Electronic Supplementary Information

Mechanistic Insights into HCO_2H Dehydrogenation and CO_2 Hydrogenation Catalyzed by Ir(Cp*) Containing Tetrahydroxy Bipyrimidine Ligand: The Role of Sodium and Proton Shuttle

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Standard state conversion[1-2]

The default parameters in Gaussian 09, standard state in gas phase at 1 atm and 298.15 K, were used for all calculations. Thus, the relative free energies of all species are converted from standard state at 1 atm, to the standard state in solution (1 M). The standard state conversion of free energy change for the reaction of reactants A and B to form product C from 1 atm to 1 M (eq. S1) can be calculated using eq. S2. In eq. S2, ΔG^{o} is the standard state free energy change at 1 atm, ΔG^{*} is the standard state free energy change at 1 M, R is the gas constant, T is the absolute temperature (in Kelvin), Q^{o} is the reaction quotient at 1 atm, and Q^{*} is the reaction quotient at 1 M. Note that ΔG^{o} and ΔG^{*} here refer to the changes in solution phase because all geometries were optimized in this phase, as mentioned in the main text. Assuming A, B, and C to be ideal gases, we can thus represent their concentrations at 1 atm and 298.15 K as (1/24.5) mol/L. Therefore, the standard state free energy change at 1 atm (ΔG^{o}) can be converted to the standard state free energy change at 1 M (ΔG^{*}), through eq. S5-S7.

$$\mathrm{A} + \mathrm{B} \rightarrow \mathrm{C} \tag{S1}$$

$$\Delta G^{*} = \Delta G^{\circ} + RT \ln \left(\frac{Q^{*}}{Q^{\circ}}\right) \tag{S2}$$

$$Q^{\circ} = \frac{[\mathrm{C}]_{1\ \mathrm{atm}}}{[\mathrm{A}]_{1\ \mathrm{atm}}[\mathrm{B}]_{1\ \mathrm{atm}}} \tag{S3}$$

$$Q^{*} = \frac{[\mathrm{C}]_{1\ \mathrm{M}}}{[\mathrm{A}]_{1\ \mathrm{M}}[\mathrm{B}]_{1\ \mathrm{M}}} \tag{S4}$$

$$\Delta G^{*} = \Delta G^{\circ} + RT \ln \left(\frac{\frac{1}{1 \cdot 1}}{\frac{24.5 \cdot 24.5}{24.5}} \right) \tag{S5}$$

$$\Delta G^{*} = \Delta G^{\circ} - RT \ln (24.5) \tag{S6}$$

$$\Delta G^{*} = \Delta G^{\circ} - 1.89\ \mathrm{kcal/mol} \tag{S7}$$

For the reaction involving a water molecule arising from water solvent, the standard state concentration for water is adjusted from 1 atm to 55.6 M, which is the standard state concentration of the bulk water. The standard state free energy change for the reaction of A with water in aqueous solution (eq. S8) can be calculated using eqs. S9-S14. Note that, in eq. S9, Q* is the reaction quotient at 1 M for all species except for water, for which the concentration was adjusted to 55.6 M (eq. S11).

$$A + H_2O \rightarrow A(H_2O) \tag{S8}$$

$$\Delta G^* = \Delta G^\circ + RT \ln \left(\frac{Q^*}{Q^\circ}\right) \tag{S9}$$

$$Q^\circ = \frac{[A(H_2O)]_{1\ atm}}{[A]_{1\ atm}[H_2O]_{1\ atm}} \tag{S10}$$

$$Q^* = \frac{[A(H_2O)]_{1\ M}}{[A]_{1\ M}[H_2O]_{55.6\ M}} \tag{S11}$$

$$\Delta G^* = \Delta G^\circ + RT\ln\left(\left(\frac{\frac{1}{1 \cdot 1}}{\frac{24.5 \cdot 24.5}{24.5}}\right)\left(\frac{1}{1 \cdot 55.6}\right)\right) \tag{S12}$$

$$\Delta G^* = \Delta G^\circ - RT \ln (24.5 \times 55.6) \tag{S13}$$

$$\Delta G^* = \Delta G^\circ - 4.27\ \text{kcal/mol} \tag{S14}$$

pH correction[3-5]

For the reaction involving a proton (H^+) transfer (eq. S15), the proton dissociation energy, corrected to pH 3.5, can be calculated from eq. S16-S18:

$$AH \rightleftharpoons A^- + H^+ \tag{S15}$$

$$\Delta G^* = \Delta G^\circ + RT ln \left(\frac{Q^*}{Q^\circ}\right) \tag{S16}$$

$$Q^{\circ} = \frac{[A^-]_{1\ atm}[H^+]_{1\ atm}}{[AH]_{1\ atm}} \quad \text{(S17)}$$

$$Q^{*} = \frac{[A^-]_{1\ M}[H^+]_{at\ pH\ 3.5}}{[AH]_{1\ M}} \quad \text{(S18)}$$

where ΔG° is the standard state free energy change at 1 atm and ΔG^{*} is the standard state free energy change at 1 M except for the proton concentration, which is adjusted corresponding to that at pH 3.5. The proton concentration [H$^+$] is taken from the pH (eq. S19-S20). Then, the standard state proton dissociation free energy at pH 3.5 (ΔG^{*}) can be calculated according to eq. S21-S23.

$$pH = 3.5 = -\log[H^+] \quad \text{(S19)}$$

$$[H^+] = 10^{-3.5} \quad \text{(S20)}$$

$$\Delta G^{*} = \Delta G^{\circ} + RTln\left(\frac{\frac{1 \cdot (10^{-3.5})}{1}}{\frac{24.5}{24.5 \cdot 24.5}}\right) \quad \text{(S21)}$$

$$\Delta G^{*} = \Delta G^{\circ} + 1.89 - 3.5\ RTln(10) \quad \text{(S22)}$$

$$\Delta G^{*} = \Delta G^{\circ} + 1.89 - 4.77\ kcal/mol\ . \quad \text{(S23)}$$

Using the same procedure above, the standard state free energy change ΔG^{*} can be adjusted for proton dissociation at pH 7.6 ($\Delta G^{*} = \Delta G^{\circ}$ + 1.89 – 10.36 kcal/mol), and 8.3 ($\Delta G^{*} = \Delta G^{\circ}$ + 1.89 – 11.31 kcal/mol).

Solvation free energy of sodium ion

Free energy change for the transfer of a sodium ion from gas phase into solution phase is the solvation free energy of sodium, $\Delta G_s^{*}(Na^+)$, which can be represented as

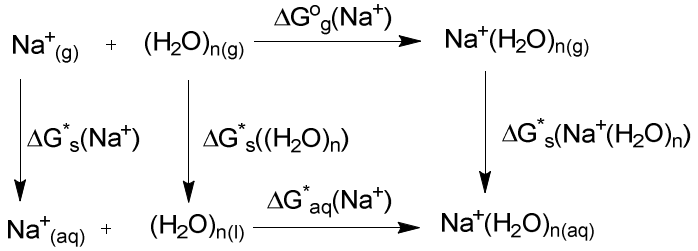
$$\Delta G_s^{*}(Na^+) = G_{aq}^{*}(Na^+) - G_g^{o}(Na^+) - \Delta G^{o\rightarrow *} \quad \text{(S24)}$$

where the $G_{aq}^{*}(Na^+)$ and $G_g^{o}(Na^+)$ are the free energies of sodium ion in aqueous and gas phases, respectively. The $\Delta G^{o\rightarrow *}$ is the free energy correction from the 1 atm standard state to 1 M as described above.

To calculate the $\Delta G_s^*(Na^+)$, a thermodynamic cycle in Scheme S1 is employed.[2] We applied a mixed cluster/continuum model in this thermodynamic cycle,[2] where the Na^+ is surrounded by a water cluster (n is the number of water molecule) to account for the interaction between the first solvation shell and the bulk. The upper leg represents the free energy change in gas phase ($\Delta G_g^{\circ}(Na^+)$), while the lower leg the free energy change in aqueous phase, $\Delta G_{aq}^*(Na^+)$. In water solvent, the $\Delta G_{aq}^*(Na^+)$ is equal to zero.[2] By relating the free energy change in gas phase ($\Delta G_g^o(Na^+)$) to the solvation free energy of each species ($\Delta G_s^*(Na^+)$, $\Delta G_s^*((H_2O)_n)$, and $\Delta G_s^*(Na^+(H_2O)_n)$, we can calculate the $\Delta G_s^*(Na^+)$ as follows:

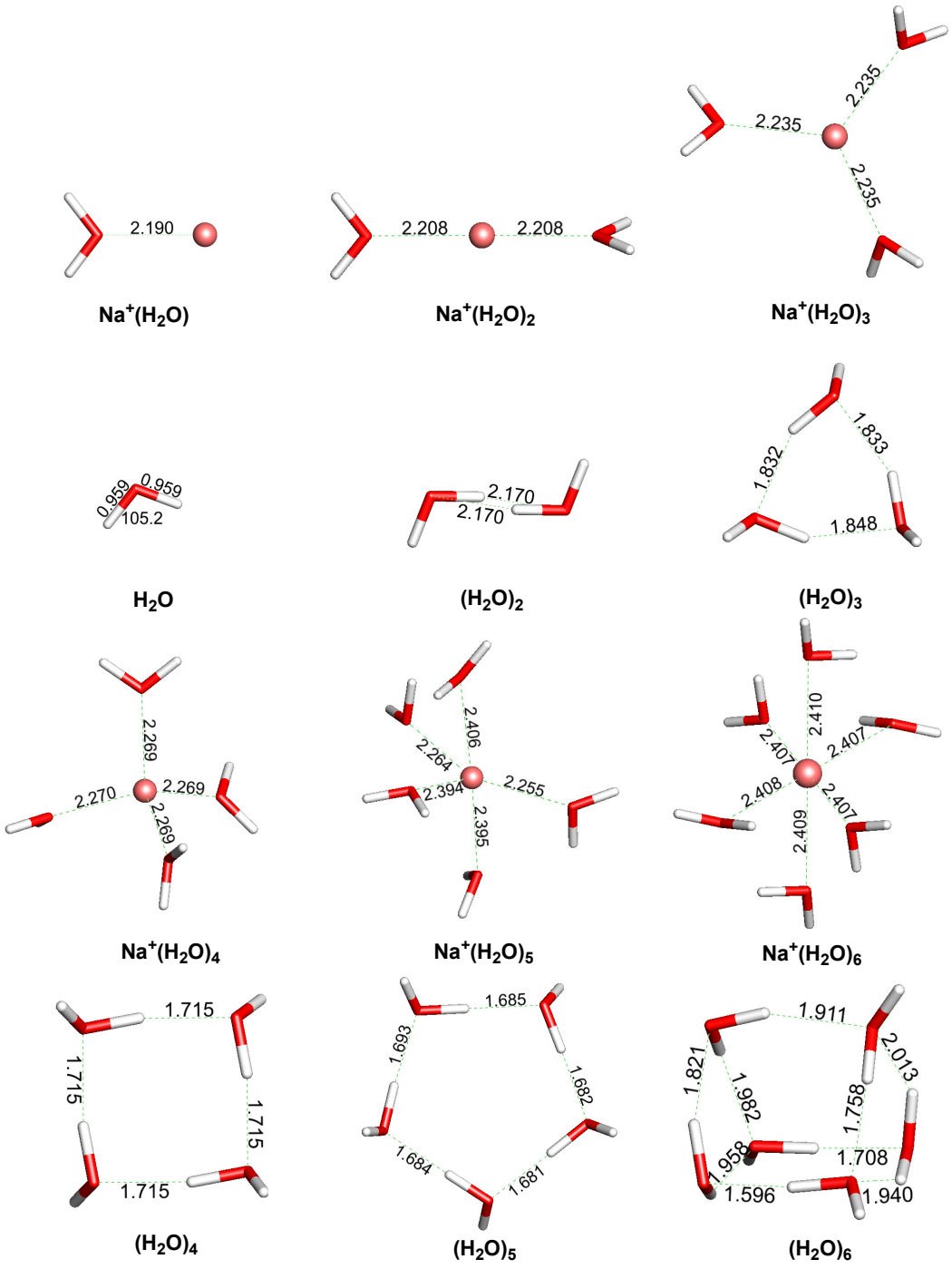
$$\Delta G_s^*(Na^+) = \Delta G_s^*(Na^+(H_2O)_n) + \Delta G_g^o(Na^+) - \Delta G_s^*((H_2O)_n) - \Delta G^{o\to *} - \Delta G_w^{*\to 55.6\,M} \quad \text{(S25)}$$

where $\Delta G_w^{*\to 55.6\,M}$, the correction for water cluster, is equal to RTln(55.6/n).



Scheme S1 Thermodynamic cycle for the calculation of solvation free energy of sodium ion.

Table S1 shows the calculated solvation free energies of Na^+. The optimized structures of Na^+ solvated by water ($Na^+(H_2O)_n$, n = 1-6) and water cluster ($(H_2O)_n$, n = 1-6) used for obtaining the calculated values in Table S1 are shown as follows:



Scheme S2. Optimized geometries of $Na^+(H_2O)_n$ and $(H_2O)_n$ (n = 1-6) clusters. The arrangement of $Na^+(H_2O)_n$ (n = 1-6) clusters were based on the report by Rempe and co-workers (J. Chem. Theory Comput. 2015, 11, 2958). The arrangement of $(H_2O)_n$ (n = 1-6) clusters were chosen from the lowest energy isomer from the study by Shields and co-workers (J. Phys. Chem. A 2011, 115, 12034).

Table S1 Calculated solvation free energies of Na^+ using the thermodynamic cycle in Scheme S1.

	Solvation free energies, kcal/mol							Exp.[a]
	n = 0	n = 1	n = 2	n = 3	n = 4	n = 5	n = 6	
Na^+	-70.5	-76.0	-81.0	-88.4	-87.2	-89.3	-92.0	-87.6

[a]Taken from ref. 6.

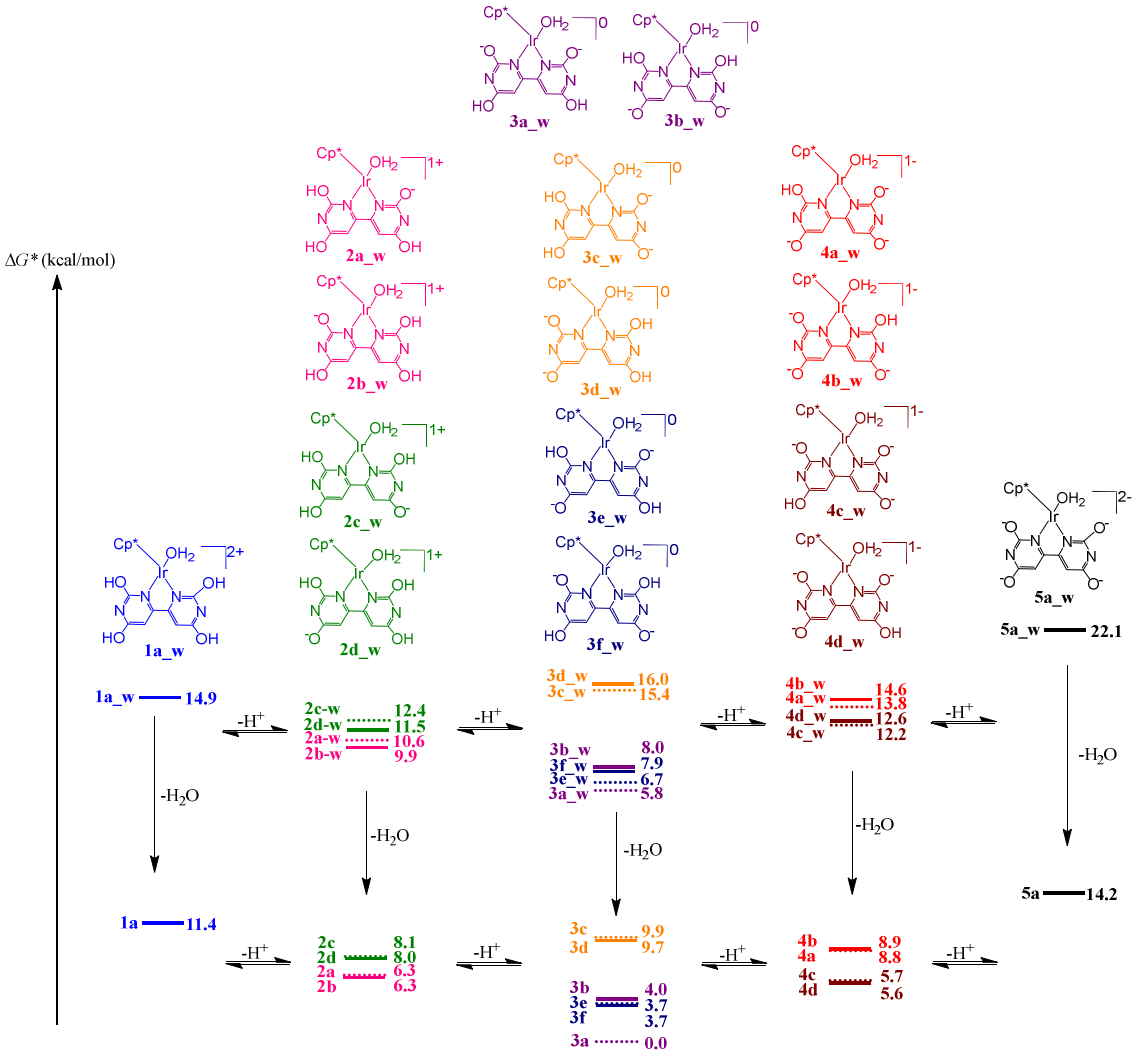


Fig. S1 Relative free energies (in kcal/mol) at pH 3.5 of $[IrCp^*(H_2O)(bpymO_4H_n)]^{n-2}$ (n = 0, 1, 2, 3, and 4) with respect to **3a** + H_2O.

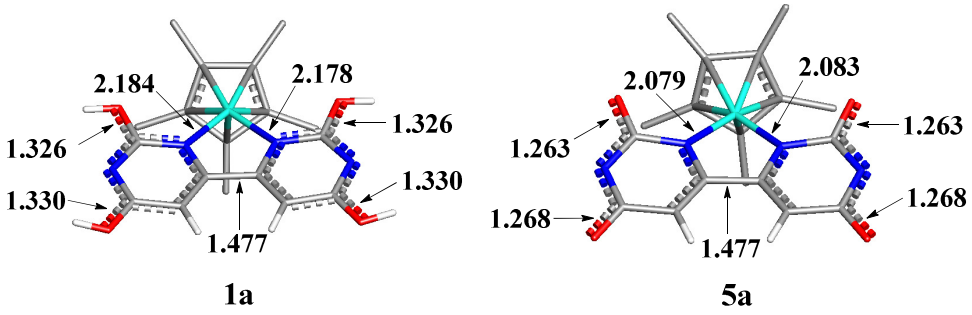


Fig. S2 Optimized geometries for tetraprotic complex $[IrCp^*(bpymO_4H_4)]^{2+}$ (**1a**) and fully deprotonated complex $[IrCp^*(bpymO_4)]^{2-}$ (**5a**). Selected geometry parameters are shown in Å. Hydrogen atoms on Cp* are omitted for clarity.

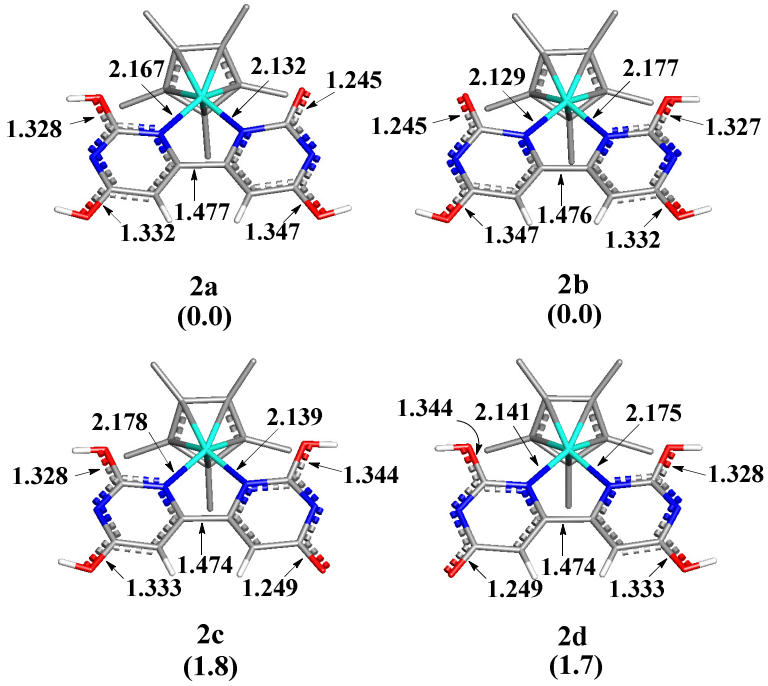


Fig. S3 Optimized geometries and relative free energies (in kcal/mol) of triprotic complexes $[IrCp^*(bpymO_4H_3)]^{1+}$ **2a**, **2b**, **2c**, and **2d**. Selected geometry parameters are shown in Å. Hydrogen atoms on Cp* are omitted for clarity.

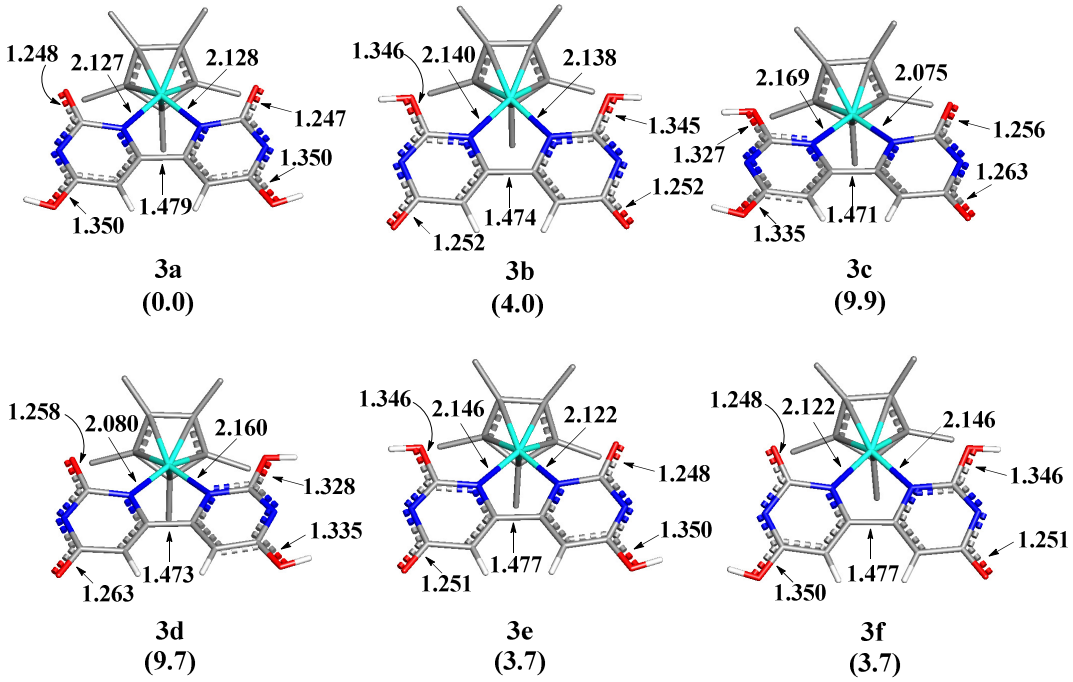


Fig. S4 Optimized geometries and relative free energies (in kcal/mol) of diprotic complexes $[IrCp^*(bpymO_4H_2)]^0$ **3a**, **3b**, **3c**, **3d**, **3e**, and **3f**. Selected geometry parameters are shown in Å. Hydrogen atoms on Cp* are omitted for clarity.

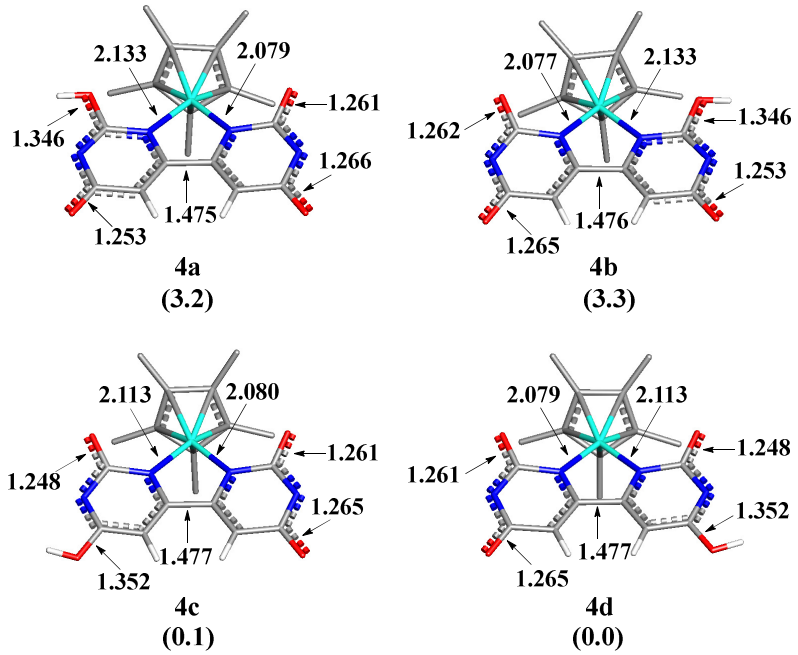


Fig. S5 Optimized geometries and relative free energies (in kcal/mol) of monoprotic complexes $[IrCp^*(bpymO_4H)]^{1-}$ **4a**, **4b**, **4c**, and **4d**. Selected geometry parameters are shown in Å. Hydrogen atoms on Cp* are omitted for clarity.

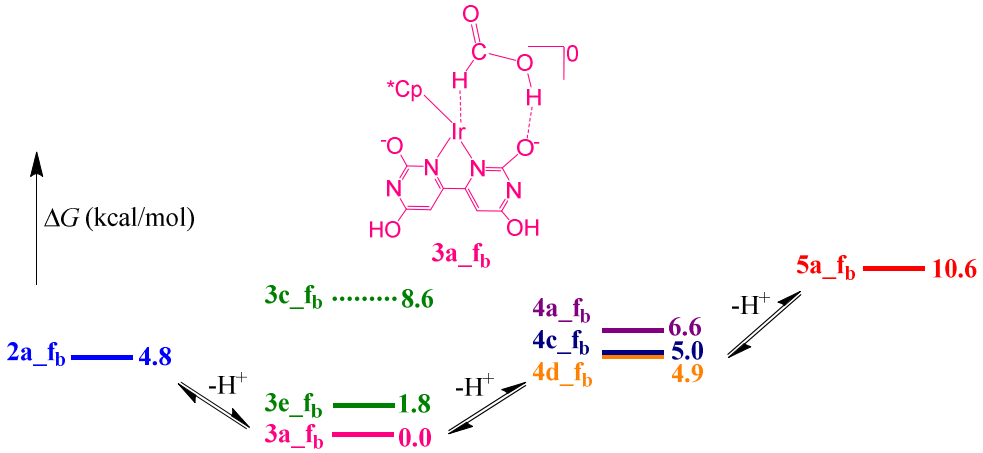


Fig. S6 Relative free energies (in kcal/mol) at pH 3.5 of H-bound Ir-HCO_2H complexes having the proton still residing on the HCO_2H moiety.

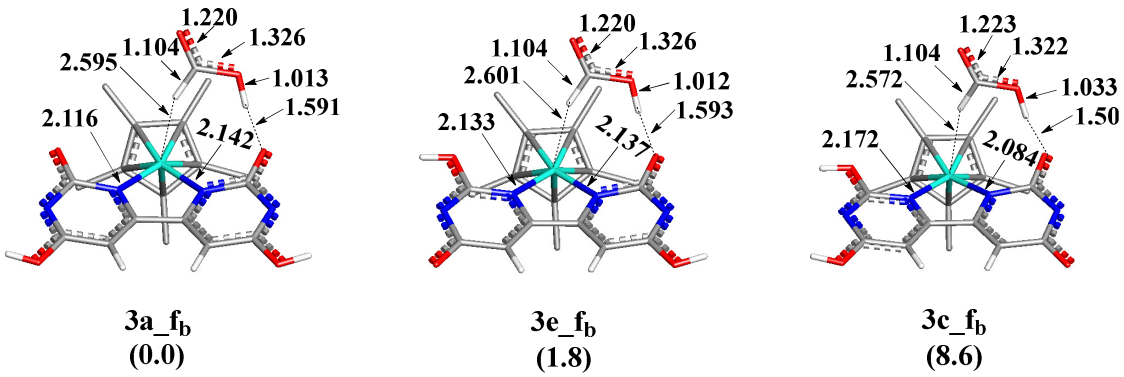


Fig. S7 Optimized geometries and relative free energies (in kcal/mol) of H-bound Ir-HCO_2H complexes **3a_fb**, **3e_fb**, and **3c_fb**. Selected geometry parameters are shown in Å. Hydrogen atoms on Cp* are omitted for clarity.

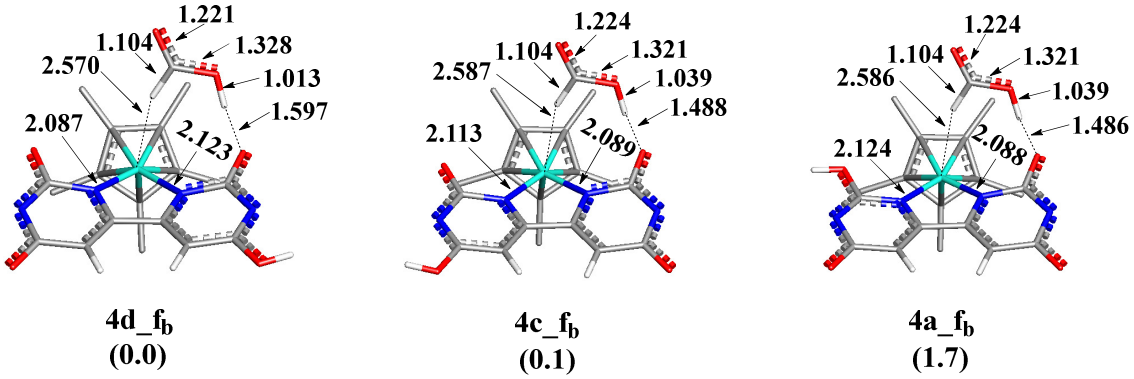


Fig. S8 Optimized geometries and relative free energies (in kcal/mol) of H-bound Ir-HCO_2H complexes **4d_fb**, **4c_fb**, and **4a_fb**. Selected geometry parameters are shown in Å. Hydrogen atoms on Cp* are omitted for clarity.

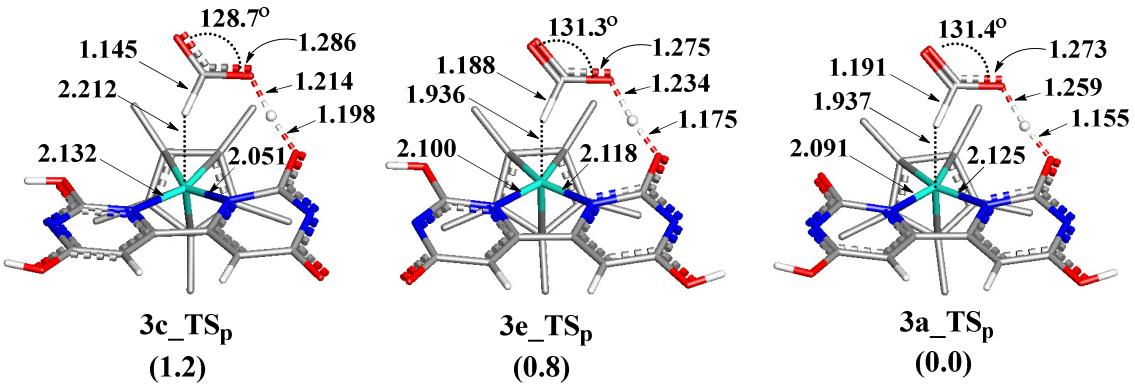


Fig. S9 Optimized geometries and relative free energies (in kcal/mol) of transition states **3c_TS$_p$**, **3e_TS$_p$**, and **3a_TS$_p$** for proton transfer from HCO_2H to the pendant O^- of the bipyrimidine ligand.

