561	-0.098040
H	-6.768304	-4.923981	0.330036
H	-8.418405	-4.348346	0.040624
H	-7.162084	-4.060697	-1.174281
C	-8.143509	-2.141692	1.276931
H	-8.296209	-1.129262	0.885945
H	-9.072232	-2.697126	1.153194
H	-7.924552	-2.070018	2.349228

$M1_{RA}$-11 (OAc^-)

O	1.837967	0.650139	-0.665439
C	0.549342	0.157317	-0.506992
O	0.525227	-1.126113	-0.447858
C	-3.898012	-0.277073	-1.026077
C	-5.223663	-0.586735	-0.865136
C	-5.771900	-0.729451	0.446968
C	-4.866545	-0.548313	1.538047
C	-3.552715	-0.239577	1.296836
N	-3.078304	-0.105103	0.036711
H	-3.445801	-0.151495	-2.002918
H	-5.834775	-0.711466	-1.748036
H	-5.192904	-0.644355	2.564227
H	-2.837055	-0.086542	2.096153
N	-7.073800	-1.015820	0.643206
C	-7.609482	-1.140144	2.000533
H	-7.477995	-0.209345	2.563227
H	-8.674458	-1.358653	1.940602
H	-7.119390	-1.953035	2.547464
C	-7.972987	-1.194880	-0.498577
H	-7.652269	-2.031913	-1.128619
H	-8.974105	-1.407711	-0.127732
H	-8.017297	-0.289094	-1.113359
H	-2.072145	0.174251	-0.123215
N	-0.518353	0.887157	-0.458712
Cu	2.152830	-2.124735	-0.461335
C	-0.586345	2.233589	-0.876508
C	-0.021021	2.676965	-2.087445
C	-1.337885	3.140867	-0.108518
C	-0.185106	4.000255	-2.499389
H	0.534973	1.979243	-2.706837
C	-1.496140	4.461892	-0.527577
H	-1.786741	2.799936	0.819940
C	-0.919549	4.900938	-1.723139
H	0.258230	4.324692	-3.437081
H	-2.074101	5.150234	0.083177
H	-1.045812	5.929433	-2.048299
C	2.267004	1.827268	0.005746
C	3.424519	1.489377	0.963931
Cl	4.026772	3.041916	1.651119
Cl	4.763529	0.663752	0.089908
Cl	2.861304	0.427168	2.309321
H	2.633679	2.544871	-0.731821
H	1.466081	2.281945	0.589812
C	3.159563	-5.844241	-0.724236
H	2.324244	-6.520876	-0.540390
H	3.556366	-6.014990	-1.730813
H	3.966241	-6.037460	-0.011027
C	2.725706	-4.421688	-0.610809
O	1.504958	-4.090673	-0.455937
O	3.574369	-3.459656	-0.676521

$M1_{RA}$-TS9

C	-3.844238	-1.745101	-0.239863
O	-3.374277	-0.404342	-0.085107
C	-2.043041	-0.206350	-0.173699
O	-1.323839	-1.230229	-0.439494
C	1.646983	1.826965	0.977823
C	2.903965	2.385964	0.977402
C	3.424837	2.954397	-0.222720
C	2.578767	2.892738	-1.370168
C	1.334709	2.311120	-1.271836
N	0.861611	1.781562	-0.122262
H	1.226148	1.398298	1.882260
H	3.472854	2.391207	1.897299
H	2.889274	3.302035	-2.321983
H	0.670014	2.263503	-2.129111
N	4.649591	3.525059	-0.267708
C	5.150860	4.109894	-1.511728
H	4.492650	4.910807	-1.866037
H	6.137924	4.531896	-1.330189
H	5.236395	3.353740	-2.300490
C	5.493172	3.560448	0.927301
H	5.718704	2.548822	1.282926
H	6.430676	4.057073	0.682607
H	5.008511	4.115958	1.737942
N	-1.589244	1.008992	0.027077
H	-0.348832	1.317656	-0.052904
Cu	0.565181	-1.423249	-0.257383
C	3.359879	-1.345309	-0.910679
C	4.689116	-1.692867	-0.859920
C	5.159153	-2.557671	0.172269
C	4.177124	-3.030266	1.093046
C	2.866872	-2.632391	0.963578
N	2.450508	-1.779593	-0.004015
H	2.989956	-0.683524	-1.686981
H	5.357761	-1.290538	-1.608670
H	4.436316	-3.699224	1.902258
H	2.109025	-2.985085	1.655843
N	6.458063	-2.915326	0.264725
C	6.906637	-3.821179	1.322890
H	6.481489	-4.824093	1.198115
H	7.992051	-3.896707	1.284474
H	6.622767	-3.440380	2.309061
C	7.422386	-2.466109	-0.740641
H	7.477883	-1.372674	-0.771119
H	8.406241	-2.854043	-0.482691
H	7.155104	-2.831293	-1.738680
C	-2.434150	2.122353	0.313380
C	-2.125655	2.911918	1.429895
C	-3.488347	2.500503	-0.531350
C	-2.875606	4.055573	1.709723
H	-1.304883	2.620273	2.078527
C	-4.236995	3.641518	-0.241731
H	-3.714661	1.905402	-1.409637
C	-3.935932	4.422685	0.878015

H	-2.630865	4.656467	2.581085
H	-5.054452	3.924418	-0.899017
H	-4.520423	5.311489	1.097269
H	-3.452078	-2.387941	0.551897
H	-3.563884	-2.148714	-1.215059
C	-5.371967	-1.712861	-0.139156
Cl	-6.084180	-0.701568	-1.447077
Cl	-5.898523	-1.070791	1.457550
Cl	-5.952112	-3.410272	-0.320107

$M1_{RA}$-TS9 (OAc^-)

C	-2.857749	0.654454	0.161966
O	-2.038210	-0.481822	-0.089809
C	-0.696984	-0.356311	0.075963
O	-0.164943	0.768830	0.340690
C	3.288511	-0.846000	-1.102003
C	4.649641	-0.629223	-1.091641
C	5.367059	-0.694470	0.137429
C	4.596703	-0.991612	1.298473
C	3.238029	-1.193258	1.184707
N	2.579055	-1.126369	0.009974
H	2.724924	-0.797794	-2.029587
H	5.150652	-0.411666	-2.025294
H	5.054454	-1.062648	2.276101
H	2.633723	-1.418403	2.058998
N	6.704834	-0.485584	0.198344
C	7.404716	-0.558194	1.479565
H	7.312568	-1.553667	1.929712
H	8.461942	-0.352523	1.317741
H	7.016400	0.180460	2.190612
C	7.458767	-0.178538	-1.015514
H	7.103613	0.746991	-1.483993
H	8.508815	-0.049244	-0.756722
H	7.383942	-0.989347	-1.749695
N	0.030386	-1.442868	-0.046315
H	1.280459	-1.278868	-0.030221
Cu	-0.466115	2.585859	-0.285382
C	-0.474437	-2.765225	-0.143696
C	0.081989	-3.612992	-1.112868
C	-1.424484	-3.275160	0.755084
C	-0.323752	-4.945962	-1.195916
H	0.825119	-3.219237	-1.799943
C	-1.828359	-4.606826	0.661658
H	-1.834523	-2.632862	1.526902
C	-1.282792	-5.447882	-0.312797
H	0.111303	-5.591265	-1.953974
H	-2.565921	-4.990318	1.361280
H	-1.597793	-6.485214	-0.378199
H	-2.745179	1.411699	-0.623832
H	-2.641331	1.092073	1.140137
C	-4.320058	0.191582	0.145671
Cl	-4.628761	-1.005260	1.451572
Cl	-4.741350	-0.540956	-1.442892
Cl	-5.344104	1.649628	0.420106
O	-0.426369	4.562673	-0.469193
C	0.802254	4.583683	-0.104940
C	1.563753	5.857691	0.026674
H	1.448766	6.226698	1.052634
H	2.625603	5.686617	-0.161009
H	1.167551	6.609133	-0.659044
O	1.326663	3.450403	0.163711

$M1_{RA}$-12

N	-2.493971	1.081241	0.233484
O	-0.879145	2.606175	0.637426
C	0.442561	2.984423	1.008385
C	1.043298	3.910498	-0.059741
H	1.094482	2.117674	1.133549
H	0.379356	3.532130	1.951039
Cl	2.688046	4.378125	0.505567
Cl	1.167135	3.060887	-1.643951
Cl	0.042289	5.391395	-0.266109
C	-4.759203	1.668216	0.835458
C	-3.567939	2.017362	0.185795
C	-3.485081	3.215912	-0.532837
C	-4.586666	4.071807	-0.571489
C	-5.774702	3.732769	0.081136
C	-5.859028	2.524595	0.777448
H	-4.815110	0.732942	1.384565
H	-2.575547	3.472135	-1.062755
H	-4.516169	5.002961	-1.126234
H	-6.628906	4.402259	0.042630
H	-6.778576	2.248603	1.285340
O	-0.384943	0.362908	0.543331
C	-1.194402	1.305444	0.466039
H	-2.746481	0.077885	0.188817
Cu	1.450597	-0.195177	0.331170
C	-2.773856	-2.671935	0.905443
C	-3.087416	-4.020445	0.834562
C	-3.983321	-4.453343	-0.179090
C	-4.512435	-3.475601	-1.062983
C	-4.128972	-2.154703	-0.891688
N	-3.277707	-1.748961	0.066953
H	-2.088760	-2.313316	1.667449
H	-2.641213	-4.707966	1.540433
H	-5.205691	-3.729624	-1.853067
H	-4.520938	-1.385966	-1.550530
N	-4.325950	-5.774967	-0.302443
C	-5.200331	-6.227411	-1.385520
H	-4.807185	-5.888053	-2.346746
H	-5.251740	-7.312515	-1.368908
H	-6.202601	-5.808806	-1.240705
C	-3.819992	-6.774848	0.638729
H	-4.022463	-6.458829	1.664615
H	-4.308344	-7.725052	0.440890
H	-2.737783	-6.882827	0.503354
C	4.000062	-0.732539	-0.899075
C	5.259022	-1.269990	-1.063072
C	5.809730	-2.112456	-0.057373
C	4.986744	-2.332676	1.082223
C	3.739154	-1.749942	1.156003
N	3.221585	-0.952912	0.189050
H	3.579711	-0.091668	-1.667004
H	5.807170	-1.036152	-1.966223
H	5.316514	-2.954268	1.904123
H	3.111610	-1.919528	2.024804
N	7.039343	-2.670512	-0.177928
C	7.569781	-3.521398	0.885413
H	6.922516	-4.388158	1.063140
H	8.552870	-3.885094	0.589491
H	7.675598	-2.969259	1.826960
C	7.854228	-2.407614	-1.362482
H	8.089314	-1.340834	-1.459552
H	8.790530	-2.957623	-1.277635
H	7.345738	-2.734516	-2.276945

$M1_{RA}$-12 (OAc^-)

C	-2.934311	0.630375	0.144138
O	-2.093930	-0.515227	-0.002790
C	-0.768330	-0.349897	0.145830
O	-0.234643	0.772706	0.361070
C	3.412022	-0.807966	-1.074125
C	4.776961	-0.583519	-1.105162
C	5.527299	-0.647994	0.100297
C	4.786557	-0.951095	1.275046
C	3.421493	-1.158829	1.188244
N	2.715110	-1.095106	0.042692
H	2.838335	-0.756790	-1.997327
H	5.251127	-0.361475	-2.052447
H	5.267537	-1.023669	2.241994
H	2.854663	-1.390236	2.087697
N	6.870972	-0.433304	0.127570
C	7.600824	-0.505218	1.389804
H	7.525390	-1.501570	1.842599
H	8.653427	-0.294496	1.204044
H	7.227726	0.229565	2.113769
C	7.590536	-0.124159	-1.104151
H	7.221755	0.800121	-1.565994
H	8.647168	0.008885	-0.873954
H	7.500600	-0.934228	-1.838366

N	-0.032747	-1.451624	0.064833
H	1.022911	-1.289920	0.052092
Cu	-0.552433	2.612196	-0.253665
C	-0.488754	-2.796165	-0.062312
C	0.182848	-3.626619	-0.968515
C	-1.516537	-3.313235	0.736004
C	-0.186652	-4.966950	-1.086596
H	0.984866	-3.218833	-1.575888
C	-1.886355	-4.651669	0.600689
H	-2.013323	-2.679663	1.461490
C	-1.225761	-5.482497	-0.308271
H	0.336599	-5.605373	-1.792486
H	-2.686723	-5.047344	1.219246
H	-1.514985	-6.524834	-0.404532
H	-2.783298	1.332268	-0.683815
H	-2.758896	1.125520	1.102401
C	-4.390266	0.152647	0.094400
Cl	-4.742621	-0.973749	1.450067
Cl	-4.741135	-0.667812	-1.467019
Cl	-5.427883	1.616964	0.248737
O	-0.501217	4.587466	-0.434541
C	0.726255	4.599728	-0.065576
C	1.497580	5.865097	0.076743
H	1.394975	6.219108	1.109354
H	2.556412	5.688323	-0.122722
H	1.100791	6.629286	-0.594279
O	1.237982	3.458535	0.198571

$M1_{RA}$-13/M1'-9/ $M2_{RA}$-10

N	-1.744002	1.586478	0.054026
O	0.153402	0.553503	-0.662752
C	1.533970	0.612378	-0.996979
C	2.353920	-0.271755	-0.045980
H	1.899226	1.637939	-0.932375
H	1.657297	0.232011	-2.013525
Cl	4.085686	-0.125889	-0.529076
Cl	2.159545	0.266733	1.661363
Cl	1.849264	-1.999201	-0.175551
C	-4.010158	0.819280	0.012744
C	-2.643242	0.493950	0.015965
C	-2.258019	-0.854284	0.027505
C	-3.236747	-1.850371	0.017431
C	-4.594707	-1.529298	0.009376
C	-4.974786	-0.184868	0.011821
H	-4.308055	1.864449	0.009873
H	-1.212878	-1.127518	0.049160
H	-2.924123	-2.890750	0.024754
H	-5.345679	-2.313405	0.005315
H	-6.026163	0.087848	0.009397
O	0.165994	2.790292	-0.191603
C	-0.424288	1.725659	-0.256179
H	-2.168856	2.481652	0.265328

$M1_{RA}$-6'

C	-0.067635	-0.166022	-0.970086
O	-0.230882	-0.471641	-2.297826
O	-0.829052	-0.956215	-0.138594
C	-2.238307	-0.908963	-0.351725
C	-2.840208	-2.229629	0.139253
H	-2.473593	-0.797001	-1.412391
H	-2.684523	-0.089041	0.218059
Cl	-4.620792	-2.136151	-0.127065
Cl	-2.512970	-2.467485	1.895397
Cl	-2.170554	-3.623637	-0.779963
C	1.704002	-1.091684	0.539317
C	3.013941	-1.295089	0.861943
C	4.061254	-0.804335	0.021139
C	3.644109	-0.101954	-1.154561
C	2.319706	0.059369	-1.430566
N	1.347766	-0.429152	-0.601471
H	0.898734	-1.444830	1.163651
H	3.228484	-1.835883	1.772709
H	4.359495	0.311412	-1.851234
H	1.981195	0.576745	-2.317623
N	5.354442	-0.988276	0.315647
C	5.745591	-1.700212	1.537524
H	5.371265	-2.728730	1.527430
H	6.831828	-1.726114	1.595249
H	5.361406	-1.190286	2.426602
C	6.402018	-0.471873	-0.572287
H	6.364424	0.620919	-0.628764
H	7.372037	-0.766555	-0.177423
H	6.298290	-0.884432	-1.580536
C	-1.250977	3.827700	-0.943349
C	-0.752807	3.280590	0.250253
C	-0.688592	4.069390	1.410618
C	-1.117110	5.392794	1.376845
C	-1.612890	5.935526	0.187356
C	-1.678633	5.153450	-0.969049
H	-1.303816	3.224138	-1.841846
H	-0.302632	3.634306	2.326079
H	-1.066462	6.000526	2.274868
H	-1.947999	6.968180	0.161688
H	-2.064511	5.576380	-1.891312
O	0.128332	1.342614	1.356600
C	-0.288143	1.879474	0.355847
O	-0.378004	1.219603	-0.862128
H	-0.620769	0.289827	-2.761944

$M1_{RA}$-TS4'

C	-0.804505	-0.052752	-0.983950
O	-0.614384	-0.677032	-2.097455
O	-1.401464	-0.645209	-0.007849
C	-1.699420	-2.072869	-0.039730
C	-3.191801	-2.252887	0.260348
H	-1.098204	-2.526492	0.748271
H	-1.454657	-2.498688	-1.010649
Cl	-3.502530	-4.021931	0.250086
Cl	-4.187000	-1.448955	-1.005551
Cl	-3.607103	-1.571421	1.869590
C	2.354948	-1.713018	-0.672849
C	3.632483	-2.050490	-0.259391
C	4.589046	-1.025410	-0.031628
C	4.137042	0.300803	-0.265520
C	2.832531	0.516517	-0.675448
N	1.922568	-0.454673	-0.886777
H	1.628635	-2.505161	-0.846659
H	3.879588	-3.094798	-0.117557
H	4.792370	1.151399	-0.129367
H	2.495387	1.536998	-0.848927
N	5.856602	-1.295568	0.387834
C	6.292310	-2.677216	0.564462
H	6.258979	-3.238937	-0.377779
H	7.319180	-2.681190	0.927996
H	5.670110	-3.201361	1.299183
C	6.818333	-0.212144	0.564827
H	6.460302	0.523603	1.294375
H	7.755308	-0.626426	0.935478
H	7.023141	0.310844	-0.378125
C	-1.173315	3.871611	-0.977549
C	-0.688713	3.342835	0.232804
C	-0.472944	4.182217	1.344214
C	-0.740034	5.540972	1.239368
C	-1.223800	6.066112	0.036127
C	-1.439907	5.233825	-1.066355
H	-1.342865	3.229845	-1.833416
H	-0.099399	3.760673	2.270861
H	-0.573329	6.191125	2.091798
H	-1.433820	7.128521	-0.042004
H	-1.816749	5.647439	-1.995811
O	-0.053294	1.311275	1.378227
C	-0.400677	1.931037	0.427521
O	-0.546405	1.203918	-0.900494
H	0.119532	-0.254965	-2.598122

$M1_{RA}$-7'

C	-0.120275	1.338145	0.547233
O	-0.550972	2.271768	1.165740
O	-0.782048	0.547010	-0.310080
C	-2.154563	0.858626	-0.570001

C	-3.039102	-0.316374	-0.133613
H	-2.264250	1.003843	-1.646220
H	-2.455684	1.759250	-0.033403
Cl	-4.739886	0.118524	-0.537094
Cl	-2.891228	-0.601920	1.639232
Cl	-2.582362	-1.822082	-1.009939
C	3.498055	-0.537731	1.048171
C	3.271374	0.172617	-0.141669
C	4.257902	0.205260	-1.140967
C	5.460752	-0.467744	-0.950688
C	5.684858	-1.174970	0.234788
C	4.704832	-1.209478	1.230696
H	2.737808	-0.565316	1.820256
H	4.069625	0.758195	-2.054894
H	6.223150	-0.441931	-1.723070
H	6.623985	-1.700202	0.382179
H	4.880910	-1.760284	2.149375
O	1.716247	1.499104	-1.407477
C	2.014025	0.900654	-0.401172
O	1.160073	0.872812	0.702033

$M1_{RA}$-TS_4''

C	0.461010	0.053291	0.982769
O	0.145366	-0.309998	2.180952
O	0.565892	-0.818851	0.043079
C	0.214731	-2.206452	0.291676
C	1.101914	-3.066737	-0.612613
H	-0.840415	-2.326513	0.043906
H	0.400970	-2.465041	1.333310
Cl	0.611836	-4.776799	-0.320078
Cl	2.826142	-2.827004	-0.177963
Cl	0.844564	-2.658610	-2.347826
C	-2.988830	0.283641	1.546217
C	-4.361264	0.455202	1.467100
C	-4.970901	0.638517	0.197907
C	-4.090123	0.626877	-0.915751
C	-2.731340	0.449495	-0.712534
N	-2.152952	0.277249	0.491623
H	-2.529195	0.141597	2.522790
H	-4.945871	0.444793	2.378230
H	-4.457163	0.758232	-1.925729
H	-2.058874	0.450864	-1.566536
N	-6.315392	0.814409	0.057427
C	-7.178560	0.840214	1.233134
H	-6.898996	1.647036	1.921942
H	-8.207062	1.008111	0.915379
H	-7.141657	-0.108078	1.783625
C	-6.896949	0.990584	-1.268864
H	-6.688652	0.130355	-1.916635
H	-7.977903	1.087801	-1.173218
H	-6.514007	1.892194	-1.763177
C	2.986205	2.924806	0.544991
C	2.075644	2.858606	-0.524467
C	2.172998	3.753028	-1.607958
C	3.168874	4.721609	-1.608478
C	4.073699	4.792328	-0.543072
C	3.986135	3.893305	0.523641
H	2.933802	2.201120	1.353165
H	1.464348	3.685190	-2.426439
H	3.242482	5.421052	-2.434935
H	4.852543	5.549249	-0.547774
H	4.700726	3.945322	1.338866
O	0.325976	1.512265	-1.495204
C	1.018053	1.857085	-0.589627
O	0.787045	1.284175	0.767553
H	0.364550	0.395114	2.825537
N	3.029882	-0.083275	2.275065
N	3.999380	-0.644064	1.877506
N	4.961248	-1.211532	1.487230

$M1_{RA}$-6''

