Supporting Information

belonging to the paper:

How Solvent Affects C-H Activation and Hydrogen Production Pathways in Homogeneous Ru-Catalysed Methanol Dehydrogenation Reactions

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Computational Methods

All static density functional theory calculations were carried out with the Turbomole[1] program coupled to the PQS Baker optimizer[2] via the BOpt package[3]. All geometries were fully optimized as minima or transition states using the BP86 functional[4,5] and the resolution-of-identity (ri)[6] method using the Turbomole def2-TZVP[7] basis for all atoms (referenced as *BP86/def2-TZVP* in the main text and SI). Grimme's dispersion corrections (D3 version)[8] were applied in all calculations. Hessian matrix calculations were performed to characterize all minima (no imaginary frequencies) and transition states (one imaginary frequency). Zero-point energy (ZPE) and gas-phase thermal corrections (298 K, 1 bar, entropy and enthalpy) were obtained from these analyses. The relative (free) energies obtained from *BP86/def2-TZVP* calculations are reported in the main text of this paper. For every transition state, the imaginary eigenvalue was followed in both directions to confirm its connection to the relative reactant and product states. Further, single-point calculations were performed using the M06[9] functional (27% HF exchange) with implicit solvent corrections for methanol ($\epsilon = 32.7$) (COSMO)[10] as implemented in the Turbomole program (referenced as *M06//def2-TZVP* in the main text and SI). The corresponding minimum energy reaction pathways (MERPs) with *M06//def2-TZVP* are reported in the SI (*vide infra*).

By calculation of the partition function of the molecules in the gas phase, the entropy of dissociation or coordination for reactions in solution is overestimated (overestimated translational entropy terms in the gas phase compared to solutions). For reactions in solution we therefore corrected the Gibbs free energies for all steps involving a change in the number of solute species (we did not apply any corrections for loss of gaseous H_2). The applied correction term is a correction for the condensed phase (CP) reference volume (1 L mol^{-1}) compared to the gas phase (GP) reference volume (24.5 L mol^{-1}). This leads to an entropy correction term ($S_{CP} = S_{GP} + Rln\{1/24.5\}$) for all species, which (combined with neglecting the RT term) corrects the relative free energies (298 K) of all associative (–2.5 kcal mol^{-1}) and dissociative steps (+2.5 kcal mol^{-1})

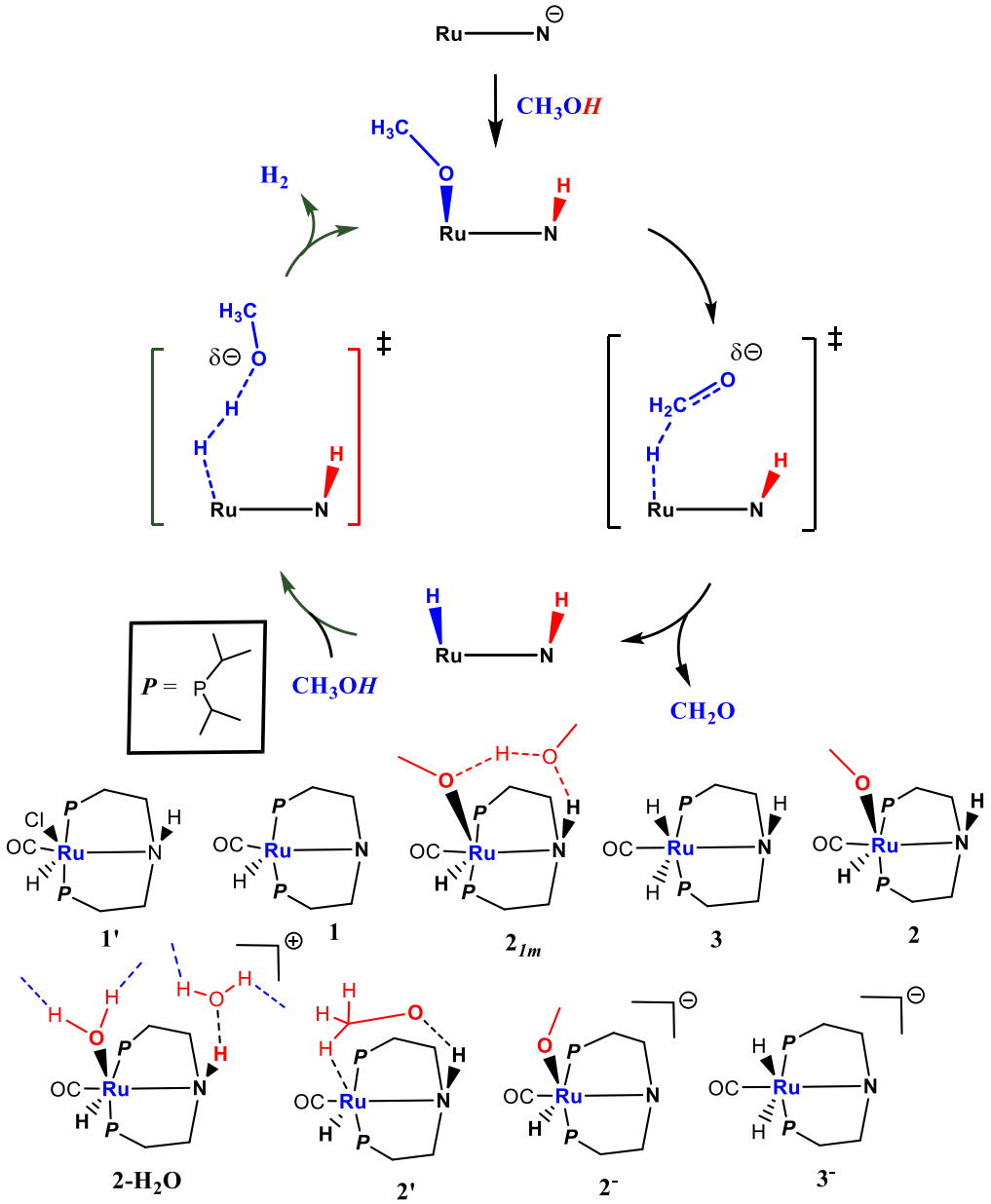
The reactions incorporating explicit methanol/water solvent were studied using DFT-based Born-Oppenheimer molecular dynamics, employing the CP2K package[11], and using the BLYP functional[5,13] supplemented by D3 dispersion corrections.[8] The system consisted of complexes **2/3** with 66 methanol molecules in a periodic cubic box (L=18 Å) in the methanol solvent system and 159 water molecules in a periodic cubic box (L=16.76 Å) for the water solvent system. A time step of 0.5 fs was used in our simulations. The electronic structure was converged to an accuracy that ensured that the energy is conserved within 0.6 kcal mol^{-1}, for trajectories up to ~ 10 ps. The temperature was controlled by a CSVR thermostat[12] and set at T = 360 K.

Goedecker–Teter–Hutter (GTH) pseudopotentials[11] were employed to account for the interactions of the nuclei and core electrons with the valence electrons. The electronic states were expanded using a TZVP-GTH basis set for ruthenium, and a DZVP-GTH basis set for all other atom types. The auxillary plane waves were expanded up to 280 Ry. In order to determine the free energy profiles along the reaction pathways, we used the constrained molecular dynamics method.[13,14] In this method, using a chosen reaction coordinate, Q, simulations are performed at several fixed values of this coordinate. The free-energy change upon changing from Q_1 to Q_2 is then computed

according to Eq. (1) Here, $\langle F(Q)\rangle$ is the average constraint force measured for each value of Q. For each value of the reaction coordinate, a 2 ps equilibration run, followed by a 5 ps production run was performed. The data from production runs was used to compute the average forces.

$$\Delta G = -\int_{Q_1}^{Q_2}\langle F(Q)\rangle dQ \qquad (1)$$

The structure of complex **1'** (RuH(CO)Cl(HN($C_2H_4P_i$-Pr_2)$_2$)) was reported in an earlier study by Beller and co-workers.[15] Complex **1** was assumed to be generated from complex **1'** by loss of HCl.[15] No simplifications were made to the geometry of complex **1** for both static and dynamic DFT calculations.



Scheme S1. Scheme 2 from main text showing the important complexes in this study. Blue dashed lines in complex **2-H$_2$O** show interactions with the solvent.

Analysis of the Frontier Orbitals

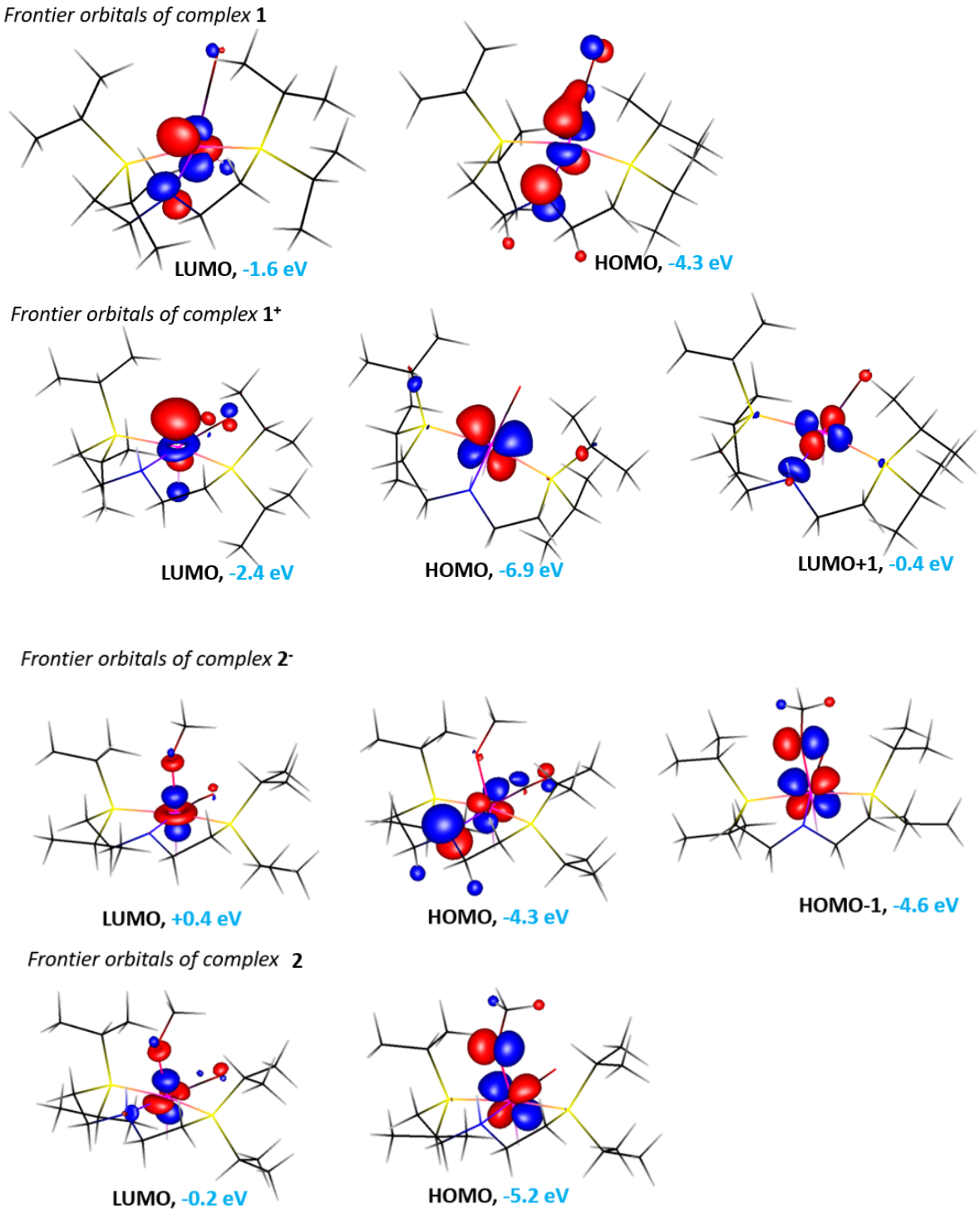


Figure S1. Frontier orbitals of complexes **1**, $\mathbf{1}^{+}$, $\mathbf{2}^{-}$ and **2**. The contour plots are made at a level of 0.08 a.u. at M06/def2-TZVP/DFT-D3 level of theory with implicit solvation correction for methanol (COSMO model).

The highest occupied molecular orbital (HOMO) in complex **1** is a π* orbital localized primarily between the C_{CO}-Ru-N centers (Figure S1). The relatively larger contribution of HOMO on the ligand nitrogen indicates presence of a relatively higher negative charge density, consistent with the observation that it makes strong hydrogen bonds with protic solvent/substrate species. Protonation of the ligand nitrogen to generate complex $\mathbf{1}^+$ increases the electrophilicity of the complex, which is manifested in the negative energies of the LUMO and LUMO+1 of complex $\mathbf{1}^+$. The HOMO and HOMO-1 are nearly degenerate in complex $\mathbf{2}^-$, which is formed upon the adsorption of a methoxy moiety on complex **1**. The HOMO in complex $\mathbf{2}^-$ also features a large negative charge density at the ligand nitrogen, indicating its high nucleophilicity. The general picture therefore is: complex **1** has strong hydrogen bond interactions with solvent molecules via the nitrogen moiety. Approach of an electron donating adsorbate species ROH/RO^- (R=H, Me) at the metal center results in a polarization effect on the HOMO of complex **1**, leading to a large negative charge density on ligand nitrogen, thereby making it highly nucleophilic. Binding of ROH/RO^- species to the metal center is followed by a spontaneous protonation of the nitrogen moiety and vice versa (put video of water being driven to metal center in cationic species). Such a sequence of events leads to the formation of complex $\mathbf{2}_{1m}$ (R=Me).

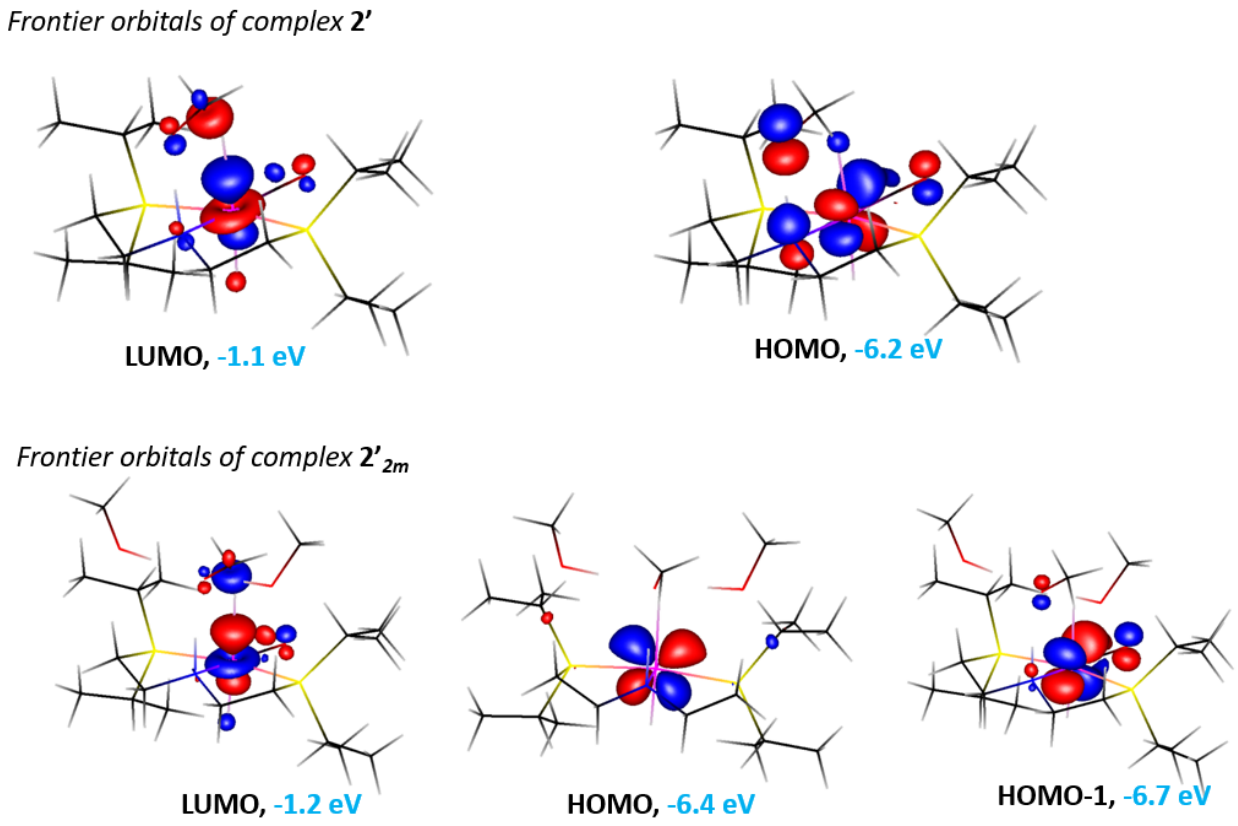


Figure S2. Frontier orbitals of the Ru-H-C adduct **2'** and $\mathbf{2'}_{2m}$. The contour plots are made at a level of 0.08 a.u. (M06//def2-TZVP)

The stabilization effect of adding explicit solvent molecules is demonstrated by comparing the frontier orbitals of complexes **2'** and **2'$_{2m}$** (Figure S2). In complex **2'**, where no explicit solvent molecules are present, there is a clear negative charge density on the hydride in the Ru-H-C adduct. However, addition of explicit methanol molecules leads to a stabilization of this adduct and a reordering of the orbitals. The HOMO in complex **2'** corresponds to the HOMO-1 in complex **2'$_{2m}$.** Further, the strong interaction between the O_{CH3O-} and the proton on the ligand nitrogen is weakened as remarked by the relatively smaller orbital lobes in HOMO-1 of complex **2'$_{2m}$.** Additionally, the negative charge density on the hydride in the Ru-H-C adduct seems to have diminished in complex **2'$_{2m}$**, resulting in increased barriers for C-H activation as discussed in the main text.