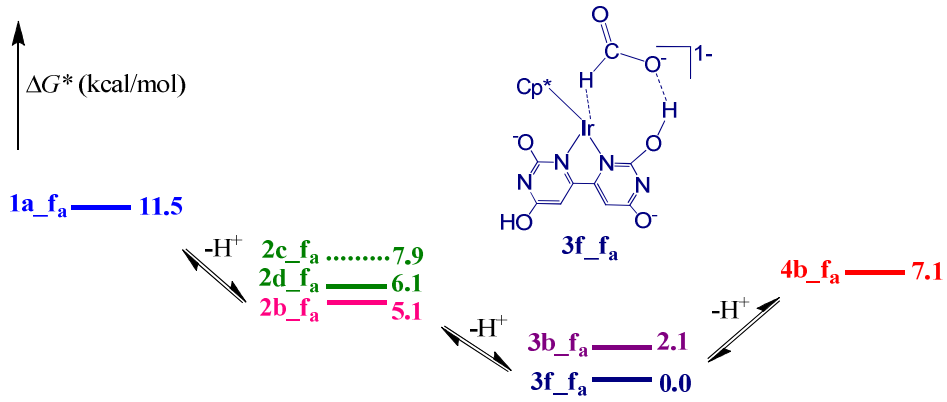


Fig. S10 Relative free energies of Ir-HCO_2^H (in kcal/mol) at pH 3.5, in which the HCO_2 moiety forms a hydrogen bond with the pendant OH on the bipyrimidine ligand.

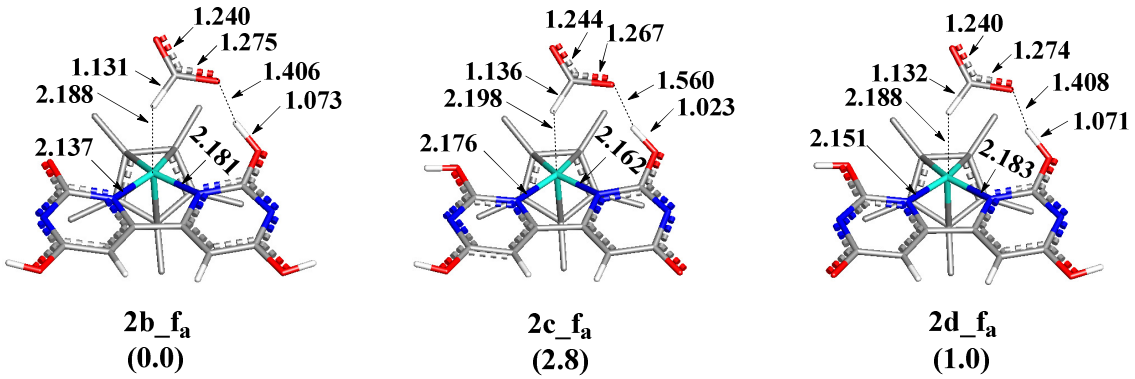
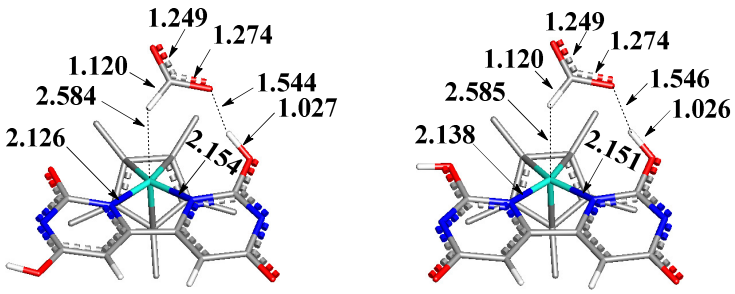


Fig. S11 Optimized geometries and relative free energies (in kcal/mol) of H-bound Ir-HCO_2^H complexes **2b_f$_a$**, **2d_f$_a$**, and **2c_f$_a$**. Selected geometry parameters are shown in Å. Hydrogen atoms on Cp* are omitted for clarity.



3f_f$_a$ (0.0) **3b_f$_a$** (2.1)

Fig. S12 Optimized geometries and relative free energies (kcal/mol) of H-bound Ir-HCO_2^H complexes **3f_f$_a$** and **3b_f$_a$**. Selected geometry parameters are shown in Å. Hydrogen atoms on Cp* are omitted for clarity.

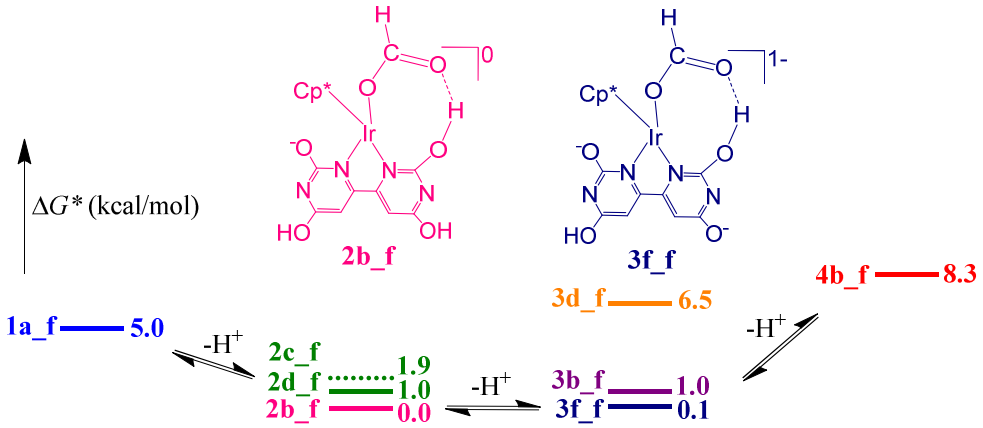
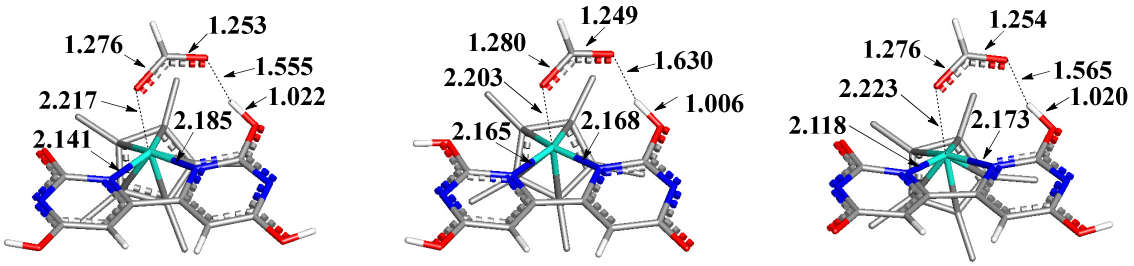
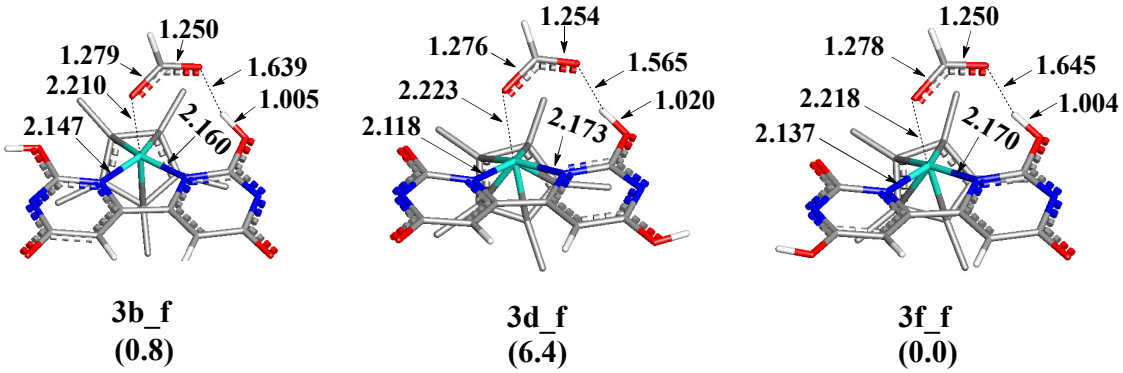


Fig. S13 Relative free energies of Ir-$OCHO^H$ (in kcal/mol) at pH 3.5, in which the HCO_2 moiety forms a hydrogen bond with the pendant OH on the bipyrimidine ligand.



2b_f (0.0) **2c_f** (1.9) **2d_f** (1.0)

Fig. S14 Optimized geometries and relative free energies (in kcal/mol) of Ir-$OCHO^H$ complexes **2b_f**, **2c_f**, and **2d_f**. Selected geometry parameters are shown in Å. Hydrogen atoms on Cp* are omitted for clarity.



3b_f (0.8) **3d_f** (6.4) **3f_f** (0.0)

Fig. S15 Optimized geometries and relative free energies (in kcal/mol) of Ir-OCHO^{H} complexes **3b_f**, **3d_f**, and **3f_f**. Selected geometry parameters are shown in Å. Hydrogen atoms on Cp* are omitted for clarity.

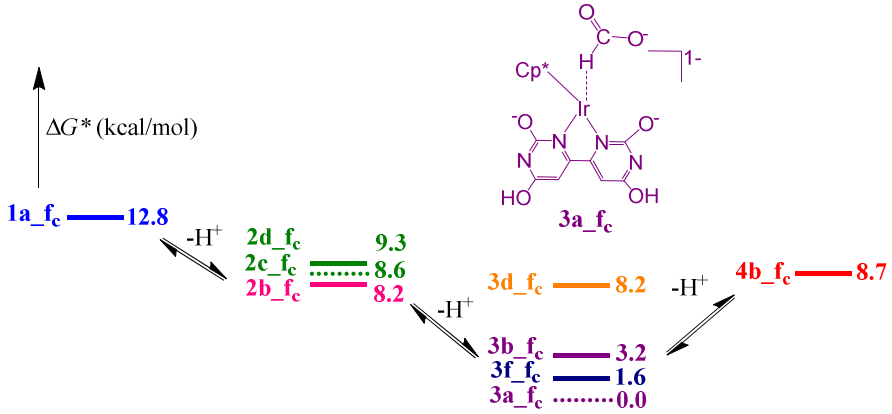
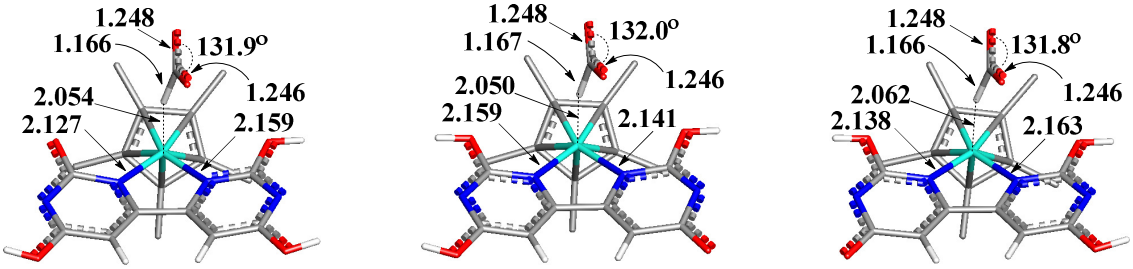


Fig. S16 Relative free energies of H-bound Ir-HCO_2 (in kcal/mol) at pH 3.5, in which the hydrogen bond between the HCO_2 moiety and the pendant OH/O$^-$ on the bipyrimidine ligand is absent.



2b_f$_c$ (0.0) **2c_f$_c$** (0.4) **2d_f$_c$** (1.1)

Fig. S17 Optimized geometries and relative free energies (in kcal/mol) of H-bound Ir-HCO_2 complexes **2b_f$_c$**, **2c_f$_c$**, and **2d_f$_c$**. Selected geometry parameters are shown in Å. Hydrogen atoms on Cp* are omitted for clarity.

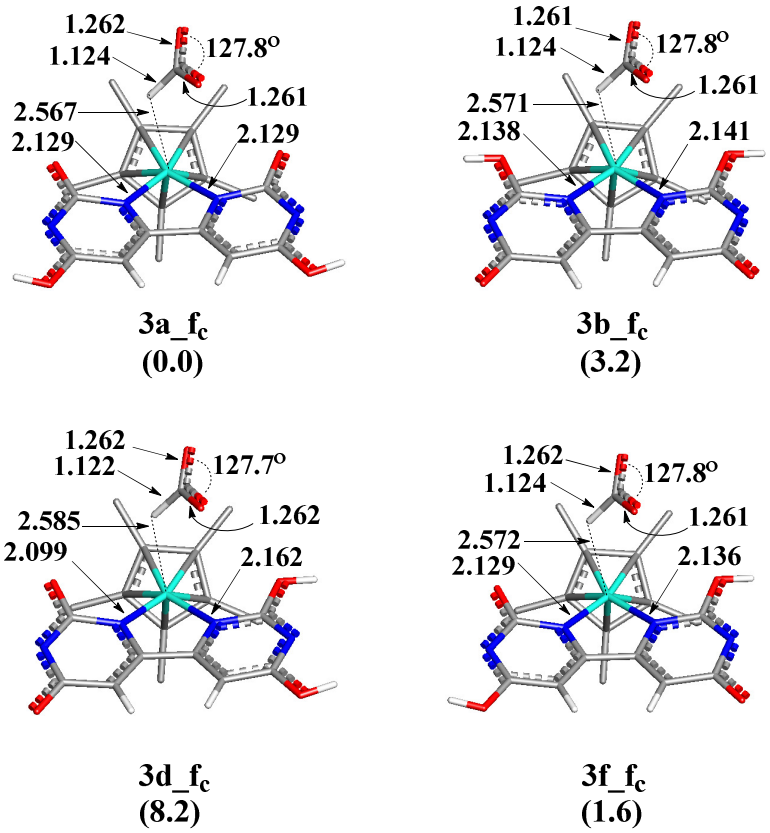


Fig. S18 Optimized geometries and relative free energies (in kcal/mol) of H-bound Ir-HCO_2 complexes **3a_f$_c$**, **3b_f$_c$**, **3d_f$_c$** and **3f_f$_c$**. Selected geometry parameters are shown in Å. Hydrogen atoms on Cp* are omitted for clarity.

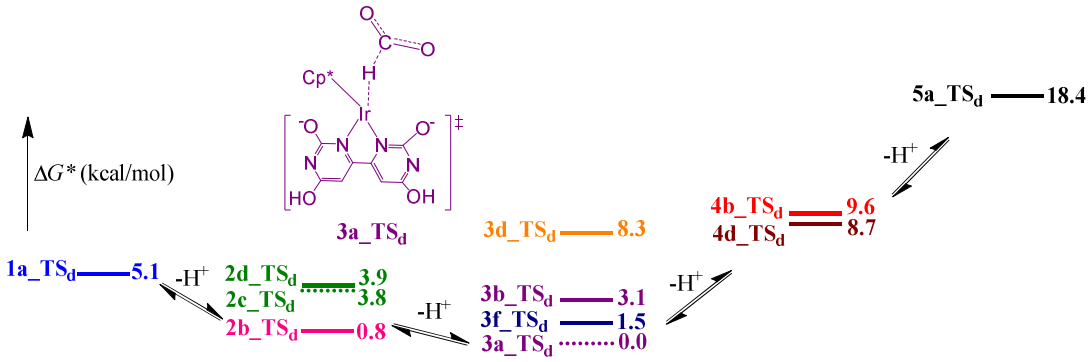
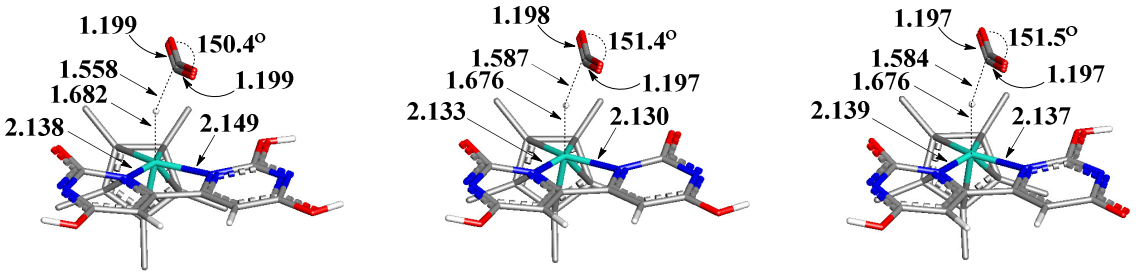


Fig. S19 Relative free energies of transition states for direct hydride transfer (in kcal/mol) at pH 3.5.



2b_TS$_d$ **3a_TS$_d$** **3f_TS$_d$**

Fig. S20 Optimized geometries of the transition states **2b_TS$_d$**, **3a_TS$_d$**, and **3f_TS$_d$** for direct hydride transfer. Selected geometry parameters are shown in Å. Hydrogen atoms on Cp* are omitted for clarity.

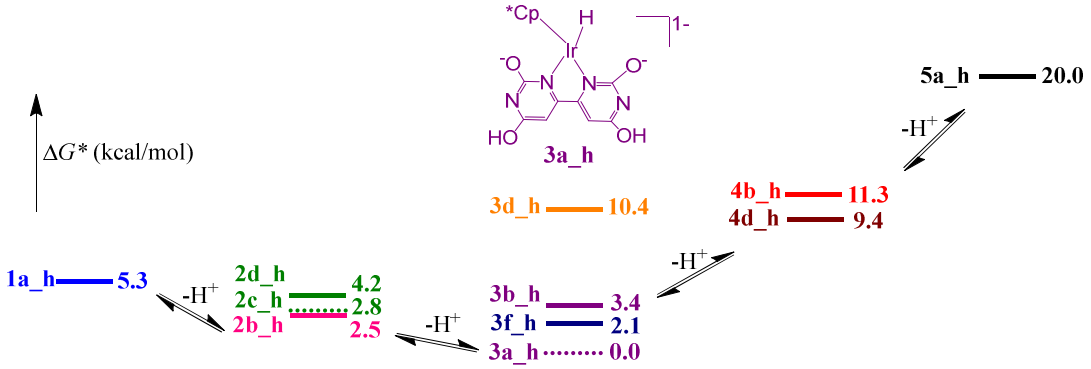
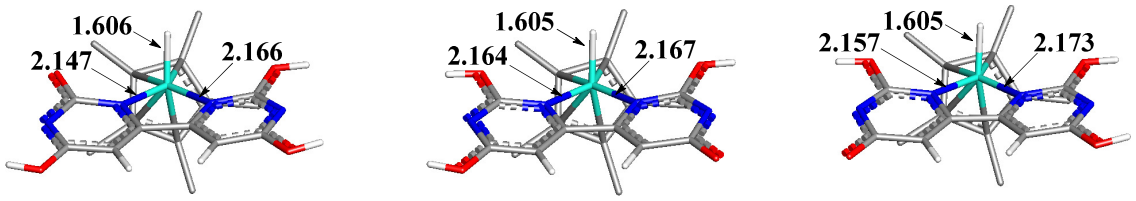


Fig. S21 Relative free energies of Ir-H complexes (in kcal/mol) at pH 3.5.



2b_h **2c_h** **2d_h**
(0.0) **(0.3)** **(1.7)**

Fig. S22 Optimized geometries and relative free energies (in kcal/mol) of Ir-H complexes **2b_h**, **2c_h**, and **2d_h**. Selected geometry parameters are shown in Å. Hydrogen atoms on Cp* are omitted for clarity.

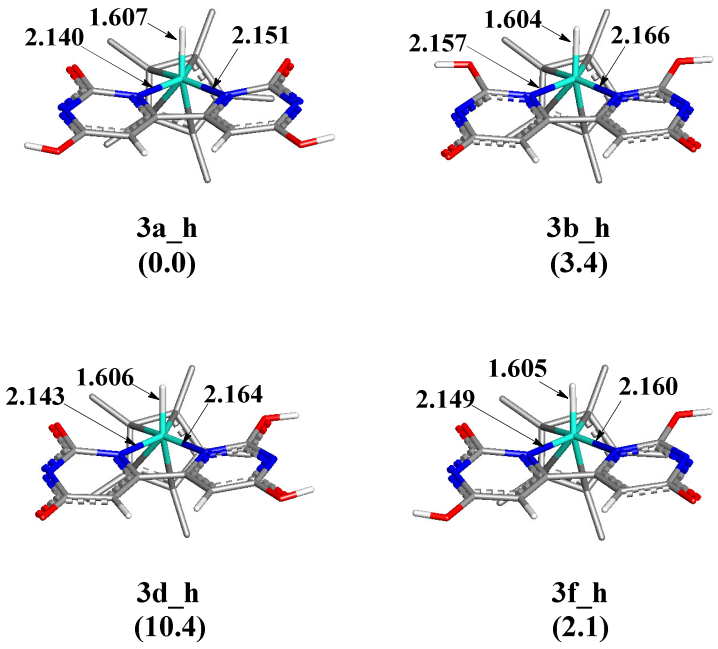


Fig. S23 Optimized geometries and relative free energies (in kcal/mol) of Ir-H complexes **3a_h**, **3b_h**, **3d_h** and **3f_h**. Selected geometry parameters are shown in Å. Hydrogen atoms on Cp* are omitted for clarity.

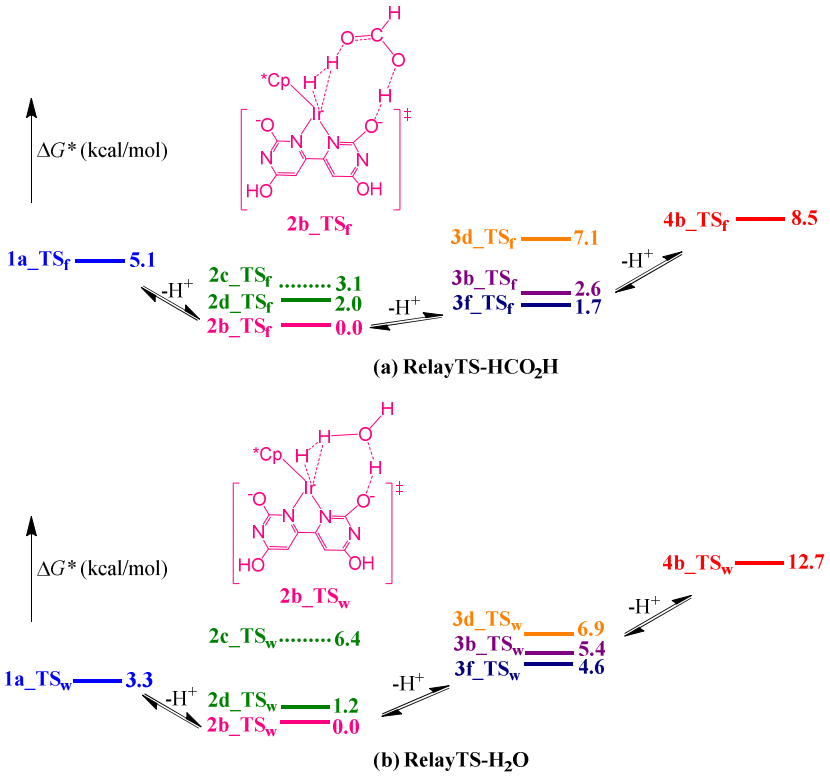


Fig. S24 Relative free energies (in kcal/mol) at pH 3.5 of the transition states for H_2 formation using (a) HCO_2H as a proton shuttle and (b) H_2O as a proton shuttle.

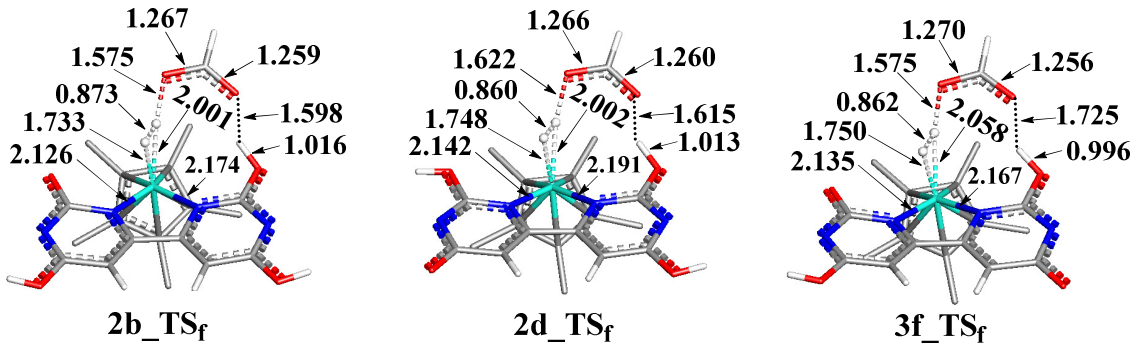


Fig. S25 Optimized geometries of the transition states for H_2 formation using HCO_2H as a proton shuttle: **2b_TS$_f$**, **2d_TS$_f$**, and **3f_TS$_f$**. Selected geometry parameters are shown in Å.

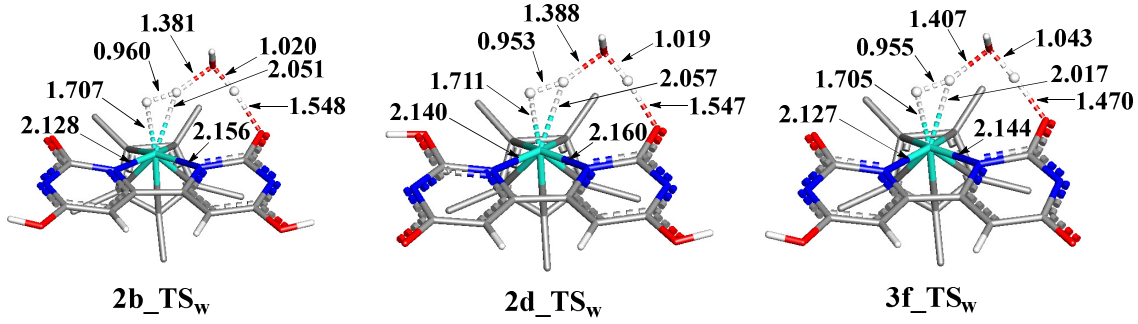


Fig. S26 Optimized geometries of the transition states for H_2 formation using H_2O as a proton shuttle: **2b_TS$_w$**, **2d_TS$_w$**, and **3f_TS$_w$**. Selected geometry parameters are shown in Å.

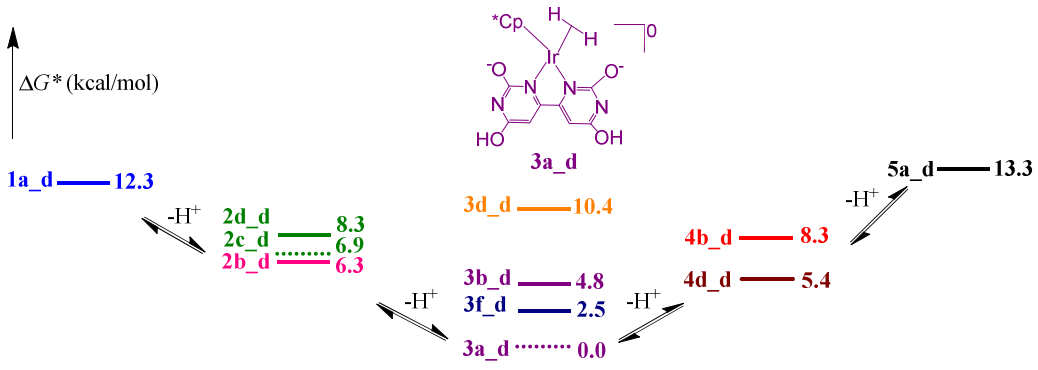


Fig. S27 Relative free energies of Ir-H_2 complexes (in kcal/mol) at pH 3.5.

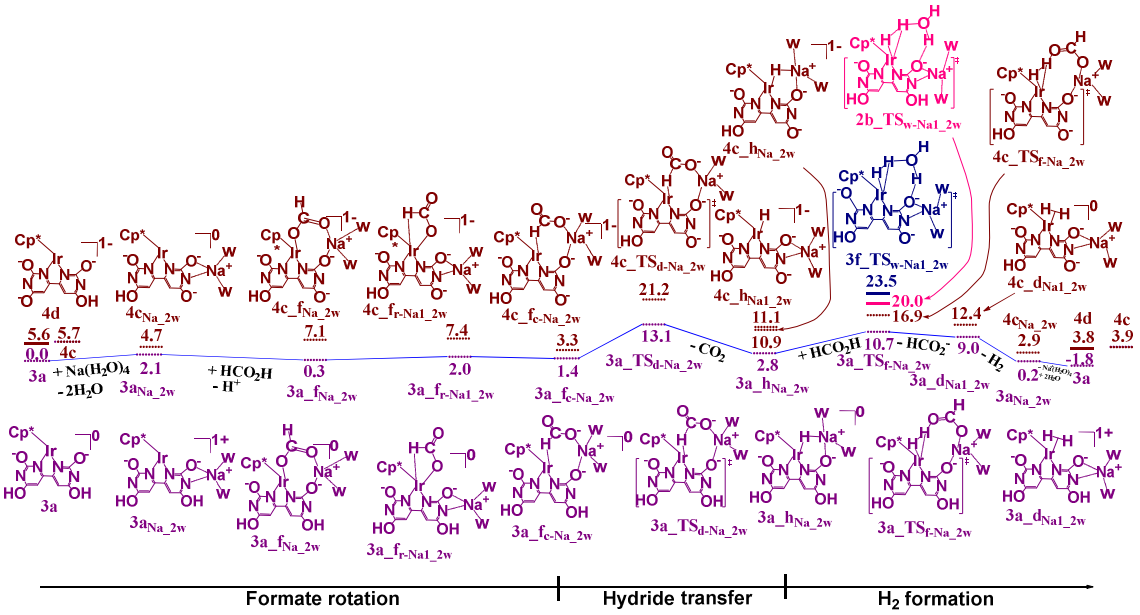


Fig. S28 Overall free energy profile (in kcal/mol) at pH 3.5 of Na^+ mediated formic acid dehydrogenation by complex **C**. A water molecule coordinated to Na^+ is labeled as w for clarity (w = H_2O).

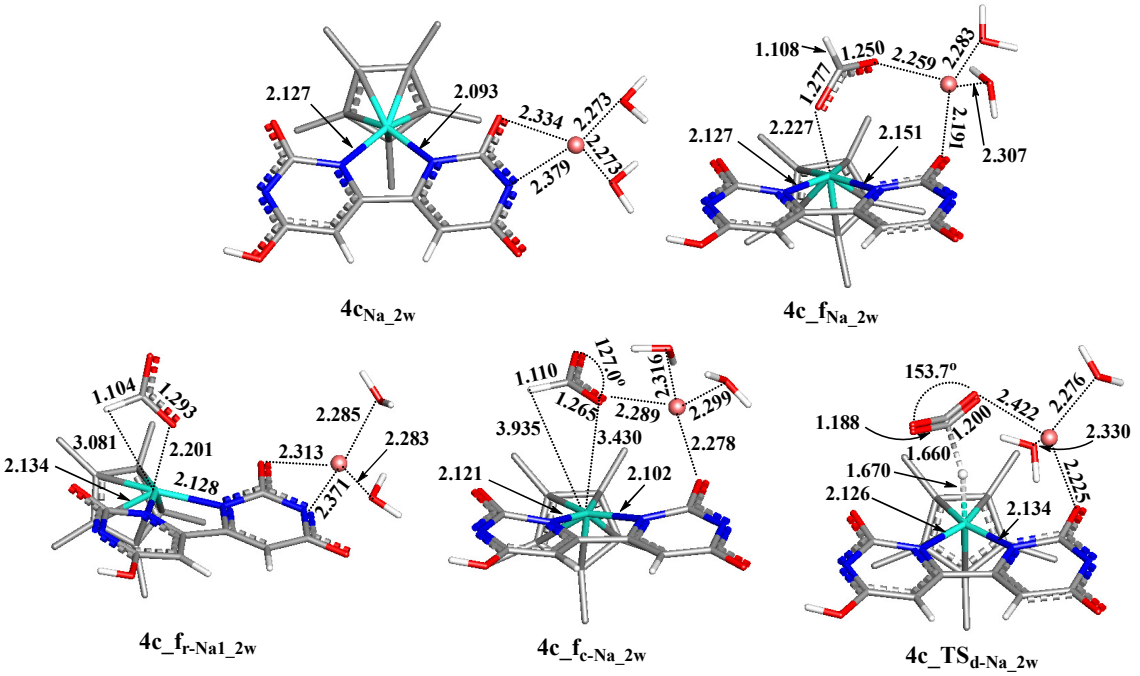


Fig. S29 Optimized geometries of intermediates and transition states for Na^+ mediated hydride transfer in formic acid dehydrogenation by complex **C**. Selected geometry parameters are shown in Å and °.