C	0.098809	0.407092	0.593700
O	-0.243774	0.709911	1.772398
O	-0.478881	1.126565	-0.495841
C	-1.049205	2.375763	-0.181235
C	-2.511875	2.427746	-0.651606
H	-0.510082	3.176104	-0.699640
H	-1.031870	2.553480	0.896485
Cl	-3.144259	4.083630	-0.288981
Cl	-3.519481	1.209117	0.206326
Cl	-2.628977	2.133913	-2.430570
C	2.425219	0.201257	1.465779
C	3.790478	0.290233	1.426491
C	4.445550	0.774724	0.253863
C	3.595823	1.139674	-0.831879
C	2.234793	1.007202	-0.725762
N	1.650198	0.546529	0.407391
H	1.889637	-0.134756	2.343704
H	4.348191	-0.004949	2.304313
H	3.998751	1.524564	-1.758295
H	1.565266	1.258091	-1.533978
N	5.786359	0.883235	0.179928
C	6.625682	0.499938	1.317029
H	6.508556	-0.562825	1.556054
H	7.668160	0.683050	1.062444
H	6.379867	1.089488	2.206738
C	6.421949	1.375890	-1.043418
H	6.101373	2.397973	-1.272519
H	7.501415	1.377528	-0.903443
H	6.185187	0.733778	-1.898795
C	-1.054103	-3.622450	0.315370
C	-0.429667	-3.063795	-0.810502
C	-0.233094	-3.848058	-1.956861
C	-0.655126	-5.175288	-1.979256
C	-1.275514	-5.729455	-0.855571
C	-1.473966	-4.952050	0.288696
H	-1.209128	-3.018462	1.202564
H	0.250805	-3.404217	-2.820302
H	-0.500561	-5.777402	-2.869701
H	-1.604063	-6.764666	-0.871930
H	-1.956471	-5.382088	1.161408
O	0.602530	-1.149057	-1.805216
C	0.048541	-1.648051	-0.842152
O	-0.200106	-1.015499	0.324940
H	-1.192101	-0.307583	2.592387
N	-1.764385	-0.964314	3.211929
N	-2.970441	-0.820021	3.058806
N	-4.113253	-0.763702	2.993511

$M1_{RB}$-1

C	1.796277	1.505149	-0.074677
O	1.789325	1.456691	1.132731
N	1.012753	2.361167	-0.887792
N	0.225991	3.085066	-0.246875
N	-0.529949	3.789363	0.212977
O	2.569197	0.791606	-0.912269
C	-1.519186	-1.061301	-1.166916
C	-2.903431	-1.133490	-1.123350
C	-3.596716	-0.602986	-0.004428
C	-2.781719	-0.040978	1.012357
C	-1.404001	-0.026307	0.855044
N	-0.744300	-0.519330	-0.209495
H	-0.998068	-1.470502	-2.031241
H	-3.431639	-1.597904	-1.946411
H	-3.211928	0.380809	1.911829
H	-0.785999	0.414580	1.635001
N	-4.960015	-0.628051	0.086802
C	-5.619442	-0.178545	1.307685
H	-5.372915	0.865404	1.532354
H	-6.698588	-0.245840	1.172363
H	-5.343254	-0.790516	2.176982
C	-5.750696	-1.299486	-0.938490
H	-5.563213	-2.381706	-0.965271
H	-6.808836	-1.140172	-0.730985
H	-5.538799	-0.891124	-1.932604
C	3.394517	-0.202247	-0.351680
C	2.824843	-1.371959	0.143359
C	4.769941	-0.004312	-0.394901
C	3.673124	-2.372874	0.620150
H	1.744807	-1.482651	0.148090

C	5.605521	-1.017454	0.082230
H	5.172090	0.920600	-0.795224
C	5.059946	-2.198483	0.590760
H	3.247337	-3.291619	1.012354
H	6.682106	-0.879133	0.055685
H	5.713492	-2.982475	0.961221

$M1_{RB}$-TS1

C	1.095375	0.827647	0.317110
O	1.125020	1.486630	1.339036
N	1.247439	1.418774	-1.020114
N	0.998956	2.629513	-1.057127
N	0.786262	3.739293	-1.187572
O	1.544353	-0.491060	0.233690
C	-1.357483	-0.515453	-0.861201
C	-2.692313	-0.861431	-0.941872
C	-3.603752	-0.390351	0.044797
C	-3.049976	0.425038	1.070230
C	-1.697719	0.711473	1.057796
N	-0.859582	0.257173	0.117719
H	-0.648277	-0.867730	-1.605062
H	-3.019869	-1.491327	-1.758393
H	-3.664314	0.828385	1.864430
H	-1.243952	1.329866	1.828923
N	-4.926312	-0.702392	0.008216
C	-5.822768	-0.230673	1.059786
H	-5.856650	0.864700	1.097448
H	-6.829253	-0.595134	0.857640
H	-5.516229	-0.600064	2.045892
C	-5.454627	-1.545499	-1.060244
H	-5.017320	-2.551370	-1.037335
H	-6.532675	-1.638652	-0.936189
H	-5.261597	-1.107953	-2.046574
C	2.910147	-0.718686	0.185527
C	3.283458	-2.028376	-0.134951
C	3.880176	0.253766	0.447505
C	4.634396	-2.365498	-0.193141
H	2.509960	-2.763473	-0.333464
C	5.230806	-0.099589	0.376378
H	3.594071	1.264145	0.713304
C	5.616561	-1.402396	0.058116
H	4.918266	-3.384261	-0.441207
H	5.983208	0.657766	0.577491
H	6.668626	-1.665814	0.008425

$M1_{RB}$-2

C	-0.745281	0.675926	-0.326156
O	-0.997269	1.428867	-1.276662
N	-1.034631	1.266198	1.157940
N	-1.252451	2.466499	1.127956
N	-1.473488	3.592772	1.124106
O	-1.342894	-0.636107	-0.243131
C	1.227617	-0.530484	0.783823
C	2.555823	-0.847158	0.891373
C	3.500734	-0.320288	-0.041823
C	2.972209	0.531898	-1.056444
C	1.628838	0.804833	-1.097647
N	0.766842	0.283471	-0.197774
H	0.488652	-0.916854	1.472503
H	2.860388	-1.505030	1.693403
H	3.609368	0.979639	-1.806435
H	1.173670	1.446241	-1.841995
N	4.814137	-0.611930	0.034347
C	5.749384	-0.080553	-0.958694
H	5.783419	1.014126	-0.926775
H	6.745902	-0.462969	-0.744219
H	5.470552	-0.393344	-1.970583
C	5.322900	-1.472496	1.103821
H	4.913941	-2.486393	1.028260
H	6.406814	-1.530221	1.022534
H	5.072820	-1.065726	2.089182
C	-2.708785	-0.770383	-0.211546
C	-3.168012	-2.071200	0.041880
C	-3.628427	0.267725	-0.415101
C	-4.535445	-2.332884	0.093532
H	-2.440268	-2.861953	0.196813
C	-4.996849	-0.011041	-0.352113
H	-3.280215	1.267137	-0.638426
C	-5.461198	-1.302799	-0.099411
H	-4.876501	-3.345603	0.290252
H	-5.704111	0.799028	-0.508933
H	-6.527038	-1.505814	-0.056224

$M1_{RB}$-TS2

C	0.699564	0.537340	0.435958
O	1.000861	1.367190	1.284759
N	0.922171	1.233546	-1.316351
N	1.209682	2.398769	-1.201241
N	1.493830	3.515576	-1.059386
O	1.361145	-0.679309	0.263428
C	-1.205249	-0.728604	-0.608540
C	-2.536800	-1.004818	-0.749293
C	-3.506721	-0.329042	0.054910
C	-2.994524	0.625758	0.985221
C	-1.648348	0.850023	1.076434
N	-0.758766	0.181621	0.299260
H	-0.449411	-1.215053	-1.208201
H	-2.828551	-1.738000	-1.488218
H	-3.649151	1.185506	1.638156
H	-1.212745	1.563039	1.763525
N	-4.823564	-0.574230	-0.060236
C	-5.788576	0.170209	0.752789
H	-5.701912	1.247640	0.577769
H	-6.794634	-0.142017	0.479410
H	-5.640962	-0.027225	1.820053
C	-5.316080	-1.568546	-1.017058
H	-4.854901	-2.545025	-0.839171
H	-6.392803	-1.671342	-0.894424
H	-5.108901	-1.263158	-2.048656
C	2.740428	-0.748362	0.216431
C	3.245674	-2.042525	0.045348
C	3.606882	0.345824	0.312196
C	4.622154	-2.245153	-0.029486
H	2.550864	-2.873256	-0.028449
C	4.984828	0.123500	0.230820
H	3.220929	1.344324	0.462617
C	5.501070	-1.161858	0.061114
H	5.005898	-3.252727	-0.161443
H	5.657188	0.973713	0.304363
H	6.573760	-1.318917	0.001786

$M1_{RB}$-3

C	-0.745281	0.675926	-0.326156
O	-0.997269	1.428867	-1.276662
N	-1.034631	1.266198	1.157940
N	-1.252451	2.466499	1.127956
N	-1.473488	3.592772	1.124106
O	-1.342894	-0.636107	-0.243131
C	1.227617	-0.530484	0.783823
C	2.555823	-0.847158	0.891373
C	3.500734	-0.320288	-0.041823
C	2.972209	0.531898	-1.056444
C	1.628838	0.804833	-1.097647
N	0.766842	0.283471	-0.197774
H	0.488652	-0.916854	1.472503
H	2.860388	-1.505030	1.693403
H	3.609368	0.979639	-1.806435
H	1.173670	1.446241	-1.841995
N	4.814137	-0.611930	0.034347
C	5.749384	-0.080553	-0.958694
H	5.783419	1.014126	-0.926775
H	6.745902	-0.462969	-0.744219
H	5.470552	-0.393344	-1.970583
C	5.322900	-1.472496	1.103821
H	4.913941	-2.486393	1.028260
H	6.406814	-1.530221	1.022534
H	5.072820	-1.065726	2.089182
C	-2.708785	-0.770383	-0.211546
C	-3.168012	-2.071200	0.041880
C	-3.628427	0.267725	-0.415101

C	-4.535445	-2.332884	0.093532
H	-2.440268	-2.861953	0.196813
C	-4.996849	-0.011041	-0.352113
H	-3.280215	1.267137	-0.638426
C	-5.461198	-1.302799	-0.099411
H	-4.876501	-3.345603	0.290252
H	-5.704111	0.799028	-0.508933
H	-6.527038	-1.505814	-0.056224

$M1_{RB}$-4 (oH_2O)

C	0.932555	-0.601840	-0.378591
O	0.925372	3.081050	-1.562517
O	1.435329	0.465217	-0.650820
H	1.183211	2.236404	-1.144358
O	1.588109	-1.701781	-0.009056
C	5.144732	-1.948206	-0.933553
C	3.752832	-1.948835	-1.048395
C	3.002516	-1.630419	0.076412
C	3.574619	-1.319697	1.303351
C	4.967963	-1.324274	1.400404
C	5.750913	-1.636725	0.286159
H	5.751734	-2.193270	-1.799521
H	3.260345	-2.192199	-1.983984
H	2.946466	-1.083727	2.155936
H	5.437831	-1.084341	2.349098
H	6.833391	-1.639353	0.368820
C	-1.296680	0.227780	-0.710291
C	-2.648547	0.086880	-0.731068
C	-3.258760	-1.169011	-0.414036
C	-2.363150	-2.253484	-0.122589
C	-1.019038	-2.065215	-0.125722
N	-0.466162	-0.836735	-0.422890
H	-0.808654	1.158151	-0.950809
H	-3.242041	0.952091	-0.987175
H	-2.732866	-3.238500	0.124603
H	-0.327006	-2.860807	0.105180
N	-4.583761	-1.323428	-0.391679
C	-5.188148	-2.634744	-0.124144
H	-5.017871	-2.940736	0.913189
H	-6.259981	-2.566199	-0.299689
H	-4.776908	-3.393085	-0.795346
C	-5.470045	-0.168510	-0.585269
H	-5.408391	0.204911	-1.612464
H	-6.493860	-0.476063	-0.383556
H	-5.202091	0.633638	0.107916
C	0.990284	4.111588	-0.686301
O	0.704311	5.228901	-1.063587
C	1.405662	3.757633	0.719696
H	0.648924	3.107936	1.180092
H	2.353838	3.209554	0.716146
H	1.514649	4.668249	1.309207
N	-0.793157	1.282707	1.970241
N	-1.962576	1.391612	2.147951
N	-3.130332	1.487663	2.318974

$M1_{RB}$-TS_3 (oH_2O)

C	-0.732157	-0.193789	-0.367373
O	-1.409913	1.726390	-1.090782
O	-1.137495	-0.512330	-1.562577
H	-1.497081	0.410348	-1.864524
O	-1.417155	-0.460910	0.709862
C	-5.075214	-0.282320	1.018150
C	-3.732874	0.105679	1.019145
C	-2.792398	-0.832482	0.619099
C	-3.110539	-2.128899	0.236915
C	-4.458229	-2.494183	0.242770
C	-5.436817	-1.575051	0.631142
H	-5.835454	0.429886	1.323209
H	-3.417226	1.102491	1.307674
H	-2.332338	-2.827602	-0.050014
H	-4.738068	-3.500267	-0.053105
H	-6.482020	-1.868345	0.635101
C	1.514144	-0.042755	-1.180875
C	2.836865	0.191987	-0.984503
C	3.343120	0.529469	0.312495
C	2.368281	0.653457	1.365356
C	1.058041	0.412475	1.129458
N	0.609034	0.056519	-0.132432
H	1.098251	-0.292770	-2.143114
H	3.494088	0.107801	-1.837270
H	2.654735	0.925296	2.371325
H	0.305276	0.497272	1.899306
N	4.640854	0.734452	0.530217
C	5.135465	1.146684	1.851191
H	5.029722	0.335456	2.578512
H	6.188682	1.404752	1.762412
H	4.593898	2.026373	2.206738
C	5.620508	0.488810	-0.536529
H	5.513769	1.222529	-1.341576
H	6.621051	0.570320	-0.117318
H	5.488489	-0.518602	-0.941388
C	-2.033055	2.725941	-0.530466
O	-1.966590	2.984493	0.674635
C	-2.869508	3.566230	-1.484670
H	-2.286259	3.844626	-2.367666
H	-3.725904	2.977420	-1.832538
H	-3.234753	4.464916	-0.983866
N	1.419787	-2.908812	-1.003248
N	2.545534	-2.881549	-0.628990
N	3.670015	-2.834975	-0.258236

$M1_{RB}$-5 (oH_2O)/ $M1_{RB}$-5

C	0.988590	-0.203497	-0.302414
O	1.233794	-1.059358	0.812581
O	1.046307	-1.017060	-1.404733
H	1.710541	-1.711076	-1.247056
O	1.849687	0.879884	-0.337842
C	5.422719	0.547876	0.464744
C	4.046281	0.720738	0.622718
C	3.222526	0.625238	-0.497433
C	3.739651	0.378530	-1.768975
C	5.118088	0.202954	-1.910598
C	5.959114	0.285034	-0.798210
H	6.073723	0.622389	1.330466
H	3.614507	0.939658	1.593282
H	3.076402	0.333897	-2.625081
H	5.532492	0.009841	-2.895452
H	7.030177	0.151930	-0.916338
C	-1.427318	-0.524777	-0.344068
C	-2.722777	-0.104431	-0.282286
C	-3.034141	1.285794	-0.138782
C	-1.907803	2.165619	-0.042133
C	-0.631801	1.685808	-0.095915
N	-0.380968	0.354435	-0.258337
H	-1.184230	-1.573940	-0.468259
H	-3.488328	-0.866490	-0.349993
H	-2.034820	3.231469	0.082003
H	0.227827	2.332428	-0.013222
N	-4.286980	1.760093	-0.094171
C	-4.535816	3.196632	0.065995
H	-4.083003	3.765253	-0.751537
H	-5.611764	3.363581	0.049179
H	-4.141821	3.562075	1.019777
C	-5.487311	0.923913	-0.145974
H	-6.021402	0.985437	0.808133
H	-6.145095	1.289324	-0.939869
H	-5.250288	-0.116684	-0.347829
C	1.137065	-0.592181	2.112422
O	0.814811	0.537638	2.386102
C	1.475897	-1.693665	3.070421
H	0.792932	-2.535997	2.923076
H	2.491696	-2.053041	2.879579
H	1.396971	-1.323624	4.092297
N	-2.150581	-3.820172	-0.725655
N	-3.287199	-3.490070	-0.640925
N	-4.425856	-3.166110	-0.556497

$M1_{RB}$-4 ($1H_2O$)

C	0.565615	-0.670400	0.272249
O	1.657948	2.173670	0.351610

O	0.964259	-0.783186	1.409685
H	1.126314	0.692261	2.747525
O	1.238614	-0.954486	-0.840929
C	4.899573	-0.852937	-1.103345
C	3.564023	-0.443247	-1.130225
C	2.593522	-1.353061	-0.729101
C	2.893163	-2.644370	-0.311915
C	4.233936	-3.034048	-0.287768
C	5.234848	-2.142164	-0.682338
H	5.675982	-0.160072	-1.413022
H	3.279786	0.554241	-1.449512
H	2.100543	-3.324281	-0.018465
H	4.491985	-4.037690	0.035683
H	6.274909	-2.453047	-0.664240
C	-1.648230	-0.088139	0.999460
C	-2.922788	0.332800	0.780665
C	-3.383326	0.617451	-0.543914
C	-2.416937	0.471688	-1.596391
C	-1.151124	0.061828	-1.325830
N	-0.747778	-0.219383	-0.038200
H	-1.269206	-0.319170	1.982125
H	-3.577104	0.424538	1.634551
H	-2.670925	0.676133	-2.626825
H	-0.407272	-0.055850	-2.099299
N	-4.639177	1.001333	-0.786119
C	-5.088331	1.298655	-2.151724
H	-5.094371	0.394002	-2.768560
H	-6.099347	1.698032	-2.106227
H	-4.441219	2.046626	-2.617181
C	-5.618955	1.059083	0.305947
H	-5.331693	1.810429	1.047972
H	-6.588505	1.329255	-0.107118
H	-5.699542	0.082246	0.793352
C	2.641424	3.008799	-0.018974
O	2.973073	3.078553	-1.188499
C	3.274216	3.820105	1.088704
H	3.745717	3.153658	1.819523
H	4.027873	4.488889	0.673170
H	2.514029	4.405601	1.616231
N	-2.127483	-2.979265	1.307910
N	-3.267261	-2.793284	1.035860
N	-4.404533	-2.597798	0.762815
H	1.541237	2.134058	1.340286
O	1.245026	1.640353	2.935041
H	2.049292	1.687431	3.475895

$M1_{RB}$-TS_3 ($1H_2O$)

C	0.762702	-0.061159	0.464130
O	1.314547	1.874753	0.730545
O	1.165412	-0.484217	1.593617
H	1.085474	0.264745	2.439781
O	1.352372	-0.430891	-0.657517
C	4.989225	-0.445016	-1.191591
C	3.668329	0.006596	-1.132428
C	2.703955	-0.860236	-0.634688
C	2.991092	-2.155090	-0.217813
C	4.316821	-2.587969	-0.284451
C	5.314205	-1.735239	-0.765821
H	5.761515	0.214274	-1.575866
H	3.380901	0.995643	-1.470574
H	2.197534	-2.803504	0.137162
H	4.565771	-3.594778	0.036326
H	6.342677	-2.079443	-0.816022
C	-1.541480	-0.296306	1.161202
C	-2.879944	-0.177091	0.938083
C	-3.370966	0.423441	-0.263319
C	-2.382639	0.941713	-1.165473
C	-1.057138	0.803875	-0.897480
N	-0.628263	0.181641	0.250876
H	-1.139743	-0.774283	2.040330
H	-3.552068	-0.570822	1.686047
H	-2.665295	1.448783	-2.077335
H	-0.273806	1.207593	-1.528850
N	-4.679142	0.502619	-0.529022
C	-5.156776	1.139786	-1.761582
H	-4.803588	0.598254	-2.644992
H	-6.244740	1.132316	-1.759459
H	-4.816413	2.177753	-1.819333
C	-5.658088	-0.097308	0.384964
H	-5.644446	0.403440	1.358237
H	-6.651361	0.007731	-0.046599
H	-5.444622	-1.161589	0.525239
C	1.584567	2.760131	-0.194649
O	1.436333	2.575563	-1.406535
C	2.111666	4.078546	0.350448
H	1.373252	4.526747	1.023539
H	3.023098	3.907046	0.932399
H	2.324795	4.769463	-0.466843
N	-0.999714	-3.156245	0.608908
N	-2.097670	-3.241437	0.165301
N	-3.196321	-3.318772	-0.273127
H	1.257915	1.914895	2.395697
O	1.089916	1.322295	3.188539
H	1.889107	1.349037	3.744185

$M1_{RB}$-5 ($1H_2O$)

C	1.171500	-0.289285	-0.199425
O	1.513797	-0.646470	1.147107
O	1.181365	-1.437721	-0.907934
H	1.035150	-2.236125	-0.320239
O	2.005028	0.668100	-0.742182
C	5.611597	0.804014	-0.054873
C	4.235374	1.007932	0.068050
C	3.376559	0.379570	-0.831835
C	3.858714	-0.432411	-1.857672
C	5.236697	-0.630613	-1.965922
C	6.113522	-0.016958	-1.067297
H	6.288581	1.290614	0.640869
H	3.827898	1.650296	0.841131
H	3.167013	-0.892754	-2.552523
H	5.623483	-1.261927	-2.760365
H	7.184042	-0.173080	-1.160260
C	-1.267766	-0.485828	0.029469
C	-2.548295	-0.016259	0.055676
C	-2.811487	1.369192	-0.186679
C	-1.670343	2.188107	-0.450501
C	-0.411420	1.657131	-0.445339
N	-0.200489	0.330502	-0.215762
H	-1.049626	-1.531596	0.202641
H	-3.338606	-0.734757	0.253920
H	-1.769367	3.245460	-0.651387
H	0.465571	2.258780	-0.624320
N	-4.054874	1.872933	-0.168744
C	-4.283435	3.288143	-0.474350
H	-3.928128	3.536372	-1.479877
H	-5.351679	3.490247	-0.426297
H	-3.774396	3.932886	0.249602
C	-5.213272	1.009879	0.086722
H	-5.070222	0.426017	0.999425
H	-6.092797	1.638173	0.218081
H	-5.393662	0.322468	-0.747520
C	1.551821	0.285436	2.162967
O	1.290946	1.454469	2.007825
C	1.961764	-0.378109	3.444237
H	2.953768	-0.825458	3.328320
H	1.978318	0.359471	4.246222
H	1.261498	-1.182325	3.689741
N	-4.668672	-2.617317	0.521674
N	-5.343196	-2.442660	-0.440729
N	-6.017414	-2.269915	-1.399790
H	1.152189	-3.612859	1.362524
O	0.594699	-3.523434	0.573180
H	0.667631	-4.373909	0.110409