Estimate of Acidity Constant of Important Complexes

The basicity of the amido function in the aliphatic PNP ligand is of prime importance in the mechanism of dehydrogenation of methanol-water mixture by complex **1**. Experimentally, the pK_a of the NH moiety of the ligand in complex **1** in water/MeOH is difficult to assess. Therefore we used a DFT-MD approach to estimate the pK_a value of the NH moiety of these complexes in a water solvent box.

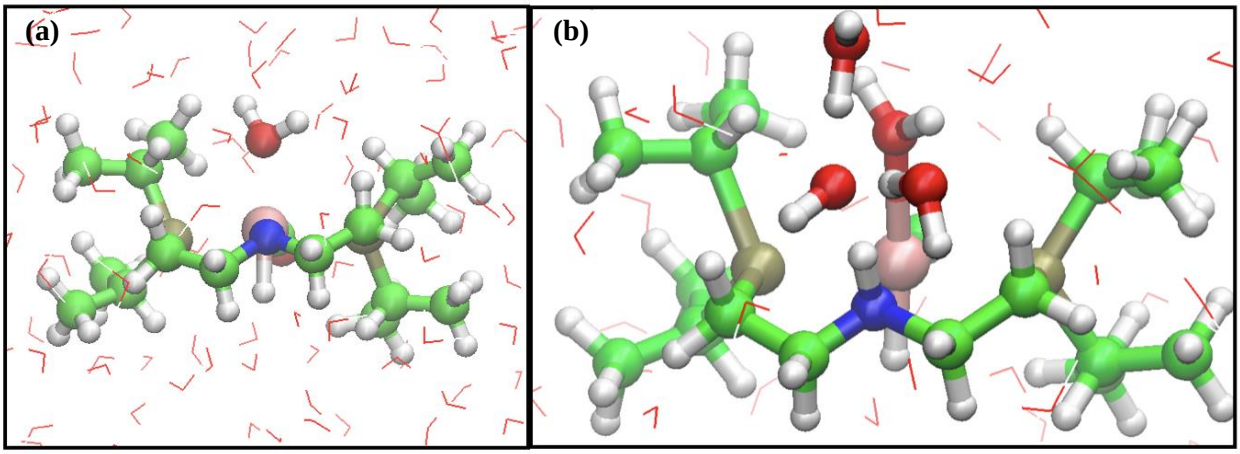


Figure S3. Two representative snapshots that show the spontaneous protonation of complex **1** by a solvent molecule. (a) Left: A water molecule gets adsorbed at the metal center (b) Right: spontaneous protonation of the amido moiety by solvent forming complex **2-H_2O** in aqueous solution

An interesting first observation in the AIMD simulations is spontaneous protonation of the amido moiety subsequent to adsorption of a solvent/substrate moiety at the metal centre (Figure S3). This indicates that adsorption of an adsorbate (e.g. water or methanol) at the metal centre increases the basicity of the amido moiety. In order to assess the basicity of this amido moiety we performed constrained molecular dynamics simulations to calculate the free energy of deprotonation of the NH moiety of complex **2-H_2O** (Figure S4), with the asymmetric stretch O-H-N as reaction coordinate for the deprotonation process, as shown in the inset of Figure S4 (b). These constrained molecular dynamics simulations started from a cationic complex (charge = +1). The resulting

free-energy profile, shown in Figure S3 (b), yields a deprotonation free energy of ~35 kcal/mol. It provides the dominant contribution to ΔG_a^0, the standard dissociation free energy, from which the pK_a can be computed using Eq. (2). Here, R is the universal gas constant. The resulting estimate for the pK_a, 25, indicates the very strong basicity of **2-H$_2$O**, which explains the spontaneous protonation that was observed (Figure S3 (a)). It is expected that the complexes **2** and **2*$_{1m}$*** will also have similar pK_a values. (Figure S5)

$$\mathrm{p}K_a = \frac{\Delta G_a^0}{2.303RT} \qquad (2)$$

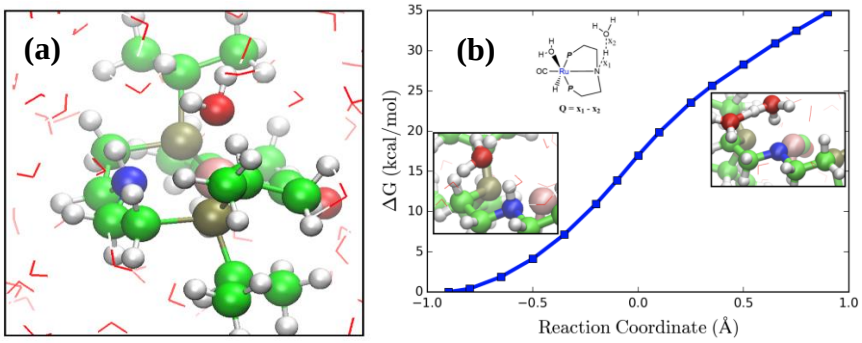


Figure S4. (a) Left: Complex **2-H$_2$O** with the protonated amido ligand, used as starting point in the constrained molecular dynamics simulations for the estimation of the acidity constant**.** (b) Right: free energy profile for the deprotonation of the NH moiety in complex **2-H$_2$O** that is a measure of its pK_a. The insets contain the representative snapshots of the initial and final state, and the chosen reaction coordinate (Q).

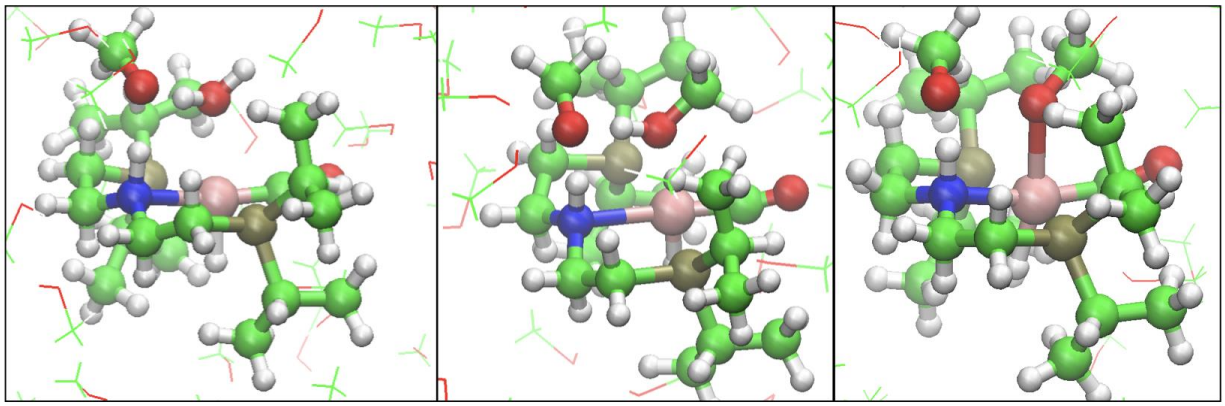
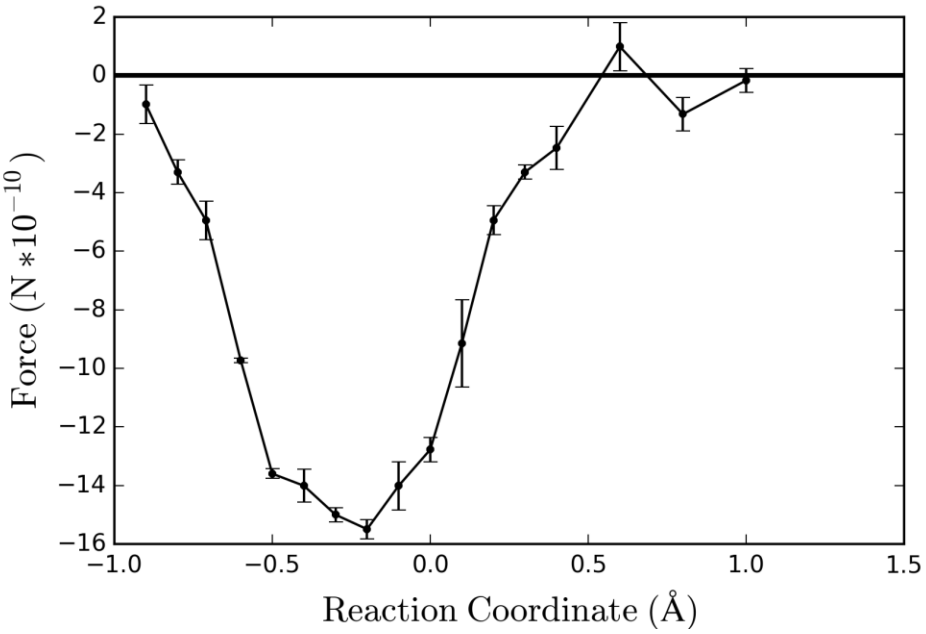


Figure S5. Snapshots from AIMD simulations showing the protonation of the ligand nitrogen by a solvent molecule upon adsorption of H_2O (left), CH_3OH (center) and CH_3O^- (right) on the metal center.

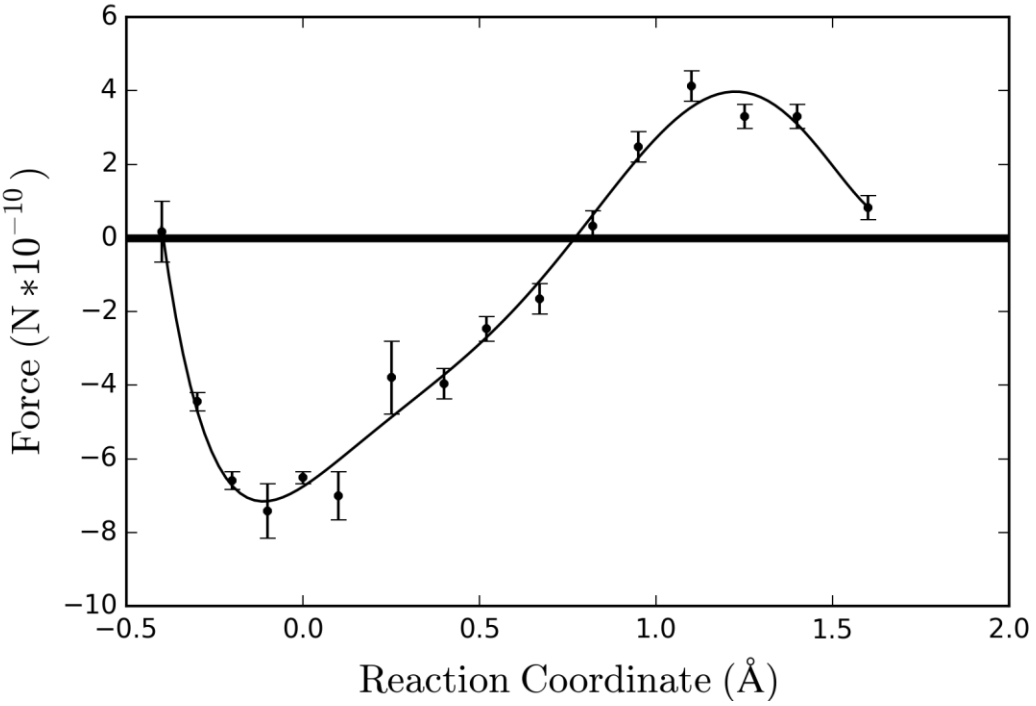
Constrained Force Profiles

The constrained force profiles used for the construction of the free energy profiles for C-H activation and H_2 production steps are provided below:

1. C-H Activation step



2. Hydrogen production



Benchmarking of the DFT methods

Resting state

DFT-MD simulations indicated spontaneous formation of complex **2** from complex **1**. Static DFT calculations (M06//def2-TZVP) further confirm that formation of complex **2** and **2_{1m}** from complexation of methanol with complex **1** is exergonic (see Table S1).

*Table S1: energy data for solvation of complexes **1** and **3**.*

Reactant => Product	**ΔG_{298}(kcal mol^{-1})***
1 + MeOH => 2	-13.9
2 + MeOH => 2_{1m}	-11.2
2_{1m} + MeOH => 2_{2m}	-5.9
3 + MeOH => 3_{1m}	-8.9
3 + $(MeOH)_2$ => 3_{2m}	-9.0

* since the substrate is also the solvent in the present case, $\Delta G_{298} \sim \Delta H_{298}$.

Benchmark Calculations

Beller and co-workers studied thermal decomposition of complex **3** using NMR.[15]

$$\mathbf{3} \rightleftharpoons \mathbf{1} + \boldsymbol{H_2}$$

$$K_{eq} = \frac{[\mathbf{1}][H_2]}{[\mathbf{3}]}$$

$$\frac{[\mathbf{3}]}{[\mathbf{1}]} \sim 4\ (experimentally\ determined)$$

The reaction starts with 62 mM of the hydrogenated complex **3** which dissociates to produce complex **1** and H_2. The reaction was monitored using NMR at 373 K. At equilibrium, 12.4 mM of complex **1** is formed (ratio of complex **1** to complex **3** was ~ 1:4).

At equilibrium:

[**1**] = [H_2] = 12.4 mM , [**3**] = 49.6 mM.

$$\Delta G^0_{373} = -RTln(K_{eq}) = -RTln\left(\frac{12.4 * 12.4}{49.6}\right) = -0.83\ kcal\ mol^{-1}$$

The results of our DFT calculations (Table S2) show that the M06 functional with corrections to the free energy by incorporating solvent effects in an implicit manner using the COSMO model and a correction to the solvent reference volume gives a free energy value that is in excellent

agreement with the experimental results. However, the results based on the BP86 functional are almost identical, and within the error margin of these calculations (see Table S2).

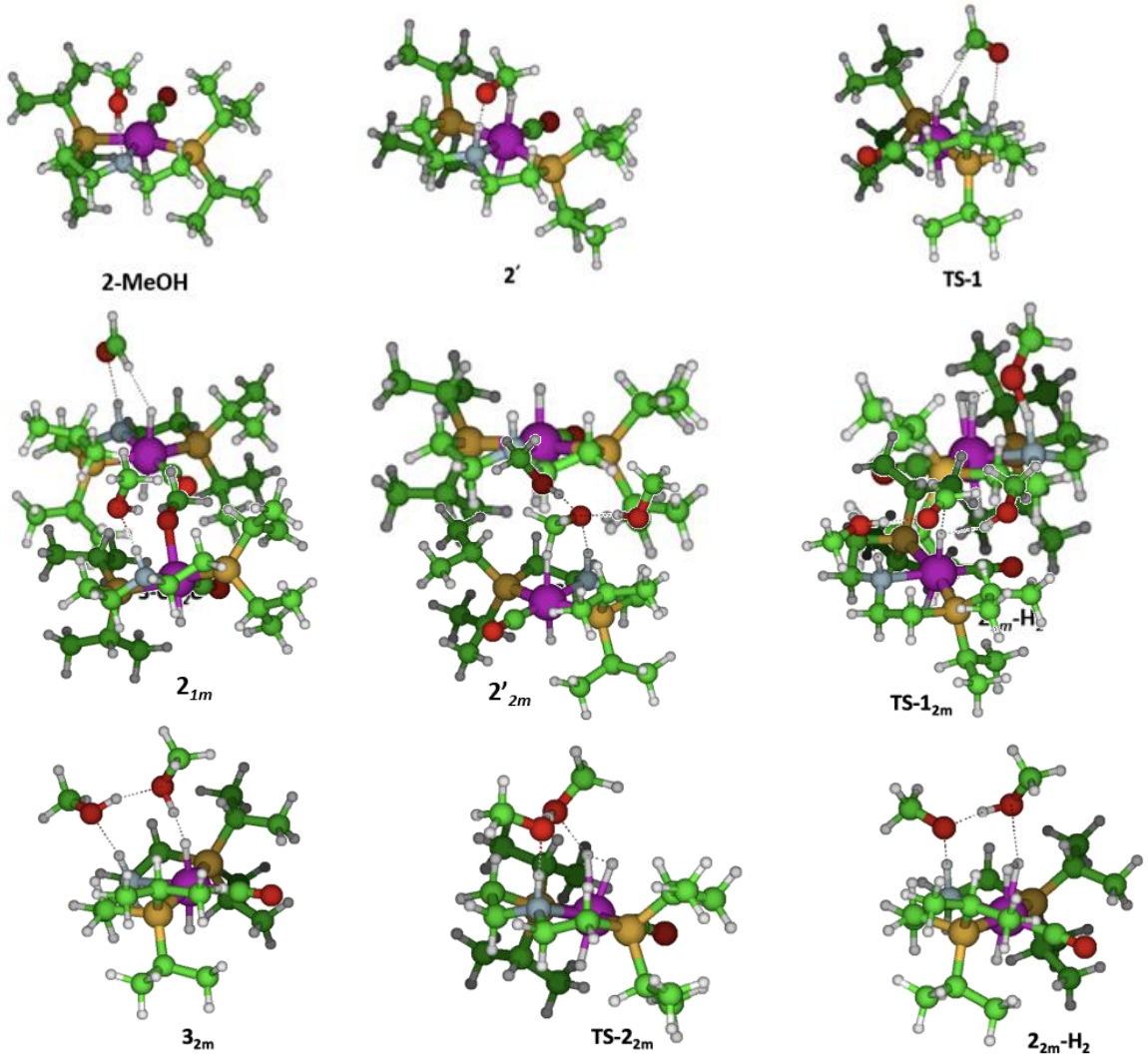
Table S2: Energy data for thermal decomposition of complex 3 obtained with different DFT methods.

