Electronic Supplementary Material (ESI) for Dalton Transactions.
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Table S2: Electronic energies, Zero-Point Vibrational Energies, Thermal Energies, Entropies and relative free energies for species calculated at B3LYP\LANL2DZ. for structures described in Figures 4 and 8. Italicized relative free energy values are in kcal mol^{-1} while values in parentheses are in kJ mol^{-1}.

Structure	Electronic energy (Hartrees)	ZPE (kcal mol^{-1})	$H_{298}^{o} - H_{0}^{o}$ (kcal mol^{-1})	Entropy (cal mol^{-1} K^{-1})	Relative free energy at 298 K
1A	-1639.2886242	312.6	19.6	196.8	*0.0* (0.0)
$TS_{(1A\rightarrow 1D)}$	-1639.2696380	312.8	19.8	200.6	*11.1* (46.4)
1D	-1639.2817215	312.8	20.0	202.8	*3.1* (13.0)
$TS_{(1D\rightarrow 1E)}$	-1639.2682464	311.8	19.8	199.7	*11.3* (47.3)
1E	-1639.285837	312.6	19.8	199.3	*1.1* (4.6)
$TS_{(1E\rightarrow 2C)}$	-1639.1570269	307.9	20.5	208.7	*75.2* (314.6)
2C	-1639.2923679	311.7	21.1	221.7	*-9.2* (-38.5)
2B + CO_2	-1639.288777	312.0	20.5	235.1	*-11.3* (-47.3)
$TS_{(2B\rightarrow 3A)}$ + CO_2	-1639.232367	309.8	20.6	241.0	*20.3* (84.9)
3A + CO_2	-1639.262436	310.4	20.9	244.4	*1.3* (5.4)
$TS_{(3A\rightarrow 4A)}$ + CO_2 + HCOOH	-1639.101313	305.2	21.1	283.6	*85.6* (358.2)
4A + CO_2 + HCOOH	-1639.229491	307.3	21.7	256.1	*7.2* (-30.1)