Supporting Information (SI) for Publication

Bimolecular sinks of Criegee intermediates derived from Hydrofluoroolefins – A Computational Analysis

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S1. Breakdown of different types of rate constants

S1.1 Conditions Applied to Calculations determined using MESMER

The purpose of this section is to provide a summary of **all MESMER calculations used** in this *HFO-sCI + co-reactants* study and this section outlines: the different *grainsizes* used for that reaction system; what channels in that system are barrierless; what channels do not use Eckart Functions; and the temperatures and pressures applied to that system.[1] Determination of the rate constants (k_{ME}) and product branching ratio (Γ_{THEO}) values are vital in determining the atmospheric chemistry of each reaction. For reactions that do not proceed via intermediate product(s) (referred to a single-step reactions) only one MESMER calculation, with a single grain size, is required to determine both the k_{ME} & Γ_{THEO} values. One examples of a reaction series which does not produce intermediate products is the sCI + MeOH reactions. However, the determination of k_{ME} & Γ_{THEO} values of multi-step reaction systems (e.g. sCI + HCHO reactions) are more complex and often require splitting MESMER calculations into two operations: a full calculation involving all stationary point structures of the reaction system to determine the Γ_{THEO} values, which are calculated using all stationary point structures of the potential energy surface (reactants, pre-reaction complexes, transition states, the intermediate products and post-reaction complexes); and those used to calculate the k_{ME} values, which only contain the stationary points in the first step of the reaction prior to the fragmentation of any intermediate product. Systems which involve larger numbers of atoms, and/or a larger number of stationary points are more computationally costly to calculate and so the grainsize for MESMER calculation is adjusted to provide greater computational efficiency. The grainsize used to calculate the k_{ME} & Γ_{THEO} values for each reaction system in this study is found in *Table S1*.

Several other factors are also noted in *Table S1* including at what temperatures and pressures these calculations were ran and whether any *barrierless* pathways and/or Eckart Functions were included into these MESMER calculations. Some systems do include bimolecular association and/or unimolecular dissociation channels that proceed between reactant(s) and product(s) via a asymptotic minimum energy pathway, with no local maximum. To determine whether these *barrierless* unimolecular dissociations contribute significantly to the fragmentation of intermediate products, a *reverse ILT method* needs to be included in the MESMER calculations of the Γ_{THEO} values. The reason that the dipole-dipole capture limits of these processes are noted in *Table S1* is because they are required to determine the Γ_{THEO} values of final products that emerge from unimolecular dissociation channels.[2,3] For more details on the dipole-dipole capture limit ($k_{d\text{-}d}$) see Section S3. Often it becomes impractical to calculate an Eckart function for certain very low transition state barriers and so, in *Table S1*, it is noted whether a *Eckart* tunneling function has been excluded from MESMER calculations and to which transition state barriers this *Eckart* tunneling function would have applied. The author also notes, in *Table S1*, under what range of temperature and pressure conditions these results were obtained. To determine the accuracy of the results calculated here, some additional temperature and pressure conditions are only applied to certain reactions, where existing k_{EXP} & Γ_{EXP} results from the literature have been obtained using equivalent conditions.

Table S1: The conditions applied to each reaction system calculated using MESMER: Including the grain sizes used for calculations; Transition States that do not apply an Eckart function; Reaction channels without TS minima referred to as "Barrierless"; and the Temperatures and Pressures applied to each system.

Reaction system	**Grain size** to determine k_{ME}	TSs without Eckart Functions	Barrierless channels and their $k_{d\text{-}d}$ value	**Grainsize** to determine Γ_{THEO}	**Temperatures (K) and Pressures (Torr)**
sCI 1 + HCHO	grainsize 10	N/A	N/A	grainsize 15	At 760 Torr: 200, 275, 298, 325 & 400 K
sCIs 2 & **3** + HCHO, and **sCI 1** + CF_3CHO	grainsize 10 (grainsize 5 **sCI 3** + HCHO)	N/A	**sCI 1** + CF_3CHO TSc 1 & 2 ($k_{d\text{-}d}$ ~ 6.50×10^{-10} cm^3 s^{-1})	grainsize 40.	At 760 Torr: 200, 275, 298, 325 & 400 K
sCIs 2 & **3** + HCHO, and **sCI 1** + CF_3CFO	**sCI 5** + HCHO – grainsize 5 **sCI 1** + CF_3CFO – grainsize 10	**sCI 26** + HCHO TSc	**sCI 4** + HCHO TSc ($k_{d\text{-}d}$ ~ 7.20×10^{-10} cm^3 s^{-1})	grainsize 40.	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 1 + SO_2	N/A	N/A	**sCI 1** + SO_2 ($k_{d\text{-}d}$ ~ 7.25×10^{-10} cm^3 s^{-1})	grainsize 20	At 760 Torr: 200, 275, 298, 325 & 400 K
sCIs 2 & **3** + SO_2	grainsize 10	**sCI 2** + SO_2	**sCI 3** + SO_2 ($k_{d\text{-}d}$ ~4.08×10^{-10} cm^3 s^{-1})	**sCI 2** + SO_2: grainsize 50 **sCI 3** + SO_2: grainsize 40.	At 760 Torr: 200, 275, 298, 325 & 400 K
sCIs 4 & **5** + SO_2	N/A	N/A	**sCIs 4** & **5** + SO_2 ($k_{d\text{-}d}$ ~ 4.51 & 4.42×10^{-10} cm^3 s^{-1})	grainsize 50	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 1 + HNO_3	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 2 + HNO_3	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 3 + HNO_3	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 4 + HNO_3	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 5 + HNO_3	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 1 + TFA	N/A	N/A	**sCI 1** + TFA TS ($k_{d\text{-}d}$ ~7.54×10^{-10} cm^3 s^{-1})	N/A	-295 K Pressures: 27, 31, 35 & 760 Torr -At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 2 + TFA	N/A	N/A	**sCI 2** + TFA TS ($k_{d\text{-}d}$ ~4.96×10^{-10} cm^3 s^{-1})	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K

sCI 3 + TFA	N/A	N/A	**sCI 3** + TFA TS ($k_{d\text{-}d}$ ~3.98 × 10^{-10} cm^3 s^{-1})	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 4 + TFA	N/A	N/A	**sCI 4** + TFA TS ($k_{d\text{-}d}$ ~4.35 × 10^{-10} cm^3 s^{-1})	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 5 + TFA	N/A	N/A	**sCI 5** + TFA TS ($k_{d\text{-}d}$ ~4.27 × 10^{-10} cm^3 s^{-1})	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 1 + H_2O	grainsize 10	N/A	N/A	N/A	-At 293 K & 50 Torr; 297 K & 760 Torr -At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 2 + H_2O	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 3 + H_2O	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 4 + H_2O	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 5 + H_2O	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 1 + $(H_2O)_2$	grainsize 25	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 2 + $(H_2O)_2$	grainsize 25	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 3 + $(H_2O)_2$	grainsize 25	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 4 + $(H_2O)_2$	grainsize 25	**sCI 4** + $(H_2O)_2$ $TS_{(H_2O)_2}$ 1, 2, 3 & 4	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 5 + $(H_2O)_2$	grainsize 25	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 1 + MeOH	grainsize 10	N/A	N/A	N/A	-At 295 K & 90 Torr; 262.1 K & 100 Torr -At 10 Torr: 254.5, 292.6 & 327.8 K -At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 2 + MeOH	grainsize 15	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 3 + MeOH	grainsize 15	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 4 + MeOH	grainsize 25	N/A	**sCI 4** + MeOH $TS_{AAAH}1$ ($k_{d\text{-}d}$ ~ 5.50×10^{-10} cm^3 s^{-1})	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 5 + MeOH	grainsize 25	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 1 + H_2S	grainsize 10	N/A	N/A	N/A	-At 100 Torr: 278, 299 & 318 K -At 299 K & 250 Torr; 299 K & 500 Torr -At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 2 + H_2S	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 3 + H_2S	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K

sCI 4 + H_2S	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 5 + H_2S	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 1 + HCl	grainsize 25	N/A	N/A	N/A	-At 295 K with 27, 31 & 35 Torr -At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 2 + HCl	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 3 + HCl	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 4 + HCl	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 5 + HCl	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 1 + HF	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 2 + HF	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 3 + HF	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 4 + HF	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K
sCI 5 + HF	grainsize 10	N/A	N/A	N/A	At 760 Torr: 200, 275, 298, 325 & 400 K

S1.2 Master Equation rate constants (k_{ME}) Calculated using MESMER

Table S2: Master Equation (k_{ME}) rate constants for all non-barrierless reactions between 200 – 400 K. (For rate constants of all barrierless reactions see Section S3)

Co-reactant	sCI	Grain size	k_{ME} (cm^3 molec.$^{-1}$ s^{-1})				
			200 K	275 K	298.15 K	325 K	400 K
HCHO	**1**	10	2.77E-11	3.48E-12	2.79E-12	2.25E-12	1.40E-12
	2	10	2.02E-12	3.69E-13	2.69E-13	1.98E-13	1.11E-13
	3	10	2.27E-11	3.32E-12	2.49E-12	1.82E-12	8.59E-13
	5	5	4.59E-11	2.12E-11	1.66E-11	1.25E-11	5.86E-12
CF_3CFO	**1**	10	2.27E-10	2.92E-12	1.98E-12	1.32E-12	5.11E-13
SO_2	**2**	10	9.81E-12	2.52E-12	1.90E-12	1.41E-12	7.20E-13
HNO_3	**1**	15	3.89E-04	5.48E-08	8.22E-09	1.21E-09	3.95E-11
	2	15	5.47E-09	5.11E-11	2.06E-11	8.69E-12	1.70E-12
	3	15	1.99E-07	3.03E-10	8.87E-11	3.29E-11	8.53E-12
	4	15	4.03E-05	2.85E-07	9.51E-08	3.07E-08	2.44E-09
	5	15	2.97E-07	8.58E-11	7.57E-11	6.64E-11	4.30E-11
HF	**1**	10	2.24E-12	4.31E-13	3.32E-13	2.62E-13	1.71E-13
	2	10	2.51E-19	3.63E-18	6.67E-18	1.24E-17	4.79E-17
	3	10	2.44E-15	2.59E-15	2.86E-15	3.23E-15	4.48E-15
	4	10	5.35E-10	2.05E-11	1.19E-11	7.20E-12	2.73E-12
	5	10	2.41E-12	4.90E-13	3.66E-13	2.78E-13	1.64E-13
HCl	**1**	5	7.60E-08	8.37E-10	4.70E-10	3.21E-10	1.99E-10
	2	5	1.46E-14	3.34E-14	4.04E-14	4.93E-14	7.76E-14
	3	5	4.26E-10	9.05E-11	7.28E-11	5.72E-11	3.23E-11
	4	5	4.18E-10	2.05E-10	1.64E-10	1.28E-10	6.67E-11
	5	5	3.92E-09	1.42E-10	1.13E-10	8.66E-11	4.51E-11
H_2S	**1**	10	4.04E-15	6.31E-15	7.06E-15	8.00E-15	1.09E-14
	2	10	2.73E-17	1.37E-16	1.96E-16	2.84E-16	6.49E-16
	3	10	4.34E-15	5.36E-15	5.72E-15	6.18E-15	7.67E-15
	4	10	3.02E-12	7.91E-13	6.08E-13	4.74E-13	3.00E-13
	5	10	1.61E-14	1.26E-14	1.23E-14	1.21E-14	1.26E-14
H_2O	**1**	10	1.35E-17	8.04E-17	1.18E-16	1.73E-16	4.00E-16
	2	10	1.63E-20	6.27E-19	1.35E-18	2.90E-18	1.47E-17
	3	10	1.61E-17	7.99E-17	1.12E-16	1.59E-16	3.37E-16
	4	10	8.71E-11	8.15E-12	5.13E-12	3.23E-12	1.24E-12
	5	10	1.43E-12	3.06E-13	2.27E-13	1.69E-13	9.66E-14
$(H_2O)_2$	**1**	25	3.18E-09	9.88E-12	3.28E-12	1.22E-12	2.18E-13
	2	25	1.15E-09	7.04E-12	2.71E-12	1.09E-12	1.62E-13
	3	25	5.60E-09	7.50E-12	3.74E-12	1.96E-12	4.00E-13
	4	35	2.71E-06	2.21E-06	1.14E-06	4.91E-07	3.65E-08
	5	45	1.05E-07	8.51E-09	1.46E-09	1.30E-09	1.91E-10
MeOH	**1**	10	2.65E-14	1.34E-14	1.20E-14	1.09E-14	9.48E-15
	2	10	2.55E-17	7.34E-17	9.43E-17	1.23E-16	2.28E-16
	3	10	1.86E-13	4.32E-14	3.30E-14	2.57E-14	1.62E-14
	4	10	*1.10E-10*	*6.08E-11*	*5.17E-11*	*4.27E-11*	*2.52E-11*
	5	20	6.92E-09	7.91E-11	3.31E-11	1.04E-11	2.22E-12

S1.3 Canonical Rate constants (k_{CAN}) calculated by MESMER

*Note: **sCI 4** + HCHO; **sCI 1** + CF_3CHO; **sCIs 1,3,4** & **5** with SO_2; and **sCIs 1 – 5** with TFA are barrierless reactions (see IRCs in section S7) and so are not included in this section*

*Table S3: Overall Canonical Rate Constants (k_{CAN}) of HCHO + **sCIs 1-3**, and **5** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, and k_2)*

sCI#	T (K)	k_{CAN} (cm^3 $molec.^{-1}$ s^{-1})	k_1 (cm^3 $molec.^{-1}$ s^{-1})	k_{-1} (s^{-1})	k_2 (s^{-1})
1	200	1.82E-09	9.99E-11	7.83E+10	1.43E+12
	275	5.66E-11	1.00E-10	2.44E+12	1.38E+12
	298	2.83E-11	1.00E-10	4.81E+12	1.36E+12
	325	1.45E-11	1.00E-10	9.29E+12	1.34E+12
	400	3.81E-12	1.00E-10	3.40E+13	1.29E+12
2	200	2.65E-12	1.01E-10	4.56E+10	1.20E+09
	275	4.17E-13	1.01E-10	9.49E+11	3.93E+09
	298	2.94E-13	1.01E-10	1.70E+12	4.98E+09
	325	2.11E-13	1.00E-10	2.99E+12	6.26E+09
	400	1.13E-13	1.00E-10	8.81E+12	9.95E+09
3	200	2.52E-10	1.01E-10	2.19E+10	5.48E+10
	275	1.15E-11	1.01E-10	9.49E+11	1.08E+11
	298	6.24E-12	1.01E-10	2.00E+12	1.24E+11
	325	3.45E-12	1.01E-10	4.11E+12	1.41E+11
	400	1.08E-12	1.00E-10	1.70E+13	1.83E+11
5	200	5.61E-08	1.01E-10	1.02E+09	5.71E+11
	275	5.31E-10	1.00E-10	9.80E+10	5.20E+11
	298	2.10E-10	1.00E-10	2.42E+11	5.07E+11
	325	8.46E-11	1.00E-10	5.83E+11	4.93E+11
	400	1.39E-11	1.00E-10	3.35E+12	4.63E+11

*Table S4: Overall Canonical Rate Constants (k_{CAN}) of CF_3CFO + **sCI 1** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, k_2, k_3, k_{-3}, and k_4))*

sCI#	T (K)	k_{CAN} (cm^3 $molec.^{-1}$ s^{-1})	k_1 (cm^3 $molec.^{-1}$ s^{-1})	k_{-1} (s^{-1})	k_2 (s^{-1})	k_3 (cm^3 $molec.^{-1}$ s^{-1})	k_{-3} (s^{-1})	k_4 (s^{-1})
1	200	1.21E-09	1.01E-10	3.17E+09	3.50E+10	1.01E-10	9.36E+09	8.14E+09
	275	1.82E-11	1.01E-10	4.48E+11	7.03E+10	1.00E-10	1.13E+12	2.68E+10
	298	7.97E-12	1.01E-10	1.20E+12	8.08E+10	1.00E-10	2.92E+12	3.41E+10
	325	3.58E-12	1.01E-10	3.11E+12	9.26E+10	1.00E-10	7.37E+12	4.33E+10
	400	7.42E-13	1.01E-10	2.08E+13	1.22E+11	1.00E-10	4.63E+13	7.04E+10

*Table S5: Overall Canonical Rate Constants (k_{CAN}) of SO_2 + **sCI 2** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, k_2, k_3, k_{-3}, and k_4)*

sCI#	T (K)	k_{CAN} (cm^3 molec.$^{-1}$ s^{-1})	k_1 (cm^3 molec.$^{-1}$ s^{-1})	k_{-1} (s^{-1})	k_2 (s^{-1})	k_3 (cm^3 molec.$^{-1}$ s^{-1})	k_{-3} (s^{-1})	k_4 (s^{-1})
2	200	7.06E-11	1.01E-10	1.78E+11	3.47E+10	1.01E-10	3.15E+11	1.59E+11
	275	5.20E-12	1.01E-10	3.95E+12	5.90E+10	1.01E-10	4.78E+12	1.76E+11
	298	3.16E-12	1.01E-10	7.18E+12	6.56E+10	1.01E-10	8.03E+12	1.79E+11
	325	1.97E-12	1.01E-10	1.28E+13	7.29E+10	1.00E-10	1.32E+13	1.82E+11
	400	7.94E-13	1.00E-10	3.87E+13	9.04E+10	1.00E-10	3.39E+13	1.89E+11

*Table S6: Overall Canonical Rate Constants (k_{CAN}) of HNO_3 + **sCIs 1-5** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, and k_2)*

sCI#	T (K)	k_{CAN} (cm^3 molec.$^{-1}$ s^{-1})	k_1 (cm^3 molec.$^{-1}$ s^{-1})	k_{-1} (s^{-1})	k_2 (s^{-1})
1	200	6.58E-03	1.01E-10	6.61E+02	4.30E+10
	275	2.66E-06	1.01E-10	3.96E+06	1.04E+11
	298	5.47E-07	1.01E-10	2.30E+07	1.25E+11
	325	1.15E-07	1.01E-10	1.30E+08	1.49E+11
	400	4.87E-09	1.00E-10	4.44E+09	2.15E+11
2	200	7.22E-09	1.00E-10	1.21E+07	8.73E+08
	275	7.72E-11	1.00E-10	2.52E+09	1.94E+09
	298	3.13E-11	1.00E-10	7.32E+09	2.28E+09
	325	1.29E-11	1.00E-10	2.08E+10	2.68E+09
	400	2.20E-12	1.00E-10	1.68E+11	3.70E+09
3	200	8.68E-07	1.01E-10	9.60E+05	8.29E+09
	275	2.95E-09	1.00E-10	7.70E+08	2.26E+10
	298	9.42E-10	1.00E-10	2.95E+09	2.77E+10
	325	3.08E-10	1.00E-10	1.11E+10	3.40E+10
	400	3.23E-11	1.00E-10	1.59E+11	5.14E+10
4	200	1.27E-01	1.00E-10	2.72E+02	3.45E+11
	275	1.42E-05	1.00E-10	1.91E+06	2.70E+11
	298	2.24E-06	1.00E-10	1.14E+07	2.56E+11
	325	3.63E-07	1.00E-10	6.68E+07	2.42E+11
	400	8.88E-09	1.00E-10	2.42E+09	2.14E+11
5	200	9.93E-03	1.01E-10	5.48E+02	5.39E+10
	275	2.13E-06	1.01E-10	3.72E+06	7.89E+10
	298	3.88E-07	1.01E-10	2.22E+07	8.56E+10
	325	7.25E-08	1.01E-10	1.29E+08	9.28E+10
	400	2.41E-09	1.00E-10	4.59E+09	1.10E+11

*Table S7: Overall Canonical Rate Constants (k_{CAN}) of HF + **sCIs 1 – 5** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, and k_2)*

sCI#	T (K)	k_{CAN} (cm^3 $molec.^{-1}$ s^{-1})	k_1 (cm^3 $molec.^{-1}$ s^{-1})	k_{-1} (s^{-1})	k_2 (s^{-1})
1	200	2.26E-12	1.01E-10	2.60E+04	5.81E+02
	275	4.37E-13	1.01E-10	2.29E+07	9.92E+04
	298	3.36E-13	1.01E-10	9.19E+07	3.07E+05
	325	2.65E-13	1.01E-10	3.64E+08	9.57E+05
	400	1.72E-13	1.01E-10	6.15E+09	1.05E+07
2	200	2.51E-19	1.01E-10	6.81E+07	1.70E-01
	275	3.63E-18	1.00E-10	5.17E+09	1.87E+02
	298	6.67E-18	1.00E-10	1.25E+10	8.28E+02
	325	1.24E-17	1.00E-10	2.96E+10	3.67E+03
	400	4.79E-17	1.00E-10	1.72E+11	8.23E+04
3	200	2.44E-15	1.01E-10	1.10E+07	2.67E+02
	275	2.59E-15	1.00E-10	2.07E+09	5.35E+04
	298	2.86E-15	1.00E-10	6.05E+09	1.72E+05
	325	3.23E-15	1.00E-10	1.74E+10	5.62E+05
	400	4.48E-15	1.00E-10	1.52E+11	6.79E+06
4	200	1.05E-09	1.01E-10	3.99E+07	4.17E+08
	275	4.61E-11	1.01E-10	5.39E+09	2.47E+09
	298	2.44E-11	1.01E-10	1.47E+10	3.57E+09
	325	1.31E-11	1.00E-10	3.94E+10	5.13E+09
	400	3.66E-12	1.00E-10	2.96E+11	1.08E+10
5	200	2.42E-12	1.01E-10	1.67E+06	4.02E+04
	275	4.93E-13	1.00E-10	4.61E+08	2.26E+06
	298	3.68E-13	1.00E-10	1.45E+09	5.31E+06
	325	2.79E-13	1.00E-10	4.50E+09	1.25E+07
	400	1.64E-13	1.00E-10	4.53E+10	7.42E+07

*Table S8: Overall Canonical Rate Constants (k_{CAN}) of HCl + **sCIs 1-5** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, and k_2)*

sCI#	T (K)	k_{CAN} (cm^3 molec.$^{-1}$ s^{-1})	k_1 (cm^3 molec.$^{-1}$ s^{-1})	k_{-1} (s^{-1})	k_2 (s^{-1})
1	200	6.60E-07	1.00E-10	2.16E+08	1.43E+12
	275	8.46E-09	1.00E-10	1.75E+10	1.48E+12
	298	3.48E-09	1.00E-10	4.29E+10	1.49E+12
	325	1.45E-09	1.00E-10	1.04E+11	1.51E+12
	400	2.46E-10	1.00E-10	6.22E+11	1.53E+12
2	200	1.46E-15	1.01E-10	1.28E+10	1.85E+05
	275	3.35E-15	1.01E-10	2.02E+11	6.70E+06
	298	4.05E-15	1.01E-10	3.49E+11	1.40E+07
	325	4.93E-15	1.01E-10	5.96E+11	2.92E+07
	400	7.76E-15	1.00E-10	1.72E+12	1.33E+08
3	200	2.80E-10	1.01E-10	1.62E+10	4.52E+10
	275	2.56E-11	1.00E-10	3.93E+11	1.00E+11
	298	1.59E-11	1.00E-10	7.46E+11	1.18E+11
	325	1.01E-11	1.00E-10	1.40E+12	1.40E+11
	400	4.05E-12	1.00E-10	4.93E+12	1.99E+11
4	200	3.30E-09	1.00E-10	9.27E+08	3.05E+10
	275	1.39E-10	1.00E-10	2.91E+10	4.03E+10
	298	7.32E-11	1.00E-10	5.81E+10	4.24E+10
	325	3.90E-11	1.00E-10	1.14E+11	4.45E+10
	400	1.10E-11	1.00E-10	4.44E+11	4.87E+10
5	200	1.38E-09	1.01E-10	1.18E+09	1.63E+10
	275	6.62E-11	1.00E-10	5.00E+10	3.30E+10
	298	3.64E-11	1.00E-10	1.06E+11	3.85E+10
	325	2.03E-11	1.00E-10	2.22E+11	4.50E+10
	400	6.41E-12	1.00E-10	9.77E+11	6.25E+10

*Table S9: Overall Canonical Rate Constants (k_{CAN}) of H_2S + **sCIs 1-5**: based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, k_2, k_3, k_{-3}, and k_4)*

sCI#	T (K)	k_{CAN} (cm^3 molec.$^{-1}$ s^{-1})	k_1 (cm^3 molec.$^{-1}$ s^{-1})	k_{-1} (s^{-1})	k_2 (s^{-1})	k_3 (cm^3 molec.$^{-1}$ s^{-1})	k_{-3} (s^{-1})	k_4 (s^{-1})
1	200	4.04E-15	1.01E-10	4.10E+11	9.05E+06	1.00E-10	4.62E+11	8.34E+06
	275	6.31E-15	1.01E-10	3.66E+12	1.24E+08	1.00E-10	3.99E+12	1.16E+08
	298	7.06E-15	1.01E-10	5.55E+12	2.09E+08	1.00E-10	6.01E+12	1.96E+08
	325	8.00E-15	1.01E-10	8.26E+12	3.51E+08	1.00E-10	8.88E+12	3.30E+08
	400	1.09E-14	1.01E-10	1.75E+13	1.01E+09	1.00E-10	1.86E+13	9.50E+08
2	200	2.73E-17	1.01E-10	5.05E+11	1.01E+05	1.00E-10	8.12E+11	5.66E+04
	275	1.37E-16	1.01E-10	1.67E+12	1.54E+06	1.00E-10	1.94E+12	8.56E+05
	298	1.96E-16	1.01E-10	2.05E+12	2.64E+06	1.00E-10	2.23E+12	1.48E+06
	325	2.84E-16	1.01E-10	2.47E+12	4.50E+06	1.00E-10	2.52E+12	2.52E+06
	400	6.49E-16	1.00E-10	3.35E+12	1.33E+07	1.00E-10	3.00E+12	7.50E+06
3	200	3.01E-10	1.01E-10	5.11E+13	1.52E+14	1.01E-10	1.52E+14	2.04E+09
	275	5.36E-15	1.01E-10	1.09E+14	3.72E+09	1.00E-10	2.42E+14	4.59E+09
	298	5.72E-15	1.01E-10	1.22E+14	4.40E+09	1.00E-10	2.56E+14	5.35E+09
	325	6.18E-15	1.01E-10	1.35E+14	5.18E+09	1.00E-10	2.67E+14	6.17E+09
	400	7.67E-15	1.01E-10	1.54E+14	7.10E+09	1.00E-10	2.69E+14	8.15E+09
4	200	2.99E-12	1.01E-10	7.85E+10	1.84E+09	1.00E-10	7.97E+10	4.96E+08
	275	7.39E-13	1.01E-10	6.78E+11	3.61E+09	1.00E-10	6.36E+11	1.29E+09
	298	5.71E-13	1.00E-10	1.02E+12	4.10E+09	1.00E-10	9.38E+11	1.56E+09
	325	4.49E-13	1.00E-10	1.50E+12	4.63E+09	1.00E-10	1.36E+12	1.87E+09
	400	2.92E-13	1.00E-10	3.07E+12	5.90E+09	1.00E-10	2.69E+12	2.68E+09
5	200	1.60E-14	1.01E-10	3.85E+10	3.70E+06	1.01E-10	3.97E+10	2.49E+06
	275	1.26E-14	1.00E-10	5.76E+11	4.19E+07	1.01E-10	5.97E+11	3.12E+07
	298	1.23E-14	1.00E-10	9.69E+11	6.82E+07	1.01E-10	1.00E+12	5.19E+07
	325	1.21E-14	1.00E-10	1.59E+12	1.10E+08	1.00E-10	1.65E+12	8.55E+07
	400	1.26E-14	1.00E-10	4.13E+12	2.92E+08	1.00E-10	4.29E+12	2.36E+08

*Table S10: Overall Canonical Rate Constants (k_{CAN}) of H_2O + **sCIs 1-5**: based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, k_2, k_3, k_{-3}, and k_4)*

sCI#	T (K)	k_{CAN} (cm^3 molec.$^{-1}$ s^{-1})	k_1 (cm^3 molec.$^{-1}$ s^{-1})	k_{-1} (s^{-1})	k_2 (s^{-1})	k_3 (cm^3 molec.$^{-1}$ s^{-1})	k_{-3} (s^{-1})	k_4 (s^{-1})
1	200	1.35E-17	1.00E-10	6.00E+07	7.04E+00	1.00E-10	6.00E+07	1.02E+00
	275	8.04E-17	1.00E-10	3.68E+09	2.38E+03	1.00E-10	3.68E+09	5.69E+02
	298	1.18E-16	1.00E-10	8.39E+09	7.79E+03	1.00E-10	8.39E+09	2.07E+03
	325	1.73E-16	1.00E-10	1.88E+10	2.51E+04	1.00E-10	1.88E+10	7.38E+03
	400	4.00E-16	1.00E-10	9.34E+10	2.73E+05	1.00E-10	9.34E+10	9.98E+04
2	200	1.63E-20	1.00E-10	1.54E+10	6.74E-01	1.00E-10	1.54E+10	1.83E+00
	275	6.27E-19	1.00E-10	1.15E+11	2.24E+02	1.00E-10	1.15E+11	4.98E+02
	298	1.35E-18	1.00E-10	1.69E+11	7.28E+02	1.00E-10	1.69E+11	1.55E+03
	325	2.90E-18	1.00E-10	2.44E+11	2.32E+03	1.00E-10	2.44E+11	4.74E+03
	400	1.47E-17	1.00E-10	4.86E+11	2.49E+04	1.00E-10	4.86E+11	4.65E+04
3	200	1.61E-17	1.01E-10	6.88E+08	9.27E+01	1.01E-10	6.88E+08	1.72E+01
	275	7.99E-17	1.00E-10	2.41E+10	1.52E+04	1.00E-10	2.41E+10	4.05E+03
	298	1.12E-16	1.00E-10	4.89E+10	4.25E+04	1.00E-10	4.89E+10	1.22E+04
	325	1.59E-16	1.00E-10	9.71E+10	1.17E+05	1.00E-10	9.71E+10	3.64E+04
	400	3.37E-16	1.00E-10	3.78E+11	9.31E+05	1.00E-10	3.78E+11	3.37E+05
4	200	1.12E-10	1.01E-10	1.29E+09	5.84E+08	1.01E-10	5.61E+08	3.69E+08
	275	8.88E-12	1.00E-10	4.52E+10	1.63E+09	1.01E-10	2.69E+10	1.40E+09
	298	5.33E-12	1.00E-10	9.11E+10	1.98E+09	1.01E-10	5.80E+10	1.81E+09
	325	3.23E-12	1.00E-10	1.80E+11	2.38E+09	1.01E-10	1.22E+11	2.31E+09
	400	1.19E-12	1.00E-10	6.89E+11	3.38E+09	1.01E-10	5.35E+11	3.71E+09
5	200	1.45E-12	1.01E-10	2.69E+08	1.25E+06	1.01E-10	2.69E+08	2.64E+06
	275	3.10E-13	1.00E-10	2.09E+10	2.46E+07	1.00E-10	2.09E+10	3.98E+07
	298	2.28E-13	1.00E-10	4.96E+10	4.46E+07	1.00E-10	4.96E+10	6.84E+07
	325	1.70E-13	1.00E-10	1.15E+11	7.99E+07	1.00E-10	1.15E+11	1.16E+08
	400	9.68E-14	1.00E-10	6.20E+11	2.60E+08	1.00E-10	6.20E+11	3.39E+08

*Table S11: Overall Canonical Rate Constants (k_{CAN}) of $(H_2O)_2$ + **sCIs 1-5** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, k_2, k_3, k_{-3}, and k_4)*

sCI#	T (K)	k_{CAN} (cm^3 $mol.^{-1}$ s^{-1})	k_1 (cm^3 $mol.^{-1}$ s^{-1})	k_{-1} (s^{-1})	k_2 (s^{-1})	k_3 (cm^3 $mol.^{-1}$ s^{-1})	k_{-3} (s^{-1})	k_4 (s^{-1})
1	200	8.04E-09	1.01E-10	1.01E+07	1.99E+08	1.01E-10	7.06E+06	1.47E+07
			1.01E-10	5.45E+06	1.62E+08	1.01E-10	9.74E+06	2.71E+08
	275	4.28E-11	1.01E-10	8.14E+09	9.31E+08	1.01E-10	5.92E+09	1.25E+08
			1.01E-10	6.10E+09	8.84E+08	1.01E-10	9.04E+09	1.30E+09
	298	1.44E-11	1.00E-10	3.19E+10	1.24E+09	1.01E-10	2.33E+10	1.88E+08
			1.01E-10	2.56E+10	1.22E+09	1.01E-10	3.65E+10	1.75E+09
	325	4.85E-12	1.00E-10	1.23E+11	1.64E+09	1.01E-10	9.00E+10	2.79E+08
			1.01E-10	1.05E+11	1.66E+09	1.01E-10	1.45E+11	2.32E+09
	400	5.09E-13	1.00E-10	1.92E+12	2.75E+09	1.01E-10	1.41E+12	5.98E+08
			1.01E-10	1.89E+12	2.99E+09	1.00E-10	2.41E+12	3.96E+09
2	200	1.57E-09	1.01E-10	5.04E+07	2.28E+08	1.01E-10	4.92E+07	2.13E+07
			1.01E-10	1.52E+07	8.51E+07	1.01E-10	4.44E+07	2.24E+08
	275	1.01E-11	1.01E-10	3.58E+10	1.09E+09	1.00E-10	4.04E+10	2.22E+08
			1.01E-10	1.53E+10	5.13E+08	1.00E-10	3.58E+10	1.12E+09
	298	3.57E-12	1.00E-10	1.36E+11	1.46E+09	1.00E-10	1.59E+11	3.51E+08
			1.01E-10	6.24E+10	7.25E+08	1.00E-10	1.39E+11	1.52E+09
	325	1.26E-12	1.00E-10	5.05E+11	1.94E+09	1.00E-10	6.10E+11	5.48E+08
			1.00E-10	2.51E+11	1.01E+09	1.00E-10	5.33E+11	2.03E+09
	400	1.48E-13	1.00E-10	7.31E+12	3.30E+09	1.00E-10	9.49E+12	1.31E+09
			1.00E-10	4.27E+12	1.94E+09	1.00E-10	8.18E+12	3.55E+09
3	200	5.86E-08	1.01E-10	2.86E+08	7.70E+09	1.01E-10	2.59E+08	8.47E+10
			1.01E-10	1.69E+08	1.55E+10	1.01E-10	1.58E+08	2.14E+10
	275	1.33E-10	1.01E-10	1.32E+11	1.32E+10	1.01E-10	1.53E+11	9.42E+10
			1.01E-10	8.35E+10	2.19E+10	1.01E-10	8.85E+10	3.05E+10
	298	3.78E-11	1.01E-10	4.58E+11	1.44E+10	1.01E-10	5.63E+11	9.40E+10
			1.00E-10	2.96E+11	2.29E+10	1.01E-10	3.21E+11	3.21E+10
	325	1.08E-11	1.00E-10	1.57E+12	1.54E+10	1.01E-10	2.03E+12	9.29E+10
			1.00E-10	1.03E+12	2.36E+10	1.01E-10	1.15E+12	3.33E+10
	400	8.15E-13	1.00E-10	1.90E+13	1.70E+10	1.00E-10	2.79E+13	8.70E+10
			1.00E-10	1.30E+13	2.42E+10	1.00E-10	1.53E+13	3.44E+10
4	200	2.87E-01	1.00E-10	1.14E+04	2.95E+12	1.01E-10	5.96E+03	8.52E+12
			1.00E-10	2.78E+04	9.32E+12	1.00E-10	2.01E+04	1.66E+13
	275	1.04E-05	1.00E-10	1.26E+08	1.61E+12	1.00E-10	8.93E+07	3.99E+12
			1.00E-10	2.77E+08	4.25E+12	1.00E-10	2.31E+08	7.07E+12
	298	1.25E-06	1.00E-10	8.51E+08	1.39E+12	1.00E-10	6.41E+08	3.34E+12
			1.00E-10	1.83E+09	3.54E+12	1.00E-10	1.57E+09	5.81E+12
	325	1.53E-07	1.00E-10	5.62E+09	1.19E+12	1.00E-10	4.52E+09	2.78E+12
			1.00E-10	1.18E+10	2.93E+12	1.00E-10	1.05E+10	4.75E+12
	400	1.99E-09	1.00E-10	2.69E+11	8.39E+11	1.00E-10	2.49E+11	1.85E+12
			1.00E-10	5.47E+11	1.93E+12	1.00E-10	5.23E+11	3.05E+12
5	200	5.33E-03	1.01E-10	2.26E+04	1.59E+11	1.01E-10	1.04E+04	4.16E+11
			1.01E-10	2.17E+04	9.18E+10	1.01E-10	2.74E+04	4.16E+10
	275	4.80E-07	1.00E-10	1.69E+08	1.47E+11	1.01E-10	1.12E+08	3.39E+11
			1.01E-10	1.53E+08	9.17E+10	1.01E-10	1.60E+08	4.41E+10
	298	7.07E-08	1.00E-10	1.04E+09	1.41E+11	1.01E-10	7.48E+08	3.18E+11
			1.01E-10	9.33E+08	8.96E+10	1.01E-10	9.39E+08	4.35E+10
	325	1.06E-08	1.00E-10	6.31E+09	1.35E+11	1.01E-10	4.89E+09	2.96E+11
			1.01E-10	5.58E+09	8.66E+10	1.00E-10	5.40E+09	4.25E+10
	400	2.12E-10	1.00E-10	2.49E+11	1.17E+11	1.00E-10	2.29E+11	2.48E+11
			1.00E-10	2.16E+11	7.77E+10	1.00E-10	1.93E+11	3.88E+10