3 => 1 + H_2				
method	Δ(SCF+ZPE)	ΔH_{298} (kcal mol^{-1})	ΔG_{298} (kcal mol^{-1}) gas phase	ΔG_{298} (kcal mol^{-1}) 'solution' [a]
BP86 (gas phase) [b]	+2.9	+5.1	-5.8	-3.3
M06 (gas phase)	+5.8	+8.0	-3.0	-0.5
BP86 (dioxane)	+5.1	+7.3	-3.6	-1.1
M06 (dioxane) [c]	***+8.2***	***+10.3***	***-0.6***	***+1.9***
BP86 (methanol)	+8.5	+10.7	-0.2	+2.3
M06 (methanol) [d]	+11.8	+14.0	+3.0	+5.5
	Δ(SCF+ZPE)	ΔH_{373} (kcal mol^{-1})	ΔG_{373} (kcal mol^{-1}) gas phase	ΔG_{373} (kcal mol^{-1}) 'solution' [a]
M06 (dioxane) [c]	***+8.6***	***+10.7***	***-3.3***	***-0.8***
CH_3OH => CH_2O + H_2				
M06 (methanol) [d]	+19.4	+21.1	+13.1	+15.6
M06 (methanol) [d, e]		*+21.29 ± 2.39*		

[a] An (entropy) correction factor of 2.5 kcal mol^{-1} is used in this column to compensate for intrinsic differences in reference volume in solution when compared to the gas phase (for dissociative processes).
[b] Method used for comparison with DFT-MD.
[c] Experimental set-up to study dehydrogenation of complex **3** using NMR, was performed in dioxane.[15]
[d] Method used in the SI for full MERP.
[e] Experimental value

Computed MERPs

Snapshots of optimized molecular complexes and Transition states are shown in Figure S6.



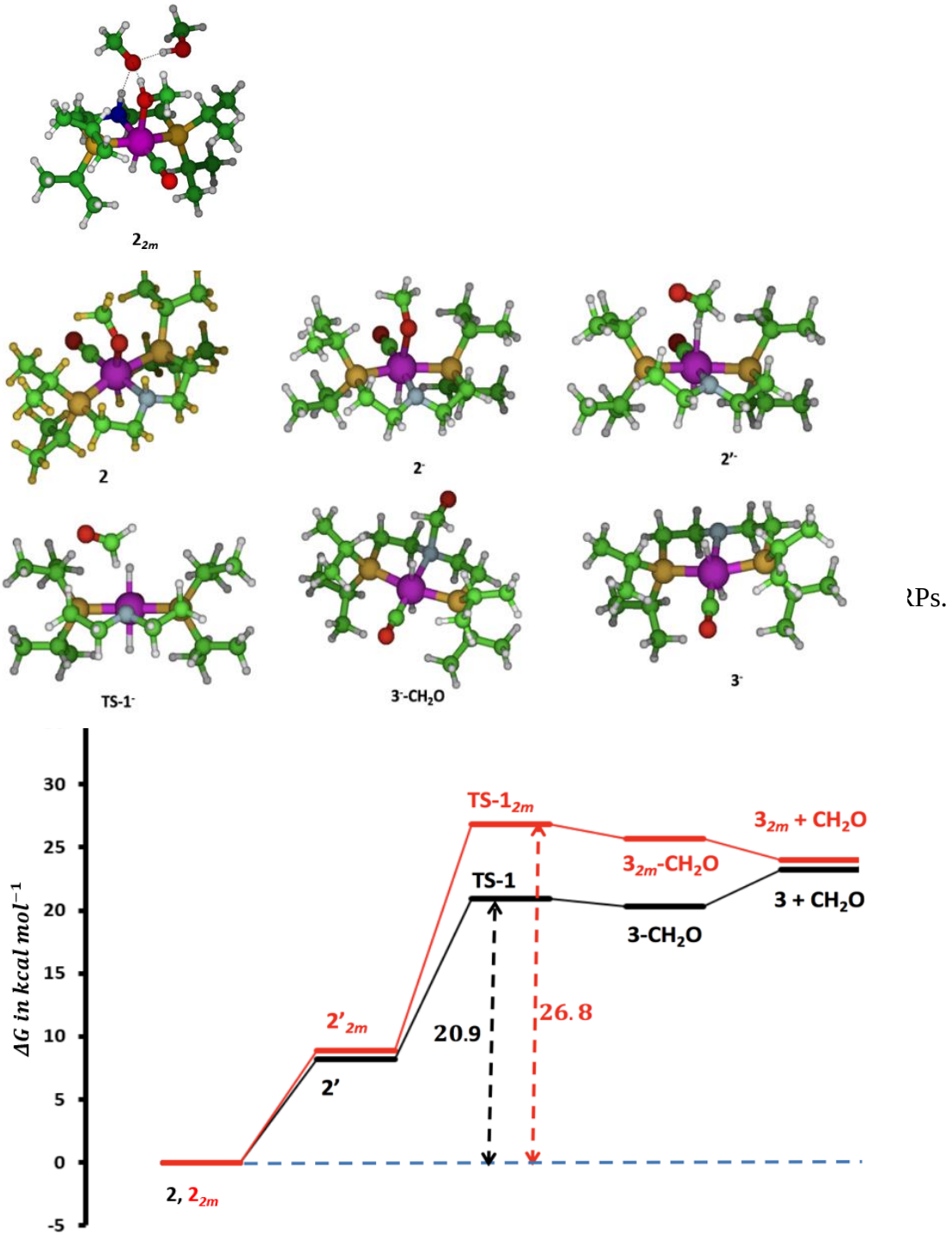


Figure S7. Computed MERP for oxidation of methanol to formaldehyde over complex **2**/**2**$_{2m}$ (*BP86/def2-TZVP*).

The rate-determining step (RDS) for methanol oxidation to formaldehyde (Figure S7) and hydrogen production (see main text) is the C-H activation step of complex **2**$_{2m}$ (*BP86/def2-TZVP).* The transition state barrier for the RDS in gas-phase is +20.9 kcal mol^{-1}. Upon introduction of explicit solvent molecules (MeOH), this barrier increases to +26.8 kcal mol^{-1}, demonstrating the crucial role of solvent in this mechanism.

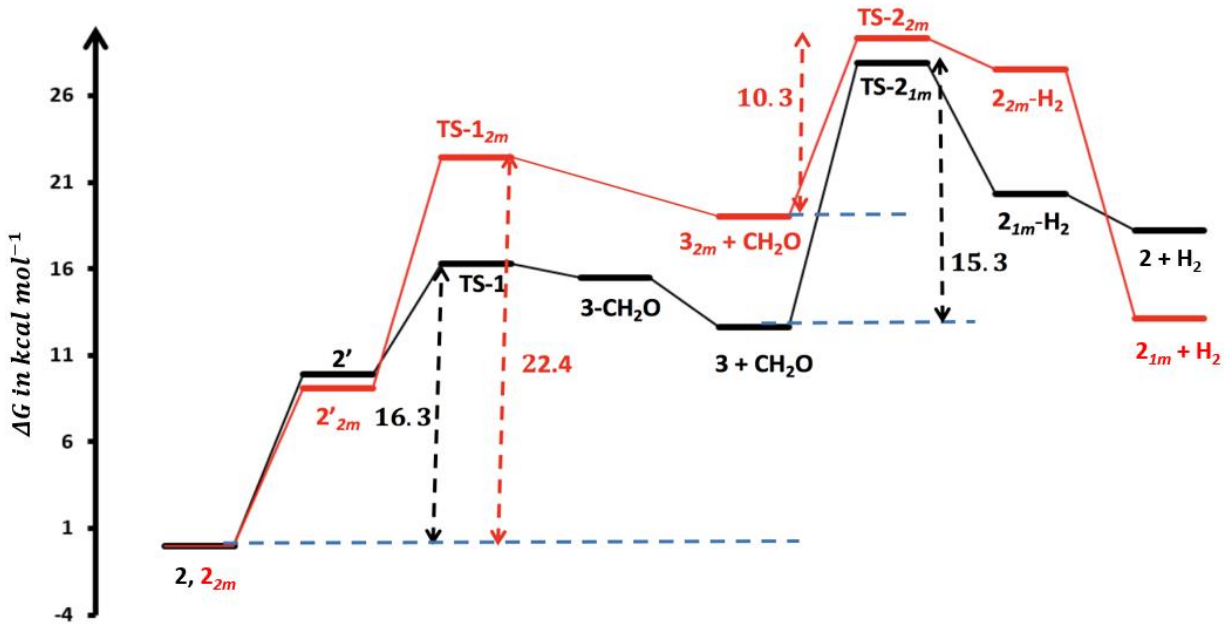


Figure S8. Computed MERP for oxidation of methanol to formaldehyde and hydrogen over complex **2**/**2**$_{2m}$ (*M06//def2-TZVP*)

Similar results were obtained with the M06 functional. The rate determining step (RDS) for methanol oxidation to formaldehyde and hydrogen production (Figure S8) is the C-H activation step (*M06//def2-TZVP).* The transition state barrier for the RDS in gas-phase is +16.3 kcal mol^{-1}. Upon introduction of explicit solvent molecules (MeOH), this barrier increases to +22.4 kcal mol^{-1}, consistent with the relatively high temperature (90° C) needed for optimal catalytic activity. It is interesting to note that while GGA functionals typically underestimate activation barriers compared to meta-GGA/hybrid functionals, but in this case we observed the opposite.

Computed MERP for the anionic pathway

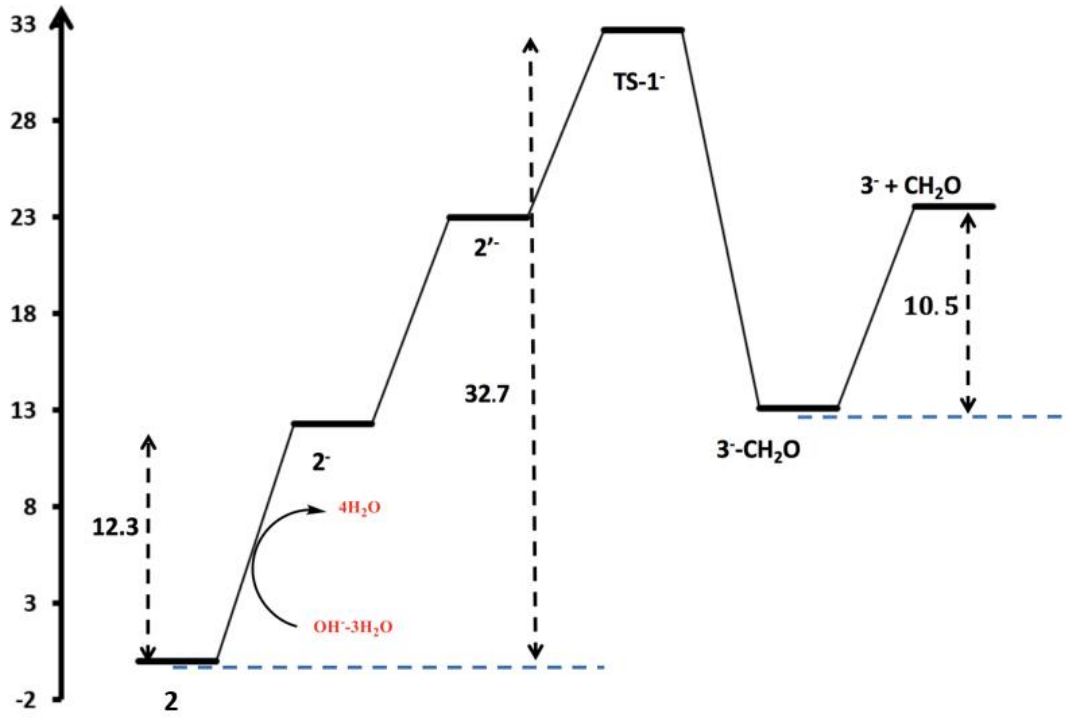


Figure S9. Computed MERP for oxidation of methanol to formaldehyde and hydrogen over complex **2** (*M06//def2-TZVP*) via an anionic pathway.

We also compute the MERP for oxidation of methanol to formaldehyde and hydrogen by complex **2** via an anionic pathway as proposed by Beller and co-workers[15] (Figure S9). The first step in the MERP that involves deprotonation of complex **2** by an incoming base (OH^-) is uphill by +12.3 kcal. Evidently, the overall barrier is quite high (+32.7 kcal mol^{-1}) to account for the reaction conditions, making this an unlikely mechanism (compared to +22.4 kcal mol^{-1} in the neutral pathway). An interesting observation is the formation of complex **3^--CH_2O** where the CH_2O moiety coordinates strongly at the ligand nitrogen, further demonstrating the high proton affinity of the ligand nitrogen.

Analysis of the transition states

IRC calculations were performed to confirm that transition states connected to their respective product and reactant states.

TS-1: The potential energy surface obtained from the IRC calculations on TS-1 is shown in Figure S10. The TS is very close to the product state. Due to the endergonic nature of the transformation, **TS-1** is a very late transition state. The formaldehyde moiety is oriented away from the Ru–N bond, and is not parallel to it as one would normally expect.

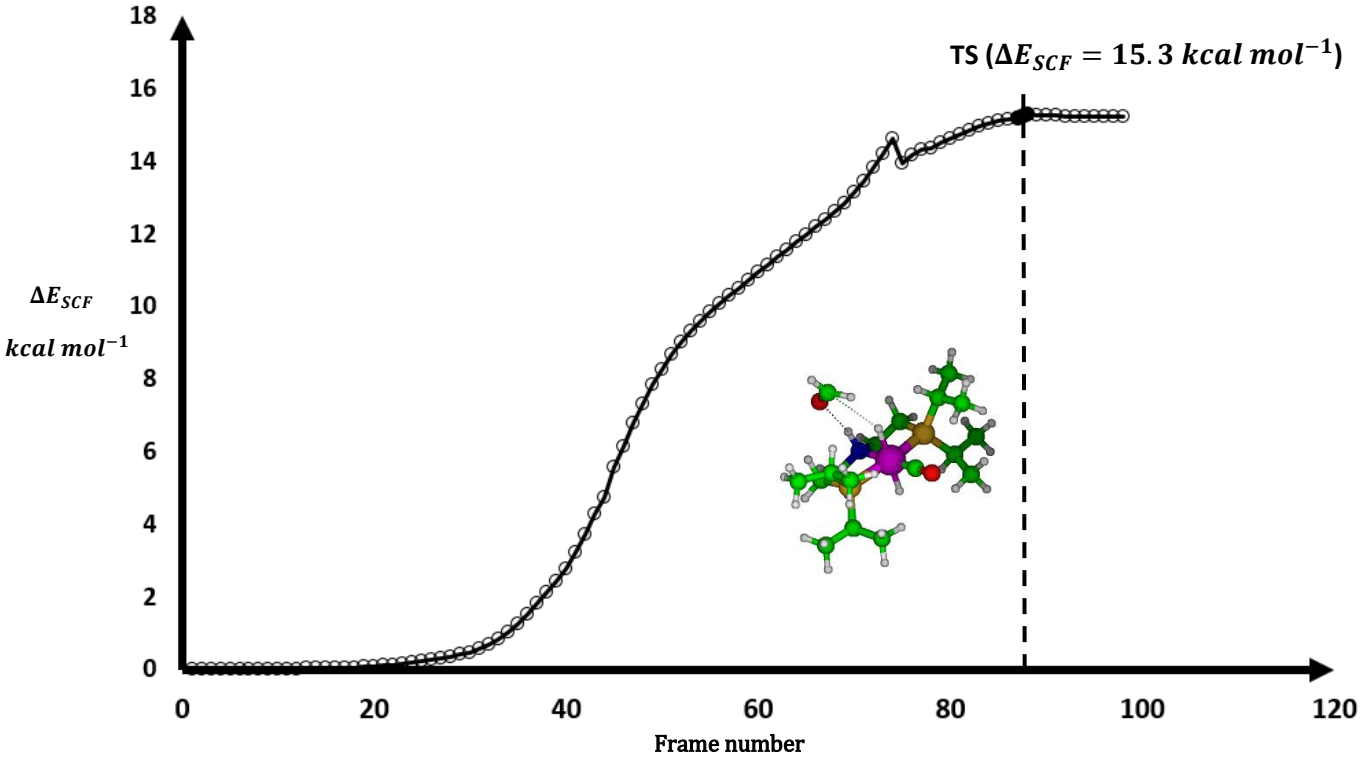


Figure S10. Potential energy surface for formation of CH_2O from the methoxide adduct **1'** obtained by IRC calculations using static DFT. Inset shows the optimized **TS-1** geometry. The vertical axis is the computed scf energy, while the horizontal axis represents the frame number of the intermediate in the trajectory.

The slight kink in the obtained PES corresponds to the movement of CH_2O moiety away from the plane of Ru–N bond. Animations generated from IRC calculations for all the TSs reported in the present study have been supplied separately.