$M1_{RB}$-4 ($2H_2O$)

C	-0.662081	0.705172	0.271838
O	-1.270583	-2.130998	0.275363
O	-1.063667	0.911414	1.394622
H	-0.947380	0.041082	3.070368
O	-1.333827	0.889247	-0.860678

C	-4.970947	0.691599	-1.284099
C	-3.623068	0.325328	-1.261594
C	-2.700081	1.252990	-0.795274
C	-3.057964	2.525187	-0.363952
C	-4.410444	2.871812	-0.390440
C	-5.364988	1.958869	-0.847327
H	-5.710602	-0.016446	-1.645275
H	-3.281929	-0.647505	-1.600210
H	-2.301730	3.223710	-0.022567
H	-4.714014	3.859368	-0.056973
H	-6.414272	2.237154	-0.867092
C	1.618365	0.440488	0.974333
C	2.919850	0.109953	0.753888
C	3.339554	-0.399844	-0.516003
C	2.306477	-0.607704	-1.490904
C	1.019349	-0.265583	-1.221287
N	0.665582	0.275380	-0.006332
H	1.265466	0.838029	1.912296
H	3.622198	0.255842	1.560984
H	2.523048	-1.035866	-2.459450
H	0.214775	-0.430356	-1.922495
N	4.620500	-0.677135	-0.774996
C	5.021244	-1.244494	-2.068093
H	4.819236	-0.542559	-2.883501
H	6.088918	-1.452935	-2.042976
H	4.490591	-2.180918	-2.262895
C	5.657813	-0.393119	0.224303
H	5.561839	-1.056555	1.090064
H	6.634131	-0.548135	-0.230300
H	5.588018	0.646350	0.556669
C	-1.671610	-2.972370	-0.682968
O	-1.737163	-2.595659	-1.842277
C	-2.011115	-4.377775	-0.239225
H	-1.114098	-4.872459	0.149146
H	-2.750253	-4.358227	0.567610
H	-2.400254	-4.948266	-1.082436
N	1.576733	3.366956	0.810016
N	2.725878	3.327614	0.514593
N	3.873298	3.279374	0.221057
H	-1.198977	-2.106056	3.238090
O	-0.926958	-0.531423	3.859223
H	-1.679736	-0.238035	4.395554
O	-1.315187	-2.964339	2.752989
H	-1.284315	-2.536625	1.198712
H	-0.527640	-3.484910	2.973191

$M1_{RB}$-TS_3 ($2H_2O$)

C	0.817898	0.105810	0.284758
O	1.353417	1.835470	0.251814
O	1.172856	-0.285675	1.421667
H	1.002978	0.326183	2.614238
O	1.349844	-0.458871	-0.831215
C	4.942454	-1.106643	-1.266404
C	3.712281	-0.443934	-1.278341
C	2.603251	-1.085872	-0.735676
C	2.681409	-2.369563	-0.199052
C	3.917385	-3.017846	-0.192056
C	5.047938	-2.388468	-0.721751
H	5.816187	-0.619115	-1.688548
H	3.602582	0.542875	-1.713326
H	1.788629	-2.844962	0.193195
H	3.993692	-4.018365	0.223131
H	6.006109	-2.899353	-0.716230
C	-1.518108	-0.151270	0.966268
C	-2.864259	-0.085131	0.746962
C	-3.376624	0.429233	-0.482776
C	-2.404692	0.889724	-1.427308
C	-1.071643	0.801578	-1.152124
N	-0.624446	0.290003	0.033528
H	-1.101469	-0.569823	1.869413
H	-3.520685	-0.453006	1.521516
H	-2.700022	1.303457	-2.381378
H	-0.300997	1.142589	-1.834294
N	-4.692836	0.473473	-0.737996
C	-5.190488	1.015747	-2.005540
H	-4.872751	0.398322	-2.852845
H	-6.278291	1.031927	-1.975708
H	-4.834258	2.038689	-2.158815
C	-5.650393	-0.089141	0.219572
H	-5.639220	0.467631	1.162496
H	-6.650028	-0.028207	-0.206558
H	-5.417537	-1.139612	0.422180
C	1.771651	2.511318	-0.815282
O	1.567276	2.185195	-1.979241
C	2.541920	3.766656	-0.449867
H	1.901220	4.458049	0.107538
H	3.392789	3.515973	0.190931
H	2.894254	4.260644	-1.356168
N	-1.287502	-3.382709	1.057164
N	-2.386359	-3.419995	0.610166
N	-3.485572	-3.460469	0.165942
H	0.928353	1.885059	3.281408
O	0.896007	0.856149	3.557172
H	1.650123	0.645224	4.138595
O	0.992838	3.117944	2.586644
H	1.117406	2.774534	1.660351
H	0.140164	3.584274	2.594218

$M1_{RB}$-5 ($2H_2O$)

C	-0.773922	-0.006650	0.195024
O	-1.410876	-1.283140	0.006290
O	-0.940527	0.309726	1.490200
H	-1.784774	-0.106576	1.883256
O	-1.243592	0.937028	-0.718417
C	-4.777140	1.200504	-1.683088
C	-3.437266	0.807812	-1.672754
C	-2.599737	1.280970	-0.663136
C	-3.067904	2.148297	0.324935
C	-4.412619	2.526743	0.306654
C	-5.267929	2.054577	-0.692388
H	-5.434628	0.838835	-2.468033
H	-3.036170	0.153258	-2.439188
H	-2.389006	2.520247	1.083060
H	-4.786765	3.200864	1.071413
H	-6.310430	2.357937	-0.703390
C	1.457140	-0.770482	0.848197
C	2.798084	-0.949063	0.671874
C	3.455463	-0.429408	-0.487262
C	2.621481	0.273030	-1.410919
C	1.280708	0.403313	-1.187092
N	0.692160	-0.111587	-0.070363
H	0.939699	-1.134478	1.724551
H	3.341311	-1.472112	1.445699
H	3.025285	0.725218	-2.305292
H	0.631468	0.917844	-1.877160
N	4.772196	-0.590748	-0.693341
C	5.432127	0.073489	-1.820106
H	5.436016	1.161284	-1.683371
H	6.460762	-0.278026	-1.879945
H	4.933999	-0.169832	-2.761762
C	5.617936	-1.185653	0.344718
H	5.247402	-2.173062	0.631643
H	6.625913	-1.303416	-0.049895
H	5.656625	-0.541045	1.230596
C	-1.367286	-1.957386	-1.192203
O	-0.725058	-1.588228	-2.147360
C	-2.239306	-3.177776	-1.126981
H	-2.245816	-3.612247	-0.125754
H	-3.266534	-2.879128	-1.367478
H	-1.904985	-3.903349	-1.869434
N	2.340619	2.659875	1.758254
N	3.488782	2.491029	1.514460
N	4.640196	2.326318	1.272580
H	-2.926709	-1.693658	2.557692
O	-3.027098	-0.710321	2.599124
H	-3.811157	-0.511669	2.064359
O	-2.604130	-3.393058	2.418542
H	-1.647995	-3.521332	2.523619
H	-2.999910	-3.929723	3.123828

$M1_{RB}$-TS_3 ($3H_2O$)

C	0.883727	-0.346156	-0.064954
O	1.290999	-1.038644	1.268294
O	1.426897	-0.991732	-0.998735
H	1.149499	-2.032714	-2.087183
O	1.179145	1.019015	0.078693
C	4.818031	1.436730	-0.474235
C	3.617188	0.808548	-0.135063
C	2.418682	1.511507	-0.289137
C	2.417643	2.825203	-0.766460
C	3.625939	3.441514	-1.091335
C	4.831800	2.749596	-0.950277
H	5.750068	0.890754	-0.357704
H	3.614525	-0.208460	0.234287
H	1.471035	3.346803	-0.869139
H	3.621145	4.463776	-1.458505
H	5.771725	3.228948	-1.206857
C	-1.434977	0.694753	0.172731
C	-2.801600	0.616601	0.111772
C	-3.447075	-0.617302	-0.194634
C	-2.587339	-1.741004	-0.393012
C	-1.230344	-1.589353	-0.327638
N	-0.648445	-0.390380	-0.060455
H	-0.933718	1.624882	0.392731
H	-3.361062	1.527478	0.280628
H	-2.981414	-2.725552	-0.602429
H	-0.557822	-2.420637	-0.483633
N	-4.785244	-0.715314	-0.292359
C	-5.418436	-1.998496	-0.602450
H	-5.285422	-2.719277	0.212601
H	-6.484798	-1.837026	-0.751056
H	-5.006173	-2.426099	-1.521387
C	-5.632486	0.448748	-0.020167
H	-5.376257	1.285488	-0.677781
H	-6.671808	0.176402	-0.195324
H	-5.529489	0.779231	1.019452
C	0.902890	-0.608778	2.498941
O	0.132449	0.308130	2.688294
C	1.546484	-1.433993	3.585196
H	1.229461	-2.478320	3.501272
H	2.635958	-1.409383	3.487816
H	1.253979	-1.042988	4.559958
N	-1.268397	4.214320	0.024051
N	-2.444378	4.103791	-0.091177
N	-3.621575	4.004271	-0.204561
H	1.498843	-3.820996	-1.944226
O	1.010759	-2.861294	-2.657758
H	1.493159	-2.736052	-3.492171
O	1.916982	-4.589338	-1.224332
H	2.272724	-4.099854	-0.368027
H	1.221796	-5.218103	-0.959860
O	2.741483	-3.371395	0.803170
H	2.251724	-2.524399	0.916516
H	3.678132	-3.127366	0.724870

$M1_{RB}$-TS_4

C	3.578043	-2.683256	0.483289
C	2.665568	-1.631529	0.612673
C	2.878521	-0.452257	-0.110666
C	3.989130	-0.338126	-0.956705
C	4.886770	-1.396790	-1.077175
C	4.686708	-2.578125	-0.356923
H	3.409234	-3.594596	1.050193
H	1.819671	-1.736175	1.278390
H	4.132732	0.584795	-1.509829
H	5.744385	-1.295280	-1.736120
H	5.386700	-3.403025	-0.448337
C	1.047546	0.898732	0.855347
O	1.473867	0.536549	2.129455
O	2.047762	0.654637	-0.119892
C	-0.072266	2.874466	-0.469955
O	-0.097643	2.197610	-1.490515
O	0.699503	2.182555	0.846888
C	0.512416	4.272029	-0.400107
H	1.560662	4.230875	-0.710032
H	-0.036401	4.914005	-1.095499
H	0.446746	4.692347	0.604357
C	-1.085646	-0.196460	1.510534
C	-2.218329	-0.930323	1.292066
C	-2.437709	-1.559529	0.028042
C	-1.428311	-1.350979	-0.957941
C	-0.325041	-0.590656	-0.675539
N	-0.135140	-0.035885	0.550039
H	-0.886620	0.283831	2.458223
H	-2.930541	-1.020632	2.100261
H	-1.511353	-1.774892	-1.948659
H	0.438633	-0.394703	-1.411203
N	-3.534482	-2.298080	-0.218145
C	-3.735204	-2.909514	-1.534006
H	-2.937072	-3.623367	-1.763994
H	-4.684862	-3.441035	-1.534415
H	-3.763984	-2.148483	-2.321104
C	-4.551110	-2.486465	0.819189
H	-4.999967	-1.531183	1.112043
H	-5.336091	-3.131805	0.428986
H	-4.123724	-2.962466	1.707906
H	1.654036	1.376555	2.584388
N	-1.579534	3.048758	0.307106
N	-2.446720	2.472913	-0.315088
N	-3.263639	1.920453	-0.916166

$M1_{RB}$-6

C	3.838565	-2.454403	-1.392847
C	2.968738	-1.487788	-0.884356
C	3.459740	-0.579050	0.049221
C	4.783070	-0.597118	0.477227
C	5.641960	-1.568567	-0.042967
C	5.172074	-2.496768	-0.975270
H	3.471953	-3.173585	-2.119358
H	1.926924	-1.433591	-1.187224
H	5.128170	0.135892	1.199293
H	6.677776	-1.596049	0.281707
H	5.843473	-3.249553	-1.377339
C	1.697262	0.246481	1.457287
O	1.737031	-0.992097	1.965615
O	2.626861	0.459365	0.507982
C	0.358209	3.614771	-0.514210
O	0.182653	3.013611	-1.554144
O	0.945785	1.126707	1.810780
C	1.678562	4.029897	0.058202
H	2.467884	3.854309	-0.672676
H	1.656092	5.083243	0.351434
H	1.868423	3.431616	0.955265
C	-1.116239	-2.341712	-0.164853
C	-2.456718	-2.580592	0.099025
C	-3.406374	-1.549216	-0.121426
C	-2.882498	-0.327808	-0.618809
C	-1.519540	-0.208709	-0.845240
N	-0.615816	-1.183444	-0.632307
H	-0.394563	-3.138256	0.010290
H	-2.755378	-3.553855	0.467777
H	-3.525346	0.518882	-0.823752
H	-1.128221	0.735043	-1.221129
N	-4.737916	-1.718930	0.128979
C	-5.681081	-0.648150	-0.171968
H	-5.684734	-0.394702	-1.240122
H	-6.684437	-0.971072	0.104212
H	-5.449896	0.262400	0.393932
C	-5.237571	-3.004971	0.600624
H	-4.751294	-3.303267	1.536875
H	-6.307909	-2.923144	0.788915
H	-5.078981	-3.803503	-0.136300
H	1.018091	-1.054153	2.619905
N	-0.726715	4.012205	0.345106
N	-1.856880	3.676806	-0.054150
N	-2.923477	3.418345	-0.334971

$M1_{RB}$-TS_5

C	-5.558507	-0.564888	2.109891

C	-4.386796	-0.221442	1.434594
C	-4.445350	0.065758	0.069519
C	-5.655772	0.022622	-0.620777
C	-6.824510	-0.317465	0.065505
C	-6.779329	-0.613912	1.429527
H	-5.517446	-0.790145	3.171796
H	-3.435093	-0.172769	1.953927
H	-5.673561	0.258606	-1.680203
H	-7.769246	-0.350185	-0.469571
H	-7.688811	-0.877629	1.961157
C	-2.272363	-0.372592	-0.874645
O	-2.481188	-1.591960	-0.531329
O	-3.315022	0.503888	-0.611462
C	0.878017	3.116779	-0.803597
O	1.982640	2.884254	-1.253698
O	-1.282443	0.115936	-1.414443
C	-0.369003	3.344333	-1.599475
H	-0.106320	3.598030	-2.627229
H	-0.945729	2.408836	-1.593017
H	-0.982730	4.130131	-1.152257
C	2.575570	-2.997039	-0.015682
C	3.829811	-2.514265	0.293686
C	4.105549	-1.124520	0.153367
C	3.029156	-0.314947	-0.306566
C	1.809998	-0.893657	-0.590887
N	1.569605	-2.213990	-0.452928
H	2.349994	-4.054862	0.085772
H	4.584589	-3.206636	0.641823
H	3.140679	0.752110	-0.444706
H	0.969948	-0.300376	-0.942360
N	5.324600	-0.602222	0.440245
C	5.561458	0.833104	0.305121
H	4.871702	1.412807	0.929533
H	6.578511	1.055158	0.625157
H	5.446933	1.164415	-0.734082
C	6.411063	-1.470058	0.887625
H	6.626895	-2.251607	0.150036
H	7.311021	-0.871204	1.021134
H	6.174221	-1.953035	1.843326
H	-1.554345	-2.328758	-0.805386
H	0.358378	-2.704035	-0.771909
O	-0.684359	-3.114859	-1.044958
H	-0.688144	-3.273215	-2.001931
N	0.611580	3.163791	0.610235
N	1.597167	2.932226	1.335257
N	2.430990	2.735826	2.076172

$M1_{RB}$-7

C	-0.435932	3.231728	1.167014
C	0.272443	2.028691	1.175753
C	0.485501	1.340605	-0.027664
C	-0.011136	1.865980	-1.226930
C	-0.711976	3.073479	-1.225209
C	-0.931625	3.761363	-0.028972
H	-0.593072	3.762301	2.102381
H	0.659936	1.622383	2.103036
H	0.166841	1.322753	-2.150207
H	-1.088834	3.473977	-2.162393
H	-1.477303	4.700266	-0.027656
C	1.120421	-0.864506	0.852010
O	0.049472	-0.907427	1.510140
O	1.253712	0.208290	-0.107626
C	6.126719	-0.746982	-0.245937
O	6.325614	-1.612208	0.580441
O	2.095502	-1.614612	0.865860
C	4.795453	-0.235518	-0.702894
H	3.986614	-0.743891	-0.173354
H	4.739615	0.844600	-0.529079
H	4.697645	-0.390930	-1.783264
C	-3.215496	0.387861	0.725287
C	-4.533342	0.368401	0.346769
C	-5.117758	-0.835679	-0.151943
C	-4.259608	-1.975106	-0.226627
C	-2.952234	-1.876609	0.174620
N	-2.439044	-0.715914	0.641285
H	-2.735443	1.281762	1.104788
H	-5.107014	1.280711	0.431044
H	-4.618032	-2.927856	-0.590229
H	-2.271197	-2.718634	0.138756
N	-6.410685	-0.893909	-0.528912
C	-6.971732	-2.136589	-1.061957
H	-6.945609	-2.936926	-0.313891
H	-8.008478	-1.961940	-1.344321
H	-6.423352	-2.468086	-1.950044
C	-7.270054	0.285413	-0.412029
H	-6.920933	1.098209	-1.058729
H	-8.280869	0.015002	-0.712123
H	-7.303066	0.648147	0.620644
H	-1.424554	-0.691151	0.950582
N	7.205700	-0.068162	-0.925932
N	8.344495	-0.440420	-0.589655
N	9.415938	-0.715628	-0.344530

$M1_{RB}$-8

C	-0.862317	-5.880883	-1.154675
C	-0.640938	-4.502904	-1.112217
C	-0.127115	-3.942132	0.055150
C	0.177409	-4.718518	1.169604
C	-0.044251	-6.097074	1.113006
C	-0.565522	-6.678757	-0.045367
H	-1.264930	-6.330083	-2.057813
H	-0.861192	-3.871441	-1.967078
H	0.582449	-4.248131	2.060233
H	0.190625	-6.712716	1.976342
H	-0.737786	-7.750224	-0.085354
C	-0.853509	-1.662453	0.179616
O	-2.027531	-2.025889	0.234629
O	0.173134	-2.573197	0.103191
C	0.611550	2.282031	1.772706
O	1.008005	1.929561	0.649091
O	-0.430288	-0.447386	0.192499
C	0.412714	1.361880	2.929620
H	-0.346576	0.622819	2.653341
H	1.348228	0.825134	3.120019
H	0.102135	1.899641	3.824685
C	-5.391545	-0.802533	0.085252
C	-6.511591	-0.042732	-0.126639
C	-6.386447	1.328537	-0.511485
C	-5.055622	1.833237	-0.649131
C	-3.982492	1.013403	-0.418444
N	-4.149992	-0.281170	-0.058296
H	-5.442668	-1.845893	0.372608
H	-7.479832	-0.506844	-0.001054
H	-4.868430	2.859555	-0.932628
H	-2.958410	1.354323	-0.511443
N	-7.465419	2.102681	-0.733141
C	-7.304525	3.497487	-1.150763
H	-6.733774	3.565343	-2.082898
H	-8.288570	3.931905	-1.318637
H	-6.792584	4.085496	-0.380783
C	-8.814784	1.560717	-0.555706
H	-8.959114	1.190190	0.464686
H	-9.539068	2.352122	-0.739710
H	-9.008630	0.742046	-1.257614
H	-3.319146	-0.886275	0.092012
N	0.309500	3.612053	2.039845
N	0.464952	4.405584	1.071894
N	0.558470	5.221830	0.302031
Cu	1.426108	-0.026504	0.056365
C	3.711277	1.076137	-1.311431
C	5.030476	1.379554	-1.554269
C	6.044444	0.908022	-0.668918
C	5.596863	0.135706	0.443365
C	4.255224	-0.118998	0.606933
N	3.310612	0.325375	-0.257077
H	2.930026	1.430273	-1.976504
H	5.272401	1.975458	-2.423843
H	6.292139	-0.263388	1.169435
H	3.901930	-0.705723	1.448871

N	7.351840	1.181864	-0.867272
C	8.358979	0.697315	0.077060
H	8.367989	-0.397772	0.118891
H	9.340495	1.037291	-0.249095
H	8.177329	1.084346	1.085946
C	7.775743	1.989024	-2.011870
H	7.370371	3.005946	-1.955388
H	8.862854	2.050595	-2.015560
H	7.454178	1.535981	-2.955830