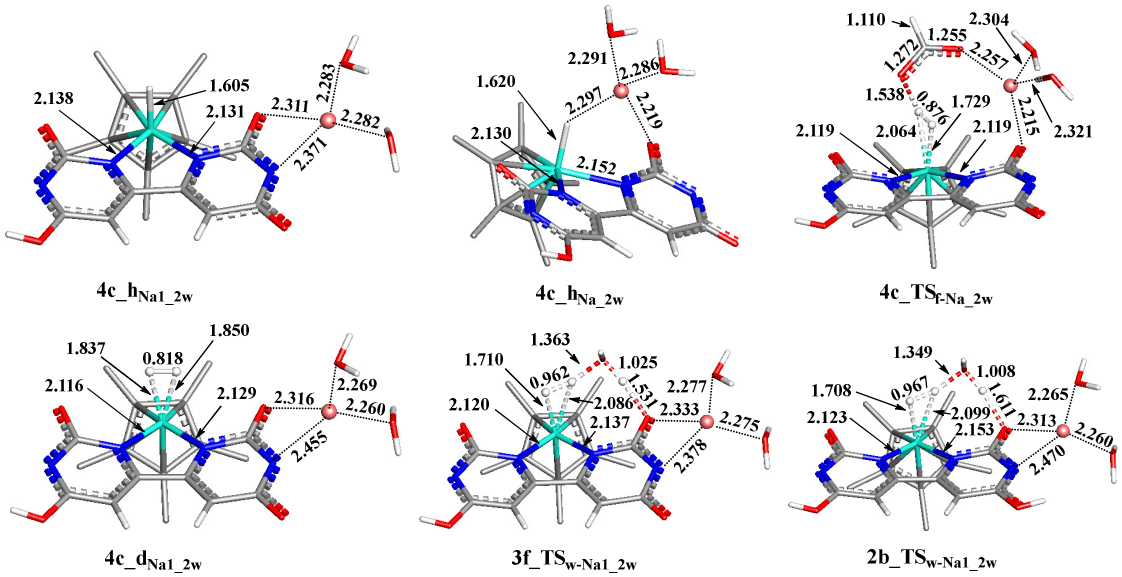


Fig. S30 Optimized geometries of intermediates and transition states for Na^+ mediated H_2 formation in formic acid dehydrogenation by complex **C**. Selected geometry parameters are shown in Å and °.

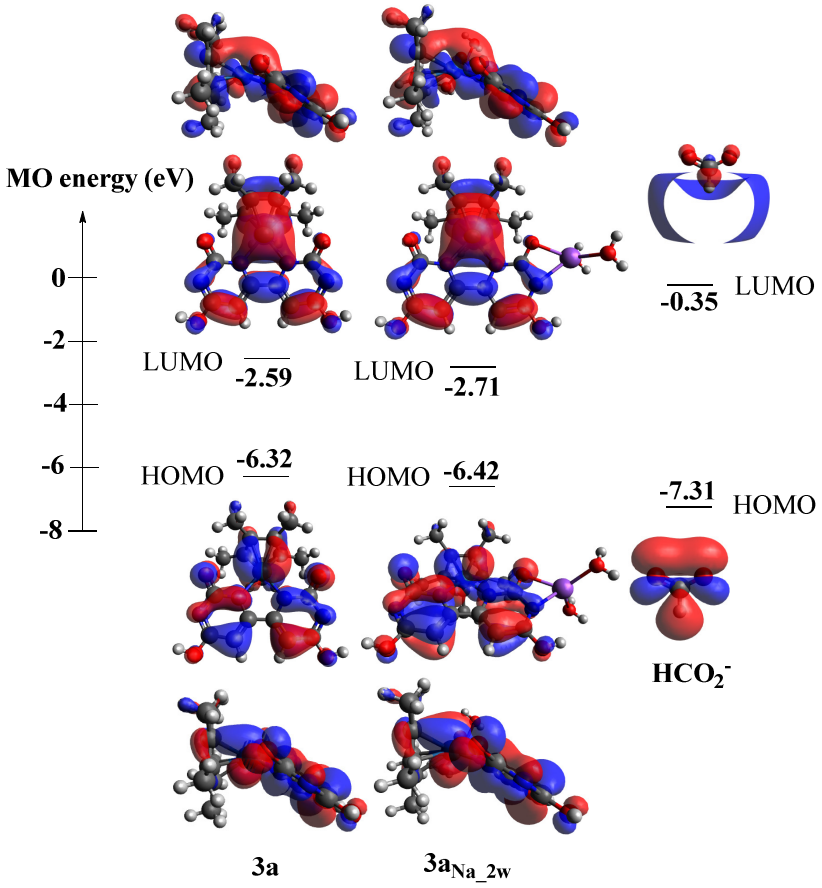


Fig. S31 Selected molecular orbitals (MOs) and MO energies of **3a**, **3a**$_{Na\_2w}$, and HCO_2^-.

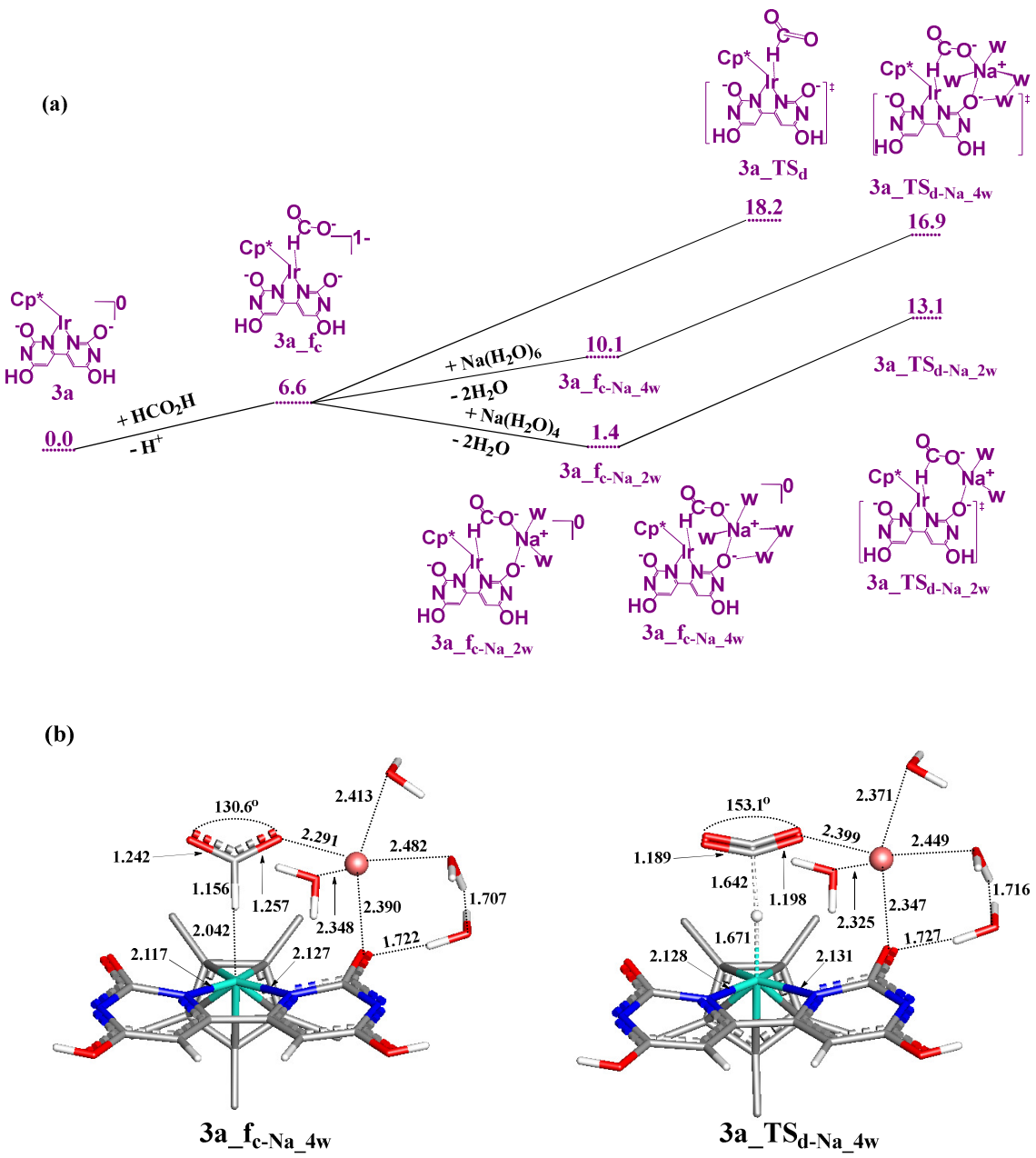


Fig. S32 (a) Free energy profile (in kcal/mol) at pH 3.5 of the hydride transfer via **3a_TS$_d$** and the Na^+ mediated hydride transfer via **3a_TS$_{d\text{-}Na_4w}$** and **3a_TS$_{d\text{-}Na_2w}$**. A water molecule coordinated to Na^+ is labeled as w for clarity (w = H_2O). (b) Optimized geometries of **3a_f$_{c\text{-}Na_4w}$** and **3a_TS$_{d\text{-}Na_4w}$**. Selected optimized geometry parameters are shown in Å and °.

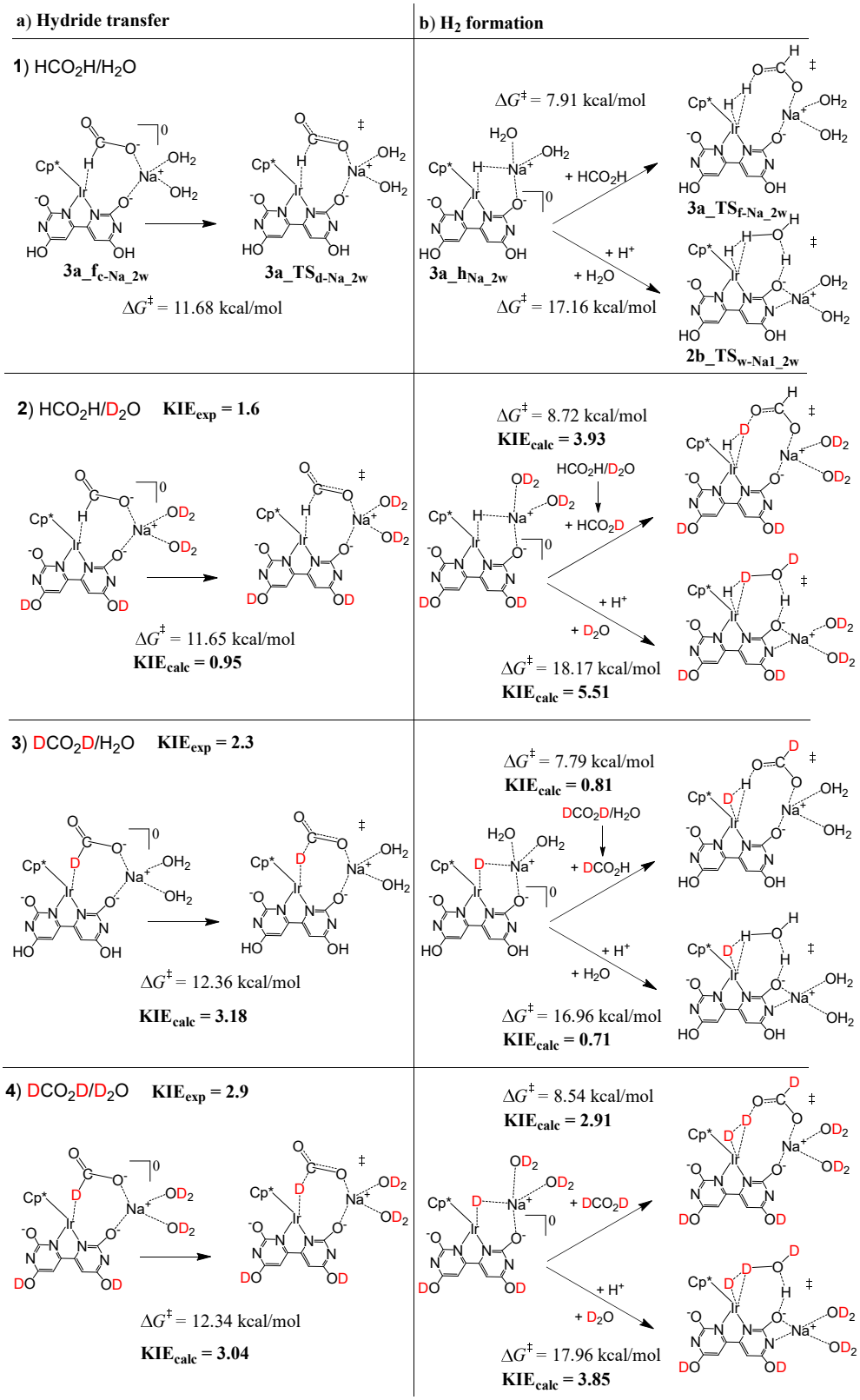


Fig. S33 Relative free energy ($\Delta G^{\neq}$) and kinetic isotope effects (KIE) in Na^+ mediated formic acid dehydrogenation at pH 3.5: (a) hydride transfer and (b) H_2 formation. KIE_{exp} was taken from reference [7]. KIE_{calc} was calculated from k_H/k_D i.e., $e^{(\Delta G^{\neq}(D)-\Delta G^{\neq}(H))/RT}$.

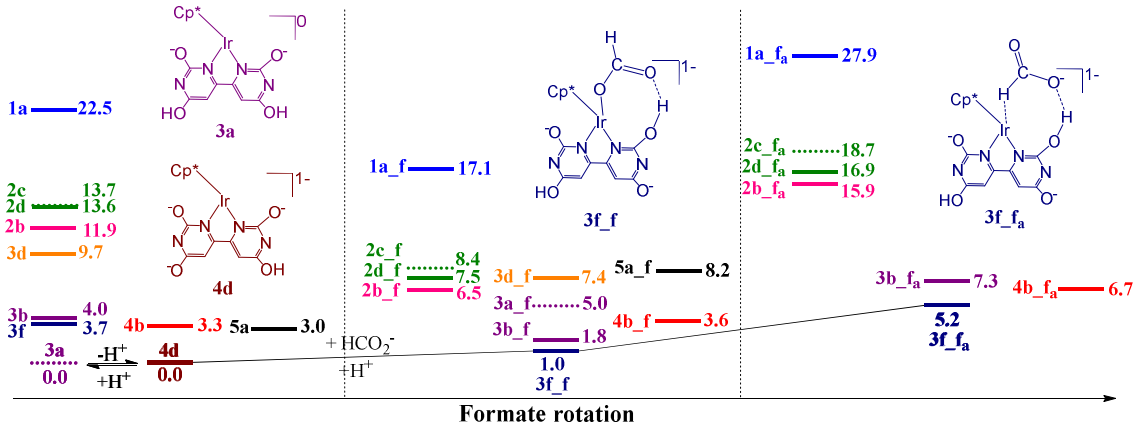


Fig. S34 Relative free energy profile (in kcal/mol) at pH 7.6 for the binding of HCO_2H to $[Ir(Cp^*)(bpymO_4H_2)]^{2-}$ **3a** to form O-bound Ir-$OCHO^H$ and H-bound Ir-HCO_2^H complexes.

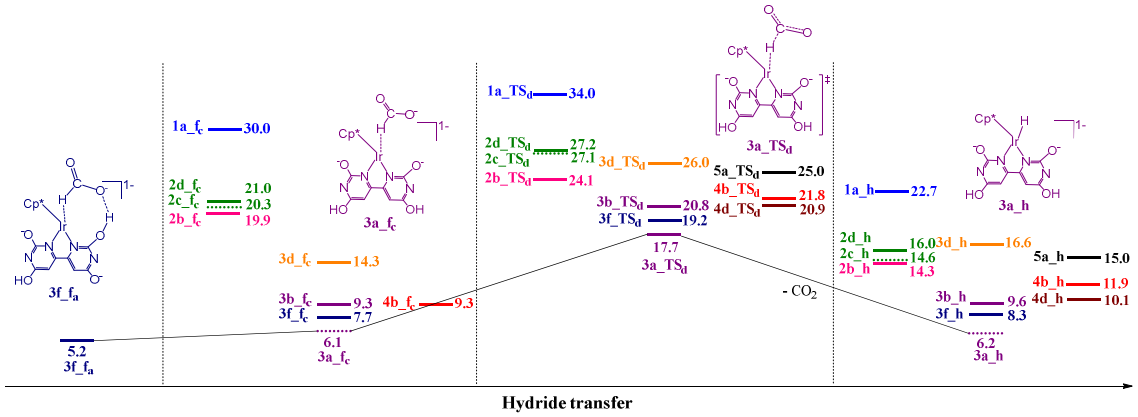


Fig. S35 Relative free energy profile (in kcal/mol) at pH 7.6 for direct hydride transfer.

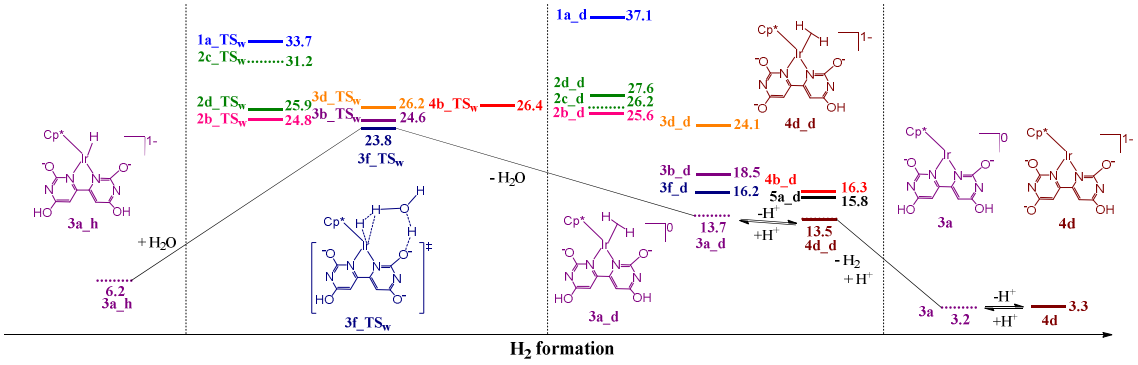


Fig. S36 Relative free energy profile (in kcal/mol) at pH 7.6 for H_2 formation *via* a water proton shuttle.

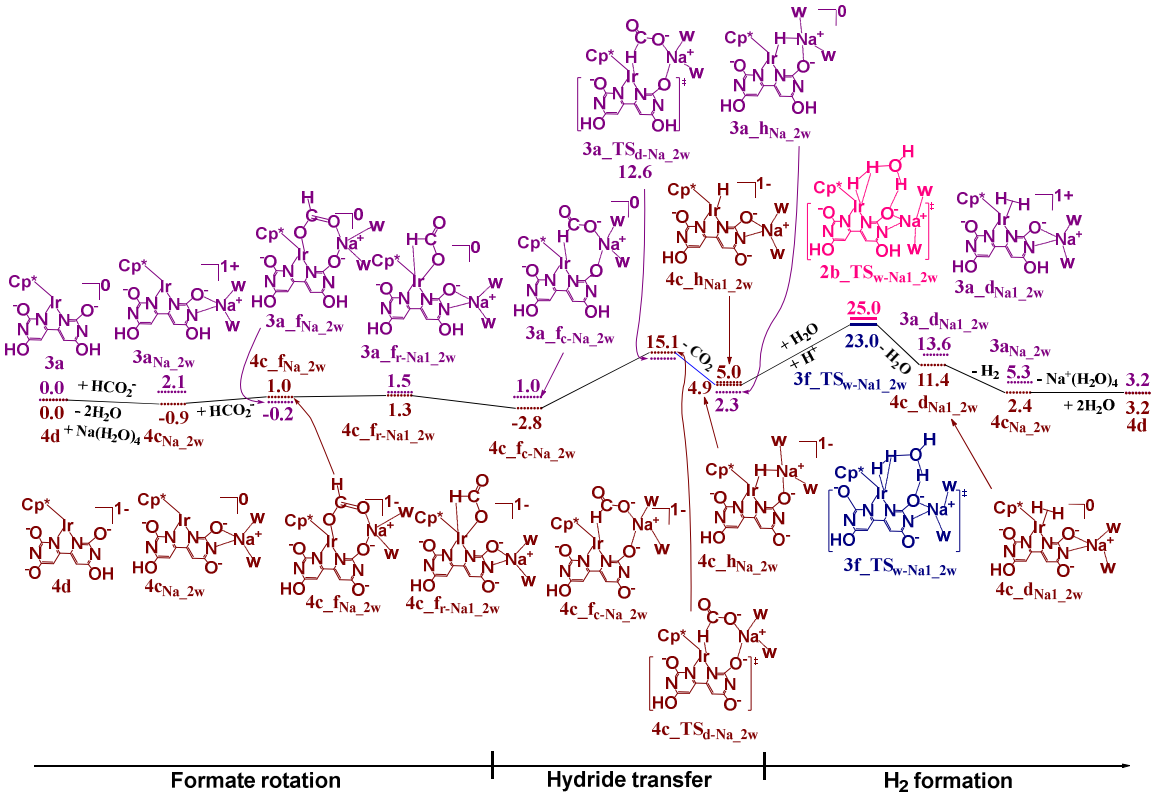


Fig. S37 Overall free energy profile (in kcal/mol) at pH 7.6 of Na^+ mediated formic acid dehydrogenation by complex **C**. A water molecule coordinated to Na^+ is labeled as w for clarity (w = H_2O).

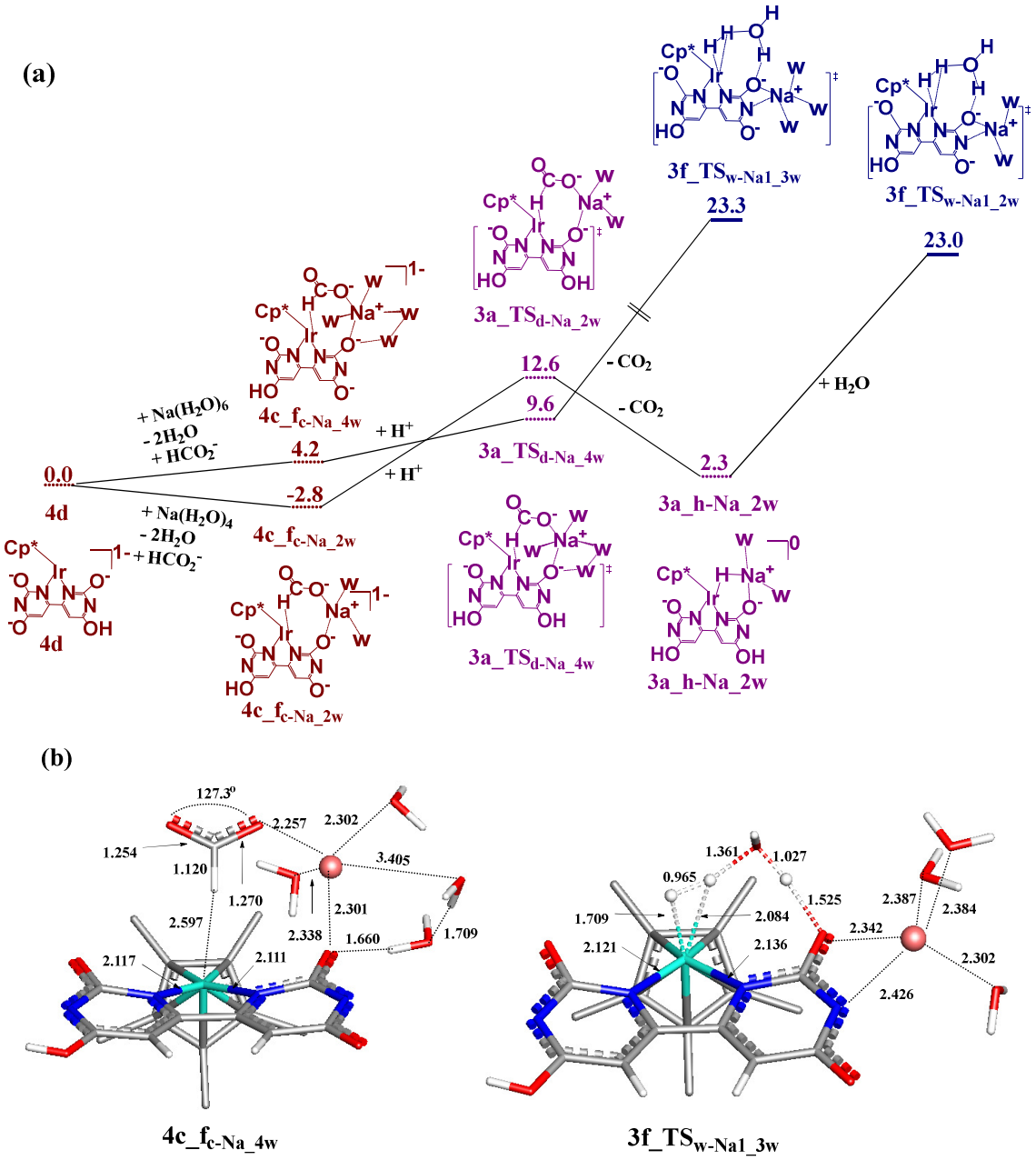


Fig. S38 (a) Free energy profile (in kcal/mol) at pH 7.6 of the Na^+ mediated H_2 formation via **3f_TS$_{w\text{-}Na1_2w}$** and **3f_TS$_{w\text{-}Na1_3w}$**. A water molecule coordinated to Na^+ is labeled as w for clarity (w = H_2O). (b) Optimized geometries of **4c_f$_{c\text{-}Na_4w}$** and **3f_TS$_{w\text{-}Na1_3w}$**. Selected optimized geometry parameters are shown in Å and °.

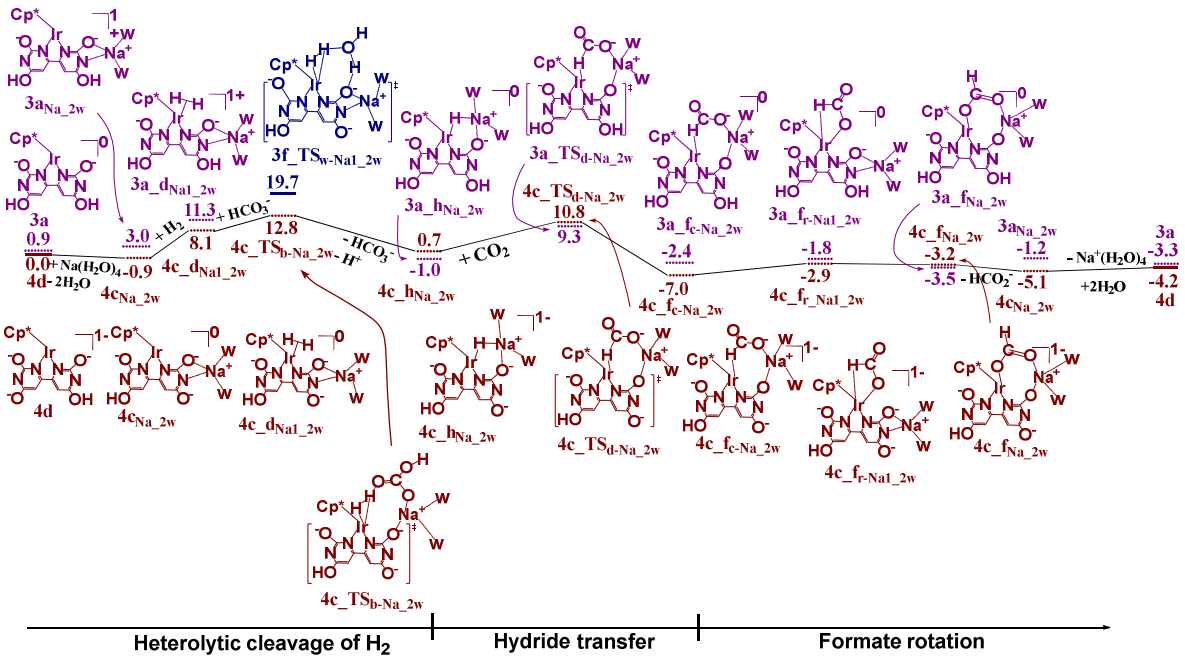


Fig. S39 Overall free energy profile (in kcal/mol) at pH 8.3 of Na^+ mediated CO_2 hydrogenation by complex **C**. A water molecule coordinated to Na^+ is labeled as w for clarity (w = H_2O).

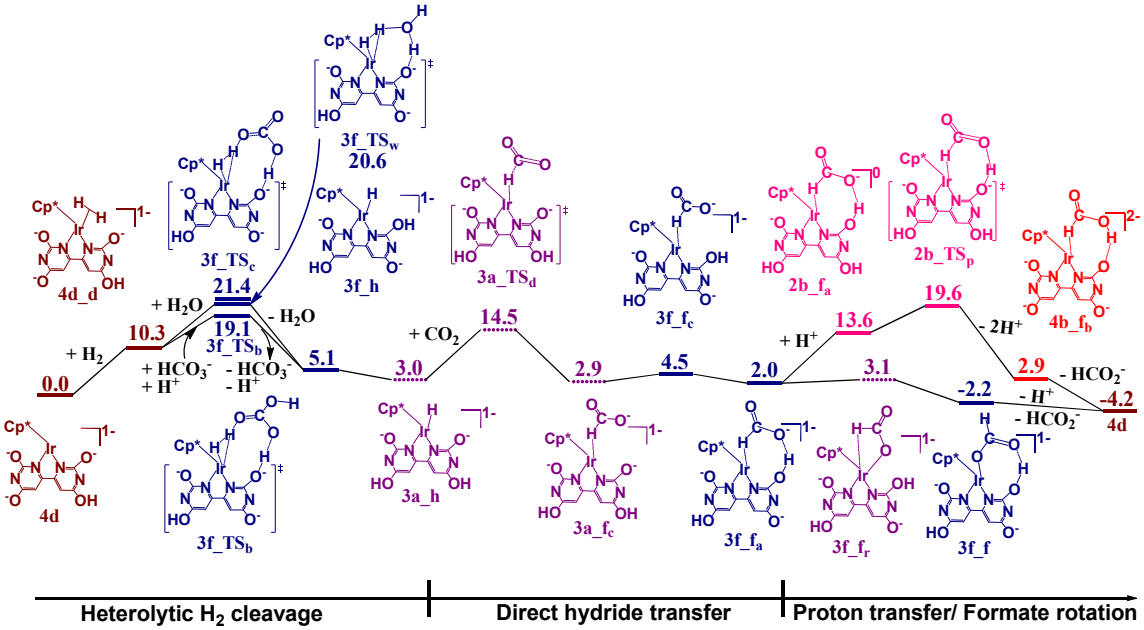


Fig. S40 Overall free energy profile (in kcal/mol) at pH 8.3 of CO_2 hydrogenation by complex **C**, in the absence of Na^+.

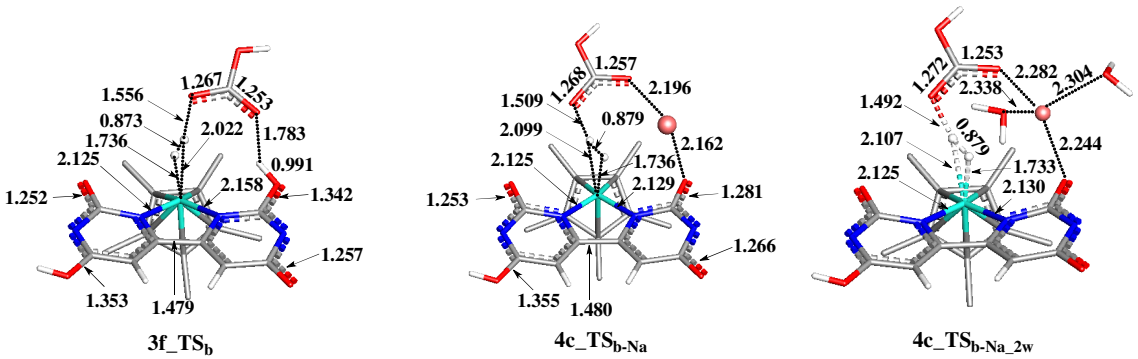


Fig. S41 Optimized geometries of transition states for H_2 heterolytic cleavage in CO_2 hydrogenation by complex **C**. Selected geometry parameters are shown in Å and °.