Selected Snapshots from AIMD Simulations

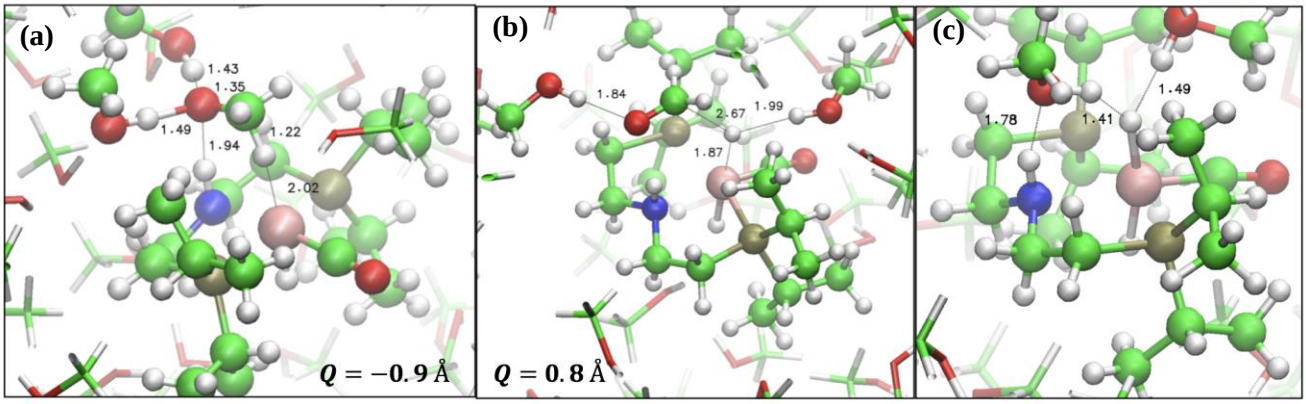


Figure S11. Selected snapshots for methanol oxidation of complex **2**. Important distances are shown in Å. (a) Left: Q= -0.9 Å corresponds to the reactant state where the methoxide adduct is stabilized by hydrogen bonds with the solvent and the protonated ligand nitrogen (NH). (b) Center: Q= 0.8 Å represents the product state, with the formation of metal hydride bond and formaldehyde. The metal hydride interacts with a solvent methanol molecule. (c) Right: The last snapshot is from an unconstrained run of the complex **3**, where the metal hydride interacts with up to two solvent molecules.

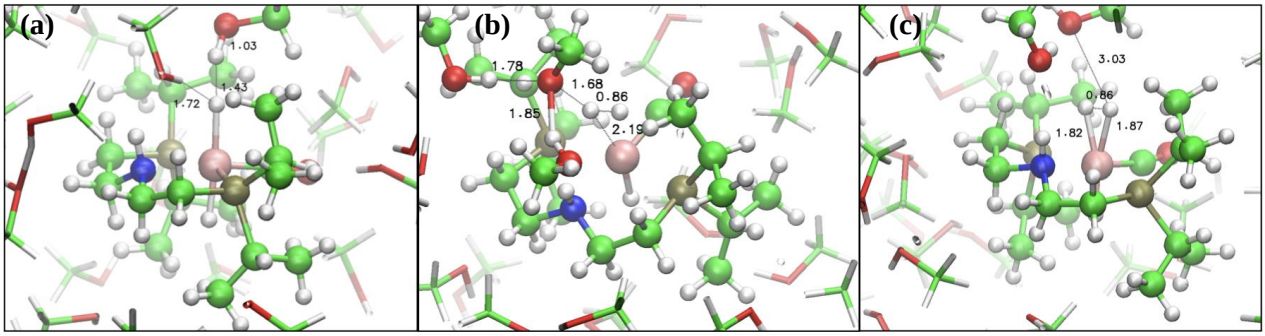


Figure S12. Selected snapshots for hydrogen production from complex **3**. Important distances are shown in Å. (a) Left: Q= -0.4 Å corresponds to the reactant state where complex **3** interacts with two solvent molecules (b) Center: Q= 0.82 Å represents a transition state geometry, with the formation of di-hydrogen bond and the Ru-H bond. (c) Right: Q= 1.6 Å. The complex **2-H$_2$** formed by protonation of the metal hydride by a solvent methanol molecule. The ligand nitrogen remains protonated throughout the reaction.

Energy Tables

Table S3: Energies for geometry optimizations with (BP86/def2-TZVP)

Species	SCF	ZPE	H_{corr}	G_{corr}	SCF+ZPE	H	G
MeOH	-115.77951	0.04957	0.05387	0.02679	-115.72994	-115.72564	-115.75272
HCHO	-114.55933	0.02557	0.02939	0.00456	-114.53376	-114.52994	-114.55477
H_2	-1.17753	0.00986	0.01307	-0.00182	-1.16767	-1.16446	-1.17935
1	-1578.47943	0.50248	0.53393	0.44253	-1577.97695	-1577.9455	-1578.0369
2_{1m}	-1810.09839	0.60817	0.64676	0.54095	-1809.49022	-1809.45163	-1809.55744
2_{2m}	-1925.90051	0.65864	0.70175	0.58432	-1925.24187	-1925.19876	-1925.31619
2-MeOH	-1694.284545	0.55366	0.58881	0.48981	-1693.730885	-1693.695735	-1693.794735
2'	-1694.272277	0.55185	0.58616	0.49065	-1693.720427	-1693.686117	-1693.781627
TS_1	-1694.24789	0.55032	0.58528	0.48648	-1693.69757	-1693.66261	-1693.76141
3-CH_2O	-1694.24785	0.5503	0.58601	0.48546	-1693.69755	-1693.66184	-1693.76239
3	-1579.67247	0.52318	0.55436	0.46554	-1579.14929	-1579.11811	-1579.20693
2' $_{2m}$	-1925.884466	0.65798	0.70136	0.58245	-1925.226486	-1925.183106	-1925.302016
TS-1_{2m}	-1925.852396	0.65429	0.69768	0.57884	-1925.198106	-1925.154716	-1925.273556
3_{2m}	-1811.282784	0.62651	0.6666	0.55559	-1810.656274	-1810.616184	-1810.727194
TS-2_{2m}	-1811.267437	0.61868	0.65804	0.54978	-1810.648757	-1810.609397	-1810.717657
2_{2m}-H_2	-1811.270395	0.62135	0.66134	0.55081	-1810.649045	-1810.609055	-1810.719585
3_{1m}	-1695.488223	0.5742	0.6101	0.50842	-1694.914023	-1694.878123	-1694.979803
TS-2_{1m}	-1695.464542	0.56774	0.60282	0.50494	-1694.896802	-1694.861722	-1694.959602
2_{1m}-H_2	-1695.470481	0.57108	0.60693	0.50654	-1694.899401	-1694.863551	-1694.963941

Table S4: Energies for geometry optimizations with (M06//def2-TZVP)

Species	SCF	ZPE	H_{corr}	G_{corr}	SCF+ZPE	H	G
1^+	-1577.986252	0.5174	0.54907	0.45682	-1577.468852	-1577.437182	-1577.529432
MeOH	-115.7070442	0.04957	0.05387	0.02679	-115.6574742	-115.6531742	-115.6802542
HCHO	-114.4910602	0.02557	0.02939	0.00456	-114.4654902	-114.4616702	-114.4865002
H_2	-1.170990116	0.00986	0.01307	-0.00182	-1.161130116	-1.157920116	-1.172810116
1	-1577.508029	0.50248	0.53393	0.44253	-1577.005549	-1576.974099	-1577.065499
2_{1m}	-1808.967182	0.60817	0.64676	0.54095	-1808.359012	-1808.320422	-1808.426232
2_{2m}	-1924.68482	0.65864	0.70175	0.58432	-1924.02618	-1923.98307	-1924.1005
2-MeOH	-1693.231637	0.55366	0.58881	0.48981	-1692.677977	-1692.642827	-1692.741827
2'	-1693.220427	0.55185	0.58616	0.49065	-1692.668577	-1692.634267	-1692.729777
TS_1	-1693.206022	0.55032	0.58528	0.48648	-1692.655702	-1692.620742	-1692.719542
3-CH_2O	-1693.206397	0.5503	0.58601	0.48546	-1692.656097	-1692.620387	-1692.720937
3	-1578.708619	0.52318	0.55436	0.46554	-1578.185439	-1578.154259	-1578.243079
2' $_{2m}$	-1924.670386	0.65798	0.70136	0.58245	-1924.012406	-1923.969026	-1924.087936
TS-1_{2m}	-1924.645686	0.65429	0.69768	0.57884	-1923.991396	-1923.948006	-1924.066846
3_{2m}	-1810.145288	0.62651	0.6666	0.55559	-1809.518778	-1809.478688	-1809.589698
TS-2_{2m}	-1810.123075	0.61868	0.65804	0.54978	-1809.504395	-1809.465035	-1809.573295
2_{2m}-H_2	-1810.126957	0.62135	0.66134	0.55081	-1809.505607	-1809.465617	-1809.576147
3_{1m}	-1694.431724	0.5742	0.6101	0.50842	-1693.857524	-1693.821624	-1693.923304
TS-2_{1m}	-1694.403294	0.56774	0.60282	0.50494	-1693.835554	-1693.800474	-1693.898354
2_{1m}-H_2	-1694.413374	0.57108	0.60693	0.50654	-1693.842294	-1693.806444	-1693.906834

Table S5: Energies for geometry optimizations with (M06//def2-TZVP) (anionic pathway)

Species	SCF	ZPE	H_{corr}	G_{corr}	SCF+ZPE	H	G
OH^--$3H_2O$	-305.262352	0.0829	0.09234	0.05228	-305.179452	-305.170012	-305.210072
$4H_2O$	-305.757399	0.09549	0.10572	0.06231	-305.661909	-305.651679	-305.695089
2^-	-1692.719618	0.53924	0.57355	0.47868	-1692.180378	-1692.146068	-1692.240938
$2'^-$	-1692.697860	0.53599	0.57049	0.47401	-1692.161870	-1692.127370	-1692.223850
TS-1^-	-1692.685055	0.53801	0.57179	0.4767	-1692.147045	-1692.113265	-1692.208355
3^--CH_2O	-1692.716382	0.53801	0.57179	0.4767	-1692.178372	-1692.144592	-1692.239682
3^-	-1578.188488	0.50585	0.53697	0.44807	-1577.682638	-1577.651518	-1577.740418

G = Gibbs Free Energy (298K)

H = Enthalpy
$\mathbf{H}_{corr}$ = Correction term to Enthalpy
$\mathbf{G}_{corr}$ = Correction term to Free Energy
All values are in atomic units.

XYZ Coordinates

1^{+}
60

Ru	15.5130078	10.5521489	5.2003823
H	16.6509802	11.6054875	5.2013361
P	15.8235563	10.2709054	2.9115233
P	14.9220350	11.3069032	7.3282246
O	17.5967533	8.5677139	6.0679037
N	14.0361646	12.0692744	4.5438803
C	14.5918234	11.4704207	2.1886988
H	14.9351997	11.8676611	1.2232048
H	13.6597425	10.9178639	1.9929533
C	14.3371236	12.6060892	3.1764831
H	15.2299940	13.2361211	3.2802972
H	13.5092209	13.2496055	2.8349399
C	13.8710342	13.1754917	5.5429644
H	13.0383330	13.8328621	5.2412447
H	14.7949679	13.7670290	5.5046096
C	13.6458189	12.6173932	6.9456232
H	12.6540164	12.1435729	7.0156144
H	13.6641412	13.4288960	7.6868061
C	16.2008120	12.1785613	8.3622139
H	15.6654478	12.5236065	9.2621481
C	17.3210120	11.2152415	8.7739729
H	17.8323503	10.8016885	7.8940144
H	16.9544859	10.3774722	9.3795213
H	18.0682600	11.7536838	9.3745257
C	16.7672456	13.4034446	7.6313458
H	17.5316559	13.8829879	8.2594284
H	16.0022787	14.1623874	7.4182026
H	17.2470805	13.1142121	6.6850158
C	13.9902522	10.1352014	8.4500545
H	13.0362802	10.0160135	7.9047262
C	14.6500710	8.7510357	8.5311259
H	15.6191199	8.7851096	9.0450464
H	14.8174021	8.3173230	7.5360453
H	14.0014928	8.0659820	9.0957450
C	13.6870864	10.7178418	9.8365026
H	12.9996052	10.0512810	10.3769195
H	13.2143902	11.7091236	9.7850975
H	14.6005593	10.8033937	10.4417006
C	15.3399581	8.6099548	2.2235106
H	16.1701136	7.9557556	2.5373548
C	14.0645429	8.1212809	2.9272915
H	14.1887053	8.0916130	4.0218478
H	13.8157300	7.1021533	2.5992053
H	13.1968953	8.7562571	2.6916985
C	15.2121887	8.5669169	0.6969468
H	16.1424833	8.8539132	0.1896199
H	14.4082938	9.2266108	0.3388999
H	14.9644267	7.5459683	0.3719622
C	17.4546003	10.6936147	2.1321734
H	17.3155944	10.5460860	1.0478191
C	17.8280850	12.1601277	2.3861383
H	17.9003620	12.3676052	3.4638858
H	17.1095412	12.8628435	1.9420727
H	18.8091467	12.3737313	1.9386422
C	18.5472214	9.7438923	2.6411298

H	18.3203941	8.6880333	2.4417111
H	18.6986208	9.8616322	3.7231610
H	19.4989060	9.9752267	2.1419879
C	16.7795669	9.3275529	5.7343617
H	13.1318226	11.5801997	4.4825373

MeOH
6

C	-3.8590733	3.0841737	-0.0120916
O	-2.4370163	3.2324798	-0.0213527
H	-4.3697979	3.9337424	0.4770286
H	-4.1835087	2.1473085	0.4766912
H	-4.1784081	3.0511241	-1.0616752
H	-2.1334510	3.2653090	0.9007050

HCHO
4

C	-1.5900409	0.0794198	0.0104328
O	-0.7108677	0.2543533	0.8211746
H	-1.3845331	0.0226609	-1.0882660
H	-2.6621931	-0.0362217	0.3098886

H_2
2

H	-0.0253553	0.0000000	0.0000000
H	0.7253553	0.0000000	0.0000000

1
59

Ru	15.3980042	10.5490630	5.2033603
H	16.9439317	10.7730840	5.4520114
P	15.7467822	10.3527306	2.9458026
P	14.9265047	11.3401653	7.3234641
O	16.0603873	7.6485323	5.7451690
N	14.2736536	12.1247227	4.6360560
C	14.5298784	11.5516168	2.2257427
H	14.8802410	11.9773868	1.2738167
H	13.6165897	10.9742169	2.0208314
C	14.2307908	12.6388847	3.2622000
H	14.9512548	13.4761988	3.1471242
H	13.2320531	13.0746795	3.0573791
C	13.7876659	13.1571420	5.5562860
H	12.8123790	13.5471668	5.2006236
H	14.4766243	14.0278764	5.5498860
C	13.6278365	12.6270450	6.9819159
H	12.6639566	12.1040191	7.0756667
H	13.6419961	13.4406238	7.7225548
C	16.2852502	12.2723648	8.2092159
H	15.8439149	12.6793921	9.1342785
C	17.4506661	11.3397622	8.5621893
H	17.8198203	10.8290013	7.6611655
H	17.1657364	10.5718051	9.2916701
H	18.2809748	11.9191043	8.9944284
C	16.7710910	13.4398232	7.3379693
H	17.6240801	13.9396163	7.8223041
H	15.9899998	14.1950917	7.1793382
H	17.0997678	13.0763378	6.3533387
C	14.0767878	10.2898563	8.6239594
H	13.1373135	10.0390773	8.1001085
C	14.7987023	8.9710750	8.9257662
H	15.7188447	9.1352633	9.5027507

H	15.0643092	8.4269478	8.0124229
H	14.1467697	8.3232460	9.5319371
C	13.7332503	11.0502086	9.9116889
H	13.0884044	10.4315338	10.5546623
H	13.2030242	11.9932364	9.7177824
H	14.6405895	11.2811454	10.4889444
C	15.3994234	8.7261483	2.0949264
H	16.1679274	8.0563431	2.5157924
C	14.0284390	8.1834535	2.5225436
H	13.9244905	8.1663091	3.6155495
H	13.8974136	7.1578248	2.1458085
H	13.2079949	8.7913866	2.1120321
C	15.5398019	8.7657253	0.5683917
H	16.5550882	9.0336455	0.2459060
H	14.8386391	9.4876193	0.1224554
H	15.3083298	7.7777050	0.1412298
C	17.4065070	10.8737300	2.2713575
H	17.3229432	10.8594744	1.1716855
C	17.7383451	12.3024017	2.7229766
H	17.7288895	12.3718898	3.8202981
H	17.0227734	13.0376813	2.3300824
H	18.7401961	12.5875695	2.3669701
C	18.4902053	9.8846383	2.7182649
H	18.3195573	8.8712523	2.3283327
H	18.5229301	9.8239489	3.8160972
H	19.4775347	10.2164776	2.3623808
C	15.8294397	8.7898140	5.5755584

2$_{Im}$
71

H	-1.1498296	-1.5682928	-0.2140818
Ru	-0.4731143	-0.1001687	-0.1384890
O	0.1264326	2.0298391	0.0354570
P	-0.8232682	-0.0842118	2.1482169
P	-0.7238883	0.0228167	-2.4354433
C	-2.4758780	0.7610926	2.2773309
C	-2.4204391	0.7623508	-2.6210920
H	-2.2754196	1.8441602	2.2806638
H	-2.2988848	1.8566677	-2.6160090
H	-3.0068079	0.5158616	3.2082272
H	-2.9005084	0.4731514	-3.5666136
C	-3.3102296	0.4031125	1.0498263
C	-3.2684898	0.3556054	-1.4180619
H	-4.2691147	0.9541701	1.0571389
H	-4.2500742	0.8639511	-1.4501936
H	-3.5443078	-0.6727588	1.0369860
H	-3.4483969	-0.7302553	-1.4038106
N	-2.5443721	0.7182789	-0.1763060
C	0.3827838	1.2262973	-3.3348133
C	0.3074534	1.0128585	3.1441433
H	0.3979641	2.0395305	-2.5872460
H	0.3962571	1.8476625	2.4252795
C	-0.8525440	-1.5888958	-3.3749677
C	-1.0993916	-1.7206661	3.0051853
H	-1.7875048	-1.9950204	-2.9467192
H	-2.0313823	-2.0546212	2.5129613
C	1.1786177	-0.8738647	-0.1200963
O	2.2335556	-1.3916104	-0.1084616
C	-1.3379985	-1.6543683	4.5185242
C	-1.0216811	-1.4654252	-4.8943107
H	-2.0886668	-0.9031099	4.8012331
H	-1.7987381	-0.7435858	-5.1819790
H	-0.4069511	-1.4215412	5.0537367
H	-0.0806374	-1.1592554	-5.3720056