*Table S12: Overall Canonical Rate Constants (k_{CAN}) of MeOH + **sCIs 1-5** based on a steady state treatment of individual canonical rate coefficients of reaction (k_1, k_{-1}, k_2, k_3, k_{-3}, and k_4).*
*Note: **sCI 4** + MeOH has one barrierless step and one with a barrier so the dipole-dipole capture rate constant is used.*

sCI#	T (K)	k_{CAN} (cm³ molec.$^{-1}$ s^{-1})	k_1 (cm³ molec.$^{-1}$ s^{-1})	k_{-1} (s^{-1})	k_2 (s^{-1})	k_3 (cm³ molec.$^{-1}$ s^{-1})	k_{-3} (s^{-1})	k_4 (s^{-1})
1	200	2.65E-14	1.01E-10	2.89E+08	6.86E+04	1.01E-10	2.89E+08	7.70E+03
	275	1.34E-14	1.00E-10	2.21E+10	2.43E+06	1.00E-10	2.21E+10	5.23E+05
	298	1.20E-14	1.00E-10	5.21E+10	5.01E+06	1.00E-10	5.21E+10	1.24E+06
	325	1.09E-14	1.00E-10	1.21E+11	1.02E+07	1.00E-10	1.21E+11	2.89E+06
	400	9.48E-15	1.00E-10	6.41E+11	4.41E+07	1.00E-10	6.41E+11	1.64E+07
2	200	**2.55E-17**	1.01E-10	2.80E+10	6.90E+03	1.01E-10	2.80E+10	1.90E+02
	275	7.34E-17	1.01E-10	2.34E+11	1.59E+05	1.01E-10	2.34E+11	1.10E+04
	298	9.43E-17	1.01E-10	3.49E+11	3.02E+05	1.01E-10	3.49E+11	2.52E+04
	325	1.23E-16	1.01E-10	5.10E+11	5.67E+05	1.01E-10	5.10E+11	5.71E+04
	400	2.28E-16	1.00E-10	1.04E+12	2.06E+06	1.00E-10	1.04E+12	3.06E+05
3	200	**1.87E-13**	1.01E-10	2.70E+09	4.53E+06	1.01E-10	2.70E+09	4.97E+05
	275	4.34E-14	1.00E-10	1.30E+11	4.62E+07	1.00E-10	1.30E+11	1.00E+07
	298	3.31E-14	1.00E-10	2.80E+11	7.38E+07	1.00E-10	2.80E+11	1.85E+07
	325	2.57E-14	1.00E-10	5.88E+11	1.17E+08	1.00E-10	5.88E+11	3.37E+07
	400	1.62E-14	1.00E-10	2.55E+12	2.98E+08	1.00E-10	2.55E+12	1.15E+08
4	200	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	1.00E-10	2.33E+08	1.41E+10
	275	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	1.00E-10	2.32E+10	1.76E+10
	298	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	1.00E-10	5.79E+10	1.82E+10
	325	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	1.00E-10	1.41E+11	1.88E+10
	400	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	>> $k_{d\text{-}d}$	1.00E-10	8.27E+11	1.98E+10
5	200	6.33E-09	1.01E-10	2.09E+08	5.93E+09	1.01E-10	1.20E+08	4.14E+09
	275	9.09E-11	1.00E-10	2.25E+10	9.23E+09	1.01E-10	1.53E+10	7.52E+09
	298	4.65E-11	1.00E-10	3.99E+10	1.00E+10	1.01E-10	3.99E+10	8.43E+09
	325	1.71E-11	1.00E-10	1.40E+11	1.09E+10	1.01E-10	1.02E+11	9.43E+09
	400	3.29E-12	1.00E-10	8.47E+11	1.26E+10	1.00E-10	6.59E+11	1.17E+10

S1.4 sCI 1 + Co-reactant Under Experimental Conditions From the Literature

*Table 13: **sCI 1** + co-reactants under experimental conditions, atmospheric pressure and temperature applied to MESMER method. The **sCI 4** + MeOH rate constant is only for TS2 as TS1 is barrierless.*

Reaction	p (Torr)	T (K)	Grain size	k_{CAN} (cm^3 molec.$^{-1}$ s^{-1})				k_{ME}
				k_1	k_{-1}	k_2	k_{TS}	
				cm^3 s^{-1}	s^{-1}	s^{-1}	cm^3 s^{-1}	
sCI 1 + HNO_3	27	295	10	1.01E-10	1.86E+07	1.22E+11	6.62E-07	6.18E-11
	31	295		1.01E-10	1.86E+07	1.22E+11	6.62E-07	6.18E-11
	35	295		1.01E-10	1.86E+07	1.22E+11	6.62E-07	6.18E-11
	760	295		1.01E-10	1.86E+07	1.22E+11	6.62E-07	1.04E-08
sCI 1 + H_2O	50	293	10	1.00E-10	7.10E+09	6.12E+03	8.64E-17	1.09E-16
				1.00E-10	7.10E+09	1.59E+03	2.24E-17	
	760	297	10	1.00E-10	8.12E+09	7.43E+03	9.17E-17	1.16E-16
				1.00E-10	8.12E+09	1.96E+03	2.42E-17	
sCI 1 + H_2S	100	299	10	1.01E-10	5.64E+12	2.14E+08	3.81E-15	7.10E-15
				1.00E-10	6.11E+12	2.00E+08	3.29E-15	
	250	299	10	1.01E-10	5.64E+12	2.14E+08	3.81E-15	7.10E-15
				1.00E-10	6.11E+12	2.00E+08	3.29E-15	
	500	299	10	1.01E-10	5.64E+12	2.14E+08	3.81E-15	7.10E-15
				1.00E-10	6.11E+12	2.00E+08	3.29E-15	
	100	278	10	1.01E-10	3.88E+12	1.33E+08	3.45E-15	6.40E-15
				1.00E-10	4.23E+12	1.24E+08	2.95E-15	
	100	318	10	1.01E-10	7.51E+12	3.10E+08	4.15E-15	7.75E-15
				1.00E-10	8.09E+12	2.91E+08	3.60E-15	
sCI 1 + MeOH	90	295	10	1.00E-10	4.70E+10	4.59E+06	9.81E-15	1.03E-13
				1.00E-10	4.70E+10	1.11E+06	2.38E-15	
	10	254.5	10	1.00E-10	8.86E+09	1.14E+06	1.29E-14	1.15E-12
				1.00E-10	8.86E+09	2.12E+05	2.41E-15	
	100	262.1	10	1.00E-10	1.27E+10	1.53E+06	1.21E-14	1.10E-13
				1.00E-10	1.27E+10	3.02E+05	2.40E-15	
	10	292.6	10	1.00E-10	4.32E+10	4.27E+06	9.94E-15	9.29E-13
				1.00E-10	4.32E+10	1.02E+06	2.38E-15	
	10	327.8	10	1.00E-10	1.30E+11	1.10E+07	8.43E-15	8.20E-13
				1.00E-10	1.30E+11	3.13E+06	2.41E-15	
sCI 1 + HCl	27	295	5	1.00E-10	3.85E+10	1.49E+12	3.88E-09	5.04E-10
	31	295		1.00E-10	3.85E+10	1.49E+12	3.88E-09	5.04E-10
	35	295		1.00E-10	3.85E+10	1.49E+12	3.88E-09	5.04E-10
	760	295		1.00E-10	3.85E+10	1.49E+12	3.88E-09	4.98E-10

S1.5 Breakdown of k_{TST} Constants using Wignar Factor for Tunneling Constant

*Table S14: Breakdown of rate constant (k_{TST}) of sCI + atmospheric co-reactant using: equilibrium rate constant (K_{eq}); **Wignar** tunneling constant (κ_{Wignar}); unimolecular rate constant (k_2); individual rate constant of transition state (k_{TS}); pathway breakdown (**Γ**); total rate constant (k_{total});*

*Note: **sCI 4** + HCHO; **sCI 1** + CF_3CFO; **sCIs 1**,**3**,**4** and **5** with SO_2; and **sCIs 1**-**5** with TFA are barrierless reactions (see IRCs in section S7) and so are not included. The **sCI 4** + MeOH rate constant is only for TS2 as TS1 is barrierless.*

Co-reactant	CI	#TS	K_{eq}	κ_{Wignar}	k_2	k_{TS}	Γ	k_{total}
			cm^3		s^{-1}	$cm^3\ s^{-1}$		$cm^3\ s^{-1}$
HCHO	1	TS_C	2.08E-23	1.01	1.37E+12	2.88E-11	1.00	2.88E-11
	2	TS_C	5.86E-23	1.00	5.00E+9	2.93E-13	1.00	2.93E-13
	3	TS_C	5.20E-23	1.00	1.21E+11	6.28E-12	1.00	6.28E-12
	5	TS_C	4.03E-22	1.00	5.15E+11	2.08E-10	1.00	2.08E-10
CF_3CFO	1	TS_{CYC} 1	5.73E-23	1.01	1.15E+11	6.69E-12	1.00	7.86E-12
		TS_{CYC} 2	4.95E-23	1.03	2.29E+10	1.17E-12	1.00	
SO_2	2	TS_{ENDO}	1.37E-23	1.00	6.73E+10	9.21E-13	1.00	3.21E-12
		TS_{EXO}	1.28E-23	1.00	1.79E+11	2.29E-12	1.00	
HNO_3	1	TS	4.30E-18	1.06	1.19E+11	5.40E-07	1.00	5.40E-7
	2	TS	1.42E-20	1.04	2.13E+9	3.15E-11	1.00	3.15E-11
	3	TS	3.32E-20	1.07	2.60E+10	9.19E-10	1.00	9.19E-10
	4	TS	8.73E-18	1.00	2.56E+11	2.24E-6	1.00	2.24E-6
	5	TS	4.41E-18	1.11	7.72E+10	3.79E-7	1.00	3.79E-7
HCl	1	TS	2.21E-21	1.01	1.66E+12	3.69E-9	1.00	3.69E-9
	2	TS	2.21E-21	1.00	6.34E+11	4.19E-15	1.00	4.19E-15
	3	TS	1.80E-21	1.13	2.05E+6	1.63E-11	1.00	1.63E-11
	4	TS	1.34E-22	1.17	1.04E+11	7.37E-11	1.00	7.37E-11
	5	TS	1.70E-21	1.01	4.31E+10	3.59E-11	1.00	3.59E-11
HF	1	TS	1.12E-18	1.67	1.46E+5	5.47E-13	1.00	5.47E-13
	2	TS	8.44E-21	1.54	4.51E+2	1.17E-17	1.00	1.17E-17
	3	TS	1.74E-20	1.70	7.82E+4	4.63E-15	1.00	4.63E-15
	4	TS	2.18E-19	1.14	1.02E+8	5.09E-11	1.00	5.09E-11
	5	TS	6.99E-20	1.43	3.38E+6	6.76E-13	1.00	6.76E-13
MeOH	1	TS_{AAAH}1	1.94E-21	1.09	4.51E+6	1.90E-14	0.80	1.19E-14
		TS_{AAAH}2	1.94E-21	1.10	1.11E+6	4.72E-15	0.20	
	2	TS_{AAAH}1	2.96E-22	1.06	2.79E+5	1.75E-16	0.92	9.47E-17
		TS_{AAAH}2	2.96E-22	1.07	2.30E+4	1.47E-17	0.08	
	3	TS_{AAAH}1	3.55E-22	1.06	7.11E+7	5.34E-14	0.80	3.34E-14
		TS_{AAAH}2	3.55E-22	1.05	1.78E+7	1.33E-14	0.20	
	4	TS_{AAAH}1	$>>k_{d\text{-}d}$	N/A	$>>k_{d\text{-}d}$	$>>k_{d\text{-}d}$	$>>k_{d\text{-}d}$	$>>k_{d\text{-}d}$
		TS_{AAAH}2	1.79E-21	1.02	1.74E+10	6.33E-11	1.00	
	5	TS_{AAAH}1	1.72E-21	1.04	9.86E+9	3.53E-11	0.46	3.88E-11
		TS_{AAAH}2	2.50E-21	1.04	8.14E+9	4.22E-11	0.54	

*Table S15: Breakdown of rate constant (k_{TST}) of sCI + atmospheric co-reactant using: equilibrium rate constant (K_{eq}); **Wignar** tunneling constant (κ_{Wignar}); unimolecular rate constant (k_2); individual rate constant of transition state (k_{TS}); pathway breakdown (Γ); total rate constant (k_{total});*

Co-reactant	CI	#TS	K_{eq}	K_{Wignar}	k_2	k_{TS}	Γ	k_{total}
			cm^3		cm^3	$cm^3\ s^{-1}$		$cm^3\ s^{-1}$
H_2S	1	TS1	1.81E-23	1.08	1.95E+8	3.80E-15	0.54	1.41E-15
		TS2	1.68E-23	1.08	1.79E+8	3.25E-15	0.46	
	2	TS1	5.14E-23	1.03	2.48E+6	1.32E-16	0.66	3.98E-16
		TS2	4.80E-23	1.04	1.35E+6	6.75E-17	0.34	
	3	TS1	8.63E-25	1.04	4.11E+9	3.70E-15	0.63	1.17E-14
		TS2	4.08E-25	1.05	5.01E+9	2.14E-15	0.37	
	4	TS1	1.01E-22	1.01	4.03E+9	4.09E-13	0.71	5.75E-13
		TS2	1.06E-22	1.01	1.55E+9	1.65E-13	0.29	
	5	TS1	1.03E-22	1.04	6.59E+7	7.11E-15	0.58	2.47E-14
		TS2	1.02E-22	1.04	4.91E+7	5.23E-15	0.42	
H_2O	1	TSH_2O 1	1.22E-20	1.18	6.40E+3	1.85E-16	0.79	1.17E-16
		TSH_2O 2	1.22E-20	1.20	1.67E+3	4.89E-17	0.21	
	2	TSH_2O 1	6.07E-22	1.11	6.55E+2	4.41E-19	0.32	1.38E-18
		TSH_2O 2	6.07E-22	1.12	1.38E+3	9.40E-19	0.68	
	3	TSH_2O 1	2.07E-21	1.11	3.82E+4	8.82E-17	0.78	1.14E-16
		TSH_2O 2	2.07E-21	1.13	1.09E+4	2.54E-17	0.22	
	4	TSH_2O 1	1.12E-21	1.03	1.94E+9	2.23E-12	0.42	5.37E-12
		TSH_2O 2	1.74E-21	1.05	1.72E+9	3.13E-12	0.58	
	5	TSH_2O 1	2.06E-21	1.08	4.09E+7	9.11E-14	0.40	2.30E-13
		TSH_2O 2	2.06E-21	1.08	6.24E+7	1.39E-13	0.60	
$(H_2O)_2$	1	$TS(H_2O)_2$ 1	3.13E-21	1.11	1.12E+9	3.87E-12	0.27	1.41E-11
		$TS(H_2O)_2$ 2	4.28E-21	1.15	1.60E+8	7.87E-13	0.06	
		$TS(H_2O)_2$ 3	3.86E-21	1.12	1.08E+9	4.68E-12	0.33	
		$TS(H_2O)_2$ 4	2.71E-21	1.10	1.60E+9	4.78E-12	0.34	
	2	$TS(H_2O)_2$ 1	1.21E-22	1.08	3.65E+9	4.79E-13	0.20	2.41E-12
		$TS(H_2O)_2$ 2	1.17E-22	1.07	1.10E+10	1.38E-12	0.57	
		$TS(H_2O)_2$ 3	4.99E-23	1.06	2.62E+9	1.39E-13	0.06	
		$TS(H_2O)_2$ 4	5.39E-23	1.06	7.17E+9	4.09E-13	0.17	
	3	$TS(H_2O)_2$ 1	2.20E-22	1.07	1.35E+10	3.17E-12	0.08	3.84E-11
		$TS(H_2O)_2$ 2	1.83E-22	1.05	8.91E+10	1.72E-11	0.45	
		$TS(H_2O)_2$ 3	3.47E-22	1.05	2.18E+10	7.95E-12	0.21	
		$TS(H_2O)_2$ 4	3.17E-22	1.05	3.01E+10	1.00E-11	0.26	
	4	$TS(H_2O)_2$ 1	1.16E-19	1.04	1.58E+12	1.90E-7	0.14	1.36E-06
		$TS(H_2O)_2$ 2	1.53E-19	1.03	3.35E+12	5.28E-7	0.39	
		$TS(H_2O)_2$ 3	5.45E-20	1.02	3.96E+12	2.21E-7	0.16	
		$TS(H_2O)_2$ 4	6.28E-20	1.02	6.59E+12	4.21E-7	0.31	
	5	$TS(H_2O)_2$ 1	9.31E-20	1.05	1.39E+11	1.36E-8	0.19	7.22E-08
		$TS(H_2O)_2$ 2	1.32E-19	1.05	3.21E+11	4.44E-8	0.61	
		$TS(H_2O)_2$ 3	1.06E-19	1.06	8.56E+10	9.60E-9	0.13	
		$TS(H_2O)_2$ 4	1.00E-19	1.07	4.35E+10	4.68E-9	0.06	

S1.5 Conventional Transition State Theory Rate Constant (k_{TST}) Equations

$$k_{TST} = K_{eq}.\, k_2 \qquad \textit{Equation S1}$$

$$K_{eq} = \frac{RT}{P_0} e^{-(G_{PRC} - (G_{CI} + G_{Co}))/RT} \qquad \textit{Equation S2}$$

$$k_2 = \kappa \frac{k_B T}{h} e^{-(G_{TS} - G_{PRC})/RT} \qquad \textit{Equation S3}$$

$$k_{total} = \sum k_{TST} \qquad \textit{Equation S4}$$

S2. MEMSER derived product branching ratios in HCHO & SO_2 reactions

S2.1 Full potential energy surfaces for HCHO & SO_2 + sCI reactions

The complexities of the HCHO & SO_2 + sCI systems are not fully expressed in the diagrams in the main manuscript, which only exhibit a condensed and lowest energy path version. The visual representation of such potential energy surfaces for HCHO and SO_2 + sCI systems are found in this section. For all the energy values on the potential energy surface, please see Section S5.

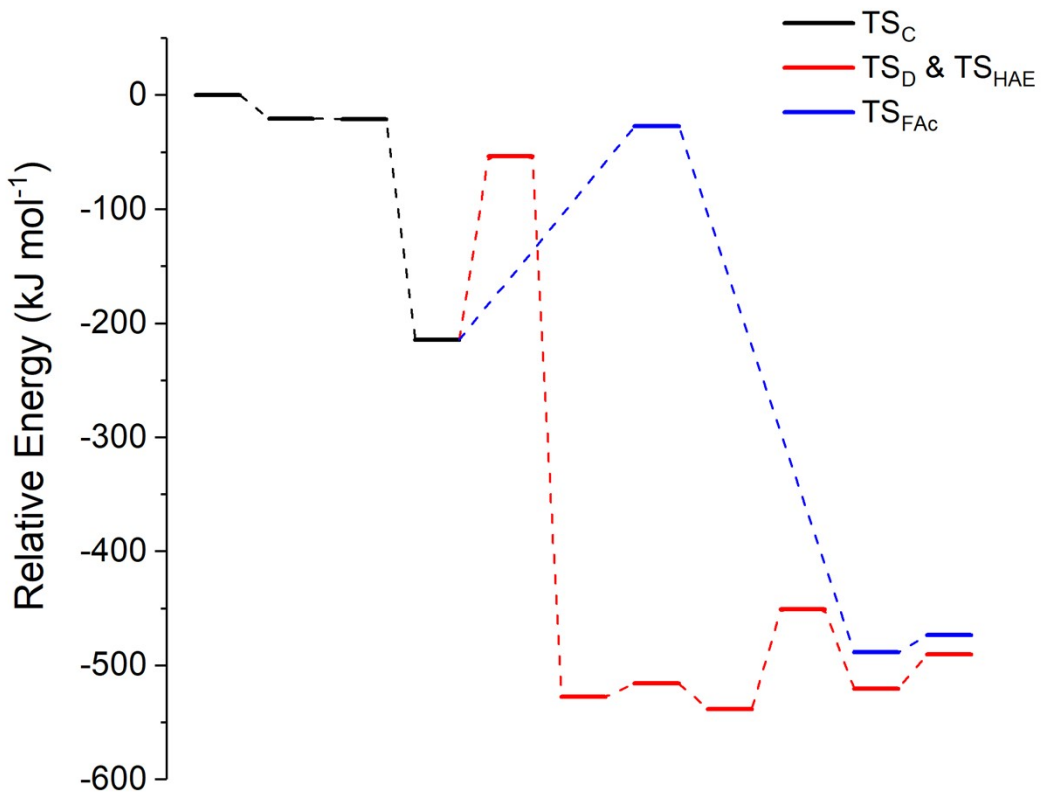

Figure S1: sCI1 + HCHO full potential energy surface with labels of channels in legend.

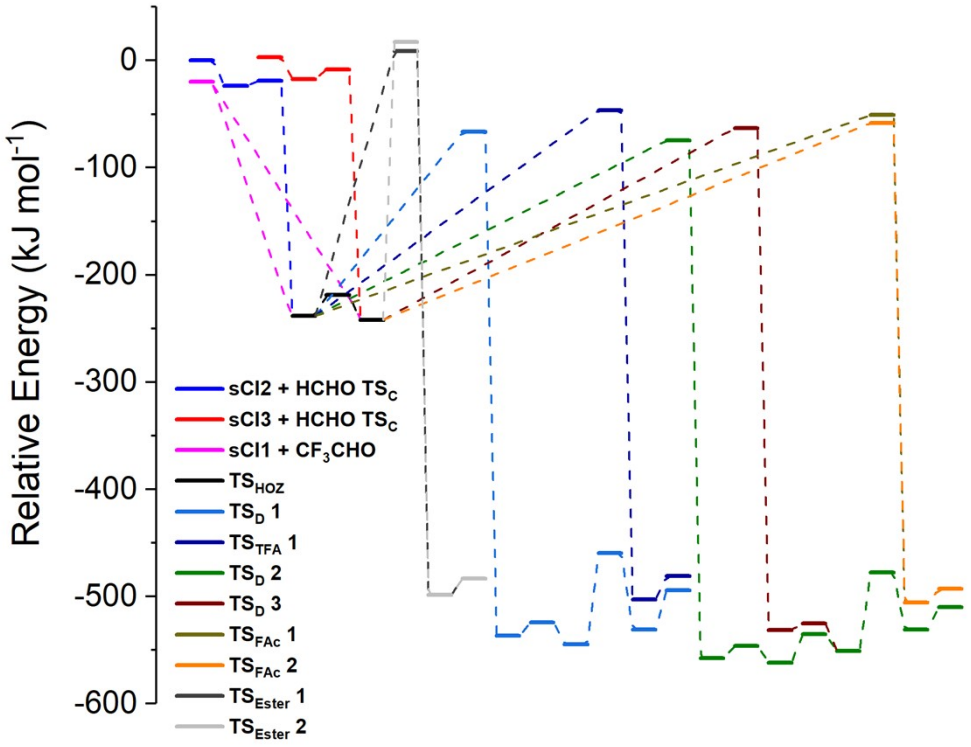

*Figure S2: Potential Energy Surface including all reactions HCHO + **sCIs 2** & **3** & **sCI1** + CF_3CHO with legend attached.*

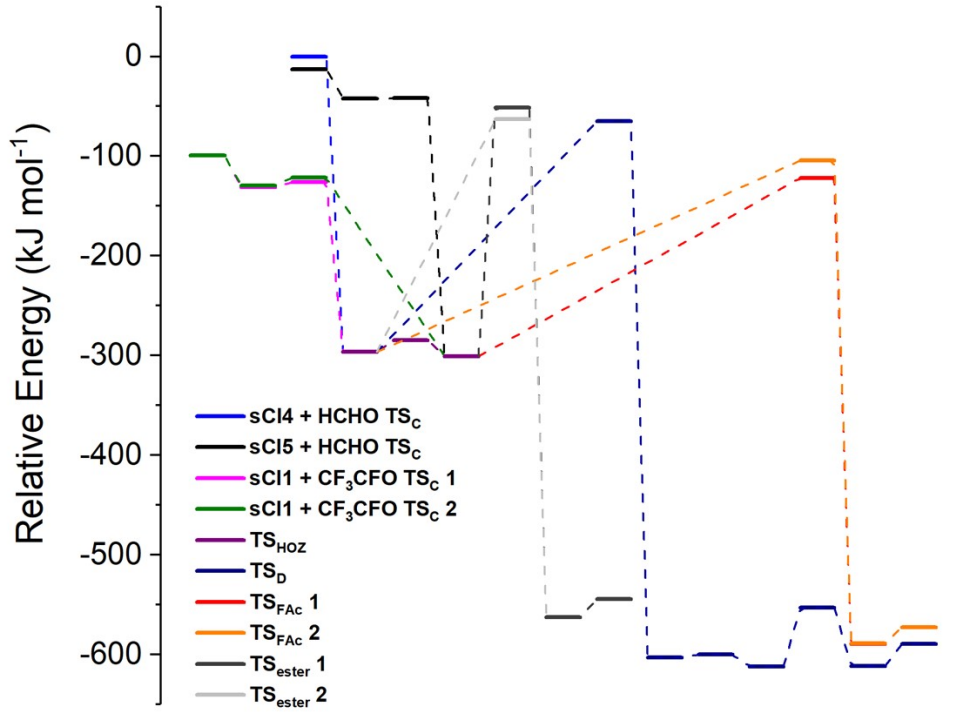

*Figure S3: Potential Energy Surface including all reactions HCHO + **sCIs 4** & **5** & **sCI1** + CF_3CFO with legend attached*

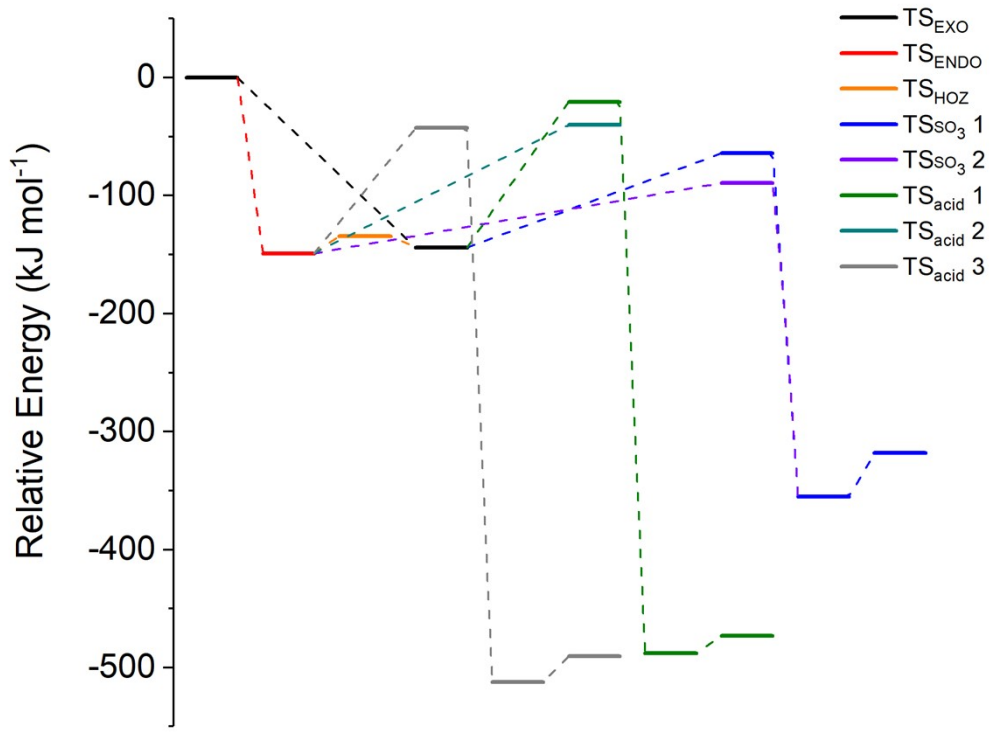

*Figure S4: Full Potential Energy Surface of **sCl1** + SO_2 with legend attached.*

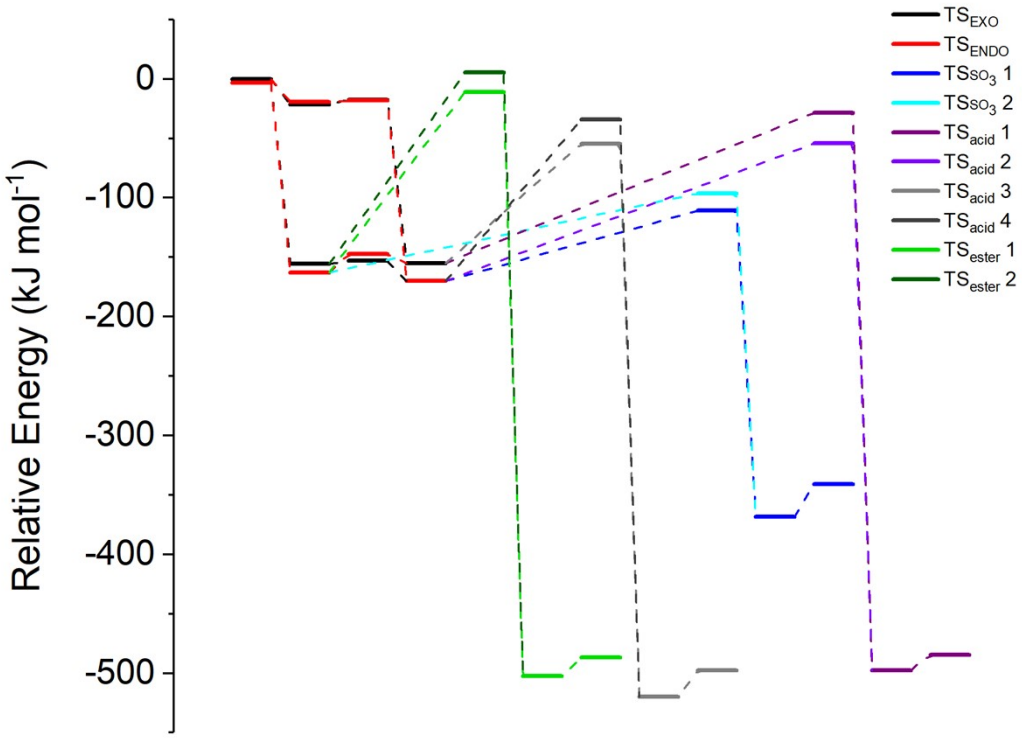

*Figure S5: Potential Energy Surface including all **sCl2** & **sCl3** + SO_2 reactions with legend attached.*

*Figure S6: Potential Energy Surface including all **sCI4** & **sCI5** + SO_2 reactions with legend attached*

S2.2 Product branching ratio of sCI 1 reactions HCHO, CF_3CHO and CF_3CFO

As seen in Figures **S2, S3, S4** & **S5,** many of these reactions lead to barrierless POZ-to-final product pathways. To determine their product branching fraction, the MESMER software employs a reverse ILT method using a user provided pre-exponential. This pre-exponential can be either a previously measured literature k_{EXP} value for the forward reaction barrierless channels or a calculated rate-limiting value. Here the product branching ratios are calculated in the following tables excluding the barrierless channels entirely for the purpose of being comprehensive and using either the dipole-dipole capture limit ($k_{d\text{-}d}$) or the collision-limiting rate constant (k_{COLL}) as the pre-exponential. The product branching ratios seen in the main body of the text uses the $k_{d\text{-}d}$ constant for the reverse ILT pre-exponential. For more details, the dipole-dipole capture limit ($k_{d\text{-}d}$) and the collision-limiting rate constant (k_{COLL}) see Section S3.

*Table S16: The product branching ratio from the **sCI 1** + HCHO reaction of: the heterozonide intermediate product (Γ_{HOZ}); direct transfer pathway ($\Gamma_{TS_{FAc}}$); hydroxyalkyl hydroperoxide pathway ($\Gamma_{TS_{HAE}}$)* using MESMER grainsize of 10.