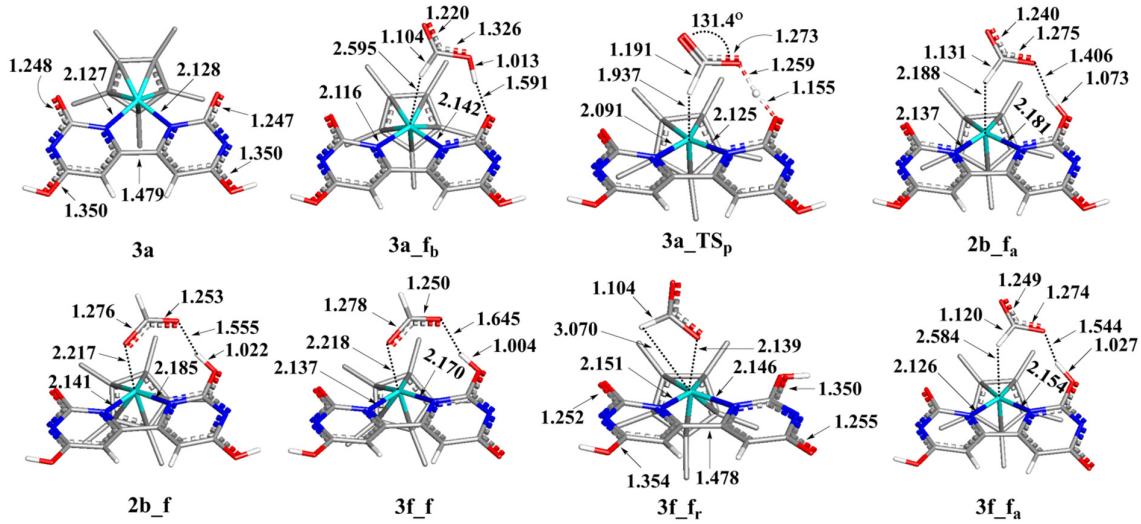


Fig. S42 Optimized geometries of the intermediates and transition states for the formation of Ir-HCO_2H, Ir-HCO_2^H, and Ir-$OCHO^H$ complexes. Selected geometry parameters are shown in Å.

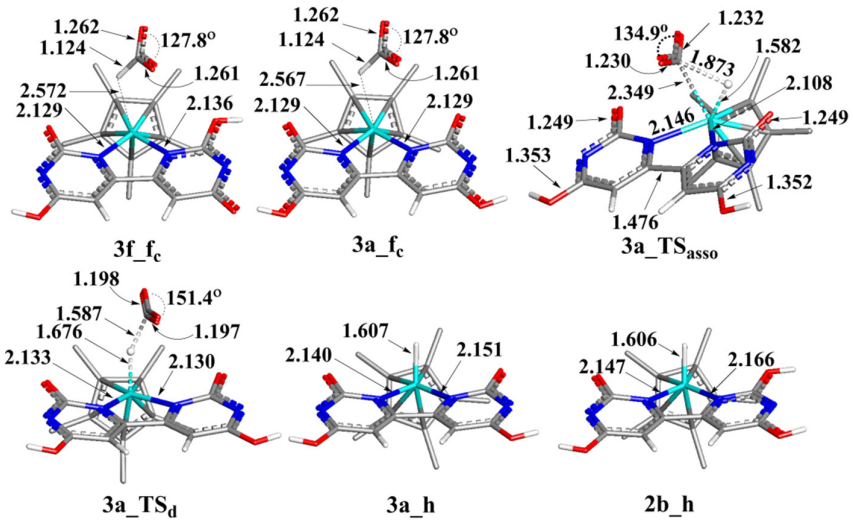


Fig. S43 Optimized geometries of intermediates and transition states for direct hydride transfer from HCO_2 to generate Ir-H complexes: **3f_f$_c$**, **3a_f$_c$**, **3a_TS$_{asso}$**, **3a_TS$_d$**, **3a_h**, and **2b_h**. Selected geometry parameters are given in Å and °.

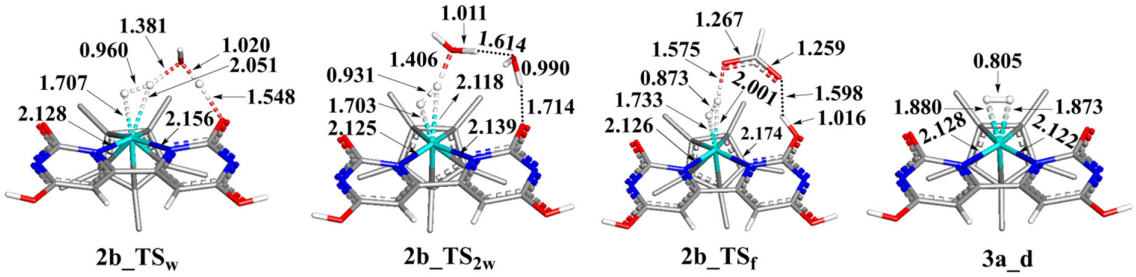


Fig. S44 Optimized geometries of intermediates and transition states in H_2 formation *via* a proton shuttle pathway: **2b_TS$_w$**, **2b_TS$_{2w}$**, **2b_TS$_f$**, and **3a_d.** Selected geometry parameters are shown in Å.

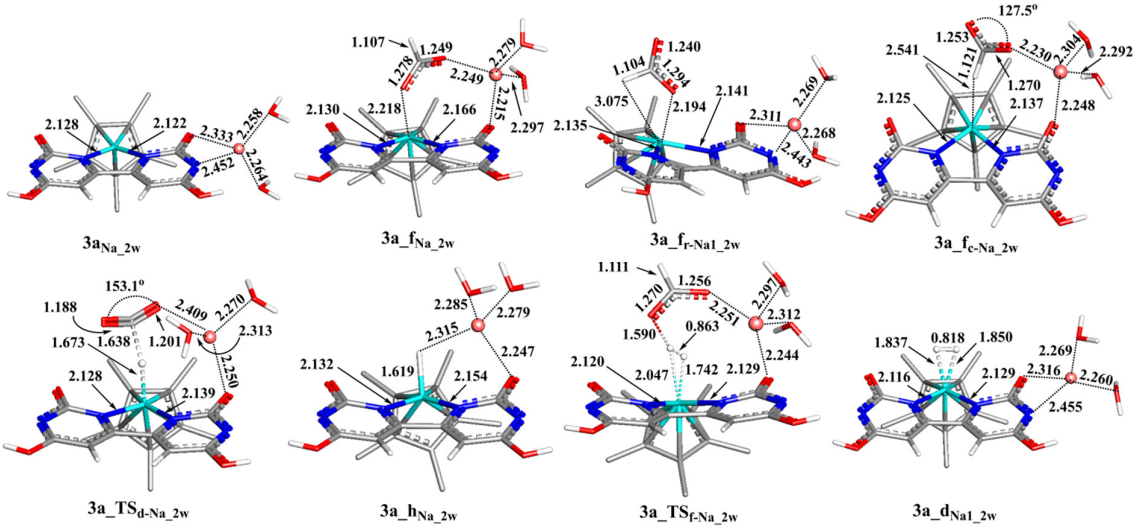


Fig. S45 Optimized geometries of intermediates and transition states for Na^+ mediated hydride transfer and H_2 formation. Selected geometry parameters are shown in Å and °.

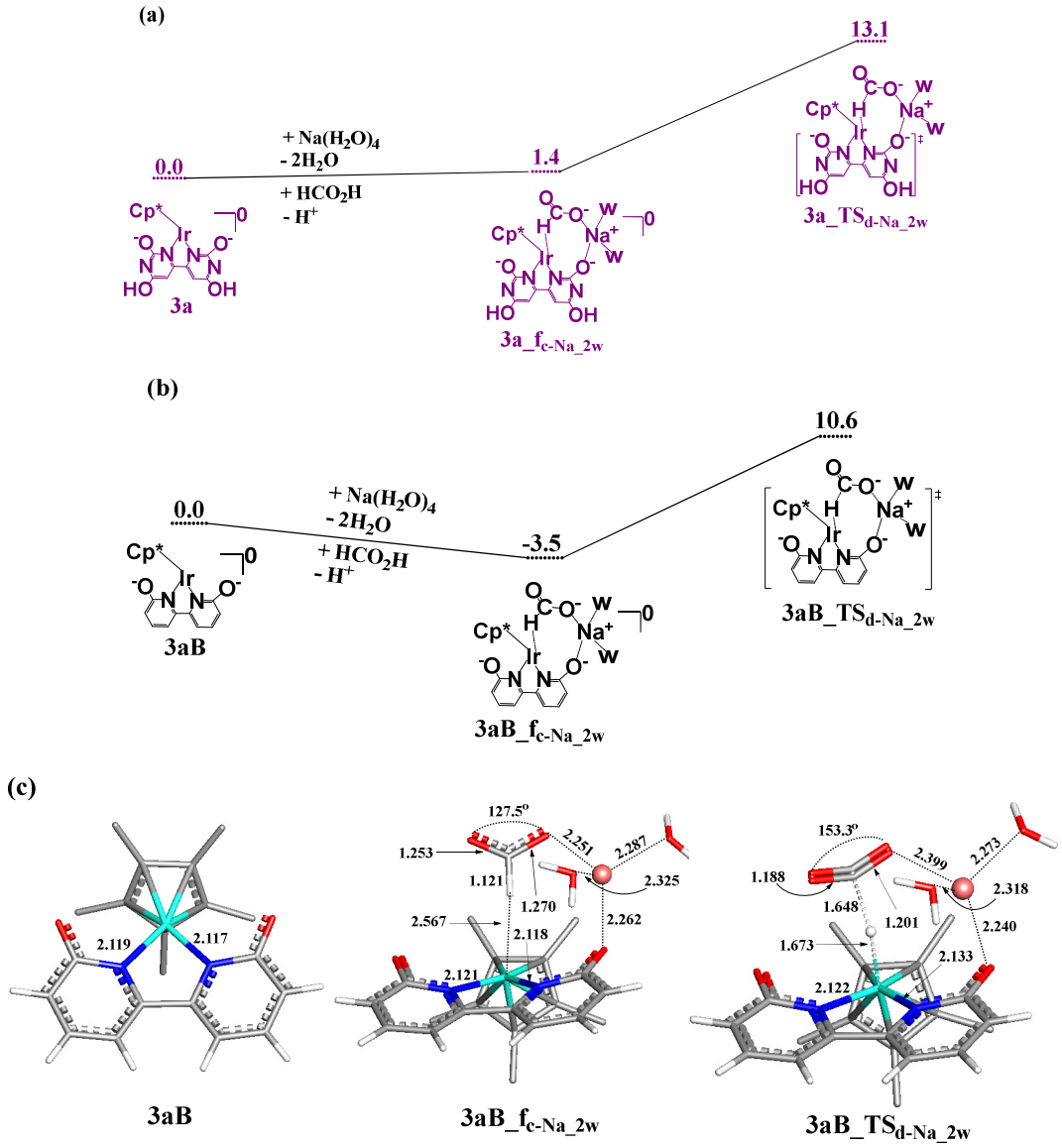


Fig. S46 (a) Free energy profile (in kcal/mol) at pH 3.5 of Na^+ mediated hydride transfer by complex **C**. (b) Free energy profile (in kcal/mol) at pH 3.5 of Na^+ mediated hydride transfer by complex **B**. A water molecule coordinated to Na^+ is labeled as w for clarity (w = H_2O). (c) Optimized geometries of **3aB**, **3aB_f$_{c\text{-}Na_2w}$**, and **3aB_TS$_{d\text{-}Na_2w}$**. Selected optimized geometry parameters are shown in Å.

Table S2 Relative free energies (in kcal/mol) of $[IrCp^*(H_2O)(bpymO_4H_n)]^{n-2}$ (n = 0, 1, 2, 3, and 4), and starting complexes $[IrCp^*(bpymO_4H_n)]^{n-2}$ (n = 3 and 4).[a]

complex	substrate	ΔG° 1atm	ΔG* 1 M [b]	ΔG* 1 M pH 3.5	ΔG* 1 M pH 7.6 [c]	ΔG* 1 M pH 8.3 [c]
1-H_2O	$2HCO_2H$	13.4	5.4	14.9	26.1	24.7
2a-H_2O	$H^+ + 2HCO_2H$	12.0	5.8	10.6	16.2	13.9
2b-H_2O	$H^+ + 2HCO_2H$	11.3	5.2	9.9	15.5	13.2
2c-H_2O	$H^+ + 2HCO_2H$	13.9	7.7	12.5	18.1	15.7
2d-H_2O	$H^+ + 2HCO_2H$	13.0	6.8	11.6	17.2	14.9
3a-H_2O	$2H^+ + 2HCO_2H$	10.1	5.8	5.8	5.8	2.5
3b-H_2O	$2H^+ + 2HCO_2H$	12.2	8.0	8.0	8.0	4.7
3c-H_2O	$2H^+ + 2HCO_2H$	19.7	15.4	15.4	15.4	12.1
3d-H_2O	$2H^+ + 2HCO_2H$	20.3	16.0	16.0	16.0	12.8
3e-H_2O	$2H^+ + 2HCO_2H$	10.9	6.7	6.7	6.7	3.4
3f-H_2O	$2H^+ + 2HCO_2H$	12.2	7.9	7.9	7.9	4.6
4a-H_2O	$3H^+ + 2HCO_2H$	20.9	18.5	13.8	8.2	4.0
4b-H_2O	$3H^+ + 2HCO_2H$	21.8	19.4	14.6	9.0	4.8
4c-H_2O	$3H^+ + 2HCO_2H$	19.4	17.0	12.2	6.6	2.4
4d-H_2O	$3H^+ + 2HCO_2H$	19.8	17.4	12.6	7.0	2.8
5a-H_2O	$4H^+ + 2HCO_2H$	32.1	31.7	22.1	10.9	5.8
1a	$H_2O + 2HCO_2H$	5.6	1.8	11.4	22.5	21.2
2a	$H^+ + H_2O + 2HCO_2H$	3.4	1.6	6.3	11.9	9.6
2b	$H^+ + H_2O + 2HCO_2H$	3.4	1.6	6.3	11.9	9.6
2c	$H^+ + H_2O + 2HCO_2H$	5.2	3.4	8.1	13.7	11.4
2d	$H^+ + H_2O + 2HCO_2H$	5.2	3.3	8.1	13.6	11.3

[a]Free energies are relative to **3a** in Table S3 at 1 atm, 1 M, pH 3.5 and pH 7.6, and relative to **4d** in Table S8 at pH 8.3. [b]For H_2O, its free energy is at 55.6 M (standard state). [c]At pH 7.6 and 8.3, the substrates HCO_2^- and H^+ were used for HCO_2H.

Table S3 Relative free energies (in kcal/mol) of starting complexes $[IrCp^*(bpymO_4H_n)]^{n-2}$ (n = 0, 1, and 2), and Ir-$OCHO^H$ complexes.[a]

complex	substrate	ΔG° 1atm	ΔG* 1 M [b]	ΔG* 1 M pH 3.5	ΔG* 1 M pH 7.6 [c]	ΔG* 1 M pH 8.3 [c]
3a	$2H^+ + H_2O + 2HCO_2H$	0.0	0.0	0.0	0.0	-3.3
3b	$2H^+ + H_2O + 2HCO_2H$	4.0	4.0	4.0	4.0	0.8
3c	$2H^+ + H_2O + 2HCO_2H$	9.9	9.9	9.9	9.9	6.7
3d	$2H^+ + H_2O + 2HCO_2H$	9.7	9.7	9.7	9.7	6.5
3e	$2H^+ + H_2O + 2HCO_2H$	3.7	3.7	3.7	3.7	0.4
3f	$2H^+ + H_2O + 2HCO_2H$	3.7	3.7	3.7	3.7	0.4
4a	$3H^+ + H_2O + 2HCO_2H$	11.7	13.6	8.8	3.3	-1.0
4b	$3H^+ + H_2O + 2HCO_2H$	11.8	13.7	8.9	3.3	-0.9
4c	$3H^+ + H_2O + 2HCO_2H$	8.6	10.5	5.7	0.1	-4.1
4d	$3H^+ + H_2O + 2HCO_2H$	8.5	10.4	5.6	0.0	-4.2
5a	$4H^+ + H_2O + 2HCO_2H$	19.9	23.7	14.2	3.0	-2.2
1a_f	$H_2O + H^+ + HCO_2H$	5.4	1.7	6.4	17.1	15.7
2b_f	$2H^+ + H_2O + HCO_2H$	3.3	1.4	1.4	6.5	4.2
2c_f	$2H^+ + H_2O + HCO_2H$	5.2	3.3	3.3	8.4	6.1
2d_f	$2H^+ + H_2O + HCO_2H$	4.3	2.4	2.4	7.5	5.2
3a_f	$3H^+ + H_2O + HCO_2H$	10.3	10.3	5.5	5.0	1.8
3b_f	$3H^+ + H_2O + HCO_2H$	7.1	7.1	2.4	1.9	-1.4
3d_f	$3H^+ + H_2O + HCO_2H$	12.7	12.7	7.9	7.4	4.2
3f_f	$3H^+ + H_2O + HCO_2H$	6.3	6.3	1.5	1.0	-2.2
4b_f	$4H^+ + H_2O + HCO_2H$	17.4	19.3	9.7	3.7	-0.6
5a_f	$5H^+ + H_2O + HCO_2H$	30.4	34.2	19.9	8.2	3.0
3a_f$_r$	$3H^+ + H_2O + HCO_2H$	10.4	10.4	5.6	5.1	1.9
3f_f$_r$	$3H^+ + H_2O + HCO_2H$	11.6	11.6	6.8	6.3	3.1

[a]Free energies are relative to **3a** at 1 atm, 1 M, pH 3.5 and pH 7.6, and relative to **4d** in Table S8 at pH 8.3. [b]For H_2O, its free energy is calculated at 55.6 M (standard state). [c]At pH 7.6 and 8.3, the substrates HCO_2^- and H^+ were used for HCO_2H.

Table S4 Relative free energies (in kcal/mol) of Ir-HCO_2^H complexes, transition states for proton transfer, and Ir-HCO_2H complexes.[a]

complex	substrate	ΔG° 1atm	ΔG* 1 M [b]	ΔG* 1 M pH 3.5	ΔG* 1 M pH 7.6 [c]	ΔG* 1 M pH 8.3 [c]
1a_f$_a$	$H_2O + H^+ + HCO_2H$	16.2	12.4	17.2	27.9	26.5
2b_f$_a$	$2H^+ + H_2O + HCO_2H$	12.7	10.8	10.8	15.9	13.6
2c_f$_a$	$2H^+ + H_2O + HCO_2H$	15.5	13.6	13.6	18.7	16.4
2d_f$_a$	$2H^+ + H_2O + HCO_2H$	13.7	11.8	11.8	16.9	14.6
3b_f$_a$	$3H^+ + H_2O + HCO_2H$	12.6	12.6	7.8	7.3	4.1
3f_f$_a$	$3H^+ + H_2O + HCO_2H$	10.5	10.5	5.7	5.2	2.0
4b_f$_a$	$4H^+ + H_2O + HCO_2H$	20.5	22.4	12.8	6.7	2.5
2a_TS$_p$	$H_2O + H^+ + HCO_2H$	22.0	18.2	23.0	33.7	32.3
3a_TS$_p$	$2H^+ + H_2O + HCO_2H$	18.7	16.8	16.8	21.9	19.6
3c_TS$_p$	$2H^+ + H_2O + HCO_2H$	19.8	18.0	18.0	23.0	20.7
3e_TS$_p$	$2H^+ + H_2O + HCO_2H$	19.5	17.6	17.6	22.7	20.4
2a_f$_b$	$H_2O + H^+ + HCO_2H$	6.4	2.6	7.4	18.0	16.7
3a_f$_b$	$2H^+ + H_2O + HCO_2H$	4.5	2.6	2.6	7.7	5.4
3c_f$_b$	$2H^+ + H_2O + HCO_2H$	13.1	11.2	11.2	16.3	13.9
3e_f$_b$	$2H^+ + H_2O + HCO_2H$	6.2	4.3	4.3	9.4	7.1
4a_f$_b$	$3H^+ + H_2O + HCO_2H$	14.0	14.0	9.2	8.8	5.5
4d_f$_b$	$3H^+ + H_2O + HCO_2H$	12.3	12.3	7.5	7.0	3.8
4c_f$_b$	$3H^+ + H_2O + HCO_2H$	12.4	12.4	7.7	7.2	3.9
5a_f$_b$	$4H^+ + H_2O + HCO_2H$	20.9	22.8	13.2	7.1	2.9

[a]Free energies are relative to **3a** in Table S3 at 1 atm, 1 M, pH 3.5 and pH 7.6, and relative to **4d** in Table S8 at pH 8.3. [b]For H_2O, its free energy is calculated at 55.6 M (standard state). [c]At pH 7.6 and 8.3, the substrates HCO_2^- and H^+ were used for HCO_2H.

Table S5 Relative free energies (in kcal/mol) of Ir-HCO_2 complexes and transition states for direct hydride transfer.[a]

complex	substrate	ΔG° 1atm	ΔG* 1 M [b]	ΔG* 1 M pH 3.5	ΔG* 1 M pH 7.6 [c]	ΔG* 1 M pH 8.3 [c]
1a_f$_c$	$H_2O + H^+ + HCO_2H$	18.4	14.6	19.4	30.1	28.7
2b_f$_c$	$2H^+ + H_2O + HCO_2H$	16.7	14.8	14.8	19.9	17.6
2c_f$_c$	$2H^+ + H_2O + HCO_2H$	17.1	15.2	15.2	20.3	18.0
2d_f$_c$	$2H^+ + H_2O + HCO_2H$	17.9	16.0	16.0	21.1	18.8
3a_f$_c$	$3H^+ + H_2O + HCO_2H$	11.4	11.4	6.6	6.1	2.9
3b_f$_c$	$3H^+ + H_2O + HCO_2H$	14.6	14.6	9.8	9.3	6.1
3d_f$_c$	$3H^+ + H_2O + HCO_2H$	19.6	19.6	14.8	14.3	11.0
3f_f$_c$	$3H^+ + H_2O + HCO_2H$	13.0	13.0	8.2	7.7	4.5
4b_f$_c$	$4H^+ + H_2O + HCO_2H$	23.0	24.9	15.4	9.3	5.1
1a_TS$_d$	$H_2O + H^+ + HCO_2H$	22.3	18.6	23.3	34.0	32.6
2b_TS$_d$	$2H^+ + H_2O + HCO_2H$	20.9	19.0	19.0	24.1	21.8
2c_TS$_d$	$2H^+ + H_2O + HCO_2H$	23.9	22.0	22.0	27.1	24.8
2d_TS$_d$	$2H^+ + H_2O + HCO_2H$	24.0	22.2	22.2	27.2	24.9

[a]Free energies are relative to **3a** in Table S3 at 1 atm, 1 M, pH 3.5 and pH 7.6, and relative to **4d** in Table S8 at pH 8.3. [b]For H_2O, its free energy is calculated at 55.6 M (standard state). [c]At pH 7.6 and 8.3, the substrates HCO_2^- and H^+ were used for HCO_2H.

Table S6 Relative free energies (in kcal/mol) of transition states for direct hydride transfer (cont.), associative transition state, and Ir-H complexes.[a]

complex	substrate	ΔG° 1atm	ΔG* 1 M [b]	ΔG* 1 M pH 3.5	ΔG* 1 M pH 7.6 [c]	ΔG* 1 M pH 8.3 [c]
3a_TS$_d$	$3H^+ + H_2O + HCO_2H$	23.0	23.0	18.2	17.7	14.5
3b_TS$_d$	$3H^+ + H_2O + HCO_2H$	26.1	26.1	21.4	20.9	17.6
3d_TS$_d$	$3H^+ + H_2O + HCO_2H$	31.3	31.3	26.5	26.0	22.8
3f_TS$_d$	$3H^+ + H_2O + HCO_2H$	24.5	24.5	19.7	19.2	16.0
4b_TS$_d$	$4H^+ + H_2O + HCO_2H$	35.5	37.4	27.8	21.8	17.5
4d_TS$_d$	$4H^+ + H_2O + HCO_2H$	34.6	36.5	27.0	20.9	16.7
5a_TS$_d$	$5H^+ + H_2O + HCO_2H$	47.2	51.0	36.7	25.0	19.8
3a_TS$_{asso}$	$3H^+ + H_2O + HCO_2H$	32.4	32.4	27.6	27.1	22.9
1a_h	$H_2O + H^+ + HCO_2H + CO_2$	9.1	7.2	12.0	22.7	21.3
2b_h	$2H^+ + H_2O + HCO_2H + CO_2$	9.2	9.2	9.2	14.3	12.0
2c_h	$2H^+ + H_2O + HCO_2H + CO_2$	9.5	9.5	9.5	14.6	12.3
2d_h	$2H^+ + H_2O + HCO_2H + CO_2$	10.9	10.9	10.9	16.0	13.7
3a_h	$3H^+ + H_2O + HCO_2H + CO_2$	9.6	11.5	6.7	6.2	3.0
3b_h	$3H^+ + H_2O + HCO_2H + CO_2$	13.0	14.8	10.1	9.6	6.3
3d_h	$3H^+ + H_2O + HCO_2H + CO_2$	19.9	21.8	17.1	16.6	13.3
3f_h	$3H^+ + H_2O + HCO_2H + CO_2$	11.7	13.6	8.8	8.3	5.1
4b_h	$4H^+ + H_2O + HCO_2H + CO_2$	23.7	27.5	18.0	11.9	7.7
4d_h	$4H^+ + H_2O + HCO_2H + CO_2$	21.9	25.7	16.1	10.0	5.8
5a_h	$5H^+ + H_2O + HCO_2H + CO_2$	35.3	41.0	26.7	15.0	9.9

[a]Free energies are relative to **3a** in Table S3 at 1 atm, 1 M, pH 3.5 and pH 7.6, and relative to **4d** in Table S8 at pH 8.3. [b]For H_2O, its free energy is calculated at 55.6 M (standard state). [c]At pH 7.6 and 8.3, the substrates HCO_2^- and H^+ were used for HCO_2H.

Table S7 Relative free energies (in kcal/mol) of transition states for H_2 formation with HCO_2H or H_2O as a proton shuttle, and Ir-H_2 complexes.[a]

complex	substrate	ΔG° 1atm	ΔG* 1 M [b]	ΔG* 1 M pH 3.5	ΔG* 1 M pH 7.6 [c]	ΔG* 1 M pH 8.3 [c]
1a_TS$_f$	$H_2O + H^+ + CO_2$	21.0	17.3	22.0	37.8	37.4
2b_TS$_f$	$2H^+ + H_2O + CO_2$	18.8	16.9	16.9	27.0	25.7
2c_TS$_f$	$2H^+ + H_2O + CO_2$	21.8	20.0	20.0	30.1	28.8
2d_TS$_f$	$2H^+ + H_2O + CO_2$	20.8	18.9	18.9	29.0	27.7
3b_TS$_f$	$3H^+ + H_2O + CO_2$	24.2	24.2	19.5	24.0	21.7
3d_TS$_f$	$3H^+ + H_2O + CO_2$	28.8	28.8	24.0	28.6	26.3
3f_TS$_f$	$3H^+ + H_2O + CO_2$	23.3	23.3	18.6	23.2	20.8
4b_TS$_f$	$4H^+ + H_2O + CO_2$	33.1	34.9	25.4	24.4	21.2
1a_TS$_w$	$H^+ + HCO_2H + CO_2$	24.5	18.3	23.1	33.8	32.4
2b_TS$_w$	$2H^+ + HCO_2H + CO_2$	24.0	19.8	19.8	24.9	22.6
2c_TS$_w$	$2H^+ + HCO_2H + CO_2$	30.5	26.2	26.2	31.3	29.0
2d_TS$_w$	$2H^+ + HCO_2H + CO_2$	25.2	20.9	20.9	26.0	23.7
3b_TS$_w$	$3H^+ + HCO_2H + CO_2$	32.3	29.9	25.1	24.6	21.4
3d_TS$_w$	$3H^+ + HCO_2H + CO_2$	33.9	31.5	26.7	26.2	23.0
3f_TS$_w$	$3H^+ + HCO_2H + CO_2$	31.5	29.1	24.3	23.8	20.6
4b_TS$_w$	$4H^+ + HCO_2H + CO_2$	42.5	42.0	32.5	26.4	22.2
1a_d	$H_2O + HCO_2H + CO_2$	15.1	11.3	20.9	37.1	36.7
2b_d	$H_2O + H^+ + HCO_2H + CO_2$	12.0	10.1	14.9	25.6	24.2
2c_d	$H_2O + H^+ + HCO_2H + CO_2$	12.6	10.7	15.5	26.1	24.8
2d_d	$H_2O + H^+ + HCO_2H + CO_2$	14.0	12.1	16.9	27.6	26.2
3a_d	$2H^+ + H_2O + HCO_2H + CO_2$	8.6	8.6	8.6	13.7	11.4
3b_d	$2H^+ + H_2O + HCO_2H + CO_2$	13.4	13.4	13.4	18.5	16.2
3d_d	$2H^+ + H_2O + HCO_2H + CO_2$	19.0	19.0	19.0	24.1	21.8
3f_d	$2H^+ + H_2O + HCO_2H + CO_2$	11.1	11.1	11.1	16.2	13.9
4b_d	$3H^+ + H_2O + HCO_2H + CO_2$	19.7	21.6	16.9	16.4	13.1
4d_d	$3H^+ + H_2O + HCO_2H + CO_2$	16.9	18.8	14.0	13.5	10.3
5a_d	$4H^+ + H_2O + HCO_2H + CO_2$	27.7	31.4	21.9	15.8	11.6

[a]Free energies are relative to **3a** in Table S3 at 1 atm, 1 M, pH 3.5 and pH 7.6, and relative to **4d** in Table S8 at pH 8.3. [b]For H_2O, its free energy is calculated at 55.6 M (standard state). [c]At pH 7.6 and 8.3, the substrates HCO_2^- and H^+ were used for HCO_2H.

Table S8 Relative free energies (in kcal/mol) of regeneration of complexes $[IrCp^*(bpymO_4H_n)]^{n-2}$ (n = 0, 1, 2, 3 and 4) in HCO_2H dehydrogenation to produce CO_2 and H_2.[a]

complex	substrate	ΔG° 1atm	ΔG* 1 M [b]	ΔG* 1 M pH 3.5	ΔG* 1 M pH 7.6 [c]	ΔG* 1 M pH 8.3 [c]
1a	$H_2O + HCO_2H + CO_2 + H_2$	1.9	0.0	9.5	25.8	25.4
2a	$H_2O + H^+ + HCO_2H + CO_2 + H_2$	-0.3	-0.3	4.5	15.2	13.8
2b	$H_2O + H^+ + HCO_2H + CO_2 + H_2$	-0.3	-0.3	4.5	15.1	13.8
2c	$H_2O + H^+ + HCO_2H + CO_2 + H_2$	1.5	1.5	6.3	17.0	15.6
2d	$H_2O + H^+ + HCO_2H + CO_2 + H_2$	1.4	1.4	6.2	16.9	15.5
3a	$2H^+ + H_2O + HCO_2H + CO_2 + H_2$	-3.7	-1.8	-1.8	3.2	0.9
3b	$2H^+ + H_2O + HCO_2H + CO_2 + H_2$	0.3	2.2	2.2	7.3	5.0
3c	$2H^+ + H_2O + HCO_2H + CO_2 + H_2$	6.2	8.1	8.1	13.2	10.9
3d	$2H^+ + H_2O + HCO_2H + CO_2 + H_2$	6.0	7.9	7.9	13.0	10.6
3e	$2H^+ + H_2O + HCO_2H + CO_2 + H_2$	0.0	1.9	1.9	6.9	4.6
3f	$2H^+ + H_2O + HCO_2H + CO_2 + H_2$	0.0	1.9	1.9	6.9	4.6
4a	$3H^+ + H_2O + HCO_2H + CO_2 + H_2$	8.0	11.8	7.0	6.5	3.2
4b	$3H^+ + H_2O + HCO_2H + CO_2 + H_2$	8.0	11.8	7.0	6.6	3.3
4c	$3H^+ + H_2O + HCO_2H + CO_2 + H_2$	4.8	8.6	3.8	3.3	0.1
4d	$3H^+ + H_2O + HCO_2H + CO_2 + H_2$	4.7	8.5	3.8	3.3	0.0
5a	$4H^+ + H_2O + HCO_2H + CO_2 + H_2$	16.2	21.9	12.3	6.2	2.0

[a]Free energies are relative to **3a** in Table S3 at 1 atm, 1 M, pH 3.5 and pH 7.6, and relative to **4d** at pH 8.3. [b]For H_2O, its free energy is calculated at 55.6 M (standard state). [c]At pH 7.6 and 8.3, the substrates HCO_2^- and H^+ were used for HCO_2H.