$M1_{RB}$-TS6

C	-1.184363	5.078679	-1.111377
C	-0.927216	3.706042	-1.157981
C	-0.620549	3.047788	0.028165
C	-0.566131	3.706432	1.253658
C	-0.819535	5.079044	1.283534
C	-1.129181	5.764507	0.104886
H	-1.425672	5.609187	-2.027531
H	-0.962729	3.154119	-2.091866
H	-0.331764	3.156094	2.159544
H	-0.778723	5.609818	2.229915
H	-1.329849	6.831230	0.135307
C	0.850150	1.091883	0.202039
O	1.854541	1.782927	0.254306
O	-0.417119	1.655270	-0.019232
C	-0.529207	-3.163952	1.193372
O	-1.096209	-2.487434	0.307588
O	0.708543	-0.178186	0.304642
C	0.125136	-2.613066	2.499061
H	0.896795	-1.920225	2.154584
H	-0.689394	-2.121118	3.037771
H	0.579320	-3.368214	3.145442
C	5.496597	1.560852	0.193618
C	6.785010	1.146364	-0.016135
C	7.053925	-0.213210	-0.369290
C	5.922381	-1.082554	-0.465848
C	4.661394	-0.597725	-0.242707
N	4.455161	0.701833	0.079532
H	5.249434	2.582594	0.455387
H	7.580549	1.870923	0.087117
H	6.033361	-2.126853	-0.721423
H	3.777182	-1.219261	-0.313636
N	8.305111	-0.650778	-0.601538
C	8.546856	-2.049747	-0.963040
H	8.023003	-2.314348	-1.887940
H	9.614611	-2.193307	-1.119035
H	8.218762	-2.726171	-0.166422
C	9.442627	0.267136	-0.503299
H	9.539001	0.671490	0.510084
H	10.354456	-0.275885	-0.745737
H	9.338513	1.099729	-1.207180
H	3.492045	1.046237	0.215331
N	-0.285633	-4.406799	1.393434
N	-1.030227	-5.278726	-0.131617
N	-1.295378	-6.137380	-0.773421
Cu	-1.206127	-0.462747	0.169058
C	-3.775087	-1.282529	-0.892436
C	-5.136129	-1.267595	-1.092240
C	-5.943841	-0.296070	-0.431627
C	-5.253378	0.618034	0.416781
C	-3.887621	0.529629	0.555332
N	-3.137300	-0.396409	-0.090308
H	-3.153779	-2.023351	-1.383911
H	-5.568970	-2.003955	-1.755939
H	-5.778171	1.391893	0.960526
H	-3.354266	1.223395	1.197725
N	-7.283719	-0.246631	-0.596777
C	-8.078261	0.758671	0.108918
H	-7.784382	1.773835	-0.181449
H	-9.128284	0.619754	-0.143554
H	-7.969346	0.661008	1.194948
C	-7.956344	-1.206307	-1.472428
H	-7.813779	-2.234433	-1.120414
H	-9.023650	-0.990166	-1.479016
H	-7.584135	-1.134592	-2.500608

$M1_{RB}$-9

C	-0.035128	-5.503859	-1.518214
C	0.172640	-4.147386	-1.256637
C	0.204360	-3.716180	0.066636
C	0.038874	-4.597094	1.131777
C	-0.169184	-5.950925	0.857379
C	-0.206612	-6.405350	-0.464149
H	-0.060949	-5.853148	-2.546212
H	0.311929	-3.432111	-2.061444
H	0.073898	-4.226192	2.151366
H	-0.300185	-6.649640	1.678396
H	-0.366495	-7.459219	-0.671744
C	-0.554618	-1.498089	0.524822
O	-1.717954	-1.894355	0.570978
O	0.488154	-2.365869	0.325707
C	-0.102105	2.713070	0.454764
O	0.990497	2.277932	0.157039
O	-0.156787	-0.280891	0.656482
C	-2.369811	3.810097	1.062071
H	-3.167282	3.067377	1.141393
H	-2.261644	4.331962	2.015878
H	-2.619488	4.527744	0.276862
C	-4.399624	-0.196502	-1.046459
C	-5.539692	0.501732	-1.344790
C	-6.278759	1.147295	-0.304931
C	-5.760977	1.015118	1.021807
C	-4.613966	0.298615	1.244356
N	-3.945955	-0.293883	0.225960
H	-3.811225	-0.699976	-1.804173
H	-5.859558	0.550197	-2.376144
H	-6.258684	1.465634	1.869063
H	-4.191805	0.169914	2.233841
N	-7.402882	1.841223	-0.562099
C	-8.129204	2.505451	0.522579
H	-7.495442	3.242382	1.027445
H	-8.991874	3.021388	0.104547
H	-8.484574	1.780148	1.262633
C	-7.910017	1.947217	-1.932129
H	-8.131267	0.958403	-2.347992
H	-8.829283	2.530220	-1.923894
H	-7.186287	2.448899	-2.583895
H	-3.081020	-0.834590	0.417059
N	-1.144734	3.157460	0.734529
Cu	1.625629	0.239396	0.315631
C	3.902063	1.445599	-1.039910
C	5.218047	1.802205	-1.220081
C	6.210227	1.362172	-0.294338
C	5.744943	0.563409	0.791532
C	4.408626	0.256483	0.892842
N	3.485767	0.669781	-0.010406
H	3.139130	1.778078	-1.736006
H	5.474260	2.417469	-2.071850
H	6.421608	0.185463	1.545670
H	4.040300	-0.349185	1.715079
N	7.513321	1.689722	-0.430601
C	8.490098	1.267746	0.574192
H	8.518962	0.176414	0.662169
H	9.477403	1.613619	0.272560
H	8.258874	1.691849	1.558214
C	7.952767	2.541825	-1.535945
H	7.526286	3.549042	-1.459692
H	9.038243	2.622702	-1.507746
H	7.665343	2.112111	-2.501046

$M1_{RB}$-TS7

C	0.674466	-3.310183	1.931455
C	0.460504	-2.041007	1.399052
C	0.833540	-1.768339	0.067398
C	1.430603	-2.778734	-0.712061
C	1.639542	-4.042613	-0.166661
C	1.263347	-4.314904	1.154350
H	0.383330	-3.517074	2.957289
H	0.008438	-1.257152	2.000743
H	1.713932	-2.553673	-1.735719

H	2.096306	-4.819685	-0.772865
H	1.428569	-5.301983	1.575491
C	-0.954014	0.543535	-0.065926
O	-1.897495	-0.158370	-0.023523
O	0.613135	-0.557783	-0.491041
C	1.514462	4.062566	0.262478
O	2.199217	3.111161	-0.046462
O	-0.378095	1.602821	-0.025769
C	0.100731	6.140252	0.901489
H	0.505510	6.606816	1.802670
H	0.126014	6.856902	0.076986
H	-0.931653	5.832500	1.084071
C	-5.573135	-1.287374	-0.564355
C	-6.928562	-1.439113	-0.671172
C	-7.807881	-0.412523	-0.201167
C	-7.191584	0.742680	0.376600
C	-5.828548	0.830035	0.453985
N	-5.038975	-0.169670	-0.011918
H	-4.870090	-2.035297	-0.909205
H	-7.309591	-2.345891	-1.119372
H	-7.781192	1.562794	0.761619
H	-5.319413	1.684153	0.882690
N	-9.143273	-0.527002	-0.298199
C	-10.017674	0.548769	0.177016
H	-9.805395	1.487083	-0.346216
H	-11.052258	0.272488	-0.018424
H	-9.897983	0.709859	1.253898
C	-9.745179	-1.729372	-0.880950
H	-9.468902	-2.623163	-0.311544
H	-10.828373	-1.626187	-0.856891
H	-9.431407	-1.862367	-1.921806
H	-4.028582	-0.079737	0.054645
N	0.883769	4.997494	0.563917
Cu	1.695142	1.063073	-0.196589
C	4.401507	0.757658	-1.216671
C	5.716253	0.351752	-1.275461
C	6.246976	-0.490733	-0.256679
C	5.340542	-0.868196	0.775523
C	4.039547	-0.415747	0.748887
N	3.558563	0.392533	-0.222698
H	3.991776	1.401806	-1.988135
H	6.323726	0.689457	-2.104410
H	5.648898	-1.507410	1.591844
H	3.340154	-0.703940	1.527214
N	7.534088	-0.907977	-0.268675
C	8.044246	-1.754744	0.808481
H	7.503576	-2.706893	0.858649
H	9.095837	-1.967448	0.622132
H	7.960483	-1.255889	1.781011
C	8.433204	-0.499602	-1.347014
H	8.556243	0.589493	-1.374086
H	9.410696	-0.951003	-1.182528
H	8.061561	-0.832315	-2.322906

$M1_{RB}$-10

C	-1.811907	4.639807	1.031234
C	-1.781951	3.326284	0.590138
C	-0.691969	2.869065	-0.199467
C	0.343451	3.781632	-0.545346
C	0.304323	5.089893	-0.081424
C	-0.770499	5.526141	0.705680
H	-2.642678	4.984732	1.639763
H	-2.573351	2.630080	0.849348
H	1.151148	3.433816	-1.184369
H	1.101434	5.779574	-0.342133
H	-0.803601	6.552334	1.058246
O	-0.636519	1.607998	-0.604028
C	0.229140	-0.549702	2.509954
O	0.477492	0.479790	1.936012
C	-0.019370	-2.696397	3.892438
H	-0.254046	-3.593790	3.315432
H	0.987710	-2.782732	4.307922
H	-0.743723	-2.598819	4.704688
C	-3.163435	-0.977523	0.343037
C	-4.282344	-1.766490	0.328678
C	-5.282402	-1.578055	-0.676494
C	-5.037490	-0.543466	-1.633386
C	-3.894252	0.206123	-1.559218
N	-2.974208	-0.009971	-0.587296
H	-2.385180	-1.086888	1.088789
H	-4.383955	-2.526023	1.091247
H	-5.741969	-0.330283	-2.425177
H	-3.671686	1.000400	-2.261308
N	-6.394721	-2.333240	-0.719953
C	-7.395140	-2.122178	-1.769559
H	-6.958194	-2.262976	-2.763923
H	-8.197240	-2.846840	-1.640552
H	-7.822692	-1.115263	-1.711465
C	-6.624205	-3.375427	0.283757
H	-6.645725	-2.951920	1.293452
H	-7.585553	-3.846888	0.087887
H	-5.844722	-4.144007	0.241091
H	-2.125433	0.577611	-0.551284
N	-0.104238	-1.548174	3.039205
Cu	1.013738	0.757690	-0.259949
C	3.539977	-0.414986	0.730674
C	4.789227	-0.988236	0.633835
C	5.355055	-1.254376	-0.645863
C	4.552189	-0.894553	-1.765537
C	3.311970	-0.329724	-1.568198
N	2.785303	-0.081722	-0.343291
H	3.112007	-0.204152	1.705080
H	5.323315	-1.220281	1.545715
H	4.891839	-1.054870	-2.780161
H	2.696620	-0.054701	-2.419191
N	6.579606	-1.812487	-0.790502
C	7.139480	-2.026521	-2.124116
H	7.228350	-1.083701	-2.676413
H	8.134339	-2.458944	-2.025451
H	6.521644	-2.715709	-2.711519
C	7.373345	-2.165601	0.385115
H	6.834532	-2.867981	1.030575
H	8.295693	-2.643089	0.057764
H	7.633583	-1.279085	0.975852

$M1_{RB}$-TS8

C	-3.394805	3.412410	0.985727
C	-2.645992	2.249408	1.138566
C	-1.499314	2.046787	0.344636
C	-1.127431	3.011984	-0.611898
C	-1.886044	4.171310	-0.751478
C	-3.019959	4.377999	0.042922
H	-4.273825	3.569110	1.604087
H	-2.923406	1.493236	1.866078
H	-0.251843	2.849865	-1.233470
H	-1.593022	4.916056	-1.485654
H	-3.607924	5.283250	-0.073606
O	-0.776469	0.913550	0.541585
C	0.978827	0.747140	-0.066437
O	0.816028	-0.161087	-0.886679
C	1.636367	2.504816	1.499705
H	1.561619	3.480061	1.009544
H	0.745487	2.339174	2.110074
H	2.516884	2.512073	2.145518
C	4.900669	-0.650110	1.033417
C	6.133580	-1.242724	0.978031
C	7.098255	-0.806124	0.016248
C	6.699097	0.259873	-0.850220
C	5.449265	0.807465	-0.737630
N	4.568989	0.356736	0.188970
H	4.139135	-0.950601	1.742563
H	6.351943	-2.042527	1.671688
H	7.367360	0.655243	-1.602246
H	5.106048	1.615669	-1.371842
N	8.316936	-1.369374	-0.068758
C	9.272453	-0.922568	-1.086031
H	9.546645	0.127632	-0.937895
H	10.173912	-1.528260	-1.011851
H	8.858272	-1.040765	-2.092887

C	8.704845	-2.439593	0.853947
H	8.064732	-3.320065	0.730615
H	9.733426	-2.728143	0.645411
H	8.644729	-2.102406	1.894056
H	3.630723	0.776775	0.248206
N	1.802257	1.460628	0.502651
Cu	-1.112340	-0.700942	-0.667750
C	-3.433171	-1.887831	0.610106
C	-4.757226	-2.184837	0.841411
C	-5.760237	-1.708069	-0.051570
C	-5.297250	-0.930370	-1.152373
C	-3.951327	-0.682290	-1.301751
N	-3.011650	-1.151001	-0.445875
H	-2.663161	-2.245313	1.286164
H	-5.009726	-2.783203	1.706460
H	-5.983073	-0.522777	-1.882908
H	-3.591287	-0.086863	-2.134578
N	-7.072738	-1.973806	0.136307
C	-8.071898	-1.454387	-0.796808
H	-7.877207	-1.799420	-1.818189
H	-9.055154	-1.813384	-0.496673
H	-8.088255	-0.357981	-0.796718
C	-7.511901	-2.747420	1.297258
H	-7.229872	-2.255172	2.235125
H	-8.596833	-2.837507	1.271008
H	-7.082304	-3.755664	1.289686

$M1_{RB}$-11

C	2.067637	5.481484	-0.409222
C	1.625107	4.294855	-0.991982
C	0.658475	3.530279	-0.332706
C	0.135111	3.931750	0.898678
C	0.587745	5.125971	1.466261
C	1.551526	5.903544	0.820462
H	2.817416	6.077919	-0.920858
H	2.012250	3.955672	-1.947659
H	-0.613286	3.332125	1.406934
H	0.181253	5.443562	2.422104
H	1.898139	6.828878	1.270146
O	0.284320	2.353198	-0.968166
C	-0.803606	1.615199	-0.499502
O	-0.473461	0.521867	0.117720
C	-2.357477	3.182923	-1.418279
H	-2.528631	3.997747	-0.704072
H	-1.585687	3.505119	-2.125370
H	-3.289846	3.028688	-1.969261
C	-4.181939	-0.875987	-1.142278
C	-5.149180	-1.837476	-0.999549
C	-5.997510	-1.833571	0.150396
C	-5.769688	-0.794618	1.104843
C	-4.781429	0.131939	0.890001
N	-4.001063	0.091230	-0.214074
H	-3.519639	-0.843841	-1.999870
H	-5.249728	-2.586669	-1.772659
H	-6.365753	-0.714253	2.003216
H	-4.579733	0.935254	1.589012
N	-6.960777	-2.760036	0.325434
C	-7.805566	-2.734607	1.521122
H	-8.365654	-1.795741	1.591358
H	-8.518520	-3.555629	1.466180
H	-7.207860	-2.855300	2.431343
C	-7.174691	-3.805268	-0.677552
H	-6.281495	-4.428233	-0.798043
H	-7.996772	-4.441585	-0.354084
H	-7.434013	-3.372478	-1.650099
H	-3.235279	0.816711	-0.361115
N	-2.019342	1.945953	-0.726284
Cu	1.217788	-0.272577	0.094140
C	3.319500	-1.953119	-0.907585
C	4.546310	-2.573006	-0.954461
C	5.486647	-2.373053	0.099051
C	5.064463	-1.522900	1.163555
C	3.817381	-0.943894	1.127182
N	2.946315	-1.136926	0.107425
H	2.595522	-2.093659	-1.704127
H	4.775209	-3.202878	-1.803406
H	5.707207	-1.313611	2.007990
H	3.484343	-0.292570	1.928978
N	6.704090	-2.958147	0.091013
C	7.641427	-2.729830	1.191199
H	7.229005	-3.080316	2.144091
H	8.560260	-3.279027	0.991639
H	7.888835	-1.666621	1.287726
C	7.101785	-3.823519	-1.019948
H	7.097495	-3.276833	-1.969745
H	8.111655	-4.187942	-0.838628
H	6.433855	-4.687390	-1.110939

$M1_{RB}$-TS_9

C	-3.284460	3.664551	-0.465484
C	-1.924645	3.678114	-0.779970
C	-1.028987	3.033857	0.070976
C	-1.479675	2.360048	1.229278
C	-2.861365	2.353972	1.518153
C	-3.757616	3.001187	0.676462
H	-3.983423	4.173463	-1.122167
H	-1.552273	4.192108	-1.659538
H	-0.767185	2.001545	1.968484
H	-3.207021	1.854709	2.417395
H	-4.818019	3.003948	0.905727
O	0.314631	3.155962	-0.207387
C	1.145423	2.058687	-0.151298
O	0.654637	0.877644	-0.120077
C	2.930340	3.667675	-0.230490
H	2.612741	4.192165	-1.138647
H	2.610605	4.257762	0.635513
H	4.021828	3.615456	-0.227739
C	4.681222	0.006863	1.059749
C	5.688356	-0.928629	1.143829
C	6.270900	-1.450918	-0.047892
C	5.747222	-0.950944	-1.275644
C	4.737046	-0.015345	-1.258086
N	4.203411	0.464710	-0.115876
H	4.225396	0.421728	1.953981
H	6.021730	-1.249812	2.121500
H	6.125307	-1.292202	-2.229789
H	4.323390	0.380707	-2.180773
N	7.266626	-2.367782	-0.015057
C	7.841628	-2.878800	-1.258664
H	8.246599	-2.065584	-1.871331
H	8.656305	-3.560247	-1.017653
H	7.097762	-3.423936	-1.852029
C	7.753239	-2.880858	1.264564
H	6.951207	-3.370395	1.829278
H	8.536030	-3.614332	1.077245
H	8.173268	-2.078716	1.882406
N	2.418217	2.301591	-0.181552
H	3.290278	1.328194	-0.149802
Cu	-1.140442	0.252978	0.103198
C	-3.737948	-0.438578	-0.915276
C	-4.902997	-1.156115	-1.053604
C	-5.204686	-2.207913	-0.138064
C	-4.261252	-2.416241	0.911627
C	-3.121886	-1.648345	0.973385
N	-2.836672	-0.682998	0.066336
H	-3.490921	0.358131	-1.609212
H	-5.566770	-0.911515	-1.871786
H	-4.410977	-3.179101	1.663512
H	-2.390729	-1.801934	1.760467
N	-6.319472	-2.960694	-0.257740
C	-6.609676	-4.014072	0.716131
H	-6.730616	-3.602414	1.724380
H	-7.536909	-4.509496	0.433035
H	-5.809604	-4.762477	0.736642
C	-7.266947	-2.715660	-1.346232
H	-6.771514	-2.783694	-2.320577
H	-8.050061	-3.471337	-1.307242
H	-7.731937	-1.726927	-1.257757

$M1_{RB}$-12

C	0.902788	4.568806	-1.757712
C	1.246820	3.759741	-0.672044
C	0.313689	3.581009	0.344112
C	-0.938039	4.186464	0.321752
C	-1.267632	4.993417	-0.770451
C	-0.351516	5.183465	-1.808689
H	1.618764	4.719601	-2.559994
H	2.218309	3.279979	-0.608422
H	-1.632053	4.032484	1.141773
H	-2.240292	5.474699	-0.804898
H	-0.612695	5.812729	-2.654181
O	0.685450	2.827157	1.477560
C	0.465024	1.503443	1.471354
O	-0.152340	0.956170	0.523999
C	1.652608	1.542844	3.641416
H	2.541807	2.059217	3.271846
H	1.006167	2.261035	4.152772
H	1.957055	0.770903	4.347715
C	-2.954716	-0.108811	-0.212554
C	-4.322885	-0.246358	-0.258984
C	-4.911525	-1.544409	-0.249543
C	-4.002435	-2.641243	-0.197245
C	-2.646589	-2.407621	-0.156595
N	-2.107548	-1.164132	-0.165414
H	-2.497291	0.873913	-0.208121
H	-4.929413	0.648588	-0.298039
H	-4.351115	-3.665149	-0.187143
H	-1.946059	-3.236637	-0.116662
N	-6.251096	-1.722719	-0.282847
C	-6.819757	-3.069880	-0.248186
H	-6.550024	-3.594681	0.675803
H	-7.905292	-2.996710	-0.296305
H	-6.477525	-3.667609	-1.100367
C	-7.147143	-0.566497	-0.308568
H	-6.965673	0.055519	-1.192024
H	-8.177135	-0.917982	-0.343414
H	-7.023118	0.053487	0.586806
N	0.941623	0.883861	2.545690
H	0.763994	-0.110231	2.612169
Cu	-0.158802	-0.985123	-0.067533
C	2.390746	-2.161178	0.552813
C	3.733774	-2.442179	0.456861
C	4.545947	-1.727153	-0.471627
C	3.882543	-0.726927	-1.241661
C	2.532509	-0.515723	-1.079335
N	1.774564	-1.222548	-0.206696
H	1.763111	-2.701164	1.254825
H	4.148668	-3.210793	1.094690
H	4.416111	-0.126518	-1.966323
H	2.018364	0.239329	-1.664985
N	5.865311	-1.982224	-0.610252
C	6.675520	-1.205886	-1.549483
H	6.674987	-0.140851	-1.291152
H	7.701733	-1.567900	-1.512229
H	6.307281	-1.316330	-2.575586
C	6.505341	-3.021175	0.197106
H	6.021103	-3.992213	0.046096
H	7.548133	-3.108743	-0.103666
H	6.472059	-2.776585	1.265208

$M1_{RB}$-13

C	2.640381	1.200317	0.131666
C	1.249320	1.246505	0.014793
C	0.554884	0.072588	-0.268467
C	1.217743	-1.141198	-0.438277
C	2.608531	-1.176434	-0.318290
C	3.321380	-0.008549	-0.033509
H	3.190064	2.111048	0.350739
H	0.703970	2.176963	0.136909
H	0.648734	-2.037566	-0.663954
H	3.133759	-2.117911	-0.449929
H	4.403075	-0.040062	0.056671
O	-0.825644	0.132857	-0.467524
C	-1.632686	-0.136858	0.617115
O	-1.207615	-0.404848	1.729188
C	-3.444680	0.238577	-1.066172
H	-3.110976	1.219765	-1.417592
H	-3.131861	-0.516527	-1.794529
H	-4.534392	0.241406	-1.015013
N	-2.933911	-0.053981	0.265900
H	-3.588167	-0.253015	1.008938