H	-1.6889785	-2.6310147	4.8861613
H	-1.2998902	-2.4418864	-5.3203152
C	-0.0041468	-2.7358072	2.6496634
C	0.2778562	-2.5611796	-3.0122874
H	0.9666838	-2.4495105	3.0769400
H	1.2543486	-2.1961471	-3.3588220
H	0.1161884	-2.8222769	1.5629486
H	0.3381966	-2.7117365	-1.9279926
H	-0.2664129	-3.7260318	3.0531736
H	0.0987248	-3.5367276	-3.4903874
C	1.8053387	0.6650712	-3.4653386
C	1.6915338	0.3711604	3.3105943
H	1.8581455	-0.1038205	-4.2503396
H	1.6702961	-0.4371687	4.0567810
H	2.1609178	0.2189519	-2.5264828
H	2.0698380	-0.0444175	2.3670122
H	2.5041774	1.4679511	-3.7448763
H	2.4142581	1.1229080	3.6624744
C	-0.1209773	1.8107221	-4.6614699
C	-0.2224748	1.5690403	4.4724781
H	-1.1414558	2.2091202	-4.5856800
H	-1.2197514	2.0194517	4.3758053
H	-0.1026403	1.0709547	-5.4715804
H	-0.2732550	0.7986188	5.2524299
H	0.5326588	2.6442720	-4.9630968
H	0.4572440	2.3566570	4.8344018
C	1.4780067	2.4003673	-0.0420927
H	1.5840888	3.4987047	0.0560672
H	2.0806280	1.9337019	0.7635425
H	1.9574468	2.1051424	-0.9984129
O	-1.8197996	3.3766876	-0.6564191
H	-0.8936358	2.9071505	-0.4183258
H	-2.3977187	1.7592103	-0.2210115
C	-2.0455131	4.4051441	0.2925551
H	-1.8775872	4.0582439	1.3321407
H	-3.0884023	4.7503480	0.2120932
H	-1.3854828	5.2763893	0.1234584

2-MeOH

65

Ru	11.1305970	9.7714601	8.9238358
H	12.3590010	10.0020626	9.8722735
P	12.6276261	9.1426002	7.2782693
P	9.8334544	11.0118970	10.3821126
O	10.8809570	7.0729054	10.2680340
N	11.1017474	11.5539071	7.8217266
C	12.4894710	10.5269209	6.0543073
H	13.4025685	10.6426978	5.4526330
H	11.6643075	10.2638688	5.3764542
C	12.1327661	11.8103648	6.8053380
H	13.0382921	12.2458306	7.2724766
H	11.7653974	12.5655251	6.0820551
C	10.7403738	12.8144657	8.4868126
H	10.4464003	13.5686473	7.7296832
H	11.6170534	13.2357932	9.0180760
C	9.5792913	12.6043846	9.4593011
H	8.6476866	12.4786558	8.8868949
H	9.4495505	13.4612854	10.1364749
C	10.5962359	11.5041545	12.0137765
H	9.8604646	12.1489241	12.5220211
C	10.8679193	10.2615173	12.8710644
H	11.5192208	9.5571507	12.3336105
H	9.9456807	9.7292646	13.1389148
H	11.3708764	10.5499196	13.8069331

C	11.8815920	12.3129387	11.7945537
H	12.3462227	12.5443762	12.7651708
H	11.6920919	13.2646353	11.2805370
H	12.6058629	11.7400958	11.1975379
C	8.0721629	10.4970031	10.7714677
H	7.5770497	10.6861146	9.8036387
C	7.9384836	8.9984073	11.0646155
H	8.3447813	8.3929551	10.2451011
H	6.8766879	8.7375392	11.1939660
H	8.4663845	8.7063684	11.9823831
C	7.3860991	11.3600965	11.8375541
H	6.3117872	11.1241776	11.8785658
H	7.4828383	12.4358404	11.6309485
H	7.8006824	11.1651703	12.8373957
C	12.3380562	7.5941145	6.2776801
H	12.9760464	7.6749524	5.3807278
C	12.7260622	6.3427349	7.0789498
H	12.5076655	5.4398080	6.4888855
H	12.1460207	6.2805412	8.0105105
H	13.7918252	6.3159055	7.3416391
C	10.8691246	7.5113651	5.8430654
H	10.7289256	6.6620845	5.1573130
H	10.5186212	8.4196231	5.3340115
H	10.2246479	7.3518057	6.7184418
C	14.4438090	9.0574948	7.7283486
H	14.4704844	8.2734053	8.5034357
C	15.3686938	8.6597798	6.5701190
H	15.1358103	7.6712941	6.1540248
H	16.4123098	8.6329318	6.9192386
H	15.3205562	9.3924700	5.7507438
C	14.9149716	10.3735112	8.3643969
H	15.9081513	10.2384982	8.8181990
H	14.2220599	10.7203415	9.1425233
H	15.0055219	11.1657649	7.6069372
C	10.9661820	8.1209435	9.7439782
C	8.4951678	9.7680045	7.0487258
H	8.2339772	8.9458502	6.3633647
H	7.6125747	9.9991778	7.6771170
O	8.9697219	10.8790209	6.3440054
H	9.7801095	11.2158501	6.8814634
H	9.2729478	9.3340449	7.7518693

2’

65

H	-1.5613509	-0.3781039	0.0020627
Ru	0.0259905	-0.1959493	-0.0002138
H	1.8875616	0.2676197	-0.0049979
P	-0.0709261	0.1006891	2.2966920
P	-0.0782080	0.1037546	-2.2964614
C	-0.0274628	1.9490063	2.4451322
C	-0.0372193	1.9522873	-2.4427719
H	1.0339195	2.2418899	2.4097605
H	1.0240643	2.2461701	-2.4112425
H	-0.4587133	2.3108851	3.3889323
H	-0.4726768	2.3148235	-3.3844407
C	-0.7333833	2.5481210	1.2300025
C	-0.7388447	2.5492099	-1.2240794
H	-0.5936212	3.6453369	1.2192003
H	-0.6000431	3.6465603	-1.2124911
H	-1.8191724	2.3553942	1.2633139
H	-1.8246262	2.3554599	-1.2531996
N	-0.1616152	1.9569116	0.0014383
H	0.9680698	2.2413977	-0.0009541
C	1.3784061	-0.4683811	-3.3174759

C	1.3879001	-0.4744590	3.3128091
H	2.2035073	-0.2132796	-2.6289625
H	2.2113261	-0.2197139	2.6221617
C	-1.6845519	-0.3785362	-3.1228860
C	-1.6754554	-0.3807034	3.1271918
H	-2.3832119	0.3060973	-2.6078108
H	-2.3748070	0.3053457	2.6149176
C	0.2459254	-2.0235551	-0.0017997
O	0.3600779	-3.1923199	-0.0027497
C	-1.7561192	-0.1232403	4.6368432
C	-1.7698694	-0.1194148	-4.6319844
H	-1.4194130	0.8841977	4.9177776
H	-1.4353123	0.8887942	-4.9126131
H	-1.1514859	-0.8520219	5.1941976
H	-1.1658878	-0.8466964	-5.1919593
H	-2.7963584	-0.2342716	4.9799868
H	-2.8109348	-0.2313993	-4.9723019
C	-2.0994649	-1.8144094	2.7782503
C	-2.1058216	-1.8131060	-2.7743778
H	-1.4445585	-2.5566773	3.2541059
H	-1.4507914	-2.5540932	-3.2521241
H	-2.0735413	-1.9847178	1.6950255
H	-2.0774888	-1.9842000	-1.6913167
H	-3.1240356	-1.9985099	3.1362951
H	-3.1308702	-1.9983633	-3.1306105
C	1.3721695	-1.9924942	-3.4977879
C	1.3801649	-1.9987518	3.4914443
H	0.6092035	-2.3023105	-4.2264857
H	0.6189049	-2.3083343	4.2219990
H	1.1808605	-2.5209362	-2.5544705
H	1.1854127	-2.5258935	2.5481112
H	2.3467690	-2.3282563	-3.8830615
H	2.3554350	-2.3362304	3.8735173
C	1.6290462	0.2599790	-4.6453079
C	1.6433143	0.2520896	4.6407096
H	1.6411134	1.3520672	-4.5310784
H	1.6558724	1.3442775	4.5278136
H	0.8768996	0.0043561	-5.4021295
H	0.8933250	-0.0038600	5.3995045
H	2.6109692	-0.0387197	-5.0445735
H	2.6262236	-0.0478572	5.0365775
O	2.3227337	2.3676034	-0.0046488
H	3.3333620	0.7885599	-0.9071836
C	2.7628785	1.1079210	-0.0033016
H	3.3304113	0.7893566	0.9028282

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H	-1.7515328	-0.0761417	-0.0225793
Ru	-0.0647120	-0.2295411	-0.0361979
H	1.6269505	-0.1636474	-0.0700608
P	-0.1074061	0.0675793	2.2400008
P	-0.1283724	0.0521555	-2.3135110
C	-0.0880439	1.9244346	2.4211121
C	-0.0365371	1.9064776	-2.4961539
H	0.9630792	2.2444413	2.4834335
H	1.0296318	2.1810373	-2.5299425
H	-0.5904922	2.2584271	3.3403596
H	-0.4988570	2.2608474	-3.4288552
C	-0.7375001	2.5459031	1.1868760
C	-0.6964165	2.5505819	-1.2793220
H	-0.6509566	3.6482880	1.2146814
H	-0.5897141	3.6511771	-1.3115203
H	-1.8049997	2.2843371	1.1358471

H	-1.7705513	2.3126418	-1.2515803
N	-0.0971843	2.0081918	-0.0376846
H	0.8962327	2.2870395	-0.0100678
C	1.3268386	-0.5520045	-3.3262368
C	1.3883830	-0.4726975	3.2321209
H	2.1429515	-0.2791378	-2.6345956
H	2.1808766	-0.1589838	2.5295951
C	-1.7292359	-0.3732094	-3.1899895
C	-1.6751219	-0.4206379	3.1437447
H	-2.4090855	0.3563583	-2.7132326
H	-2.3888624	0.2852235	2.6809892
C	-0.0413236	-2.0540349	-0.0308015
O	-0.0210260	-3.2305967	-0.0269188
C	-1.6899924	-0.2135339	4.6625868
C	-1.7648908	-0.1631347	-4.7080911
H	-1.3239254	0.7778500	4.9650725
H	-1.3705083	0.8155952	-5.0161755
H	-1.0773627	-0.9712450	5.1707578
H	-1.1881625	-0.9404557	-5.2283868
H	-2.7174316	-0.3190783	5.0445460
H	-2.8022005	-0.2324557	-5.0712870
C	-2.1282051	-1.8364803	2.7633801
C	-2.2257103	-1.7727533	-2.8024110
H	-1.4353313	-2.6009115	3.1416690
H	-1.5744391	-2.5608698	-3.2051789
H	-2.1939094	-1.9446741	1.6737963
H	-2.2628613	-1.8838068	-1.7115889
H	-3.1194340	-2.0415965	3.1971207
H	-3.2365169	-1.9370829	-3.2073344
C	1.3100930	-2.0819962	-3.4429337
C	1.4444319	-2.0023181	3.3374134
H	0.5327858	-2.4179095	-4.1447199
H	0.6913286	-2.3781074	4.0454028
H	1.1293526	-2.5640822	-2.4730405
H	1.2733474	-2.4839568	2.3654651
H	2.2761706	-2.4424070	-3.8285126
H	2.4302358	-2.3216857	3.7091139
C	1.5924264	0.1164698	-4.6822306
C	1.6451990	0.1999704	4.5875730
H	1.5733836	1.2137212	-4.6263557
H	1.5681115	1.2950909	4.5400076
H	0.8671044	-0.1947847	-5.4437378
H	0.9508998	-0.1534343	5.3594438
H	2.5906563	-0.1759292	-5.0450832
H	2.6634703	-0.0431551	4.9308434
O	2.7462572	2.8155068	0.5338129
H	3.1812836	0.8816324	0.0841058
C	3.4866231	1.8473242	0.5517679
H	4.4746831	1.8965696	1.0724273

3$_{CH2O}$
65

H	0.2116750	-1.4990923	-0.1365670
Ru	-0.1837795	0.1477689	-0.1220936
H	-0.3601551	1.8323896	-0.0858895
P	0.1174127	0.1413064	-2.3974847
P	0.1036676	0.1183731	2.1561251
C	1.9481645	0.4545237	-2.5745175
C	1.9272447	0.4658945	2.3414065
H	2.0963710	1.5444321	-2.6224377
H	2.0513263	1.5594922	2.3833730
H	2.3592754	0.0237434	-3.4989462
H	2.3420020	0.0499568	3.2710970
C	2.6623709	-0.1036192	-1.3457625

C	2.6574529	-0.0886429	1.1206371
H	3.7394622	0.1468465	-1.3732421
H	3.7321703	0.1712728	1.1551433
H	2.5646133	-1.1988566	-1.3041982
H	2.5719472	-1.1853023	1.0843660
N	2.0363857	0.4388294	-0.1166417
H	2.1700528	1.4621571	-0.1313846
C	-0.6974640	1.4718611	3.1730496
C	-0.6511359	1.5220170	-3.4055143
H	-0.5373914	2.3208132	2.4855852
H	-0.4775498	2.3618752	-2.7095554
C	-0.0955552	-1.5294976	3.0261077
C	-0.1109381	-1.4909518	-3.2900415
H	0.7225318	-2.0990335	2.5483417
H	0.6959961	-2.0803704	-2.8173828
C	-1.9922877	-0.0929449	-0.1299855
O	-3.1593246	-0.2440459	-0.1362296
C	0.1046190	-1.4861288	-4.8077291
C	0.1156518	-1.5405108	4.5443844
H	1.0274619	-0.9706062	-5.1095047
H	1.0285932	-1.0129765	4.8553642
H	-0.7374516	-1.0058554	-5.3252834
H	-0.7358722	-1.0810845	5.0653182
H	0.1653408	-2.5206632	-5.1802625
H	0.1930899	-2.5785038	4.9040479
C	-1.4393683	-2.1593651	-2.9113370
C	-1.4115157	-2.2153694	2.6346723
H	-2.3016453	-1.6018459	-3.3027657
H	-2.2835955	-1.6803602	3.0356609
H	-1.5433154	-2.2285086	-1.8215614
H	-1.5137210	-2.2667085	1.5436350
H	-1.4805104	-3.1755178	-3.3335929
H	-1.4344703	-3.2394224	3.0388455
C	-2.2108560	1.2439235	3.2846617
C	-2.1685710	1.3270492	-3.5227808
H	-2.4382815	0.4237060	3.9811748
H	-2.4101536	0.5186663	-4.2281935
H	-2.6608094	1.0041415	2.3120475
H	-2.6248238	1.0855358	-2.5534655
H	-2.7019223	2.1489740	3.6740820
H	-2.6409677	2.2454529	-3.9039480
C	-0.0754918	1.8203856	4.5324530
C	-0.0178089	1.8743742	-4.7585579
H	1.0145130	1.9495454	4.4808075
H	1.0746259	1.9787572	-4.7022716
H	-0.2889103	1.0571583	5.2906763
H	-0.2450673	1.1246735	-5.5260468
H	-0.5010133	2.7688648	4.8969056
H	-0.4220899	2.8356811	-5.1136753
O	2.4806372	3.4126162	-0.4626788
H	0.4581477	3.4177277	-0.6295979
C	1.4195575	3.9864074	-0.6350517
H	1.3904533	5.0935912	-0.7867904

3
61

H	0.2432101	-1.5037117	0.0000022
Ru	-0.1263953	0.1536413	0.0000013
H	-0.2195690	1.8462526	0.0000011
P	0.1558094	0.1346443	-2.2769550
P	0.1558105	0.1346423	2.2769581
C	1.9867384	0.4596636	-2.4620498
C	1.9867419	0.4596473	2.4620535
H	2.1228982	1.5515055	-2.5189155

H	2.1229105	1.5514869	2.5189278
H	2.3983583	0.0298061	-3.3867750
H	2.3983591	0.0297760	3.3867733
C	2.7137978	-0.0925965	-1.2381158
C	2.7137951	-0.0926033	1.2381103
H	3.7911334	0.1578859	-1.2705982
H	3.7911333	0.1578677	1.2705978
H	2.6179425	-1.1877884	-1.1942724
H	2.6179255	-1.1877927	1.1942470
N	2.0915490	0.4355704	0.0000048
H	2.1768929	1.4575300	-0.0000615
C	-0.6260818	1.5008983	3.2912808
C	-0.6260910	1.5008960	-3.2912775
H	-0.4607462	2.3454523	2.5997986
H	-0.4607606	2.3454504	-2.5997948
C	-0.0595857	-1.5076419	3.1548595
C	-0.0595732	-1.5076414	-3.1548569
H	0.7501717	-2.0890900	2.6770150
H	0.7501867	-2.0890838	-2.6770099
C	-1.9389425	-0.0456742	0.0000032
O	-3.1090393	-0.1731067	0.0000069
C	0.1543627	-1.5157384	-4.6728028
C	0.1543461	-1.5157387	4.6728060
H	1.0743523	-0.9984574	-4.9806773
H	1.0743384	-0.9984636	4.9806824
H	-0.6903688	-1.0438903	-5.1936132
H	-0.6903837	-1.0438844	5.1936137
H	0.2195508	-2.5533684	-5.0361094
H	0.2195262	-2.5533688	5.0361138
C	-1.3846501	-2.1788862	-2.7683852
C	-1.3846660	-2.1788784	2.7683855
H	-2.2490607	-1.6347015	-3.1736482
H	-2.2490743	-1.6346857	3.1736427
H	-1.4914831	-2.2285210	-1.6775886
H	-1.4914954	-2.2285172	1.6775888
H	-1.4168406	-3.2029386	-3.1720480
H	-1.4168656	-3.2029289	3.1720525
C	-2.1414207	1.2870810	3.4086403
C	-2.1414287	1.2870701	-3.4086370
H	-2.3747181	0.4733070	4.1109088
H	-2.3747214	0.4732953	-4.1109062
H	-2.5972389	1.0467468	2.4388954
H	-2.5972452	1.0467325	-2.4388922
H	-2.6220610	2.1994654	3.7937231
H	-2.6220742	2.1994519	-3.7937188
C	0.0022646	1.8479523	4.6482975
C	0.0022537	1.8479546	-4.6482938
H	1.0932504	1.9692393	4.5943652
H	1.0932387	1.9692482	-4.5943613
H	-0.2151145	1.0888790	5.4097081
H	-0.2151207	1.0888805	-5.4097050
H	-0.4148945	2.8010281	5.0102996
H	-0.4149111	2.8010281	-5.0102954