Table S9 Relative free energies (in kcal/mol) of intermediates and transition states with starting $Na^+(H_2O)_4$ substrate in the formate rotation and hydride transfer pathways.[a]

complex	substrate	ΔG° 1 atm	ΔG* 1 M [b]	ΔG* 1 M pH 3.5	ΔG* 1 M pH 7.6 [c]	ΔG* 1 M pH 8.3 [c]
3a	$2HCO_2H + Na(H_2O)_4 + HCO_3^-$	0.0	0.0	0.0	0.0	-3.3
4c	$2HCO_2H + Na(H_2O)_4 + HCO_3^- + H^+$	8.6	10.5	5.7	0.1	-4.1
4d	$2HCO_2H + Na(H_2O)_4 + HCO_3^- + H^+$	8.5	10.4	5.6	0.0	-4.2
3a$_{Na_2w}$	$2HCO_2H + 2H_2O + HCO_3^-$	-4.6	2.1	2.1	2.1	-1.2
4c$_{Na_2w}$	$2HCO_2H + H^+ + 2H_2O + HCO_3^-$	1.0	9.5	4.7	-0.9	-5.1
3a_f$_{Na_2w}$	$HCO_2H + H^+ + 2H_2O + HCO_3^-$	-1.6	5.1	0.3	-0.2	-3.5
4c_f$_{Na_2w}$	$HCO_2H + 2H^+ + 2H_2O + HCO_3^-$	8.1	16.7	7.1	1.0	-3.2
3a_f$_{r_Na1_2w}$	$HCO_2H + H^+ + 2H_2O + HCO_3^-$	0.1	6.7	2.0	1.3	-1.8
4c_f$_{r_Na1_2w}$	$HCO_2H + 2H^+ + 2H_2O + HCO_3^-$	8.4	16.9	7.4	1.5	-2.9
3a_f$_{c\text{-}Na_2w}$	$HCO_2H + H^+ + 2H_2O + HCO_3^-$	-0.4	6.2	1.4	1.0	-2.4
4c-f$_{c\text{-}Na_2w}$	$HCO_2H + 2H^+ + 2H_2O + HCO_3^-$	4.3	12.8	3.3	-2.8	-7.0
3a_TS$_{d\text{-}Na_2w}$	$HCO_2H + H^+ + 2H_2O + HCO_3^-$	11.2	17.9	13.1	15.1	9.3
4c_TS$_{d\text{-}Na_2w}$	$HCO_2H + 2H^+ + 2H_2O + HCO_3^-$	22.2	30.7	21.2	12.6	10.8
3a_h$_{Na_2w}$	$HCO_2H + H^+ + CO_2 + 2H_2O + HCO_3^-$	-1.0	7.6	2.8	2.3	-1.0
3a_h$_{Na1_2w}$	$HCO_2H + H^+ + CO_2 + 2H_2O + HCO_3^-$	2.3	10.9	6.1	5.6	7.4
4c_h$_{Na_2w}$	$HCO_2H + 2H^+ + CO_2 + 2H_2O + HCO_3^-$	10.0	20.5	10.9	4.9	0.6
4c_h$_{Na1_2w}$	$HCO_2H + 2H^+ + CO_2 + 2H_2O + HCO_3^-$	10.2	20.6	11.1	5.0	0.7

[a]Free energies are relative to **3a** at 1 atm, 1 M, pH 3.5 and pH 7.6, and relative to **4d** in Table S10 at pH 8.3. [b]For H_2O, its free energy is calculated at 55.6 M (standard state). [c]At pH 7.6 and 8.3, the substrates HCO_2^- and H^+ were used for HCO_2H.

Table S10 Relative free energies (in kcal/mol) of intermediates and transition states with starting $Na^+(H_2O)_4$ substrate in the H_2 formation pathway for pH 3.5 and pH 7.6 and heterolytic cleavage of H_2 for pH 8.3.[a]

complex	Substrate	ΔG° 1 atm	ΔG* 1 M [b]	ΔG* 1 M pH 3.5	ΔG* 1 M pH 7.6 [c]	ΔG* 1 M pH 8.3 [c]
2b_TS$_{w_Na1_2w}$	$HCO_2H + CO_2 + H_2O + HCO_3^-$	17.6	20.0	20.0	25.0	22.7
3f_TS$_{w_Na1_2w}$	$HCO_2H + H^+ + CO_2 + H_2O + HCO_3^-$	24.0	28.3	23.5	23.0	19.7
3a_TS$_{f_Na_2w}$	$H^+ + CO_2 + 2H_2O + HCO_3^-$	8.8	15.5	10.7	15.3	17.1
4c_TS$_{f_Na_2w}$	$2H^+ + CO_2 + 2H_2O + HCO_3^-$	17.9	26.4	16.9	15.9	16.8
4c_TS$_{b\text{-}Na_2w}$	$HCO_2H + H^+ + CO_2 + 2H_2O$	11.3	16.1	16.6	16.1	12.8
3a_d$_{Na1_2w}$	$H^+ + CO_2 + 2H_2O + HCO_3^- + HCO_2^-$	5.2	13.8	9.0	13.6	11.3
4c_d$_{Na1_2w}$	$2H^+ + CO_2 + 2H_2O + HCO_3^- + HCO_2^-$	11.5	21.9	12.4	11.4	8.1
3a$_{Na_2w}$	$CO_2 + 2H_2O + HCO_3^- + HCO_2H + H_2$	-8.3	0.2	0.2	5.3	3.0
4c$_{Na_2w}$	$H^+ + CO_2 + 2H_2O + HCO_3^- + HCO_2H + H_2$	-2.8	7.7	2.9	2.4	-0.9
3a	$CO_2 + HCO_3^- + HCO_2H + H_2 + Na(H_2O)_4$	-3.7	-1.8	-1.8	3.2	0.9
4c	$H^+ + CO_2 + HCO_3^- + HCO_2H + H_2 + Na(H_2O)_4$	4.8	8.6	3.9	3.3	0.1
4d	$H^+ + CO_2 + HCO_3^- + HCO_2H + H_2 + Na(H_2O)_4$	4.7	8.5	3.8	3.2	0.0

[a]Free energies are relative to **3a** in Table S9 at 1 atm, 1 M, pH 3.5 and pH 7.6, and relative to **4d** at pH 8.3. [b]For H_2O, its free energy is calculated at 55.6 M (standard state). [c]At pH 7.6 and 8.3, the substrates HCO_2^- and H^+ were used for HCO_2H.

Table S11. APT charge and Mulliken charge population of **3a_f$_c$**, **3a_f$_{c\text{-}Na_2w}$** and **3aB_f$_{c\text{-}Na_2w}$**.

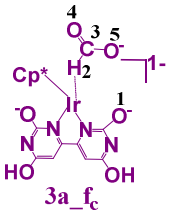
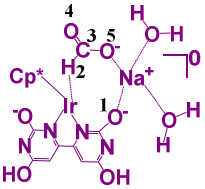
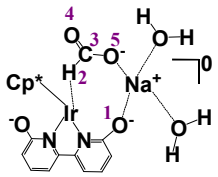
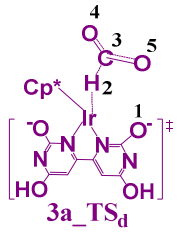
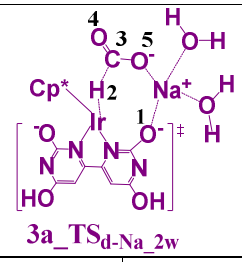
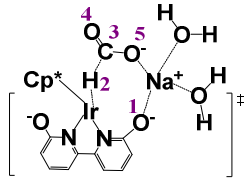
Atom	 3a_f$_c$		 3a_f$_{c\text{-}Na_2w}$		 3aB_f$_{c\text{-}Na_2w}$	
	APT charge	**Mulliken charge**	**APT charge**	**Mulliken charge**	**APT charge**	**Mulliken charge**
O1	-1.27	-0.60	-1.36	-0.58	-1.37	-0.62
Ir	0.75	0.32	0.79	0.46	0.72	0.43
H2	0.11	0.15	-0.24	0.05	-0.22	0.03
C3	1.74	0.39	1.83	0.41	1.78	0.43
O4	-1.33	-0.64	-1.30	-0.60	-1.24	-0.62
O5	-1.24	-0.63	-1.33	-0.57	-1.32	-0.58
Na$^+$	-	-	0.92	0.32	0.92	0.33

Table S12. APT charge and Mulliken charge population of **3a_TS$_d$**, **3a_TS$_{d\text{-}Na_2w}$** and **3aB_TS$_{d\text{-}Na_2w}$**.

Atom	 3a_TS$_d$		 3a_TS$_{d\text{-}Na_2w}$		 3aB_TS$_{d\text{-}Na_2w}$	
	APT charge	**Mulliken charge**	**APT charge**	**Mulliken charge**	**APT charge**	**Mulliken charge**
O1	-1.31	-0.61	-1.35	-0.60	-1.37	-0.64
Ir	0.28	0.07	0.33	0.25	0.29	0.21
H2	-0.66	-0.10	-0.70	-0.16	-0.69	-0.16
C3	2.91	0.60	2.88	0.64	2.86	0.65
O4	-1.38	-0.42	-1.34	-0.38	-1.34	-0.38
O5	-1.41	-0.41	-1.40	-0.40	-1.39	-0.40
Na$^+$	-	-	0.94	0.36	0.94	0.37

Optimized geometries

3a

Ir	0.688966811	-0.003005093	-0.199042949
N	-0.984791682	1.307378007	-0.305080216
N	-0.989043312	-1.308716624	-0.272735329
C	-2.197546624	0.743574205	-0.047183723
C	-2.202953807	-0.735347286	-0.045264806
C	-3.327403877	1.507201662	0.137221849
C	-3.343126821	-1.490306733	0.110361693
C	-3.135904680	2.902540253	0.046391895
C	-3.159850511	-2.887155480	0.025149943
N	-1.996610814	3.479483865	-0.269388827
N	-2.016916500	-3.472755374	-0.259830973
C	-0.904057893	2.683893572	-0.532237876
C	-0.913031862	-2.685488194	-0.497639191
C	2.790722285	0.708008536	-0.450104668
C	2.780868062	-0.761021033	-0.416125641
C	2.295511802	1.185421807	0.795652677
C	1.893422220	0.026697047	1.583541826
C	2.275216461	-1.172911131	0.848308038
C	3.338386062	1.522804906	-1.576741631
C	3.319307511	-1.634995759	-1.502061046
C	2.268765021	2.595520796	1.292494608
C	1.409286179	0.062825242	2.996210784
C	2.219042339	-2.559286279	1.405562603
O	0.142355823	-3.193460294	-0.927153982
O	0.145167493	3.184079488	-0.984824586
O	-4.208217687	3.684449352	0.292019083
O	-4.244601881	-3.660965016	0.240117617
H	-4.300615356	1.087096603	0.346680831
H	-4.319759880	-1.062937726	0.286701041
H	2.983314005	2.553594303	-1.539391117
H	3.064111882	1.094351255	-2.544363451
H	4.434285789	1.536833785	-1.522122553
H	3.031607460	-1.263732875	-2.489371726
H	2.338285374	3.317446078	0.479573262
H	2.970602115	-2.663757572	-1.403262043
H	1.361732926	2.805079058	1.864543539
H	4.415827773	-1.640174105	-1.460029369
H	3.124329330	2.747639996	1.962215574
H	0.797431405	-0.810106941	3.234079772
H	1.320785982	-2.714932613	2.007913564
H	0.827333086	0.964932801	3.197447097
H	2.246997161	-3.317052291	0.623453073
H	2.271871497	0.062116946	3.675362880
H	3.085834995	-2.708952839	2.061250250
H	-3.934784729	4.610387428	0.169862272
H	-3.975640410	-4.588853279	0.122522536

4c

Ir	0.644203950	-0.026743323	-0.154979872
N	-0.860018736	1.396639494	-0.344611416
N	-1.101730829	-1.201952667	-0.342181593
C	-2.135845490	0.939727852	-0.095769481
C	-2.265620477	-0.531285448	-0.100126306
C	-3.176783995	1.795471076	0.102968562
C	-3.455323320	-1.199907736	0.093181459
C	-2.920409777	3.227347270	0.073077450
C	-3.377452136	-2.604337583	0.043271527
N	-1.678288729	3.662480352	-0.280105783
N	-2.288494481	-3.283408678	-0.254653750
C	-0.680157083	2.781663484	-0.532241961
C	-1.133962016	-2.588623609	-0.528485090
C	2.794437880	0.477234611	-0.494318130
C	2.650537990	-0.983465136	-0.465218440
C	2.395777847	0.995567503	0.772006070
C	1.925031899	-0.128639594	1.569682225
C	2.163122776	-1.353266797	0.820469428
C	3.363571162	1.244284048	-1.643744764
C	3.065210935	-1.895846888	-1.574844960
C	2.521763391	2.400222600	1.272046944
C	1.489447143	-0.054750459	2.996666448
C	1.987854469	-2.730350248	1.378448759
O	-0.124488653	-3.188687890	-0.951882196
O	0.435233246	3.179807977	-0.964150376
O	-3.844898914	4.045112487	0.352280042
O	-4.509392844	-3.292947665	0.312145425
H	-4.180597044	1.444731856	0.307658318
H	-4.390285145	-0.696579498	0.293949718
H	3.065865506	2.293304451	-1.614974839
H	3.043442107	0.819622760	-2.598710543
H	4.459580133	1.198167046	-1.613123185

H	2.789905236	-1.485901742	-2.550240073
H	2.635895144	3.114516203	0.457305898
H	2.613389717	-2.883526442	-1.475495064
H	1.653002250	2.695721842	1.865829894
H	4.155670839	-2.018358592	-1.565882332
H	3.405783632	2.470999897	1.917823953
H	0.819815555	-0.878292540	3.254035894
H	1.066532976	-2.812254386	1.961225320
H	0.983922964	0.889430113	3.211175727
H	1.968493449	-3.489047919	0.596862749
H	2.369085063	-0.120461025	3.650384382
H	2.824825874	-2.951272115	2.052323034
H	-4.307132764	-4.240422536	0.224607510

4d

Ir	-0.643955269	-0.027030298	-0.154382585
N	1.102374774	-1.201853822	-0.341106317
N	0.859400768	1.396724818	-0.344907588
C	2.266057847	-0.530461741	-0.100022784
C	2.135446073	0.940464731	-0.095664966
C	3.456350966	-1.198269542	0.092381461
C	3.175809595	1.796733189	0.103678667
C	3.379413335	-2.602745803	0.042586914
C	2.918691529	3.228485927	0.074030659
N	2.290596933	-3.282568546	-0.254059421
N	1.676534920	3.663027701	-0.279705347
C	1.135277677	-2.588608908	-0.526792210
C	0.678979627	2.781743733	-0.532459215
C	-2.649769762	-0.983967192	-0.466882517
C	-2.793873873	0.476717926	-0.495648486
C	-2.163949187	-1.354109517	0.819306318
C	-1.926610016	-0.129765429	1.569061850
C	-2.396487150	0.994702267	0.771225650
C	-3.063135323	-1.896059421	-1.577226098
C	-3.362262560	1.244053296	-1.645254267
C	-1.989496273	-2.731258030	1.377415282
C	-1.492594577	-0.056530382	2.996544150
C	-2.522796795	2.399282210	1.271411842
O	-0.436342527	3.179415428	-0.964881561
O	0.125737574	-3.189609182	-0.948609067
O	4.512182750	-3.290517891	0.310149943
O	3.842610869	4.046625997	0.353937395
H	4.391162325	-0.694303502	0.292230111
H	4.179713695	1.446511849	0.308800986
H	-2.611372013	-2.883745378	-1.477632145
H	-2.786702757	-1.485862340	-2.552196525
H	-4.153602091	-2.018577835	-1.569549243
H	-3.042778646	0.818700627	-2.600119741
H	-1.971554543	-3.490144924	0.595985183
H	-3.063327266	2.292722679	-1.616867245
H	-1.067778029	-2.813957812	1.959454222
H	-4.458322718	1.199244894	-1.614421928
H	-2.826135884	-2.951207482	2.052016890
H	-0.988218558	0.887959519	3.212367624
H	-1.654462535	2.694577788	1.865932448
H	-0.822471823	-0.879660357	3.253972975
H	-2.636141745	3.113701673	0.456671500
H	-2.372883671	-0.123653648	3.649241010
H	-3.407345202	2.470097348	1.916458036
H	4.310609176	-4.238140000	0.222638366

3a_f$_b$

C	-1.379048957	-1.382668644	-0.164414023
C	-1.346556150	1.618738139	0.106343054
C	-0.230793164	-0.629479833	-0.066243662
C	-0.211203743	0.842920757	0.068395628
N	0.998189914	-1.212696060	-0.004979530
N	1.030901075	1.378970194	0.230580693
C	1.088790165	-2.584408412	0.135747262
C	1.156224016	2.726433148	0.576119313
N	-0.016440198	-3.369889985	-0.024486506
N	0.047692417	3.541502557	0.539840319
C	-1.187019117	-2.779416879	-0.181030548
C	-1.129287970	2.998196595	0.314749395
O	-2.216325147	3.796951916	0.290849443
O	-2.279223019	-3.550417163	-0.339066847
O	2.199384842	-3.116068279	0.427164391
O	2.263312508	3.179732352	0.931530207
Ir	2.665131289	0.114014041	-0.224868942
C	3.970290177	1.407271411	-1.472555983
C	4.728950493	0.946113034	-0.357664064
C	4.809489401	-0.518129223	-0.437245478

C	4.083211506	-0.948923811	-1.580294917
C	3.492404102	0.233309467	-2.197610913
C	3.990360051	-2.334533547	-2.135003649
C	5.634629493	-1.372578826	0.469299449
C	5.439646978	1.775944884	0.662824287
C	3.731395311	2.818848243	-1.902904966
C	2.736237528	0.252116908	-3.485952196
O	3.252574492	-2.536612934	2.730348163
C	3.337607119	-1.246914519	3.027354454
O	3.842053185	-0.841470426	4.061919371
H	5.243358708	-2.388496530	0.542281079
H	2.985273251	-2.551499604	-2.505512958
H	4.257643469	-3.088195775	-1.394248503
H	4.681808882	-2.426209197	-2.981656755
H	5.703712545	-0.947688823	1.472874780
H	6.654875235	-1.433331034	0.068887320
H	5.327533475	1.352295266	1.664826371
H	5.069684499	2.801673021	0.676850467
H	6.512167152	1.801813865	0.433527099
H	3.905051972	3.528900567	-1.095178856
H	2.713493087	2.957446981	-2.275972417
H	4.418455534	3.055438121	-2.724772495
H	2.144327552	-0.657179101	-3.612459367
H	3.442998719	0.312536331	-4.323618797
H	2.069760120	1.115212687	-3.546665912
H	2.832437509	-2.682205603	1.820337860
H	2.917779339	-0.565996749	2.267150455
H	-1.920823402	4.709447648	0.455501690
H	-1.999699747	-4.481946719	-0.300821984
H	-2.369473321	-0.953570281	-0.217827049
H	-2.343889184	1.220735868	-0.014559080

3a_TS$_p$

C	3.199150312	1.791081706	-0.260733216
C	3.542088092	-1.204562462	0.145704742
C	2.176524491	0.903261006	-0.007835701
C	2.325846625	-0.562015735	0.104992269
N	0.902354536	1.345127791	0.206156181
N	1.153035476	-1.232959121	0.240428806
C	0.690345592	2.687357136	0.365758064
C	1.149330232	-2.617325688	0.513352428
N	1.628969480	3.596631201	0.043139267
N	2.360687993	-3.284538704	0.494764708
C	2.830927545	3.149721846	-0.286100690
C	3.467906689	-2.605885140	0.326394662
O	4.637790416	-3.284464249	0.325593728
O	3.765375597	4.047800616	-0.635004309
O	-0.434730175	3.090806221	0.847387175
O	0.087748749	-3.194042113	0.758575124
Ir	-0.601613309	-0.134063849	-0.052191847
C	-1.676384316	-1.466265058	-1.470090441
C	-2.523486482	-1.187979595	-0.353800664
C	-2.793021252	0.257114855	-0.339915740
C	-2.068499716	0.856167745	-1.408489428
C	-1.323546259	-0.197857382	-2.096063059
C	-2.094944596	2.297011876	-1.812399591
C	-3.760529018	0.944062553	0.573395596
C	-3.108279942	-2.188525050	0.592581147
C	-1.256226330	-2.815053753	-1.958706564
C	-0.547251511	-0.031432802	-3.364095275
O	-1.278912016	1.794812959	2.690721977
C	-1.274187888	0.523117438	2.750345693
O	-1.778972940	-0.245095819	3.543608126
H	-3.482090808	1.982496462	0.759443810
H	-1.140376641	2.611526342	-2.241107585
H	-2.306227154	2.951048030	-0.966365940
H	-2.866965408	2.453752907	-2.575419611
H	-3.840303641	0.437668650	1.536729262
H	-4.756699536	0.939865729	0.113399910
H	-3.202259719	-1.771126505	1.598237251
H	-2.465324690	-3.066373066	0.663223948
H	-4.105385562	-2.498486155	0.256023615
H	-1.134969590	-3.517531231	-1.134953519
H	-0.310307793	-2.768484129	-2.503009496
H	-2.016893978	-3.195824519	-2.651634556
H	-0.071859467	0.950152597	-3.421495215
H	-1.214229007	-0.126770902	-4.230232382
H	0.232800614	-0.789156003	-3.462100898
H	-0.840674035	2.396764735	1.675930267
H	-0.654985456	-0.003182316	1.879685103
H	4.403444545	-4.216098001	0.469068675

H	3.352944113	4.925188492	-0.575856762
H	4.216701194	1.484136958	-0.454741087
H	4.491583859	-0.696981794	0.059704747

2b_f$_a$

C	-1.238686890	-1.391209873	-0.552282217
C	-1.299170012	1.601177755	-0.064509353
C	-0.157766161	-0.641318602	-0.144577023
C	-0.162394151	0.827922415	0.024741442
N	1.020886263	-1.236380335	0.197857137
N	1.039697574	1.358978946	0.362791279
C	1.057712357	-2.585136544	0.283825144
C	1.127883492	2.696159329	0.734194886
N	0.065095073	-3.378616897	-0.145433233
N	0.024601873	3.508525474	0.603512737
C	-1.039565375	-2.784218239	-0.584004680
C	-1.115563929	2.970976936	0.220476112
O	-2.197447710	3.769540230	0.100916876
O	-2.033823377	-3.547791164	-1.054534945
O	2.102835011	-3.170058758	0.811867137
O	2.200048160	3.147354731	1.194724654
Ir	2.742676289	0.097704713	0.086259366
C	3.875658227	1.354505394	-1.343016888
C	4.784533700	0.882822401	-0.347524688
C	4.837470699	-0.580580370	-0.430337744
C	3.938097541	-1.000156193	-1.447560725
C	3.276546385	0.188344551	-1.985449677
C	3.737471379	-2.391622400	-1.954414097
C	5.770797478	-1.452395207	0.348581808
C	5.639582590	1.713095870	0.556077062
C	3.607985852	2.772579197	-1.731488639
C	2.346493725	0.214794318	-3.155197680
O	3.294696018	-2.151075734	2.704619795
C	3.577341149	-0.925010794	2.911246389
O	4.333920275	-0.462838049	3.777873022
H	5.384818420	-2.468225872	0.451750206
H	2.704054073	-2.564507923	-2.263326479
H	4.012110072	-3.139791887	-1.210257671
H	4.374026632	-2.538846913	-2.835686005
H	5.962734844	-1.050248162	1.345157848
H	6.732409297	-1.510453597	-0.176939357
H	5.720937680	1.261823599	1.548506800
H	5.242937954	2.723679141	0.668009888
H	6.652759427	1.789009708	0.141974151
H	3.886792613	3.472158187	-0.943778083
H	2.556557345	2.930671488	-1.982611871
H	4.200082876	3.008246740	-2.624456358
H	1.735762209	-0.689594473	-3.201028991
H	2.927413747	0.273768922	-4.084347437
H	1.683742168	1.082165748	-3.119844470
H	2.607701175	-2.589194411	1.559062987
H	3.080209028	-0.169070842	2.231804389
H	-1.929458258	4.674566126	0.337023710
H	-1.761999980	-4.481114726	-1.003861713
H	-2.183728140	-0.955985948	-0.845851747
H	-2.271422670	1.203908129	-0.318846610

2b_f

C	-1.347188448	-1.282645873	-0.381739880
C	-1.290656009	1.689012094	0.126121348
C	-0.216995963	-0.575856439	-0.031972949
C	-0.164051821	0.893161424	0.117418809
N	0.958189880	-1.208843387	0.248912304
N	1.077510091	1.396215787	0.315324931
C	0.943120681	-2.556968643	0.299286290
C	1.231839859	2.743810432	0.628954599
N	-0.096606402	-3.315292101	-0.068286539
N	0.135143629	3.575918679	0.597167682
C	-1.206523369	-2.680143131	-0.430919177
C	-1.051383554	3.057664178	0.357502125
O	-2.122744999	3.881228915	0.341292012
O	-2.255089590	-3.404502124	-0.840892495
O	2.003057153	-3.202777487	0.739490837
O	2.356705883	3.193413382	0.940479961
Ir	2.726696943	0.058435469	0.045018296
C	3.656890909	1.127004169	-1.645061472
C	4.642631767	0.942826549	-0.608667408
C	4.864829760	-0.492638185	-0.462125683
C	4.000369476	-1.174376301	-1.362754026
C	3.203397650	-0.177169413	-2.073022475
C	3.977584046	-2.642459685	-1.645359780
C	5.897932624	-1.104576378	0.430540636

C	5.467917467	2.005123494	0.049612549
C	3.207250059	2.431133760	-2.223790353
C	2.256089904	-0.467385465	-3.196801570
O	3.403709788	-2.053338107	2.525933454
C	3.203216561	-0.885573884	2.934232976
O	2.810375982	0.123825145	2.259214795
H	5.701645000	-2.161548845	0.617115062
H	2.982135951	-2.984825297	-1.935172962
H	4.315253643	-3.231778090	-0.791857944
H	4.653663054	-2.847821033	-2.485251602
H	5.952831457	-0.586025120	1.390990963
H	6.883561724	-1.021220443	-0.044370987
H	5.688584964	1.748239261	1.089014399
H	4.967025396	2.974125582	0.035882373
H	6.425874420	2.112125380	-0.474893424
H	3.340588608	3.253886359	-1.520991638
H	2.157751127	2.397627971	-2.525248932
H	3.802728502	2.647520930	-3.119252348
H	1.695430497	-1.388196115	-3.016755504
H	2.809857870	-0.593464047	-4.135419929
H	1.541844980	0.346931771	-3.339038273
H	2.606231635	-2.609182426	1.312794991
H	3.378138510	-0.677195110	4.004418977
H	-2.015784426	-4.347619569	-0.813708324
H	-1.805293241	4.782369251	0.525492316
H	-2.287598230	-0.808166444	-0.625103656
H	-2.291033821	1.304854860	-0.012621302

3f_f

C	-1.342398835	-1.239198631	-0.428629543
C	-1.278509407	1.714932707	0.210399059
C	-0.224853783	-0.556971567	-0.041129284
C	-0.159158859	0.906646532	0.152054469
N	0.952238104	-1.205559648	0.251098701
N	1.089806265	1.400712342	0.331090683
C	0.900081758	-2.558281616	0.249906107
C	1.261792499	2.741551433	0.665371560
N	-0.118491598	-3.305223190	-0.135004873
N	0.172809904	3.581178778	0.682167246
C	-1.278608644	-2.680152248	-0.548762179
C	-1.023991426	3.073095778	0.463444451
O	-2.088292322	3.909728468	0.495743799
O	-2.246490157	-3.355691256	-0.982149951
O	1.975766495	-3.219827406	0.696073975
O	2.399561960	3.179761933	0.952663970
Ir	2.714304639	0.043179296	0.040116858
C	3.656274762	1.112607046	-1.643692428
C	4.646046821	0.921783704	-0.614530551
C	4.854510645	-0.514777550	-0.467953892
C	3.986361970	-1.191429485	-1.369417147
C	3.192741550	-0.188984541	-2.074488359
C	3.966313650	-2.657748323	-1.663633775
C	5.886641416	-1.133792563	0.421571048
C	5.485079154	1.976725634	0.039249320
C	3.211195243	2.420222675	-2.219760358
C	2.247557724	-0.471543204	-3.202641885
O	3.418927849	-2.053530320	2.535636841
C	3.184818817	-0.893540379	2.939589835
O	2.793707187	0.113074966	2.255358047
H	5.684866649	-2.189838393	0.607739882
H	2.971774560	-2.999931830	-1.956628851
H	4.302921808	-3.253395717	-0.814051738
H	4.644019428	-2.856796860	-2.503859794
H	5.946749626	-0.617152195	1.382784709
H	6.872103084	-1.055775199	-0.054753553
H	5.699624126	1.724511308	1.081230136
H	4.997889158	2.952677250	0.018426927
H	6.446298270	2.069064930	-0.482324202
H	3.349376211	3.241193885	-1.515706705
H	2.160263617	2.391881411	-2.517097908
H	3.803525522	2.637036055	-3.117239110
H	1.679504201	-1.388429043	-3.025080882
H	2.802188466	-0.600690123	-4.140493773
H	1.538669394	0.347299376	-3.346259480
H	2.563469148	-2.625046973	1.251598518
H	3.322017908	-0.679618073	4.015521708
H	-1.752255249	4.801182415	0.692843329
H	-2.268217953	-0.730633520	-0.667572047
H	-2.284435228	1.338718981	0.091066173

3f_f_r

C	3.313798377	1.667753429	-0.177687931

C	3.431659562	-1.330966083	-0.337324397
C	2.221391673	0.853730816	-0.063127547
C	2.259822242	-0.621121901	-0.158703738
N	0.978536392	1.360106135	0.236161803
N	1.063310674	-1.240015622	0.009527299
C	0.940449057	2.669982964	0.537263137
C	1.019824072	-2.630749135	0.108355704
N	1.924896472	3.539527838	0.453039043
N	2.165724321	-3.365744397	-0.093831823
C	3.164737820	3.091717220	0.031332632
C	3.297551680	-2.728773163	-0.314414943
O	4.416966710	-3.463052988	-0.518811694
O	4.112252988	3.898712516	-0.128899519
O	-0.251032737	3.107426972	0.997205735
O	-0.053155446	-3.215671461	0.379859122
Ir	-0.682434581	0.016506744	0.028928650
C	-2.772922691	-0.718792713	-0.255591751
C	-2.781456941	0.741740188	-0.155640688
C	-2.026401050	1.258093414	-1.255894705
C	-1.487542641	0.138926659	-2.007792107
C	-2.025657647	-1.074799832	-1.420981657
C	-0.759072328	0.232641392	-3.314389309
C	-1.865884674	2.691584392	-1.654030896
C	-3.553207153	1.526660558	0.859886976
C	-3.537910054	-1.647973179	0.635577418
C	-1.893364608	-2.435586457	-2.027326930
C	-0.709529465	-1.075915146	2.910376714
O	-0.778341885	-1.091963910	4.148823326
O	-0.481382830	-0.007736908	2.213024262
H	-0.842228170	2.911505146	-1.967434206
H	-0.132087755	-0.645932888	-3.485795528
H	-0.121618572	1.119491205	-3.350846508
H	-1.472221273	0.299881982	-4.145927976
H	-2.139186592	3.376364450	-0.851883025
H	-2.520840575	2.892144867	-2.511126531
H	-3.179402611	2.548648419	0.948698540
H	-3.499434833	1.057191673	1.845852711
H	-4.611607906	1.578118772	0.575844130
H	-3.567475734	-1.279552949	1.664346799
H	-3.100683516	-2.648547485	0.641552091
H	-4.574669251	-1.734802462	0.286805167
H	-0.892412777	-2.608146139	-2.429256574
H	-2.599481548	-2.507186989	-2.864637077
H	-2.127480546	-3.228899616	-1.318155406
H	-0.832377090	-2.007966789	2.331795077
H	4.165677354	-4.401386374	-0.468231113
H	4.295671584	1.278041297	-0.413834227
H	4.395120855	-0.860625130	-0.470171967
H	-0.163239109	4.062887638	1.151699585