M1'-1

C	-2.683139	0.676865	-0.371440
O	-1.658190	1.366459	-0.035367
O	-2.487326	-0.418575	-0.997426
C	-4.052385	1.137686	-0.040535
C	-5.161596	0.359706	-0.405700
C	-6.448477	0.791932	-0.090049
C	-6.633058	2.000046	0.589874
C	-5.529547	2.777799	0.955058
C	-4.240815	2.349124	0.641863
H	-5.005282	-0.575920	-0.932173
H	-7.306760	0.189144	-0.371981
H	-7.636901	2.334953	0.835669
H	-5.675174	3.715680	1.482933
H	-3.376495	2.943207	0.919429
O	0.186309	-1.592785	-1.861265
C	0.866601	-2.623156	-1.439321
O	1.637463	-3.256239	-2.167409
C	0.685272	-3.061802	-0.000881
C	-0.493812	-2.813975	0.718562
C	1.723501	-3.772834	0.619739
C	-0.622882	-3.254832	2.038281
C	1.602422	-4.197044	1.942672
H	2.623700	-3.982421	0.050812
C	0.427239	-3.938661	2.655935
H	-1.545156	-3.067522	2.581634
H	2.420575	-4.731742	2.417432
H	0.329148	-4.273413	3.684975
H	-1.322647	-2.296034	0.244422
Cu	-0.456181	-0.077601	-0.854111
C	1.453869	1.650351	0.568170
C	2.641909	2.274437	0.884520
C	3.823421	1.966512	0.152254
C	3.676934	1.006005	-0.887591
C	2.447421	0.431459	-1.126782
N	1.334863	0.732583	-0.418481
H	0.545780	1.887049	1.112771
H	2.650626	2.994955	1.691847
H	4.514359	0.711363	-1.506044
H	2.325388	-0.303909	-1.913932
N	5.013852	2.552314	0.426977
C	6.202509	2.205885	-0.349602
H	6.083320	2.469297	-1.407486
H	7.055813	2.755133	0.045929
H	6.424277	1.134644	-0.282445
C	5.115298	3.552720	1.487414
H	4.845342	3.130785	2.462496
H	6.143604	3.908041	1.540769
H	4.464550	4.412651	1.289762

M1'-TS1

C	-1.930072	1.358959	-0.193470
O	-0.868426	1.076296	0.434093
O	-2.630756	0.466668	-0.806770
C	-2.409737	2.767917	-0.241096
C	-3.608804	3.085213	-0.897944
C	-4.049867	4.406641	-0.942288
C	-3.298904	5.416066	-0.332184
C	-2.103936	5.103425	0.323504
C	-1.658404	3.783762	0.369249
H	-4.184990	2.295448	-1.367241
H	-4.977769	4.649803	-1.451542
H	-3.644221	6.445435	-0.368284
H	-1.520972	5.887929	0.796914
H	-0.732153	3.531179	0.873661
O	0.093019	-2.326704	-1.263877
C	-0.777269	-3.299698	-1.187595

O	-0.734378	-4.314314	-1.886566	O	-1.479340	-4.400493	-1.681593	C	-4.720434	-0.267139	0.103672
C	-1.833022	-3.101718	-0.130801	C	-2.451645	-2.866999	-0.109407	C	-4.065418	-0.872347	-1.004080
C	-2.038792	-1.799843	0.376088	C	-2.219801	-1.652476	0.565151	C	-2.723579	-1.184936	-0.925869
C	-2.514200	-4.201743	0.397720	C	-3.632007	-3.592789	0.076564	N	-1.955105	-0.945523	0.162824
C	-2.909461	-1.653967	1.472312	C	-3.206336	-1.191190	1.449590	H	-1.951204	-0.188609	2.094238
C	-3.386585	-4.027787	1.473607	C	-4.606181	-3.114273	0.956251	H	-4.313416	0.413555	2.145175
H	-2.334519	-5.186229	-0.024846	H	-3.771802	-4.525664	-0.463501	H	-4.597289	-1.100862	-1.918384
C	-3.576768	-2.753908	2.019590	C	-4.391630	-1.916557	1.644959	H	-2.216717	-1.661790	-1.757473
H	-3.100003	-0.664177	1.883168	H	-3.069032	-0.259326	1.996501	N	-6.035635	0.065901	0.072968
H	-3.910460	-4.882518	1.892937	H	-5.526486	-3.672089	1.108819	C	-6.837331	-0.211591	-1.116261
H	-4.250994	-2.618849	2.861267	H	-5.146404	-1.545309	2.334413	H	-6.882121	-1.286343	-1.330532
H	-2.246225	-0.620120	-0.391117	H	-2.585365	0.202674	-0.486994	H	-7.852784	0.146713	-0.951164
Cu	-0.186551	-0.822010	-0.021117	Cu	-0.376683	-1.012462	0.161338	H	-6.433061	0.299335	-1.997836
C	2.175331	0.856346	0.636219	C	2.212958	0.321146	0.823969	C	-6.671098	0.665576	1.243745
C	3.499970	1.222498	0.751753	C	3.576389	0.523980	0.889279	H	-6.183302	1.606104	1.525083
C	4.512332	0.430267	0.141951	C	4.452101	-0.291006	0.119924	H	-7.713150	0.879880	1.009801
C	4.057239	-0.718622	-0.563210	C	3.825196	-1.285463	-0.680568	H	-6.644665	-0.009289	2.108080
C	2.708897	-1.003808	-0.620975	C	2.451010	-1.413751	-0.671930	N	1.911442	1.432672	3.068975
N	1.756888	-0.241171	-0.035407	N	1.627304	-0.631166	0.062543	N	1.586305	0.708992	4.038282
H	1.398558	1.458842	1.093222	H	1.542653	0.946833	1.403016	N	1.389900	0.137427	4.990869
H	3.743692	2.115030	1.312931	H	3.953670	1.308016	1.532666	O	0.401612	0.253002	1.730406
H	4.748702	-1.386444	-1.060132	H	4.404463	-1.959566	-1.297949	C	1.247962	1.121325	1.876554
H	2.345843	-1.876879	-1.151886	H	1.960021	-2.178671	-1.263688	O	1.698443	1.945941	0.931967
N	5.827301	0.751495	0.227512	N	5.800199	-0.131906	0.151190	C	1.115668	1.797758	-0.370972
C	6.837257	-0.107184	-0.386963	C	6.663345	-1.013916	-0.630380	H	0.028549	1.726826	-0.300317
H	6.683229	-0.192968	-1.468840	H	6.403456	-0.981877	-1.694107	H	1.515608	0.905228	-0.858234
H	7.821412	0.326967	-0.215917	H	7.695912	-0.683128	-0.524820	C	1.492770	3.036470	-1.187148
H	6.825248	-1.115245	0.045046	H	6.596872	-2.054848	-0.289068	Cl	0.775421	2.825896	-2.824868
C	6.249910	1.930813	0.979598	C	6.404821	0.852935	1.044937	Cl	0.826604	4.525737	-0.426971
H	5.984835	1.848512	2.040856	H	6.165786	0.645070	2.095219	Cl	3.279121	3.192557	-1.332930
H	7.332039	2.030002	0.903100	H	7.487440	0.819585	0.928010				
H	5.793026	2.842959	0.578939	H	6.067602	1.868728	0.808077	**M1'-TS2**			
								O	0.680828	-2.769598	-1.299263
M1'-2				**M1'-3**				C	1.891777	-3.128938	-1.641086
C	-1.636886	1.792015	-0.123066	O	-0.149105	-2.608766	-1.494025	O	2.141218	-3.829840	-2.627798
O	-0.732687	1.185153	0.465264	C	0.944447	-3.258958	-1.803711	C	2.973953	-2.618299	-0.726612
O	-2.659967	1.163902	-0.696697	O	1.041308	-3.987560	-2.796331	C	2.565335	-1.815803	0.352944
C	-1.669017	3.265711	-0.249883	C	2.084457	-3.051175	-0.843192	C	4.322173	-2.927993	-0.939660
C	-2.749268	3.919023	-0.865826	C	1.848657	-2.196695	0.248873	C	3.546672	-1.329905	1.225826
C	-2.747910	5.308247	-0.972316	C	3.318608	-3.685084	-1.026731	C	5.288849	-2.436313	-0.060717
C	-1.674554	6.048797	-0.468006	C	2.888390	-1.998989	1.166722	H	4.596181	-3.549634	-1.788426
C	-0.598094	5.400401	0.145975	C	4.345409	-3.473747	-0.105255	C	4.899580	-1.639130	1.022033
C	-0.593216	4.012364	0.256506	H	3.457272	-4.336232	-1.886147	H	3.274126	-0.705751	2.074972
H	-3.581004	3.342647	-1.254948	C	4.127535	-2.632595	0.991653	H	6.339138	-2.670754	-0.214403
H	-3.583053	5.813173	-1.448089	H	2.755694	-1.355598	2.034531	H	5.652055	-1.256636	1.708385
H	-1.676632	7.131658	-0.553770	H	5.308352	-3.960787	-0.235705	Cu	0.605899	-1.590726	0.320349
H	0.235057	5.977012	0.536191	H	4.924651	-2.469702	1.713817	C	-2.171497	-1.153291	1.409095
H	0.236942	3.498091	0.728219	Cu	0.003513	-1.508277	0.169339	C	-3.549999	-1.090034	1.420343
O	-0.278352	-2.626392	-1.022785	C	-2.571724	-0.377444	1.225145	C	-4.283749	-1.390499	0.239478
C	-1.355282	-3.367445	-1.015499	C	-3.907683	-0.033234	1.247143	C	-3.505972	-1.762419	-0.891556

C	-2.129637	-1.805244	-0.798170
N	-1.439429	-1.499649	0.325498
H	-1.612968	-0.911118	2.306905
H	-4.049488	-0.806823	2.337644
H	-3.969978	-2.019923	-1.834811
H	-1.526602	-2.106038	-1.647961
N	-5.638742	-1.326050	0.195956
C	-6.351360	-1.643268	-1.039126
H	-6.175299	-2.679753	-1.351321
H	-7.420302	-1.512836	-0.874673
H	-6.047805	-0.979891	-1.857578
C	-6.396910	-0.960264	1.390004
H	-6.120672	0.038322	1.748604
H	-7.458877	-0.953019	1.147353
H	-6.235506	-1.676555	2.204662
N	1.182199	2.386043	2.214630
N	1.122543	1.974908	4.127016
N	1.211000	2.225031	5.199248
O	0.605265	0.088601	1.883972
C	0.903692	1.240242	1.638757
O	1.095378	1.820718	0.354377
C	-0.115051	2.144156	-0.365688
H	-0.902225	2.455523	0.324937
H	-0.428899	1.255371	-0.919806
C	0.192851	3.277832	-1.348068
Cl	-1.321449	3.601806	-2.266959
Cl	0.696770	4.766110	-0.474506
Cl	1.494520	2.787646	-2.488424

M1'-4

O	1.561971	2.274593	-1.104690
C	0.525982	3.072384	-1.200715
O	0.377984	3.876062	-2.126080
C	-0.475476	2.933277	-0.084344
C	-0.185932	1.985661	0.913543
C	-1.637525	3.711382	-0.037829
C	-1.092561	1.831291	1.969312
C	-2.532130	3.548168	1.021630
H	-1.826290	4.433870	-0.827852
C	-2.258805	2.608996	2.023399
H	-0.906886	1.109061	2.762905
H	-3.437685	4.147301	1.070751
H	-2.956203	2.482505	2.848483
Cu	1.524376	1.129233	0.521057
C	3.810309	-0.614896	1.201412
C	5.022942	-1.260536	1.078380
C	5.812625	-1.066478	-0.089171
C	5.268644	-0.187149	-1.066623
C	4.045821	0.413288	-0.849655
N	3.302274	0.217490	0.263418
H	3.205153	-0.762108	2.091548
H	5.351486	-1.907684	1.880803
H	5.796163	0.027620	-1.986679
H	3.620750	1.090136	-1.583471
N	7.010140	-1.681089	-0.258852
C	7.789817	-1.451387	-1.473189
H	8.064268	-0.395131	-1.580669
H	8.706142	-2.038301	-1.422655
H	7.235589	-1.757177	-2.368414
C	7.538401	-2.563780	0.778890
H	6.867736	-3.411309	0.963728
H	8.501219	-2.955725	0.453664
H	7.687122	-2.028292	1.724226
N	-2.035559	-2.582823	-0.140177
O	0.142456	-2.236123	0.799945
C	-0.911847	-2.313093	0.287369
O	-2.629956	-1.718384	-1.092012
C	-3.971351	-2.105709	-1.330892
H	-4.095222	-3.188296	-1.252539
H	-4.181406	-1.782214	-2.353580
C	-4.986834	-1.405950	-0.401693
Cl	-6.636844	-1.857125	-0.985744
Cl	-4.809798	-1.927380	1.311310
Cl	-4.786824	0.380442	-0.492501

M1'-TS3

O	1.492397	-2.469806	-1.718366
C	2.322515	-3.347612	-1.238476
O	2.443311	-4.511289	-1.632088
C	3.239497	-2.839368	-0.141816
C	3.168198	-1.558237	0.372215
C	4.234885	-3.667738	0.411165
C	3.969329	-1.031386	1.361734
C	5.078975	-3.193650	1.417042
H	4.324111	-4.681668	0.030691
C	4.952704	-1.884063	1.894892
H	3.860019	-0.010745	1.718330
H	5.841440	-3.846424	1.832738
H	5.613276	-1.520118	2.677985
Cu	-0.212780	-2.019941	-1.107927
C	-2.806032	-2.423855	0.104086
C	-4.092757	-2.130231	0.506554
C	-4.657731	-0.858235	0.212786
C	-3.818930	0.037655	-0.506139
C	-2.544008	-0.348144	-0.864400
N	-2.012567	-1.561002	-0.575436
H	-2.374987	-3.393647	0.329976
H	-4.650842	-2.885100	1.044925
H	-4.155805	1.028253	-0.782108
H	-1.902218	0.337897	-1.406763
N	-5.915067	-0.519072	0.594388
C	-6.458185	0.793800	0.253207
H	-6.507414	0.939825	-0.832643
H	-7.467626	0.874473	0.654482
H	-5.852939	1.600756	0.682795
C	-6.747923	-1.474397	1.321423
H	-6.271551	-1.786198	2.258122
H	-7.699268	-1.002255	1.564352
H	-6.951436	-2.370301	0.722275
N	0.637567	0.929018	0.614666
O	-0.057200	-0.650613	2.283329
C	0.355381	0.144845	1.526369
O	1.741210	1.799944	0.816561
C	1.946626	2.599317	-0.333923
H	1.689271	2.057868	-1.247062
H	3.014159	2.831808	-0.331271
C	1.179272	3.938942	-0.295067
Cl	1.742613	4.912814	-1.709540
Cl	-0.600798	3.707141	-0.413867
Cl	1.552553	4.825310	1.227662

M1'-5

O	-0.306545	1.754876	-0.118283
C	-0.148809	2.991395	0.230356
O	-1.022508	3.741079	0.689164
C	1.256065	3.514745	0.030164
C	2.280664	2.749646	-0.494930
C	1.588700	4.840076	0.370246
C	3.575855	3.165733	-0.711548
C	2.884722	5.320816	0.175819
H	0.807984	5.472030	0.784614
C	3.877974	4.494167	-0.362094
H	4.336187	2.512721	-1.131684
H	3.124899	6.345897	0.443531
H	4.885453	4.874292	-0.512343
Cu	-2.029805	1.001216	-0.023388
C	-4.827800	0.736159	0.605275
C	-6.084343	0.170840	0.670836
C	-6.321080	-1.106089	0.090951
C	-5.198296	-1.718411	-0.531657
C	-3.979570	-1.071970	-0.545593
N	-3.763478	0.145457	0.009285
H	-4.647955	1.710328	1.048267
H	-6.872949	0.719633	1.168500
H	-5.272532	-2.690819	-1.000597
H	-3.123594	-1.540381	-1.019863
N	-7.539825	-1.701649	0.130743
C	-7.736134	-3.017970	-0.471614
H	-7.109804	-3.778853	0.009781
H	-8.779191	-3.309724	-0.354602

H	-7.502510	-3.005795	-1.542640
C	-8.657101	-1.046032	0.806107
H	-8.893811	-0.080247	0.344259
H	-9.537733	-1.682996	0.733417
H	-8.442102	-0.877799	1.868284
N	1.915167	-1.105550	-0.297278
O	0.146045	-0.975357	-1.910046
C	1.069827	-0.974425	-1.185885
O	3.215908	-0.586371	-0.518376
C	4.059972	-0.915141	0.569122
H	3.505547	-0.949984	1.509785
H	4.802621	-0.114552	0.606900
C	4.818997	-2.245236	0.372363
Cl	5.997193	-2.390870	1.735063
Cl	3.716650	-3.666371	0.395608
Cl	5.714376	-2.225728	-1.190894

M1'-TS4

O	-0.294545	-1.623810	0.054943
C	-0.092543	-2.827327	-0.374181
O	-0.946853	-3.603058	-0.819567
C	1.353182	-3.269876	-0.298353
C	2.381150	-2.491512	0.191934
C	1.735689	-4.548186	-0.749014
C	3.710984	-2.829182	0.283166
C	3.065988	-4.962943	-0.686854
H	0.956547	-5.194321	-1.144084
C	4.052720	-4.114135	-0.174621
H	4.462928	-2.156126	0.682320
H	3.338438	-5.952992	-1.040387
H	5.089071	-4.437832	-0.127058
Cu	-2.031295	-0.897271	-0.004403
C	-4.038440	1.091427	-0.653466
C	-5.284872	1.681003	-0.703958
C	-6.392511	1.059703	-0.062954
C	-6.111168	-0.163337	0.606431
C	-4.829966	-0.673679	0.600836
N	-3.781027	-0.075586	-0.014925
H	-3.194172	1.565168	-1.143571
H	-5.392982	2.616046	-1.237944
H	-6.884131	-0.713406	1.126584
H	-4.615717	-1.607420	1.110493
N	-7.637727	1.598273	-0.086957
C	-8.738946	0.937210	0.609643
H	-8.549717	0.869020	1.687875
H	-9.650531	1.514122	0.458628
H	-8.907193	-0.074838	0.223356
C	-7.879432	2.863756	-0.775595
H	-7.626897	2.793959	-1.840116
H	-8.935912	3.116103	-0.692996
H	-7.294785	3.680182	-0.334562
N	2.238816	0.189386	0.322990
O	1.576092	-0.882070	2.392222
C	1.904497	-0.497022	1.325657
O	2.408734	1.579382	0.777326
C	2.945819	2.352873	-0.264260
H	2.520583	3.354858	-0.149024
H	2.676047	1.952237	-1.244960
C	4.482743	2.504668	-0.192154
Cl	4.965295	3.699396	-1.463026
Cl	4.972946	3.129673	1.426235
Cl	5.334627	0.951365	-0.497771

M1'-6

O	0.418519	-1.846206	0.261393
C	0.918152	-2.611414	-0.660749
O	0.306264	-3.068986	-1.633990
C	2.370019	-2.976657	-0.442072
C	3.216939	-2.234840	0.405808
C	2.862034	-4.141435	-1.042033
C	4.515949	-2.691422	0.666366
C	4.162219	-4.582081	-0.794970
H	2.198605	-4.700784	-1.693328
C	4.989603	-3.859080	0.067945
H	5.157264	-2.115834	1.327060
H	4.525795	-5.491037	-1.265693
H	6.000722	-4.199160	0.271818
Cu	-1.385551	-1.304810	0.109325
C	-3.598047	0.403490	-0.622922
C	-4.893019	0.876221	-0.672006
C	-5.926580	0.192502	0.026388
C	-5.523601	-0.966838	0.745134
C	-4.201476	-1.359885	0.734578
N	-3.223374	-0.701629	0.066054
H	-2.809891	0.924063	-1.156878
H	-5.096538	1.767626	-1.250634
H	-6.233971	-1.556139	1.309769
H	-3.894159	-2.243542	1.284280
N	-7.214531	0.618398	0.008480
C	-8.245316	-0.125249	0.728993
H	-8.045315	-0.147687	1.807083
H	-9.207808	0.359595	0.570275
H	-8.318396	-1.158240	0.369215
C	-7.581804	1.824473	-0.729738
H	-7.383390	1.715411	-1.802861
H	-8.646795	2.010480	-0.595905
H	-7.032874	2.700516	-0.364474
N	2.373645	0.004320	0.083596
O	2.971630	-0.693326	2.231053
C	2.806815	-0.941792	1.044325
O	1.935103	1.112712	0.731327
C	1.603117	2.153591	-0.185247
H	0.659523	2.589827	0.150101
H	1.501308	1.752342	-1.195124
C	2.677424	3.254575	-0.174898
Cl	2.122392	4.549291	-1.301508
Cl	2.863382	3.940494	1.479848
Cl	4.266581	2.619976	-0.727147

M1'-TS5

O	0.642822	-1.438124	0.132540
C	1.209161	-2.228432	-0.715598
O	0.662406	-2.814194	-1.658961
C	2.697901	-2.432856	-0.489236
C	3.457722	-1.771281	0.507497
C	3.365780	-3.357462	-1.295723
C	4.848086	-1.971380	0.621067
C	4.735436	-3.594555	-1.157127
H	2.783593	-3.880456	-2.046433
C	5.480003	-2.900689	-0.195721
H	5.407418	-1.406745	1.359808
H	5.225966	-4.309869	-1.810427
H	6.546748	-3.074201	-0.093978
Cu	-1.208118	-1.087471	0.016146
C	-3.549603	0.591992	-0.149686
C	-4.885672	0.934841	-0.148269
C	-5.878147	-0.072137	0.007427
C	-5.391956	-1.401129	0.150867
C	-4.034203	-1.644055	0.136217
N	-3.095527	-0.677200	-0.009880
H	-2.792686	1.360699	-0.265953
H	-5.152030	1.977215	-0.264552
H	-6.065963	-2.238682	0.273557
H	-3.663325	-2.657886	0.246451
N	-7.203653	0.216956	0.019432
C	-8.188292	-0.846693	0.202626
H	-8.056397	-1.354915	1.165452
H	-9.187219	-0.412831	0.179205
H	-8.121877	-1.596470	-0.594547
C	-7.655854	1.599319	-0.118014
H	-7.328922	2.033876	-1.069977
H	-8.744625	1.619599	-0.090261
H	-7.278964	2.228900	0.697039
N	3.034735	-0.100808	1.157948
O	2.196608	-1.674003	2.793868
C	2.689929	-1.140156	1.835971
O	1.883880	1.192074	1.443460
C	1.435882	1.736947	0.257197
H	0.416056	2.115717	0.421072
H	1.386341	0.993213	-0.545201