T (K)	Γ_{HOZ}	$\Gamma_{TS_{FAc}}$	$\Gamma_{TS_{HAE}}$
200	1.000	0.000	0.000
275	0.000	0.025	0.975
298.15	0.000	0.027	0.973
325	0.000	0.030	0.970
400	0.000	0.038	0.962

*Table S17: The product branching ratio of the **sCI 1** + CF_3CHO reaction with **CI 2 + HCHO** and **CI 3 + HCHO** as sinks (not barrierless) using MESMER grainsize of 40.*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
CI 2 + HCHO (TS_{CYC} 1)	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
CI 3 + HCHO (TS_{CYC} 2)	<0.0001	<0.0001	<0.0001	<0.0001	0.0001
HCOOH + CF_3CHO	0.8447	0.8282	0.8232	0.8176	0.8051
TS_{HAE} 2	0.6908	0.6479	0.6344	0.6195	0.5862
TS_{HAE} 3	0.0969	0.1084	0.1118	0.1155	0.1234
TS_{FAc} 1	0.0097	0.0142	0.0158	0.0177	0.0222
TS_{FAc} 2	0.0473	0.0578	0.0611	0.0648	0.0733
CF_3COOH + HCHO	0.1553	0.1717	0.1768	0.1824	0.1948
TS_{HAE} 1	0.1499	0.1624	0.1659	0.1696	0.1771
TS_{TFA} 1	0.0054	0.0094	0.0109	0.0128	0.0177
CF_3OCHO + HCHO	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table S18: the product branching ratio of the **sCI 1** + CF_3CFO reaction with **CI 4 + HCHO** and **CI 5 + HCHO** as sinks for barrierless exit channel using the $k_{d\text{-}d}$ as pre-exponential factors (7.20×10^{-10} cm^3 $molec^{-1}$ s^{-1}). MESMER grainsize = 40*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
CI 4 + HCHO (TS_{CYC} 1)	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
CI 5 + HCHO (TS_{CYC} 2)	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
HCOOH + CF_3CFO	1.0000	1.0000	1.0000	1.0000	1.0000
TS_{HAE} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{FAc} 1	0.9940	0.9839	0.9784	0.9705	0.9419
TS_{FAc} 2	0.0060	0.0161	0.0216	0.0295	0.0581
CF_3OCFO + HCHO	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table S19: The product branching ratio of the **sCI 1** + CF_3CFO reaction with **CI 4 + HCHO** and **CI 5 + HCHO** as sinks using the k_{COLL} as pre-exponential factor (1.49×10^{-10} cm^3 $molec^{-1}$ s^{-1}) for barrierless exit channels. MESMER grainsize = 40*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
CI 4 + HCHO (TS_{CYC} 1)	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
CI 5 + HCHO (TS_{CYC} 2)	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
HCOOH + CF_3CFO	**1.0000**	**1.0000**	**1.0000**	**1.0000**	**1.0000**
TS_{HAE} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{FAc} 1	0.9940	0.9839	0.9784	0.9705	0.9419
TS_{FAc} 2	0.0060	0.0161	0.0216	0.0295	0.0581
CF_3OCFO + HCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

(Due to the very low yield of **CI 4 + HCHO** & **CI 5 + HCHO**, no models were ran excluding these pathways for **sCI 1** + CF_3CFO reactions, as they would yield the same results)

S2.3 Product branching ratio of HCHO reactions with sCIs 2 & 3

*Table S20: the product branching ratio of the **sCI 2** + HCHO reaction with **CI 1 + CF_3CHO** and **CI 3 + HCHO** as sinks using the $k_{d\text{-}d}$ as pre-exponential factor (6.50×10^{-10} cm^3 $molec^{-1}$ s^{-1}) for barrierless exit channels – using a MESMER grainsize of 40.*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
CI 1 + CF_3CHO	**0.9809**	**0.9915**	**0.9931**	**0.9944**	**0.9965**
TS_{cyc} 3 (barrierless)	0.4914	0.4965	0.4973	0.4980	0.4998
TS_{cyc} 4 (barrierless)	0.4895	0.4950	0.4958	0.4963	0.4967
CI 3 + HCHO (TS_{CYC} 2)	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
HCOOH + CF_3CHO	**0.0158**	**0.0069**	**0.0056**	**0.0046**	**0.0028**
TS_{HAE} 2	0.0121	0.0052	0.0042	0.0033	0.0020
TS_{HAE} 3	0.0022	0.0010	0.0008	0.0007	0.0004
TS_{FAc} 1	0.0003	0.0002	0.0001	0.0001	0.0001
TS_{FAc} 2	0.0012	0.0006	0.0005	0.0004	0.0003
CF_3COOH + HCHO	**0.0034**	**0.0016**	**0.0013**	**0.0011**	**0.0007**
TS_{HAE} 1	0.0032	0.0015	0.0012	0.0010	0.0006
TS_{TFA} 1	0.0002	0.0001	0.0001	0.0001	0.0001
CF_3OCHO + HCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table S21: the product branching ratio of the **sCI 2** + HCHO reaction with **CI 1 + CF_3CHO** and **CI 3 + HCHO** as sinks using the k_{COLL} as pre-exponential factor (1.52×10^{-10} cm^3 $molec^{-1}$ s^{-1}) for barrierless exit channels – using a MESMER grainsize of 40.*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
CI 1 + CF_3CHO	**0.9251**	**0.9695**	**0.9758**	**0.9809**	**0.9884**
TS_{cyc} 3 (barrierless)	0.4634	0.4853	0.4885	0.4910	0.4949
TS_{cyc} 4 (barrierless)	0.4617	0.4841	0.4873	0.4899	0.4935
CI 3 + HCHO (TS_{CYC} 2)	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
HCOOH + CF_3CHO	**0.0617**	**0.0248**	**0.0195**	**0.0153**	**0.0092**
TS_{HAE} 2	0.0475	0.0184	0.0144	0.0111	0.0065
TS_{HAE} 3	0.0084	0.0037	0.0029	0.0024	0.0015
TS_{FAc} 1	0.0012	0.0006	0.0005	0.0004	0.0003
TS_{FAc} 2	0.0046	0.0021	0.0017	0.0014	0.0009
CF_3COOH + HCHO	**0.0133**	**0.0058**	**0.0046**	**0.0037**	**0.0024**
TS_{HAE} 1	0.0125	0.0053	0.0042	0.0034	0.0021
TS_{TFA} 1	0.0008	0.0004	0.0004	0.0003	0.0003
CF_3OCHO + HCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table S22: the product branching ratio of the **sCI 2** + HCHO reaction with no reference to **CI 1 + CF_3CHO** and **CI 3 + HCHO** as sinks using a MESMER grainsize of 30.*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
HCOOH + CF_3CHO	**0.8227**	**0.8101**	**0.8054**	**0.7996**	**0.7836**
TS_{HAE} 2	0.6331	0.5992	0.5867	0.5712	0.5284
TS_{HAE} 3	0.1125	0.1206	0.1235	0.1269	0.1356
TS_{FAc} 1	0.0157	0.0202	0.0220	0.0244	0.0315
TS_{FAc} 2	0.0614	0.0700	0.0732	0.0771	0.0881
CF_3COOH + HCHO	**0.1773**	**0.1899**	**0.1946**	**0.2004**	**0.2164**
TS_{HAE} 1	0.1667	0.1745	0.1771	0.1801	0.1870
TS_{TFA} 1	0.0106	0.0154	0.0175	0.0203	0.0294
CF_3OCHO + HCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table S23: the product branching ratio of **sCI 3** + HCHO with **CI 1 + CF_3CHO** and **CI 2 + HCHO** as sinks using the $k_{d\text{-}d}$ as pre-exponential factor (6.50×10^{-10} cm^3 $molec^{-1}$ s^{-1}) for barrierless exit channels – using a MESMER grainsize of 40.*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
CI 1 + CF_3CHO	**0.9749**	**0.9888**	**0.9910**	**0.9928**	**0.9956**
TS_{cyc} 3	0.4873	0.4943	0.4953	0.4961	0.4970
TS_{cyc} 4	0.4876	0.4945	0.4956	0.4966	0.4985
CI 2 + HCHO (TS_{CYC} 1)	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
HCOOH + CF_3CHO	**0.0207**	**0.0091**	**0.0074**	**0.0059**	**0.0036**
TS_{HAE} 2	0.0161	0.0069	0.0055	0.0044	0.0026
TS_{HAE} 3	0.0028	0.0013	0.0011	0.0009	0.0005
TS_{FAc} 1	0.0004	0.0002	0.0002	0.0001	0.0001
TS_{FAc} 2	0.0015	0.0007	0.0006	0.0005	0.0003
CF_3COOH + HCHO	**0.0044**	**0.0020**	**0.0017**	**0.0014**	**0.0009**
TS_{HAE} 1	0.0041	0.0019	0.0016	0.0013	0.0008
TS_{TFA} 1	0.0002	0.0001	0.0001	0.0001	0.0001
CF_3OCHO + HCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table S24: the product branching ratio of **sCI 3** + HCHO with **CI 1 + CF_3CHO** and **CI 3 + HCHO** as sinks using the k_{COLL} as pre-exponential factor (1.52×10^{-10} cm^3 $molec^{-1}$ s^{-1}) for barrierless exit channels – using a MESMER grainsize of 40.*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
CI 1 + CF_3CHO	**0.9027**	**0.9593**	**0.9683**	**0.9756**	**0.9858**
TS_{cyc} 3 (barrierless)	0.4512	0.4796	0.4841	0.4877	0.4927
TS_{cyc} 4 (barrierless)	0.4515	0.4797	0.4842	0.4878	0.4931
CI 2 + HCHO (TS_{CYC} 1)	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
HCOOH + CF_3CHO	**0.0803**	**0.0332**	**0.0257**	**0.0197**	**0.0113**
TS_{HAE} 2	0.0624	0.0250	0.0192	0.0145	0.0081
TS_{HAE} 3	0.0107	0.0047	0.0038	0.0030	0.0018
TS_{FAc} 1	0.0014	0.0007	0.0006	0.0005	0.0003
TS_{FAc} 2	0.0058	0.0027	0.0022	0.0017	0.0011
CF_3COOH + HCHO	**0.0170**	**0.0075**	**0.0059**	**0.0047**	**0.0028**
TS_{HAE} 1	0.0160	0.0070	0.0055	0.0043	0.0026
TS_{TFA} 1	0.0009	0.0005	0.0005	0.0004	0.0003
CF_3OCHO + HCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table S25: the product branching ratio of **sCI 3** + HCHO **without** using **CI 1 + CF_3CHO** and **CI 2 + HCHO** as sinks – using a MESMER grainsize of 40.*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
HCOOH + CF_3CHO	**0.8250**	**0.8154**	**0.8116**	**0.8065**	**0.7907**
TS_{HAE} 2	0.6398	0.6142	0.6037	0.5901	0.5478
TS_{HAE} 3	0.1107	0.1170	0.1195	0.1226	0.1317
TS_{FAc} 1	0.0149	0.0182	0.0196	0.0216	0.0283
TS_{FAc} 2	0.0595	0.0660	0.0687	0.0722	0.0830
CF_3COOH + HCHO	**0.1750**	**0.1846**	**0.1884**	**0.1935**	**0.2093**
TS_{HAE} 1	0.1652	0.1714	0.1737	0.1765	0.1840
TS_{TFA} 1	0.0098	0.0132	0.0148	0.0170	0.0252
CF_3OCHO + HCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

S2.4 Product branching ratio of HCHO reactions with sCIs 4 & 5

*Table S26: the product branching ratio of **sCI 4 + HCHO** with **CI 1** + CF_3CFO and **CI 5** + HCHO no barrierless exit channels.*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
CI 1 + CF_3CFO	**0.8441**	**0.8437**	**0.8436**	**0.8435**	**0.8429**
TS_{CYC} 3	0.5708	0.5701	0.5698	0.5695	0.5683
TS_{CYC} 4	0.2732	0.2737	0.2738	0.2740	0.2746
CI 5 + HCHO (TS_{CYC} 2)	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
HCOOH + CF_3CFO	**0.1559**	**0.1562**	**0.1564**	**0.1565**	**0.1570**
TS_{HAE} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{FAc} 1	0.1354	0.1353	0.1353	0.1353	0.1353
TS_{FAc} 2	0.0205	0.0209	0.0210	0.0212	0.0217
CF_3OCFO + HCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table S27: The product branching ratio of **sCI 4 + HCHO** with no **CI 1** + CF_3CFO and **CI 4** + HCHO exit channels using a MESMER grainsize of 20*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
HCOOH + CF_3CFO	**0.9996**	**0.9992**	**0.9990**	**0.9988**	**0.9978**
TS_{HAE} 2	0.0004	0.0006	0.0007	0.0009	0.0016
TS_{FAc} 1	0.8450	0.8271	0.8209	0.8133	0.7910
TS_{FAc} 2	0.1542	0.1715	0.1774	0.1845	0.2053
CF_3OCFO + HCHO	**0.0004**	**0.0008**	**0.0010**	**0.0012**	**0.0022**
TS_{ESTER} 1	<0.0001	0.0001	0.0001	0.0002	0.0004
TS_{ESTER} 2	0.0004	0.0007	0.0008	0.0011	0.0019

Table S28: the product branching ratio of sCI 5 ***+ HCHO*** *with* ***CI 1*** *+ CF_3CFO and* ***CI 4*** *+ HCHO as sinks using the $k_{d\text{-}d}$ as pre-exponential factor (7.20×10^{-10} cm^3 $molec^{-1}$ s^{-1}) for barrierless exit channels using MESMER grainsize of 40*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
CI 1 + CF_3CFO	**0.8456**	**0.8432**	**0.8421**	**0.8406**	**0.8355**
TS_{CYC} 3	0.5750	0.5693	0.5669	0.5637	0.5541
TS_{CYC} 4	0.2705	0.2740	0.2753	0.2769	0.2813
CI 4 + HCHO (TS_{CYC} 1)	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**0.0002**
HCOOH + CF_3CFO	**0.1544**	**0.1567**	**0.1578**	**0.1593**	**0.1641**
TS_{HAE} 2	<0.0001	<0.0001	<0.0001	0.0001	0.0001
TS_{FAc} 1	0.1356	0.1354	0.1354	0.1354	0.1356
TS_{FAc} 2	0.0188	0.0213	0.0224	0.0238	0.0284
CF_3OCFO + HCHO	**<0.0001**	**<0.0001**	**<0.0001**	**0.0001**	**0.0002**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	0.0001	0.0001

Table S29: the product branching ratio of sCI 5 ***+ HCHO*** *with* ***CI 1*** *+ CF_3CFO and* ***CI 4*** *+ HCHO as sinks using the k_{COLL} as pre-exponential factor (1.49×10^{-10} cm^3 $molec^{-1}$ s^{-1}) for barrierless exit channels using MESMER grainsize of 40.*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
CI 1 + CF_3CFO	**0.8455**	**0.8432**	**0.8422**	**0.8407**	**0.8356**
TS_{CYC} 3	0.5748	0.5693	0.5669	0.5637	0.5542
TS_{CYC} 4	0.2706	0.2740	0.2753	0.2769	0.2814
CI 4 + HCHO (TS_{CYC} 1)	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**0.0001**
HCOOH + CF_3CFO	**0.1545**	**0.1567**	**0.1578**	**0.1593**	**0.1642**
TS_{HAE} 2	<0.0001	<0.0001	<0.0001	0.0001	0.0001
TS_{FAc} 1	0.1357	0.1354	0.1354	0.1354	0.1356
TS_{FAc} 2	0.0188	0.0213	0.0224	0.0238	0.0285
CF_3OCFO + HCHO	**<0.0001**	**<0.0001**	**<0.0001**	**0.0001**	**0.0002**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ESTER} 2	<0.0001	<0.0001	<0.0001	0.0001	0.0001

Table S30: product branching ratios of ***sCI 5 + HCHO*** *with no* ***CI*** *+ aldehyde exit channels using MESMER grainsize of 30*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
HCOOH + CF_3CFO	**0.9999**	**0.9998**	**0.9997**	**0.9996**	**0.9992**
TS_{HAE} 2	0.0001	0.0002	0.0003	0.0003	0.0006
TS_{FAc} 1	0.8735	0.8624	0.8581	0.8524	0.8324
TS_{FAc} 2	0.1263	0.1372	0.1414	0.1470	0.1662
CF_3OCFO + HCHO	**0.0001**	**0.0002**	**0.0003**	**0.0004**	**0.0008**
TS_{ESTER} 1	<0.0001	<0.0001	<0.0001	<0.0001	0.0001
TS_{ESTER} 2	0.0001	0.0002	0.0003	0.0003	0.0007

S2.5 sCI 1 + HCHO & SO_2 yields of the HOZ/SOZ intermediate products

*Table S31: Yields from the first step of the **sCI** + CF_3CHO & SO_2 reactions.*

Intermediate Product branching ratio (*Γ*)	Temperature (K)				
	200	**275**	**298**	**325**	**400**
sCI 1 + CF_3CFO					
TS_{cyc} 1	0.7486	0.7647	0.7663	0.7668	0.7609
TS_{cyc} 2	0.2514	0.2353	0.2337	0.2332	0.2391
sCI 2 + SO_2					
TS_{EXO}	0.3278	0.3102	0.3070	0.3042	0.3001
TS_{ENDO}	0.6722	0.6898	0.6930	0.6958	0.6999
sCI 3 + SO_2					
TS_{EXO}	0.4871	0.4991	0.4987	0.4975	0.4905
TS_{ENDO}	0.5129	0.5009	0.5013	0.5025	0.5095
sCI 4 + SO_2					
TS_{EXO}	0.0027	0.4981	0.4990	0.4994	0.4998
TS_{ENDO}	0.9973	0.5019	0.5010	0.5006	0.5002
sCI 5 + SO_2					
TS_{EXO}	0.4715	0.4905	0.4938	0.4962	0.4986
TS_{ENDO}	0.5285	0.5095	0.5062	0.5038	0.5014

(All other sCI + aldehyde/ketone and sCI + SO_2 reactions in this study produce one HOZ or SOZ conformer at 100% efficiency)

S2.6 Product branching ratio of SO_2 reactions with sCI 1

*Table S32: SOZ fragmentation branching ratios (**Γ**) of **sCI 1** + SO_2 reaction all identified pathways included (grainsize=20)*

Product branching ratio (*Γ*)	Temperature (K)				
	200	**275**	**298**	**325**	**400**
SO_3 + HCHO	**0.9949**	**0.9936**	**0.9931**	**0.9926**	**0.9908**
TS_{SO_3} 1	0.0649	0.0694	0.0709	0.0725	0.0771
TS_{SO_3} 2	0.9106	0.9001	0.8966	0.8925	0.8803
SO_2 + HCOOH	**0.0051**	**0.0064**	**0.0069**	**0.0074**	**0.0092**
TS_{acid} 1	0.0001	0.0001	0.0002	0.0002	0.0003
TS_{acid} 2	0.0049	0.0061	0.0065	0.0070	0.0086
TS_{acid} 3	0.0196	0.0242	0.0258	0.0278	0.0337

*Table S33: SOZ decomposition branching ratios (**Γ**) of **sCI 1** + SO_2 reaction with some pathways included (grainsize=10)*

Product branching ratio (*Γ*)	Temperature (K)				
	200	**275**	**298**	**325**	**400**
SO_3 + HCHO	**0.9947**	**0.9933**	**0.9928**	**0.9922**	**0.9903**
TS_{SO_3} 1	0.0640	0.0686	0.0700	0.0717	0.0764
TS_{SO_3} 2	0.9307	0.9247	0.9227	0.9204	0.9138
SO_2 + HCOOH	**0.0053**	**0.0067**	**0.0072**	**0.0078**	**0.0097**
TS_{acid} 1	0.0001	0.0001	0.0002	0.0002	0.0003
TS_{acid} 2	0.0052	0.0066	0.0071	0.0076	0.0094

S2.7 SO_2 reactions with sCIs 2 & 3

*Table S34: SOZ decomposition branching ratios (**Γ**) of **sCI 2** + SO_2 reaction all identified pathways included (grainsize=50), using the $k_{d\text{-}d}$ as pre-exponential factor (4.08×10^{-10} cm^3 $molec^{-1}$ s^{-1}) for cyclo-reversion pathway.*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
sCI 3 + SO_2	**0.0001**	**0.0012**	**0.0023**	**0.0046**	**0.0224**
TS_{EXO}	0.0001	0.0009	0.0017	0.0032	0.0148
TS_{ENDO}	<0.0001	0.0003	0.0007	0.0013	0.0076
SO_3 + CF_3CHO	**0.9988**	**0.9971**	**0.9958**	**0.9931**	**0.9733**
TS_{SO_3} 1	0.6907	0.6910	0.6909	0.6923	0.6883
TS_{SO_3} 2	0.3081	0.3061	0.3048	0.3008	0.2850
SO_2 + CF_3COOH	**0.0011**	**0.0016**	**0.0019**	**0.0024**	**0.0043**
TS_{acid} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{acid} 2	0.0002	0.0003	0.0004	0.0004	0.0008
TS_{acid} 3	0.0008	0.0013	0.0015	0.0018	0.0032
TS_{acid} 4	<0.0001	<0.0001	0.0001	0.0001	0.0002
SO_2 + CF_3OCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ester} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ester} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table S35: SOZ decomposition branching ratios (**Γ**) of **sCI 2** + SO_2 reaction without cyclo-revision pathway to **CI 3** + SO_2 revision. Grainsize = 40.*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
SO_3 + CF_3CHO	**0.9989**	**0.9984**	**0.9981**	**0.9976**	**0.9955**
TS_{SO_3} 1	0.6910	0.6901	0.6914	0.6936	0.6958
TS_{SO_3} 2	0.3080	0.3082	0.3067	0.3040	0.2997
SO_2 + CF_3COOH	**0.0011**	**0.0016**	**0.0019**	**0.0024**	**0.0045**
TS_{acid} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{acid} 2	0.0002	0.0003	0.0004	0.0005	0.0008
TS_{acid} 3	0.0008	0.0013	0.0015	0.0018	0.0034
TS_{acid} 4	<0.0001	<0.0001	0.0001	0.0001	0.0003
SO_2 + CF_3OCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ester} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ester} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table S36: SOZ decomposition branching ratios (**Γ**) of **sCI 2** + SO_2 reaction without sCI pathways and with only pathways that lead directly to SOZs included. Grainsize = 30.*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
SO_3 + CF_3CHO	**0.9998**	**0.9997**	**0.9996**	**0.9995**	**0.9992**
TS_{SO_3} 1	0.6921	0.6903	0.6928	0.6955	0.6992
TS_{SO_3} 2	0.3077	0.3094	0.3069	0.3041	0.3000
SO_2 + CF_3COOH	**0.0002**	**0.0003**	**0.0004**	**0.0005**	**0.0008**
TS_{acid} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{acid} 2	0.0002	0.0003	0.0004	0.0005	0.0008

*Table S37: **sCI 3** + SO_2 SOZ fragmentation branching ratios (**Γ**) with all identified pathways included. Grainsize = 50*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
sCI 2 + SO_2	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{EXO}	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ENDO}	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
SO_3 + CF_3CHO	**0.9987**	**0.9977**	**0.9973**	**0.9966**	**0.9941**
TS_{SO_3} 1	0.5088	0.4989	0.4989	0.4995	0.5045
TS_{SO_3} 2	0.4899	0.4989	0.4984	0.4971	0.4896
SO_2 + CF_3COOH	**0.0013**	**0.0023**	**0.0027**	**0.0033**	**0.0059**
TS_{acid} 1	<0.0001	<0.0001	<0.0001	<0.0001	0.0001
TS_{acid} 2	0.0002	0.0004	0.0005	0.0006	0.0010
TS_{acid} 3	0.0010	0.0016	0.0019	0.0024	0.0040
TS_{acid} 4	0.0001	0.0002	0.0003	0.0004	0.0008
SO_2 + CF_3OCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ester} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ester} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table S38: SOZ fragmentation branching ratios (**Γ**) of the **sCI 3** + SO_2 reaction with all identified pathways except cyclo-reversion pathways **CI 2** + SO_2. Grainsize = 40*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
SO_3 + CF_3CHO	**0.9987**	**0.9977**	**0.9973**	**0.9967**	**0.9941**
TS_{SO_3} 1	0.5117	0.4989	0.4989	0.4995	0.5045
TS_{SO_3} 2	0.4870	0.4989	0.4984	0.4971	0.4896
SO_2 + CF_3COOH	**0.0013**	**0.0023**	**0.0027**	**0.0033**	**0.0059**
TS_{acid} 1	<0.0001	<0.0001	<0.0001	<0.0001	0.0001
TS_{acid} 2	0.0002	0.0004	0.0005	0.0006	0.0010
TS_{acid} 3	0.0010	0.0016	0.0019	0.0024	0.0040
TS_{acid} 4	0.0001	0.0002	0.0003	0.0004	0.0008
SO_2 + CF_3OCHO	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**
TS_{ester} 1	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ester} 2	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001

*Table S39: SOZ decomposition branching ratios (**Γ**) of **sCI 2** + SO_2 reaction without sCI pathways and with only pathways that lead directly to SOZs included. Grainsize =30*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
SO_3 + CF_3CHO	**0.9997**	**0.9996**	**0.9995**	**0.9994**	**0.9990**
TS_{SO_3} 1	0.5102	0.5005	0.5008	0.5019	0.5086
TS_{SO_3} 2	0.4895	0.4991	0.4987	0.4975	0.4904
SO_2 + CF_3COOH	**0.0003**	**0.0004**	**0.0005**	**0.0006**	**0.0010**
TS_{acid} 1	<0.0001	<0.0001	<0.0001	<0.0001	0.0001
TS_{acid} 2	0.0002	0.0004	0.0005	0.0006	0.0010

S2.8 SO_2 reactions with sCIs 4 & 5

*Table S40: SOZ decomposition branching ratios (**Γ**) of **sCI 4** + SO_2 reaction with all identified pathways included. Grainsize = 50. The $k_{d\text{-}d}$ (4.42 × 10^{-10} cm^3 $molec^{-1}$ s^{-1}) used as pre-exponential factor for cyclo-reversion pathway.*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
sCI 5 + SO_2	**<0.0001**	**0.0010**	**0.0017**	**0.0029**	**0.0107**
TS_{EXO}	<0.0001	0.0002	0.0003	0.0005	0.0020
TS_{ENDO}	<0.0001	0.0009	0.0014	0.0024	0.0087
SO_3 + CF_3CHO	**1.0000**	**0.9913**	**0.9892**	**0.9861**	**0.9716**
TS_{SO_3} 1	<0.0001	0.1025	0.1052	0.1082	0.1147
TS_{SO_3} 2	1.0000	0.4995	0.4984	0.4972	0.4936
TS_{SO_3} 3	<0.0001	0.3892	0.3856	0.3807	0.3633
SO_2 + CF_3OCHO	**<0.0001**	**0.0077**	**0.0091**	**0.0110**	**0.0177**
TS_{ester} 1	<0.0001	0.0021	0.0024	0.0029	0.0045
TS_{ester} 2	<0.0001	0.0056	0.0067	0.0081	0.0132

*Table S41: SOZ decomposition branching ratios (**Γ**) of **sCI 4** + SO_2 reaction without cyclo-revision to **CI 5** + SO_2 revision. Grainsize = 50*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
SO_3 + CF_3CHO	**1.0000**	**0.9923**	**0.9909**	**0.9889**	**0.9818**
TS_{SO_3} 1	0.0005	0.1027	0.1056	0.1087	0.1169
TS_{SO_3} 2	0.9973	0.4998	0.4986	0.4977	0.4956
TS_{SO_3} 3	0.0022	0.3897	0.3867	0.3825	0.3693
SO_2 + CF_3OCHO	**<0.0001**	**0.0077**	**0.0091**	**0.0111**	**0.0182**
TS_{ester} 1	<0.0001	0.0021	0.0024	0.0029	0.0046
TS_{ester} 2	<0.0001	0.0057	0.0067	0.0082	0.0136

*Table S42: SOZ decomposition branching ratios (**Γ**) of **sCI 4** + SO_2 reaction without **CI 5** + SO_2 cyclo-revision pathways and with only pathways that lead directly to SOZs included. Grainsize =30*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
SO_3 + CF_3CHO	**1.000**	**1.000**	**1.000**	**1.000**	**1.000**
TS_{SO_3} 1	0.0057	0.0886	0.0924	0.0965	0.1071
TS_{SO_3} 2	0.9643	0.5095	0.5062	0.5039	0.5014
TS_{SO_3} 3	0.0300	0.4019	0.4014	0.3996	0.3915

*Table S43: SOZ decomposition branching ratios (**Γ**) of **sCI 5** + SO_2 reaction with all identified pathways included. Grainsize = 50. The $k_{d\text{-}d}$ (4.51×10^{-10} cm^3 $molec^{-1}$ s^{-1}) used as pre-exponential factor for cyclo-reversion pathway.*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
sCI 4 + SO_2	**<0.0001**	**<0.0001**	**<0.0001**	**<0.0001**	**0.0001**
TS_{EXO}	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
TS_{ENDO}	<0.0001	<0.0001	<0.0001	<0.0001	0.0001
SO_3 + CF_3CHO	**0.9998**	**0.9963**	**0.9955**	**0.9943**	**0.9895**
TS_{SO_3} 1	0.0076	0.0881	0.0917	0.0957	0.1053
TS_{SO_3} 2	0.9523	0.5083	0.5049	0.5023	0.4987
TS_{SO_3} 3	0.0399	0.3999	0.3988	0.3963	0.3856
SO_2 + CF_3OCHO	**0.0002**	**0.0037**	**0.0045**	**0.0057**	**0.0103**
TS_{ester} 1	0.0001	0.0011	0.0013	0.0016	0.0027
TS_{ester} 2	0.0001	0.0026	0.0032	0.0041	0.0077

*Table S44: SOZ decomposition branching ratios (**Γ**) of **sCI 5** + SO_2 reaction without cyclo-revision to **CI 4** + SO_2 revision. Grainsize = 50*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
SO_3 + CF_3CHO	**0.9981**	**0.9963**	**0.9955**	**0.9943**	**0.9897**
TS_{SO_3} 1	0.0753	0.0881	0.0917	0.0957	0.1053
TS_{SO_3} 2	0.5279	0.5084	0.5049	0.5023	0.4987
TS_{SO_3} 3	0.3950	0.3998	0.3988	0.3964	0.3856
SO_2 + CF_3OCHO	**0.0019**	**0.0037**	**0.0045**	**0.0057**	**0.0103**
TS_{ester} 1	0.0007	0.0011	0.0013	0.0016	0.0027
TS_{ester} 2	0.0012	0.0026	0.0032	0.0041	0.0076

*Table S45: SOZ decomposition branching ratios (**Γ**) of **sCI 5** + SO_2 reaction without **CI 4** pathways and with only pathways that lead directly to SOZs included. Grainsize =30*

Product branching ratio (*Γ*)	**Temperature (K)**				
	200	**275**	**298**	**325**	**400**
SO_3 + CF_3CHO	**1.000**	**1.000**	**1.000**	**1.000**	**1.000**
TS_{SO_3} 1	0.0042	0.0886	0.0924	0.0965	0.1071
TS_{SO_3} 2	0.9740	0.5096	0.5063	0.5039	0.5014
TS_{SO_3} 3	0.0219	0.4018	0.4014	0.3996	0.3915

*Table S46: Pathway Distribution (Γ) of **sCIs 1-5** reactions with H_2S, H_2O and MeOH.*

sCI	T (K)	H_2S		H_2O		MeOH	
		Γ_{TS1}	Γ_{TS2}	Γ_{TS1}	Γ_{TS2}	Γ_{TS1}	Γ_{TS2}
1	**200**	0.551	0.449	0.874	0.126	0.899	0.101
	275	0.539	0.461	0.807	0.193	0.823	0.177
	298.15	0.537	0.463	0.790	0.210	0.802	0.198
	325	0.534	0.466	0.773	0.227	0.780	0.220
	400	0.529	0.471	0.732	0.268	0.728	0.272
2	**200**	0.743	0.257	0.270	0.730	0.973	0.027
	275	0.677	0.323	0.311	0.689	0.935	0.065
	298.15	0.662	0.338	0.320	0.680	0.923	0.077
	325	0.647	0.353	0.329	0.671	0.908	0.092
	400	0.614	0.386	0.348	0.652	0.871	0.129
3	**200**	0.689	0.311	0.843	0.157	0.900	0.100
	275	0.644	0.356	0.789	0.211	0.821	0.179
	298.15	0.634	0.366	0.777	0.223	0.799	0.201
	325	0.624	0.376	0.763	0.237	0.776	0.224
	400	0.604	0.396	0.734	0.266	0.721	0.279
4	**200**	0.734	0.266	0.438	0.562	N/A	N/A
	275	0.710	0.290	0.424	0.576	N/A	N/A
	298.15	0.700	0.300	0.422	0.578	N/A	N/A
	325	0.688	0.312	0.420	0.580	N/A	N/A
	400	0.658	0.342	0.417	0.583	N/A	N/A
5	**200**	0.604	0.396	0.325	0.675	0.472	0.528
	275	0.581	0.419	0.383	0.617	0.465	0.535
	298.15	0.576	0.424	0.396	0.604	0.464	0.536
	325	0.571	0.429	0.408	0.592	0.462	0.538
	400	0.561	0.439	0.435	0.565	0.459	0.541

Table S47: Branching Ratios (Γ) for $(H_2O)_2$ reaction with ***sCIs 1 – 5***

sCI	T (K)	Γ_{TS1}	Γ_{TS2}	Γ_{TS3}	Γ_{TS4}
1	**200**	0.273	0.171	0.275	0.281
	275	0.279	0.143	0.283	0.295
	298.15	0.281	0.137	0.284	0.298
	325	0.282	0.133	0.286	0.300
	400	0.284	0.126	0.286	0.304
2	**200**	0.273	0.154	0.314	0.259
	275	0.289	0.122	0.315	0.274
	298.15	0.292	0.117	0.314	0.277
	325	0.296	0.113	0.311	0.280
	400	0.302	0.111	0.303	0.284
3	**200**	0.161	0.316	0.249	0.274
	275	0.144	0.333	0.246	0.277
	298.15	0.140	0.336	0.245	0.278
	325	0.138	0.339	0.245	0.279
	400	0.134	0.341	0.245	0.280
4	**200**	0.241	0.259	0.244	0.255
	275	0.228	0.273	0.235	0.264
	298.15	0.225	0.277	0.232	0.266
	325	0.220	0.282	0.229	0.269
	400	0.211	0.292	0.222	0.275
5	**200**	0.254	0.287	0.243	0.216
	275	0.256	0.324	0.233	0.188
	298.15	0.256	0.333	0.230	0.181
	325	0.256	0.344	0.227	0.174
	400	0.256	0.366	0.219	0.159

S3. Collision Frequency Rate-Limiting Coefficients

S3.1. Equations

Often, when k_{ME} values ≥ 10^{-10} cm^3 molec.$^{-1}$ s^{-1} each collision leads to a reaction which means the main limit to reaction is the number of collisions. One way to model the collision frequency is using the collision-limited reaction rate coefficient (k_{COLL}), which is modelled using the assumption that molecules have no attractive or repulsive forces and the only interactions between molecules are the momentum from elastic collisions. Another model is the dipole–dipole capture limit ($k_{d\text{-}d}$), which incorporates the changes to collision frequency caused by significant permanent dipoles within the reactants. These approaches have been used in a variety of different studies that examine bimolecular reactions involving Criegee intermediates.[4–6]

Collision Limit Rate Equation (k_{COLL}):

$$k_{COLL} = \left(\frac{8k_BT}{\pi\mu}\right)^{1/2} \pi(r_1 + r_2)^2 \qquad \textit{Equation S5}$$

$$\mu = \frac{m_1 m_2}{m_1 + m_2} \qquad \textit{Equation S6}$$

k_B is the Boltzmann constant, T is the temperature, μ are the reduced mass of reactants, r_1 and r_2 are the covalent radii of reactants and m_1 and m_2 are the masses.