3a_f$_r$

C	-3.422240630	-1.421124942	-0.156815677
C	-3.314794764	1.560043107	-0.369701463
C	-2.247226766	-0.697625072	-0.081591705
C	-2.192646683	0.776986800	-0.182566957
N	-1.055643635	-1.291488664	0.166418589
N	-0.959387720	1.313798560	-0.005487558
C	-1.021502992	-2.641332586	0.509230432
C	-0.827109483	2.697425252	0.107225084
N	-2.158574622	-3.405250661	0.369479523
N	-1.920410088	3.506434114	-0.107957535
C	-3.286756712	-2.805723119	0.046519619
C	-3.089083104	2.947037784	-0.342957704
O	-4.155159919	3.753108274	-0.559058133
O	-4.402169349	-3.562294424	-0.085235464
O	0.031527465	-3.156683111	0.945824024
O	0.275468386	3.209700884	0.403413329
Ir	0.685463553	-0.064500347	0.027641669
C	2.842082463	0.519211585	-0.183005512
C	2.732155721	-0.939699308	-0.120548762
C	1.973361925	-1.369191765	-1.254712296
C	1.540264254	-0.192445507	-1.986484954
C	2.156921578	0.960984210	-1.354401655
C	0.846330313	-0.193917119	-3.315327582
C	1.721647122	-2.775004003	-1.701010129
C	3.414521392	-1.806551777	0.892406072
C	3.652755878	1.362315729	0.752486688
C	2.147647243	2.340997930	-1.931394633
C	0.724052966	0.979878337	2.926311048
O	0.769953075	0.976957158	4.166079650
O	0.433998704	-0.060407795	2.210733746

H	0.703800012	-2.900947663	-2.078589433
H	0.288584322	0.732204704	-3.475761025
H	0.148547013	-1.030810131	-3.398533987
H	1.577021116	-0.286908120	-4.129067016
H	1.884761048	-3.498184493	-0.902929847
H	2.408491044	-3.010591735	-2.523689474
H	2.959662804	-2.797403398	0.946505287
H	3.372074486	-1.357692395	1.888532958
H	4.472818278	-1.933859577	0.632592833
H	3.619958096	0.970783626	1.772588235
H	3.300090607	2.395668704	0.769478403
H	4.703694531	1.370179390	0.436857798
H	1.171092615	2.604319168	-2.343927211
H	2.871500461	2.372981367	-2.755915848
H	2.433076549	3.096985437	-1.200415069
H	0.925052123	1.907996046	2.362901604
H	-3.843984607	4.673059548	-0.503251681
H	-4.385524468	-0.972485205	-0.352030867
H	-4.305664255	1.154270856	-0.514023776
H	-4.158857977	-4.484133993	0.107081779

3f_f$_a$

C	2.881205239	2.259016067	-0.143246571
C	3.712324491	-0.632172106	0.333234983
C	2.024560255	1.237480526	0.144349984
C	2.408896150	-0.182753678	0.285280323
N	0.686732112	1.468012236	0.381458753
N	1.360973573	-1.032791496	0.435556173
C	0.300351659	2.766232920	0.463505086
C	1.585708424	-2.368033827	0.757040235
N	1.050498447	3.813167789	0.176193803
N	2.869915073	-2.858181822	0.751509224
C	2.360424087	3.610644766	-0.212906706
C	3.863982285	-2.016483109	0.542567766
O	5.125584985	-2.503142420	0.543761023
O	3.072436154	4.579226777	-0.576096235
O	-0.943182283	3.017991868	0.878108408
O	0.622341251	-3.107782293	1.062088196
Ir	-0.554495913	-0.240835807	-0.039488500
C	-1.191387616	-1.687699004	-1.595805730
C	-2.286310080	-1.502107042	-0.702547308
C	-2.695248641	-0.094840929	-0.762445101
C	-1.831516359	0.582065685	-1.665407524
C	-0.837512817	-0.379113961	-2.143224260
C	-1.940416514	2.000296939	-2.125745026
C	-3.902156093	0.476226076	-0.087335805
C	-2.989432836	-2.552049689	0.098448469
C	-0.533539085	-2.974863360	-1.978494916
C	0.182647495	-0.121672505	-3.205663517
O	-2.129561069	1.563430665	2.593724134
C	-2.022929448	0.318470057	2.843870193
O	-2.852545610	-0.395505943	3.446329105
H	-3.801775899	1.549453847	0.084293851
H	-0.959487448	2.437024151	-2.327044369
H	-2.459192434	2.625934884	-1.398685435
H	-2.510921883	2.024439407	-3.062536363
H	-4.098545055	-0.011191009	0.869200750
H	-4.779638775	0.319429616	-0.727710663
H	-3.221795891	-2.190421605	1.104153359
H	-2.387963516	-3.458284891	0.189022087
H	-3.937117785	-2.818580072	-0.385692300
H	-0.721352813	-3.763002270	-1.249488473
H	0.547082381	-2.858005061	-2.091552550
H	-0.933608381	-3.301236651	-2.946440957
H	0.569904309	0.898155982	-3.148062770
H	-0.274102127	-0.251483491	-4.195094235
H	1.021780567	-0.816975775	-3.131241562
H	-1.322162816	2.293413112	1.499147535
H	-1.084209863	-0.178660422	2.488529515
H	5.074700108	-3.459948862	0.712064455
H	3.931881203	2.086601633	-0.340933848
H	4.567386066	0.020635487	0.229496282

3a_f$_c$

C	3.334579703	1.577413194	-0.315083500
C	3.467242651	-1.415194524	-0.052785294
C	2.227005796	0.774688854	-0.149262516
C	2.291164348	-0.698424728	-0.028464361
N	0.979297263	1.296888195	-0.013526189
N	1.090159358	-1.300934081	0.183248503
C	0.818814120	2.676731812	0.105814627
C	1.052362224	-2.650466551	0.534053520

N	1.892721367	3.504364815	-0.132307489
N	2.198764990	-3.407814095	0.444345403
C	3.075443752	2.963283661	-0.334565653
C	3.332978233	-2.802674197	0.161070207
O	4.458032634	-3.546254593	0.081320383
O	4.125610077	3.781210001	-0.566378979
O	-0.286403155	3.154250061	0.437953636
O	-0.011604582	-3.163955490	0.939155764
Ir	-0.634323200	-0.088885470	-0.116167187
C	-2.768850616	-0.781242246	-0.073902711
C	-2.728730808	0.671816840	-0.288740799
C	-2.039042957	0.913934194	-1.511744334
C	-1.579301049	-0.371261257	-2.029637978
C	-2.107031210	-1.416872359	-1.161718789
C	-0.916343944	-0.591280382	-3.350557789
C	-1.868284291	2.216842809	-2.225102431
C	-3.427557498	1.674695173	0.573751029
C	-3.474233831	-1.445096295	1.065024101
C	-2.027181015	-2.880212238	-1.459781248
C	-0.928413217	0.479477014	3.207059158
O	-2.050263414	0.665706470	3.753163520
O	0.152861524	1.087005003	3.435472928
H	-0.889429578	2.286839146	-2.705911590
H	-0.308545701	-1.498941071	-3.345516696
H	-0.279854286	0.252997196	-3.624418825
H	-1.680850411	-0.703062483	-4.130264607
H	-1.987575016	3.069452199	-1.557502142
H	-2.627734038	2.286858038	-3.013882692
H	-3.109462039	2.693086530	0.345911719
H	-3.245505915	1.483522187	1.634042774
H	-4.509761040	1.611660513	0.403823835
H	-3.316610974	-0.904185832	2.002107423
H	-3.143699367	-2.477072700	1.197330284
H	-4.553620786	-1.458611333	0.867097150
H	-1.043153973	-3.157360310	-1.845795607
H	-2.768131936	-3.124887898	-2.230989229
H	-2.236813764	-3.489630130	-0.581043601
H	-0.887403984	-0.329083350	2.427245987
H	4.217909839	-4.470482650	0.268015578
H	3.799365016	4.697243075	-0.532700086
H	4.337937676	1.192256250	-0.426999948
H	4.435638652	-0.964594382	-0.216047333

3a_TS$_{asso}$

C	3.461180109	-1.162089287	0.213941427
C	3.095805377	1.797967177	0.385903931
C	2.244511141	-0.536111060	0.029137641
C	2.062255126	0.926776107	0.107538693
N	1.126778025	-1.229107681	-0.304245114
N	0.807047292	1.363587786	-0.175465159
C	1.223366867	-2.590493424	-0.606915456
C	0.567254407	2.734311292	-0.283361642
N	2.406350533	-3.249214107	-0.364613688
N	1.572033475	3.625594937	0.018097398
C	3.453883917	-2.556192959	0.032898156
C	2.761156869	3.162806054	0.340913749
O	3.739800996	4.048548973	0.635827825
O	4.611164990	-3.215544379	0.267294290
O	0.252993150	-3.204808955	-1.097432065
O	-0.547692924	3.156932930	-0.654001557
Ir	-0.694067167	-0.168621644	-0.235224418
C	-2.590297433	0.754966015	0.703965555
C	-2.867112017	-0.558949286	0.208405862
C	-2.063326820	-1.497493206	0.965811198
C	-1.366262273	-0.754643249	2.000513119
C	-1.669576957	0.618223715	1.830909213
C	-0.489434246	-1.376555184	3.042945485
C	-2.198216345	-2.989475948	0.936578307
C	-3.917035455	-0.920290594	-0.796614298
C	-3.360575258	1.989407117	0.343247667
C	-1.195631901	1.752499977	2.683068654
C	-0.743885250	0.541290608	-2.474315810
O	0.361505831	0.509007864	-3.013111374
O	-1.869193602	0.902935927	-2.820317609
H	-1.264128477	-3.486530634	1.204342885
H	0.137065994	-0.634378023	3.542107830
H	0.161813856	-2.141423249	2.608851738
H	-1.102172433	-1.867340911	3.809218366
H	-2.510410661	-3.349030177	-0.045218196
H	-2.961060503	-3.294743348	1.664205794
H	-3.681408018	-1.859831133	-1.300812291

H	-4.037787185	-0.142149891	-1.551816855
H	-4.880306884	-1.044796274	-0.286418760
H	-3.611802452	2.005857097	-0.719627151
H	-2.806067899	2.898753986	0.576155646
H	-4.300804527	2.012300198	0.909072158
H	-0.249449162	1.523111061	3.178080807
H	-1.938683819	1.961904090	3.462943115
H	-1.071061408	2.666214885	2.098161754
H	-0.954281077	-1.055809876	-1.519082140
H	3.365199678	4.942900961	0.555902899
H	4.458727115	-4.158819204	0.085441192
H	4.366557812	-0.634693200	0.476797633
H	4.100779986	1.474041526	0.614054885

3a_TS$_d$

C	-3.331342674	-1.446911838	-0.511649843
C	-3.358220516	1.545407579	-0.267773445
C	-2.196067484	-0.692080393	-0.280937060
C	-2.211265664	0.780819111	-0.157310052
N	-0.984946074	-1.262347982	-0.066663410
N	-1.012873512	1.327466582	0.159856206
C	-0.901437732	-2.644728896	0.087886025
C	-0.952060867	2.667307519	0.537682404
N	-1.992518133	-3.426790504	-0.212084190
N	-2.055425229	3.471219020	0.367530362
C	-3.135824319	-2.837755367	-0.500995036
C	-3.187558261	2.918067550	-0.021378978
O	-4.269528261	3.717470378	-0.180765951
O	-4.203290244	-3.619377007	-0.791955508
O	0.155904698	-3.172276486	0.502714110
O	0.097057743	3.135253343	1.035738483
Ir	0.689980571	0.049532466	0.030487710
C	2.812205606	0.757397329	0.011174681
C	2.783117281	-0.692548614	-0.163320483
C	2.126875189	-0.963526048	-1.412855948
C	1.728031621	0.287817025	-2.008398089
C	2.168648601	1.345783076	-1.126787625
C	1.134928256	0.469973872	-3.372850709
C	1.976863035	-2.299572881	-2.073690350
C	3.498562871	-1.683212467	0.705684697
C	3.532179945	1.482246293	1.109037536
C	2.080672337	2.805235715	-1.454112566
C	0.312411474	-0.752998535	3.105392668
O	1.424213219	-0.825592978	3.544350789
O	-0.870465086	-0.906232377	3.208309434
H	1.037981627	-2.371673639	-2.629119477
H	0.530777162	1.379295966	-3.429164286
H	0.500935887	-0.375441176	-3.652486913
H	1.925728481	0.553169795	-4.130407606
H	2.015390719	-3.119534976	-1.356692742
H	2.794224881	-2.438380310	-2.792667778
H	3.081151228	-2.686907743	0.601702375
H	3.446690840	-1.402237192	1.760159650
H	4.559683191	-1.733002101	0.429011257
H	3.448398219	0.948056722	2.058987844
H	3.137764716	2.490902540	1.251140743
H	4.600243285	1.570509297	0.872139709
H	1.117790415	3.062023601	-1.903680962
H	2.860751897	3.053634056	-2.184815133
H	2.228981029	3.433102723	-0.575711476
H	0.497479171	-0.055714408	1.692198665
H	-4.000773730	4.624278716	0.046236614
H	-3.914997906	-4.545552361	-0.720029315
H	-4.306483353	-1.014582839	-0.684046608
H	-4.325329716	1.132944483	-0.516698743

3a_h

C	3.408083642	-1.344386858	0.171332308
C	3.242681036	1.636476438	0.195962198
C	2.224537381	-0.655334136	-0.030760243
C	2.149095601	0.820492098	-0.039980612
N	1.056659110	-1.286505653	-0.303650649
N	0.932893515	1.321751809	-0.361079363
C	1.074236782	-2.662706828	-0.534637445
C	0.791483451	2.696726019	-0.551356390
N	2.210784389	-3.386959579	-0.256477315
N	1.843242894	3.538044613	-0.275463113
C	3.308716939	-2.740572191	0.081031311
C	2.998716935	3.012892105	0.082514783
O	4.025938203	3.856471465	0.349891459
O	4.423791544	-3.465787642	0.344199721
O	0.063312468	-3.240054254	-0.995752514

O	-0.287682521	3.165512308	-0.982301369
Ir	-0.705235887	-0.054642967	-0.364429211
C	-2.716734693	0.876799007	-0.090274755
C	-2.882981776	-0.533637893	-0.385340354
C	-2.300716766	-1.277879686	0.692990540
C	-1.834571880	-0.338464064	1.704802370
C	-2.099831265	0.970377334	1.225243614
C	-1.274698126	-0.724886134	3.041914198
C	-2.397297902	-2.759657256	0.899525159
C	-3.664169675	-1.101335576	-1.534435846
C	-3.392333683	2.000392758	-0.822536615
C	-1.846298569	2.253103388	1.957582275
H	-1.507325711	-3.163924195	1.387814764
H	-0.681883073	0.081602323	3.480897635
H	-0.636209139	-1.610042444	2.967993384
H	-2.079395920	-0.965472287	3.749463964
H	-2.541060540	-3.294289224	-0.040393726
H	-3.256111083	-2.979200908	1.547402762
H	-3.296860548	-2.088966875	-1.823620249
H	-3.615855180	-0.451832065	-2.411778524
H	-4.721455141	-1.207058161	-1.258883322
H	-3.422660823	1.816655343	-1.899864860
H	-2.887750984	2.954121644	-0.658185018
H	-4.429229864	2.110520471	-0.477356904
H	-1.111338641	2.127157965	2.756453311
H	-2.777712685	2.607190033	2.417649648
H	-1.493570120	3.036525097	1.283630734
H	-0.540763637	-0.127684915	-1.960914259
H	3.698934625	4.762474270	0.213294733
H	4.197995628	-4.402908732	0.214899430
H	4.349334244	-0.858833914	0.384672147
H	4.220640615	1.257630612	0.454809370

3f_h

C	-3.328785082	1.539248298	0.206690979
C	-3.326574461	-1.459410205	0.210294000
C	-2.210310495	0.782211317	-0.016183004
C	-2.201051432	-0.695354998	-0.046064440
N	-0.997658023	1.356833080	-0.319023568
N	-1.017942795	-1.254966375	-0.401875874
C	-1.027811089	2.687603187	-0.508456612
C	-0.954399576	-2.632016562	-0.617524645
N	-2.039674487	3.507758845	-0.311461394
N	-2.036748736	-3.422894671	-0.313780555
C	-3.243907647	2.978531107	0.114557745
C	-3.152664779	-2.844887297	0.086095963
O	-4.210421227	-3.636840583	0.390041729
O	-4.213983525	3.732917118	0.377375433
O	0.125838086	3.217989860	-0.972717371
O	0.083260850	-3.149734589	-1.093378717
Ir	0.705051188	0.028139301	-0.364699102
C	2.650480220	-1.017923126	-0.092354385
C	2.904174034	0.390056790	-0.336568663
C	2.344905299	1.128889442	0.758302772
C	1.811777125	0.185996902	1.731942340
C	2.000047131	-1.118704748	1.207529033
C	1.256722899	0.556510786	3.075535538
C	2.503717969	2.598436635	1.011276255
C	3.740773555	0.946281704	-1.451626821
C	3.267948809	-2.157213494	-0.851783831
C	1.644681878	-2.402792342	1.894403192
H	1.610685224	3.032256189	1.468321435
H	0.608845502	-0.227470650	3.475853218
H	0.676620958	1.482746403	3.028379242
H	2.064705686	0.718640199	3.801458679
H	2.721648017	3.149906778	0.095399657
H	3.338688984	2.758312749	1.705766583
H	3.460062556	1.973467528	-1.695885621
H	3.650048211	0.345068865	-2.359392112
H	4.799679608	0.950841310	-1.162289316
H	3.371816216	-1.920632141	-1.913944392
H	2.675486828	-3.069859051	-0.766644740
H	4.271655007	-2.374160368	-0.462293555
H	0.823043593	-2.268140280	2.602439896
H	2.509897687	-2.774623599	2.457898654
H	1.358934495	-3.176357420	1.179268150
H	0.568056174	0.145713902	-1.959755187
H	-3.934043722	-4.559217568	0.253735319
H	-0.013856166	4.176861647	-1.048625552
H	-4.285133368	1.089766090	0.441141325
H	-4.277514351	-1.034397829	0.497027798

2b_h

C	3.436819710	-1.285218234	0.179867138
C	3.208097700	1.696464811	0.218518344
C	2.247964751	-0.607841569	-0.014719752
C	2.135590348	0.862904703	-0.038054698
N	1.084775321	-1.270657151	-0.281503756
N	0.914043410	1.333605538	-0.389877991
C	1.180026969	-2.598918208	-0.453292972
C	0.758045851	2.703549561	-0.610196142
N	2.274614470	-3.333943050	-0.272001668
N	1.782310264	3.565902163	-0.294551281
C	3.386323847	-2.680428828	0.064689122
C	2.935739389	3.069851738	0.103897059
O	3.933492934	3.928608974	0.417560053
O	4.505181205	-3.381593285	0.277780351
O	0.071300483	-3.214737908	-0.863046723
O	-0.305263272	3.147163603	-1.098050647
Ir	-0.713345995	-0.065872356	-0.356605326
C	-2.722878433	0.842460283	-0.135374477
C	-2.882385531	-0.582011307	-0.365544871
C	-2.297475461	-1.268346769	0.748167551
C	-1.846788962	-0.281032227	1.720923742
C	-2.112693134	1.001947515	1.179934273
C	-1.294108460	-0.600744892	3.078177777
C	-2.361160299	-2.742106783	1.015113021
C	-3.653660776	-1.205501031	-1.491466880
C	-3.398420156	1.927460980	-0.923659461
C	-1.861684390	2.314399886	1.857970039
H	-1.453245118	-3.108886538	1.500280767
H	-0.711877465	0.230424785	3.483755847
H	-0.650291957	-1.484624489	3.051262655
H	-2.104792151	-0.812841410	3.787785221
H	-2.519108600	-3.317394547	0.101723980
H	-3.200709595	-2.948613768	1.691511381
H	-3.295361966	-2.212006147	-1.719527942
H	-3.586930704	-0.606367943	-2.402537908
H	-4.715045559	-1.282637596	-1.222610207
H	-3.441029027	1.681303085	-1.987809431
H	-2.884629601	2.884407797	-0.819035527
H	-4.430299336	2.062252692	-0.573358057
H	-1.050324803	2.244068257	2.586636083
H	-2.764375112	2.631470832	2.395436422
H	-1.612671083	3.097349341	1.139480819
H	-0.556003840	-0.180208749	-1.951172692
H	3.596874278	4.832268932	0.290434710
H	0.257672436	-4.166117211	-0.945450018
H	4.319615145	-4.327011003	0.140069446
H	4.370762134	-0.784795759	0.392091999
H	4.187400859	1.338909400	0.501548283

2b_TS$_w$

Ir	2.805851900	0.045472789	0.258443466
N	1.094606392	-1.265452615	0.259294637
N	1.125593103	1.339751945	0.431690414
C	-0.072787182	-0.657468238	-0.087404440
C	-0.066450952	0.815570376	0.055816998
C	-1.180212763	-1.379736353	-0.481079262
C	-1.188900627	1.604278457	-0.101521531
C	-1.011996158	-2.775157348	-0.505442308
C	-0.997483505	2.975287385	0.153063221
N	0.081740631	-3.395972998	-0.103670967
N	0.131324528	3.506301507	0.579073634
C	1.136173807	-2.646037689	0.332402988
C	1.215386878	2.683582829	0.782084373
C	4.909371466	-0.602838475	-0.252874947
C	4.844503108	0.855287687	-0.204327343
C	4.045493611	-1.045422803	-1.302062726
C	3.407486429	0.116644672	-1.894686456
C	3.955841380	1.286308709	-1.245247262
C	5.833811400	-1.455636326	0.561260769
C	5.708799049	1.732252930	0.650534569
C	3.891173167	-2.449095636	-1.795716471
C	2.520603705	0.111473197	-3.102836970
C	3.687492643	2.698455152	-1.659874518
O	2.270927921	3.136392645	1.279414940
O	2.153110403	-3.234422620	0.809332099
O	-2.043955635	-3.519014471	-0.953929031
O	-2.057007119	3.792195356	-0.045046339
O	3.146063376	-1.974623822	2.806355438
H	5.444554884	-2.468277032	0.686357566

H	6.003996734	-1.028217428	1.551992203
H	6.807981171	-1.531673431	0.061972950
H	5.261989867	2.717909562	0.796321261
H	4.139284249	-3.182681127	-1.028441762
H	6.688381718	1.873811238	0.176909039
H	2.876538797	-2.644732241	-2.150285276
H	5.878447109	1.286918718	1.633815122
H	4.571468604	-2.600829923	-2.643277549
H	1.836467116	0.963694067	-3.100502527
H	2.662335229	2.830118433	-2.014138395
H	1.924908595	-0.802894174	-3.157247611
H	3.870405769	3.406057333	-0.851362188
H	3.120471492	0.169739276	-4.019943479
H	4.357037146	2.951343591	-2.491658940
H	2.808365877	0.146912608	1.962453074
H	2.974534006	-0.784706588	2.126103654
H	2.765720069	-2.547714131	2.053817705
H	2.476627784	-1.985865044	3.510364978
H	-1.782942096	4.695522293	0.189590999
H	-1.781083166	-4.454743477	-0.908553416
H	-2.116228925	-0.922178861	-0.767878865
H	-2.154250901	1.216094509	-0.392651331

3f_TS$_w$

Ir	2.814771506	0.058397457	0.273457656
N	1.132885956	-1.269456310	0.330543154
N	1.119563427	1.333621551	0.427850466
C	-0.037940508	-0.689890055	-0.088952746
C	-0.062495919	0.782485463	0.055007888
C	-1.094499832	-1.435722777	-0.532144535
C	-1.199034012	1.555388842	-0.098453252
C	-0.956075871	-2.876448932	-0.568404944
C	-1.032379966	2.926506886	0.156116689
N	0.179364496	-3.430615951	-0.039375046
N	0.088902539	3.482077012	0.576114582
C	1.176862850	-2.649970342	0.412334350
C	1.188611538	2.680347054	0.770019148
C	4.902552236	-0.618423151	-0.262120153
C	4.870088672	0.840855919	-0.218433562
C	4.021139414	-1.045672506	-1.305221653
C	3.393650911	0.125094491	-1.884390608
C	3.971332322	1.287592471	-1.238881606
C	5.828064695	-1.487831291	0.533842283
C	5.753180964	1.701952810	0.633934657
C	3.837325984	-2.446876935	-1.796576410
C	2.494404120	0.139915502	-3.084036984
C	3.719198246	2.704357413	-1.650868862
O	2.242252788	3.155777435	1.255063506
O	2.211172863	-3.203251333	0.948189990
O	-1.866778756	-3.611873123	-1.049954844
O	-2.108689418	3.727937673	-0.031072021
O	3.132827304	-1.881405039	2.873502877
H	5.432369101	-2.499075229	0.650092558
H	6.009235903	-1.074282471	1.528667695
H	6.798181394	-1.565869346	0.026728560
H	5.317661414	2.691128416	0.791130124
H	4.061862225	-3.183172098	-1.024585570
H	6.730162146	1.837450883	0.153066049
H	2.820181743	-2.620141571	-2.155534553
H	5.927355287	1.248104140	1.612606465
H	4.518784021	-2.618952642	-2.639297159
H	1.820874800	1.000622726	-3.068944607
H	2.686207446	2.855527523	-1.973770217
H	1.885414528	-0.765798511	-3.137672465
H	3.939559784	3.410612806	-0.850272295
H	3.084033274	0.197220458	-4.007941433
H	4.367351969	2.944719862	-2.503098133
H	2.826414078	0.236024572	1.968637444
H	2.976957859	-0.691239901	2.138718345
H	2.746626166	-2.472996852	2.106444633
H	2.448246926	-1.860818572	3.561474343
H	-1.844096838	4.633551770	0.205104832
H	-2.019061265	-0.980715130	-0.865441958
H	-2.157766309	1.145684726	-0.382605908

2b_TS$_f$

C	-2.703224879	2.481513797	0.157593426
C	-3.758416961	-0.288291056	-0.387456812
C	-1.905170685	1.395088307	-0.124762927
C	-2.416373474	0.025268004	-0.345930540
N	-0.553180940	1.526708946	-0.278196136
N	-1.456711757	-0.902983278	-0.581870795

C	-0.035097723	2.771535480	-0.252201474
C	-1.813152144	-2.182115838	-0.998170054
N	-0.742371925	3.870488421	0.041185828
N	-3.140608751	-2.545008026	-0.981070678
C	-2.041874445	3.716552435	0.267467437
C	-4.046338442	-1.637422712	-0.679328492
O	-5.344838570	-2.006982488	-0.655780713
O	-2.766055122	4.794275072	0.590990377
O	1.238337369	2.981249648	-0.512026089
O	-0.937037014	-2.986915901	-1.382510357
Ir	0.528179424	-0.347171109	-0.060959093
C	1.905384033	-1.928813858	0.730550534
C	2.605233062	-0.653929525	0.872109911
C	1.842726873	0.175444343	1.744126862
C	0.652197481	-0.557533690	2.149017320
C	0.739375227	-1.877958207	1.570240692
C	-0.357566961	-0.102848719	3.158652232
C	2.228769178	1.529466747	2.247415846
C	3.962816986	-0.348022783	0.321960051
C	2.431030481	-3.129539019	0.006644295
C	-0.196804498	-3.005934734	1.865350946
C	3.228082752	0.944215818	-2.784736732
O	2.670631761	-0.193169957	-2.809247147
O	2.909890432	1.944981782	-2.089670320
H	1.358012113	2.173209578	2.391924221
H	-1.333936390	-0.559513342	2.978379324
H	-0.479165619	0.982805299	3.142714093
H	-0.038833886	-0.385820844	4.169590967
H	2.928514287	2.029015306	1.576292164
H	2.719350426	1.416213751	3.222439825
H	4.107615175	0.722535805	0.166589772
H	4.138537654	-0.860915299	-0.624731597
H	4.724623203	-0.690830323	1.033444173
H	2.979472191	-2.840690643	-0.893183735
H	1.623776867	-3.802979205	-0.287601794
H	3.119364570	-3.688600936	0.652695061
H	-1.226969181	-2.660224697	1.976947232
H	0.101081470	-3.462617216	2.817496297
H	-0.166436485	-3.777675866	1.096499973
H	0.558594463	-0.319365648	-1.793051784
H	1.730977163	2.286113200	-1.065597364
H	1.425225736	-0.230149730	-1.846021307
H	4.099434453	1.069064537	-3.459947587
H	-3.772670153	2.408177776	0.296793359
H	-4.544899602	0.432578521	-0.216363578
H	-5.390412881	-2.950231737	-0.890530229
H	-2.177963704	5.570080697	0.603433927

3f_TS$_b$

C	-2.600811079	2.714920087	-0.054557181
C	-3.821668949	0.049526724	-0.813620115
C	-1.883229964	1.574716164	-0.272088734
C	-2.473922092	0.257902376	-0.595471480
N	-0.505181782	1.579793834	-0.264199547
N	-1.572584274	-0.747322513	-0.727457331
C	0.088934617	2.785769463	-0.130904790
C	-1.973599203	-1.989702340	-1.208909746
N	-0.517740046	3.936078619	0.092569001
N	-3.315034481	-2.245184338	-1.367504299
C	-1.894807701	3.953617720	0.196754071
C	-4.175471605	-1.266176260	-1.163337954
O	-5.493757708	-1.532857575	-1.310625244
O	-2.499643951	5.020847220	0.468890089
O	1.425043429	2.854427734	-0.234775761
O	-1.119999078	-2.860457505	-1.494293225
Ir	0.356119572	-0.367963705	0.081083470
C	1.486155980	-2.060580016	1.038007642
C	2.237425043	-0.836409827	1.314160570
C	1.405673450	0.031999621	2.078782435
C	0.120301946	-0.619629082	2.272633681
C	0.210931306	-1.938744463	1.683969397
C	-0.998784296	-0.113070318	3.131331601
C	1.799902123	1.348236885	2.669877996
C	3.682671942	-0.615703419	0.990862263
C	2.038196739	-3.284383560	0.373310119
C	-0.834668056	-3.000913273	1.807769408
C	3.545057198	0.496185809	-2.237714973
O	2.872346900	-0.574550716	-2.321260851
O	3.243152935	1.564844097	-1.656851234
O	4.762986141	0.432930735	-2.883644353
H	0.966416545	2.054503979	2.682258997

H	-1.963536463	-0.507804761	2.803063650
H	-1.053477269	0.978128100	3.115599979
H	-0.849923441	-0.422122051	4.173575654
H	2.635448418	1.800959610	2.134410325
H	2.112009474	1.190134816	3.709948206
H	3.913336211	0.442972341	0.858656809
H	3.980086111	-1.148904424	0.086653809
H	4.299881753	-0.992405576	1.816312664
H	2.733382496	-3.021061714	-0.427554819
H	1.242731131	-3.897415328	-0.055182099
H	2.583750000	-3.898598838	1.100613520
H	-1.843249176	-2.584057716	1.759867534
H	-0.725545922	-3.484192699	2.786773630
H	-0.735729420	-3.767468227	1.039341887
H	0.655488872	-0.311261024	-1.628195363
H	1.839810446	2.072362036	-0.680568052
H	1.523877569	-0.376675250	-1.570100185
H	-3.683623772	2.718202641	-0.056375324
H	-4.563142453	0.830739515	-0.725953193
H	-5.579538252	-2.467045368	-1.568113596
H	5.193370219	1.293810285	-2.756956612

3a_d

C	-1.126497456	-1.340310131	-0.865458273
C	-1.040758013	1.661076094	-0.551788696
C	-0.018436230	-0.642202952	-0.431906911
C	0.025955780	0.828182325	-0.283494951
N	1.105113059	-1.279897100	-0.013890723
N	1.186314952	1.303161340	0.236501795
C	1.103411088	-2.664698539	0.135627252
C	1.271736386	2.630821532	0.647275775
N	0.040470695	-3.389371531	-0.351278539
N	0.253291182	3.498522590	0.327993562
C	-1.003307267	-2.742913863	-0.829884010
C	-0.832953406	3.019407475	-0.243652901
O	-1.832069248	3.879738430	-0.541894198
O	-2.041321968	-3.466218450	-1.305196639
O	2.052184782	-3.238219540	0.713112437
O	2.256748555	3.022996549	1.310357385
Ir	2.806840720	-0.069974138	0.361572666
C	4.988089189	0.536402288	0.493935899
C	4.900945395	-0.920166279	0.342354073
C	4.288886201	-1.197526075	-0.914279180
C	3.894940399	0.070893796	-1.513500265
C	4.417869766	1.135952563	-0.665820148
C	3.342031219	0.244887668	-2.894646731
C	4.121673815	-2.527384616	-1.576436259
C	5.493018289	-1.917961380	1.288166501
C	5.682155938	1.243414177	1.615783993
C	4.406747233	2.586949478	-1.025426083
H	3.132934753	-2.633868999	-2.029376639
H	2.769430573	1.171280303	-2.981504442
H	2.691156584	-0.588230412	-3.169928316
H	4.159542388	0.286299689	-3.625042344
H	4.280612508	-3.354543778	-0.885094015
H	4.860721032	-2.605591230	-2.383671986
H	5.002389700	-2.889464840	1.205649502
H	5.416947243	-1.578964884	2.323696282
H	6.557582657	-2.056373207	1.062119766
H	5.540436464	0.723896975	2.566118140
H	5.325384699	2.269321467	1.725662363
H	6.760338253	1.280419223	1.416059295
H	3.472940962	2.874046744	-1.514877284
H	5.222112923	2.776807586	-1.734807436
H	4.556543864	3.227436812	-0.156583921
H	2.401613928	0.156606744	2.183248531
H	2.342659292	-0.640333513	2.084511998
H	-1.552363590	4.766560579	-0.255647074
H	-1.816613528	-4.407372054	-1.202530046
H	-2.035593458	-0.862665092	-1.201360010
H	-1.979840110	1.312304169	-0.956767182