2'$_{2m}$
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H	-0.0215017	-1.2352867	-0.2980669
Ru	0.2186748	0.3376322	-0.3111261
H	0.6255234	2.1973762	-0.2663905
P	0.5738338	0.1748361	-2.6068636
P	0.4391434	0.2206162	2.0091529
C	2.4140910	0.0172192	-2.7225114
C	2.2693470	0.0372552	2.2367611
H	2.8165746	1.0374993	-2.8334206

H	2.6834504	1.0488344	2.3731042
H	2.7208114	-0.5573179	-3.6082643
H	2.5093057	-0.5418403	3.1400764
C	2.9492468	-0.6237164	-1.4478961
C	2.8716011	-0.6178762	0.9993928
H	4.0516100	-0.5552573	-1.4237178
H	3.9744259	-0.5608122	1.0381794
H	2.6821582	-1.6911072	-1.3980001
H	2.5972949	-1.6829797	0.9426853
N	2.3784637	0.0364166	-0.2424653
H	2.6862400	1.0646562	-0.2376216
C	0.0166329	1.7448715	2.9981800
C	0.1851035	1.6755508	-3.6495096
H	0.4534991	2.5219807	2.3478223
H	0.4998862	2.4754652	-2.9572786
C	-0.2732817	-1.3152728	2.8040868
C	-0.0691963	-1.3795265	-3.4238975
H	0.3480386	-2.0935708	2.3237898
H	0.5341835	-2.1418439	-2.8971912
C	-1.5981659	0.6080905	-0.3751612
O	-2.7592094	0.7632177	-0.4203101
C	0.2017611	-1.4976693	-4.9289280
C	-0.0983542	-1.4190369	4.3242715
H	1.2455064	-1.2796129	-5.1935911
H	0.9257082	-1.1967511	4.6541854
H	-0.4435261	-0.8168998	-5.5010942
H	-0.7794347	-0.7327906	4.8460429
H	-0.0212797	-2.5206922	-5.2690283
H	-0.3431108	-2.4388917	4.6589448
C	-1.5438896	-1.6509871	-3.0962734
C	-1.7303659	-1.5669034	2.3924330
H	-2.2063755	-0.9094112	-3.5625139
H	-2.4041264	-0.8006529	2.7991580
H	-1.7239234	-1.6317519	-2.0147543
H	-1.8444062	-1.5718138	1.3019328
H	-1.8339085	-2.6416693	-3.4787859
H	-2.0636553	-2.5416653	2.7805586
C	-1.5008339	1.9576150	3.0711608
C	-1.3245606	1.8185083	-3.8829967
H	-1.9686967	1.2511801	3.7723531
H	-1.6837512	1.0889193	-4.6229066
H	-1.9857586	1.8389387	2.0926635
H	-1.9027707	1.6820242	-2.9589553
H	-1.7186296	2.9722830	3.4371620
H	-1.5486033	2.8207465	-4.2782844
C	0.6892806	1.8949744	4.3691204
C	0.9939151	1.8509136	-4.9416359
H	1.7797512	1.7998633	4.3005136
H	2.0746813	1.8341438	-4.7524463
H	0.3079428	1.1746629	5.1034940
H	0.7510848	1.0880212	-5.6915850
H	0.4809876	2.9044246	4.7565753
H	0.7571848	2.8320917	-5.3822126
O	2.7045758	2.7278740	-0.2544969
H	1.1025996	3.5734135	-1.2826711
C	1.3948418	3.0884013	-0.3298618
H	1.0485779	3.7164639	0.5156375
H	4.8948315	4.1595737	2.3025341
C	3.8383341	4.2733491	2.6117073
H	3.4436088	5.1937663	2.1406857
H	3.8168588	4.4151936	3.7026499
H	2.0502333	4.3338399	-3.3843730
C	3.1463499	4.2700095	-3.2203477
H	3.6371600	4.4427123	-4.1904174
H	3.4331413	5.0921557	-2.5398635

O	3.0565521	3.1314070	2.2988673
H	3.0463347	3.0074054	1.2913872
O	3.5498327	3.0026277	-2.7314660
H	3.3075397	2.9425859	-1.7500881

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H	0.2726502	-1.1643709	-0.2491412
Ru	-0.0848104	0.4721071	-0.2067117
H	-0.1301040	2.1774959	-0.0995502
P	0.3809324	0.5365734	-2.4675561
P	0.0479619	0.3534239	2.0865989
C	2.2089549	0.8956072	-2.4725003
C	1.8588177	0.6514697	2.4054464
H	2.3202391	1.9901172	-2.4115341
H	2.0107474	1.7400614	2.4715862
H	2.7020152	0.5592665	-3.3959118
H	2.1980752	0.2048549	3.3509653
C	2.8339040	0.2424460	-1.2417084
C	2.6501309	0.1063447	1.2179125
H	3.9102005	0.4884067	-1.1719293
H	3.7260026	0.3392141	1.3291084
H	2.7393052	-0.8531344	-1.2880362
H	2.5423455	-0.9860479	1.1377309
N	2.1230107	0.7069619	-0.0287388
H	2.3054290	1.7268065	0.0484579
C	-0.8169604	1.6789092	3.0857264
C	-0.3528719	1.8957288	-3.5192545
H	-0.6357847	2.5438161	2.4236111
H	-0.3117613	2.7330688	-2.8052132
C	-0.2350000	-1.3211242	2.8780372
C	0.2782169	-1.0948963	-3.3845650
H	0.6101634	-1.8853031	2.4428537
H	1.0522870	-1.6709189	-2.8455632
C	-1.8845815	0.1765536	-0.3364630
O	-3.0388508	-0.0382557	-0.4068027
C	0.6359272	-1.0659065	-4.8752261
C	-0.1301281	-1.3812241	4.4065998
H	1.5744433	-0.5320191	-5.0811005
H	0.7679654	-0.8808325	4.7954071
H	-0.1606894	-0.5914917	-5.4647512
H	-1.0076572	-0.9216901	4.8822531
H	0.7496378	-2.0944469	-5.2519708
H	-0.0950769	-2.4307283	4.7380275
C	-1.0616785	-1.8027946	-3.1412101
C	-1.5252901	-1.9820728	2.3750378
H	-1.8964096	-1.2665328	-3.6125556
H	-2.4198725	-1.4491793	2.7253516
H	-1.2711399	-1.8859984	-2.0678481
H	-1.5508416	-2.0071286	1.2789571
H	-1.0314982	-2.8161624	-3.5709920
H	-1.5858509	-3.0156011	2.7499994
C	-2.3300064	1.4247074	3.1207387
C	-1.8312701	1.6146971	-3.8186031
H	-2.5787451	0.6070391	3.8125690
H	-1.9411197	0.8219782	-4.5730486
H	-2.7249617	1.1668724	2.1292401
H	-2.3830831	1.3259452	-2.9148637
H	-2.8580879	2.3240869	3.4725252
H	-2.3086107	2.5226083	-4.2151461
C	-0.2627896	2.0082132	4.4782291
C	0.4179031	2.3169124	-4.7776733
H	0.8226966	2.1769999	4.4713744
H	1.4768341	2.5252208	-4.5732029

H	-0.4779380	1.2156248	5.2053135
H	0.3640586	1.5610452	-5.5707219
H	-0.7356238	2.9304269	4.8514445
H	-0.0239306	3.2431512	-5.1770469
O	1.3715766	4.4980148	-1.5191560
H	-0.6080816	4.9718016	-1.4138220
C	0.3201990	4.6504962	-0.9063515
H	0.2498113	4.4700819	0.1870577
H	4.5463944	2.9415881	-1.2509892
C	4.4477536	3.4035562	-0.2514085
H	4.8525996	4.4290311	-0.3001506
H	5.0558968	2.8255471	0.4579894
O	3.1007327	3.3866396	0.2207070
H	2.5315368	3.8676909	-0.4429967
H	-3.7198947	2.5137014	0.2391666
C	-3.1066102	3.4188729	0.0842691
H	-2.5599025	3.6283037	1.0234926
H	-3.7766412	4.2654224	-0.1223936
O	-2.2280841	3.2744748	-1.0256327
H	-1.5341175	2.6078752	-0.7577436

3$_{2m}$
73

H	-0.6623595	-1.2546009	-0.2027240
Ru	-1.0237405	0.3797471	-0.2229986
H	-1.2304874	2.0739479	-0.3689732
P	-0.7195616	0.2882761	-2.5054894
P	-0.7242185	0.3334462	2.0631975
C	1.1133787	0.5648781	-2.6865582
C	1.0845203	0.7449232	2.2222228
H	1.2797428	1.6515974	-2.7498364
H	1.1559541	1.8442928	2.2108736
H	1.5180288	0.1072108	-3.6006476
H	1.5205510	0.3861453	3.1659639
C	1.8109764	0.0236354	-1.4409589
C	1.8226752	0.1595470	1.0204997
H	2.8930555	0.2505271	-1.4741047
H	2.8920183	0.4414078	1.0438701
H	1.6901171	-1.0673783	-1.3624388
H	1.7639623	-0.9396455	1.0269395
N	1.1971332	0.6339860	-0.2368495
H	1.3965416	1.6519692	-0.3109362
C	-1.5681216	1.6062859	3.1451839
C	-1.4723701	1.6472549	-3.5473833
H	-1.4766479	2.4910954	2.4955252
H	-1.2729497	2.5054920	-2.8822376
C	-0.8457141	-1.3527256	2.8740785
C	-0.9775708	-1.3737359	-3.3289513
H	-0.0265821	-1.8780645	2.3505806
H	-0.1801583	-1.9596205	-2.8362809
C	-2.8335251	0.1329339	-0.2044282
O	-3.9980206	-0.0261253	-0.1888482
C	-0.7624839	-1.4268036	-4.8460337
C	-0.5825639	-1.4114676	4.3832478
H	0.1683033	-0.9373843	-5.1656428
H	0.3248129	-0.8682349	4.6827054
H	-1.5968416	-0.9512187	-5.3799960
H	-1.4285757	-0.9983479	4.9497776
H	-0.7190430	-2.4749053	-5.1809681
H	-0.4618119	-2.4591022	4.7003955
C	-2.3176533	-2.0055044	-2.9289832
C	-2.1501222	-2.0717591	2.5034279
H	-3.1696758	-1.4452073	-3.3382520
H	-3.0245021	-1.5904341	2.9622465

H	-2.4246951	-2.0395051	-1.8380932
H	-2.2952762	-2.0818654	1.4162912
H	-2.3772436	-3.0334584	-3.3191769
H	-2.1173704	-3.1123686	2.8619565
C	-3.0597331	1.2843892	3.3065437
C	-2.9941020	1.4770147	-3.6462733
H	-3.2143423	0.4407599	3.9947951
H	-3.2584058	0.6513141	-4.3230551
H	-3.5330235	1.0354575	2.3470427
H	-3.4469874	1.2766597	-2.6659567
H	-3.5880127	2.1519612	3.7308312
H	-3.4511089	2.3921290	-4.0528877
C	-0.9090138	1.9508850	4.4878168
C	-0.8418672	1.9384825	-4.9160321
H	0.1589574	2.1849224	4.3826479
H	0.2521510	2.0269805	-4.8679005
H	-1.0107399	1.1422941	5.2216949
H	-1.0874282	1.1666433	-5.6556057
H	-1.3972470	2.8417057	4.9134157
H	-1.2310125	2.8943448	-5.3008359
C	3.1858064	3.5795463	0.3149993
H	4.0427091	3.0873735	-0.1660208
H	3.0539382	3.1410859	1.3217935
H	3.4248998	4.6509782	0.4343626
O	2.0436164	3.3791427	-0.5147999
H	1.2356051	3.7067078	-0.0157290
C	-1.0404212	4.8886173	0.7788249
H	-1.9370310	4.7539805	1.4080459
H	-1.3650784	5.0437916	-0.2639475
H	-0.5040053	5.7839361	1.1203037
O	-0.1552701	3.7718591	0.8982351
H	-0.6137386	2.9659016	0.4494978

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73

H	-1.8844029	-0.0362768	0.4740176
Ru	-0.2582293	-0.0248530	0.4916911
H	1.4872689	0.3013099	0.5793564
P	-0.4469665	2.2805919	0.7519622
P	-0.3789856	-2.1958864	-0.3596627
C	-0.4802390	2.8766531	-1.0036994
C	-0.2420084	-1.8808791	-2.1795412
H	0.5674206	2.9964929	-1.3230991
H	0.8364341	-1.7878282	-2.3830932
H	-0.9916894	3.8436929	-1.1085313
H	-0.6440488	-2.7085765	-2.7808122
C	-1.1313227	1.7964803	-1.8644898
C	-0.9531655	-0.5684398	-2.4986013
H	-1.0790135	2.0802936	-2.9319077
H	-0.8151570	-0.3091672	-3.5643322
H	-2.1935731	1.6618452	-1.6034141
H	-2.0374559	-0.6542084	-2.3163775
N	-0.4184344	0.5182940	-1.6472076
H	0.6014524	0.7064064	-1.9675380
C	1.0064976	-3.3770806	0.0283623
C	1.0050429	3.1804689	1.5069750
H	1.8546897	-2.6753076	-0.0397046
H	1.8315787	2.6450849	1.0071447
C	-2.0394587	-3.0344798	-0.1717327
C	-2.0590659	2.9024105	1.4641926
H	-2.6834698	-2.3456080	-0.7478859
H	-2.7631341	2.5661834	0.6811373
C	-0.2535916	-0.5011166	2.2684377
O	-0.2819879	-0.8080394	3.3979057

C	-2.1823402	4.4237585	1.6141793
C	-2.1447541	-4.4350373	-0.7882995
H	-1.8647818	4.9712460	0.7161075
H	-1.7574730	-4.4804993	-1.8154078
H	-1.5850293	4.7855073	2.4624275
H	-1.5981884	-5.1736552	-0.1859988
H	-3.2301485	4.6939749	1.8161529
H	-3.1986690	-4.7523798	-0.8152617
C	-2.4382135	2.1797084	2.7638893
C	-2.5406107	-3.0236595	1.2790498
H	-1.7419339	2.4179960	3.5795234
H	-1.9259823	-3.6641790	1.9256430
H	-2.4422496	1.0918218	2.6289382
H	-2.5307932	-2.0095966	1.6961312
H	-3.4438144	2.4933197	3.0835631
H	-3.5726138	-3.4049988	1.3186657
C	0.9059515	-3.9150909	1.4609604
C	1.1025518	2.9050675	3.0132595
H	0.1106427	-4.6692535	1.5549524
H	0.3287707	3.4556387	3.5676972
H	0.7105228	-3.1186648	2.1916726
H	0.9945077	1.8365133	3.2436495
H	1.8519794	-4.4027480	1.7407323
H	2.0790882	3.2386194	3.3949005
C	1.2628816	-4.4955291	-0.9904806
C	1.1530353	4.6747024	1.1882304
H	1.3699540	-4.1079091	-2.0118894
H	1.0503385	4.8886998	0.1160290
H	0.4734519	-5.2577224	-0.9878403
H	0.4219294	5.2859341	1.7310237
H	2.2079540	-4.9999996	-0.7360806
H	2.1549141	5.0125636	1.4950856
C	2.2473910	0.9018644	-3.7933282
H	1.5683342	1.5758857	-4.3498735
H	2.0409999	-0.1340329	-4.1372699
H	3.2808335	1.1474433	-4.1061236
O	2.0678554	1.0541513	-2.4021416
H	2.4693644	0.0836820	-1.8281881
C	3.9515976	-0.8327636	-0.5410947
H	4.3250266	-1.8282707	-0.2332255
H	3.9054955	-0.2048823	0.3788739
H	4.7183585	-0.3793863	-1.1992931
O	2.7020915	-0.9413686	-1.1783504
H	1.5868188	-0.3308416	-0.0284026

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73

H	-1.8561371	-0.0437891	0.5018716
Ru	-0.2374895	-0.0270628	0.4914231
H	1.4984267	0.4130193	0.4233688
P	-0.4548664	2.2869858	0.7263199
P	-0.3878762	-2.2059959	-0.3464710
C	-0.4807198	2.8595157	-1.0323949
C	-0.2422289	-1.9112852	-2.1654465
H	0.5711957	2.9732103	-1.3399974
H	0.8363752	-1.8427439	-2.3737711
H	-0.9966073	3.8220760	-1.1536856
H	-0.6594846	-2.7391090	-2.7561676
C	-1.1177329	1.7586539	-1.8773696
C	-0.9301566	-0.5888494	-2.4935288
H	-1.0574472	2.0288164	-2.9483791
H	-0.7655832	-0.3350731	-3.5574653
H	-2.1876180	1.6373378	-1.6283494
H	-2.0226288	-0.6731054	-2.3452715