Dipole-Dipole Capture Limit ($k_{d\text{-}d}$):

$$k_{d\text{-}d} = C\sqrt{\pi/\mu}\,(\mu_{D1}\mu_{D2})^{(2/3)}(k_BT)^{-1/6} \qquad \textit{Equation S7}$$

μ_{D1} and μ_{D2}, the dipole moments of reactants, μ, reduced mass, k_B, the Boltzmann constant, T, temperature, and, C, isotropic, adiabatic or non-adiabatic anisotropic constant which depends on the anisotropy of the capture potential model.

S3.2. Properties of Criegee intermediates 1-5 and co-reactants

Table S48: Reactants Dipole moments (μ_D, Debye), mass (m, amu), radii (r, Å) and C-O-O bond ratios

Reactant	Dipole Moment (μ_D, Debye)	Mass (m, amu)	radii (r, Å)	C=O-O Bond Ratio
HCHOO	4.3104	46.005	3.209	1.078
Syn-CF_3CHOO	3.4822	113.993	4.082	1.064
Anti-CF_3CHOO	2.5055	113.993	4.418	1.071
Syn-CF_3CFOO	3.016	131.983	4.099	1.114
Anti-CF_3CFOO	2.9299	131.983	4.447	1.101
HCHO	2.3887	30.011	2.017	N/A
HNO_3	2.2588	62.996	2.938	N/A
SO_2	1.8065	63.962	2.491	N/A
CF_3COOH	2.2289	113.993	4.237	N/A
HCl	1.1157	35.977	1.284	N/A
H_2O	1.8472	18.011	1.536	N/A
$(H_2O)_2$	2.631	36.021	3.911	N/A
H_2S	0.9902	33.988	1.944	N/A
HF	1.8124	20.006	0.924	N/A
MeOH	1.6556	32.026	2.829	N/A

S3.3 Gas-collision limit

Table S49: Gas-Collision Limit for Criegee intermediates reactions in this study.

Reaction	**Collision Limit (10^{-10} cm^3 $molec.^{-1}$ s^{-1})**				
T (K)	**200**	**275**	**298.15**	**325**	**400**
sCI 1 + HCHO	1.04	1.21	1.26	1.32	1.46
sCI 1 + HNO_3	1.18	1.39	1.45	1.51	1.67
sCI 1 + SO_2	1.02	1.19	1.24	1.29	1.44
sCI 1 + CF_3COOH	1.57	1.84	1.91	2.00	2.21
sCI 1 + HCl	0.73	0.85	0.89	0.93	1.03
sCI 1 + H_2O	1.01	1.19	1.23	1.29	1.43
sCI 1 + $(H_2O)_2$	1.82	2.14	2.23	2.32	2.58
sCI 1 + H_2S	0.97	1.14	1.19	1.24	1.37
sCI 1 + HF	0.74	0.87	0.90	0.94	1.05
sCI 1 + MeOH	1.36	1.59	1.66	1.73	1.92
sCI 1 + CF_3CHO	1.24	1.46	1.52	1.58	1.76
sCI 1 + CF_3CFO	1.27	1.49	1.55	1.62	1.80
sCI 2 + HCHO	1.23	1.45	1.51	1.57	1.74
sCI 2 + HNO_3	1.25	1.47	1.53	1.59	1.77
sCI 2 + SO_2	1.09	1.28	1.33	1.39	1.54
sCI 2 + CF_3COOH	1.48	1.74	1.81	1.89	2.10
sCI 2 + HCl	0.89	1.04	1.09	1.13	1.26
sCI 2 + H_2O	1.29	1.52	1.58	1.65	1.83
sCI 2 + $(H_2O)_2$	1.97	2.31	2.41	2.52	2.79
sCI 2 + H_2S	1.15	1.34	1.40	1.46	1.62
sCI 2 + HF	0.98	1.15	1.20	1.25	1.39
sCI 2 + MeOH	1.54	1.81	1.88	1.97	2.18
sCI 3 + HCHO	1.37	1.61	1.68	1.75	1.94
sCI 3 + HNO_3	1.37	1.61	1.68	1.75	1.94
sCI 3 + SO_2	1.21	1.41	1.47	1.54	1.70
sCI 3 + CF_3COOH	1.60	1.88	1.96	2.04	2.27
sCI 3 + HCl	1.00	1.18	1.23	1.28	1.42
sCI 3 + H_2O	1.45	1.70	1.77	1.85	2.05
sCI 3 + $(H_2O)_2$	2.14	2.51	2.62	2.73	3.03
sCI 3 + H_2S	1.28	1.50	1.56	1.63	1.81
sCI 3 + HF	1.12	1.31	1.36	1.43	1.58
sCI 3 + MeOH	1.70	1.99	2.07	2.16	2.40
sCI 4 + HCHO	1.22	1.43	1.49	1.56	1.73
sCI 4 + HNO_3	1.23	1.44	1.50	1.56	1.73
sCI 4 + SO_2	1.07	1.25	1.31	1.36	1.51
sCI 4 + CF_3COOH	1.44	1.68	1.75	1.83	2.03
sCI 4 + HCl	0.88	1.03	1.08	1.12	1.25
sCI 4 + H_2O	1.29	1.51	1.57	1.64	1.82
sCI 4 + $(H_2O)_2$	1.95	2.29	2.38	2.48	2.76
sCI 4 + H_2S	1.14	1.33	1.39	1.45	1.61
sCI 4 + HF	0.98	1.15	1.19	1.25	1.38
sCI 4 + MeOH	1.53	1.79	1.87	1.95	2.16
sCI 5 + HCHO	1.37	1.60	1.67	1.74	1.93
sCI 5 + HNO_3	1.35	1.58	1.65	1.72	1.91
sCI 5 + SO_2	1.19	1.39	1.45	1.51	1.68
sCI 5 + CF_3COOH	1.56	1.83	1.90	1.99	2.20
sCI 5 + HCl	1.00	1.17	1.22	1.27	1.41
sCI 5 + H_2O	1.45	1.70	1.77	1.85	2.06
sCI 5 + $(H_2O)_2$	2.12	2.49	2.59	2.71	3.00
sCI 5 + H_2S	1.27	1.49	1.55	1.62	1.80
sCI 5 + HF	1.12	1.31	1.37	1.43	1.58
sCI 5 + MeOH	1.69	1.98	2.06	2.15	2.38

S3.4 Isotropic dipole-dipole capture moment

Table S50: Isotropic Dipole-Dipole Capture Limit for Criegee intermediates reactions in this study

Reaction	**Isotropic Dipole-Dipole Capture Limit (10^{-10} cm^3 molec.$^{-1}$ s^{-1})**				
T (K)	**200**	**275**	**298.15**	**325**	**400**
sCI 1 + HCHO	11.34	10.75	10.61	10.45	10.10
sCI 1 + HNO_3	9.03	8.56	8.45	8.32	8.04
sCI 1 + SO_2	7.75	7.35	7.25	7.15	6.91
sCI 1 + CF_3COOH	8.06	7.64	7.54	7.43	7.18
sCI 1 + HCl	6.47	6.14	6.06	5.97	5.77
sCI 1 + H_2O	11.31	10.73	10.58	10.43	10.08
sCI 1 + $(H_2O)_2$	11.46	10.87	10.73	10.57	10.21
sCI 1 + H_2S	6.07	5.76	5.68	5.60	5.41
sCI 1 + HF	10.76	10.21	10.07	9.93	9.59
sCI 1 + MeOH	8.71	8.26	8.15	8.03	7.76
sCI 1 + CF_3CHO	6.95	6.59	6.50	6.41	6.19
sCI 1 + CF_3CFO	3.57	3.38	3.34	3.29	3.18
sCI 2 + HCHO	8.60	8.15	8.04	7.93	7.66
sCI 2 + HNO_3	6.34	6.01	5.93	5.85	5.65
sCI 2 + SO_2	5.43	5.15	5.08	5.01	4.84
sCI 2 + CF_3COOH	5.30	5.03	4.96	4.89	4.72
sCI 2 + HCl	4.82	4.57	4.51	4.45	4.30
sCI 2 + H_2O	8.95	8.49	8.38	8.26	7.98
sCI 2 + $(H_2O)_2$	8.54	8.10	7.99	7.88	7.61
sCI 2 + H_2S	4.55	4.32	4.26	4.20	4.06
sCI 2 + HF	8.45	8.01	7.91	7.79	7.53
sCI 2 + MeOH	6.56	6.22	6.14	6.05	5.85
sCI 3 + HCHO	6.90	6.55	6.46	6.37	6.15
sCI 3 + HNO_3	5.09	4.83	4.76	4.69	4.53
sCI 3 + SO_2	4.36	4.14	4.08	4.02	3.89
sCI 3 + CF_3COOH	4.26	4.04	3.98	3.93	3.79
sCI 3 + HCl	3.87	3.67	3.62	3.57	3.45
sCI 3 + H_2O	7.19	6.82	6.73	6.63	6.40
sCI 3 + $(H_2O)_2$	6.86	6.50	6.42	6.33	6.11
sCI 3 + H_2S	3.66	3.47	3.42	3.37	3.26
sCI 3 + HF	6.79	6.43	6.35	6.26	6.04
sCI 3 + MeOH	5.27	5.00	4.93	4.86	4.70
sCI 4 + HCHO	7.70	7.30	7.20	7.10	6.86
sCI 4 + HNO_3	5.62	5.33	5.26	5.18	5.00
sCI 4 + SO_2	4.82	4.57	4.51	4.44	4.29
sCI 4 + CF_3COOH	4.65	4.41	4.35	4.29	4.14
sCI 4 + HCl	4.31	4.09	4.03	3.98	3.84
sCI 4 + H_2O	8.06	7.64	7.54	7.43	7.18
sCI 4 + $(H_2O)_2$	7.63	7.24	7.14	7.04	6.80
sCI 4 + H_2S	4.07	3.86	3.81	3.76	3.63
sCI 4 + HF	7.60	7.21	7.11	7.01	6.77
sCI 4 + MeOH	5.87	5.57	5.50	5.42	5.23
sCI 5 + HCHO	7.55	7.16	7.07	6.97	6.73
sCI 5 + HNO_3	5.51	5.23	5.16	5.08	4.91
sCI 5 + SO_2	4.72	4.48	4.42	4.36	4.21
sCI 5 + CF_3COOH	4.56	4.32	4.27	4.21	4.06
sCI 5 + HCl	4.23	4.01	3.96	3.90	3.77
sCI 5 + H_2O	7.90	7.50	7.40	7.29	7.04
sCI 5 + $(H_2O)_2$	7.49	7.10	7.01	6.91	6.67
sCI 5 + H_2S	3.99	3.79	3.74	3.68	3.56
sCI 5 + HF	7.45	7.07	6.97	6.87	6.64
sCI 5 + MeOH	5.76	5.46	5.39	5.31	5.13

S3.5 Adiabatic anisotropic dipole-dipole capture moment

Table S51: Adiabatic anisotropic Dipole-Dipole Capture Limit for Criegee intermediates reactions in this study

Reaction	**Adiabatic anisotropic Dipole-Dipole Capture Limit (10^{-10} cm^3 molec.$^{-1}$ s^{-1})**				
T (K)	**200**	**275**	**298.15**	**325**	**400**
sCI 1 + HCHO	7.45	7.06	6.97	6.87	6.63
sCI 1 + HNO_3	5.93	5.62	5.55	5.47	5.28
sCI 1 + SO_2	5.09	4.83	4.76	4.70	4.54
sCI 1 + CF_3COOH	5.29	5.02	4.95	4.88	4.72
sCI 1 + HCl	4.25	4.03	3.98	3.92	3.79
sCI 1 + H_2O	7.43	7.05	6.95	6.85	6.62
sCI 1 + $(H_2O)_2$	7.53	7.14	7.05	6.94	6.71
sCI 1 + H_2S	3.99	3.78	3.73	3.68	3.56
sCI 1 + HF	7.07	6.70	6.61	6.52	6.30
sCI 1 + MeOH	5.72	5.42	5.35	5.27	5.10
sCI 1 + CF_3CHO	4.57	4.33	4.27	4.21	4.07
sCI 1 + CF_3CFO	2.34	2.22	2.19	2.16	2.09
sCI 2 + HCHO	5.65	5.36	5.28	5.21	5.03
sCI 2 + HNO_3	4.16	3.95	3.90	3.84	3.71
sCI 2 + SO_2	3.57	3.39	3.34	3.29	3.18
sCI 2 + CF_3COOH	3.48	3.30	3.26	3.21	3.10
sCI 2 + HCl	3.17	3.00	2.96	2.92	2.82
sCI 2 + H_2O	5.88	5.58	5.50	5.42	5.24
sCI 2 + $(H_2O)_2$	5.61	5.32	5.25	5.18	5.00
sCI 2 + H_2S	2.99	2.84	2.80	2.76	2.66
sCI 2 + HF	5.55	5.26	5.19	5.12	4.94
sCI 2 + MeOH	4.31	4.09	4.03	3.98	3.84
sCI 3 + HCHO	4.53	4.30	4.24	4.18	4.04
sCI 3 + HNO_3	3.34	3.17	3.13	3.08	2.98
sCI 3 + SO_2	2.87	2.72	2.68	2.64	2.55
sCI 3 + CF_3COOH	2.80	2.65	2.62	2.58	2.49
sCI 3 + HCl	2.54	2.41	2.38	2.35	2.27
sCI 3 + H_2O	4.72	4.48	4.42	4.35	4.21
sCI 3 + $(H_2O)_2$	4.51	4.27	4.22	4.16	4.01
sCI 3 + H_2S	2.40	2.28	2.25	2.21	2.14
sCI 3 + HF	4.46	4.23	4.17	4.11	3.97
sCI 3 + MeOH	3.46	3.28	3.24	3.19	3.08
sCI 4 + HCHO	5.06	4.80	4.73	4.66	4.51
sCI 4 + HNO_3	3.69	3.50	3.45	3.40	3.29
sCI 4 + SO_2	3.16	3.00	2.96	2.92	2.82
sCI 4 + CF_3COOH	3.05	2.90	2.86	2.82	2.72
sCI 4 + HCl	2.83	2.69	2.65	2.61	2.52
sCI 4 + H_2O	5.29	5.02	4.95	4.88	4.72
sCI 4 + $(H_2O)_2$	5.01	4.76	4.69	4.62	4.47
sCI 4 + H_2S	2.67	2.54	2.50	2.47	2.38
sCI 4 + HF	4.99	4.73	4.67	4.60	4.45
sCI 4 + MeOH	3.86	3.66	3.61	3.56	3.44
sCI 5 + HCHO	4.96	4.70	4.64	4.58	4.42
sCI 5 + HNO_3	3.62	3.43	3.39	3.34	3.22
sCI 5 + SO_2	3.10	2.94	2.90	2.86	2.76
sCI 5 + CF_3COOH	3.00	2.84	2.80	2.76	2.67
sCI 5 + HCl	2.78	2.63	2.60	2.56	2.47
sCI 5 + H_2O	5.19	4.92	4.86	4.79	4.63
sCI 5 + $(H_2O)_2$	4.92	4.66	4.60	4.54	4.38
sCI 5 + H_2S	2.62	2.49	2.45	2.42	2.34
sCI 5 + HF	4.90	4.64	4.58	4.52	4.36
sCI 5 + MeOH	3.78	3.59	3.54	3.49	3.37

S3.6 Non-adiabatic anisotropic dipole-dipole capture moment

Table S52: Non-adiabatic anisotropic Dipole-Dipole Capture Limit for Criegee intermediate reactions in this study

Reaction	Non-adiabatic anisotropic Dipole-Dipole Capture Limit (10^{-10} cm^3 $molec.^{-1}$ s^{-1})				
T (K)	200	275	298.15	325	400
sCI 1 + HCHO	5.43	5.15	5.08	5.00	4.83
sCI 1 + HNO_3	4.32	4.10	4.04	3.98	3.85
sCI 1 + SO_2	3.71	3.52	3.47	3.42	3.31
sCI 1 + CF_3COOH	3.86	3.66	3.61	3.56	3.44
sCI 1 + HCl	3.10	2.94	2.90	2.86	2.76
sCI 1 + H_2O	5.42	5.14	5.07	4.99	4.82
sCI 1 + $(H_2O)_2$	5.49	5.20	5.13	5.06	4.89
sCI 1 + H_2S	2.91	2.76	2.72	2.68	2.59
sCI 1 + HF	5.15	4.89	4.82	4.75	4.59
sCI 1 + MeOH	4.17	3.95	3.90	3.84	3.71
sCI 1 + CF_3CHO	3.33	3.16	3.11	3.07	2.96
sCI 1 + CF_3CFO	1.71	1.62	1.60	1.57	1.52
sCI 2 + HCHO	4.12	3.90	3.85	3.80	3.67
sCI 2 + HNO_3	3.03	2.88	2.84	2.80	2.70
sCI 2 + SO_2	2.60	2.47	2.43	2.40	2.32
sCI 2 + CF_3COOH	2.54	2.41	2.37	2.34	2.26
sCI 2 + HCl	2.31	2.19	2.16	2.13	2.06
sCI 2 + H_2O	4.29	4.06	4.01	3.95	3.82
sCI 2 + $(H_2O)_2$	4.09	3.88	3.83	3.77	3.64
sCI 2 + H_2S	2.18	2.07	2.04	2.01	1.94
sCI 2 + HF	4.04	3.84	3.78	3.73	3.60
sCI 2 + MeOH	3.14	2.98	2.94	2.90	2.80
sCI 3 + HCHO	3.30	3.13	3.09	3.05	2.94
sCI 3 + HNO_3	2.44	2.31	2.28	2.25	2.17
sCI 3 + SO_2	2.09	1.98	1.95	1.93	1.86
sCI 3 + CF_3COOH	2.04	1.93	1.91	1.88	1.81
sCI 3 + HCl	1.85	1.76	1.73	1.71	1.65
sCI 3 + H_2O	3.44	3.26	3.22	3.17	3.07
sCI 3 + $(H_2O)_2$	3.28	3.11	3.07	3.03	2.93
sCI 3 + H_2S	1.75	1.66	1.64	1.61	1.56
sCI 3 + HF	3.25	3.08	3.04	3.00	2.89
sCI 3 + MeOH	2.52	2.39	2.36	2.33	2.25
sCI 4 + HCHO	3.69	3.50	3.45	3.40	3.28
sCI 4 + HNO_3	2.69	2.55	2.52	2.48	2.40
sCI 4 + SO_2	2.30	2.19	2.16	2.13	2.05
sCI 4 + CF_3COOH	2.23	2.11	2.08	2.05	1.98
sCI 4 + HCl	2.06	1.96	1.93	1.90	1.84
sCI 4 + H_2O	3.86	3.66	3.61	3.56	3.44
sCI 4 + $(H_2O)_2$	3.65	3.47	3.42	3.37	3.26
sCI 4 + H_2S	1.95	1.85	1.82	1.80	1.74
sCI 4 + HF	3.64	3.45	3.40	3.35	3.24
sCI 4 + MeOH	2.81	2.67	2.63	2.59	2.51
sCI 5 + HCHO	3.62	3.43	3.38	3.33	3.22
sCI 5 + HNO_3	2.64	2.50	2.47	2.43	2.35
sCI 5 + SO_2	2.26	2.14	2.12	2.09	2.01
sCI 5 + CF_3COOH	2.18	2.07	2.04	2.01	1.94
sCI 5 + HCl	2.02	1.92	1.89	1.87	1.80
sCI 5 + H_2O	3.78	3.59	3.54	3.49	3.37
sCI 5 + $(H_2O)_2$	3.58	3.40	3.35	3.31	3.19
sCI 5 + H_2S	1.91	1.81	1.79	1.76	1.70
sCI 5 + HF	3.57	3.38	3.34	3.29	3.18
sCI 5 + MeOH	2.76	2.62	2.58	2.54	2.46

S4. Effective Rate Constants (k_{EFF})

S4.1 The formula for the Effective Rate Constants (k_{EFF})

The main approach in this study to determine the atmospheric impact of these sCI + co-reactant reactions is the effective rate constant (k_{EFF}), which is seen in Equation S8.

$$k_{EFF} = k_{ME}\,[\text{co-reactant}] \qquad \textit{Equation 8}$$

By incorporating the local co-reactant abundance, [co-reactant], the k_{EFF} constant produces a single measure of sCI loss path contribution. This k_{EFF} constant can be used to compare the tropospheric impact that reaction with each trace gas has on the local sCI population. This approach has been adopted in various other sCI studies as a modest measure of the atmospheric impact of each reaction.[6–8] The significant variety of local co-reactant abundances in many different environments and the range of effective rate constants produced from these values is covered in this section.

S4.2 Literature Abundances of Atmospheric Co-reactants Across Environments

Table S53: Representative abundances of atmospheric co-reactants across different environments in the literature.

Co-reactant Environment	Abundance (Original units)	Study	Ref
Formaldehyde (HCHO)			
Mean of European homes	23.1 µg/m^3	Salthammer *et al.*	9
Range of European homes	20–30 µg/m^3	Salthammer *et al.*	9
Mean of Rural European sites	3.49 ppb	Salthammer *et al.*	9
Range of Rural European sites	0.4–5.5 ppb	Salthammer *et al.*	9
Homes with particle floorboards	32.0 µg/m^3	Raw *et al.*	10
Homes without particle floorboards	20.3 µg/m^3	Raw *et al.*	10
Homes with particle floorboards in main bedroom England	37.7 µg/m^3	Raw *et al.*	10
Homes without particle floorboards in main bedroom England	23.2 µg/m^3	Raw *et al.*	10
New homes	128 & 135 µg/m^3	Raw *et al.*	10
Average home	22.2 µg/m^3	Raw *et al.*	10
Minimum	1 µg/m^3	Raw *et al.*	10
Maximum	171 µg/m^3	Raw *et al.*	10
In buildings in the absent of ozone	<30 µg/m^3	Uhde *et al.*	11
Highest found with ozone present	148 µg/m^3	Uhde *et al.*	11
General	0.5 µg/m^3	WHO Regional Publications	12
Urban general	1—20 µg/m^3	WHO Regional Publications	12
Heavy traffic	100 µg/m^3	WHO Regional Publications	12
Mobile Home	490 µg/m^3	WHO Regional Publications	12
São Paulo, Brazil	5.0±2.8 ppbv	Nguyen *et al.*	13
Osaka, Japan	1.9±0.9 ppbv	Nguyen *et al.*	13
Acetaldehyde (CH_3CHO)			
São Paulo, Brazil	5.4±2.8 ppbv	Nguyen *et al.*	13
Osaka, Japan	1.5±0.8 ppbv	Nguyen *et al.*	13

General Aldehydes and Ketones (from Vereecken *et al.*)			
$R_1R_2C=O$ – Boreal Forest	1.2×10^{11}	Vereecken *et al.*	8
$R_1R_2C=O$ – Tropical Forest	1.9×10^{10}	Vereecken *et al.*	8
$R_1R_2C=O$ – Mega city	5.1×10^{11}	Vereecken *et al.*	8
$R_1R_2C=O$ – Rural Europe	6.6×10^{10}	Vereecken *et al.*	8
Sulphur Dioxide (SO_2)			
Beijing urban area, China	16.8 ± 13.1 ppb	Lin *et al.*	14
Gucheng rural area, China	14.8 ± 9.4 ppb	Lin *et al.*	14
Shangdianzi, China	7.5 ± 4.0 ppb	Lin *et al.*	14
London Bloomsbury, UK	2 µg/m^3	*defra*	15
London Marylebone Road, UK	7 µg/m^3	*defra*	15
London N. Kensington, UK	14 µg/m^3	*defra*	15
Grangemouth, Falkirk, UK	18 µg/m^3	*defra*	15
Londonderry Rosemount, NI, UK	18 µg/m^3	*defra*	15
0.1 km from Volcanic vents (Mount Etna)	~10,000 µg/m^3	Aiuppa *et al.*	16
10 km from Volcanic vents (Mount Etna)	7 µg/m^3	Aiuppa *et al.*	16
Sao Paulo citywide concentrations	4.94+2.99 ppb	Bravo *et al.*	17
Typical indoor	22.9 (≤50) ppb	Salthammer *et al.*	18
Typical urban concentrations	15 ppbv	Hunter *et al.*	19
SO_2 – Boreal Forest	1.7×10^{10}	Vereecken *et al.*	8
SO_2 – Tropical Forest	~0	Vereecken *et al.*	8
SO_2 – Mega city	9×10^{10}	Vereecken *et al.*	8
SO_2– Rural Europe	6.6×10^{9}	Vereecken *et al.*	8
Nitric Acid (HNO_3) 1.1×10^{11}			
Houston, TX	~4.5 ppb	Leong *et al.*	20
Los Angeles Southern California	20 ppbv	Foreman *et al.*	21
Southern California rural	0.1-8.0 ppb	Crisp *et al.*	22
Houston, TX	0.4-4.6 ppb	Leong *et al.*	20
HNO_3	*~10^{11}*	*Kumar and Fransisco*	7
Trifluoroacetic acid (CF_3COOH)			
Beijing (04/14-04/15)	1459 ± 223 pg/m^3	Zhang *et al.*	23
Beijing (04/14-04/15)	1162 ± 173 pg/m^3	Zhang *et al.*	23
lowest abundance of local TFA	283 pg/m^3	Zhang *et al.*	23
highest abundance of local TFA	6317 pg/m^3	Zhang *et al.*	23
Average Beijing (05/12-04/13)	1580 ± 558 pg/m^3	Wu *et al.*	24
Europe projected future abundance	0.06 — 0.94 ppt	Henne *et al.*	25
Carboxylic acid (RCOOH)			
RCOOH – Boreal Forest	1×10^{11}	Vereecken *et al.*	8
RCOOH – Tropical Forest	5×10^{10}	Vereecken *et al.*	8
RCOOH – Mega city	N/A	Vereecken *et al.*	8
RCOOH – Rural Europe	N/A	Vereecken *et al.*	8
Hydrofluoric acid (HF)			
Stratosphere	0.1-0.5 ppb	Mankin *et al.*	26
vicinity of volcano by ambient T (K)	up to 15 ppbv	Cheng *et al.*	27
At source of volcano	900 ug m^{-3}	Cheng *et al.*	27

Hydrochloric acid (HCl)			
Southern California (overall)	1.3 ppb	Crisp *et al.*	22
Southern California (halfway range)	8 ppb	Crisp *et al.*	22
Southern California (Mean)	2.2 ± 2.3 ppb	Crisp *et al.*	22
Southern California (lowest)	~0 ppb	Crisp *et al.*	22
Southern California (highest)	16 ppb	Crisp *et al.*	22
Los Angeles (Daytime)	5 ppb	Crisp *et al.*	22
Los Angeles (Nighttime)	3 ppb	Crisp *et al.*	22
San Francisco Bay	3.9 ppb	Crisp *et al.*	22
Standard tropospheric range	100 - 300 pptv	Sanhueza *et al.*	28
Industrial or marine environments	1.5 - 3 ppb	Graedel and Keene	29
Hydrogen sulphide (H_2S)			
Volcanoes	500 ppb	Kumar *et al.*	30
construction and demolition waste emissions - average	7 — 100 ppm	Kumar *et al.*	30
construction and demolition waste emissions- highest end	5,000–12,000 ppm	Kumar *et al.*	30
ambient air range	0.11–0.33 ppb	Abdollahi and Hosseini	31
industrial landfill, Terre Haute, Indiana, USA	2.0 – 300 ppb	Levels *et al.*	32
Dakota City 1999	≥ 90 ppb	Inserra *et al.*	33
Methanol (CH_3OH)			
Troposphere over Remote oceans	1 ppbv	Heikes *et al.*	34
Average Urban areas and forest	20 ppbv	Heikes *et al.*	34
São Paulo, Brazil	**34.1±9.2 ppb**	**Nguyen *et al.***	13
Osaka, Japan	5.8±3.8	Nguyen *et al.*	13
wooded North Carolina industrial area	78.5—297 ppbv	Kelly *et al.*	34,35

S4.3 Effective Rate Constants Used in Manuscript

*Table S54: Co-reactant and their chosen atmospheric concentration ([**co-reactant**]); Criegee Intermediate number [sCI); computational master equation rate constant (k_{ME})*; dipole-dipole capture limit ($k_{d\text{-}d}$); literature experimental rate constant (k_{EXP}); and effective rate constants (kEFF = rate constant × [**co-reactant**]).*

[**Co-reactant**] (molec./cm^3)	**sCI**	k_{ME} (cm^3 s^{-1})	$k_{d\text{-}d}$ (cm^3 s^{-1})	k_{EXP} (cm^3 s^{-1})	k_{EFF} (s^{-1})
HCHO	1	**2.79×10^{-12}**	1.06×10^{-9}	-	5.60
	23	**2.69×10^{-13}**	8.04×10^{-10}	-	0.54
2.0×10^{12}	24	**2.49×10^{-12}**	6.46×10^{-10}	-	5.0
(Urban Heavy	25	» $k_{d\text{-}d}$	**7.20×10^{-10}**	-	1447
traffic) [12]	26	**1.66×10^{-11}**	7.07×10^{-10}	-	33.4
CF_3CHO	1	» $k_{d\text{-}d}$	6.50×10^{-10}	-	-
CF_3CFO	1	**1.98×10^{-12}**	3.34×10^{-10}	-	-
SO_2	1	» $k_{d\text{-}d}$	**7.25×10^{-10}**	3.80×10^{-11}	300
	23	**1.90×10^{-12}**	5.08×10^{-10}	-	0.79
4.1×10^{11}	24	» $k_{d\text{-}d}$	**4.08×10^{-10}**	-	169
(Beijing urban	25	» $k_{d\text{-}d}$	**4.51×10^{-10}**	-	186
area) [14]	26	» $k_{d\text{-}d}$	**4.42×10^{-10}**	-	183
HNO_3	1	8.22×10^{-9}	**8.45×10^{-10}**	5.1×10^{-10}	94
	23	**2.06×10^{-11}**	5.93×10^{-10}	-	2.3
1.1×10^{11}	24	**8.87×10^{-11}**	4.76×10^{-10}	-	9.8
(Houston,	25	9.25×10^{-8}	**5.26×10^{-10}**	-	58
Texas) [20]	26	**7.53×10^{-11}**	5.16×10^{-10}	-	8.4
TFA	1	» $k_{d\text{-}d}$	**7.54×10^{-10}**	3.50×10^{-10}	2.5×10^{-2}
	23	» $k_{d\text{-}d}$	**4.96×10^{-10}**	-	1.7×10^{-2}
3.3×10^{7}	24	» $k_{d\text{-}d}$	**3.98×10^{-10}**	-	1.3×10^{-2}
(Beijing higher	25	» $k_{d\text{-}d}$	**4.35×10^{-10}**	-	1.5×10^{-2}
emission areas)	26	» $k_{d\text{-}d}$	**4.27×10^{-10}**	-	1.4×10^{-2}
H_2O	1	**1.18×10^{-16}**	1.06×10^{-9}	*2.4×10^{-16}*	73
	23	**1.35×10^{-18}**	8.38×10^{-10}	-	0.83
6.2×10^{17}	24	**1.12×10^{-16}**	6.73×10^{-10}	-	70
(~80% humidity	25	**5.13×10^{-12}**	7.54×10^{-10}	-	3.2×10^{6}
Sao Paulo) [17,36]	26	**2.27×10^{-13}**	7.40×10^{-10}	-	1.4×10^{5}
$(H_2O)_2$	1	**3.28×10^{-12}**	1.07×10^{-9}	7.50×10^{-12}	2.9×10^{3}
	23	**2.71×10^{-12}**	7.99×10^{-10}	-	2.4×10^{3}
8.7×10^{14}	24	**3.74×10^{-12}**	6.42×10^{-10}	-	3.3×10^{3}
(~80% humidity	25	1.14×10^{-6}	**7.14×10^{-10}**	-	6.2×10^{5}
Sao Paulo) [17,36]	26	1.46×10^{-9}	**7.01×10^{-10}**	-	6.1×10^{5}
MeOH	1	**1.20×10^{-14}**	8.15×10^{-10}	1.1×10^{-13}	0.010
	23	**9.43×10^{-17}**	6.14×10^{-10}	-	7.9×10^{-5}
8.4×10^{11}	24	**3.30×10^{-14}**	4.93×10^{-10}	-	0.028
(Sao Paulo,	25	» $k_{d\text{-}d}$	**5.50×10^{-10}**	-	462
Brazil) [13]	26	**3.31×10^{-11}**	5.39×10^{-10}	-	28
H_2S	1	**7.06×10^{-15}**	5.68×10^{-10}	1.7×10^{-13}	0.052
	23	**1.96×10^{-16}**	4.26×10^{-10}	-	1.4×10^{-3}
1.2×10^{13}	24	**5.72×10^{-15}**	3.42×10^{-10}	-	0.042
(Industrial	25	**6.08×10^{-13}**	3.81×10^{-10}	-	4.5
landfill) [32]	26	**1.23×10^{-14}**	3.74×10^{-10}	-	0.091
HCl	1	**4.70×10^{-10}**	6.06×10^{-10}	4.1×10^{-11}	58
	23	**4.04×10^{-15}**	4.51×10^{-10}	-	5.0×10^{-3}
1.2×10^{11}	24	**7.28×10^{-11}**	3.62×10^{-10}	-	8.96
(Daytime	25	**1.64×10^{-10}**	4.03×10^{-10}	-	20
Los Angeles) [22]	26	**1.13×10^{-10}**	3.96×10^{-10}	-	14
HF	1	**3.32×10^{-13}**	8.15×10^{-10}	-	0.12
3.7×10^{11}	23	**6.67×10^{-18}**	6.14×10^{-10}	-	2.5×10^{-6}
(near Volcano	24	**2.86×10^{-15}**	4.93×10^{-10}	-	1.1×10^{-3}
vicinity	25	**1.19×10^{-11}**	5.50×10^{-10}	-	4.4
ambient T) [27]	26	**3.66×10^{-13}**	5.39×10^{-10}	-	0.14