4d_d

C	-1.114288856	-1.298130406	-0.851943018
C	-0.983936960	1.710183634	-0.534561159
C	-0.003323927	-0.603061227	-0.411809049
C	0.057421801	0.865944094	-0.264540904
N	1.110213521	-1.255724622	0.011618074
N	1.226957635	1.322030934	0.278924941
C	1.098046646	-2.640656816	0.158065230
C	1.296625686	2.647402812	0.707534891
N	0.030759671	-3.357159013	-0.326982995

N	0.311575636	3.529670435	0.402816984
C	-1.005022679	-2.698085554	-0.811361286
C	-0.823887297	3.119769290	-0.236173902
O	-1.734381428	3.950895073	-0.537786779
O	-2.049051742	-3.417683908	-1.286959395
O	2.044908249	-3.222900675	0.734593690
O	2.295647340	3.004900119	1.401752566
Ir	2.823754000	-0.063442535	0.385774614
C	5.018205727	0.511571693	0.495321192
C	4.915564296	-0.941442116	0.327796686
C	4.280044759	-1.196157633	-0.920210090
C	3.888307732	0.084491891	-1.498669254
C	4.436368037	1.133263989	-0.647253042
C	3.316979286	0.279018575	-2.870038678
C	4.085065107	-2.516460794	-1.595215465
C	5.513234861	-1.957150911	1.251687483
C	5.737081018	1.197293771	1.615212953
C	4.444198603	2.588840640	-0.990598759
H	3.088264526	-2.604112350	-2.034535496
H	2.748318152	1.209394065	-2.938253049
H	2.656520447	-0.546506943	-3.145716685
H	4.122848541	0.323997058	-3.613194224
H	4.240115370	-3.353639044	-0.914918897
H	4.810892440	-2.598961267	-2.413911954
H	5.007251784	-2.920975563	1.169407043
H	5.460682663	-1.629059985	2.292310593
H	6.571660353	-2.109120205	1.006019596
H	5.602867919	0.668577960	2.561664237
H	5.393385796	2.225658183	1.742586666
H	6.812979088	1.225164587	1.401722879
H	3.520827855	2.889843027	-1.491344730
H	5.272728132	2.782046989	-1.683659140
H	4.582472796	3.217947367	-0.111352458
H	2.422611095	0.161216843	2.202301062
H	2.374227156	-0.638078076	2.104061665
H	-1.829318829	-4.358920009	-1.176463221
H	-2.016701458	-0.811607602	-1.193380222
H	-1.919007192	1.355737885	-0.950233529

3a$_{Na_2w}$

C	2.564373004	2.457813838	0.022763909
C	-0.121237114	3.780633865	0.150713259
C	1.375751973	1.783031712	-0.137741576
C	0.049250339	2.432262796	-0.055089966
N	1.336116843	0.447913795	-0.424019378
N	-1.008858731	1.594007391	-0.246023707
C	2.524390660	-0.219525610	-0.665597545
C	-2.292116390	2.131756381	-0.377225382
N	3.728443905	0.407166820	-0.448793991
N	-2.501923471	3.462663296	-0.090451295
C	3.735097978	1.683493894	-0.112208974
C	-1.462183844	4.226718630	0.159802400
O	-1.665680034	5.531053415	0.434699273
O	4.911786385	2.288821597	0.109288812
O	2.525654705	-1.403757443	-1.086493871
O	-3.237051540	1.415115682	-0.759670822
Ir	-0.554287359	-0.484168053	-0.179060002
C	-2.158396845	-2.025398249	-0.368811151
C	-0.853396652	-2.687700604	-0.481770037
C	-0.147115844	-2.494239409	0.737893204
C	-0.965060195	-1.641368902	1.589406652
C	-2.242426548	-1.424399923	0.920513721
C	-0.646628190	-1.259283158	2.996797620
C	1.147887822	-3.111138466	1.159508454
C	-0.414236392	-3.493705856	-1.660836159
C	-3.228402756	-2.087865964	-1.409578639
C	-3.432847014	-0.773894406	1.549461276
Na	4.806328611	-1.772484796	-0.764186374
O	6.086718687	-2.096445670	-2.595401160
O	5.509642437	-2.666558284	1.193070177
H	1.786678297	-2.393430132	1.680193819
H	-1.138593474	-0.325455355	3.277683174
H	0.429616203	-1.150641511	3.147812708
H	-1.004532302	-2.044162093	3.675813390
H	1.698695371	-3.522885962	0.314216528
H	0.932672711	-3.929235773	1.858137243
H	0.667418485	-3.636978640	-1.671626856
H	-0.713174685	-3.018488850	-2.598831523
H	-0.888270342	-4.482682265	-1.627408260

H	-2.809206829	-1.999018548	-2.415286078
H	-3.973913071	-1.303438375	-1.272348289
H	-3.739410781	-3.057109272	-1.350054847
H	-3.144282388	0.078532495	2.169216636
H	-3.929949612	-1.503092332	2.201014051
H	-4.151627228	-0.432152009	0.805693811
H	-2.622852571	5.701653729	0.392892660
H	5.623033479	1.638474457	-0.028838058
H	2.626953449	3.510334286	0.257632261
H	0.694364099	4.471223170	0.308113093
H	6.084158476	-3.002923950	-2.935641661
H	7.024954694	-1.892542013	-2.469424050
H	5.422720299	-3.629443895	1.248750032
H	6.438852219	-2.499161374	1.408634148

4c$_{Na\_2w}$

C	1.088352219	3.210571592	0.257500701
C	-1.900058909	3.458617834	0.107767383
C	0.255818034	2.158734962	0.016863277
C	-1.216311879	2.271991403	-0.042869726
N	0.735313662	0.888785014	-0.235121759
N	-1.867614337	1.102731540	-0.306313891
C	2.113052832	0.732415989	-0.356746862
C	-3.240500488	1.126467705	-0.573589873
N	2.973424565	1.742094648	-0.075604028
N	-3.955389537	2.279989860	-0.350565248
C	2.523691935	2.987240086	0.261621723
C	-3.299955175	3.373967188	-0.023176129
O	-4.005628643	4.506532458	0.189682544
O	3.328721115	3.914536316	0.547241827
O	2.576189918	-0.382237930	-0.751800097
O	-3.810890322	0.111686870	-1.022337822
Ir	-0.677423132	-0.652519845	-0.149018596
C	-1.593714243	-2.657002612	-0.545726773
C	-0.131961401	-2.793889668	-0.523615202
C	0.333506902	-2.428824209	0.771324723
C	-0.820093342	-1.984156766	1.539018370
C	-2.015309363	-2.206446211	0.738021720
C	-0.801268521	-1.584950712	2.978009334
C	1.713807105	-2.570381089	1.330624023
C	0.685524287	-3.327874966	-1.654873599
C	-2.460875910	-3.060143081	-1.694280347
C	-3.414529748	-2.068176907	1.249497850
Na	4.776860677	0.197938161	-0.232696357
O	6.241633297	0.265314907	-1.969751128
O	5.660651985	-0.400618497	1.773916739
H	2.005832226	-1.692760386	1.913089231
H	-1.627511878	-0.911169667	3.215543247
H	0.138950336	-1.097117718	3.244662793
H	-0.906627148	-2.478997359	3.606384420
H	2.455907181	-2.733099360	0.549375734
H	1.732399326	-3.435431499	2.005112757
H	1.736369725	-3.049997848	-1.559375085
H	0.315087251	-2.966962436	-2.617858394
H	0.623530111	-4.423439588	-1.667798102
H	-2.007349715	-2.785981700	-2.650364833
H	-3.449750060	-2.603617188	-1.636198488
H	-2.589117453	-4.150051757	-1.690896572
H	-3.524786761	-1.185538834	1.884631241
H	-3.656765028	-2.946295952	1.860738724
H	-4.141095664	-2.002013092	0.440645344
H	-4.946102313	4.301359634	0.048124210
H	0.717679336	4.206820454	0.460248651
H	-1.416113213	4.400806016	0.320422868
H	6.773089409	-0.535595245	-2.085790416
H	6.895673579	0.977138433	-1.910039055
H	6.250615547	-1.168249283	1.755695825
H	6.195593945	0.301019200	2.173132212

3a_f$_{Na\_2w}$

C	-2.861426328	2.399892759	0.407721074
C	-3.832404442	-0.362136027	-0.173965271
C	-2.009764736	1.340838171	0.163781299
C	-2.492793787	-0.029366611	-0.116555830
N	-0.662395728	1.498134817	0.095535371
N	-1.519052580	-0.932746452	-0.380323063
C	-0.130664538	2.776022198	0.183842883
C	-1.864405921	-2.191899802	-0.868040085
N	-0.941019213	3.848898688	0.451398640
N	-3.184968352	-2.580270777	-0.858578702
C	-2.240620547	3.649966596	0.562641137
C	-4.102704481	-1.698013151	-0.519315407

O	-5.398156908	-2.088724602	-0.513614101
O	-3.032210415	4.710463694	0.830661610
O	1.104407385	2.958346476	0.020427864
O	-0.986415329	-2.962909871	-1.313786299
Ir	0.489399151	-0.334064954	0.000302682
C	0.997507228	-2.026264454	1.338659692
C	1.992196314	-1.952150903	0.306257332
C	2.700665900	-0.683212196	0.466377843
C	2.118728128	0.019025072	1.557337393
C	1.007895015	-0.773851342	2.069426178
C	2.619138595	1.278072460	2.190735063
C	3.931081215	-0.302679949	-0.295846638
C	2.402331963	-3.038198952	-0.640245225
C	0.142233376	-3.205594195	1.681032988
C	0.217904346	-0.474401882	3.307205355
O	2.187835421	1.167909694	-2.695942281
C	1.156140602	0.526390180	-2.985713950
O	0.359924380	-0.091656846	-2.200296190
Na	2.448373500	3.180345859	-1.725725208
O	1.898355171	4.864266836	-3.159029736
O	4.523655270	3.472425734	-0.785536972
H	4.128412207	0.770009120	-0.252204002
H	1.799837405	1.923325652	2.514857912
H	3.266146295	1.848667837	1.522374986
H	3.203385246	1.012275082	3.081119885
H	3.862527086	-0.600108954	-1.344219781
H	4.796152532	-0.820982206	0.137897178
H	2.693608801	-2.627405038	-1.610726347
H	1.599943418	-3.759187221	-0.802470509
H	3.268269586	-3.579813527	-0.238959053
H	0.068978788	-3.911798142	0.854993957
H	-0.867139447	-2.906168026	1.973497882
H	0.591520665	-3.724485682	2.537056898
H	0.076879488	0.600951261	3.440834867
H	0.740150964	-0.854034363	4.194461138
H	-0.766984630	-0.946637941	3.272110220
H	0.861469702	0.456379394	-4.050731092
H	-5.425452123	-3.022206657	-0.785774583
H	-3.935174997	2.297315925	0.466698107
H	-4.630256770	0.337415786	0.028697940
H	-2.464104631	5.497767335	0.893432294
H	2.060200263	5.739910686	-2.778502524
H	2.430551935	4.856030984	-3.967990226
H	4.454649764	3.414321274	0.179152331
H	5.139514966	2.762323726	-1.018917238

4c_f$_{Na_2w}$

C	-2.839418735	2.399030766	0.445331606
C	-3.826102256	-0.357600703	-0.181413449
C	-2.002290212	1.349243650	0.181071598
C	-2.486029926	-0.016351861	-0.117706576
N	-0.643711191	1.501798696	0.098372277
N	-1.513712925	-0.919961318	-0.390304824
C	-0.131348062	2.789744763	0.198283750
C	-1.855200400	-2.176567084	-0.887316702
N	-0.916840153	3.856781425	0.472609077
N	-3.173661464	-2.566337902	-0.892208096
C	-2.266508277	3.712747822	0.632627092
C	-4.092603249	-1.685993700	-0.543798674
O	-5.389176510	-2.082307584	-0.550487334
O	-2.994324310	4.709501931	0.922671366
O	1.121281924	2.958171155	0.023285879
O	-0.971810584	-2.945946504	-1.330959817
Ir	0.490027642	-0.324278842	0.003729840
C	0.991599073	-2.026008771	1.336840794
C	1.995653967	-1.956364824	0.316538152
C	2.701247461	-0.686461406	0.479313848
C	2.116892418	0.016253444	1.568547400
C	0.998319515	-0.772389130	2.069423469
C	2.625959322	1.266897782	2.212530424
C	3.935711926	-0.305420649	-0.277159902
C	2.411609875	-3.044013433	-0.626144886
C	0.130019419	-3.202699560	1.674568435
C	0.203974050	-0.475583240	3.305505554
O	2.225691067	1.147815854	-2.716720977
C	1.183038208	0.518378988	-2.998246232
O	0.378733832	-0.079270765	-2.206935324
Na	2.403467445	3.176402183	-1.739954191
O	1.850466288	4.830666028	-3.212672562
O	4.496356659	3.484766073	-0.818552151
H	4.127708227	0.768539987	-0.238939161

H	1.811672708	1.915329777	2.542806273
H	3.275014687	1.839736822	1.547861087
H	3.210194056	0.990822162	3.099922237
H	3.874309307	-0.607898699	-1.324606719
H	4.801096929	-0.817237014	0.163735094
H	2.712446661	-2.634944699	-1.594568927
H	1.607819715	-3.761917690	-0.796085756
H	3.271962781	-3.590175697	-0.218683883
H	0.057543763	-3.908392031	0.847869091
H	-0.880010005	-2.899239601	1.960853986
H	0.570992275	-3.724479491	2.533220449
H	0.071689073	0.600051808	3.446187291
H	0.716289198	-0.866239365	4.193916123
H	-0.785445583	-0.937655272	3.260878391
H	0.887440116	0.443003898	-4.063169414
H	-5.408163857	-3.012345243	-0.834167169
H	-3.913332158	2.277410847	0.507182088
H	-4.624886074	0.338562807	0.029462115
H	1.990572920	5.713787864	-2.840730781
H	2.398700391	4.820051224	-4.010731614
H	4.417871211	3.416607429	0.144836861
H	5.107152242	2.770927710	-1.053630619

3a_f$_{\text{r-Na1\_2w}}$

C	-2.828214502	2.252261472	-0.392890814
C	-0.215778197	3.711009560	-0.228195970
C	-1.615802884	1.621586445	-0.189749119
C	-0.322767884	2.338681003	-0.120636147
N	-1.529302025	0.286644790	0.040546375
N	0.750331673	1.550282998	0.136711731
C	-2.686651240	-0.434783779	0.241400862
C	1.985077470	2.139744668	0.403735421
N	-3.910269339	0.143802671	-0.002561888
N	2.135810104	3.500191497	0.253808319
C	-3.962597351	1.426759836	-0.319070604
C	1.080567131	4.227082725	-0.049744422
O	1.237631849	5.563582401	-0.189174786
O	-5.163886356	1.983008965	-0.563783324
O	-2.650102969	-1.625454057	0.656332693
O	2.951814437	1.441834221	0.781241034
Ir	0.437964171	-0.558725826	0.031970353
C	2.148368639	-1.973196917	-0.203233207
C	0.902324516	-2.740107489	-0.173654711
C	0.112789341	-2.340894154	-1.293536531
C	0.822725479	-1.286589067	-2.002513291
C	2.108647015	-1.122408320	-1.355944497
C	0.414383059	-0.697621490	-3.318951693
C	-1.168027711	-2.955289241	-1.764168457
C	0.577524489	-3.812896183	0.819061589
C	3.319703558	-2.188639612	0.704976680
C	3.220757651	-0.271134902	-1.882596248
C	1.093768462	-0.418160207	3.041176367
O	0.956734977	-0.529129150	4.268712566
O	0.111901071	-0.441176240	2.198185055
Na	-4.935292348	-1.966279838	0.681065203
O	-6.053799909	-2.072319728	2.652379536
O	-5.934404189	-3.186462759	-0.948888165
H	-1.866216532	-2.203436179	-2.140046235
H	0.868334091	0.283566652	-3.478359422
H	-0.670764704	-0.586234589	-3.385056510
H	0.732128328	-1.349536602	-4.142672818
H	-1.662133511	-3.529158572	-0.980545222
H	-0.941368259	-3.636532978	-2.594237288
H	-0.498021715	-3.991977327	0.878746987
H	0.936990795	-3.552014230	1.818281615
H	1.061317015	-4.754393439	0.530798695
H	3.000930535	-2.487956612	1.706381223
H	3.928818697	-1.287042518	0.794454478
H	3.959198945	-2.988134506	0.309661595
H	2.847826987	0.660267722	-2.315608431
H	3.732845970	-0.821865455	-2.681870502
H	3.953114833	-0.027632091	-1.113900027
H	2.098145423	-0.276202391	2.605084607
H	2.173671089	5.769599739	-0.022537093
H	-2.923276705	3.310149124	-0.590353380
H	-1.055783380	4.361433648	-0.424427326
H	-5.845049266	1.295176292	-0.463304589
H	-5.523124703	-2.433685282	3.377554384
H	-6.338023945	-1.205494369	2.977562761
H	-6.846143722	-2.912246656	-1.126677752
H	-6.009496575	-4.127239609	-0.731232760

4c_f$_{r\text{-}Na1_2w}$

C	-2.851215926	2.202222993	-0.416014289
C	-0.252812329	3.698255432	-0.257580806
C	-1.641396059	1.592465041	-0.222033665
C	-0.356636892	2.323438906	-0.143610274
N	-1.532819427	0.247084141	0.011708134
N	0.723939494	1.549414132	0.128515176
C	-2.693523519	-0.468123344	0.220665140
C	1.950766015	2.149568241	0.407688571
N	-3.916784455	0.084387199	0.001752665
N	2.093833022	3.509118645	0.257855543
C	-4.053471975	1.400731392	-0.343004466
C	1.033735088	4.224216152	-0.064547324
O	1.185890578	5.563738085	-0.205903153
O	-5.196337659	1.900157759	-0.558403858
O	-2.627932210	-1.672563172	0.640513385
O	2.919942900	1.458310639	0.797291523
Ir	0.435238381	-0.562306502	0.015181685
C	2.162542676	-1.982468432	-0.198111524
C	0.911559030	-2.742803900	-0.202370922
C	0.147078033	-2.329548292	-1.335207283
C	0.872703659	-1.265447461	-2.011878581
C	2.149293630	-1.117246410	-1.336600527
C	0.498676684	-0.662094975	-3.332491702
C	-1.121424956	-2.939798007	-1.844849740
C	0.568211752	-3.831680210	0.766843070
C	3.313251986	-2.213431432	0.733125875
C	3.273492960	-0.263114486	-1.833380676
C	1.074460793	-0.434936253	3.035158317
O	0.934611203	-0.554647009	4.262533319
O	0.098081215	-0.457554341	2.187975521
Na	-4.924474346	-1.937259915	0.722307766
O	-6.004159137	-2.025920367	2.734549363
O	-6.025187044	-3.216246205	-0.814761497
H	-1.807040356	-2.184375525	-2.236826358
H	0.953161190	0.322542626	-3.468293253
H	-0.584625050	-0.552008014	-3.426448793
H	0.840206275	-1.301974999	-4.156310725
H	-1.640663567	-3.512233052	-1.076501067
H	-0.875428206	-3.620037033	-2.670183114
H	-0.507218477	-4.018418767	0.797053007
H	0.900136866	-3.582819359	1.778802397
H	1.064896109	-4.766629393	0.478629123
H	2.971784900	-2.512007495	1.727324069
H	3.930878709	-1.319011064	0.837768594
H	3.952681368	-3.018913917	0.349705749
H	2.912374579	0.684104806	-2.241820641
H	3.785692316	-0.795282021	-2.645141517
H	4.004090120	-0.047330599	-1.054709299
H	2.080458524	-0.284822785	2.604928002
H	2.118511795	5.772220699	-0.024884723
H	-2.939343757	3.265406855	-0.598412259
H	-1.095851805	4.340118716	-0.468759455
H	-5.425531287	-2.335264721	3.447041748
H	-6.268151519	-1.137709092	3.016603472
H	-6.831012276	-2.781057576	-1.130174352
H	-6.338233975	-4.060968207	-0.459290398

3a_f$_{c\text{-}Na_2w}$

C	2.963457215	2.189197602	-0.140494387
C	3.781651705	-0.684110373	0.216034951
C	2.069763253	1.154813548	0.027121012
C	2.472267191	-0.256928281	0.206926267
N	0.727709600	1.372701738	0.100121814
N	1.438548846	-1.112533676	0.424936231
C	0.254176024	2.674335958	0.144079735
C	1.700482280	-2.430793113	0.795091009
N	1.103906794	3.723465604	-0.086260984
N	2.990303597	-2.905755347	0.733909051
C	2.391532487	3.473250043	-0.232029425
C	3.962476455	-2.062652712	0.454500409
O	5.226759939	-2.533186386	0.397130803
O	3.225080191	4.504591219	-0.469631741
O	-0.959946483	2.888391547	0.400108653
O	0.771286527	-3.167904818	1.188276071
Ir	-0.489654943	-0.374180055	-0.078985691
C	-2.200502770	-1.794271818	-0.395431351
C	-2.716127331	-0.426936280	-0.521284365
C	-2.037731831	0.212564761	-1.592852811
C	-1.045331610	-0.723452418	-2.114816965
C	-1.215557368	-1.990698362	-1.406960626

C	-0.215017814	-0.513360799	-3.339433388
C	-2.334451000	1.555848041	-2.180026431
C	-3.840736889	0.131322800	0.291176039
C	-2.723754126	-2.809911751	0.570500707
C	-0.521711217	-3.263805343	-1.771260175
C	-1.720638135	0.233094334	3.239732144
O	-2.509865381	-0.643300550	3.662090507
O	-1.573497972	1.415656850	3.677598981
Na	-1.932243280	3.208741925	2.401004919
O	-4.154971939	3.470814406	1.854610966
O	-1.173241327	5.100464492	3.448581997
H	-1.424409872	2.067659510	-2.501585708
H	0.690444162	-1.123986617	-3.320343772
H	0.072339689	0.534340656	-3.452516338
H	-0.794545470	-0.799887014	-4.226516934
H	-2.867227859	2.199039046	-1.478732791
H	-2.967657213	1.419683596	-3.065610771
H	-3.849665412	1.222966740	0.282215921
H	-3.793932305	-0.210097680	1.327371992
H	-4.794100056	-0.215824548	-0.127777736
H	-2.849036976	-2.380139407	1.568161529
H	-2.058134694	-3.670875634	0.647325978
H	-3.705969599	-3.168383749	0.238060419
H	0.502707372	-3.081168940	-2.104156763
H	-1.060948470	-3.731434957	-2.604424882
H	-0.496748638	-3.968888022	-0.940934693
H	-1.066758050	-0.049366324	2.373716775
H	5.198702688	-3.485747108	0.593860887
H	2.695967655	5.320909767	-0.497867083
H	4.032526774	2.046217152	-0.205604591
H	4.623250086	-0.028817426	0.043281977
H	-4.648929532	2.677461542	2.109588262
H	-4.244655862	3.497731290	0.890553725
H	-0.745123143	5.706278472	2.825958154
H	-0.475967554	4.889366627	4.086747858

4c_f$_{c\text{-}Na_2w}$

C	1.258931774	3.407187883	-0.836129066
C	3.351844330	1.920311873	0.769391073
C	1.131890907	2.115193077	-0.417764523
C	2.160599449	1.373135140	0.340701581
N	-0.027151252	1.404014253	-0.618353680
N	1.812626846	0.095048433	0.657014802
C	-1.141000626	2.089375653	-1.100505652
C	2.600110560	-0.636633089	1.547130014
N	-1.047619719	3.347240368	-1.576925309
N	3.827378858	-0.146021658	1.924806993
C	0.137669264	4.029978813	-1.518224466
C	4.165390741	1.068968888	1.540327099
O	5.371568727	1.548220870	1.920978673
O	0.243425962	5.185304414	-2.018021988
O	-2.270341408	1.493421109	-1.056365268
O	2.182703590	-1.722468209	2.006286403
Ir	0.125789766	-0.677282868	-0.370360036
C	-0.439915846	-2.855998506	-0.249103743
C	-1.494072627	-2.127656318	-0.966161894
C	-0.926373372	-1.553052113	-2.136864135
C	0.501671845	-1.852734536	-2.125395954
C	0.768340524	-2.725041740	-0.987255752
C	1.464073133	-1.539285150	-3.225036153
C	-1.634214413	-0.843824750	-3.247641139
C	-2.934801529	-2.117483467	-0.565676222
C	-0.661318413	-3.690747802	0.971836572
C	2.076364620	-3.404279203	-0.731819215
C	-1.557156796	-0.661033155	3.037019560
O	-2.643533793	-1.295446728	3.163322118
O	-1.393440799	0.465249122	2.484285965
Na	-2.967016020	1.400778155	1.110665216
O	-4.635713088	-0.015930487	1.867558900
O	-3.450902036	3.552603447	1.759506550
H	-1.047380689	-0.002689749	-3.625496161
H	2.492977142	-1.513328658	-2.859074512
H	1.234778738	-0.580256514	-3.695196191
H	1.402612711	-2.315343244	-3.999016079
H	-2.610790103	-0.470695150	-2.938582927
H	-1.784698307	-1.542867419	-4.079532794
H	-3.487935351	-1.319478513	-1.064226515
H	-3.050425984	-2.002176825	0.514403812
H	-3.396349613	-3.073516416	-0.844631094
H	-1.383134436	-3.231096256	1.650901126
H	0.268542507	-3.859810736	1.517545103

H	-1.062425673	-4.669709673	0.679334017
H	2.919619446	-2.730385200	-0.903452107
H	2.181480440	-4.248287837	-1.424608266
H	2.144301585	-3.788359236	0.285707532
H	-0.650872184	-1.144032217	3.459076895
H	5.806911533	0.861808582	2.455442606
H	2.169676490	3.974149401	-0.689100618
H	3.654435507	2.931711289	0.538066020
H	-3.951638815	-0.531764702	2.378160396
H	-4.893891122	-0.607240186	1.146218983
H	-3.309142249	4.171266924	1.028021236
H	-2.850268996	3.866436513	2.451266474

3a_TS$_{d\text{-}Na_2w}$

C	3.142480424	2.057101815	-0.328011373
C	3.590222185	-0.889017910	-0.007789112
C	2.117198362	1.145987378	-0.159078948
C	2.335461384	-0.309641732	-0.016964634
N	0.821852501	1.536985796	-0.043477801
N	1.206166366	-1.035997351	0.174689504
C	0.535849657	2.890314714	0.055720079
C	1.308250319	-2.387482997	0.505727864
N	1.510812458	3.820275033	-0.178765373
N	2.538202984	-3.003582982	0.470037388
C	2.749895194	3.404378286	-0.372527817
C	3.607304294	-2.276474987	0.215891345
O	4.810872432	-2.895191964	0.177571346
O	3.708086424	4.326658511	-0.608020113
O	-0.626628188	3.267599013	0.374838000
O	0.290671988	-3.038398865	0.830739917
Ir	-0.640904871	-0.022306194	-0.120373479
C	-2.549901294	-1.130754489	-0.445500965
C	-2.836114993	0.299277349	-0.509206798
C	-2.130948486	0.833451669	-1.635506277
C	-1.403971199	-0.238413811	-2.282272957
C	-1.694748118	-1.450371057	-1.555154014
C	-0.662939991	-0.140793734	-3.581211364
C	-2.238147845	2.226723523	-2.175420336
C	-3.821598679	1.028410228	0.354782702
C	-3.207892750	-2.108516483	0.482640907
C	-1.269384231	-2.820263363	-1.985514195
C	-0.963094276	-0.301097287	3.116219862
O	-0.170403484	-1.137964356	3.405633108
O	-1.866297083	0.450405514	3.364551600
O	-2.856299661	3.983068293	3.333643102
Na	-1.322537838	2.591687946	2.404411623
O	0.730385336	2.526006724	3.468728025
H	-1.284370085	2.587178665	-2.568571970
H	0.142464653	-0.877340466	-3.642662520
H	-0.227612311	0.851990866	-3.721324231
H	-1.341063388	-0.323941143	-4.425431087
H	-2.591915788	2.933168859	-1.424290315
H	-2.956788876	2.229231853	-3.004873221
H	-3.607895802	2.099940741	0.391858935
H	-3.826239932	0.638411071	1.375571634
H	-4.837080669	0.911874118	-0.045565655
H	-3.413607599	-1.657083368	1.456498319
H	-2.583090021	-2.989313248	0.643208727
H	-4.164825421	-2.447085362	0.065038447
H	-0.269061851	-2.813621430	-2.425946672
H	-1.963760141	-3.182776718	-2.754154799
H	-1.277433828	-3.530998748	-1.159563435
H	-0.634071851	0.052758427	1.551340320
H	4.663625942	-3.839043750	0.360555977
H	3.288609514	5.204471094	-0.604992686
H	4.179935399	1.772567750	-0.426998473
H	4.504340109	-0.333165799	-0.158144309
H	-3.628697877	3.528651478	3.700885727
H	-3.231493086	4.617568926	2.705541886
H	1.474476837	2.466099776	2.851973962
H	0.878848838	1.797522928	4.088843806

4c_TS$_{d\text{-}Na_2w}$

C	3.101592134	2.104964234	-0.235651754
C	3.574122678	-0.844174965	0.010446285
C	2.088105883	1.189429640	-0.129301362
C	2.315652040	-0.266518237	-0.002603572
N	0.774728262	1.566052584	-0.048023859
N	1.192184858	-1.007743115	0.168187683
C	0.497488355	2.922351873	0.061687194
C	1.301217710	-2.360213988	0.493332683
N	1.454251645	3.862733311	-0.094430918

N	2.533294941	-2.969811646	0.462183951
C	2.765389005	3.509771644	-0.270455362
C	3.598799075	-2.230306363	0.220155982
O	4.807321432	-2.845393381	0.184885607
O	3.657277304	4.396362087	-0.431345973
O	-0.703196290	3.276316124	0.334300850
O	0.285243258	-3.019595481	0.812157713
Ir	-0.659885375	-0.011544295	-0.142241634
C	-2.584505665	-1.109577556	-0.457886548
C	-2.843519184	0.323627294	-0.565100482
C	-2.124217953	0.810726443	-1.706120460
C	-1.402418345	-0.287961540	-2.305255707
C	-1.718136673	-1.473500765	-1.541340341
C	-0.644078520	-0.250934932	-3.597738276
C	-2.215204525	2.184126340	-2.297889579
C	-3.828088897	1.096011675	0.262749579
C	-3.264111265	-2.049183321	0.494639560
C	-1.310742409	-2.861049633	-1.933847443
C	-0.970977601	-0.305393630	3.110044885
O	-0.172290841	-1.142193676	3.379640796
O	-1.871376600	0.444777418	3.367702103
O	-2.710667886	3.888629360	3.527172735
Na	-1.267361161	2.565602901	2.365811506
O	0.835935774	2.490193739	3.366270616
H	-1.268447958	2.499466376	-2.743696510
H	0.140757158	-1.011592137	-3.622819097
H	-0.177662757	0.723908506	-3.762259226
H	-1.314522050	-0.442520503	-4.446383543
H	-2.516270396	2.930781085	-1.563345124
H	-2.966636870	2.174957206	-3.097888398
H	-3.592088137	2.163290134	0.273299117
H	-3.853444741	0.736776005	1.294883149
H	-4.841342269	0.988142875	-0.145991624
H	-3.507474539	-1.553201743	1.437676948
H	-2.636959282	-2.914159731	0.720562609
H	-4.203782152	-2.419369483	0.064567929
H	-0.272005382	-2.900296633	-2.272648101
H	-1.939546488	-3.193606315	-2.769584384
H	-1.431289459	-3.571608527	-1.116668485
H	-0.656397861	0.074605645	1.525334197
H	4.659449455	-3.790270178	0.360965343
H	4.141116138	1.808080443	-0.291326464
H	4.484637971	-0.279491419	-0.128755271
H	-3.312185884	3.387827826	4.097631494
H	-3.298399157	4.405504376	2.957030916
H	1.533509172	2.604732921	2.703556821
H	1.083751284	1.676114600	3.828543042