C	2.272366	2.943133	-0.243040
Cl	1.434692	3.643346	-1.688604
Cl	2.376039	4.204695	1.045039
Cl	3.940768	2.461864	-0.716904

M1'-7

O	0.904264	-1.131406	0.116120
C	1.484170	-1.784842	-0.853197
O	0.923689	-2.120520	-1.902567
C	2.941589	-2.115800	-0.641928
C	3.598391	-2.144759	0.613220
C	3.691314	-2.433865	-1.785764
C	4.960509	-2.483338	0.677797
C	5.043758	-2.754079	-1.718924
H	3.173197	-2.422778	-2.738595
C	5.680564	-2.778643	-0.475022
H	5.436974	-2.508870	1.652594
H	5.594951	-2.985792	-2.625323
H	6.734253	-3.031342	-0.400121
Cu	-0.981195	-0.891230	-0.020443
C	-3.463744	0.548819	-0.378169
C	-4.824810	0.771648	-0.403199
C	-5.723570	-0.274949	-0.056873
C	-5.120833	-1.515618	0.290705
C	-3.747049	-1.640049	0.287518
N	-2.898352	-0.634917	-0.038630
H	-2.779139	1.347918	-0.642254
H	-5.182522	1.751302	-0.691474
H	-5.716688	-2.376947	0.562655
H	-3.287440	-2.585860	0.555308
N	-7.069324	-0.100931	-0.058494
C	-7.956466	-1.218107	0.255973
H	-7.750149	-1.621414	1.253829
H	-8.987148	-0.866216	0.239193
H	-7.857701	-2.031317	-0.473954
C	-7.646096	1.179882	-0.460832
H	-7.403111	1.423953	-1.502456
H	-8.729920	1.125198	-0.365722
H	-7.287813	1.995371	0.177765
N	2.990300	-1.890408	1.842944
O	1.028714	-1.199868	2.997198
C	1.936466	-1.520406	2.314247
O	2.945308	1.543220	1.726948
C	1.836961	1.777132	1.004201
H	0.976295	2.013683	1.658468
H	1.541603	0.825854	0.497848
C	1.990648	2.899842	-0.057419
Cl	0.440417	3.066183	-0.963356
Cl	2.377351	4.463174	0.756624
Cl	3.318352	2.492296	-1.202753

M1'-TS6

O	0.340261	-1.882704	0.465642
C	0.958650	-2.313297	-0.588737
O	0.447467	-2.508351	-1.697451
C	2.420886	-2.641266	-0.378655
C	3.231291	-2.100325	0.666615
C	3.007375	-3.556302	-1.254467
C	4.576955	-2.525217	0.800920
C	4.333405	-3.970646	-1.110295
H	2.393453	-3.948581	-2.057742
C	5.119998	-3.453557	-0.071485
H	5.167908	-2.092718	1.601647
H	4.751236	-4.695005	-1.802848
H	6.151832	-3.769699	0.045601
Cu	-1.462887	-1.325010	0.260672
C	-3.558317	0.632225	-0.025933
C	-4.834248	1.144079	-0.138355
C	-5.957615	0.273578	-0.080565
C	-5.660372	-1.105438	0.102950
C	-4.348908	-1.521058	0.205418
N	-3.284827	-0.684213	0.144042
H	-2.701814	1.296783	-0.071399
H	-4.953312	2.211640	-0.268430
H	-6.444463	-1.848776	0.164216
H	-4.122601	-2.573396	0.342612
N	-7.230865	0.728819	-0.194251
C	-8.355642	-0.197207	-0.083657
H	-8.379840	-0.687085	0.897405
H	-9.284493	0.357142	-0.212079
H	-8.310813	-0.973412	-0.856344
C	-7.490380	2.156806	-0.363939
H	-6.985648	2.548714	-1.254236
H	-8.561918	2.309901	-0.487370
H	-7.156702	2.735504	0.506294
N	2.822310	-1.169020	1.581346
O	1.042556	0.285785	2.174080
C	1.842134	-0.386908	1.628037
O	2.314575	0.511968	-0.200578
C	1.810199	1.769325	-0.241042
H	1.146215	1.973905	0.619497
H	1.193061	1.917276	-1.146786
C	2.895890	2.880993	-0.252553
Cl	2.080591	4.494936	-0.321122
Cl	3.906158	2.791718	1.240199
Cl	3.970229	2.699565	-1.690640

M1'-8

O	-1.122415	-0.809200	-1.295041
C	-1.148447	-1.574027	-0.267609
O	-0.025889	-1.777116	0.315724
C	-2.373670	-2.248760	0.207086
C	-3.670151	-1.956599	-0.273949
C	-2.209182	-3.294858	1.132388
C	-4.746257	-2.752546	0.133264
C	-3.287800	-4.070703	1.541989
H	-1.212112	-3.504344	1.503524
C	-4.558838	-3.806095	1.026248
H	-5.736692	-2.524485	-0.248924
H	-3.138044	-4.880318	2.248977
H	-5.409721	-4.409225	1.328619
Cu	0.825585	-0.557479	-1.114791
C	3.326030	-1.484997	-0.000076
C	4.653475	-1.462695	0.361367
C	5.462289	-0.335226	0.036919
C	4.808808	0.720247	-0.663578
C	3.475631	0.608918	-0.987755
N	2.724915	-0.473036	-0.670078
H	2.701120	-2.335967	0.250406
H	5.056919	-2.311786	0.896233
H	5.337031	1.618879	-0.952617
H	2.969902	1.407893	-1.520781
N	6.769289	-0.270299	0.376512
C	7.555941	0.921930	0.062314
H	7.139791	1.813048	0.546360
H	8.573244	0.779815	0.424274
H	7.596586	1.099310	-1.018321
C	7.401008	-1.375110	1.097586
H	7.325206	-2.311313	0.533545
H	8.456218	-1.146376	1.238709
H	6.944476	-1.523507	2.083346
N	-3.943457	-0.914801	-1.199869
O	-4.212926	1.263578	-1.812491
C	-3.818210	0.431236	-1.016583
O	-3.231150	0.727619	0.184492
C	-3.230435	2.095674	0.565701
H	-3.675545	2.164549	1.561076
H	-3.804094	2.692429	-0.145183
C	-1.804178	2.662004	0.645386
Cl	-1.939140	4.354102	1.261469
Cl	-0.792219	1.700886	1.785309
Cl	-1.013415	2.685567	-0.970698
H	-4.537374	-1.153617	-1.985285

M1'-TS7

O	-0.773664	-2.204364	1.077747
C	-1.709745	-1.698562	1.637261
O	-2.305530	-1.218743	2.533697
C	-3.280359	-1.789602	0.116251
C	-2.943103	-1.763859	-1.233257

C	-4.445592	-2.294077	0.651378
C	-3.821474	-2.463286	-2.085059
C	-5.303089	-2.974445	-0.224291
H	-4.668006	-2.216221	1.710574
C	-4.976260	-3.058834	-1.581571
H	-3.594120	-2.501327	-3.147497
H	-6.208265	-3.434174	0.160321
H	-5.641842	-3.576148	-2.265635
Cu	1.105309	-1.587595	0.798218
C	3.169973	-0.167668	-0.633962
C	4.434071	0.267899	-0.971285
C	5.555250	-0.120824	-0.185822
C	5.267851	-0.955468	0.930397
C	3.969087	-1.340286	1.187967
N	2.909611	-0.967068	0.429763
H	2.312547	0.127320	-1.230422
H	4.545655	0.903978	-1.839566
H	6.049938	-1.301653	1.593215
H	3.749682	-1.977009	2.038779
N	6.816563	0.278000	-0.481959
C	7.940968	-0.155287	0.344637
H	8.013265	-1.248571	0.377612
H	8.864040	0.234343	-0.082627
H	7.852193	0.216892	1.372462
C	7.064242	1.148617	-1.629228
H	6.516648	2.093998	-1.539174
H	8.128532	1.374990	-1.677146
H	6.771352	0.666515	-2.569601
N	-1.796932	-1.166352	-1.775146
O	-0.151082	0.402876	-1.934727
C	-1.120138	-0.055393	-1.358121
O	-1.662438	0.460592	-0.215028
C	-1.084167	1.660689	0.293942
H	-0.219727	1.951280	-0.304569
H	-0.784090	1.483715	1.328692
C	-2.120360	2.793896	0.267366
Cl	-1.334861	4.254129	0.972770
Cl	-2.636232	3.143625	-1.422072
Cl	-3.569811	2.367901	1.245996
H	-1.492314	-1.509799	-2.679279

$M2_{RA'}$-4/ $M1_{RA'}$-4

C	0.463711	-0.730131	-0.989611
O	0.557139	-0.475868	-2.161930
N	3.536069	-2.607574	-2.354789
N	2.516454	-3.160067	-2.097044
N	1.503772	-3.721603	-1.842898
O	1.418552	-0.603916	-0.063443
C	2.568842	0.122556	-0.507196
C	3.491209	0.321800	0.694163
H	2.262334	1.097438	-0.890626
H	3.093438	-0.458746	-1.273864
Cl	2.691725	1.281113	1.991936
Cl	4.017873	-1.260325	1.379359
Cl	4.940287	1.220954	0.100768
C	-0.895479	-1.473841	0.916788
C	-1.991929	-2.102806	1.424753
C	-2.954856	-2.706889	0.554065
C	-2.700490	-2.586538	-0.848221
C	-1.590487	-1.935461	-1.295428
N	-0.675897	-1.407148	-0.430656
H	-0.158519	-0.998157	1.545116
H	-2.113176	-2.121160	2.498551
H	-3.378061	-2.999431	-1.581769
H	-1.360511	-1.818236	-2.344560
N	-4.035576	-3.342500	1.026909
C	-5.016941	-3.927608	0.106984
H	-4.563299	-4.718150	-0.499550
H	-5.828790	-4.359194	0.688945
H	-5.433367	-3.164225	-0.557484
C	-4.260974	-3.459709	2.471508
H	-4.402341	-2.474856	2.928808
H	-5.158208	-4.052204	2.638475
H	-3.418969	-3.960211	2.959204
C	-0.981865	4.264472	0.081084
C	-1.288802	5.621706	0.199100
C	-2.562333	6.083937	-0.147397
C	-3.523350	5.180465	-0.612264
C	-3.208775	3.825150	-0.728956
C	-1.936322	3.349700	-0.384185
H	0.000508	3.886953	0.346934
H	-0.537978	6.319975	0.560853
H	-2.803920	7.139690	-0.056211
H	-4.515108	5.534405	-0.883148
H	-3.940187	3.107995	-1.088590
C	-1.601939	1.855392	-0.513405
O	-2.510156	1.110301	-0.957648
O	-0.435655	1.517930	-0.149166

$M2_{RA'}$-TS3/ $M1_{RA'}$-TS3

C	0.091975	0.320299	0.909117
O	0.259536	0.340049	2.114745
N	2.111238	3.761150	2.335701
N	0.950051	3.916358	2.137110
N	-0.207070	4.087781	1.944857
O	1.020252	0.797526	-0.000008
C	2.348806	0.795617	0.494921
C	3.294637	1.033810	-0.682583
H	2.601021	-0.165098	0.951157
H	2.489053	1.606119	1.221914
Cl	3.176815	-0.285321	-1.908099
Cl	2.941024	2.607284	-1.493142
Cl	4.978586	1.075163	-0.028300
C	-1.513356	0.610214	-0.981679
C	-2.739631	0.948926	-1.482227
C	-3.775032	1.408742	-0.610471
C	-3.443913	1.481496	0.776013
C	-2.196424	1.121961	1.208701
N	-1.240440	0.699663	0.346535
H	-0.711127	0.249189	-1.608771
H	-2.900041	0.853733	-2.546952
H	-4.161204	1.819915	1.510369
H	-1.896079	1.155790	2.246561
N	-4.992504	1.749177	-1.071710
C	-6.037879	2.190475	-0.145647
H	-5.738476	3.102738	0.381273
H	-6.944185	2.399679	-0.711062
H	-6.262282	1.414875	0.594334
C	-5.298046	1.660811	-2.501571
H	-5.243569	0.625635	-2.856153
H	-6.307960	2.031176	-2.668033
H	-4.606029	2.271609	-3.090294
C	0.771949	-4.102741	-0.262769
C	1.046215	-5.442806	-0.541206
C	0.181919	-6.443898	-0.088968
C	-0.957971	-6.099297	0.643894
C	-1.229680	-4.759705	0.921561
C	-0.368624	-3.749564	0.471373
H	1.436894	-3.319674	-0.609989
H	1.933386	-5.706775	-1.110451
H	0.395511	-7.486915	-0.305968
H	-1.632060	-6.874616	0.997839
H	-2.108411	-4.473248	1.490229
C	-0.696056	-2.302922	0.794846
O	-1.698191	-2.040523	1.471188
O	0.142661	-1.444888	0.292687

$M2_{RA'}$-5/ $M1_{RA'}$-5

C	-0.412540	-0.405008	0.844725
O	-0.232373	-0.492133	2.062605
N	3.985677	0.151739	1.745008
N	3.552576	0.847248	2.603500
N	3.127399	1.547303	3.462190
O	0.112079	-1.430644	-0.026367
C	1.294562	-1.997898	0.486289
C	1.785566	-3.056885	-0.500099
H	1.119565	-2.488456	1.449438
H	2.099113	-1.260604	0.618742
Cl	0.549297	-4.354219	-0.732335
Cl	2.169407	-2.329463	-2.108360

Cl	3.289305	-3.798522	0.176570
C	0.071785	1.213421	-1.118277
C	0.595793	2.356687	-1.665735
C	1.283591	3.297050	-0.840263
C	1.384845	2.962321	0.540437
C	0.822735	1.801716	1.013160
N	0.175804	0.942082	0.203038
H	-0.444742	0.475745	-1.718419
H	0.480427	2.516550	-2.728866
H	1.912497	3.593480	1.242013
H	0.884432	1.502218	2.052186
N	1.812873	4.433877	-1.343068
C	2.552665	5.349046	-0.474035
H	3.449171	4.872308	-0.060825
H	2.860795	6.216854	-1.055075
H	1.928102	5.695306	0.356162
C	1.731526	4.718563	-2.775575
H	0.690862	4.738680	-3.115250
H	2.170123	5.696621	-2.966722
H	2.277389	3.972413	-3.364947
C	-4.418777	-1.001862	-0.389819
C	-5.737894	-1.262325	-0.760570
C	-6.760701	-0.391820	-0.374427
C	-6.462443	0.743327	0.385360
C	-5.145511	1.006090	0.756784
C	-4.114909	0.136524	0.371527
H	-3.623726	-1.676340	-0.686453
H	-5.967985	-2.145272	-1.349679
H	-7.787224	-0.597438	-0.664203
H	-7.255762	1.420824	0.687348
H	-4.897829	1.882368	1.346506
C	-2.716672	0.464228	0.800177
O	-2.443879	1.436309	1.484201
O	-1.827501	-0.422605	0.324006

$M2_{RA'}$-TS4/ $M1_{RA'}$-TS4

C	-0.482490	-0.675177	0.949331
O	-0.202689	-0.644083	2.133543
N	4.046693	0.268606	1.535298
N	3.640815	0.895715	2.457823
N	3.243317	1.527782	3.379807
O	0.116008	-1.550540	0.050308
C	1.379161	-2.016472	0.488128
C	1.896667	-3.011209	-0.550593
H	1.297163	-2.532483	1.449331
H	2.109624	-1.202842	0.586923
Cl	0.758513	-4.400181	-0.744157
Cl	2.123894	-2.218222	-2.155719
Cl	3.488826	-3.635841	0.027186
C	-0.055220	1.345912	-1.108774
C	0.406993	2.535427	-1.634815
C	1.128994	3.440117	-0.805430
C	1.324763	3.033205	0.542685
C	0.811224	1.826418	0.975293
N	0.134528	0.993580	0.173891
H	-0.601416	0.639559	-1.726809
H	0.214842	2.755258	-2.676674
H	1.877081	3.642296	1.245877
H	0.948335	1.490526	1.999000
N	1.603972	4.622815	-1.277126
C	2.365860	5.509626	-0.402427
H	3.275727	5.022895	-0.031542
H	2.657667	6.396464	-0.963810
H	1.770997	5.830777	0.461013
C	1.372960	5.007058	-2.666358
H	0.301739	5.063646	-2.892991
H	1.809184	5.989992	-2.839635
H	1.835546	4.298716	-3.364458
C	-4.366526	-1.097837	-0.448363
C	-5.663989	-1.304688	-0.915313
C	-6.701605	-0.465081	-0.501499
C	-6.441406	0.585821	0.383345
C	-5.147063	0.795622	0.852689
C	-4.101710	-0.044259	0.440021
H	-3.561690	-1.749407	-0.768299
H	-5.865412	-2.121649	-1.601742
H	-7.711158	-0.629218	-0.867178
H	-7.246677	1.239070	0.705850
H	-4.929342	1.606420	1.539671
C	-2.735967	0.227612	0.978771
O	-2.480088	1.116451	1.763166
O	-1.823522	-0.638069	0.457134

$M2_{RA'}$-6/ $M1_{RA'}$-6

C	0.442817	0.427753	1.173088
O	0.580620	1.596563	1.411730
O	1.432531	-0.493178	1.068870
C	2.770211	-0.019425	1.196815
C	3.524467	-0.218732	-0.125856
H	3.263428	-0.610257	1.971341
H	2.784834	1.038191	1.463729
Cl	3.543164	-1.958743	-0.595749
Cl	2.760725	0.736663	-1.447159
Cl	5.217040	0.347471	0.127508
O	-0.698645	-0.261518	0.945973
C	-3.770940	-2.400630	-0.803448
C	-2.731691	-1.668238	-0.234797
C	-3.018695	-0.512789	0.510049
C	-4.350579	-0.098966	0.673887
C	-5.384352	-0.834728	0.099374
C	-5.096304	-1.986126	-0.638201
H	-3.547540	-3.294801	-1.377398
H	-1.704988	-1.988292	-0.366372
H	-4.559607	0.796149	1.248900
H	-6.412908	-0.510939	0.226085
H	-5.903137	-2.560266	-1.084431
C	-1.970364	0.303766	1.162564
O	-2.148911	1.256441	1.875711
N	-1.626706	1.655245	-1.543401
N	-2.646473	2.252012	-1.429253
N	-3.667972	2.844282	-1.315799

$M2_{RA'}$-TS5/ $M1_{RA'}$-TS5

C	-0.270157	0.584518	-0.718356
O	-0.490825	1.775554	-0.649886
O	-1.255816	-0.350024	-1.002541
C	-2.571971	0.142228	-1.150749
C	-3.476668	-0.387083	-0.027071
H	-2.975006	-0.215665	-2.102126
H	-2.585065	1.233658	-1.125225
Cl	-3.531870	-2.190969	-0.041212
Cl	-2.891334	0.162822	1.585789
Cl	-5.140977	0.255821	-0.310622
O	0.846854	-0.077762	-0.566862
C	3.957429	-2.322779	1.043283
C	2.986811	-1.353961	0.789013
C	3.224249	-0.351228	-0.159783
C	4.442962	-0.328944	-0.844790
C	5.416197	-1.297782	-0.588806
C	5.175486	-2.297451	0.355537
H	3.764791	-3.099246	1.778534
H	2.042680	-1.374373	1.322550
H	4.613133	0.452796	-1.577937
H	6.359267	-1.271890	-1.127885
H	5.930075	-3.053051	0.555608
C	2.220099	0.741209	-0.481267
O	2.404177	1.558430	-1.374259
N	1.945220	1.454190	1.109475
N	1.936243	2.658164	0.993922
N	1.944175	3.806984	0.860254

$M2_{RA'}$-7/$M1_{RA'}$-7

C	-0.426405	0.493892	-0.893639
O	-0.542795	1.592832	-0.327445
O	-1.690619	-0.152248	-1.319398
C	-2.872240	0.489024	-0.969315
C	-3.702130	-0.355646	0.016172
H	-3.508879	0.646000	-1.850525
H	-2.663967	1.451106	-0.489499
Cl	-4.133387	-1.959973	-0.704714

Cl	-2.800526	-0.645563	1.552682
Cl	-5.236857	0.536500	0.394908
O	0.545233	-0.200256	-1.209843
C	4.153893	-2.138821	1.386984
C	3.548724	-0.896193	1.205063
C	3.815165	-0.150517	0.046931
C	4.690191	-0.661923	-0.923922
C	5.292512	-1.903326	-0.738188
C	5.025349	-2.643345	0.417921
H	3.945105	-2.713806	2.284124
H	2.871170	-0.505115	1.955973
H	4.888056	-0.075389	-1.814744
H	5.969563	-2.294585	-1.491630
H	5.496169	-3.611433	0.563074
C	3.211042	1.183688	-0.197722
O	3.413157	1.861323	-1.190274
N	2.408933	1.634213	0.895180
N	1.880850	2.745177	0.722202
N	1.380139	3.758128	0.666662