** "» $k_{d\text{-}d}$" refers to barrierless reactions that yield no k_{ME} and that the $k_{d\text{-}d}$ should be used instead.*

S4.4 Lower Range of Effective Rate Constants

*Table S55: Co-reactant and their chosen atmospheric concentration ([**co-reactant**]); Criegee Intermediate number [sCI]; computational master equation rate constant (k_{ME})*; dipole-dipole capture limit ($k_{d\text{-}d}$); literature experimental rate constant (k_{EXP}); and effective rate constants (k_{EFF} = **k_{ME}** or **$k_{d\text{-}d}$** × [**co-reactant**]).*

[**Co-reactant**] (molec./cm^3)	**sCI**	k_{ME} (cm^3 s^{-1})	$k_{d\text{-}d}$ (cm^3 s^{-1})	k_{EXP} (cm^3 s^{-1})	k_{EFF} (s^{-1})
HCHO	1	**2.79×10^{-12}**	1.06×10^{-9}	-	1.3
	23	**2.69×10^{-13}**	8.04×10^{-10}	-	0.12
4.6×10^{11}	24	**2.49×10^{-12}**	6.46×10^{-10}	-	1.2
(European	25	» $k_{d\text{-}d}$	**7.20×10^{-10}**	-	334
Home average) [9]	26	**1.66×10^{-11}**	7.07×10^{-10}	-	7.7
CF_3CHO	1	» $k_{d\text{-}d}$	6.50×10^{-10}	-	-
CF_3CFO	1	**1.98×10^{-12}**	3.34×10^{-10}	-	-
SO_2	1	» $k_{d\text{-}d}$	**7.25×10^{-10}**	3.80×10^{-11}	88.3
	23	**1.90×10^{-12}**	5.08×10^{-10}	-	0.23
1.2×10^{11}	24	» $k_{d\text{-}d}$	**4.08×10^{-10}**	-	49.7
(Sao Paulo,	25	» $k_{d\text{-}d}$	**4.51×10^{-10}**	-	54.8
Brazil) [17]	26	» $k_{d\text{-}d}$	**4.42×10^{-10}**	-	53.8
HNO_3	1	8.22×10^{-9}	**8.45×10^{-10}**	5.1×10^{-10}	60
9.9×10^{9}	23	**2.06×10^{-11}**	5.93×10^{-10}	-	9.8
(Houston,	24	**8.87×10^{-11}**	4.76×10^{-10}	-	53
Texas, lower	25	9.25×10^{-8}	**5.26×10^{-10}**	-	58
boundary) [20]	26	**7.53×10^{-11}**	5.16×10^{-10}	-	57
TFA	1	» $k_{d\text{-}d}$	**7.54×10^{-10}**	3.50×10^{-10}	1.7×10^{-3}
	23	» $k_{d\text{-}d}$	**4.96×10^{-10}**	-	1.1×10^{-3}
2.3×10^{6}	24	» $k_{d\text{-}d}$	**3.98×10^{-10}**	-	9.2×10^{-4}
(Europe urban	25	» $k_{d\text{-}d}$	**4.35×10^{-10}**	-	1.0×10^{-3}
projected) [25]	26	» $k_{d\text{-}d}$	**4.27×10^{-10}**	-	9.9×10^{-4}
H_2O	1	**1.18×10^{-16}**	1.06×10^{-9}	*2.4×10^{-16}*	28
	23	**1.35×10^{-18}**	8.38×10^{-10}	-	0.32
2.4×10^{17}	24	**1.12×10^{-16}**	6.73×10^{-10}	-	27
(Mega city) [8]	25	**5.13×10^{-12}**	7.54×10^{-10}	-	1.2×10^{6}
	26	**2.27×10^{-13}**	7.40×10^{-10}	-	5.44×10^{4}
$(H_2O)_2$	1	**3.28×10^{-12}**	1.07×10^{-9}	7.50×10^{-12}	279
	23	**2.71×10^{-12}**	7.99×10^{-10}	-	231
8.5×10^{13}	24	**3.74×10^{-12}**	6.42×10^{-10}	-	318
(Mega city) [8]	25	1.14×10^{-6}	**7.14×10^{-10}**	-	6.1×10^{4}
	26	1.46×10^{-9}	**7.01×10^{-10}**	-	6.0×10^{4}
MeOH	1	**1.20×10^{-14}**	8.15×10^{-10}	1.1×10^{-13}	1.7×10^{-3}
	23	**9.43×10^{-17}**	6.14×10^{-10}	-	1.3×10^{-5}
1.4×10^{11}	24	**3.30×10^{-14}**	4.93×10^{-10}	-	4.7×10^{-3}
(Osaka, Japan) [13]	25	» $k_{d\text{-}d}$	**5.50×10^{-10}**	-	79
	26	**3.31×10^{-11}**	5.39×10^{-10}	-	4.7
H_2S	1	**7.06×10^{-15}**	5.68×10^{-10}	1.7×10^{-13}	5.7×10^{-5}
	23	**1.96×10^{-16}**	4.26×10^{-10}	-	1.6×10^{-6}
1.2×10^{9}	24	**5.72×10^{-15}**	3.42×10^{-10}	-	4.6×10^{-5}
(ambient air	25	**6.08×10^{-13}**	3.81×10^{-10}	-	4.9×10^{-3}
range) [31]	26	**1.23×10^{-14}**	3.74×10^{-10}	-	1.0×10^{-4}
HCl	1	**4.70×10^{-10}**	6.06×10^{-10}	4.1×10^{-11}	3.5
	23	**4.04×10^{-15}**	4.51×10^{-10}	-	3.0×10^{-4}
7.4×10^{9}	24	**7.28×10^{-11}**	3.62×10^{-10}	-	0.54
(Standard	25	**1.64×10^{-10}**	4.03×10^{-10}	-	1.2
troposphere) [28]	26	**1.13×10^{-10}**	3.96×10^{-10}	-	0.83
HF	1	**3.32×10^{-13}**	8.15×10^{-10}	-	0.12
3.7×10^{11}	23	**6.67×10^{-18}**	6.14×10^{-10}	-	2.5×10^{-6}
(near Volcano	24	**2.86×10^{-15}**	4.93×10^{-10}	-	1.1×10^{-3}
vicinity	25	**1.19×10^{-11}**	5.50×10^{-10}	-	4.4
ambient T) [27]	26	**3.66×10^{-13}**	5.39×10^{-10}	-	0.14

** "» $k_{d\text{-}d}$" refers to barrierless reactions that yield no k_{ME} and that the $k_{d\text{-}d}$ should be used instead.*

S4.5 Medium Range of Effective Rate Constants

*Table S56: Co-reactant and their chosen atmospheric concentration ([**co-reactant**]); Criegee Intermediate number [sCI); computational master equation rate constant (k_{ME})*; dipole-dipole capture limit ($k_{d\text{-}d}$); literature experimental rate constant (k_{EXP}); and effective rate constants (k_{EFF} = **k_{ME}** or **$k_{d\text{-}d}$** × [**co-reactant**]).*

[**Co-reactant**] (molec./cm^3)	**sCI**	k_{ME} (cm^3 s^{-1})	$k_{d\text{-}d}$ (cm^3 s^{-1})	k_{EXP} (cm^3 s^{-1})	k_{EFF} (s^{-1})
HCHO	1	**2.79×10^{-12}**	1.06×10^{-9}	-	5.60
	23	**2.69×10^{-13}**	8.04×10^{-10}	-	0.54
2.0×10^{12}	24	**2.49×10^{-12}**	6.46×10^{-10}	-	5.0
(Heavy traffic) [12]	25	» $k_{d\text{-}d}$	**7.20×10^{-10}**	-	1447
	26	**1.66×10^{-11}**	7.07×10^{-10}	-	33.4
CF_3CHO	1	» $k_{d\text{-}d}$	6.50×10^{-10}	-	-
CF_3CFO	1	**1.98×10^{-12}**	3.34×10^{-10}	-	-
SO_2	1	» $k_{d\text{-}d}$	**7.25×10^{-10}**	3.80×10^{-11}	300
	23	**1.90×10^{-12}**	5.08×10^{-10}	-	0.79
4.1×10^{11}	24	» $k_{d\text{-}d}$	**4.08×10^{-10}**	-	169
(Beijing urban	25	» $k_{d\text{-}d}$	**4.51×10^{-10}**	-	186
area) [14]	26	» $k_{d\text{-}d}$	**4.42×10^{-10}**	-	183
HNO_3	1	8.22×10^{-9}	**8.45×10^{-10}**	5.1×10^{-10}	60
	23	**2.06×10^{-11}**	5.93×10^{-10}	-	9.8
1.1×10^{11}	24	**8.87×10^{-11}**	4.76×10^{-10}	-	53
(Houston,	25	9.25×10^{-8}	**5.26×10^{-10}**	-	58
Texas) [20]	26	**7.53×10^{-11}**	5.16×10^{-10}	-	8.4
TFA	1	» $k_{d\text{-}d}$	**7.54×10^{-10}**	3.50×10^{-10}	4.6×10^{-3}
	23	» $k_{d\text{-}d}$	**4.96×10^{-10}**	-	3.0×10^{-3}
6.1×10^{6}	24	» $k_{d\text{-}d}$	**3.98×10^{-10}**	-	2.4×10^{-3}
(Beijing average	25	» $k_{d\text{-}d}$	**4.35×10^{-10}**	-	2.7×10^{-3}
emission areas) [23]	26	» $k_{d\text{-}d}$	**4.27×10^{-10}**	-	2.6×10^{-3}
H_2O	1	**1.18×10^{-16}**	1.06×10^{-9}	*2.4×10^{-16}*	73
6.2×10^{17}	23	**1.35×10^{-18}**	8.38×10^{-10}	-	0.83
(~80%	24	**1.12×10^{-16}**	6.73×10^{-10}	-	70
humidity,	25	**5.13×10^{-12}**	7.54×10^{-10}	-	3.2×10^{6}
Sao Paulo) [17,36]	26	**2.27×10^{-13}**	7.40×10^{-10}	-	1.4×10^{5}
$(H_2O)_2$	1	**3.28×10^{-12}**	1.07×10^{-9}	7.50×10^{-12}	2.9×10^{3}
8.7×10^{14}	23	**2.71×10^{-12}**	7.99×10^{-10}	-	2.4×10^{3}
(~80%	24	**3.74×10^{-12}**	6.42×10^{-10}	-	3.3×10^{3}
humidity,	25	1.14×10^{-6}	**7.14×10^{-10}**	-	6.2×10^{5}
Sao Paulo) [17,36]	26	1.46×10^{-9}	**7.01×10^{-10}**	-	6.1×10^{5}
MeOH	1	**1.20×10^{-14}**	8.15×10^{-10}	1.1×10^{-13}	0.010
	23	**9.43×10^{-17}**	6.14×10^{-10}	-	7.9×10^{-5}
8.4×10^{11}	24	**3.30×10^{-14}**	4.93×10^{-10}	-	0.028
(Sao Paulo,	25	» $k_{d\text{-}d}$	**5.50×10^{-10}**	-	462
Brazil) [13]	26	**3.31×10^{-11}**	5.39×10^{-10}	-	28
H_2S	1	**7.06×10^{-15}**	5.68×10^{-10}	1.7×10^{-13}	0.052
	23	**1.96×10^{-16}**	4.26×10^{-10}	-	1.4×10^{-3}
1.2×10^{13}	24	**5.72×10^{-15}**	3.42×10^{-10}	-	0.042
(Industrial	25	**6.08×10^{-13}**	3.81×10^{-10}	-	4.5
landfill) [32]	26	**1.23×10^{-14}**	3.74×10^{-10}	-	0.091
HCl	1	**4.70×10^{-10}**	6.06×10^{-10}	4.1×10^{-11}	19
3.2×10^{10}	23	**4.04×10^{-15}**	4.51×10^{-10}	-	1.3×10^{-4}
(Southern	24	**7.28×10^{-11}**	3.62×10^{-10}	-	0.24
California	25	**1.64×10^{-10}**	4.03×10^{-10}	-	0.53
Overall) [22]	26	**1.13×10^{-10}**	3.96×10^{-10}	-	0.36
HF	1	**3.32×10^{-13}**	8.15×10^{-10}	-	9.0
	23	**6.67×10^{-18}**	6.14×10^{-10}	-	1.8×10^{-4}
2.7×10^{13}	24	**2.86×10^{-15}**	4.93×10^{-10}	-	0.076
(At Volcanic	25	**1.19×10^{-11}**	5.50×10^{-10}	-	320
source) [27]	26	**3.66×10^{-13}**	5.39×10^{-10}	-	9.9

** "» $k_{d\text{-}d}$" refers to barrierless reactions that yield no k_{ME} and that the $k_{d\text{-}d}$ should be used instead.*

S4.6 Higher Range of Effective Rate Constants

*Table S57: Co-reactant and their chosen atmospheric concentration ([**co-reactant**]); Criegee Intermediate number [sCI); computational master equation rate constant (k_{ME})*; dipole-dipole capture limit ($k_{d\text{-}d}$); literature experimental rate constant (k_{EXP}); and effective rate constants (k_{EFF} = **k_{ME}** or **$k_{d\text{-}d}$** × [**co-reactant**]).*

[**Co-reactant**] (molec./cm^3)	**sCI**	k_{ME} (cm^3 s^{-1})	$k_{d\text{-}d}$ (cm^3 s^{-1})	k_{EXP} (cm^3 s^{-1})	k_{EFF} (s^{-1})
HCHO	1	**2.79×10^{-12}**	1.06×10^{-9}	-	27.4
	23	**2.69×10^{-13}**	8.04×10^{-10}	-	2.64
9.8×10^{12}	24	**2.49×10^{-12}**	6.46×10^{-10}	-	24.5
(Caravan/	25	» $k_{d\text{-}d}$	**7.20×10^{-10}**	-	7088
mobile home) [12]	26	**1.66×10^{-11}**	7.07×10^{-10}	-	164
CF_3CHO	1	» $k_{d\text{-}d}$	6.50×10^{-10}	-	-
CF_3CFO	1	**1.98×10^{-12}**	3.34×10^{-10}	-	-
SO_2	1	» $k_{d\text{-}d}$	**7.25×10^{-10}**	3.80×10^{-11}	68217
	23	**1.90×10^{-12}**	5.08×10^{-10}	-	178
9.4×10^{13}	24	» $k_{d\text{-}d}$	**4.08×10^{-10}**	-	38398
(0.1 km from	25	» $k_{d\text{-}d}$	**4.51×10^{-10}**	-	42373
Mt. Etna) [16]	26	» $k_{d\text{-}d}$	**4.42×10^{-10}**	-	41563
HNO_3	1	8.22×10^{-9}	**8.45×10^{-10}**	5.1×10^{-10}	416
	23	**2.06×10^{-11}**	5.93×10^{-10}	-	10.1
4.9×10^{11}	24	**8.87×10^{-11}**	4.76×10^{-10}	-	43.7
(Southern	25	9.25×10^{-8}	**5.26×10^{-10}**	-	259
California rural) [22]	26	**7.53×10^{-11}**	5.16×10^{-10}	-	37.3
TFA	1	» $k_{d\text{-}d}$	**7.54×10^{-10}**	3.50×10^{-10}	2.5×10^{-2}
	23	» $k_{d\text{-}d}$	**4.96×10^{-10}**	-	1.7×10^{-2}
3.3×10^{7}	24	» $k_{d\text{-}d}$	**3.98×10^{-10}**	-	1.3×10^{-2}
(Beijing higher	25	» $k_{d\text{-}d}$	**4.35×10^{-10}**	-	1.5×10^{-2}
emission areas) [14]	26	» $k_{d\text{-}d}$	**4.27×10^{-10}**	-	1.4×10^{-2}
H_2O	1	**1.18×10^{-16}**	1.06×10^{-9}	*2.4×10^{-16}*	91
7.7×10^{17}	23	**1.35×10^{-18}**	8.38×10^{-10}	-	1.0
(~100%	24	**1.12×10^{-16}**	6.73×10^{-10}	-	87
Sao Paulo	25	**5.13×10^{-12}**	7.54×10^{-10}	-	4.0×10^{6}
outside) [17,36]	26	**2.27×10^{-13}**	7.40×10^{-10}	-	1.8×10^{5}
$(H_2O)_2$	1	**3.28×10^{-12}**	1.07×10^{-9}	7.50×10^{-12}	4.5×10^{3}
1.4×10^{15}	23	**2.71×10^{-12}**	7.99×10^{-10}	-	3.7×10^{3}
(~100%	24	**3.74×10^{-12}**	6.42×10^{-10}	-	5.1×10^{3}
Sao Paulo	25	1.14×10^{-6}	**7.14×10^{-10}**	-	9.7×10^{5}
outside) [17,36]	26	1.46×10^{-9}	**7.01×10^{-10}**	-	9.5×10^{5}
MeOH	1	**1.20×10^{-14}**	8.15×10^{-10}	1.1×10^{-13}	0.088
	23	**9.43×10^{-17}**	6.14×10^{-10}	-	6.9×10^{-4}
7.3×10^{12}	24	**3.30×10^{-14}**	4.93×10^{-10}	-	0.24
(North Carolina	25	» $k_{d\text{-}d}$	**5.50×10^{-10}**	-	4.0×10^{3}
Industrial zone) [35]	26	**3.31×10^{-11}**	5.39×10^{-10}	-	242
H_2S	1	**7.06×10^{-15}**	5.68×10^{-10}	1.7×10^{-13}	2100
	23	**1.96×10^{-16}**	4.26×10^{-10}	-	58
3.0×10^{17}	24	**5.72×10^{-15}**	3.42×10^{-10}	-	1700
(construction	25	**6.08×10^{-13}**	3.81×10^{-10}	-	1.8×10^{5}
Waste- peak) [30]	26	**1.23×10^{-14}**	3.74×10^{-10}	-	1500
HCl	1	**4.70×10^{-10}**	6.06×10^{-10}	4.1×10^{-11}	190
3.9×10^{11}	23	**4.04×10^{-15}**	4.51×10^{-10}	-	0.016
(Southern	24	**7.28×10^{-11}**	3.62×10^{-10}	-	29
California	25	**1.64×10^{-10}**	4.03×10^{-10}	-	65
Highest) [22]	26	**1.13×10^{-10}**	3.96×10^{-10}	-	44
HF	1	**3.32×10^{-13}**	8.15×10^{-10}	-	9.0
	23	**6.67×10^{-18}**	6.14×10^{-10}	-	1.8×10^{-4}
2.7×10^{13}	24	**2.86×10^{-15}**	4.93×10^{-10}	-	0.076
(At Volcanic	25	**1.19×10^{-11}**	5.50×10^{-10}	-	320
source) [27]	26	**3.66×10^{-13}**	5.39×10^{-10}	-	9.9

** "» $k_{d\text{-}d}$" refers to barrierless reactions that yield no k_{ME} and that the $k_{d\text{-}d}$ should be used instead.*

S4.7 Effective Rate Constants Using General Abundances in Forest/City/Rural Environments

*Table S58: Co-reactant and their chosen atmospheric concentration ([**co-reactant**]); Criegee Intermediate number [sCI]; computational master equation rate constant (k_{ME})*; dipole-dipole capture limit ($k_{d\text{-}d}$); literature experimental rate constant (k_{EXP}); and effective rate constants (k_{EFF} = **k_{ME}** or **$k_{d\text{-}d}$** × [**co-reactant**]). Abundance obtained from study by Vereecken et al..* [8]

[**Co-reactant**] (molec./cm^3)	**sCI**	k_{ME} (cm^3 s^{-1})	$k_{d\text{-}d}$ (cm^3 s^{-1})	k_{EXP} (cm^3 s^{-1})	k_{EFF} (s^{-1})
H_2O	1	**1.18×10^{-16}**	1.06×10^{-9}	*2.4×10^{-16}*	46
	23	**1.35×10^{-18}**	8.38×10^{-10}	-	0.53
3.9×10^{17}	24	**1.12×10^{-16}**	6.73×10^{-10}	-	44
(Boreal	25	**5.13×10^{-12}**	7.54×10^{-10}	-	2.0×10^{6}
Forest)	26	**2.27×10^{-13}**	7.40×10^{-10}	-	8.8×10^{4}
H_2O	1	**1.18×10^{-16}**	1.06×10^{-9}	*2.4×10^{-16}*	72
	23	**1.35×10^{-18}**	8.38×10^{-10}	-	0.82
6.1×10^{17}	24	**1.12×10^{-16}**	6.73×10^{-10}	-	69
(Tropical	25	**5.13×10^{-12}**	7.54×10^{-10}	-	3.1×10^{6}
Forest)	26	**2.27×10^{-13}**	7.40×10^{-10}	-	1.4×10^{5}
H_2O	1	**1.18×10^{-16}**	1.06×10^{-9}	*2.4×10^{-16}*	28
	23	**1.35×10^{-18}**	8.38×10^{-10}	-	0.32
2.4×10^{17}	24	**1.12×10^{-16}**	6.73×10^{-10}	-	27
(Mega city)	25	**5.13×10^{-12}**	7.54×10^{-10}	-	1.2×10^{6}
	26	**2.27×10^{-13}**	7.40×10^{-10}	-	5.44×10^{4}
H_2O	1	**1.18×10^{-16}**	1.06×10^{-9}	*2.4×10^{-16}*	45
	23	**1.35×10^{-18}**	8.38×10^{-10}	-	0.51
3.8×10^{17}	24	**1.12×10^{-16}**	6.73×10^{-10}	-	43
(Rural	25	**5.13×10^{-12}**	7.54×10^{-10}	-	1.9×10^{6}
Europe)	26	**2.27×10^{-13}**	7.40×10^{-10}	-	8.6×10^{4}
$(H_2O)_2$	1	**3.28×10^{-12}**	1.07×10^{-9}	7.50×10^{-12}	754
	23	**2.71×10^{-12}**	7.99×10^{-10}	-	624
2.3×10^{14}	24	**3.74×10^{-12}**	6.42×10^{-10}	-	861
(Boreal	25	1.14×10^{-6}	**7.14×10^{-10}**	-	1.6×10^{5}
Forest)	26	1.46×10^{-9}	**7.01×10^{-10}**	-	1.6×10^{5}
$(H_2O)_2$	1	**3.28×10^{-12}**	1.07×10^{-9}	7.50×10^{-12}	1.8×10^{3}
	23	**2.71×10^{-12}**	7.99×10^{-10}	-	1.5×10^{3}
5.5×10^{14}	24	**3.74×10^{-12}**	6.42×10^{-10}	-	2.1×10^{3}
(Tropical	25	1.14×10^{-6}	**7.14×10^{-10}**	-	3.9×10^{5}
Forest)	26	1.46×10^{-9}	**7.01×10^{-10}**	-	3.9×10^{5}
$(H_2O)_2$	1	**3.28×10^{-12}**	1.07×10^{-9}	7.50×10^{-12}	279
	23	**2.71×10^{-12}**	7.99×10^{-10}	-	231
8.5×10^{13}	24	**3.74×10^{-12}**	6.42×10^{-10}	-	318
(Mega city)	25	1.14×10^{-6}	**7.14×10^{-10}**	-	6.1×10^{4}
	26	1.46×10^{-9}	**7.01×10^{-10}**	-	6.0×10^{4}
$(H_2O)_2$	1	**3.11×10^{-12}**	1.07×10^{-9}	7.50×10^{-12}	688
	23	**2.25×10^{-12}**	7.99×10^{-10}	-	570
2.1×10^{14}	24	**6.64×10^{-10}**	6.42×10^{-10}	-	786
(Rural	25	1.14×10^{-6}	**7.14×10^{-10}**	-	1.5×10^{5}
Europe)	26	1.46×10^{-9}	**7.01×10^{-10}**	-	1.5×10^{5}

** "» $k_{d\text{-}d}$" refers to barrierless reactions that yield no k_{ME} and that the $k_{d\text{-}d}$ should be used instead.*

*Table S59: Co-reactant and their chosen atmospheric concentration ([**co-reactant**]); Criegee Intermediate number [sCI); computational master equation rate constant (k_{ME})*; dipole-dipole capture limit ($k_{d\text{-}d}$); literature experimental rate constant (k_{EXP}); and effective rate constants (k_{EFF} = $\boldsymbol{k_{ME}}$ or $\boldsymbol{k_{d\text{-}d}}$ × [**co-reactant**]). Abundance obtained from study by Vereecken et al.. [8]*

[**Co-reactant**] (molec./cm^3)	**sCI**	$\boldsymbol{k_{ME}}$ (cm^3 s^{-1})	$\boldsymbol{k_{d\text{-}d}}$ (cm^3 s^{-1})	$\boldsymbol{k_{EXP}}$ (cm^3 s^{-1})	$\boldsymbol{k_{EFF}}$ (s^{-1})
SO_2	1	» $k_{d\text{-}d}$	**7.25×10^{-10}**	3.80×10^{-11}	12
	23	**1.90×10^{-12}**	5.08×10^{-10}	-	0.032
1.7×10^{10}	24	» $k_{d\text{-}d}$	**4.08×10^{-10}**	-	6.9
(Boreal	25	» $k_{d\text{-}d}$	**4.51×10^{-10}**	-	7.7
Forest)	26	» $k_{d\text{-}d}$	**4.42×10^{-10}**	-	7.5
SO_2	1	» $k_{d\text{-}d}$	**7.25×10^{-10}**	3.80×10^{-11}	65
	23	**1.90×10^{-12}**	5.08×10^{-10}	-	0.17
9.0×10^{10}	24	» $k_{d\text{-}d}$	**4.08×10^{-10}**	-	37
(Mega city)	25	» $k_{d\text{-}d}$	**4.51×10^{-10}**	-	41
	26	» $k_{d\text{-}d}$	**4.42×10^{-10}**	-	40
SO_2	1	» $k_{d\text{-}d}$	**7.25×10^{-10}**	3.80×10^{-11}	4.8
	23	**1.90×10^{-12}**	5.08×10^{-10}	-	0.013
6.6×10^{9}	24	» $k_{d\text{-}d}$	**4.08×10^{-10}**	-	2.7
(Rural	25	» $k_{d\text{-}d}$	**4.51×10^{-10}**	-	3.0
Europe)	26	» $k_{d\text{-}d}$	**4.42×10^{-10}**	-	2.9
$R_1R_2C=O$	1	**2.79×10^{-12}**	1.06×10^{-9}	-	0.33
1.2×10^{11}	23	**2.69×10^{-13}**	8.04×10^{-10}	-	0.032
	24	**2.49×10^{-12}**	6.46×10^{-10}	-	0.30
(R_1R_2CO: Boreal	25	» $k_{d\text{-}d}$	**7.20×10^{-10}**	-	86
Forest)	26	**1.66×10^{-11}**	7.07×10^{-10}	-	2.0
$R_1R_2C=O$	1	**2.79×10^{-12}**	1.06×10^{-9}	-	0.053
1.9×10^{10}	23	**2.69×10^{-13}**	8.04×10^{-10}	-	5.1×10^{-3}
(R_1R_2CO:	24	**2.49×10^{-12}**	6.46×10^{-10}	-	0.047
Tropical	25	» $k_{d\text{-}d}$	**7.20×10^{-10}**	-	14
Forest)	26	**1.66×10^{-11}**	7.07×10^{-10}	-	0.32
$R_1R_2C=O$	1	**2.79×10^{-12}**	1.06×10^{-9}	-	1.4
5.1×10^{11}	23	**2.69×10^{-13}**	8.04×10^{-10}	-	0.14
	24	**2.49×10^{-12}**	6.46×10^{-10}	-	1.3
(R_1R_2CO: Mega	25	» $k_{d\text{-}d}$	**7.20×10^{-10}**	-	367
city)	26	**1.66×10^{-11}**	7.07×10^{-10}	-	8.5
$R_1R_2C=O$	1	**2.79×10^{-12}**	1.06×10^{-9}	-	0.18
6.6×10^{10}	23	**2.69×10^{-13}**	8.04×10^{-10}	-	0.018
	24	**2.49×10^{-12}**	6.46×10^{-10}	-	0.16
(R_1R_2CO: Rural	25	» $k_{d\text{-}d}$	**7.20×10^{-10}**	-	48
Europe)	26	**1.66×10^{-11}**	7.07×10^{-10}	-	1.1
RCOOH	1	» $k_{d\text{-}d}$	**7.54×10^{-10}**	3.50×10^{-10}	75
1.0×10^{11}	23	» $k_{d\text{-}d}$	**4.96×10^{-10}**	-	50
(RCOOH:	24	» $k_{d\text{-}d}$	**3.98×10^{-10}**	-	40
Boreal	25	» $k_{d\text{-}d}$	**4.35×10^{-10}**	-	43
Forest)	26	» $k_{d\text{-}d}$	**4.27×10^{-10}**	-	43
RCOOH	1	» $k_{d\text{-}d}$	**7.54×10^{-10}**	3.50×10^{-10}	38
5.0×10^{10}	23	» $k_{d\text{-}d}$	**4.96×10^{-10}**	-	25
(RCOOH:	24	» $k_{d\text{-}d}$	**3.98×10^{-10}**	-	20
Tropical	25	» $k_{d\text{-}d}$	**4.35×10^{-10}**	-	22
Forest)	26	» $k_{d\text{-}d}$	**4.27×10^{-10}**	-	21

** "» $k_{d\text{-}d}$" refers to barrierless reactions that yield no k_{ME} and that the $k_{d\text{-}d}$ should be used instead.*

S5. Relative Energies, Enthalpies and Gibbs Free Energies

*Table S60: **sCI 1** + HCHO relative energies (ΔE), zero-point corrected energy (ΔZPE), enthalpies ($\Delta H_{298.15}$) and Gibbs free energies ($\Delta G_{298.15}$) [units=kJ mol^{-1}]*

#sCI	Stationary Point	ΔE	ΔZPE	$\Delta H_{298.15}$	$\Delta G_{298.15}$
1	**sCI 1 + HCHO Cycloaddition**				
	PRC	-30.01	-20.697	-22.37	18.78
	TS_C	-31.24	-20.771	-25.26	22.54
	HOZ	-240.60	-214.398	-221.72	-167.46
	HOZ to FAc pathway instant				
	HOZ	-240.60	-214.398	-221.72	-167.46
	TS_{FAc} 1	-31.27	-27.221	-32.64	18.22
	C_{FAc} 2	-499.21	-488.439	-487.37	-455.44
	HCHO + HCOOH con 2	-479.10	-473.302	-473.41	-473.31
	HOZ to FAc pathway via HAE				
	HOZ	-240.60	-214.398	-221.72	-167.46
	TS_d	-55.03	-53.629	-60.17	-7.28
	HAE con 1	-552.41	-527.558	-532.15	-484.81
	TS_{iso}	-538.07	-515.748	-521.06	-473.82
	HAE con 2	-564.24	-537.972	-543.27	-493.49
	TS_{HAE}	-461.21	-450.820	-456.96	-405.34
	C_{FAc} 1	-534.87	-520.548	-521.48	-483.02
	HCHO + HCOOH con 1	-496.94	-490.251	-490.54	-490.25

*Table S61: **sCIs 2** & **3** + HCHO relative energies (ΔE), zero-point corrected energy (ΔZPE), enthalpies ($\Delta H_{298.15}$) and Gibbs free energies ($\Delta G_{298.15}$) [units=kJ mol^{-1}]*

#sCI	Stationary Point	ΔE	ΔZPE	$\Delta H_{298.15}$	$\Delta G_{298.15}$
2 & 3	**sCI 2 + HCHO Cycloaddition**				
	sCI 2+ HCHO PRC	-25.46	-20.762	-19.54	16.22
	sCI 2+ HCHO TS_c1	-19.91	-11.620	-15.07	33.88
	HOZ 1	-269.20	-245.226	-251.81	-196.12
	sCI 3 + HCHO Cycloaddition				
	sCI 3+ HCHO	-2.54	-3.384	-2.84	-5.13
	sCI 3+ HCHO PRC2	-33.92	-26.983	-27.12	11.38
	sCI 3+ HCHO TS_c2	-30.86	-22.337	-25.61	21.15
	HOZ 2	-265.64	-241.572	-248.03	-192.96
	sCI 1 + CF_3CHO Cycloaddition (barrierless to both HOZ 1 and HOZ 2)				
	sCI 1 + CF_3CHO	-25.58	-23.031	-23.88	-28.29
	HOZ 1	-269.20	-245.226	-251.81	-196.12
	HOZ 2	-265.64	-241.572	-248.03	-192.96
	HOZ interconversion				
	HOZ 1	-269.20	-245.226	-251.81	-196.12
	TS_{HOZ}	-244.72	-222.160	-229.91	-172.06
	HOZ 2	-265.64	-241.572	-248.03	-192.96
	HOZ to TFA pathway via HAE				
	HOZ 2	-69.21	-69.80	-75.28	-21.27
	TS_d 1	-563.17	-540.11	-543.46	-497.71

	HAE1	-563.17	-540.11	-543.46	-497.71
	TS_{iso} 1	-548.18	-527.55	-531.87	-484.43
	HAE2	-572.00	-547.90	-551.77	-504.07
	TS_{HAE} 2	-470.55	-462.94	-467.47	-419.42
	C_{TFA} 1	-546.45	-534.10	-534.02	-497.41
	HCHO + TFA con 1	-503.26	-497.58	-497.56	-499.29
	HOZ to TFA pathway instant				
	HOZ 1	-269.20	-245.226	-251.81	-196.12
	TS_{acid} 1	-51.64	-49.669	-53.97	-2.98
	C_{TFA} 2	-515.99	-506.127	-504.67	-470.12
	HCHO + TFA con 2	-490.02	-484.350	-484.35	-486.57
	HOZ to FAc pathway via HAE 1				
	HOZ 2	-265.64	-241.572	-248.03	-192.96
	TS_d 2	-78.75	-77.785	-83.39	-29.16
	HAE3	-583.13	-561.064	-564.90	-516.69
	TS_{iso} 2	-569.16	-549.560	-554.18	-505.61
	HAE5	-587.81	-565.054	-569.35	-518.55
	TS_{iso} 3	-559.56	-538.677	-544.96	-489.08
	HAE6	-577.33	-554.290	-558.81	-507.64
	TS_{HAE} 2	-490.71	-481.145	-486.71	-433.25
	C_{FAc} 1	-547.63	-534.425	-533.65	-501.21
	CF_3CHO + HCOOH con 1	-522.52	-513.282	-514.42	-518.54
	HOZ to FAc pathway via HAE 2				
	HOZ 1	-269.20	-245.226	-251.81	-196.12
	TS_d 3	-66.82	-66.612	-72.08	-18.28
	HAE4	-556.17	-534.737	-538.48	-488.78
	TS_{iso} 4	-547.52	-528.525	-533.16	-482.92
	HAE6	-577.33	-554.290	-558.81	-507.64
	TS_{HAE} 2	-490.71	-481.145	-486.71	-433.25
	C_{FAc} 1	-547.63	-534.425	-533.65	-501.21
	CF_3CHO + HCOOH con 1	-522.52	-513.282	-514.42	-518.54
	HOZ to FAc pathway instant 1				
	HOZ 2	-265.64	-241.572	-248.03	-192.96
	TS_{FAc} 2	-57.38	-54.01	-58.84	-6.25
	C_{FAc} 2	-519.30	-508.906	-506.27	-489.77
	CF_3CHO + HCOOH con 2	-504.68	-496.333	-497.29	-501.59
	HOZ to FAc pathway instant 2				
	HOZ 1	-269.20	-245.226	-251.81	-196.12
	TS_{FAc} 3	-64.58	-61.516	-66.49	-13.52
	C_{FAc} 1	-519.30	-508.906	-506.27	-489.77
	CF_3CHO + HCOOH con 2	-504.68	-496.333	-497.29	-501.59
	HOZ to Ester pathway 1				
	HOZ 1	-269.20	-245.226	-251.81	-196.12
	TSester 2	8.61	14.232	10.93	59.39
	Cester 1	-509.42	-501.720	-499.59	-471.59
	SO_2 + CF_3OCHO	-491.39	-486.849	-487.23	-486.48
	HOZ to Ester pathway 2				
	HOZ 2	-265.64	-241.572	-248.03	-192.96
	TSester 1	-1.75	5.375	2.10	49.25
	Cester 1	-509.42	-501.720	-499.59	-471.59