N	-0.4036615	0.4905196	-1.6374625
H	0.7140776	0.6905765	-1.9203601
C	0.9839974	-3.3957803	0.0635376
C	0.9774859	3.2126808	1.4864460
H	1.8438154	-2.7089008	-0.0126553
H	1.8161524	2.6930364	0.9899369
C	-2.0593616	-3.0163472	-0.1431153
C	-2.0822532	2.8809708	1.4249202
H	-2.6932781	-2.3224196	-0.7244751
H	-2.7749360	2.5185065	0.6434241
C	-0.2099877	-0.4720815	2.2821839
O	-0.2353785	-0.7565802	3.4172837
C	-2.2380734	4.4017161	1.5503293
C	-2.1868450	-4.4201392	-0.7482728
H	-1.9256030	4.9415394	0.6459885
H	-1.8032771	-4.4791178	-1.7759672
H	-1.6549289	4.7889052	2.3971890
H	-1.6498363	-5.1620217	-0.1413760
H	-3.2928257	4.6524789	1.7405826
H	-3.2454741	-4.7215701	-0.7698974
C	-2.4525522	2.1719999	2.7346565
C	-2.5566096	-2.9872628	1.3087582
H	-1.7662758	2.4392727	3.5497315
H	-1.9548118	-3.6383230	1.9568202
H	-2.4329916	1.0820810	2.6193732
H	-2.5239813	-1.9721979	1.7222934
H	-3.4663777	2.4693146	3.0436104
H	-3.5965383	-3.3457726	1.3522136
C	0.8743754	-3.9157736	1.5021157
C	1.0752656	2.9509539	2.9949275
H	0.0703056	-4.6597044	1.6015656
H	0.2897672	3.4921229	3.5420061
H	0.6853919	-3.1095232	2.2237158
H	0.9852773	1.8829261	3.2350608
H	1.8138147	-4.4114579	1.7897203
H	2.0441131	3.3058518	3.3769355
C	1.2281472	-4.5282035	-0.9428257
C	1.0966977	4.7074368	1.1571993
H	1.3531676	-4.1496759	-1.9652988
H	0.9934732	4.9106941	0.0831020
H	0.4242827	-5.2751485	-0.9401931
H	0.3515311	5.3075750	1.6931450
H	2.1612081	-5.0475797	-0.6747227
H	2.0905178	5.0671933	1.4651671
C	2.2107408	1.2921131	-3.5271818
H	1.2785487	1.6655497	-4.0089420
H	2.5362641	0.4065175	-4.1148262
H	2.9783192	2.0780735	-3.6783730
O	2.0246852	0.9993244	-2.1659200
H	2.6115311	-0.3136908	-1.7736067
C	4.1754366	-1.1305312	-0.8227397
H	4.4901561	-2.1167550	-0.4442191
H	4.1566949	-0.4298067	0.0372344
H	4.9532105	-0.7740705	-1.5247909
O	2.9098333	-1.2602837	-1.4409747
H	1.4981820	-0.3877224	0.1346765

3$_{Im}$
67

Ru	0.0168828	-0.2381836	-0.1688675
H	0.0145612	-1.6084891	0.7935615
H	0.0125740	1.2386238	-1.0357426
P	2.3024965	-0.2528131	0.0279742
P	-2.2446996	-0.0423243	0.1995343

O	-0.1208077	-1.7966459	-2.7316066
N	0.1276369	0.8967740	1.7602983
H	0.0784318	1.8866426	1.4565006
C	2.5922800	0.8040808	1.5378064
H	3.5323142	0.5529733	2.0501022
H	2.6784516	1.8436933	1.1823131
C	1.4011955	0.6762473	2.4859067
H	1.3590297	-0.3355699	2.9117146
H	1.4926940	1.3919123	3.3243121
C	-1.0581269	0.6442495	2.6177512
H	-1.0301159	1.2973986	3.5102918
H	-0.9964116	-0.3998943	2.9549521
C	-2.3389337	0.8832382	1.8204624
H	-2.4252476	1.9520098	1.5725973
H	-3.2245129	0.5985975	2.4065963
C	-3.2954226	-1.5626147	0.4873649
H	-4.3222008	-1.2017120	0.6663606
C	-3.2760850	-2.4640745	-0.7539027
H	-3.8789421	-3.3674824	-0.5739112
H	-2.2486345	-2.7791502	-0.9844229
H	-3.6810057	-1.9637097	-1.6428522
C	-2.8226882	-2.3382241	1.7231594
H	-3.4115727	-3.2621354	1.8303583
H	-2.9429238	-1.7625821	2.6520352
H	-1.7620454	-2.6109751	1.6197645
C	-3.2439753	1.0738731	-0.9246857
H	-2.7659841	2.0466432	-0.7120758
C	-3.0155832	0.7712912	-2.4103704
H	-3.4620220	1.5677787	-3.0256629
H	-3.4805622	-0.1769516	-2.7137410
H	-1.9437565	0.7153632	-2.6392720
C	-4.7342912	1.1665987	-0.5772739
H	-5.2077238	1.9743080	-1.1565648
H	-4.9053169	1.3787481	0.4883847
H	-5.2624028	0.2348287	-0.8285824
C	3.4498868	0.4961993	-1.2570619
H	3.5186239	-0.2989692	-2.0190346
C	4.8611639	0.8034404	-0.7345075
H	5.5090662	1.1234023	-1.5649058
H	5.3424990	-0.0613565	-0.2581570
H	4.8422305	1.6253845	-0.0035237
C	2.8311609	1.7327087	-1.9159167
H	3.4815343	2.0922942	-2.7282673
H	2.7225854	2.5555653	-1.1924605
H	1.8338345	1.5189877	-2.3173330
C	3.1626776	-1.8806981	0.3775203
H	4.2466847	-1.6823452	0.3413950
C	2.8122194	-2.4452184	1.7580169
H	3.2696203	-3.4387404	1.8828055
H	1.7217312	-2.5561458	1.8563695
H	3.1784604	-1.8099248	2.5772871
C	2.7934792	-2.8859176	-0.7226186
H	3.3554263	-3.8221064	-0.5828226
H	3.0121047	-2.5123692	-1.7329635
H	1.7196687	-3.1146467	-0.6782118
C	-0.0706867	-1.1872754	-1.7296846
C	0.4095956	4.2715373	-0.1466614
H	0.1280333	5.1940476	0.3796317
H	0.3889061	4.4671075	-1.2323667
O	-0.5141240	3.2539720	0.2282427
H	-0.3365643	2.4388880	-0.3510307
H	1.4491362	4.0167158	0.1354852

TS-2*1m*
67

Ru	0.0224137	-0.1768437	-0.2210818
H	0.0385813	-1.5522025	0.6190120
H	0.1852235	1.3253895	-1.2479157
P	2.3227794	-0.1954729	0.0139914
P	-2.2586463	-0.0344833	0.2180789
O	-0.1326058	-1.8313348	-2.7405203
N	0.1127189	0.9122484	1.6812708
H	-0.1519970	2.0155918	1.2125269
C	2.5764369	0.9903113	1.4179858
H	3.5392550	0.8397989	1.9275096
H	2.5891244	1.9935301	0.9617142
C	1.4017700	0.8827901	2.3901494
H	1.4802246	-0.0529982	2.9697910
H	1.4462313	1.7138737	3.1198721
C	-0.9927147	0.5867684	2.6012498
H	-0.9511147	1.2507035	3.4866416
H	-0.8815070	-0.4511158	2.9623605
C	-2.3334383	0.7748039	1.8909086
H	-2.4964908	1.8471693	1.7093643
H	-3.1686765	0.3875770	2.4910530
C	-3.2762097	-1.5842592	0.4091570
H	-4.2800329	-1.2418697	0.7144692
C	-3.3819169	-2.3553988	-0.9121036
H	-3.9543893	-3.2833013	-0.7601856
H	-2.3864322	-2.6308039	-1.2871045
H	-3.8885394	-1.7762983	-1.6943939
C	-2.7027789	-2.4770037	1.5172241
H	-3.3207713	-3.3816438	1.6233585
H	-2.6797656	-1.9733313	2.4935229
H	-1.6769310	-2.7860289	1.2711782
C	-3.2329374	1.1579750	-0.8360597
H	-2.7147449	2.0989686	-0.5721132
C	-3.0491469	0.9315831	-2.3416073
H	-3.4633510	1.7869050	-2.8967793
H	-3.5697601	0.0295827	-2.6917674
H	-1.9890808	0.8333682	-2.6079864
C	-4.7119934	1.2645920	-0.4474544
H	-5.1813900	2.1055881	-0.9803075
H	-4.8499129	1.4376613	0.6295440
H	-5.2661594	0.3543697	-0.7220955
C	3.4882727	0.4124301	-1.3233896
H	3.6241604	-0.4751264	-1.9642001
C	4.8599807	0.8435840	-0.7824519
H	5.5472031	1.0429323	-1.6185520
H	5.3293373	0.0805683	-0.1459582
H	4.7802688	1.7709985	-0.1972259
C	2.8586837	1.5216579	-2.1722104
H	3.5648634	1.8446088	-2.9523284
H	2.6088694	2.4037646	-1.5635215
H	1.9368538	1.1830422	-2.6612194
C	3.1339025	-1.8091048	0.4955002
H	4.2216109	-1.6283728	0.4626394
C	2.7543583	-2.2647262	1.9083727
H	3.1894131	-3.2555804	2.1098591
H	1.6619198	-2.3489473	2.0070644
H	3.1227364	-1.5774162	2.6820400
C	2.7703210	-2.8868800	-0.5360766
H	3.3214892	-3.8147293	-0.3203437
H	3.0079454	-2.5896461	-1.5671142
H	1.6943815	-3.1052587	-0.4938034
C	-0.0782598	-1.1678487	-1.7781925
C	0.3642911	3.9577692	0.2457616
H	-0.0594055	4.9721124	0.1100798
H	0.9226780	3.7225750	-0.6936820

O	-0.6291828	3.0197245	0.5349805
H	-0.2754501	1.6973664	-0.6377782
H	1.1329420	4.0406224	1.0490865

2_{1m}-H_2

67

Ru	0.0244694	-0.1048703	-0.2631090
H	0.0199255	-1.4813220	0.5720320
H	0.4274677	1.4573784	-1.0814784
P	2.3225235	-0.1954475	0.0117656
P	-2.2530684	-0.0236699	0.2134702
O	-0.1044960	-1.7451951	-2.8021775
N	0.1184699	0.9506502	1.6332578
H	-0.3070347	2.4493125	1.1290958
C	2.5889154	0.9767357	1.4178666
H	3.5390127	0.7981752	1.9422234
H	2.6344403	1.9796805	0.9625897
C	1.3874140	0.8897621	2.3591970
H	1.4611522	-0.0448908	2.9543878
H	1.4429167	1.7203830	3.0932058
C	-0.9675530	0.6247987	2.5601322
H	-0.9267928	1.2993166	3.4402877
H	-0.8631853	-0.4099047	2.9539008
C	-2.3263560	0.7895546	1.8780643
H	-2.5231961	1.8571304	1.7014791
H	-3.1461155	0.3835540	2.4878174
C	-3.2081338	-1.6114568	0.4206172
H	-4.2201069	-1.3027491	0.7346471
C	-3.2996984	-2.3932340	-0.8955313
H	-3.8327408	-3.3423117	-0.7314450
H	-2.2986695	-2.6305009	-1.2815752
H	-3.8389604	-1.8398288	-1.6745872
C	-2.5969975	-2.4796642	1.5277924
H	-3.1914786	-3.3982294	1.6485069
H	-2.5705194	-1.9671668	2.4990419
H	-1.5676980	-2.7665919	1.2699207
C	-3.2980540	1.1155787	-0.8364414
H	-2.8270453	2.0841375	-0.5852146
C	-3.1294891	0.8913501	-2.3442854
H	-3.5856963	1.7266858	-2.8970140
H	-3.6206287	-0.0319806	-2.6803599
H	-2.0712655	0.8290338	-2.6296783
C	-4.7746308	1.1578527	-0.4255581
H	-5.2897972	1.9748861	-0.9533013
H	-4.9029096	1.3268499	0.6531224
H	-5.2900270	0.2225449	-0.6903083
C	3.5147711	0.3759444	-1.3183054
H	3.6189580	-0.5083192	-1.9691134
C	4.8990864	0.7487245	-0.7657681
H	5.5974606	0.9355001	-1.5955011
H	5.3364765	-0.0410162	-0.1394054
H	4.8503156	1.6684811	-0.1650674
C	2.9335090	1.5179688	-2.1583088
H	3.6564971	1.8251139	-2.9292057
H	2.7172564	2.4033254	-1.5400602
H	2.0045147	1.2192248	-2.6603895
C	3.0669499	-1.8412770	0.4870059
H	4.1603005	-1.6950574	0.4748656
C	2.6491848	-2.2999436	1.8880562
H	3.0505717	-3.3060752	2.0842338
H	1.5533873	-2.3503104	1.9689433
H	3.0227297	-1.6315176	2.6752014
C	2.6878176	-2.8961186	-0.5626853
H	3.2052104	-3.8430256	-0.3461337

H	2.9529685	-2.5973290	-1.5864695
H	1.6049895	-3.0808332	-0.5419867
C	-0.0638716	-1.0756172	-1.8417245
C	0.4094966	4.1235535	0.3429860
H	0.0441461	5.1115182	0.0226899
H	0.9486816	3.6740795	-0.5201679
O	-0.6862713	3.3433368	0.7665648
H	-0.3999522	1.5239627	-0.9399727
H	1.1559606	4.2862486	1.1471555

OH^--$3H_2O$
11

O	-2.1001031	-0.0155222	-1.0224792
H	-2.1159860	0.3493752	-1.9191158
H	-0.9000433	-0.8726137	-0.2840004
H	-3.1289319	-1.1195083	-0.3613140
O	-0.4735692	-1.4709014	0.4259236
H	-1.2699790	-1.9837783	0.6679053
O	-3.5783192	-1.6617291	0.3791879
H	-3.5072422	-0.9999712	1.0951682
O	-2.1915586	0.9220716	1.4217234
H	-1.4567931	0.3035273	1.6038615
H	-2.2397358	0.7902786	0.4100076

4-H_2O
12

O	-1.1879870	0.6599880	-1.0543955
H	-0.4010859	1.2171148	-0.9449120
H	-3.3531348	-2.3365374	1.3806609
O	-0.5581053	-1.8299179	-0.2797338
H	-1.2797240	-1.9485088	0.4092778
O	-2.5647674	-1.7865168	1.5138738
H	-2.8625710	-0.8457153	1.3200721
O	-3.1673421	0.7199101	0.7693932
H	-3.0006658	1.4132039	1.4276639
H	-2.4557213	0.8323482	0.0690575
H	-0.8805574	-0.2757518	-0.8519041
H	-0.6933885	-2.5389149	-0.9282202

2^-
64

H	-0.5910964	-1.6761472	0.0000337
Ru	0.0407238	-0.1693948	-0.0001054
O	0.5605952	1.9951407	-0.0003932
P	-0.2838616	-0.0570881	2.2642006
P	-0.2839282	-0.0571493	-2.2643928
C	-1.9701919	0.6928456	2.4128901
C	-1.9702677	0.6927837	-2.4130280
H	-1.8252993	1.7818485	2.3426531
H	-1.8253724	1.7817862	-2.3427895
H	-2.4656865	0.4530958	3.3669675
H	-2.4657908	0.4530392	-3.3670891
C	-2.7665252	0.2297155	1.1893715
C	-2.7665668	0.2296640	-1.1894836
H	-3.7474067	0.7625619	1.1735360
H	-3.7474586	0.7624972	-1.1736447
H	-3.0260129	-0.8602363	1.3102822
H	-3.0260420	-0.8602885	-1.3103614
N	-2.0097904	0.5150660	-0.0000725
C	0.8238359	1.1230504	-3.2001149
C	0.8238194	1.1227996	3.2003428
H	0.8701581	1.9183281	-2.4323577

H	0.8703496	1.9183384	2.4329214
C	-0.4529181	-1.6656529	-3.2155896
C	-0.4528858	-1.6654595	3.2155978
H	-1.3838792	-2.0551043	-2.7634700
H	-1.3838865	-2.0550397	2.7636214
C	1.7331739	-0.8750248	-0.0001982
O	2.7911204	-1.4125686	-0.0002651
C	-0.6552779	-1.5444855	4.7306209
C	-0.6555429	-1.5451435	-4.7305826
H	-1.4358117	-0.8165240	4.9946931
H	-1.4361062	-0.8172469	-4.9947666
H	0.2759464	-1.2374695	5.2294541
H	0.2755828	-1.2383373	-5.2296310
H	-0.9469823	-2.5191972	5.1575866
H	-0.9473097	-2.5199604	-5.1571748
C	0.6715756	-2.6510084	2.8742337
C	0.6715235	-2.6511691	-2.8739985
H	1.6392952	-2.3150057	3.2743071
H	1.6392247	-2.3153636	-3.2742076
H	0.7751182	-2.7550048	1.7866738
H	0.7751304	-2.7548549	-1.7864252
H	0.4555933	-3.6418993	3.3088841
H	0.4554801	-3.6421593	-3.3083375
C	2.2310592	0.5414427	-3.3801779
C	2.2308887	0.5408882	3.3806619
H	2.2487185	-0.2253437	-4.1718218
H	2.2481611	-0.2261863	4.1719942
H	2.6001793	0.0861149	-2.4510195
H	2.6002729	0.0858545	2.4515061
H	2.9386138	1.3344733	-3.6728576
H	2.9384430	1.3336602	3.6738671
C	0.2930657	1.7329288	-4.5038984
C	0.2927814	1.7320606	4.5042565
H	-0.7242918	2.1327751	-4.3921069
H	-0.7245274	2.1320137	4.3924466
H	0.2809524	1.0041875	-5.3266715
H	0.2804474	1.0029286	5.3266346
H	0.9436369	2.5679973	-4.8159418
H	0.9433180	2.5669021	4.8168393
C	1.9025996	2.3311991	-0.0008996
H	2.0329361	3.4418413	-0.0012062
H	2.4806545	1.9538829	0.8829758
H	2.4800462	1.9531262	-0.8849729