$M2_{RA'}$-TS6

C	2.201476	2.115279	-0.306299
C	2.719194	0.842917	-0.061144
C	4.086561	0.703135	0.216103
C	4.944323	1.813860	0.198166
C	4.415677	3.079390	-0.047099
C	3.046640	3.229132	-0.298537
H	1.137518	2.204900	-0.510114
H	2.046647	-0.013269	-0.078093
H	6.005919	1.684222	0.386219
H	5.069735	3.946258	-0.050916
H	2.642238	4.217692	-0.497846
C	4.637617	-0.668820	0.669124
O	4.715618	-1.087429	1.816908
N	4.938293	-1.102593	-0.537696
N	5.598745	-2.686087	-0.335847
N	6.035897	-3.602911	-0.781160
C	-0.904626	-0.182692	-0.599503
O	-0.918920	1.045763	-0.791445
O	-2.178494	-0.884955	-0.796123
C	-3.292237	-0.107259	-1.100509
C	-4.343293	-0.167898	0.022993
H	-3.786694	-0.478941	-2.007398
H	-3.009263	0.941007	-1.237358
Cl	-4.901009	-1.867587	0.300047
Cl	-3.683017	0.476141	1.573568
Cl	-5.771588	0.835052	-0.471321
O	-0.010602	-0.978917	-0.281882

$M2_{RA'}$-8

C	0.145315	1.529022	0.402681
O	0.320975	1.545692	1.629601
O	0.879937	0.490895	-0.349404
C	1.747131	-0.315578	0.378771
C	3.207124	-0.122140	-0.072546
H	1.516210	-1.377704	0.224933
H	1.692293	-0.076801	1.445992
Cl	3.405383	-0.537235	-1.823719
Cl	3.750755	1.580784	0.175262
Cl	4.266100	-1.225329	0.904723
O	-0.545700	2.215756	-0.363072
C	-4.925440	1.521546	-0.281546
C	-3.661894	0.938830	-0.176923
C	-3.561786	-0.448825	-0.012400
C	-4.713437	-1.248074	0.046352
C	-5.967258	-0.648670	-0.060851
C	-6.079136	0.735256	-0.224575
H	-5.006916	2.597251	-0.409071
H	-2.750675	1.532064	-0.221918
H	-4.616629	-2.321963	0.174795
H	-6.858891	-1.267429	-0.016672
H	-7.059121	1.195807	-0.306733
C	-1.664139	-2.028134	0.205483
O	-0.937192	-2.955529	0.319005
N	-2.285336	-1.006413	0.090918

$M2_{RA'}$-TS7

C	-0.943004	2.700161	0.318969
O	-2.046333	3.070760	0.002958
O	-0.811243	0.946882	-0.005944
C	-1.855238	0.423810	-0.751747
C	-2.547154	-0.753564	-0.034185
H	-1.512915	0.052147	-1.727567
H	-2.627198	1.184319	-0.918874
Cl	-1.409533	-2.132570	0.225636
Cl	-3.201040	-0.239621	1.568573
Cl	-3.923503	-1.328247	-1.070251
O	0.120664	3.028406	0.772285
C	4.933345	-0.957852	1.294789
C	3.581733	-0.617134	1.299176
C	2.960010	-0.128268	0.136492
C	3.732362	0.013710	-1.032330
C	5.085317	-0.327198	-1.027181
C	5.695433	-0.815035	0.131578
H	5.392643	-1.335184	2.204552
H	2.984375	-0.723277	2.199972
H	3.272492	0.390226	-1.940172
H	5.665761	-0.209212	-1.938553
H	6.748984	-1.078622	0.128194
C	0.942197	0.561914	-0.773370
O	0.802356	0.785884	-1.939425
N	1.588798	0.195479	0.239005

$M2_{RA'}$-9/ $M1_{RA'}$-12/ $M2_{RA'}$-5

O	0.575812	-0.544840	-0.858582
C	1.721854	0.220285	-1.081016
C	2.765457	-0.005798	0.027343
H	1.481075	1.286885	-1.106538
H	2.194069	-0.076025	-2.025217
Cl	2.134654	0.511296	1.635811
Cl	3.239568	-1.748266	0.128539
Cl	4.237509	0.972414	-0.373463
C	-5.204785	-1.089460	0.248143
C	-3.862183	-1.346116	-0.010380
C	-2.908943	-0.305249	-0.166609
C	-3.399998	1.022727	-0.043407
C	-4.749232	1.270052	0.217685
C	-5.667475	0.227079	0.366147
H	-5.896582	-1.921730	0.358733
H	-3.507141	-2.369992	-0.100690
H	-2.705487	1.844376	-0.157950
H	-5.086919	2.301059	0.305871
H	-6.714951	0.432486	0.568376
C	-0.644097	0.175963	-0.621897
O	-0.605246	1.415050	-0.666258
N	-1.604512	-0.711167	-0.415001

$M2_{RA'}$-TS6'

C	0.580968	-2.415119	-1.590256
O	0.760860	-2.897939	-0.538237
O	-0.118077	-0.078687	-0.546584
C	-0.722526	-0.255512	0.657366
C	-2.270014	-0.341254	0.530204
H	-0.559928	0.574796	1.367104
H	-0.439419	-1.190828	1.179071
Cl	-2.956656	1.172041	-0.183275
Cl	-2.766940	-1.735267	-0.517851
Cl	-3.002736	-0.585088	2.184141
O	0.440001	-2.071635	-2.699772
C	3.419469	0.109740	2.248599
C	2.411405	0.751755	1.523996
C	2.299652	0.556488	0.141126
C	3.223405	-0.278697	-0.503679
C	4.226936	-0.920849	0.219625
C	4.328078	-0.730029	1.601458
H	3.496118	0.271942	3.320334
H	1.720946	1.414255	2.033781
H	3.139829	-0.410117	-1.577550
H	4.934237	-1.566617	-0.293932
H	5.111479	-1.227307	2.166544

C	1.248283	1.216458	-0.719635
O	1.392770	1.368066	-1.929149
N	0.580126	2.338910	0.082430
N	-0.078659	3.097335	-0.614522
N	-0.692037	3.840737	-1.232120

$M2_{RA'}$-8'

O	0.140771	-0.168610	1.106353
C	0.619798	-0.041215	-0.230261
C	2.000959	-0.703828	-0.319289
H	0.715969	1.022608	-0.483481
H	-0.035621	-0.534215	-0.950500
Cl	3.168818	0.080375	0.807057
Cl	1.904594	-2.464417	0.070733
Cl	2.587976	-0.503382	-2.015015
C	-3.485385	0.825217	-1.140116
C	-2.363457	0.672018	-0.324488
C	-2.213056	-0.498614	0.435873
C	-3.192578	-1.502569	0.375736
C	-4.297443	-1.351492	-0.458121
C	-4.446821	-0.185029	-1.214790
H	-3.606893	1.737193	-1.717005
H	-1.627105	1.471439	-0.272916
H	-3.075252	-2.396051	0.980226
H	-5.044986	-2.137203	-0.512586
H	-5.313493	-0.062922	-1.858004
C	-1.093263	-0.681171	1.404688
O	-1.234962	-1.211445	2.485690
N	0.102106	3.188627	-0.719701
N	0.348947	3.893842	0.207044
N	0.595345	4.606945	1.117710

$M1_{RA'}$-8

C	1.987801	-1.775924	1.108315
O	2.604262	-2.797674	1.346384
N	-2.255914	-2.633474	1.850071
N	-1.678148	-1.915957	2.693768
N	-1.193988	-1.372557	3.557059
O	2.621586	-0.555879	0.892174
C	4.037252	-0.546574	0.842165
C	4.521438	-0.148726	-0.561144
H	4.430636	-1.535540	1.085355
H	4.411701	0.190976	1.556648
Cl	6.323699	-0.139983	-0.539709
Cl	3.941979	-1.325221	-1.796644
Cl	3.930125	1.497349	-1.005700
C	-3.771628	-4.157030	0.097600
C	-3.136983	-2.986499	-0.358125
C	-3.237949	-2.611624	-1.711001
C	-3.964433	-3.401250	-2.595296
C	-4.594171	-4.564525	-2.138564
C	-4.496903	-4.940561	-0.794938
H	-3.696613	-4.445427	1.140120
H	-2.745136	-1.708660	-2.053775
H	-4.040913	-3.113850	-3.639225
H	-5.161256	-5.179142	-2.831590
H	-4.987004	-5.843369	-0.444461
O	-1.872476	-1.047564	0.184597
C	-2.364132	-2.131460	0.551512
O	0.704095	-1.641494	1.034031
Cu	-0.119904	0.016020	0.614780
C	-0.778292	2.744011	1.175638
C	-1.323090	3.998938	1.034639
C	-2.077848	4.318746	-0.131560
C	-2.220987	3.272656	-1.090351
C	-1.640460	2.045584	-0.864307
N	-0.914003	1.769011	0.244269
H	-0.200857	2.489483	2.059311
H	-1.161863	4.722885	1.821775
H	-2.779459	3.418882	-2.005212
H	-1.746383	1.243529	-1.586861
N	-2.627861	5.539444	-0.313821
C	-3.418942	5.824378	-1.511063
H	-4.314777	5.194146	-1.557982
H	-3.733430	6.866748	-1.487862
H	-2.830527	5.663039	-2.420886
C	-2.477357	6.576412	0.707511
H	-1.421027	6.808233	0.883357
H	-2.974457	7.483149	0.366961
H	-2.930293	6.270182	1.657522

$M1_{RA'}$-TS6

C	1.981963	-1.931273	-0.119237
O	2.561906	-2.975818	-0.359557
N	-1.753934	-2.724479	1.457554
N	-0.488209	-1.845243	2.233418
N	0.256378	-1.814024	3.054322
O	2.610764	-0.870019	0.524762
C	4.002543	-0.975193	0.756009
C	4.770162	0.046754	-0.098563
H	4.354503	-1.978505	0.508608
H	4.201471	-0.755024	1.807808
Cl	6.523824	-0.118218	0.287021
Cl	4.512837	-0.260641	-1.855535
Cl	4.238876	1.729493	0.281071
C	-4.497769	-3.073843	0.719323
C	-3.285759	-3.027730	0.011551
C	-3.066544	-3.837065	-1.117864
C	-4.095824	-4.657133	-1.565659
C	-5.317580	-4.689916	-0.878851
C	-5.519013	-3.902075	0.258102
H	-4.629784	-2.465194	1.607840
H	-2.110974	-3.808442	-1.632045
H	-3.947334	-5.278398	-2.443238
H	-6.112159	-5.342074	-1.229071
H	-6.464082	-3.941609	0.790188
O	-1.929725	-0.990733	-0.171839
C	-2.193569	-2.055691	0.430162
O	0.746905	-1.657717	-0.379630
Cu	-0.125529	0.019601	-0.207778
C	-1.165893	2.430851	0.994144
C	-1.883743	3.600731	1.086023
C	-2.445133	4.185402	-0.087041
C	-2.199573	3.494328	-1.309866
C	-1.469933	2.328049	-1.305418
N	-0.942406	1.790282	-0.179013
H	-0.742081	1.972004	1.881753
H	-2.009699	4.055713	2.059255
H	-2.581665	3.861931	-2.252639
H	-1.287919	1.787131	-2.228813
N	-3.174207	5.322155	-0.041770
C	-3.757331	5.875003	-1.264266
H	-4.490722	5.188640	-1.703946
H	-4.261569	6.809872	-1.024000
H	-2.983647	6.083853	-2.010648
C	-3.454424	5.970810	1.239696
H	-2.528358	6.266356	1.744949
H	-4.046771	6.866421	1.059182
H	-4.020662	5.309499	1.905963

$M1_{RA'}$-9

C	-1.004762	-2.173177	0.259272
O	-1.767815	-3.120118	0.228712
O	0.320359	-2.293934	0.665829
C	-2.747041	1.531462	-0.623054
O	-1.577561	1.807933	-0.634113
O	-1.277117	-0.946951	-0.052755
N	-3.890953	1.243659	-0.719677
Cu	0.005804	0.422404	0.029325
C	1.884813	2.251071	-1.128553
C	2.867596	3.210897	-1.186401
C	3.404434	3.752855	0.018584
C	2.850054	3.252235	1.233729
C	1.867274	2.290394	1.195869
N	1.389894	1.771814	0.038693
H	1.468667	1.829212	-2.037923
H	3.216675	3.535549	-2.157213
H	3.189082	3.607981	2.197151
H	1.438943	1.898317	2.112704

N	4.377715	4.689124	0.009097
C	4.871363	5.255055	1.265225
H	5.304469	4.478473	1.905352
H	5.644866	5.987836	1.041733
H	4.068743	5.756715	1.817532
C	4.915921	5.184898	-1.258320
H	4.152979	5.720154	-1.835630
H	5.736133	5.869793	-1.049311
H	5.303667	4.362436	-1.868685
C	-5.213318	1.222243	-0.279453
C	-6.161973	0.524692	-1.036464
C	-5.574316	1.893625	0.897904
C	-7.487320	0.499537	-0.604332
H	-5.854881	0.014341	-1.943237
C	-6.903435	1.859590	1.313390
H	-4.819273	2.428786	1.464938
C	-7.860741	1.164829	0.566648
H	-8.228492	-0.040695	-1.185289
H	-7.191067	2.378251	2.222911
H	-8.894753	1.143192	0.897120
C	0.781189	-3.582803	1.033924
H	1.171591	-3.541251	2.054027
H	-0.034101	-4.306465	0.974093
C	1.916942	-4.031656	0.102627
Cl	3.310384	-2.888538	0.190656
Cl	2.458540	-5.662999	0.645708
Cl	1.348655	-4.125785	-1.603566

$M1_{RA'}$-TS7

C	-1.004762	-2.173177	0.259272
O	-1.767815	-3.120118	0.228712
O	0.320359	-2.293934	0.665829
C	-2.747041	1.531462	-0.623054
O	-1.577561	1.807933	-0.634113
O	-1.277117	-0.946951	-0.052755
N	-3.890953	1.243659	-0.719677
Cu	0.005804	0.422404	0.029325
C	1.884813	2.251071	-1.128553
C	2.867596	3.210897	-1.186401
C	3.404434	3.752855	0.018584
C	2.850054	3.252235	1.233729
C	1.867274	2.290394	1.195869
N	1.389894	1.771814	0.038693
H	1.468667	1.829212	-2.037923
H	3.216675	3.535549	-2.157213
H	3.189082	3.607981	2.197151
H	1.438943	1.898317	2.112704
N	4.377715	4.689124	0.009097
C	4.871363	5.255055	1.265225
H	5.304469	4.478473	1.905352
H	5.644866	5.987836	1.041733
H	4.068743	5.756715	1.817532
C	4.915921	5.184898	-1.258320
H	4.152979	5.720154	-1.835630
H	5.736133	5.869793	-1.049311
H	5.303667	4.362436	-1.868685
C	-5.213318	1.222243	-0.279453
C	-6.161973	0.524692	-1.036464
C	-5.574316	1.893625	0.897904
C	-7.487320	0.499537	-0.604332
H	-5.854881	0.014341	-1.943237
C	-6.903435	1.859590	1.313390
H	-4.819273	2.428786	1.464938
C	-7.860741	1.164829	0.566648
H	-8.228492	-0.040695	-1.185289
H	-7.191067	2.378251	2.222911
H	-8.894753	1.143192	0.897120
C	0.781189	-3.582803	1.033924
H	1.171591	-3.541251	2.054027
H	-0.034101	-4.306465	0.974093
C	1.916942	-4.031656	0.102627
Cl	3.310384	-2.888538	0.190656
Cl	2.458540	-5.662999	0.645708
Cl	1.348655	-4.125785	-1.603566

$M1_{RA'}$-10

O	1.070608	0.499034	0.757820
C	0.975420	-1.972861	-0.607590
O	-0.181899	-1.673224	-0.521267
N	2.092908	-2.311801	-0.823195
Cu	-0.732650	0.263168	0.534886
C	-3.393413	-0.573435	1.319630
C	-4.736387	-0.850085	1.198947
C	-5.424263	-0.523627	-0.005699
C	-4.641059	0.094029	-1.023710
C	-3.302048	0.331797	-0.812177
N	-2.664261	0.013401	0.340062
H	-2.859383	-0.825807	2.230371
H	-5.243423	-1.322020	2.029920
H	-5.074012	0.380588	-1.972604
H	-2.696504	0.794452	-1.585185
N	-6.739420	-0.788766	-0.176005
C	-7.393284	-0.485970	-1.448911
H	-6.928542	-1.033827	-2.276945
H	-8.439680	-0.781291	-1.387917
H	-7.350253	0.585842	-1.672527
C	-7.503978	-1.444990	0.883981
H	-7.464806	-0.868339	1.814378
H	-8.545474	-1.519522	0.574448
H	-7.127849	-2.455534	1.083651
C	3.389863	-2.576423	-0.379349
C	3.734829	-2.371585	0.964573
C	4.333198	-3.040355	-1.303076
C	5.039338	-2.636613	1.376550
H	2.987964	-2.003591	1.660546
C	5.633921	-3.302660	-0.873334
H	4.041873	-3.188674	-2.337642
C	5.990264	-3.102117	0.462786
H	5.312507	-2.477199	2.415485
H	6.369241	-3.663389	-1.586150
H	7.004949	-3.305989	0.791345
C	1.533833	1.724446	1.176562
C	2.119527	2.585629	0.023564
Cl	2.757720	4.127695	0.719667
Cl	0.846151	2.983019	-1.201158
Cl	3.459827	1.711166	-0.803806
H	0.758280	2.346362	1.655995
H	2.350256	1.606711	1.906252

$M1_{RA'}$-TS8

O	-1.068014	0.050386	-0.494610
C	-1.057866	-1.531553	0.381434
O	0.166083	-1.655201	0.457577
N	-2.126318	-2.033219	0.718605
Cu	0.869131	0.107246	-0.497076
C	3.368587	-1.321810	-0.134162
C	4.724211	-1.503537	0.014739
C	5.599293	-0.378937	0.010176
C	4.980083	0.893733	-0.159275
C	3.613582	0.980048	-0.301506
N	2.799920	-0.102837	-0.293568
H	2.694812	-2.171778	-0.126492
H	5.099611	-2.510633	0.136597
H	5.560031	1.806681	-0.179315
H	3.131866	1.944363	-0.429176
N	6.936219	-0.512719	0.160278
C	7.799689	0.667802	0.172395
H	7.532951	1.348148	0.989257
H	8.831132	0.349396	0.315831
H	7.736823	1.216708	-0.774151
C	7.530304	-1.838668	0.331443
H	7.309948	-2.485435	-0.525245
H	8.611387	-1.734116	0.410678
H	7.161827	-2.326961	1.241029
C	-3.441086	-2.133031	0.284049
C	-3.755339	-2.267248	-1.082699
C	-4.466709	-2.168739	1.244758
C	-5.085401	-2.402771	-1.474059
H	-2.955616	-2.266152	-1.817279
C	-5.792134	-2.303814	0.837977

H	-4.209522	-2.082029	2.295574
C	-6.108228	-2.419332	-0.519621
H	-5.323454	-2.498792	-2.529490
H	-6.581015	-2.320442	1.584378
H	-7.142791	-2.526281	-0.831497
C	-2.115555	0.881337	-0.890760
C	-2.339357	2.086548	0.052394
Cl	-3.796402	2.981171	-0.526747
Cl	-0.920652	3.207282	0.017565
Cl	-2.603690	1.545910	1.747803
H	-1.935999	1.287036	-1.894021
H	-3.051896	0.315748	-0.912651

$M1_{RA'}$-11

O	1.651140	0.690993	0.051535
C	2.013865	-0.571497	-0.226866
O	1.102452	-1.410370	-0.378404
N	3.324877	-0.805386	-0.442512
Cu	-0.793278	-1.135174	-0.250188
C	-3.563369	-1.622740	-0.904656
C	-4.935413	-1.495494	-0.855267
C	-5.533747	-0.591701	0.066732
C	-4.631618	0.135164	0.892894
C	-3.272385	-0.061242	0.769298
N	-2.712582	-0.925582	-0.112193
H	-3.107185	-2.311319	-1.608234
H	-5.534674	-2.093633	-1.528840
H	-4.986201	0.848284	1.625205
H	-2.584507	0.493416	1.398858
N	-6.877696	-0.433906	0.152033
C	-7.449826	0.515691	1.104009
H	-7.116629	1.540154	0.898981
H	-8.535834	0.487588	1.023229
H	-7.176485	0.262063	2.134944
C	-7.765362	-1.196459	-0.723271
H	-7.640761	-2.275582	-0.575755
H	-8.797732	-0.937973	-0.492069
H	-7.581473	-0.967661	-1.779877
C	3.961245	-1.928521	-0.075347
C	3.462582	-2.865998	0.892289
C	5.249280	-2.162385	-0.662403
C	4.212066	-3.976180	1.221415
H	2.501764	-2.688527	1.361783
C	5.978193	-3.283333	-0.322847
H	5.618897	-1.439378	-1.382067
C	5.466478	-4.196718	0.618031
H	3.836474	-4.683711	1.953847
H	6.947090	-3.461511	-0.778097
H	6.044733	-5.075446	0.886347
C	2.660084	1.697291	0.210970
C	1.992493	3.061051	0.011899
Cl	3.272425	4.311428	0.218978
Cl	0.694195	3.330909	1.230447
Cl	1.288962	3.191196	-1.639963
H	3.082416	1.649492	1.217815
H	3.451948	1.571274	-0.529119