*Table S62: **sCIs 4** & **5** + HCHO relative energies (ΔE), zero-point corrected energy (ΔZPE), enthalpies ($\Delta H_{298.15}$) and Gibbs free energies ($\Delta G_{298.15}$) [units=kJ mol^{-1}]*

#sCI	Stationary Point	ΔE	ΔZPE	$\Delta H_{298.15}$	$\Delta G_{298.15}$
4 & 5	**sCI 4 + HCHO Cycloaddition**				
	sCI 4 + HCHO	0.00	0.00	0.00	0.00
	HOZ 1	-319.80	-296.57	-303.49	-246.27
	sCI 5 + HCHO Cycloaddition				
	sCI 5 + HCHO	-13.71	-13.00	-12.94	-14.17
	sCI 5 + HCHO PRC2	-49.26	-42.03	-41.98	-2.73
	sCI 5 + HCHO TSc2	-50.58	-41.87	-45.21	3.44
	HOZ 2	-324.11	-300.82	-307.87	-250.07
	sCI 1 + CF_3CFO Cycloaddition (barrierless) and interconversion				
	sCI 1 + CF_3CFO	-104.69	-99.204	-100.88	-104.39
	sCI 1 + CF_3CFO PRC 1	-142.02	-130.881	-132.56	-88.12
	sCI 1 + CF_3CFO TSc 3	-137.70	-125.889	-130.53	-78.24
	HOZ 1	-319.80	-296.57	-303.49	-246.27
	sCI 1 + CF_3CFO PRC 2	-140.32	-129.582	-130.88	-87.76
	sCI 1 + CF_3CFO TSc 4	-133.79	-121.601	-126.45	-73.87
	HOZ 2	-324.11	-300.82	-307.87	-250.07
	HOZ interconversion				
	HOZ 1	-319.80	-296.57	-303.49	-246.27
	TS_{HOZ}	-306.38	-284.60	-292.77	-233.16
	HOZ 2	-324.11	-300.82	-307.87	-250.07
	HOZ to FAc pathway via HAE				
	HOZ 1	-319.80	-296.57	-303.49	-246.27
	TS_d 3	-62.48	-64.96	-69.63	-17.20
	HAE4	-623.96	-603.09	-608.14	-554.75
	TS_{iso} 4	-620.09	-600.04	-607.14	-548.57
	HAE6	-633.12	-611.96	-616.94	-563.57
	TS_{HAE} 2	-562.48	-552.91	-558.75	-505.22
	C_{FAc} 1	-627.18	-611.53	-611.33	-578.03
	CF_3CFO + HCOOH con 1	-601.63	-589.46	-591.42	-594.65
	HOZ to FAc pathway instant 1				
	HOZ 2	-324.11	-300.82	-307.87	-250.07
	TS_{FAc} 1	-125.35	-121.86	-127.32	-72.20
	C_{FAc} 2	-602.46	-589.07	-587.71	-562.25
	CF_3CFO + HCOOH con 2	-583.79	-572.51	-574.29	-577.70
	HOZ to FAc pathway instant 2				
	HOZ 1	-319.80	-296.57	-303.49	-246.27
	TS_{FAc} 2	-107.18	-104.33	-109.25	-56.05
	C_{FAc} 3	-602.30	-588.97	-587.54	-563.31
	HOZ to Ester pathway 1				
	HOZ 2	-324.11	-300.82	-307.87	-250.07
	TSester 1	-58.73	-51.48	-55.19	-5.01
	Cester 1	-572.76	-562.29	-561.57	-527.35
	SO_2 + CF_3OCHO	-550.95	-544.10	-545.28	-543.71
	HOZ to Ester pathway 2				
	HOZ 1	-319.80	-296.57	-303.49	-246.27
	TSester 1	-70.99	-62.91	-66.83	-16.40
	Cester 1	-572.76	-562.29	-561.57	-527.35

Table S63:sCI + SO_2 relative energies (ΔE), zero-point corrected energy (ΔZPE), enthalpies ($ΔH_{298.15}$) and Gibbs free energies ($ΔG_{298.15}$) [units=kJ mol^{-1}]

#sCI	Stationary Point	ΔE	ΔZPE	$ΔH_{298.15}$	$ΔG_{298.15}$
1	**SOZ interconversion**				
	SOZ 1	-159.88	-143.95	-149.04	-94.15
	TS_{SOZ}	-148.79	-134.22	-140.76	-83.16
	SOZ 2	-164.58	-148.85	-154.01	-98.88
	SOZ to C_{SO_3} pathway 1				
	SOZ 1	-159.88	-143.95	-149.04	-94.15
	TS_{SO_3} 1	-71.81	-63.96	-68.44	-15.15
	C_{SO_3}	-364.76	-355.00	-355.80	-311.56
	HCHO + SO_3	-319.41	-317.93	-317.75	-315.70
	SOZ to C_{SO_3} pathway 2				
	SOZ 2	-164.58	-148.85	-154.01	-98.88
	TS_{SO_3} 2	-96.60	-89.19	-93.94	-39.79
	C_{SO_3}	-364.76	-355.00	-355.80	-311.56
	SOZ to C_{acid} pathway 1				
	SOZ 2	-164.58	-148.85	-154.01	-98.88
	TS_{acid} 1	-18.91	-20.42	-23.58	27.15
	C_{acid} 2	-496.42	-488.05	-485.39	-459.81
	SO_2 + FA con 2	-479.10	-473.30	-473.41	-473.31
	SOZ to C_{acid} pathway 2				
	SOZ 1	-164.58	-148.85	-154.01	-98.88
	TS_{acid} 2	-38.71	-39.84	-43.17	8.09
	C_{acid} 2	-496.42	-488.05	-485.39	-459.81
	SOZ to C_{acid} pathway 3				
	SOZ 1	-159.88	-143.95	-149.04	-94.15
	TS_{acid} 3	-38.10	-42.54	-44.69	3.51
	C_{acid} 1	-523.27	-512.07	-511.27	-474.88
	SO_2 + FA con 1	-447.56	-444.39	-448.56	-397.19
2 & **3**	**sCI 2 + SO_2 Cycloaddition 1**				
	PRC 1	-25.32	-21.41	-19.94	19.83
	TS_{cyc}1	-22.24	-17.56	-19.25	31.05
	SOZ 1	-167.41	-154.97	-158.68	-103.21
	sCI 2 + SO_2 Cycloaddition 2				
	PRC 2	-22.93	-19.35	-17.58	19.99
	TS_{cyc} 2	-22.44	-18.26	-19.50	28.79
	SOZ 2	-182.52	-169.97	-173.88	-117.93
	SOZ interconversion 1				
	SOZ 1	-167.41	-154.97	-158.68	-103.21
	TS_{SOZ} 1	-158.48	-147.23	-152.55	-93.32
	SOZ3	-175.58	-162.78	-166.61	-110.95
	SOZ interconversion 2				
	SOZ 2	-182.52	-169.97	-173.88	-117.93
	TS_{SOZ} 2	-164.88	-153.08	-158.54	-99.10
	SOZ4	-168.13	-155.49	-159.08	-103.90
	SOZ to C_{SO_3} pathway 1				
	SOZ3	-175.58	-162.78	-166.61	-110.95
	TS_{SO_3} 1	-102.70	-96.16	-99.88	-44.28
	C_{SO_3} 1	-376.65	-368.24	-367.24	-328.61

	$CF_3CHO + SO_3$	-345.00	-340.98	-341.64	-343.99
	SOZ to C_{SO_3} pathway 2				
	SOZ 2	-182.52	-169.97	-173.88	-117.93
	TS_{SO_3} 2	-102.70	-96.16	-99.88	-44.28
	C_{SO_3} 1	-376.65	-368.24	-367.24	-328.61
	SOZ to C_{acid} pathway 1				
	SOZ 1	-167.41	-154.97	-158.68	-103.21
	TS_{acid} 1	-24.22	-28.27	-29.89	20.72
	C_{acid} 2	-503.48	-496.08	-492.63	-472.03
	SO_2 + TFA con 2	-490.02	-484.35	-484.35	-486.57
	SOZ to C_{acid} pathway 2				
	SOZ 2	-182.52	-169.97	-173.88	-117.93
	TS_{acid} 2	-51.12	-54.28	-56.40	-4.50
	C_{acid} 3	-504.21	-496.76	-493.37	-472.07
	SOZ to C_{acid} pathway 3				
	SOZ 2	-182.52	-169.97	-173.88	-117.93
	TS_{acid} 3	-48.54	-54.58	-55.50	-7.46
	C_{acid} 3	-504.21	-496.76	-493.37	-472.07
	SOZ to C_{acid} pathway 4				
	SOZ 1	-167.41	-154.97	-158.68	-103.21
	TS_{acid} 4	-27.66	-33.91	-34.58	12.63
	C_{acid} 1	-528.65	-520.00	-517.52	-488.76
	SO_2 + TFA con 1	-503.26	-497.58	-497.56	-499.29
	SOZ to C_{ester} pathway 1				
	SOZ3	-175.58	-162.78	-166.61	-110.95
	TS_{ester} 1	-11.45	-11.06	-11.57	35.51
	C_{ester} 1	-509.50	-502.18	-499.90	-467.54
	$SO_2 + CF_3OCFO$	-491.39	-486.85	-487.23	-486.48
	SOZ to C_{ester} pathway 2				
	SOZ4	-168.13	-155.49	-159.08	-103.90
	TS_{ester} 2	5.96	5.63	5.37	48.87
	C_{ester} 1	-509.50	-502.18	-499.90	-467.54
4&5	**SOZ interconversion 1**				
	SOZ 1	-203.93	-193.02	-196.79	-140.53
	TS_{SOZ} 1	-196.71	-187.24	-192.42	-134.96
	SOZ3	-226.47	-215.04	-219.25	-161.44
	SOZ interconversion 2				
	SOZ 2	-215.60	-204.39	-208.40	-151.49
	TS_{SOZ} 2	-210.99	-200.86	-206.57	-145.35
	SOZ4	-211.13	-200.27	-203.99	-147.93
	SOZ to C_{SO_3} pathway 1				
	SOZ 2	-215.60	-204.39	-208.40	-151.49
	TS_{SO_3} 1	-117.49	-112.23	-115.98	-60.87
	C_{SO_3} 1	-443.42	-434.24	-432.59	-402.54
	$CF_3CHO + SO_3$	-424.10	-417.15	-418.64	-420.10
	SOZ to C_{SO_3} pathway 2				
	SOZ3	-226.47	-215.04	-219.25	-161.44
	TS_{SO_3} 2	-157.94	-152.16	-156.41	-98.42
	C_{SO_3} 2	-443.42	-434.24	-432.59	-402.54

	SOZ to C_{SO_3} pathway 3				
	SOZ4	-211.13	-200.27	-203.99	-147.93
	TS_{SO_3} 3	-134.70	-129.54	-133.57	-76.21
	C_{SO_3} 3	-443.42	-434.24	-432.59	-402.54
	SOZ to C_{ester} pathway 1				
	SOZ 2	-215.60	-204.39	-208.40	-151.49
	TS_{ester} 1	-85.28	-83.91	-85.02	-35.78
	C_{ester} 1	-561.50	-553.32	-550.70	-531.54
	$SO_2 + CF_3OCHO$	-550.95	-544.10	-545.28	-543.71
	SOZ to C_{ester} pathway 2				
	SOZ 1	-203.93	-193.02	-196.79	-140.53
	TS_{ester} 2	-69.69	-69.29	-69.92	-24.46
	C_{ester} 2	-561.72	-553.43	-550.90	-529.31

Table S64: sCI + HNO_3 relative energies (ΔE), zero-point corrected energy (ΔZPE), enthalpies ($\Delta H_{298.15}$) and Gibbs free energies ($\Delta G_{298.15}$) [units=kJ mol^{-1}]

#sCI	Stationary Point	ΔE	ΔZPE	$\Delta H_{298.15}$	$\Delta G_{298.15}$
1	PRC	-58.97	-54.38	-54.44	-11.56
	TS	-48.34	-48.32	-51.29	-1.74
	Pr	-192.76	-179.86	-181.93	-132.29
2	PRC	-39.46	-35.47	-33.82	2.60
	TS	-28.94	-29.05	-31.33	22.38
	Pr	-205.61	-196.26	-196.60	-147.26
3	PRC	-47.09	-42.96	-42.10	0.50
	TS	-34.54	-35.92	-38.21	14.08
	Pr	-200.32	-190.26	-191.08	-139.84
4	PRC	-60.66	-56.31	-55.35	-13.31
	TS	-59.30	-57.16	-59.45	-5.41
	Pr	-220.67	-213.94	-214.08	-164.68
5	PRC	-60.27	-56.03	-55.16	-11.62
	TS	-49.84	-52.49	-54.68	-0.74
	Pr	-209.83	-203.44	-203.90	-152.16

Table S65: sCI + TFA relative energies (ΔE), zero-point corrected energy (ΔZPE), enthalpies ($\Delta H_{298.15}$) and Gibbs free energies ($\Delta G_{298.15}$) [units=kJ mol^{-1}]

#sCI	Stationary Point	ΔE	ΔZPE	$\Delta H_{298.15}$	$\Delta G_{298.15}$
1	PRC	-45.19	-41.91	-40.16	-5.73
	Pr	-194.67	-180.21	-182.57	-130.73
2	PRC	-33.09	-30.30	-27.81	5.36
	Pr	-195.66	-184.09	-185.55	-130.37
3	PRC	-34.83	-31.94	-29.55	173.58
	Pr	-204.27	-192.57	-193.93	-138.83
4	PRC	-41.65	-38.73	-36.27	-2.79
	Pr	-224.07	-214.23	-215.92	-158.97
5	PRC	-40.48	-37.60	-35.19	0.04
	Pr	-216.16	-207.43	-208.82	-153.23

Table S66:sCI + HF relative energies (ΔE), zero-point corrected energy (ΔZPE), enthalpies ($\Delta H_{298.15}$) and Gibbs free energies ($\Delta G_{298.15}$) [units=kJ mol^{-1}]

#sCI	Stationary Point	ΔE	ΔZPE	$\Delta H_{298.15}$	$\Delta G_{298.15}$
1	PRC	-49.75	-39.94	-43.70	-8.23
	TS	-5.74	-1.52	-8.35	35.32
	Pr	-198.52	-178.46	-183.89	-142.94
2	PRC	-34.78	-26.13	-28.54	3.90
	TS	20.19	22.62	16.53	61.77
	Pr	-209.51	-192.00	-196.73	-154.41
3	PRC	-40.17	-30.95	-34.22	2.10
	TS	5.75	8.86	2.69	47.20
	Pr	-211.14	-192.83	-197.92	-153.99
4	PRC	-37.88	-29.10	-32.14	4.34
	TS	-21.37	-16.75	-23.08	23.14
	Pr	-251.93	-235.33	-240.46	-197.01
5	PRC	-42.30	-33.68	-36.44	-1.35
	TS	-7.91	-4.96	-11.10	34.41
	Pr	-244.40	-228.59	-233.72	-188.66

Table S67:sCI + HCl relative energies (ΔE), zero-point corrected energy (ΔZPE), enthalpies ($\Delta H_{298.15}$) and Gibbs free energies ($\Delta G_{298.15}$) [units=kJ mol^{-1}]

#sCI	Stationary Point	ΔE	ΔZPE	$\Delta H_{298.15}$	$\Delta G_{298.15}$
1	PRC	-31.56	-25.70	-28.93	7.08
	TS	-30.45	-25.83	-31.26	10.50
	Pr	-202.76	-180.51	-185.15	-144.07
2	PRC	-23.31	-17.26	-18.64	12.23
	TS	3.34	6.03	1.41	44.79
	Pr	-213.79	-194.13	-197.86	-154.89
3	PRC	-25.24	-19.12	-21.40	14.04
	TS	-15.75	-13.43	-18.13	24.28
	Pr	-213.84	-193.33	-197.47	-152.83
4	PRC	-27.68	-21.39	-22.89	7.87
	TS	-24.08	-19.06	-23.84	20.19
	Pr	-231.78	-213.42	-217.41	-172.92
5	PRC	-28.93	-22.96	-24.70	9.23
	TS	-18.59	-16.50	-21.07	22.66
	Pr	-225.22	-207.62	-211.63	-165.72

Table S68:sCI + H_2S relative energies (ΔE), zero-point corrected energy (ΔZPE), enthalpies ($ΔH_{298.15}$) and Gibbs free energies ($ΔG_{298.15}$) [units=kJ mol^{-1}]

#sCI	Stationary Point	ΔE	ΔZPE	$ΔH_{298.15}$	$ΔG_{298.15}$
1	PRC1	-20.13	-13.92	-14.65	19.13
	TS1	-2.57	4.26	-1.18	44.84
	Pr 1	-210.81	-188.36	-192.97	-148.26
	PRC2	-19.88	-13.71	-14.42	19.32
	TS2	-2.20	4.61	-0.87	45.24
	Pr 2	-209.59	-187.39	-191.75	-147.66
2	PRC1	-13.67	-9.89	-8.34	16.54
	TS1	2.81	9.95	5.34	53.07
	Pr 1	-226.11	-205.92	-209.55	-163.12
	PRC2	-11.88	-7.98	-6.42	16.71
	TS2	5.08	11.86	7.37	54.74
	Pr 2	-229.42	-209.23	-212.81	-166.63
3	PRC1	-11.12	-6.04	-5.77	26.67
	TS1	-5.20	1.73	-3.10	44.82
	Pr 1	-228.05	-207.02	-211.14	-162.81
	PRC2	-9.33	-4.25	-3.99	28.53
	TS2	-3.89	3.00	-1.86	46.19
	Pr 2	-222.85	-202.41	-206.02	-159.23
4	PRC1	-19.79	-15.27	-14.27	14.87
	TS1	-15.76	-9.16	-12.98	33.07
	Pr1	-240.02	-221.25	-225.09	-177.10
	PRC2	-19.28	-14.83	-13.77	14.75
	TS2	-13.31	-6.89	-10.74	35.32
	Pr2	-238.68	-220.07	-223.56	-177.03
5	PRC1	-23.07	-18.27	-17.64	14.81
	TS1	-7.06	-1.01	-5.53	43.20
	Pr1	-236.10	-218.41	-222.02	-173.29
	PRC2	-23.07	-18.31	-17.65	14.84
	TS2	-6.51	-0.41	-4.94	43.97
	Pr2	-235.98	-218.50	-221.90	-174.09

Table S69:sCI + H_2O relative energies (ΔE), zero-point corrected energy (ΔZPE), enthalpies ($ΔH_{298.15}$) and Gibbs free energies ($ΔG_{298.15}$) [units=kJ mol^{-1}]

#sCI	Stationary Point	ΔE	ΔZPE	$ΔH_{298.15}$	$ΔG_{298.15}$
1	PRC	-33.45	-25.23	-26.71	2.98
	TS1	3.66	14.28	6.75	54.28
	Pr 1	-198.40	-177.58	-183.33	-139.24
	TS2	7.30	17.54	9.95	57.61
	Pr 2	-197.78	-177.21	-182.69	-139.24
2	PRC	-20.02	-13.83	-13.66	10.42
	TS1	16.17	25.70	19.17	67.37
	Pr 1	-216.28	-198.27	-203.24	-157.68
	TS2	14.94	24.60	18.00	65.52
	Pr 2	-210.94	-194.29	-198.52	-155.45
3	PRC	-29.63	-22.29	-23.22	7.38
	TS1	1.92	12.20	5.33	54.25
	Pr 1	-220.98	-201.72	-207.21	-159.98
	TS2	4.56	14.62	7.62	57.37
	Pr 2	-216.01	-197.85	-202.59	-157.32
4	PRC1	-29.54	-22.47	-23.08	8.91
	TS1	-23.47	-13.40	-19.82	28.92
	Pr1	-262.27	-245.71	-250.98	-204.25
	PRC2	-31.47	-24.20	-25.02	7.81
	TS2	-23.25	-13.34	-19.86	28.12
	Pr2	-262.26	-245.48	-250.81	-204.05
5	PRC	-34.39	-26.80	-27.95	7.40
	TS1	-15.50	-5.89	-12.48	36.97
	Pr1	-248.73	-233.05	-238.13	-190.76
	TS2	-17.18	-7.47	-14.07	35.93
	Pr2	-257.20	-241.56	-246.67	-198.96

Table S70:sCI + $(H_2O)_2$ relative energies (ΔE), zero-point corrected energy (ΔZPE), enthalpies ($ΔH_{298.15}$) and Gibbs free energies ($ΔG_{298.15}$) [units=kJ mol^{-1}]

#sCI	Stationary Point	ΔE	ΔZPE	$ΔH_{298.15}$	$ΔG_{298.15}$
1	PRC1.1	-49.94	-39.05	-42.86	6.35
	TS1.1	-37.08	-26.33	-36.42	27.73
	Pr1.1	-209.63	-187.13	-193.79	-136.65
	AAAH- con 1 + H_2O	-178.18	-166.33	-170.00	-151.72
	PRC1.2	-49.71	-39.63	-42.97	5.58
	TS1.2	-31.89	-22.56	-32.71	31.77
	Pr1.2	-212.35	-190.79	-196.74	-140.82
	AAAH- con 2 + H_2O	-177.56	-165.96	-169.36	-151.71
	PRC1.3	-52.02	-40.84	-44.84	5.83
	TS1.3	-37.47	-27.17	-37.34	27.30
	Pr1.3	-215.73	-193.17	-199.71	-142.41
	AAAH- con 2 + H_2O	-177.56	-165.96	-169.36	-151.71
	PRC1.4	-50.89	-39.70	-43.73	6.71
	TS1.4	-38.06	-27.03	-37.10	27.20
	Pr1.4	-211.93	-189.14	-195.99	-138.25
	AAAH- con 1 + H_2O	-178.18	-166.33	-170.00	-151.72
2	PRC1.1	-44.07	-34.62	-37.44	14.41
	TS1.1	-33.71	-24.33	-33.38	32.85
	Pr1.1	-225.49	-207.53	-212.46	-155.75
	AAAH- con 2 + H_2O	-190.73	-183.04	-185.19	-167.93
	PRC1.2	-45.59	-35.42	-38.62	14.50
	TS1.2	-37.16	-27.10	-36.10	30.21
	Pr1.2	-227.04	-208.90	-213.81	-157.22
	AAAH- con 2 + H_2O	-190.73	-183.04	-185.19	-167.93
	PRC1.3	-41.52	-32.45	-34.99	16.62
	TS1.3	-32.06	-21.91	-30.89	35.88
	Pr1.3	-225.79	-207.51	-212.36	-155.73
	AAAH- con 1 + H_2O	-196.06	-187.02	-189.91	-170.15
	PRC1.4	-42.99	-33.27	-36.24	16.42
	TS1.4	-35.14	-24.60	-33.56	33.19
	Pr1.4	-230.34	-211.42	-216.72	-158.84
	AAAH- con 1 + H_2O	-196.06	-187.02	-189.91	-170.15
3	PRC1.1	-45.80	-36.24	-39.29	12.94
	TS1.1	-39.81	-29.91	-39.16	28.14
	Pr1.1	-230.20	-211.29	-216.65	-157.80
	AAAH con 2 + H_2O	-195.79	-186.60	-189.25	-169.79
	PRC1.2	-47.90	-37.15	-40.95	13.39
	TS1.2	-44.92	-34.20	-43.41	23.91
	Pr1.2	-234.30	-214.87	-220.32	-162.09
	AAAH con 2 + H_2O	-195.79	-186.60	-189.25	-169.79
	PRC1.3	-46.58	-36.49	-39.81	11.81
	TS1.3	-42.62	-31.73	-40.88	25.82
	Pr1.3	-232.92	-212.74	-218.65	-158.95
	AAAH con 2 + H_2O	-200.76	-190.47	-193.88	-172.45
	PRC1.4	-47.44	-37.11	-40.58	12.03
	TS1.4	-43.44	-32.44	-41.56	25.24
	Pr1.4	-234.79	-214.44	-220.45	-160.33
	AAAH con 2 + H_2O	-200.76	-190.47	-193.88	-172.45

4	PRC1.1	-65.71	-54.79	-58.92	-2.60
	TS1.1	-67.51	-57.30	-66.16	0.80
	Pr1.1	-278.44	-261.06	-266.52	-208.19
	AAAH- con 2 + H_2O	-242.05	-234.23	-237.48	-216.53
	PRC1.2	-67.94	-56.28	-60.84	-3.29
	TS1.2	-70.81	-59.93	-68.72	-1.75
	Pr1.2	-278.44	-261.06	-266.52	-208.19
	AAAH- con 2 + H_2O	-242.05	-234.23	-237.48	-216.53
	PRC1.3	-65.12	-53.83	-58.33	-0.73
	TS1.3	-69.10	-58.00	-66.66	0.38
	Pr1.3	-283.44	-266.55	-271.62	-214.61
	AAAH- con 1 + H_2O	-242.05	-234.46	-237.64	-216.72
	PRC1.4	-66.14	-54.49	-59.28	-1.08
	TS1.4	-70.78	-59.46	-68.03	-1.22
	Pr1.4	-283.44	-266.55	-271.62	-214.61
	AAAH- con 1 + H_2O	-242.05	-234.46	-237.64	-216.72
5	PRC1.1	-62.87	-53.00	-56.31	-2.06
	TS1.1	-60.67	-51.06	-59.89	7.37
	Pr1.1	-271.27	-255.42	-260.48	-201.38
	AAAH con 2 + H_2O	-236.98	-230.31	-233.34	-211.43
	PRC1.2	-65.55	-54.87	-58.65	-2.92
	TS1.2	-64.48	-54.26	-63.06	4.42
	Pr1.2	-273.87	-257.64	-262.87	-203.30
	AAAH con 2 + H_2O	-236.98	-230.31	-233.34	-211.43
	PRC1.3	-62.79	-52.60	-55.99	-2.37
	TS1.3	-59.52	-50.09	-59.06	8.25
	Pr1.3	-271.91	-255.94	-260.97	-202.54
	AAAH con 1 + H_2O	-228.51	-221.80	-224.80	-203.23
	PRC1.4	-61.51	-51.64	-54.83	-2.24
	TS1.4	-57.37	-48.45	-57.53	10.05
	Pr1.3	-271.91	-255.94	-260.97	-202.54
	AAAH con 1 + H_2O	-228.51	-221.80	-224.80	-203.23

Table 71: sCI + MeOH relative energies (ΔE), zero-point corrected energy (ΔZPE), enthalpies ($\Delta H_{298.15}$) and Gibbs free energies ($\Delta G_{298.15}$) [units=kJ mol^{-1}]

#sCI	Stationary Point	ΔE	ΔZPE	$\Delta H_{298.15}$	$\Delta G_{298.15}$
1	PRC	-34.19	-28.02	-27.75	7.54
	TS1	-12.01	-3.82	-8.37	42.59
	Con 1	-214.74	-199.05	-202.39	-153.88
	TS2	-7.16	0.10	-4.34	46.06
	Con 2	-205.71	-190.64	-193.87	-146.25
2	PRC 1	-20.14	-16.11	-14.10	12.20
	TS1	-0.87	5.80	2.56	54.13
	Pr1	-234.32	-221.49	-223.71	-173.78
	TS2	6.00	11.67	8.27	60.32
3	PRC	-31.11	-25.71	-24.89	11.75
	TS1	-16.83	-9.41	-13.27	39.95
	Pr1	-229.68	-215.37	-218.26	-165.47
	TS2	-12.45	-5.49	-9.13	43.38
	Pr2	-230.78	-216.98	-219.65	-168.36
4	PRC1	-30.26	-25.74	-24.07	8.00
	TS1	N/A	N/A	N/A	N/A
	Pr1	-278.79	-266.92	-269.31	-218.19
	PRC2	-35.73	-30.11	-29.29	7.75
	TS2	-33.98	-27.30	-30.75	22.32
	Pr2	-274.66	-262.01	-264.94	-212.13
5	PRC	-35.99	-30.77	-29.72	7.83
	TS1	-32.60	-26.18	-29.59	23.81
	Pr1	-258.18	-247.21	-249.63	-197.29
	PRC2	-36.93	-31.82	-30.73	6.91
	TS2	-32.73	-26.39	-29.66	23.37
	Pr2	-267.52	-256.12	-258.66	-206.58

S6. Partially Barrierless sCI 4 + MeOH Reaction

As noted in the main body of the text, many of the bimolecular HFO-sCIs reactions, such as **sCI 4** + HCHO and **sCI 3** + TFA, are barrierless and other, such as **sCI 1** + HNO_3 and **sCI 4** + $(H_2O)_2$, have large rate constants ($k_{ME} \geq 10^{-10}$ cm^3 s^{-1}). In these conditions nearly every collision would lead to a reaction meaning that the only constraint to reaction is collision frequency. This leads to employing a rate-limiting collision model, such as: the collision-limited rate coefficient (k_{COLL}), calculated using the ideal gas laws; or the often-larger dipole-dipole capture limit ($k_{d\text{-}d}$), which also includes the impact of dipole-dipole interactions.

However, the **sCI 4** (*syn*-CF_3CFOO) reaction with MeOH shows an unusual phenomenon because there is a verified TS_{AAAH} 2 structure (seen in Figure S7), but the current *B3LYP/aug-cc-pVTZ* method is unable to produce a fixed TS_{AAAH} 1 structure. This is unusual because nearly all other sCI + MeOH reactions in both this study and the Watson *et al.* study produce two TS_{AAAH} channels.[6,37] To identify other reaction channel TS_{AAAH} 1, like a structure shown in Figure S7, a minimum energy pathway (MEP) between products and reactants using the Gaussian09 *modredundant* operation. This profile is seen in Figure S7:

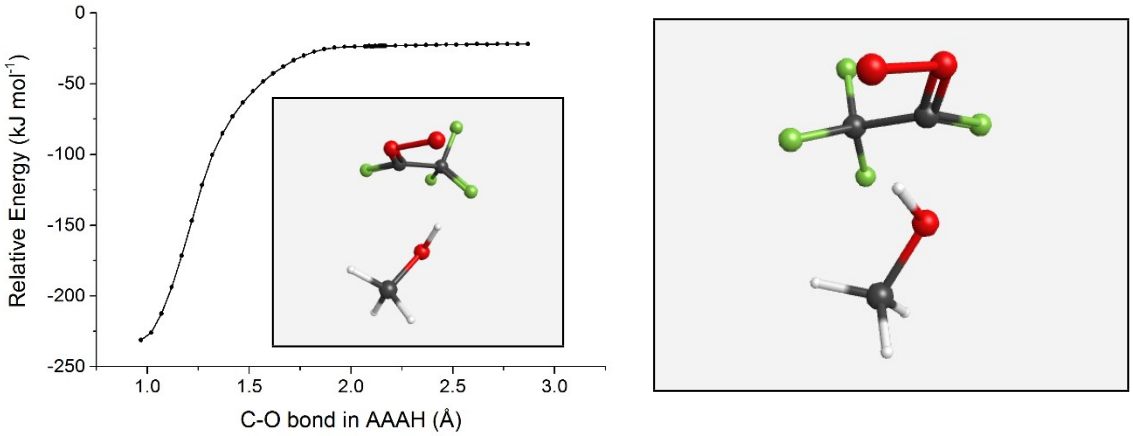

*Figure S7: The minimum energy profile (MEP) of the barrierless **sCI 4** + MeOH TS_{AAAH} 1 channel (left) with a graphic of an expected TS_{AAAH} 1; and the **sCI 4** + MeOH TS_{AAAH} 2 structure (right). Graphics of **sCI 4** + MeOH TS_{AAAH} 1 & 2 are generated using WebMO software.*[38]

This MEP generated for the **sCI 4** + MeOH TS_{AAAH} 1 channel, shown in Figure S7, has no TS inversion point meaning that it is barrierless. The TS_{AAAH} 2 barrier does have a low energy (-27.3 kJ mol^{-1}) which if it were the only barrier would produce a rate constant of ~5.17×10^{-11} cm^3 s^{-1}. However, as the TS_{AAAH} 1 channel is barrierless, the $k_{d\text{-}d}$ constant (5.50×10^{-10} cm^3 s^{-1}) is employed as the rate constant. By the inclusion of the barrierless channel, this increases the rate constant by an order of magnitude proving that identifying TS_{AAAH} 1 channel as barrierless is important.