2'$^{-}$
64

N	-0.1441569	0.1614269	-2.1629462
Ru	0.0743075	-0.0225157	-0.0471927
P	-0.0781631	-2.2427354	-0.5821310
P	0.1126098	2.2826025	-0.1735558
H	-1.7832676	0.1964043	0.0189210
C	-2.9662567	0.3357133	-0.4233271
H	1.6878420	-0.0952006	-0.2619716
C	-0.3527087	-2.2377059	-2.4166839
C	-0.4004324	2.5646347	-1.9253913
H	-1.4412486	-2.1761390	-2.5704735
H	-1.5006732	2.4703875	-1.9040666
H	0.0245897	-3.1496140	-2.9055342
H	-0.1215545	3.5610569	-2.3027293
C	0.2898602	-0.9560234	-2.9605035
C	0.1964318	1.4293630	-2.7611713
H	-0.0175447	-0.8239937	-4.0236672
H	-0.2061512	1.4916133	-3.7986544

H	1.4062233	-1.0854731	-2.9869630
H	1.3050440	1.5880905	-2.8657186
C	-1.1509444	3.2073062	0.8247662
C	-1.5595477	-3.1768601	0.0904636
H	-2.0336043	2.5493705	0.6432576
H	-2.3321867	-2.3968232	-0.0390035
C	1.7956264	3.1006649	-0.0490027
C	1.4658988	-3.2951514	-0.3908320
H	2.2973901	2.6521448	-0.9262407
H	2.1137192	-2.8069344	-1.1425835
C	0.2528416	-0.1986869	1.7770956
O	0.4238720	-0.3261464	2.9421901
C	1.3397138	-4.7816620	-0.7438260
C	1.8180094	4.6266359	-0.1938013
H	0.8292705	-4.9473305	-1.7033533
H	1.2381224	4.9756406	-1.0599580
H	0.7830597	-5.3249015	0.0337405
H	1.4079564	5.1118068	0.7037836
H	2.3387582	-5.2442101	-0.8109369
H	2.8543919	4.9850729	-0.3154427
C	2.1237944	-3.0982826	0.9808737
C	2.5551738	2.6445055	1.2035143
H	1.5170598	-3.5361058	1.7867868
H	2.1011383	3.0522773	2.1183546
H	2.2517152	-2.0306123	1.1992193
H	2.5489400	1.5494693	1.2815562
H	3.1120771	-3.5874989	1.0031007
H	3.6011030	2.9929864	1.1654253
C	-0.8168075	3.2159729	2.3200051
C	-1.4174755	-3.4381989	1.5947159
H	-0.0072008	3.9275247	2.5528544
H	-0.6928940	-4.2435979	1.7910488
H	-0.5138303	2.2231077	2.6782463
H	-1.0858013	-2.5384901	2.1300119
H	-1.7018770	3.5273021	2.8987594
H	-2.3836153	-3.7537073	2.0206137
C	-1.5534412	4.6011072	0.3248322
C	-2.0238282	-4.4324011	-0.6608544
H	-1.7981991	4.5962656	-0.7455243
H	-2.0840972	-4.2713171	-1.7462886
H	-0.7748279	5.3577461	0.5012214
H	-1.3572273	-5.2870086	-0.4824924
H	-2.4605120	4.9263218	0.8607236
H	-3.0294334	-4.7225119	-0.3127243
H	-2.8003853	-0.1435797	-1.4248347
H	-3.4591590	-0.4056020	0.2762008
O	-3.3906601	1.5626627	-0.3956823

TS-1^{-}
64

N	-0.3705148	0.1530993	-2.0929547
Ru	0.0682379	-0.0482893	0.0467516
P	-0.1214322	-2.2613406	-0.4602737
P	0.1217169	2.2342708	-0.1116633
H	-1.6065918	0.0010844	0.3475126
C	-3.3753663	0.8659593	-1.7364343
H	1.6915079	-0.0748449	-0.4623284
C	-0.6662911	-2.2562126	-2.2344166
C	-0.2673360	2.5790303	-1.8928908
H	-1.7628981	-2.1498766	-2.2297637
H	-1.3582625	2.7054209	-1.9726656
H	-0.4050655	-3.1838726	-2.7674751
H	0.2129799	3.5033512	-2.2500255
C	-0.0476047	-1.0124075	-2.8777239

C	0.1703937	1.3499085	-2.6953330
H	-0.4301388	-0.9109382	-3.9204571
H	-0.1862691	1.4594758	-3.7460511
H	1.0609592	-1.1694743	-2.9773658
H	1.2912333	1.3262157	-2.7519168
C	-1.1888147	3.2061407	0.8171982
C	-1.4487779	-3.2674586	0.4116513
H	-2.0536712	2.5548734	0.6040955
H	-2.2479101	-2.5063336	0.4229735
C	1.7910489	3.0718394	0.1156474
C	1.4606141	-3.2794260	-0.5235525
H	2.3189518	2.6592393	-0.7635350
H	1.9695108	-2.7644851	-1.3588120
C	0.4423991	-0.2130780	1.8345590
O	0.7041512	-0.3250507	2.9857473
C	1.3299247	-4.7670587	-0.8690207
C	1.8199964	4.6022630	0.0355561
H	0.6854813	-4.9442257	-1.7422788
H	1.2628422	4.9920705	-0.8284712
H	0.9171184	-5.3355023	-0.0224925
H	1.3935721	5.0528706	0.9437173
H	2.3216386	-5.1954282	-1.0931306
H	2.8603586	4.9603616	-0.0465800
C	2.3183260	-3.0657490	0.7297246
C	2.5198160	2.5617871	1.3644834
H	1.8640744	-3.5306998	1.6169677
H	2.0186110	2.8857813	2.2882917
H	2.4365397	-1.9925962	0.9295425
H	2.5537095	1.4649290	1.3644735
H	3.3160874	-3.5154990	0.5905388
H	3.5518609	2.9512452	1.3892901
C	-0.9338136	3.1697741	2.3283576
C	-1.0598198	-3.5526842	1.8671661
H	-0.0924690	3.8239198	2.6062048
H	-0.2800470	-4.3278088	1.9254833
H	-0.7047855	2.1511023	2.6700949
H	-0.6840753	-2.6492743	2.3664434
H	-1.8213322	3.5269032	2.8766266
H	-1.9312745	-3.9217193	2.4331440
C	-1.5290906	4.6203139	0.3282484
C	-1.9844518	-4.5239879	-0.2887430
H	-1.6804128	4.6561847	-0.7589633
H	-2.2337522	-4.3387624	-1.3429965
H	-0.7508081	5.3486093	0.5929611
H	-1.2664560	-5.3540048	-0.2532526
H	-2.4676054	4.9572182	0.7995743
H	-2.9046750	-4.8673910	0.2139825
H	-2.3386783	0.6264921	-1.4225792
H	-4.0546132	-0.0233618	-1.8848805
O	-3.7917295	1.9972699	-1.9617612

3^{-}-CH_2O
64

N	-0.7099340	0.2195905	-2.0430029
Ru	-0.0312448	-0.0141936	0.0581688
P	-0.1844754	-2.2322191	-0.4700759
P	0.0638102	2.2663119	-0.0494317
H	-1.6603339	0.0354740	0.4849200
C	-2.4704394	0.3364381	-2.2592318
H	1.5337992	-0.0361161	-0.6264562
C	-0.7047390	-2.2526730	-2.2533244
C	-0.4335591	2.6726089	-1.7923993
H	-1.7976517	-2.3583245	-2.2867218
H	-1.5082295	2.9008053	-1.7939985

H	-0.2692383	-3.1027884	-2.8008499
H	0.0970537	3.5569739	-2.1779231
C	-0.3013576	-0.9230726	-2.8888706
C	-0.1713349	1.4476629	-2.6673549
H	-0.7926634	-0.8170052	-3.8755206
H	-0.6620616	1.5799397	-3.6511865
H	0.7939455	-0.8872445	-3.0268648
H	0.9148283	1.3191826	-2.8216725
C	-1.1488751	3.2537204	0.9916197
C	-1.5087181	-3.2561793	0.3825690
H	-2.0450422	2.6330869	0.8160731
H	-2.3300081	-2.5198399	0.3327113
C	1.7670479	3.0561627	0.0815085
C	1.4209366	-3.2141820	-0.5040431
H	2.2245945	2.6513429	-0.8393475
H	1.9296250	-2.6988832	-1.3388463
C	0.4653434	-0.2045416	1.8067423
O	0.7765987	-0.3272456	2.9435051
C	1.3171005	-4.7074258	-0.8348116
C	1.8300297	4.5869784	0.0331069
H	0.6751183	-4.9067170	-1.7049708
H	1.2220168	5.0121280	-0.7784248
H	0.9148904	-5.2729453	0.0183958
H	1.4838173	5.0258094	0.9802379
H	2.3165194	-5.1192637	-1.0544047
H	2.8704636	4.9208866	-0.1175181
C	2.2628743	-2.9773588	0.7552970
C	2.5656223	2.5001017	1.2663962
H	1.7897890	-3.4115929	1.6480300
H	2.1340212	2.8106654	2.2290211
H	2.3933814	-1.9019829	0.9303768
H	2.5762216	1.4032081	1.2382711
H	3.2562923	-3.4436900	0.6424938
H	3.6050118	2.8680486	1.2312292
C	-0.8003044	3.1594829	2.4815534
C	-1.1682038	-3.4765698	1.8610330
H	0.0796186	3.7757229	2.7235657
H	-0.3636852	-4.2195059	1.9770853
H	-0.5869653	2.1237215	2.7781272
H	-0.8458835	-2.5427572	2.3411131
H	-1.6377347	3.5286336	3.0963610
H	-2.0476485	-3.8584117	2.4053734
C	-1.4699344	4.6960156	0.5751845
C	-1.9803274	-4.5534247	-0.2894178
H	-1.6581041	4.7886749	-0.5034831
H	-2.1655558	-4.4248333	-1.3648789
H	-0.6612499	5.3905649	0.8383371
H	-1.2550095	-5.3685536	-0.1662927
H	-2.3778696	5.0398743	1.0987420
H	-2.9258805	-4.8866918	0.1703974
H	-2.6411663	1.1825521	-1.5376235
H	-2.7389718	-0.6051323	-1.7050202
O	-2.7991436	0.4691584	-3.4873584

3^{-}
60

H	0.2120383	-1.5589037	-0.0000011
Ru	-0.1718715	0.1077138	-0.0000010
H	-0.2786066	1.7965997	-0.0000011
P	0.1696154	0.1349724	-2.2519212
P	0.1696189	0.1349730	2.2519188
C	1.9894630	0.4526463	-2.4256044
C	1.9894664	0.4526478	2.4256000
H	2.1253631	1.5454664	-2.4077296

H	2.1253663	1.5454679	2.4077242
H	2.4060730	0.0574919	-3.3658205
H	2.4060778	0.0574942	3.3658158
C	2.6527941	-0.1495308	-1.1825853
C	2.6527959	-0.1495299	1.1825802
H	3.7428381	0.0972380	-1.1987178
H	3.7428399	0.0972390	1.1987111
H	2.5989717	-1.2739583	-1.2547475
H	2.5989736	-1.2739575	1.2547433
N	2.0217851	0.3680137	-0.0000023
C	-0.6240605	1.5092143	3.2622319
C	-0.6240601	1.5092177	-3.2622319
H	-0.4627627	2.3405807	2.5545074
H	-0.4627625	2.3405804	-2.5545031
C	-0.0455020	-1.4898888	3.1796197
C	-0.0455041	-1.4898920	-3.1796184
H	0.7692443	-2.0691332	2.7077237
H	0.7692439	-2.0691329	-2.7077209
C	-1.9899662	-0.1211756	-0.0000014
O	-3.1653121	-0.2930162	-0.0000042
C	0.1771250	-1.4715059	-4.6959853
C	0.1771268	-1.4714959	4.6959866
H	1.0975708	-0.9420956	-4.9823138
H	1.0975734	-0.9420860	4.9823129
H	-0.6655051	-0.9903132	-5.2143854
H	-0.6655026	-0.9902989	5.2143843
H	0.2494440	-2.5019390	-5.0842108
H	0.2494440	-2.5019273	5.0842174
C	-1.3637174	-2.1821096	-2.8133748
C	-1.3637179	-2.1821036	2.8133808
H	-2.2330705	-1.6427129	-3.2175525
H	-2.2330685	-1.6427027	3.2175586
H	-1.4724160	-2.2345498	-1.7221707
H	-1.4724184	-2.2345468	1.7221772
H	-1.3843083	-3.2058202	-3.2247585
H	-1.3843111	-3.2058128	3.2247680
C	-2.1370261	1.2962708	3.3899068
C	-2.1370260	1.2962797	-3.3899110
H	-2.3659068	0.4898146	4.1039115
H	-2.3659074	0.4898277	-4.1039201
H	-2.5858956	1.0351438	2.4217417
H	-2.5858989	1.0351496	-2.4217484
H	-2.6263356	2.2120690	3.7619419
H	-2.6263315	2.2120812	-3.7619428
C	0.0116648	1.8857813	4.6077273
C	0.0116704	1.8857918	-4.6077227
H	1.1030331	1.9947681	4.5353339
H	1.1030388	1.9947759	-4.5353249
H	-0.2011567	1.1420250	5.3871498
H	-0.2011499	1.1420410	-5.3871506
H	-0.3961345	2.8498484	4.9576176
H	-0.3961258	2.8498620	-4.9576084

2$_{2m}$
77

H	-1.1021674	-1.4865050	-0.2557883
Ru	-0.4465900	-0.0276122	-0.1512447
O	0.2005419	2.1138750	0.1640724
P	-0.8286926	-0.0602931	2.1357707
P	-0.6999506	0.0378878	-2.4618261
C	-2.4684131	0.8068276	2.2572887
C	-2.3975797	0.7612251	-2.6615634
H	-2.2549341	1.8869706	2.2736803
H	-2.2528139	1.8511469	-2.7279547

H	-3.0136356	0.5584379	3.1791731
H	-2.8839761	0.4265892	-3.5886928
C	-3.2928130	0.4704168	1.0169236
C	-3.2427781	0.4125427	-1.4410541
H	-4.2426963	1.0363705	1.0196585
H	-4.2124880	0.9423763	-1.4825019
H	-3.5461008	-0.6014142	0.9966099
H	-3.4524973	-0.6679703	-1.4002414
N	-2.5145393	0.7839643	-0.2037144
C	0.3735588	1.1957289	-3.4507419
C	0.3062865	0.9855219	3.1821365
H	0.3145773	2.0912156	-2.8092816
H	0.4305713	1.8387332	2.4913595
C	-0.8296091	-1.6303226	-3.3004121
C	-1.1434308	-1.7180874	2.9351934
H	-1.7445368	-2.0246055	-2.8213348
H	-2.0705225	-2.0234200	2.4160169
C	1.2161561	-0.7846945	-0.1172144
O	2.2763134	-1.2895207	-0.0901445
C	-1.4116063	-1.6920849	4.4448736
C	-1.0456135	-1.5975776	-4.8185567
H	-2.1556879	-0.9370600	4.7344690
H	-1.8248168	-0.8873517	-5.1273717
H	-0.4880774	-1.4906765	5.0050799
H	-0.1174807	-1.3290027	-5.3413259
H	-1.7857441	-2.6730606	4.7760927
H	-1.3431188	-2.5962116	-5.1741726
C	-0.0561491	-2.7393564	2.5719398
C	0.3272222	-2.5662111	-2.9254601
H	0.9097033	-2.4812823	3.0273387
H	1.2884206	-2.1957153	-3.3074218
H	0.0865895	-2.7966270	1.4860435
H	0.4159176	-2.6777211	-1.8387378
H	-0.3418052	-3.7366157	2.9405512
H	0.1578095	-3.5621617	-3.3633860
C	1.8256663	0.7039722	-3.4907171
C	1.6755890	0.3146306	3.3564477
H	1.9404868	-0.1435481	-4.1824897
H	1.6244380	-0.5215646	4.0692927
H	2.1819134	0.3849421	-2.5014928
H	2.0710828	-0.0698164	2.4068373
H	2.4857512	1.5092020	-3.8474035
H	2.4000629	1.0403617	3.7560342
C	-0.1277440	1.6275967	-4.8346582
C	-0.2425081	1.5121509	4.5147754
H	-1.1755200	1.9502528	-4.8118601
H	-1.2300590	1.9814782	4.4102920
H	-0.0141820	0.8345917	-5.5841792
H	-0.3217623	0.7204746	5.2705730
H	0.4618626	2.4942557	-5.1697517
H	0.4418052	2.2776724	4.9132729
C	1.4786761	2.6073431	-0.2059531
H	1.6056654	3.6423858	0.1548567
H	2.2552879	1.9758587	0.2524848
H	1.6339261	2.6017593	-1.2989176
H	-1.4980121	3.8459104	-1.8966352
O	-1.2893076	3.9624570	-2.8802338
O	-1.7814721	3.4106989	-0.3678252
H	-0.6413207	2.8027171	-0.1061270
H	-2.3666768	1.8368571	-0.2291669
C	-2.4080496	4.5689539	-3.5013561
H	-2.6220681	5.5782972	-3.1009457
H	-3.3335549	3.9645395	-3.4013946
H	-2.1912631	4.6718308	-4.5755128
C	-2.0570420	4.4167305	0.5811244

H	-1.8274054	4.0830836	1.6154643
H	-3.1243595	4.7070278	0.5560487
H	-1.4607095	5.3322286	0.3989883

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