$M2_{RA}$-TS6

C	-0.011237	0.722230	1.874746
C	-0.310631	1.571451	0.808663
C	-0.958404	2.788163	1.064383
C	-1.352573	3.136754	2.365176
C	-1.045196	2.282607	3.421763
C	-0.375640	1.078109	3.176684
H	0.494379	-0.217997	1.678373
H	-0.037989	1.291790	-0.205109
H	-1.879167	4.069642	2.542402
H	-1.333836	2.549819	4.433785
H	-0.146857	0.411727	4.003320
C	-1.135591	3.818594	-0.075983
O	-0.389276	4.749822	-0.346855
N	-2.269827	3.325186	-0.527527
N	-2.724299	4.312421	-1.878668
N	-3.434322	4.551253	-2.696056
C	1.426533	-1.060520	-1.213767
O	1.149155	-1.894537	-0.305561
O	2.793366	-0.938826	-1.571687
C	3.740057	-1.697239	-0.864038
C	4.762700	-0.779119	-0.175663
H	4.297869	-2.337091	-1.556918
H	3.260428	-2.313138	-0.100563
Cl	5.620853	0.254583	-1.384193
Cl	3.961746	0.291251	1.034153
Cl	5.977836	-1.822257	0.667116
O	0.682025	-0.327977	-1.876569
H	-0.450603	-2.013912	-0.216906
C	-2.244899	-1.366445	-1.065684
C	-3.615110	-1.430042	-1.076004
C	-4.300572	-2.268436	-0.145116
C	-3.484771	-3.013526	0.760488
C	-2.119077	-2.897824	0.708272
N	-1.511666	-2.087659	-0.187052
H	-1.668077	-0.746567	-1.742127
H	-4.154084	-0.833539	-1.798819
H	-3.918784	-3.676191	1.495942
H	-1.467389	-3.445977	1.378631
N	-5.646599	-2.352047	-0.121616
C	-6.319273	-3.220205	0.845894
H	-6.062576	-2.940605	1.873324
H	-7.395956	-3.118025	0.721346
H	-6.051170	-4.271427	0.691009
C	-6.452478	-1.582338	-1.070525
H	-6.221353	-1.859302	-2.104910
H	-7.505261	-1.788858	-0.886437
H	-6.285142	-0.506372	-0.950541

$M2_{RA}$-8

C	-0.166732	1.350832	1.557611
C	-0.212067	2.026033	0.336657
C	-0.550262	3.384153	0.312821
C	-0.838722	4.065625	1.504960
C	-0.787823	3.378781	2.716608
C	-0.452655	2.021743	2.749059
H	0.097043	0.297695	1.565383
H	0.008762	1.505202	-0.590083
H	-1.098618	5.119531	1.472932
H	-1.010979	3.908655	3.638175
H	-0.414821	1.492950	3.696746
C	-0.832239	5.119027	-1.399565
O	-1.039217	6.118650	-1.993188
N	-0.591838	4.033815	-0.929027
C	1.105288	-1.220254	-1.080207
O	0.722457	-1.811498	-0.030502
O	2.479940	-1.333302	-1.409267
C	3.320566	-2.040298	-0.534574
C	4.447707	-1.131842	-0.018300
H	3.794629	-2.873655	-1.065275
H	2.764389	-2.420616	0.324733
Cl	5.440081	-0.488767	-1.384926
Cl	3.781089	0.258768	0.915215
Cl	5.513283	-2.117931	1.062015
O	0.459714	-0.561301	-1.903979
H	-0.878272	-1.780342	0.009949
C	-2.570712	-1.141502	-1.030026
C	-3.939373	-1.102376	-1.112666
C	-4.735924	-1.732363	-0.108869
C	-4.029158	-2.381912	0.949081
C	-2.657664	-2.376236	0.963603
N	-1.942807	-1.766118	-0.007695
H	-1.911613	-0.687472	-1.760992
H	-4.391037	-0.594711	-1.953458
H	-4.551802	-2.881311	1.752579
H	-2.087375	-2.856304	1.750212
N	-6.083910	-1.716505	-0.156983
C	-6.871122	-2.416484	0.859372
H	-6.736084	-1.967388	1.850002
H	-7.924831	-2.353976	0.593052
H	-6.593461	-3.474314	0.913290
C	-6.779048	-1.005606	-1.231515
H	-6.586608	-1.467973	-2.206504

H	-7.850138	-1.037313	-1.038891
H	-6.468521	0.043466	-1.273900

$M2_{RA}$-TS7

C	-0.876409	-1.289738	2.645712
O	-0.877855	-2.421641	3.062839
O	-1.225907	-1.284428	0.935175
C	-1.551266	-2.531609	0.409494
C	-0.630314	-2.926760	-0.759928
H	-2.581793	-2.549373	0.032348
H	-1.447239	-3.304258	1.178606
Cl	-0.787847	-1.769363	-2.139613
Cl	1.096807	-2.975280	-0.240008
Cl	-1.115879	-4.576439	-1.333445
O	-0.718910	-0.133381	2.960511
C	-2.157792	4.730871	-0.333203
C	-1.646904	3.480000	0.011454
C	-2.463013	2.338773	-0.042624
C	-3.801165	2.476363	-0.450308
C	-4.302428	3.732109	-0.794192
C	-3.487718	4.865666	-0.739020
H	-1.511388	5.602629	-0.282743
H	-0.615411	3.379048	0.332859
H	-4.447156	1.606304	-0.500220
H	-5.338712	3.820825	-1.108557
H	-3.883917	5.840086	-1.008537
C	-2.587989	0.083916	0.491742
O	-3.619045	-0.506684	0.543984
N	-1.862262	1.096334	0.307050
H	0.019377	0.898748	0.481820
C	1.893078	0.747739	1.383847
C	3.249494	0.862995	1.226326
C	3.799380	1.234959	-0.038955
C	2.864392	1.473508	-1.092981
C	1.520633	1.339516	-0.862344
N	1.046222	0.980717	0.353659
H	1.428050	0.466660	2.320186
H	3.883920	0.666372	2.079094
H	3.190201	1.760375	-2.082811
H	0.779160	1.512753	-1.632288
N	5.127650	1.355453	-0.226679
C	5.660824	1.757514	-1.530221
H	5.288063	2.745154	-1.822863
H	6.746464	1.804814	-1.466286
H	5.390365	1.035885	-2.308610
C	6.058190	1.095492	0.873708
H	5.945973	0.074044	1.252602
H	7.076058	1.215168	0.507432
H	5.902112	1.796819	1.700778

$M2_{RA}$-9

O	1.261645	-0.694959	-0.829420
C	1.933993	-1.890937	-1.120813
C	1.729777	-2.926206	-0.000964
H	3.006640	-1.715577	-1.234161
H	1.529234	-2.324519	-2.041260
Cl	2.369797	-2.317826	1.570906
Cl	-0.021179	-3.324044	0.203732
Cl	2.618733	-4.432687	-0.462374
C	1.179920	5.034355	0.645007
C	0.812345	3.715194	0.394152
C	1.751107	2.755889	-0.054760
C	3.084332	3.193991	-0.239017
C	3.440609	4.519848	0.015237
C	2.501152	5.453312	0.458124
H	0.427696	5.739510	0.990176
H	-0.218283	3.407671	0.546110
H	3.827528	2.485610	-0.577896
H	4.473951	4.823504	-0.137331
H	2.789902	6.481951	0.653888
C	2.068771	0.453304	-0.622124
O	3.289235	0.373398	-0.773857
N	1.265130	1.464871	-0.286763
H	-0.231979	1.146319	-0.201490
C	-2.114375	1.096971	-1.229613
C	-3.457133	0.807265	-1.213451
C	-4.058715	0.288260	-0.028129
C	-3.194724	0.104890	1.092747
C	-1.862093	0.421826	0.989941
N	-1.327755	0.910147	-0.149097
H	-1.623805	1.489699	-2.113573
H	-4.034874	0.976899	-2.111429
H	-3.565813	-0.279780	2.032441
H	-1.176696	0.293761	1.820483
N	-5.374141	-0.013123	0.030387
C	-5.954611	-0.552340	1.260360
H	-5.870212	0.162185	2.087223
H	-7.009996	-0.759260	1.090849
H	-5.463233	-1.486335	1.554173
C	-6.235396	0.205328	-1.131740
H	-5.914735	-0.402890	-1.985098
H	-7.254743	-0.076095	-0.872756
H	-6.234991	1.258350	-1.434044

$M2_{RA}$-TS8

O	-1.790865	-0.527897	0.484755
C	-2.566243	-1.505489	1.130945
C	-3.293621	-2.390065	0.105408
H	-3.312806	-1.044342	1.781534
H	-1.912167	-2.155334	1.720660
Cl	-4.431163	-1.416506	-0.898249
Cl	-2.117077	-3.216524	-0.987310
Cl	-4.225832	-3.643830	1.016677
C	-0.338652	5.068503	-0.741797
C	-0.366412	3.678052	-0.682591
C	-1.389816	2.992989	0.010964
C	-2.385551	3.768016	0.645166
C	-2.344809	5.162188	0.578674
C	-1.328724	5.827499	-0.110330
H	0.464538	5.561313	-1.283851
H	0.408063	3.096888	-1.172453
H	-3.179069	3.269347	1.183818
H	-3.125145	5.733577	1.075835
H	-1.307591	6.912504	-0.154413
C	-2.147375	0.812000	0.712173
O	-3.062439	1.092918	1.484310
N	-1.328389	1.592484	-0.006202
H	-0.463271	1.045744	-0.789000
C	3.462550	0.915999	-0.050438
C	4.724181	0.579300	0.380760
C	5.252502	-0.713831	0.093214
C	4.407145	-1.590193	-0.649284
C	3.158749	-1.168235	-1.040035
N	2.686636	0.061824	-0.749479
H	3.034384	1.891070	0.156744
H	5.295679	1.309905	0.936636
H	4.724392	-2.589273	-0.914670
H	2.491571	-1.812091	-1.603110
N	6.485166	-1.089511	0.503024
C	6.995878	-2.421669	0.180780
H	7.067328	-2.571860	-0.902592
H	7.991416	-2.530964	0.607860
H	6.354063	-3.205037	0.599378
C	7.328988	-0.161459	1.255461
H	6.840586	0.154597	2.183885
H	8.261537	-0.661268	1.513204
H	7.567088	0.731344	0.665835
O	0.362897	0.570731	-1.532046
H	0.342839	1.054588	-2.368904
H	1.622430	0.354709	-1.107374

$M2_{RB}$'-7

C	2.705626	1.051529	-0.566597
C	4.101382	0.760875	-0.120954
O	4.805984	1.467142	0.570043
N	4.541970	-0.531933	-0.598893
N	5.685506	-0.855342	-0.231846
N	6.716900	-1.227425	0.055095
C	-0.623602	-0.160290	0.303843
O	-0.727306	0.806462	-0.459203

O	-1.873143	-0.899825	0.616085
C	-3.094650	-0.423848	0.251282
O	0.337854	-0.695994	0.874310
H	2.587555	0.824184	-1.630147
H	1.991735	0.417274	-0.015543
H	2.474204	2.100375	-0.377154
C	-3.479145	0.921592	0.382769
C	-4.038358	-1.362758	-0.194998
H	-3.732683	-2.400822	-0.290186
H	-2.752791	1.650084	0.719971
C	-5.341977	-0.968476	-0.499867
C	-4.783128	1.306431	0.067796
H	-6.059337	-1.710876	-0.840366
C	-5.723207	0.370108	-0.374333
H	-5.067713	2.350412	0.174447
H	-6.736359	0.679009	-0.615039

$M2_{RB'}$-TS6

C	2.658062	0.838761	-0.469741
C	4.052578	0.481851	0.168635
O	4.330184	0.621297	1.353482
N	4.644378	0.062819	-0.918749
N	6.292158	-0.422762	-0.365193
N	7.305258	-0.827740	-0.553164
C	-0.699352	-0.190764	0.364163
O	-0.757273	0.756089	-0.428281
O	-1.973260	-0.883651	0.673085
C	-3.172552	-0.404104	0.242776
O	0.234970	-0.736583	0.970613
H	2.552034	0.628436	-1.535760
H	1.915037	0.252906	0.090061
H	2.535666	1.912484	-0.305099
C	-3.536254	0.952227	0.294412
C	-4.116690	-1.348373	-0.190852
H	-3.827072	-2.394851	-0.222854
H	-2.808951	1.684209	0.621675
C	-5.400385	-0.947921	-0.564250
C	-4.820142	1.342838	-0.089202
H	-6.118608	-1.694255	-0.894145
C	-5.760451	0.401623	-0.520104
H	-5.088721	2.395540	-0.045665
H	-6.757792	0.715263	-0.814691

$M2_{RB'}$-8

C	-3.374989	0.738994	0.768947
C	-5.653154	0.138933	-0.084496
O	-6.597685	-0.169233	-0.736589
N	-4.794973	0.456377	0.690497
C	-0.130075	-0.534013	-0.085849
O	-0.126726	0.584791	0.441929
O	1.200279	-1.164471	-0.304199
C	2.352097	-0.455023	-0.162380
O	-1.028930	-1.295311	-0.466924
H	-3.089291	0.808488	1.820286
H	-2.779767	-0.044854	0.290193
H	-3.158391	1.698420	0.289710
C	2.528193	0.846442	-0.662999
C	3.439733	-1.107597	0.439425
H	3.294955	-2.114433	0.820935
H	1.689518	1.354936	-1.122232
C	4.680810	-0.475923	0.535719
C	3.770786	1.471860	-0.554778
H	5.512205	-0.998621	1.001838
C	4.854556	0.820035	0.042813
H	3.893740	2.478535	-0.946891
H	5.818595	1.314440	0.120537

$M3_{RA'}$-1

C	1.990870	-0.389095	-0.089928
O	2.251056	-1.570137	-0.127768
N	2.906082	0.682329	-0.005265
N	4.102183	0.324443	0.028842
N	5.215829	0.138089	0.067341
O	0.762295	0.152164	-0.119905
C	-0.311129	-0.790591	-0.208293
C	-1.617720	-0.021429	-0.003940
H	-0.218482	-1.555968	0.564937
H	-0.322173	-1.263939	-1.193325
Cl	-1.654457	0.754647	1.620667
Cl	-1.823184	1.243451	-1.269393
Cl	-2.963944	-1.212429	-0.128550

$M3_{RA'}$-TS1

C	2.009653	0.918519	-0.024660
O	2.496859	1.914014	-0.484542
N	2.259833	-0.338174	0.304137
N	4.107471	-0.544885	-0.072047
N	5.042922	-1.132118	-0.117367
O	0.645485	0.754486	0.431221
C	-0.314971	0.617309	-0.627652
C	-1.561507	-0.076931	-0.072363
H	0.091517	0.024081	-1.450645
H	-0.590437	1.612742	-0.987467
Cl	-1.172625	-1.737734	0.499972
Cl	-2.259782	0.869639	1.291345
Cl	-2.762325	-0.169080	-1.414278

$M3_{RA'}$-2

C	-3.198200	-0.062749	0.117456
O	-4.266971	-0.029290	-0.365990
N	-2.120593	-0.311511	0.664110
O	-1.207356	0.754336	0.877034
C	0.058514	0.238447	1.248859
C	0.996409	-0.005119	0.046859
H	-0.040153	-0.684280	1.825073
H	0.512394	1.016059	1.868230
Cl	0.412082	-1.338154	-1.011412
Cl	1.151279	1.496972	-0.936083
Cl	2.614650	-0.451467	0.717526

$M3_{RA'}$-TS2

C	2.663545	-0.037423	0.103420
O	3.003430	1.132199	-0.037869
N	3.420332	-1.008517	0.487048
O	1.425094	-0.594674	-0.148866
C	0.385034	-0.327000	0.817256
C	-0.913390	-0.010989	0.060770
H	0.651592	0.522032	1.448991
H	0.236345	-1.222392	1.423496
Cl	-0.727985	1.468458	-0.941799
Cl	-1.384253	-1.390096	-0.993299
Cl	-2.185973	0.257653	1.307062

$M3_{RA'}$-3

C	0.011005	-0.536579	1.255416
O	0.390143	-1.489834	1.949430
N	-1.036880	0.225062	1.555342
O	0.679465	-0.230140	0.038967
C	1.814211	-1.003723	-0.243763
C	3.078556	-0.130034	-0.281404
H	1.709767	-1.464067	-1.232083
H	1.952089	-1.779294	0.514855
Cl	2.936627	1.163856	-1.536284
Cl	3.380815	0.648319	1.316422
Cl	4.484587	-1.192871	-0.699000
C	-4.638448	0.649450	0.041957
C	-3.271119	0.404153	-0.141396
C	-2.851094	-0.854962	-0.595429
C	-3.789680	-1.854309	-0.850671
C	-5.150357	-1.614314	-0.635541
C	-5.573289	-0.360948	-0.186646
H	-4.961044	1.632478	0.370677
H	-1.796967	-1.040475	-0.768365
H	-3.458884	-2.823067	-1.214165
H	-5.877233	-2.399669	-0.822586
H	-6.629594	-0.167088	-0.023597
O	-1.129611	1.360713	0.610572
C	-2.317881	1.549852	0.025497
O	-2.588234	2.665021	-0.401416

$M3_{RA'}$-TS3

C	0.023983	0.679459	-1.302918

O	0.494875	0.992696	-2.432416
N	-1.216023	0.359062	-1.489564
O	0.683789	0.721501	-0.128789
C	2.026532	1.200138	-0.179209
C	3.010394	0.092084	0.224837
H	2.117048	2.021101	0.535077
H	2.281653	1.551479	-1.181085
Cl	2.645973	-0.515449	1.881061
Cl	2.947298	-1.283331	-0.933260
Cl	4.665406	0.813873	0.209677
C	-4.582793	-0.282419	-0.003004
C	-3.232272	-0.498298	0.292577
C	-2.456728	0.583983	0.754155
C	-3.022852	1.860361	0.895826
C	-4.359849	2.066918	0.566625
C	-5.140938	0.990195	0.117969
H	-5.174831	-1.126019	-0.343196
H	-1.438877	0.391091	1.069887
H	-2.417789	2.683093	1.267357
H	-4.803097	3.053718	0.667122
H	-6.185380	1.151948	-0.136079
O	-1.335417	-1.925335	0.188665
C	-2.593958	-1.880092	0.101628
O	-3.379895	-2.835163	-0.119981

$M3_{RA'}$-4

C	-0.026445	-1.384017	-0.591363
O	0.440704	-2.481771	-0.824478
N	-1.287416	-1.128768	-0.106688
O	0.676052	-0.210468	-0.694184
C	2.044835	-0.305564	-1.057141
C	2.932668	0.212925	0.083872
H	2.213013	0.322813	-1.934844
H	2.317433	-1.339044	-1.278110
Cl	2.530013	1.923568	0.486177
Cl	2.731309	-0.797981	1.561953
Cl	4.647556	0.124647	-0.473494
C	-3.896699	0.046450	1.005943
C	-3.108217	0.609008	0.055468
C	-2.261806	-0.263848	-0.782802
C	-2.459224	-1.795736	-0.667715
C	-3.485251	-2.263493	0.280589
C	-4.092259	-1.387702	1.115732
H	-4.494684	0.709124	1.624969
H	-1.943145	0.154527	-1.731808
H	-2.263276	-2.403893	-1.547673
H	-3.766110	-3.312682	0.260881
H	-4.831785	-1.748534	1.826799
O	-2.609068	2.440681	-1.354202
C	-3.146894	2.111945	-0.261301
O	-3.717024	2.849716	0.581626

$M3_{RA'}$-TS4

C	-0.427977	-1.303154	-0.741275
O	0.129758	-2.172222	-1.412904
N	-1.741655	-1.029536	-0.846920
O	0.314404	-0.579422	0.216668
C	1.599520	-1.081057	0.509334
C	2.706555	-0.059050	0.212945
H	1.799813	-1.975569	-0.084269
H	1.656717	-1.317427	1.576792
Cl	2.752440	0.384043	-1.529296
Cl	2.501589	1.436290	1.199824
Cl	4.284216	-0.836402	0.663256
C	-2.417547	-0.503051	1.059951
C	-2.353467	0.198465	-0.216108
C	-3.683962	0.457209	-0.828704
C	-4.841494	0.052275	-0.248944
C	-4.808353	-0.713845	0.965329
C	-3.620676	-1.007051	1.596410
H	-1.485841	-0.629729	1.595605
H	-3.685847	1.008905	-1.764450
H	-5.802062	0.282281	-0.699919
H	-5.745661	-1.068877	1.385426
H	-3.606312	-1.599249	2.505839
O	-1.097941	1.766916	-1.502474
C	-1.512997	1.563387	-0.343847
O	-1.462095	2.254079	0.692276

$M3_{RB'}$-1

C	1.358249	-0.006548	0.013455
O	1.272713	0.784695	0.922262
N	2.553355	-0.513642	-0.552762
N	3.591567	-0.070320	-0.020414
N	4.601477	0.253281	0.370756
O	0.348725	-0.592086	-0.657019
C	-0.972125	-0.257341	-0.305895
C	-1.787234	-1.290922	0.143419
C	-1.450553	1.036805	-0.492321
H	-1.376396	-2.287621	0.266624
H	-0.792559	1.818370	-0.856167
C	-3.127679	-1.014559	0.422240
C	-2.791122	1.298642	-0.203531
H	-3.775764	-1.812237	0.772309
C	-3.629660	0.277770	0.252698
H	-4.671758	0.488865	0.472304
H	-3.179077	2.303437	-0.340468

$M3_{RB'}$-TS1

C	1.412099	0.001241	0.753274
O	1.697111	0.911833	1.485640
N	1.864777	-0.696220	-0.275149
N	3.531393	0.042289	-0.649301
N	4.439591	0.035669	-1.281915
O	0.219777	-0.816968	0.836121
C	-0.975183	-0.329882	0.311447
C	-1.965544	-1.289973	0.092501
C	-1.195369	1.025489	0.055826
H	-1.752559	-2.333817	0.297777
H	-0.420249	1.760517	0.239378
C	-3.209852	-0.878573	-0.381500
C	-2.444073	1.416222	-0.429059
H	-3.988286	-1.616627	-0.548544
C	-3.451456	0.472615	-0.646806
H	-4.419944	0.789021	-1.021341
H	-2.628119	2.466983	-0.630896

$M3_{RB'}$-2

C	-3.066525	0.089667	0.000187
O	-4.239080	0.053010	-0.001340
N	-1.861778	0.349140	0.003089
O	-0.941644	-0.718306	-0.000807
C	0.374281	-0.273127	-0.000166
C	1.320131	-1.302130	0.000181
C	0.753129	1.066622	-0.000430
H	0.989724	-2.335779	0.000513
H	0.005174	1.850078	-0.000510
C	2.673975	-0.972611	0.000086
C	2.117309	1.375326	-0.000355
H	3.412708	-1.768740	0.000322
C	3.080105	0.365865	-0.000190
H	4.136253	0.616742	-0.000180
H	2.419933	2.418421	-0.000479