Only one other sCI + MeOH reaction has no identified TS_{AAAH} 1 barrier and one TS_{AAAH} 2 barrier, which is the CF_2OO + MeOH reaction in the Watson *et al.* study.[6,37] This CF_2OO + MeOH significantly with the **sCI 4** + MeOH reaction in one way because, even if there were another TS_{AAAH} 1 barrier for the CF_2OO + MeOH reaction, the overall k_{ME} at 298 K constant from the TS_{AAAH} 2 barrier is so high (1.96×10^{-8} cm^3 s^{-1}) that it exceeds any likely $k_{d\text{-}d}$ or k_{COLL} values.[6,37]

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S8. Catersian coordinates for all structures and IRCs:

S8.1 Criegee intermediates

Compound: sCI 1 (HCHOO)	**Energy (kJ mol^{-1}):** -189.400847568329
Reaction Coordinates: 6 -1.068412 0.202194 -0.000000 8 -0.003231 -0.459294 -0.000000 8 1.179333 0.194958 0.000000 1 -1.021445 1.284352 -0.000000 1 -1.976903 -0.382830 0.000002	**Frequencies (cm^{-1}):** 527.7609,673.7578, 912.8476, 951.0664, 1242.0554, 1402.0013, 1543.5428, 3118.1651, 3267.9600

Compound: sCI 2 (*Syn*-CF_3CHOO)	**Energy (kJ mol^{-1}):** -526.2050097
Reaction Coordinates: 6 0.544326 0.408563 0.000000 6 -0.965669 0.489858 0.000000 8 -1.720767 -0.517005 -0.000000 8 -1.205470 -1.752491 -0.000000 1 -1.466000 1.447260 0.000000 9 1.014961 -0.207422 1.087387 9 1.014961 -0.207422 -1.087387 9 1.014961 1.672420 0.000000	**Frequencies (cm^{-1}):** 83.4264, 179.3385, 247.1426, .2827, 478.5065, 507.3023, ,536.2006, 591.5612, 758.0400, 772.8798, 885.1813, 947.2031, 1151.7894, 1176.1918, 1243.1084, 1364.7774, 1539.7613, ,3220.6741

Compound: sCI 3 (*Anti*-CF_3CHOO)	**Energy (kJ mol^{-1}):** -526.2059784
Reaction Coordinates: 6 -0.814124 -0.010987 0.000000 6 0.599627 -0.529934 0.000001 8 1.532385 0.307937 -0.000000 8 2.803565 -0.122750 -0.000000 1 0.814702 -1.591587 0.000002 9 -0.871266 1.317793 -0.000001 9 -1.465219 -0.472475 -1.084562 9 -1.465219 -0.472472 1.084563	**Frequencies (cm^{-1}):** 53.4225, 186.5103, 191.8874, 388.9843, 394.1412, 416.4183, 552.7580, 560.7356, 699.8777, 883.4653, 889.1822, 988.9465, 1131.2630, 1171.7198, 1270.0033, 1355.9541, 1546.1599, 3188.0668

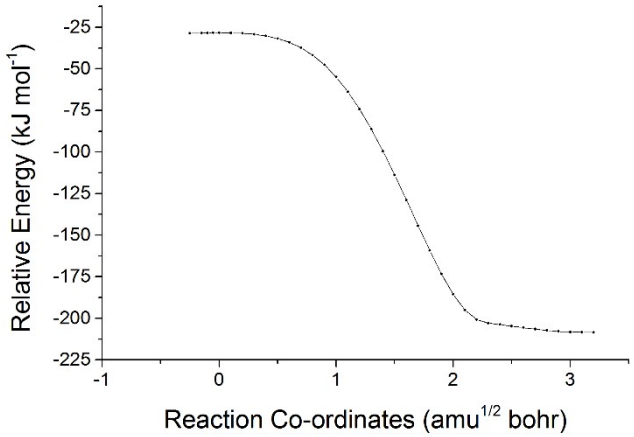
Compound: sCI 4 (*Syn*-CF_3CFOO)	**Energy (kJ mol^{-1}):** -625.3731138
Reaction Coordinates: 6 0.267347 0.734443 0.000000 6 -0.668190 -0.480912 0.000000 8 -0.317071 -1.670141 0.000000 8 1.031885 -1.966693 0.000000 9 -1.951916 -0.250006 0.000000 9 1.031885 0.735046 1.087938 9 1.031885 0.735046 -1.087938 9 -0.480015 1.843635 0.000000	**Frequencies (cm^{-1}):** 58.8820, 180.2110, 218.4479, 269.2791, 292.9260, ,363.8515, 484.2548, 493.0742, 582.0033, 631.0249, 653.9584, 780.2000, 927.2456, 1158.8972, 1195.1079, 1198.3764, 1398.0465, 1580.9318

Compound: sCI 5 (*Anti*-CF_3CFOO)	**Energy (kJ mol^{-1}):** -625.3783361
Reaction Coordinates: 6 -0.277404 -0.919423 0.000000 6 0.018963 0.571292 0.000000 8 1.190937 0.987253 0.000000 8 1.417147 2.337638 0.000000 9 -0.997920 1.369496 0.000000 9 0.847756 -1.621862 0.000000 9 -0.997920 -1.235503 1.084149 9 -0.997920 -1.235503 -1.084149	**Frequencies (cm^{-1}):** 41.8080, 154.2443, 183.9192, 293.0541, 346.5294, 372.3393, 406.8758, 515.4784, 576.4030, 659.0393, 728.8220, .5490, 906.9387, 1155.2541, 1155.7283, 1229.1869, 1400.7892, 1601.0242

S8.2 Reactions with HCHO

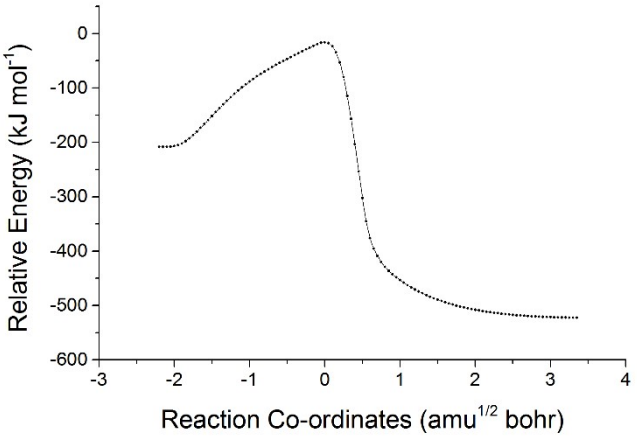
Compound: HCHO	**Energy (kJ mol^{-1}):** -114.386051813463
Reaction Coordinates: 6 -0.000000 -0.526970 -0.000000 8 0.000000 0.673271 0.000000 1 -0.000000 -1.112173 0.938294 1 -0.000000 -1.112173 -0.938294	**Frequencies (cm^{-1}):** 1198.1780, 1262.9587, 1530.2218, 1813.2454, 2885.3911, 2940.0951

Compound: sCI 1 + HCHO PRC	**Energy (kJ mol^{-1}):** -303.798329359066
Reaction Coordinates: 6 -1.568793 0.372025 -0.025055 8 -1.363160 -0.828477 -0.072239 1 -1.657461 0.978246 -0.937211 1 -1.783433 0.887713 0.921406 6 1.125843 -0.947653 0.216022 1 1.548975 -1.796415 -0.304241 1 0.693612 -0.991078 1.204393 8 1.223576 0.146118 -0.385058 8 0.621585 1.229271 0.203528	**Frequencies (cm^{-1}):** 74.8509, 103.5754, 200.3540, 278.7803, 321.9694, 483.9337, 530.6353, 685.8280, 894.8752, 1002.3931, 1157.3881, 1239.1392, 1254.7518, 1413.4948, 1517.9212, 1564.5284, 1716.1748, 2949.5550, 3015.1791, 3137.8091, 3282.9945

Compound: sCI 1 + HCHO TS_c	**Energy (kJ mol^{-1}):** -303.798797734635
Reaction Coordinates: 6 -1.487001 0.353271 0.010278 6 1.049308 -0.925024 0.242888 8 -1.242190 -0.844058 -0.122774 1 -1.676186 0.993769 -0.859690 1 -1.706764 0.792026 0.991823 1 1.451806 -1.797973 -0.253471 1 0.671776 -0.928437 1.253159 8 1.183806 0.153845 -0.385267 8 0.544074 1.236604 0.176688	**Frequencies (cm^{-1}):** -118.7612, 95.7382, 234.5586, 345.4726, 399.7370, 537.6674, 590.3087, 710.8836, ,903.1654, 1013.8378, 1146.8734, 1233.3069, 1247.5743, 1407.0484, 1501.0072, 1558.8347,6 1669.3075, 2963.4503, 3032.3718, 3142.2215, 3285.8554
IRC:  	

Compound: sCI 1 + HCHO HOZ	**Energy (kJ mol^{-1}):** -303.878537225920
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.118320 0.321848 -0.133769 8 0.000001 1.185457 -0.000005 1 -1.921112 0.617737 -0.541368 1 -1.444573 0.296995 1.177335 6 -1.118317 0.321850 0.133776 1 1.921105 0.617728 0.541390 1 1.444593 0.296997 -1.177322 8 0.669522 -0.948459 0.290933 8 -0.669527 -0.948454 -0.290938	163.2068, 371.3640, 708.1220, 750.0747, 861.2831, 925.9772, 954.1919, 1041.1937, 1086.5608, 1142.2906, 1145.0755, 1218.3662, 1222.1489, 1370.6921, 1414.6761, 1519.1635, 1529.2393, 3014.9743, 3016.9237, 3096.0501, 3097.3415

Compound: sCI 1 + HCHO TS_d	**Energy (kJ mol^{-1}):** -303.807859688040
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.204271 0.195038 -0.204006 6 1.013769 0.309599 0.311038 8 -0.063824 1.098505 -0.089969 1 -2.002883 0.746061 0.330078 1 -1.513034 0.164053 -1.270020 1 1.829321 0.907119 0.746096 1 0.499372 -0.213545 1.248177 8 1.327196 -0.694146 -0.413719 8 -0.972093 -0.983297 0.291623	-963.8912, 228.1363, 313.3548, 468.8414, 547.0783, 739.8412, 811.6421, 907.5403, 946.3363, 992.9338, 1120.5118, 1130.5080, 1233.0628, 1263.7100, 1269.1727, 1337.9092, 1376.8823, 2112.8107, 2855.1673, 2878.1255, 2969.9759
IRC:	



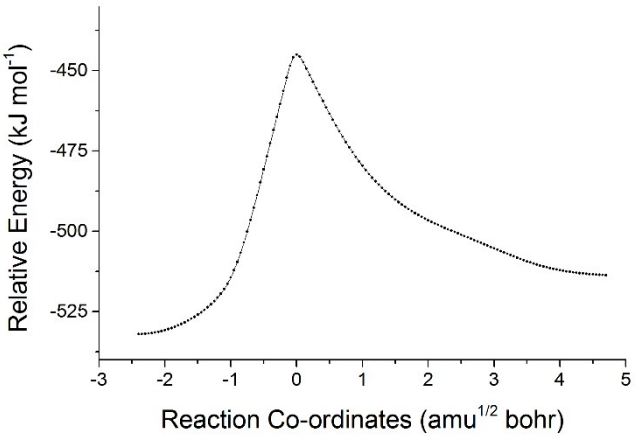
Compound: sCI 1 + HCHO HAE con 1	**Energy (kJ mol^{-1}):** -303.997300763222
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.305850 0.289288 -0.231552 6 0.940582 0.108875 0.562488 8 -0.113961 0.892842 -0.041694 1 2.217403 0.120005 -0.894036 1 -1.978441 0.989618 -0.741641 1 0.504100 -0.659409 1.192085 1 1.510830 0.833055 1.143035 8 1.709527 -0.532334 -0.400318 8 -1.603351 -0.819539 0.106380	70.4857, 248.4112, 299.0854, 381.9429, 547.6482, 755.4857, 887.0359, 1041.6181, 1059.1008, 1083.6745, 1160.7621, 1288.9470, 1396.6575, 1400.1716, 1435.6149, 1511.3613, 1800.1743, 3033.9528, 3065.1750, 3152.7357, 3803.4239

Compound: sCI 1 + HCHO TS_{ISO}	**Energy (kJ mol^{-1}):** -303.991840303773
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.312004 0.313671 -0.206358 6 -0.930064 0.023397 0.582096 8 0.087792 0.853126 -0.000989 1 -1.526009 -0.131808 -1.262605 1 1.954963 1.077031 -0.660097 1 -0.464130 -0.834440 1.062866 1 -1.444117 0.655822 1.304341 8 -1.842940 -0.400862 -0.395533 8 1.653606 -0.800891 0.059156	-422.7115, 38.5836, 260.2890, 315.7944, ,510.8464, 752.0342, 886.7029, 1041.3061, 1062.2173, 1136.1380, 1174.7639, 1275.0176, 1301.7533, 1400.7928, 1454.4948, 1531.3924, 1804.1671, 3042.0345, 3062.5202, 3115.8914, 3834.6789

Compound: sCI 1 + HCHO HAE con 2	**Energy (kJ mol^{-1}):** -304.001807069015
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.260600 -0.237487 -0.167386 6 1.023485 -0.390383 0.400595 8 -0.168614 -1.005790 -0.171215 1 0.907472 1.414099 -0.227820 1 -2.108826 -0.788602 -0.589538 1 1.764187 -1.182273 0.386199 1 0.774725 -0.093172 1.420070 8 1.496495 0.660749 -0.360576 8 -1.317239 0.897188 0.233271	134.0932, 255.9643, 311.9088, 498.3134, 561.1357, 795.3260, 864.0522, 1045.5382, 1057.3010, 1110.4985, 1185.2944, 1293.0581, 1394.8699, 1405.6822, 1444.0186, 1510.2254, 1767.9081, 3044.7503, 3055.0210, 3155.2797, 3770.5265

Compound: sCI 1 + HCHO TS_{HAE}	**Energy (kJ mol^{-1}):** -303.962565700012
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.259724 0.228825 -0.065861 6 -1.300930 0.415269 0.217050 8 0.390711 1.135692 -0.108964 1 -0.140029 -1.130261 0.047319 1 2.302132 0.521079 -0.236182 1 -1.881506 1.181054 -0.297803 1 -1.172603 0.572406 1.291527 8 -1.283919 -0.759522 -0.264454 8 1.035612 -1.002275 0.159419	-1115.5862, 186.3394, 274.1524, 418.1722, 517.4046, 579.7763, 825.7630, 933.1747, 1065.4507, 1221.2134, 1269.0745, 1326.4903, 1369.5579, 1384.3739, 1426.3933, 1614.5353, 1664.1975, 1769.6394, 3013.1948, 3043.6088, 3103.6379

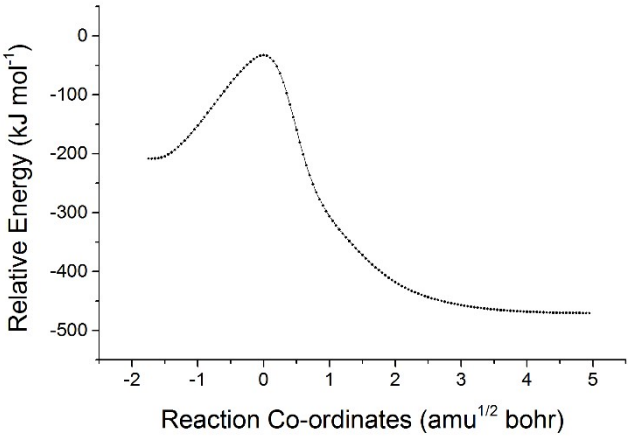
IRC:



Compound: sCI 1 + HCHO $C_{FA}1$	**Energy (kJ mol^{-1}):** -303.990619638538
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.657241 0.078650 -0.000000 8 1.043083 -1.098158 -0.000000 1 0.062756 -0.961278 0.000000 1 2.745848 -0.055528 0.000001 8 1.117502 1.158015 -0.000000 6 -2.029026 0.516294 -0.000000 1 -3.098216 0.781136 -0.000000 1 -1.289414 1.329652 0.000001 8 -1.684368 -0.642813 0.000000	79.6236, 129.7900, 169.6478, 170.9258, 222.4930, 278.0783, 683.5053, 929.9644, 1069.2322, 1203.2888, 1228.4469, 1278.6536, 1380.1043, 1433.9700, 1520.6897, 1759.5075, 1791.2246, 2935.6401, 3032.6033, 3035.6839, 3329.9795

Compound: sCI 1 + HCHO TS_{FAc}	**Energy (kJ mol^{-1}):** -303.798809356950
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.240479 0.362821 -0.185443 6 1.098625 0.163043 0.257745 8 0.375297 1.190354 -0.047479 1 -1.744598 1.114643 0.430772 1 -1.336379 0.488679 -1.266462 1 1.536373 0.118717 1.267026 1 1.992081 -0.143278 -0.499480 8 0.778126 -0.994917 -0.319869 8 -1.102967 -0.787180 0.321638	-1096.7712, 206.5170, 256.9022, 324.0747, 431.0549, 572.4996, 727.5382, 839.5537, 918.9246, 1138.6108, 1158.0605, 1191.6131, 1205.9149, 1326.2421, 1374.7565, 1428.0091, 1525.1102, 2292.9905, 2959.8703, 2995.5443, 3072.2430

IRC:

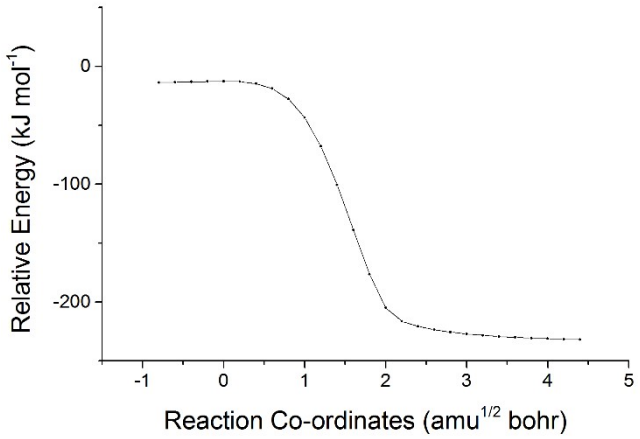


Compound: sCI 1 + HCHO $C_{FA}2$	**Energy (kJ mol^{-1}):** -303.977039930179
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.065592 -0.087673 -0.000001 8 -0.608544 1.017095 -0.000001 1 -0.449781 -0.999539 -0.000001 8 -2.394409 -0.311317 0.000001 1 -2.569904 -1.260625 0.000001 6 2.137059 0.348295 0.000001 1 2.195113 0.930061 0.935342 1 2.195122 0.930065 -0.935336 8 2.028034 -0.851239 -0.000001	62.0233, 85.0729, 96.4283, 104.1922, 151.3635, 200.7762, 548.5041, 664.7080, 1053.7673, 1121.0790, 1195.0673, 1262.7951, 1275.3896, 1425.0166, 1531.7929, 1794.9661, 1835.5258, 2912.6865, 2973.8170, 2995.6876, 3779.8452

Compound: HCOOH conformer 1	**Energy (kJ mol^{-1}):** -189.590120303627
Reaction Coordinates: 6 0.000000 0.421050 -0.000000 8 1.158545 0.117329 -0.000000 8 -1.028178 -0.446131 0.000000 1 -0.659713 -1.343779 0.000000 1 -0.383224 1.447894 -0.000000	**Frequencies (cm^{-1}):** 628.6127, 676.8905, 1051.6911, 1121.3699, ,1298.0934, 1401.7983, 1811.5029, 3048.9648, 3717.6132

Compound: HCOOH conformer 2	**Energy (kJ mol^{-1}):** -189.583325855473
Reaction Coordinates: 6 0.133997 0.361764 -0.000000 8 1.173188 -0.220201 0.000000 8 -1.056592 -0.278816 -0.000000 1 -1.779073 0.361263 0.000001 1 0.042323 1.460290 -0.000000	**Frequencies (cm^{-1}):** 530.6018, 659.6880, 1032.5549, 1103.7723, 1268.4932, 1413.8078, 1855.6257, 2962.7301, 3780.4926

Compound: sCI 2 + HCHO PRC	**Energy (kJ mol^{-1}):** -640.600757425560
Reaction Coordinates: 6 -1.180344 -0.230641 -0.046857 6 -0.299183 0.435311 0.995105 1 -0.446023 0.217189 2.043332 8 0.555870 1.315583 0.742164 8 0.850811 1.621339 -0.538900 9 -1.964927 -1.112890 0.600682 9 -0.513822 -0.882972 -0.993276 9 -1.975264 0.679816 -0.627729 8 2.104802 -1.100010 0.536169 6 2.603324 -0.596540 -0.440591 1 2.258798 -0.835449 -1.459457 1 3.438696 0.118587 -0.362384	**Frequencies (cm^{-1}):** 37.0708, 60.8826, 81.7946, 97.3619, 111.0942, 164.0783, 188.0260, 210.5000, 265.4560, 327.3318, 475.0201, 506.6223, 536.7568, 585.0303, 757.4736, 803.4917, 880.2936, 928.3002, 1153.7845, 1170.7827, 1191.6829, 1250.4028, 1262.9443, 1368.9269, 1530.1666, 1560.6252, 1782.9473, 2922.5875, 2988.1962, 3218.3068

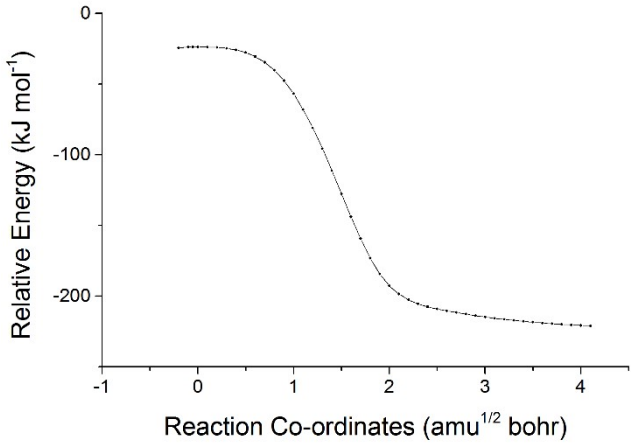
Compound: sCI 2 + HCHO TS_c	**Energy (kJ mol^{-1}):** -640.598646446407
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.092215 -0.129997 0.058184 6 0.100620 0.466841 -0.934798 1 0.343043 0.361471 -1.984193 8 -0.797561 1.308568 -0.687912 8 -1.272647 1.384786 0.588980 9 1.764815 -1.099970 -0.580750 9 0.611298 -0.619326 1.188676 9 1.973002 0.848592 0.363137 8 -1.513961 -1.198018 -0.587087 6 -2.163773 -0.843793 0.385501 1 -1.799910 -0.986918 1.408525 1 -3.186182 -0.459212 0.270934	-101.5617, 38.4107, 137.2510, 151.3563, 177.4183, 217.1369, 308.7619, 321.1385, 348.7483, 452.6528, 476.9346, 513.6888, 538.4700, 575.6568, 755.0955, 846.8308, 874.2992, 926.7008, 1124.3981, 1158.5445, 1168.3125, 1255.2191, 1280.9832, 1368.3635, 1515.2006, 1562.4061, .6061, 2970.6576, 3052.7393, 3203.3552
IRC  	

Compound: sCI 2 + HCHO HOZ 1	**Energy (kJ mol^{-1}):** -640.693594205454
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.139558 0.021002 0.054719 6 0.170641 0.051083 -0.760444 1 -0.090393 0.101412 -1.820168 8 0.948084 -1.114764 -0.588504 8 1.785506 -0.749925 0.551876 6 2.154623 0.552911 0.174737 8 0.968223 1.133091 -0.357516 1 2.456979 1.080978 1.077043 1 2.936113 0.542263 -0.589467 9 -1.845283 1.141421 -0.185469 9 -0.938327 -0.072135 1.371621 9 -1.886550 -1.027268 -0.333743	59.1063, 109.3494, 182.6206, 246.9681, 316.5757, 361.0581, 425.8088, 520.4651, 571.5285, 674.7369, 736.3570, 797.4111, 848.6080, 871.4982, 946.6412, 997.2191, 1056.8708, 1107.0675, 1149.2593, 1160.3118, 1162.8976, 1228.4602, 1290.9247, 1296.5657, 1398.3701, 1404.9809, 1520.9829, 3026.1795, 3063.2864, 3121.7528

Compound: sCI 3 + HCHO PRC	**Energy (kJ mol^{-1}):** -640.603980608439
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.395048 0.105593 -0.002788 6 0.022720 -0.321612 -0.476169 1 -0.363411 0.002589 -1.431854 8 -0.599263 -1.140283 0.236215 8 -1.841748 -1.515337 -0.175639 9 1.542932 1.421931 -0.179678 9 2.330250 -0.518267 -0.749247 9 1.608632 -0.193064 1.275855 6 -2.809371 0.706607 0.105628 8 -1.810139 1.383829 -0.036680 1 -3.152938 0.385323 1.099579 1 -3.461164 0.447480 -0.741295	26.0215, 58.6615, 71.4215, 113.1524, 179.8264, 198.8805, 262.8157, 292.8331, 389.0975, 416.4647, 420.4978, 428.0257, 552.7682, 565.6375, 701.5734, 881.9017, 894.2454, 960.3389, 1133.9182, 1171.0645, 1189.3448, 1257.3784, 1269.2401, 1357.9965, 1522.7347, 1562.6462, 1734.2093, 2944.3504, 3012.1390, 3219.1546

Compound: sCI 3 + HCHO TS_c	**Energy (kJ mol^{-1}):** -640.602817064141
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.347878 0.073175 -0.009024 6 -0.042885 -0.314571 -0.470147 1 -0.382351 -0.053128 -1.460716 8 -0.678629 -1.118670 0.253750 8 -1.961632 -1.378830 -0.150523 9 1.599343 1.337368 -0.356012 9 2.249777 -0.714834 -0.632407 9 1.505896 -0.065064 1.303663 6 -2.631041 0.764258 0.033598 8 -1.548350 1.343408 0.050311 1 -3.151648 0.509727 0.964824 1 -3.195983 0.621731 -0.896167	-108.4983, 34.2541, 80.4906, 101.0591, 190.0208, 216.2135, 336.3818, 353.9170, 404.2459, 441.4964, 451.1272, 553.6226, 559.5445, 576.7438, 703.4921, 876.6809, 909.8247, 958.9078, 1132.4025, 1154.0451, 1193.3540, 1247.9350, 1271.4011, 1352.7332, 1504.1140, 1552.4877, 1673.8982, 2966.5520, 3039.4073, 3229.4170

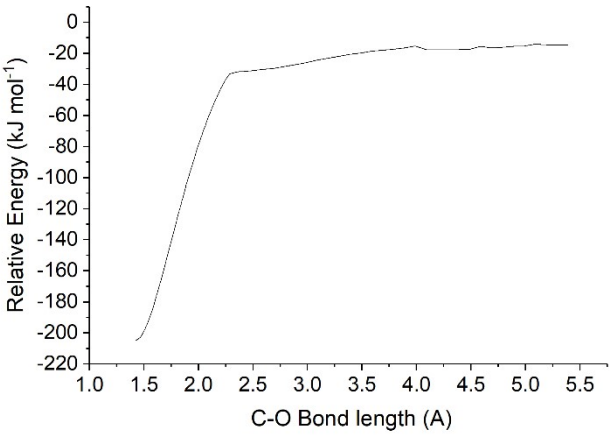
IRC



Compound: sCI 2 + HCHO HOZ 2	**Energy (kJ mol^{-1}):** -640.692237225941
Reaction Coordinates: 6 -1.199474 -0.006887 0.025742 6 0.188982 0.075516 -0.632497 1 0.066771 0.219589 -1.709669 8 0.886315 1.153776 -0.023764 8 2.263774 0.688372 -0.073467 9 -1.912002 -0.986844 -0.552341 9 -1.865454 1.147074 -0.144863 9 -1.122709 -0.261077 1.336176 6 2.082671 -0.644790 0.338694 8 0.942805 -1.084525 -0.386997 1 1.899865 -0.705867 1.413986 1 2.958623 -1.210111 0.027110	**Frequencies (cm^{-1}):** 69.3077, 77.4879, 179.4407, 253.9583, 338.8035, 359.3502, 394.3628, 520.8056, 560.9398, 693.6963, 725.0348, 762.4881, 855.7256, 889.6512, 943.1106, 1019.7862, 1053.9849, 1110.1529, 1156.8169, 1164.3491, 1169.6625, 1229.0507, 1279.8213, 1324.1151, 1395.3592, 1417.9899, 1520.2746, 3034.5928, 3042.4603, 3125.6720

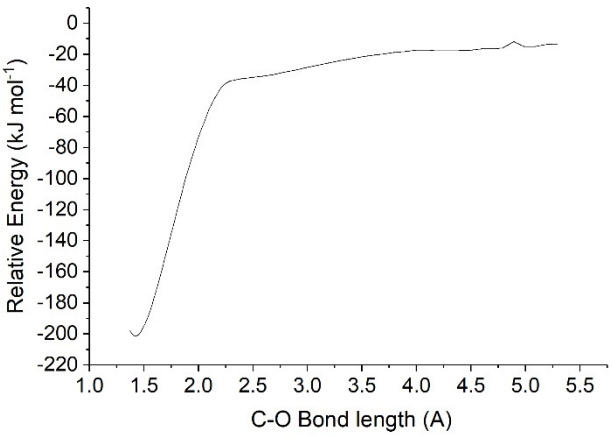
Compound: **sCI 1** + CF_3CHO TS_C 3 reaction profile

IRC



Compound: **sCI 1** + CF_3CHO TS_C 4 reaction profile

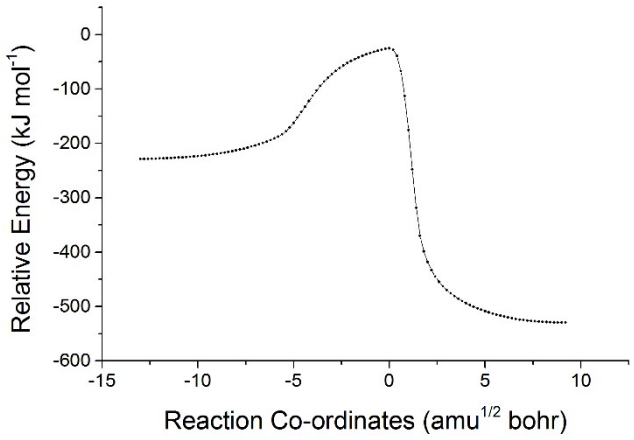
IRC



Compound: sCI 2 + HCHO TS_{HOZ}	**Energy (kJ mol^{-1}):** -640.684269884806
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.234099 -0.016283 0.006992 6 0.217213 -0.006609 -0.495282 1 0.218277 -0.049061 -1.592572 8 0.855493 1.160309 -0.027043 8 2.258508 0.764235 0.099653 9 -1.857504 -1.113969 -0.452291 9 -1.882837 1.059394 -0.467529 9 -1.314504 -0.008957 1.336003 8 0.921671 -1.073107 0.066267 6 2.262564 -0.669437 -0.024369 1 2.695489 -0.937726 -0.993919 1 2.820401 -1.098946 0.805786	-165.8267, 67.5700, 127.7216, 175.6983, 283.1192, 342.4707, 385.5527, 523.0921, 560.2367, 704.2322, 737.7067, 743.3313, 872.9650, 886.7348, 969.5435, 1045.4194, 1080.9912, 1104.8589, 1149.3572, 1169.1195, 1171.0625, 1213.1812, 1288.3676, 1324.0129, 1403.4090, 1440.7109, 1542.0138, 2991.1447, 3001.7444, 3106.4815

Compound: sCI 2 + HCHO TS_d1	**Energy (kJ mol^{-1}):** -640.617420542433
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.272566 -0.064462 -0.073317 6 -0.244352 0.274927 0.044246 1 -0.645217 0.341103 -1.063275 8 -0.552453 1.411193 0.535921 8 -2.503654 0.476103 -0.643557 9 1.439852 -1.233548 -0.702036 9 1.827864 -0.156384 1.139634 9 1.903380 0.887839 -0.761182 8 -0.981873 -0.842524 0.464269 6 -2.354325 -0.570621 0.105257 1 -2.947279 -0.507834 1.045947 1 -2.686871 -1.511682 -0.380590	-741.0428, 59.4313, 151.2334, 186.1966, 243.5673, 303.5509, 339.1981, 349.3825, 404.0339, 518.6383, 563.2478, 592.0433, 701.5788, 748.6722, 795.3978, 867.4294, 908.7148, 1011.7064, 1059.6639, 1109.0522, 1182.1362, 1200.4362, 1205.6404, 1237.9073, 1274.6459, 1307.2383, 1361.3928, 2176.3273, 2823.9085, 2857.7175

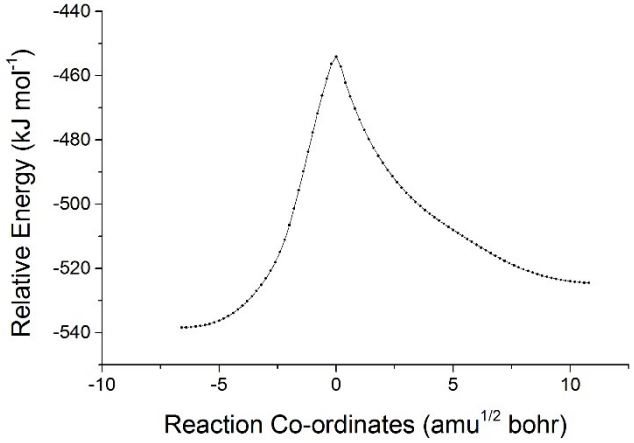
IRC



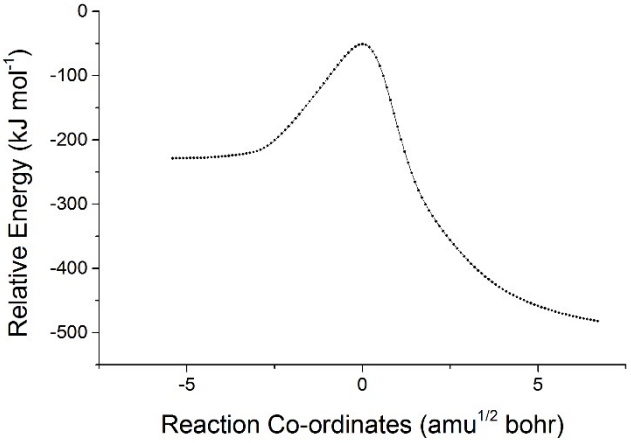
Compound: sCI 2 + HCHO HAE1	**Energy (kJ mol^{-1}):** -640.805561786150
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.351795 -0.125467 0.048198 6 0.065137 0.490331 -0.114630 8 0.286253 1.656338 0.015812 8 0.932103 -0.477171 -0.423884 6 2.335472 -0.103488 -0.537474 8 2.973678 -0.179972 0.685937 1 3.074254 -1.101793 0.946812 1 2.399971 0.923885 -0.880158 1 2.725373 -0.805410 -1.272305 9 -1.357699 -1.041318 1.031295 9 -1.738702 -0.730048 -1.087855 9 -2.240127 0.818198 0.346133	27.9049, 64.9955, 82.2236, 179.2410, 252.1594, 310.6391, 345.4473, 394.3004, 414.0244, 511.8310, 545.7231, 597.1920, 729.1634, 784.3867, 829.9422, 904.5459, 1062.5305, 1093.5179, 1149.6677, 1155.4669, 1212.3045, 1289.3237, 1330.8387, 1400.0656, 1440.7955, 1512.2298, 1841.2052, 3075.9799, 3157.7365, 3800.2458

Compound: sCI 2 + HCHO $TS_{ISO}1$	**Energy (kJ mol^{-1}):** -640.799853308352
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.306299 -0.187066 -0.541446 1 -2.717596 -0.973662 -1.173786 1 -2.373790 0.790343 -1.020955 8 -2.873212 -0.183469 0.739477 1 -3.832746 -0.200502 0.667780 8 -0.929146 -0.531110 -0.379707 6 -0.075965 0.469745 -0.131854 6 1.350154 -0.115599 0.056431 9 2.220727 0.857467 0.311018 9 1.376565 -0.988847 1.073888 9 1.743814 -0.756991 -1.057586 8 -0.316787 1.636664 -0.074482	-238.4497, 25.7190, 72.3081, 88.5166, 183.0110, 252.5813, 326.5163, 348.8901, 412.3888, 509.5526, 542.9971, 591.4858, 730.3949, 782.7179, 829.1229, 963.6820, 1080.2566, 1134.6460, 1154.5610, 1155.6226, 1212.5796, 1256.2745, 1300.2406, 1335.7964, 1469.5455, 1523.2246, 1846.9871, 3041.7344, 3095.0383, 3824.0172