3a_h$_{Na_2w}$

C	-3.216851102	1.539475622	0.453764780
C	-3.377247921	-1.374874947	-0.204740977
C	-2.124267844	0.790115645	0.059568591
C	-2.195080082	-0.658290335	-0.227189738
N	-0.906771894	1.349758349	-0.160619296
N	-1.018583348	-1.221313173	-0.595471458
C	-0.802187484	2.733303818	-0.155074413
C	-1.006264716	-2.533403629	-1.064902846
N	-1.836691905	3.504136295	0.300571804
N	-2.153732419	-3.289601277	-1.004304073
C	-2.978835940	2.914367306	0.604629475
C	-3.268080082	-2.721841140	-0.587318090
O	-4.391709123	-3.475862415	-0.533490142
O	-3.991899580	3.678487813	1.069534552
O	0.250602475	3.287372225	-0.578965205
O	0.041358992	-3.022922083	-1.547726835
Ir	0.731423396	-0.043191502	-0.290664496
C	2.606508135	-1.184269439	0.080906086
C	2.937524811	0.230392208	0.080204358
C	2.249638056	0.839139570	1.180124385
C	1.532076463	-0.192265878	1.911466362
C	1.763781475	-1.427699051	1.238210240
C	0.790813179	0.012561641	3.199151090
C	2.411787578	2.252435794	1.652999815
C	3.954883993	0.885158988	-0.807344330
C	3.282697544	-2.235771708	-0.750571009
C	1.263043230	-2.770526197	1.675108227
Na	1.019315433	2.374547054	-2.483425809
O	2.864781590	3.582519744	-3.057267803
O	-0.548608533	2.501547523	-4.141189598
H	1.486809736	2.651563202	2.075823901
H	0.057013835	-0.778808709	3.372051271

H	0.263698844	0.970713647	3.212014705
H	1.483541634	0.011180949	4.050949875
H	2.743133736	2.918034646	0.854143580
H	3.171038260	2.279190581	2.445359821
H	3.772342302	1.956725759	-0.915017916
H	3.967874172	0.436604823	-1.803852514
H	4.958610379	0.763136460	-0.379364109
H	3.512759044	-1.865903910	-1.753138122
H	2.662715490	-3.128171134	-0.854265872
H	4.229217155	-2.540001794	-0.284639706
H	0.339386825	-2.688517230	2.253315810
H	2.012360397	-3.254649110	2.313786998
H	1.078302634	-3.427263027	0.823384336
H	0.725453078	0.154664322	-1.897871244
H	-4.158801805	-4.373129687	-0.827766080
H	-3.677538168	4.598232899	1.108071788
H	-4.190769477	1.112526125	0.645528396
H	-4.327055966	-0.943909250	0.077099103
H	3.287793285	3.347872163	-3.895978084
H	2.688302521	4.531599397	-3.134667390
H	-0.834363346	3.413734940	-4.297746926
H	-0.231443934	2.200296328	-5.005311186

3a_h$_{Na1_2w}$

C	2.320574418	2.752307940	0.033555586
C	-0.510174232	3.699362734	-0.101901864
C	1.245634746	1.901528227	-0.159953019
C	-0.154294400	2.368560839	-0.228097051
N	1.404369071	0.571382898	-0.376510349
N	-1.062510161	1.399752420	-0.499362976
C	2.682777691	0.079752886	-0.554870687
C	-2.382434998	1.764247415	-0.767357694
N	3.775825139	0.877591582	-0.315158120
N	-2.782042422	3.067571255	-0.586050700
C	3.587291005	2.154794663	-0.023848014
C	-1.877086833	3.971567282	-0.267114194
O	-2.281383093	5.253546159	-0.097325835
O	4.666147105	2.927534293	0.214578980
O	2.873519065	-1.105320226	-0.946193342
O	-3.200511821	0.911070796	-1.182558086
Ir	-0.380056763	-0.624383753	-0.379940448
C	-1.962022234	-2.163912859	-0.057157481
C	-0.692731392	-2.836476738	-0.264242965
C	0.166812375	-2.489929987	0.829437274
C	-0.581682889	-1.664095149	1.765900014
C	-1.877098215	-1.469108956	1.218725757
C	-0.078894870	-1.197512755	3.100084361
C	1.514780497	-3.076528708	1.123615039
C	-0.405474973	-3.844606560	-1.338528271
C	-3.224153454	-2.439000463	-0.823582428
C	-3.005076171	-0.719251182	1.861369816
Na	5.170335362	-1.048480219	-0.946156765
O	6.389217374	-2.152992355	0.617096943
O	6.231248567	-0.970666286	-2.950870078
H	2.188145143	-2.342967908	1.574384878
H	-0.619310306	-0.313697527	3.448915463
H	0.985719128	-0.948784410	3.063477282
H	-0.201783996	-1.979825039	3.861023530
H	1.992402619	-3.475119610	0.227378604
H	1.400727413	-3.901250697	1.839175619
H	0.663164844	-3.912008437	-1.555704903
H	-0.926176370	-3.601172624	-2.267685685
H	-0.743167500	-4.839978331	-1.021538727
H	-3.017658973	-2.629442624	-1.880125462
H	-3.927028412	-1.605947407	-0.764361447
H	-3.728800597	-3.327778566	-0.421358343
H	-2.643809875	0.011364258	2.589391090
H	-3.661853150	-1.418918867	2.393878715
H	-3.612017409	-0.196263855	1.119724239
H	-0.248065197	-0.592215840	-1.977322344
H	-3.240779428	5.282742886	-0.254092303
H	5.461927976	2.377869486	0.109152465
H	2.213650993	3.812355523	0.212015582
H	0.199118945	4.486681642	0.107744000
H	5.981209683	-2.982151710	0.907052961
H	6.523098732	-1.657141969	1.438118715
H	7.176518554	-0.772141211	-2.879017362
H	6.202902090	-1.815666761	-3.423269334

4c_h$_{Na_2w}$

C	-3.181867153	1.554890325	0.394168886
C	-3.346889053	-1.361954249	-0.265278285

C	-2.095591176	0.809912378	0.019356023
C	-2.165239394	-0.638799773	-0.269991819
N	-0.862892934	1.369078299	-0.189515736
N	-0.985582299	-1.210110306	-0.615636828
C	-0.779548636	2.756316535	-0.165490948
C	-0.966035807	-2.522934105	-1.082033819
N	-1.807761825	3.530652619	0.245042875
N	-2.110832775	-3.281573725	-1.034081339
C	-3.014038344	2.977904557	0.577467476
C	-3.231049440	-2.708686800	-0.634775974
O	-4.354923257	-3.467780724	-0.591462937
O	-3.962945624	3.703511345	1.003934564
O	0.309856303	3.304892672	-0.558291811
O	0.089545142	-3.012129947	-1.552624554
Ir	0.761833954	-0.038823440	-0.283582514
C	2.637073335	-1.188909295	0.119157614
C	2.962518153	0.226965108	0.123745626
C	2.257580685	0.834338945	1.214470999
C	1.523054069	-0.196574570	1.926849463
C	1.767198329	-1.431633609	1.253427883
C	0.762270853	0.002562606	3.204362583
C	2.423277313	2.242944925	1.701222525
C	3.993498637	0.886962703	-0.744464000
C	3.328586810	-2.240386688	-0.700226988
C	1.258344080	-2.774931320	1.681140967
Na	0.924006914	2.369218617	-2.474838256
O	2.840541585	3.303885584	-3.299552408
O	-0.741472335	2.599709052	-4.030805525
H	1.495691527	2.645310245	2.115294669
H	0.023355524	-0.787759727	3.360548688
H	0.236339019	0.961502517	3.214042495
H	1.439416480	-0.005209935	4.068845917
H	2.768595606	2.913583161	0.912441152
H	3.173030347	2.258834591	2.503040712
H	3.799702033	1.955326790	-0.863218844
H	4.033305315	0.433497163	-1.737953097
H	4.989466277	0.779456914	-0.294678032
H	3.597473989	-1.863119656	-1.690470897
H	2.701846939	-3.123932162	-0.835537579
H	4.255500588	-2.562276299	-0.207095735
H	0.317845519	-2.694036837	2.231894889
H	1.989316511	-3.254141740	2.344474343
H	1.100791291	-3.436279923	0.827616947
H	0.773042447	0.152570391	-1.892597445
H	-4.112049885	-4.365192937	-0.876464583
H	-4.154540570	1.109171904	0.560526932
H	-4.301181645	-0.930239941	-0.000292398
H	2.994875903	3.174188535	-4.246634577
H	2.841014891	4.265841718	-3.187682808
H	-1.174790350	3.460951377	-3.937340675
H	-0.439229594	2.584408465	-4.950638539

4c_h$_{Na1_2w}$

C	2.470149224	2.628820344	0.101132411
C	-0.313788881	3.755843770	0.096354887
C	1.345979676	1.859892401	-0.057377810
C	-0.027556396	2.409024232	-0.062932963
N	1.409489208	0.516862017	-0.318008691
N	-0.999731629	1.499561706	-0.316401044
C	2.652381986	-0.029310024	-0.566776624
C	-2.297382162	1.939825121	-0.570937929
N	3.796035964	0.681497049	-0.381228557
N	-2.626901103	3.256612705	-0.353469803
C	3.765280768	2.002022543	-0.022927111
C	-1.666060512	4.100996102	-0.028002923
O	-2.004391499	5.398788587	0.182586609
O	4.839656845	2.645136283	0.169229867
O	2.739005187	-1.231930358	-0.994343316
O	-3.161648501	1.141219155	-1.005259364
Ir	-0.429049828	-0.560366248	-0.275080074
C	-1.815639609	-2.309516180	-0.154486186
C	-0.437459663	-2.776491519	-0.073756800
C	0.106523233	-2.291284027	1.174962031
C	-0.895289785	-1.535413654	1.863280594
C	-2.072189921	-1.530805660	1.026246567
C	-0.799748015	-0.959323964	3.245741939
C	1.457961027	-2.633373832	1.727360482
C	0.200103562	-3.799227288	-0.970320135
C	-2.833203387	-2.741563266	-1.170405584
C	-3.394517846	-0.957219385	1.441661799
Na	5.024371279	-1.115972109	-1.320671791

O	6.557501640	-2.355566951	-0.171597842
O	5.581740739	-1.071478690	-3.534251774
H	1.844391531	-1.839254477	2.372064436
H	-1.390733926	-0.043920706	3.341542767
H	0.233283307	-0.721694545	3.514073847
H	-1.176876874	-1.668384531	3.995565861
H	2.185856897	-2.816794243	0.936460713
H	1.385304538	-3.543741214	2.336266490
H	1.280518380	-3.653090429	-1.040466653
H	-0.209754742	-3.753517619	-1.982650405
H	0.025577066	-4.813912845	-0.588192168
H	-2.371568502	-2.939364061	-2.141063991
H	-3.607843160	-1.984539493	-1.316203971
H	-3.330325363	-3.665808140	-0.846936194
H	-3.282251379	0.019116976	1.921698782
H	-3.865781937	-1.627142777	2.172414764
H	-4.077838237	-0.846452934	0.599309928
H	-0.398548856	-0.449064188	-1.876348679
H	-2.963733477	5.474542232	0.042286494
H	2.417493710	3.691162957	0.301839560
H	0.441786480	4.501183234	0.298226361
H	6.181245680	-3.178035303	0.174866352
H	6.884459682	-1.895571922	0.615641595
H	6.436197073	-0.650861024	-3.709674611
H	5.672420986	-1.956685897	-3.916267831

3a_TS$_{f\text{-}Na_2w}$

C	-3.414955085	1.815507924	-0.191718589
C	-3.800900947	-1.171044830	-0.387330264
C	-2.379361125	0.903741350	-0.199752800
C	-2.566412277	-0.559696834	-0.311294209
N	-1.081016592	1.301517949	-0.200660998
N	-1.411689140	-1.263398504	-0.424532793
C	-0.775471751	2.644698765	-0.337746075
C	-1.452473261	-2.615954871	-0.749412868
N	-1.773180976	3.580391584	-0.274188475
N	-2.665289963	-3.265187050	-0.773441743
C	-3.025199656	3.167069173	-0.192041389
C	-3.766137850	-2.563993907	-0.588881501
O	-4.952775451	-3.212268943	-0.603879435
O	-4.002323325	4.094513811	-0.121681488
O	0.417699544	3.003191989	-0.521906275
O	-0.396882136	-3.231520355	-1.019511435
Ir	0.353061907	-0.234533494	0.142223616
C	2.117869771	-1.343451448	1.045838567
C	2.380352538	0.094110256	1.130997355
C	1.368687481	0.676545561	1.951055808
C	0.437846767	-0.371190927	2.342260917
C	0.955152399	-1.623603827	1.830552410
C	-0.696587224	-0.217779902	3.309311464
C	1.305665289	2.090806664	2.434869856
C	3.585931152	0.780097350	0.563194133
C	3.022479448	-2.350518343	0.405164243
C	0.382702103	-2.970100249	2.141818158
C	2.903411411	-0.244874561	-3.366098982
O	2.242135035	-1.103169413	-2.703705541
O	2.867298107	1.004997670	-3.242646851
Na	1.836753518	2.736656514	-2.239972776
O	3.689318918	3.936586174	-1.553272817
O	0.878570803	3.852044862	-4.004223525
H	0.279525105	2.464704426	2.470748829
H	-1.472745804	-0.967795252	3.137737612
H	-1.154883902	0.771230550	3.233073463
H	-0.338705706	-0.339036275	4.339466304
H	1.899528690	2.762522014	1.814589886
H	1.704566791	2.130234754	3.456324153
H	3.436436004	1.858720390	0.475922537
H	3.843930261	0.383728165	-0.422194517
H	4.449584148	0.616421893	1.220125748
H	3.483429610	-1.955504810	-0.502133072
H	2.482978739	-3.263211241	0.143315010
H	3.828189171	-2.622396685	1.098703127
H	-0.710011376	-2.951773892	2.152663624
H	0.715654614	-3.273428490	3.142255974
H	0.711112275	-3.728567320	1.431245944
H	0.512955917	0.073844908	-1.564481738
H	1.193825752	-0.434479775	-1.713453340
H	3.586540039	-0.661554325	-4.136210101
H	-4.457533392	1.531306933	-0.196993865
H	-4.735944324	-0.636467097	-0.301458443
H	-4.775430808	-4.155390793	-0.762091918

H	-3.583598132	4.971987196	-0.154945016
H	3.453937078	4.533335399	-0.827790412
H	4.330553905	3.328880371	-1.155876791
H	-0.056239832	4.053430927	-3.852313610
H	0.876666977	3.312563902	-4.808435487

4c_TS$_{f\text{-}Na_2w}$

C	-3.385541062	1.831644811	-0.188259618
C	-3.797785492	-1.159904744	-0.391965167
C	-2.368521405	0.917015454	-0.196741191
C	-2.561825906	-0.544973113	-0.315491173
N	-1.055844468	1.303333312	-0.203093920
N	-1.411162545	-1.256619567	-0.430345117
C	-0.762279516	2.649589816	-0.351772603
C	-1.455625954	-2.608252017	-0.757726541
N	-1.729784033	3.592686737	-0.311059656
N	-2.667655527	-3.255558151	-0.786156422
C	-3.047592939	3.239848759	-0.188587364
C	-3.766473189	-2.548685758	-0.597677830
O	-4.955150885	-3.199022447	-0.615671176
O	-3.948613896	4.126958060	-0.107629332
O	0.456137523	2.984898424	-0.533582499
O	-0.399336602	-3.226771949	-1.028348452
Ir	0.355373471	-0.238189855	0.145842179
C	2.124613164	-1.350860693	1.058719005
C	2.376342255	0.088591451	1.143543628
C	1.360818095	0.664415416	1.965466859
C	0.434265577	-0.387170575	2.350004195
C	0.958552604	-1.636124652	1.833564893
C	-0.702523537	-0.243260566	3.316539196
C	1.294868888	2.075600557	2.459761384
C	3.578650486	0.784151650	0.578248081
C	3.041563777	-2.351969542	0.424727762
C	0.389297245	-2.986282725	2.138660061
C	2.894507351	-0.238792625	-3.350518397
O	2.240811410	-1.091195973	-2.668588979
O	2.839040886	1.011157264	-3.258827608
Na	1.804563003	2.760383678	-2.275961596
O	3.681528940	3.945819027	-1.597544796
O	0.843688672	3.852244494	-4.062525432
H	0.268442091	2.449252267	2.492020051
H	-1.477555600	-0.992846645	3.137054883
H	-1.163128046	0.745226311	3.245536586
H	-0.349514013	-0.371097660	4.347768176
H	1.890208369	2.752611021	1.846576916
H	1.688883451	2.109707724	3.483350424
H	3.412333547	1.858574041	0.469483114
H	3.852587686	0.376522979	-0.398353868
H	4.439335715	0.646481004	1.245162789
H	3.497408085	-1.958686238	-0.486055899
H	2.514167892	-3.273741869	0.169459095
H	3.852005407	-2.610126552	1.118290164
H	-0.703609657	-2.971987199	2.143821733
H	0.717555328	-3.294585071	3.139189218
H	0.722482580	-3.741317903	1.426329112
H	0.532415875	0.070385638	-1.546414815
H	1.221971390	-0.442035397	-1.716312896
H	3.586226650	-0.668404617	-4.104886125
H	-4.427071959	1.535262436	-0.195856574
H	-4.731189991	-0.622785363	-0.302932800
H	-4.773746321	-4.140225570	-0.779282534
H	3.431027841	4.540978160	-0.875700885
H	4.298351976	3.324865098	-1.182265700
H	-0.080193142	4.074267991	-3.875677457
H	0.793891608	3.270506269	-4.835180923

2b_TS$_{w\text{-}Na1_2w}$

Ir	-0.326312658	-0.733037042	-0.172307932
N	1.240780611	0.743840756	-0.151580657
N	-1.323224308	1.123718134	-0.426301569
C	0.832941791	2.026963063	0.055892270
C	-0.622026174	2.239902416	-0.105448096
C	1.730965849	3.042222380	0.317220450
C	-1.222985055	3.479501539	-0.017333283
C	3.086436272	2.673985034	0.333941821
C	-2.606075581	3.492942958	-0.279648215
N	3.507181021	1.448383225	0.055756313
N	-3.302583984	2.441238136	-0.658730944
C	2.584730432	0.485013893	-0.232675069
C	-2.660317001	1.233078932	-0.801930140
C	-0.097331087	-2.937013806	0.261429210
C	-1.513614604	-2.583205593	0.205921368

C	0.489861398	-2.222641943	1.349662986
C	-0.535794480	-1.398434743	1.968869710
C	-1.776777845	-1.669927145	1.285022750
C	0.572256696	-3.970275461	-0.591457894
C	-2.537323825	-3.227464181	-0.679351919
C	1.882856370	-2.377414876	1.873101881
C	-0.370535722	-0.599422178	3.225607278
C	-3.112710095	-1.132238037	1.691309627
O	-3.267573078	0.245987624	-1.272174481
O	3.011429190	-0.662106421	-0.596432941
O	3.995384518	3.619226472	0.620595258
O	-3.248775091	4.674236163	-0.142091394
O	1.657753111	-1.387533532	-2.703088605
Na	5.265231377	-0.144641104	-0.630219083
O	6.811905864	-0.971664674	0.794511772
O	6.107598794	0.215889236	-2.701407870
H	1.647791179	-3.795150376	-0.663486801
H	0.157414781	-3.987009440	-1.601692512
H	0.423225417	-4.966253891	-0.155760719
H	-3.380408346	-2.559528542	-0.866042331
H	2.559674923	-2.788406469	1.123191761
H	-2.925427613	-4.137491715	-0.205039058
H	2.291031662	-1.430516987	2.234166032
H	-2.107478158	-3.513094044	-1.642364464
H	1.860792822	-3.070858592	2.723459618
H	-1.099025682	0.213042166	3.282618114
H	-3.039025214	-0.108132982	2.065725865
H	0.630208097	-0.165365212	3.295135563
H	-3.827540331	-1.149190809	0.868922170
H	-0.515777565	-1.238547373	4.105780090
H	-3.511499433	-1.752186207	2.503922411
H	-0.366473066	-0.699165332	-1.879097134
H	0.525724057	-1.019494152	-2.069033788
H	2.280193260	-1.154444881	-1.945309528
H	1.818545918	-0.723979854	-3.394880628
H	-4.184084252	4.530090359	-0.368015781
H	4.883063017	3.221656617	0.577726767
H	1.434806925	4.067031342	0.488187452
H	-0.689872254	4.385302891	0.232934595
H	6.725334729	-1.921111078	0.964436544
H	6.803606940	-0.571711909	1.676461634
H	6.948042997	0.696983572	-2.696550734
H	6.301378279	-0.592984596	-3.197604639

3f_TS$_{w\text{-}Na1_2w}$

Ir	-0.344810762	-0.753877588	-0.197775426
N	1.269518600	0.646404448	-0.174535963
N	-1.272068228	1.139106098	-0.421186402
C	0.905417661	1.934158160	0.145221720
C	-0.539081505	2.208708184	-0.024071479
C	1.825747927	2.880472270	0.499629937
C	-1.111667154	3.458227502	0.126073177
C	3.226047749	2.518310035	0.528757118
C	-2.487210991	3.525576377	-0.152233568
N	3.558087144	1.252439539	0.114698855
N	-3.210335335	2.521356878	-0.610467615
C	2.608434768	0.364618054	-0.243170749
C	-2.595902692	1.309195773	-0.817408922
C	-0.066633247	-2.911519445	0.343802188
C	-1.496310633	-2.644077162	0.193705428
C	0.411291493	-2.122448020	1.439793862
C	-0.683178741	-1.313673669	1.936272925
C	-1.870437401	-1.691022199	1.193896407
C	0.699703135	-3.965124383	-0.398108120
C	-2.423148638	-3.378461779	-0.727554921
C	1.781223498	-2.155006788	2.042449369
C	-0.638766323	-0.416191470	3.136395201
C	-3.254802973	-1.212572609	1.500870265
O	-3.216687788	0.366775001	-1.361512804
O	2.995404853	-0.791113249	-0.683539497
O	4.118563540	3.331458532	0.893696190
O	-3.103198573	4.713846157	0.054165734
O	1.621804736	-1.429829655	-2.735847551
Na	5.236955179	-0.155097719	-0.808958521
O	6.937164229	-0.974381198	0.461895158
O	5.944558831	0.272021446	-2.930798612
H	1.769881976	-3.747632133	-0.417757996
H	0.351400173	-4.060785302	-1.429171460
H	0.565508917	-4.940335500	0.086948287
H	-3.303005542	-2.781668500	-0.977475058
H	2.509619472	-2.619802040	1.377472809

H	-2.769930307	-4.303326949	-0.249486608
H	2.134796767	-1.153045234	2.300404482
H	-1.922729582	-3.656464318	-1.658244854
H	1.746233458	-2.738942188	2.970596442
H	-1.395075744	0.370117208	3.073596279
H	-3.267364286	-0.153926676	1.771719442
H	0.339219026	0.061082025	3.239570857
H	-3.936600674	-1.366036352	0.664216118
H	-0.828719519	-0.986350674	4.054667889
H	-3.639453024	-1.775644025	2.360484201
H	-0.405470193	-0.730720829	-1.906769329
H	0.482010013	-1.053770872	-2.089180440
H	2.243903598	-1.196510811	-1.954870756
H	1.781623106	-0.756033449	-3.416955009
H	-4.038157953	4.606942105	-0.191764958
H	1.540797553	3.895084960	0.746251491
H	-0.556342635	4.332243387	0.434750685
H	6.858135031	-1.922632108	0.642147764
H	6.953285924	-0.568531306	1.341179405
H	6.648874791	0.935972473	-2.967205884
H	6.326377870	-0.500617290	-3.372553518

4c_TS$_{b\text{-}Na_2w}$

C	-3.178511885	2.093944546	-0.819430431
C	-3.601060121	-0.879417661	-1.157493967
C	-2.223365339	1.154012130	-0.544646770
C	-2.412975681	-0.299390312	-0.749574125
N	-0.956358393	1.507430716	-0.163314746
N	-1.286814745	-1.039411532	-0.595442925
C	-0.597103901	2.845701516	-0.232611113
C	-1.267433722	-2.374735208	-0.989478290
N	-1.514056282	3.810846649	-0.462184083
N	-2.443422980	-2.990007078	-1.345011732
C	-2.822334700	3.492989346	-0.710608176
C	-3.541763664	-2.259927067	-1.408273154
O	-4.697034321	-2.876937500	-1.756349089
O	-3.688990855	4.402544039	-0.872868841
O	0.635072133	3.151491345	-0.077561105
O	-0.183598077	-3.003236974	-1.026339056
Ir	0.329701033	-0.092216185	0.406840853
C	1.875545256	-1.298036319	1.549752255
C	2.113745302	0.130104064	1.768368683
C	0.969231634	0.669888207	2.433511088
C	-0.017995684	-0.386900629	2.570691912
C	0.585657987	-1.610333671	2.079807472
C	-1.315250309	-0.286838151	3.315611718
C	0.816498267	2.049418080	2.993708592
C	3.410337322	0.837015279	1.512498972
C	2.886627456	-2.273130477	1.028130114
C	-0.038080761	-2.965741206	2.198585028
C	3.560126010	-0.174562531	-2.337332999
O	2.540066846	-0.917163449	-2.176027562
O	3.696515641	1.032193844	-2.029176711
Na	2.076273146	2.606755859	-1.709667031
O	4.619142425	-0.824131915	-2.925068038
O	3.284494872	4.539170238	-2.049516211
O	0.666518085	1.877229197	-3.426867277
H	-0.200781912	2.427457478	2.864998219
H	-2.044313914	-1.012280940	2.945560084
H	-1.752270600	0.710635910	3.224135404
H	-1.162570108	-0.484912185	4.384167887
H	1.509745643	2.757688786	2.539131457
H	1.020152024	2.018191372	4.071519276
H	3.268489401	1.917278779	1.430495444
H	3.888148312	0.482859238	0.596784902
H	4.104299860	0.653275489	2.342692323
H	3.536470618	-1.815209230	0.279455302
H	2.407658960	-3.143656303	0.575182818
H	3.522626210	-2.628658437	1.848865734
H	-1.110459710	-2.938019782	1.987505625
H	0.082650469	-3.318756490	3.230551998
H	0.427492735	-3.693649269	1.534219820
H	0.829985581	0.303781637	-1.204844899
H	1.483137978	-0.267226464	-1.347153062
H	-4.178618976	1.823625478	-1.134262160
H	-4.517987151	-0.322168220	-1.285811383
H	-4.491726811	-3.812816198	-1.923384079
H	5.337335157	-0.175916665	-3.008187811
H	4.109216137	4.524237927	-1.541553864
H	2.793131511	5.284329894	-1.673368235
H	-0.247858294	1.892802919	-3.106665084

H	0.866580874	0.932509449	-3.512645493

3a_d$_{Na1_2w}$

C	2.375799817	2.522981604	0.400217333
C	-0.461516915	3.556161713	0.259763730
C	1.284426855	1.743734901	0.077192203
C	-0.100973637	2.253326790	-0.010741923
N	1.421637667	0.443174912	-0.294413141
N	-0.996474444	1.348546459	-0.483245940
C	2.680487249	-0.080679114	-0.494334795
C	-2.281211021	1.755334328	-0.833172168
N	3.788227751	0.653085874	-0.146643142
N	-2.683996920	3.034016438	-0.525850122
C	3.628784789	1.892517047	0.288732221
C	-1.811461423	3.868881422	0.001169883
O	-2.221043379	5.119828423	0.303134285
O	4.719106155	2.603647330	0.622656800
O	2.833486708	-1.222020900	-1.008353558
O	-3.052141115	0.967422124	-1.423259177
Ir	-0.383859270	-0.676190885	-0.435697516
C	-1.915259720	-2.335808826	-0.069877301
C	-0.572435685	-2.921594245	-0.018811519
C	0.138674193	-2.307731811	1.050583464
C	-0.717422071	-1.276549304	1.629909198
C	-2.015782722	-1.376062319	0.980418013
C	-0.422499267	-0.496716355	2.874876097
C	1.486486583	-2.687728369	1.574303930
C	-0.093292867	-4.046554494	-0.881648099
C	-3.016232587	-2.783213385	-0.980105412
C	-3.238974485	-0.631599674	1.406875968
Na	5.132404341	-1.078191179	-1.251792917
O	6.565751139	-2.534327482	-0.284905759
O	5.823307341	-0.424776309	-3.312047097
H	2.058275201	-1.811941588	1.888989093
H	-1.003070948	0.427699942	2.914434586
H	0.637525684	-0.242689633	2.947348093
H	-0.683077044	-1.092401481	3.758542768
H	2.069302843	-3.245587668	0.840767710
H	1.349898438	-3.325556171	2.456531859
H	0.995559740	-4.053500318	-0.962697145
H	-0.514262371	-3.985067027	-1.887693376
H	-0.406554968	-5.004555955	-0.448743924
H	-2.626154847	-3.105671962	-1.947980781
H	-3.744245998	-1.987763001	-1.150451314
H	-3.544054402	-3.635086525	-0.533915193
H	-3.000617416	0.383697784	1.731973117
H	-3.680967637	-1.155559190	2.263687282
H	-3.987265270	-0.581702929	0.616044971
H	-0.625653704	-0.561699911	-2.253318879
H	0.134862405	-0.857533667	-2.201718512
H	-3.159043410	5.192953805	0.055000863
H	5.505403623	2.049456049	0.474564954
H	2.297955578	3.559289757	0.695773212
H	0.228360014	4.299323471	0.633614844
H	6.232138167	-3.443407059	-0.274221521
H	6.779070802	-2.348575089	0.641257488
H	6.755045266	-0.162185899	-3.342263035
H	5.752690417	-1.123411550	-3.979437240

4c_d$_{Na1_2w}$

C	2.389183185	2.462349049	0.435465562
C	-0.438997502	3.543657080	0.257602484
C	1.299207811	1.712848686	0.092097530
C	-0.079602447	2.237502535	-0.011140624
N	1.419029772	0.405569925	-0.304819827
N	-0.982776660	1.343365605	-0.491460160
C	2.680520106	-0.111750980	-0.507220470
C	-2.263087301	1.758091732	-0.847043363
N	3.789709325	0.585559312	-0.151447828
N	-2.659023290	3.039244548	-0.547809290
C	3.703850653	1.857341006	0.350268470
C	-1.780658967	3.866178672	-0.013148349
O	-2.186473674	5.122802621	0.281725267
O	4.742794701	2.487962734	0.694829600
O	2.808319833	-1.258405581	-1.054295429
O	-3.038119719	0.971834349	-1.438245300
Ir	-0.390738820	-0.685110550	-0.437471321
C	-1.932752247	-2.343082771	-0.059039516
C	-0.588136055	-2.924031512	-0.003358952
C	0.120929549	-2.301886898	1.063745747
C	-0.736038168	-1.266773394	1.631515346
C	-2.033948654	-1.372553722	0.978707586

C	-0.446747381	-0.478180603	2.872855275
C	1.467815097	-2.678073011	1.594059187
C	-0.107931608	-4.059360488	-0.852821315
C	-3.032277171	-2.799922747	-0.967110904
C	-3.256326648	-0.619534158	1.395417846
Na	5.108443202	-1.037956036	-1.282379141
O	6.602958951	-2.482087166	-0.356061485
O	5.788279529	-0.399773572	-3.364429408
H	2.038266463	-1.799345551	1.903054051
H	-1.026396567	0.447292880	2.903147129
H	0.612982375	-0.223717827	2.948730484
H	-0.711852123	-1.065983981	3.760564192
H	2.053557758	-3.238952037	0.864974875
H	1.331701861	-3.310779184	2.480019454
H	0.981167036	-4.068562907	-0.930873758
H	-0.525103901	-4.007937533	-1.861118472
H	-0.423328054	-5.013056783	-0.411855914
H	-2.640981762	-3.128721785	-1.932467376
H	-3.761159305	-2.006703818	-1.144956107
H	-3.560741681	-3.649273364	-0.516699461
H	-3.018368499	0.405880357	1.688173449
H	-3.691481500	-1.117936944	2.270726215
H	-4.011178578	-0.592968287	0.609495131
H	-0.628564733	-0.572784328	-2.246346940
H	0.135817398	-0.866598131	-2.191611073
H	-3.120728953	5.198384009	0.021401764
H	2.303156991	3.498084870	0.738005696
H	0.253951146	4.280575345	0.638157786
H	6.268675194	-3.390757360	-0.334496835
H	6.796342134	-2.279074411	0.570986587
H	6.624814543	0.087527741	-3.343543580
H	5.961757508	-1.138423735	-3.965996594

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