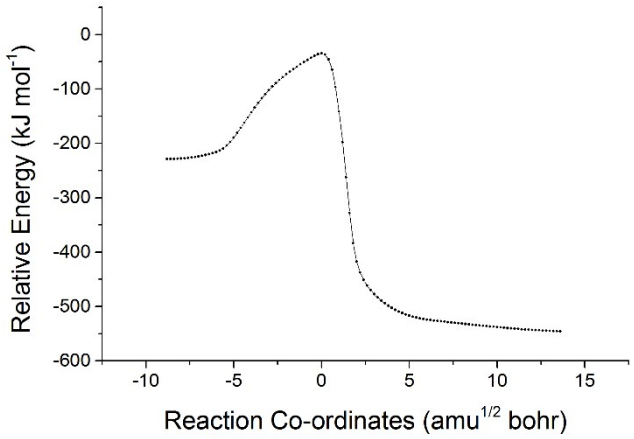
Compound: sCI 2 + HCHO HAE2	**Energy (kJ mol^{-1}):** -640.808924257914
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.318124 -0.533342 -0.393417 1 -2.737399 -1.532535 -0.416846 1 -2.393672 -0.038330 -1.361679 8 -2.916957 0.172141 0.624254 1 -2.679712 1.103745 0.538181 8 -0.888763 -0.765465 -0.148492 6 -0.130277 0.319304 -0.178029 6 1.358012 -0.057160 0.056207 9 2.122069 1.031756 0.040807 9 1.510068 -0.668874 1.240348 9 1.786173 -0.891063 -0.906048 8 -0.495740 1.449316 -0.356285	27.6747, 80.3699, 121.4909, 183.6917, 250.5901, 295.7323, 345.1689, 415.1064, 509.5916, 513.2878, 551.7353, 590.8439, 739.6659, 792.6490, 838.9950, 890.4196, 1055.1402, 1117.6863, 1154.7276, 1163.8789, 1213.1588, 1290.4440, 1345.6009, 1406.7222, 1448.6631, 1511.0362, 1811.0926, 3062.8440, 3165.5278, 3776.0480

Compound: sCI 2 + HCHO $TS_{HAE}1$	**Energy (kJ mol^{-1}):** -640.770283337633
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.390799 0.035220 0.021329 6 0.155415 -0.046897 -0.116251 1 1.833446 -1.112235 -0.029863 8 0.626879 -1.209964 -0.281780 8 2.801207 -0.543215 0.375049 9 -1.988022 -0.775715 -0.858875 9 -1.746400 -0.348928 1.259495 9 -1.836261 1.276977 -0.177237 8 0.797982 1.019752 -0.026542 6 2.702880 0.589884 -0.173390 1 3.096326 1.459636 0.350032 1 2.592859 0.679766 -1.254562	-1089.5421, 16.5601, 76.9026, 165.4483, 216.2266, 266.7990, 281.1986, 388.8310, 462.6379, 475.7872, 517.5003, 574.2078, 636.4659, 747.7625, 804.0394, 858.0309, 881.8098, 1156.5163, 1189.1043, 1208.1041, 1220.3110, 1246.2111, 1347.3573, 1438.7791, 1465.4423, 1624.4152, 1668.6753, 1790.7038, 3045.2640, 3141.5807
IRC  	

Compound: sCI 2 + HCHO $C_{TFA}1$	**Energy (kJ mol^{-1}):** -640.799194296748
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.584811 0.005077 -0.000001 6 -0.039654 0.156627 0.000008 1 1.529652 -0.913874 0.000007 8 0.540782 -1.026051 0.000005 8 3.222675 -0.659518 0.000004 9 -1.992953 -0.669392 -1.087888 9 -1.992964 -0.669470 1.087833 9 -2.176496 1.197977 0.000039 8 0.498638 1.231972 0.000014 6 3.647165 0.473450 -0.000009 1 4.731211 0.662243 -0.000012 1 2.967885 1.337445 -0.000019	25.6546, 47.4526, 85.6725, 89.5655, 138.7878, 212.8202, 239.2894, 272.2450, 275.9329, 398.0737, 430.5026, 516.2915, 588.3812, 699.8772, 781.4965, 807.0049, 948.7741, 1152.7095, 1171.4562, 1205.8043, 1228.0063, 1276.9303, 1322.5883, 1468.8858, 1522.6090, 1770.4123, 1819.6128, 2945.5541, 3040.2391, 3222.9658

Compound: sCI 2 + HCHO $TS_{acid}1$	**Energy (kJ mol^{-1}):** -640.610730401605
Reaction Coordinates: 6 1.170040 -0.019333 0.102506 6 -0.168113 -0.057013 -0.702440 1 0.095200 0.410473 -1.787063 8 -0.833645 1.094628 -0.827126 8 -1.972031 0.668468 0.724614 9 1.933853 -1.065833 -0.239568 9 0.934323 -0.078480 1.416071 9 1.854340 1.102900 -0.157453 8 -0.842555 -1.144501 -0.647246 6 -2.345900 -0.451047 0.296177 1 -2.344359 -1.284700 1.006253 1 -3.003801 -0.537460 -0.570039	**Frequencies (cm^{-1}):** -1053.5436, 42.5106, 105.4209, 173.6081, 261.0965, 263.0094, 289.2795, 345.4982, 404.0330, 428.2578, 517.2237, 537.4321, 592.1376, 704.0861, 797.1483, 818.3344, 854.2981, 933.9543, 1132.9398, 1155.0775, 1183.1777, 1194.8084, 1196.7304, 1273.4821, 1394.2535, 1446.8064, 1542.9920, 2285.7600, 3003.4676, 3093.2029
IRC  	

Compound: sCI 2 + HCHO $C_{TFA}2$	**Energy (kJ mol^{-1}):** -640.787589964388
Reaction Coordinates: 6 1.019299 -0.360811 -0.053058 6 0.148131 0.922496 -0.173713 8 0.046381 1.641340 0.947305 1 0.368706 1.141827 1.710470 8 -0.304737 1.263154 -1.223148 9 2.273904 -0.073288 -0.444518 9 0.557232 -1.344920 -0.812178 9 1.087654 -0.796104 1.225627 8 -2.080165 -0.612552 0.614197 6 -2.894107 -0.391330 -0.244657 1 -2.637248 0.185901 -1.148649 1 -3.932339 -0.756588 -0.160453	**Frequencies (cm^{-1}):** 43.6805, 46.0995, 76.9727, 88.5261, 90.8361, 152.1740, 182.0909, 250.5153, 254.9155, 383.7001, 426.9844, 506.3784, 531.5898, 586.9922, 689.0061, 762.0313, 796.3404, 1125.2518, 1139.2762, 1210.1226, 1212.7643, 1246.2164, 1270.1461, 1372.0470, 1527.1554, 1799.1525, 1869.7527, 2909.7687, 2982.7885, 3755.1592

Compound: sCI 2 + HCHO TS_d2	**Energy (kJ mol^{-1}):** -640.621055369406
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.175640 0.329999 -0.502393 1 -0.058554 0.493890 -1.591676 6 1.274700 -0.031924 0.005777 9 1.738207 -1.102156 -0.647013 9 2.091775 0.995729 -0.230496 9 1.276257 -0.294315 1.313791 8 -0.688512 1.334729 0.131328 8 -0.918574 -0.908852 -0.312853 6 -2.105447 -0.552757 0.321201 1 -2.608572 -1.415811 0.787748 8 -2.842231 0.328488 -0.233668 1 -1.656171 0.021768 1.251429	-858.3901, 83.4451, 100.7020, 167.0216, 224.4556, 310.1539, 342.4178, 408.5183, 472.7327, 531.3920, 566.5172, 584.1015, 720.7180, 750.4830, 808.8318, 848.8824, 940.9329, 988.9430, 1105.4595, 1136.6271, 1147.7638, 1181.9117, 1219.2248, 1243.8147, 1252.5114, 1271.6928, 1375.0411, 2178.8550, 2883.0314, 2954.8922
IRC  	

Compound: sCI 2 + HCHO HAE3	**Energy (kJ mol^{-1}):** -640.813164616868
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.189522 0.476776 -0.240249 1 -0.577133 0.286665 -1.237829 6 1.154475 -0.250359 -0.066579 9 1.008237 -1.579445 -0.146258 9 2.013485 0.132641 -1.021670 9 1.710486 0.040828 1.127511 8 -0.061070 1.841415 -0.086936 1 0.325339 2.036387 0.776578 8 -1.067326 -0.079665 0.744616 6 -2.334230 -0.377776 0.357102 1 -2.884504 -0.748554 1.228277 8 -2.776342 -0.263320 -0.745795	32.0458, 66.2195, 177.5694, 205.0507, 255.5542, 262.8436, 365.1985, 385.3922, 425.7036, 513.8521, 562.9730, 589.7024, 680.8692, 764.7864, 881.3630, , 959.4360, 1038.3529, 1099.5497, 1146.6269, 1158.8844, 1191.1342, 1265.9866, 1318.5849, 1370.9634, 1396.6574, 1449.4686, 1809.0497, 3057.9653, 3129.6457, 3768.2098

Compound: sCI 2 + HCHO $TS_{ISO}2$	**Energy (kJ mol^{-1}):** -640.807843829511
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.158204 0.531709 -0.275737 1 -0.562091 0.254605 -1.249995 6 1.125250 -0.280012 -0.029274 9 0.857357 -1.595448 -0.127519 9 2.045912 0.026063 -0.954538 9 1.649418 -0.050709 1.179213 8 0.151353 1.885728 -0.204465 1 -0.525151 2.338407 0.308813 8 -1.086252 0.178143 0.746633 6 -2.303982 -0.305716 0.373145 1 -2.874678 -0.526092 1.281221 8 -2.688933 -0.459116 -0.745074	-339.0386, 21.8885, 66.0356, 174.9537, 209.7879, 258.4835, 271.7906, 375.9960, 408.9945, 504.7021, 546.2406, 581.1835, 686.3237, 766.7458, 880.0458, 961.8218, 1037.9249, 1108.4232, 1140.8063, 1167.3180, 1179.8049, 1245.5598, 1311.0747, 1381.8595, 1398.2379, 1447.5863, 1812.9194, 3061.1220, 3082.6758, 3827.1680

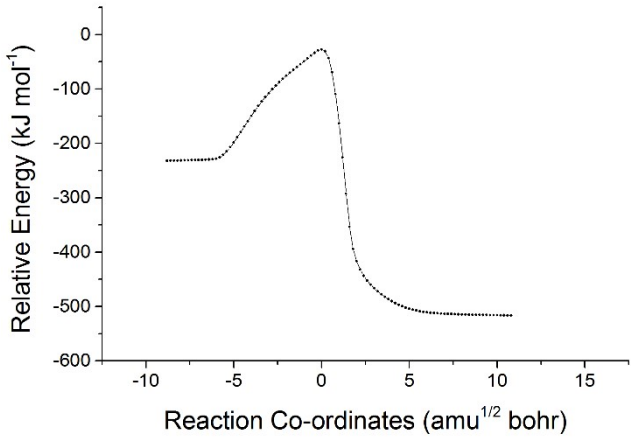
Compound: sCI 2 + HCHO HAE5	**Energy (kJ mol^{-1}):** -640.814946031998
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.210661 0.309903 -0.247637 1 -0.430875 0.333422 -1.316440 6 1.255880 -0.101420 -0.059852 9 1.476777 -1.299065 -0.627801 9 2.055084 0.793281 -0.660280 9 1.600789 -0.177441 1.228334 8 -0.407314 1.523418 0.368428 1 -1.252566 1.879199 0.066418 8 -0.991056 -0.750088 0.345904 6 -2.314706 -0.652497 0.145899 1 -2.822176 -1.505794 0.607070 8 -2.860544 0.239956 -0.445556	67.4596, 75.6599, 159.7185, 229.0168, 251.3286, 282.3992, 355.7306, 403.4892, 457.7356, 527.4247, 560.9981, 577.8060, 696.8742, 787.0476, 887.3511, 953.7355, 1043.7123, 1129.5545, 1144.6425, 1176.4830, 1194.2838, 1253.9800, 1297.3140, 1377.7165, 1392.9043, 1480.8655, 1775.7436, 3064.0576, 3066.2607, 3773.3065

Compound: sCI 2 + HCHO $TS_{ISO}3$	**Energy (kJ mol^{-1}):** -640.804184792221
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.073278 0.304727 -0.670768 1 0.145021 0.312637 -1.742577 6 1.228980 -0.082193 0.065831 9 1.719098 -1.237879 -0.414811 9 2.152502 0.869287 -0.121552 9 1.029377 -0.227967 1.382204 8 -0.506133 1.534381 -0.234289 1 -1.419321 1.457247 0.096643 8 -0.969506 -0.814841 -0.472175 6 -2.201526 -0.704448 0.034236 1 -2.648110 -1.702810 0.087808 8 -2.763291 0.304641 0.377683	-120.2227, 72.1141, 163.1147, 205.5213, 279.6381, 290.2422, 338.0677, 391.7004, 464.5542, 508.5861, 544.2558, 572.1653, 707.8013, 809.6028, 847.6336, 904.6825, 1041.7221, 1151.3840, 1158.4978, 1180.9676, 1190.4618, 1269.3497, 1350.4665, 1397.6865, 1413.3643, 1458.0097, 1760.0678, 3036.0700, 3060.7974, 3562.0744

Compound: sCI 2 + HCHO HAE6	**Energy (kJ mol^{-1}):** -640.810954254638
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.023422 0.519662 -0.759457 1 0.400592 0.711002 -1.742809 6 1.089680 -0.149560 0.081852 9 1.464574 -1.316150 -0.468800 9 2.162028 0.656306 0.113136 9 0.712418 -0.388332 1.346300 8 -0.451637 1.712395 -0.239187 8 -1.072358 -0.448844 -1.004296 6 -2.066917 -0.604329 -0.113028 1 -2.765359 -1.357094 -0.494272 8 -2.195222 -0.019867 0.928208 1 -0.928721 1.535550 0.587345	41.6872, 104.5853, 181.4384, 230.9965, 246.0566, 278.7974, 363.6505, 415.0763, 499.4583, 530.9290, 571.2800, 580.2686, 703.3542, 796.4718, 852.6964, 921.4691, 1041.5112, 1135.0504, 1154.7981, 1157.9586, 1177.1062, 1277.2267, 1350.7516, 1389.9819, 1406.1744, 1453.7478, 1778.4832, 3055.5168, 3113.8394, 3681.8234

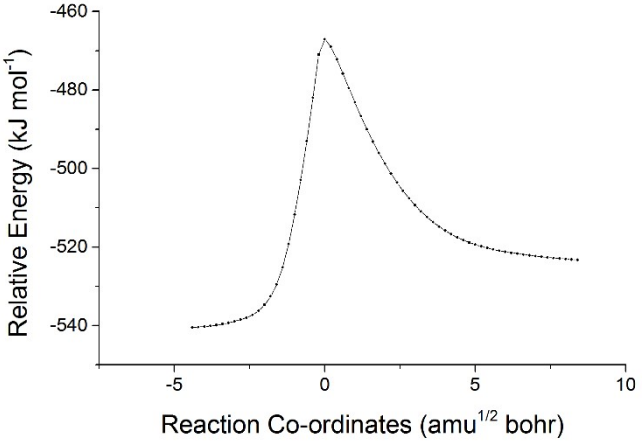
Compound: sCI 2 + HCHO TS_d3	**Energy (kJ mol^{-1}):** -640.616512703843
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.102613 0.190000 -0.770855 1 -0.221783 0.041157 -1.817708 6 -1.189442 -0.051158 0.089343 9 -0.942064 0.021767 1.393584 9 -2.103225 0.872153 -0.231028 9 -1.703562 -1.260393 -0.183258 8 0.671612 1.336675 -0.574015 8 1.026313 -0.941670 -0.577476 6 2.201564 -0.395027 -0.087848 1 3.079946 -1.035607 -0.266433 8 2.157626 0.272677 0.997020 1 2.348680 0.488346 -0.877614	-1048.6305, 61.4215, 108.2979, 187.4575, 233.9898, 294.4733, 349.9156, 393.7248, 454.9065, 519.6814, 543.1833, 575.9719, 711.6622, 736.8896, 814.5896, 855.4579, 938.4998, 990.7274, 1096.1528, 1126.2765, 1171.0636, 1177.9754, 1221.2983, 1244.8104, 1256.5281, 1292.2984, 1372.3378, 2085.0301, 2895.7780, 2964.750

IRC

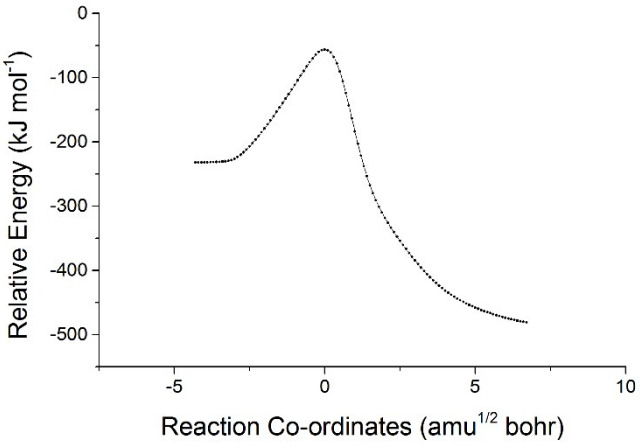


Compound: sCI 2 + HCHO HAE4	**Energy (kJ mol^{-1}):** -640.802893876772
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.003320 0.869526 -0.446611 1 -0.448004 1.351622 -1.313680 6 -0.990751 -0.244810 -0.023382 9 -0.907543 -0.608257 1.249326 9 -2.241268 0.226824 -0.231581 9 -0.836126 -1.331722 -0.797407 8 0.156092 1.730646 0.621894 1 0.442813 2.592697 0.303624 8 1.246046 0.388794 -0.977262 6 2.085126 -0.380418 -0.232513 1 2.989831 -0.555784 -0.827072 8 1.884565 -0.798931 0.864007	45.2715, 100.4461, 159.7963, 195.2888, 256.9147, 262.5438, 317.4227, 378.9325, 414.6407, 510.0905, 550.3725, 586.8127, 671.2922, 776.2965, 868.9183, 962.7327, 1037.1402, 1097.2875, 1122.7443, 1153.0702, 1173.1465, 1241.1347, 1311.4807, 1397.6599, 1415.5469, 1461.4654, 1825.1669, 3037.6121, 3078.2371, 3813.5831

Compound: sCI 2 + HCHO $TS_{ISO}4$	**Energy (kJ mol^{-1}):** -640.799602135995
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.008981 0.703216 -0.618432 1 0.454897 1.055477 -1.544508 6 1.044954 -0.226075 0.029517 9 1.450361 -1.148558 -0.855586 9 2.120492 0.537396 0.353339 9 0.648222 -0.849616 1.135229 8 -0.386453 1.757944 0.201981 1 0.360995 2.058173 0.730998 8 -1.152087 0.002061 -1.068513 6 -2.125534 -0.449922 -0.219502 1 -2.923603 -0.860758 -0.849254 8 -2.127285 -0.418657 0.968585	-205.8349, 29.6258, 111.6347, 163.0098, 198.8716, 233.8819, 261.6935, 365.4356, 414.8042, 501.7893, 544.4509, 579.2414, 686.6904, 777.6938, 869.5887, 961.1872, 1032.4184, 1105.0513, 1120.2350, 1153.8295, 1180.0968, 1249.2081, 1329.0742, 1390.0135, 1408.1359, 1439.4732, 1830.9429, 3032.2077, 3040.2313, 3805.9390

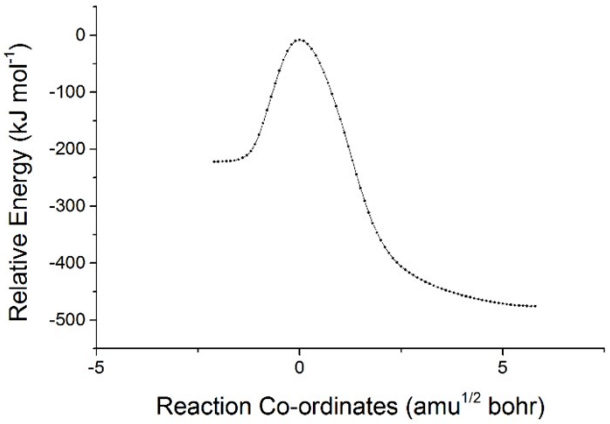
Compound: sCI 2 + HCHO $TS_{HAE}2$	**Energy (kJ mol^{-1}):** -640.777964091842
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.152459 0.080578 0.088526 6 -0.033283 -0.462620 -0.831746 1 -0.299276 -0.321810 -1.883881 8 0.573899 -1.523208 -0.483750 8 2.298411 -0.380018 0.678641 9 -1.608559 1.271322 -0.327484 9 -0.751636 0.201253 1.362196 9 -2.178307 -0.787312 0.053382 8 1.065071 0.900315 -0.699501 6 2.074660 0.682226 0.028917 1 2.814064 1.484922 0.095223 1 1.499183 -1.108300 0.318517	-968.8390, 66.1525, 81.9851, 177.5996, 246.6260, 280.8294, 330.3906, 389.7532, 484.2083, 522.6232, 557.7775, 587.2552, 662.2032, 745.8993, 846.9394, 864.7260, 1062.9738, 1129.9689, 1171.0954, 1194.3591, 1240.7771, 1274.2240, 1359.3244, 1379.3200, 1386.7151, 1574.1782, 1699.5035, 1801.5823, 3041.8683, 3078.8532
IRC  	

Compound: sCI 2 + HCHO $C_{FAc}1$	**Energy (kJ mol^{-1}):** -640.799644233095
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.829574 -0.075226 0.000000 6 0.291807 0.035526 -0.000003 8 -0.263422 1.100263 -0.000005 1 -0.249851 -0.921563 -0.000003 9 2.218400 -0.762929 -1.089059 9 2.432490 1.107775 -0.000003 9 2.218396 -0.762921 1.089067 1 -2.123558 1.071582 -0.000002 8 -3.099430 0.950319 0.000002 6 -3.378418 -0.349903 0.000002 1 -4.462694 -0.509946 0.000007 8 -2.567803 -1.243054 -0.000003	28.8611, 44.0666, 71.4606, 106.0397, 119.5735, 145.4401, 190.5235, 279.0593, 330.0197, 433.6041, 524.6309, 528.5168, 671.6616, 704.5942, 839.6375, 867.8719, 1012.6684, 1066.0493, 1162.4944, 1180.2903, 1189.8676, 1287.0851, 1365.2464, 1402.9839, 1421.8376, 1773.3347, 1819.2331, 3016.2653, 3046.6481, 3453.4462

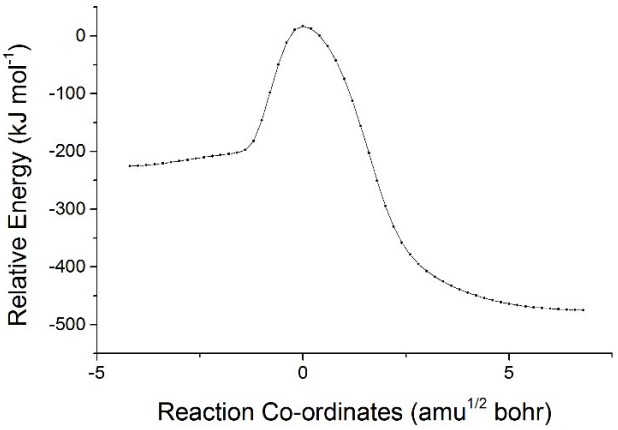
Compound: sCI 2 + HCHO $TS_{FAc}1$	**Energy (kJ mol^{-1}):** -640.612916191139
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.240405 -0.026036 0.011886 6 0.135836 0.407482 -0.547764 1 0.137618 0.408999 -1.642472 8 0.718010 1.333292 0.105212 8 2.531811 0.535366 -0.129761 9 -1.702755 -1.106895 -0.631309 9 -2.115923 0.974405 -0.195571 9 -1.203698 -0.285322 1.319510 8 0.991060 -1.056635 -0.286017 6 2.064870 -0.626086 0.301543 1 3.149347 -0.774754 -0.253715 1 2.225567 -0.902282 1.353046	-1193.8039, 72.1271, 92.5885, 172.7720, 246.7119, 259.0645, 304.4696, 372.7167, 439.4271, 457.7900, 523.2859, 566.3051, 662.7034, 705.8703, 756.4539, 845.5288, 868.5412, 1116.5453, 1148.5230, 1163.0003, 1187.5554, 1221.3952, 1249.2538, 1315.7469, 1334.6176, 1406.7356, 1461.4554, 2235.1404, 2988.7376, 3028.7966
IRC  	

Compound: sCI 2 + HCHO $C_{FAc}2$	**Energy (kJ mol^{-1}):** -640.788851617549
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.761049 -0.285003 0.062007 6 0.767135 0.875943 -0.175926 1 -0.257265 0.540397 -0.401807 8 1.105685 2.020870 -0.112233 9 1.319382 -1.051507 1.080043 9 2.990040 0.134105 0.349675 9 1.818020 -1.060276 -1.039329 8 -2.419881 -0.169238 -0.879313 6 -3.495306 -0.228361 -0.363768 8 -3.693042 0.103780 0.926100 1 -4.622004 -0.005565 1.165569 1 -4.407068 -0.554496 -0.887567	7.7036, 15.0143, 16.8036, 26.8905, 62.3992, 79.8049, 94.8453, 252.0524, 314.0173, 421.4039, 518.3137, 525.3090, 541.7266, 664.0237, 700.2285, 829.9758, 995.0095, 1037.5429, 1118.4110, 1152.2179, 1173.2951, 1271.6813, 1282.9539, 1414.6775, 1423.2612, 1831.9042, 1845.8547, 2982.1286, 2998.3238, 3779.6741

Compound: sCI 2 + HCHO $TS_{FAc}2$	**Energy (kJ mol^{-1}):** -640.615657587046
Reaction Coordinates: 6 1.147981 -0.047437 0.071635 6 -0.076256 0.257681 -0.819982 1 0.131984 -0.008703 -1.863370 8 -0.731916 1.334815 -0.635515 8 -1.928481 0.546508 0.772565 9 1.667176 -1.252307 -0.222732 9 0.876371 -0.014318 1.378858 9 2.094288 0.876690 -0.181581 8 -1.080636 -1.067320 -0.500936 6 -2.141677 -0.496699 -0.009589 1 -2.458690 -0.736594 1.153285 1 -3.065839 -0.538569 -0.602108	**Frequencies (cm^{-1}):** -1223.3404, 55.2869, 120.1231, 182.4610, 242.8627, 279.4588, 308.6175, 372.9038, 441.0465, 453.2497, 518.5714, 571.7535, 649.2592, 714.2083, 781.7622, 841.9288, 847.1269, 1080.7267, 1144.2891, 1156.3786, 1162.0579, 1222.3706, 1266.8167, 1291.5830, 1322.0916, 1407.5412, 1473.0139, 2243.0956, 2991.9693, 3009.3838
IRC 	

Compound: sCI 2 + HCHO $TS_{ester}1$	**Energy (kJ mol^{-1}):** -640.591726379101
Reaction Coordinates: 6 1.366331 -0.026686 0.061260 6 -0.368759 0.156879 -0.654823 1 -0.095006 0.135080 -1.722017 8 -0.528243 -0.990651 -0.039830 8 -2.562658 -0.772364 -0.186019 9 1.910254 1.083396 -0.410810 9 1.342257 -0.001711 1.364600 9 2.005600 -1.065334 -0.417362 6 -2.540376 0.329368 0.410312 8 -0.975599 1.192560 -0.211818 1 -2.239606 0.402513 1.457551 1 -3.199567 1.121523 0.037456	**Frequencies (cm^{-1}):** -560.5388, 50.0694, 60.3894, 102.9234, 178.5244, 242.8272, 256.1040, 306.1896, 352.1444, 491.3535, 533.1564, 542.4147, 573.0182, 711.7424, 738.2562, 847.6028, 946.0872, 1055.5919, 1141.1780, 1188.2539, 1222.2839, 1262.1485, 1301.4676, 1344.3947, 1391.0679, 1441.0526, 1534.6863, 2949.1530, 2992.2289, 3074.1389
IRC  	

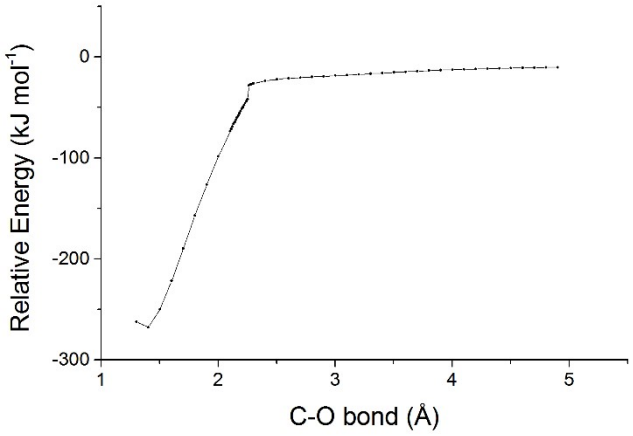
Compound: sCI 2 + HCHO $C_{ester}1$	**Energy (kJ mol^{-1}):** -640.785087532247
Reaction Coordinates: 6 1.791858 0.065785 -0.000001 8 0.650662 0.840112 -0.000017 6 -0.593997 0.236702 -0.000007 1 -1.352802 1.022550 -0.000021 8 -0.791968 -0.935019 0.000015 9 1.871240 -0.706996 -1.084234 9 2.825281 0.904836 -0.000020 9 1.871241 -0.706947 1.084267 6 -4.178424 -0.338090 -0.000012 8 -3.745980 0.785560 0.000010 1 -3.510320 -1.215360 -0.000071 1 -5.265067 -0.536821 0.000027	**Frequencies (cm^{-1}):** 17.6764, 39.3605, 53.9006, 79.8186, 93.9123, 111.7895, 112.6025, 188.4592, 231.1980, 373.5513, 441.8426, 547.8735, 581.2838, 619.1427, 818.3698, 840.7698, 1056.6360, 1094.8676, 1160.5880, 1205.7308, 1212.1275, 1237.8546, 1270.3234, 1396.9949, 1529.3276, 1796.6426, 1829.5309, 2903.8149, 2979.3096, 3101.5598

Compound: sCI 2 + HCHO $TS_{ester}2$	**Energy (kJ mol^{-1}):** -640.587782961932
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.378359 0.010001 0.025154 6 -0.332347 -0.141342 -0.462417 1 -0.200721 -0.278102 -1.556026 8 -0.824975 -1.139154 0.189235 8 -2.605340 0.761834 0.178537 9 1.471795 0.194651 1.310528 9 1.966170 0.961699 -0.661715 9 1.884549 -1.158456 -0.319820 6 -2.709063 -0.441339 -0.112929 8 -0.558469 1.084594 -0.065633 1 -3.097189 -1.143606 0.633883 1 -2.716139 -0.781448 -1.154760	-462.6014, 72.7718, 82.3414, 102.8373, 171.3199, 249.8559, 274.1585, 312.0720, 324.4221, 443.0121, 521.3093, 547.7848, 576.1725, 709.5628, 721.9533, 744.0114, 933.7447, 1091.5664, 1150.9995, 1197.9039, 1221.0053, 1231.3293, 1303.8615, 1330.7661, 1377.2627, 1441.3485, 1573.5282, 2855.4590, 2970.3282, 3047.9176
IRC	
	

Compound: CF_3COOH conformer 2	**Energy (kJ mol^{-1}):** -526.391647939292
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.581404 -0.010401 -0.000000 6 0.970727 -0.156509 -0.000004 8 1.477110 -1.232961 0.000000 8 1.654341 0.993148 -0.000001 1 1.057725 1.754791 -0.000017 9 -1.102989 -0.583142 -1.084628 9 -1.102975 -0.583095 1.084656 9 -0.954622 1.295701 -0.000023	21.6602, 251.5689, 256.7023, 383.9419, 424.0892, 504.2317, 558.0545, 581.8488, 686.6362, 774.0185, 789.5230, 1111.2671, 1173.1962, 1190.7699, 1238.1250, 1367.2329, ,1882.0972, 3753.0385

Compound: CF_3CHO	**Energy (kJ mol^{-1}):** -451.199957828211
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.015009 0.360282 0.000000 6 0.501814 -1.106406 -0.000000 8 -0.245475 -2.035870 -0.000000 1 1.601864 -1.198064 -0.000000 9 0.501814 0.987869 1.088491 9 0.501814 0.987869 -1.088491 9 -1.307962 0.464459 0.000000	73.5798, 250.7650, 307.2813, 422.6928, 518.9491, 524.0490, 701.8523, 834.5377, 974.2730, 1150.4161, 1174.8562, 1288.1325, 1403.3576, 1849.8517, 2955.8187

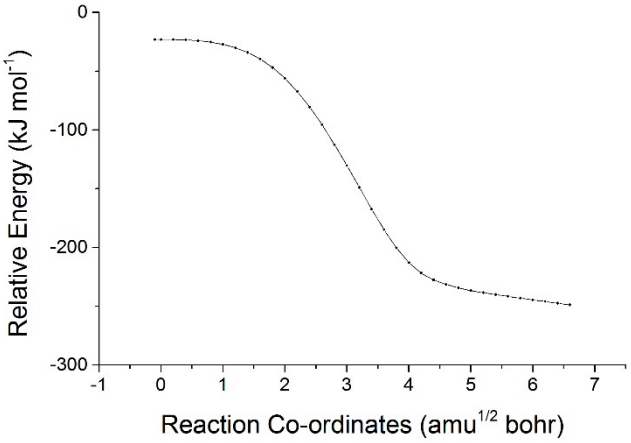
Compound: CF_3OCHO	**Energy (kJ mol^{-1}):** -526.392169685219
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.663849 -0.000032 0.000000 8 0.336896 0.952890 -0.000000 6 1.661196 0.558397 0.000000 8 2.058027 -0.558385 0.000000 1 2.265245 1.470480 0.000000 9 -0.613300 -0.773286 1.084140 9 -0.613300 -0.773286 -1.084140 9 -1.818813 0.660272 0.000000	88.2784, 182.4643, 213.8832, 372.9073, 440.5306, 548.4446, 580.4343, 618.6761, 819.4841, 841.6604, 1029.7431, ,1099.7328, 1158.7538, 1210.5947, 1240.5018, 1402.5579, 1846.9478, 3073.3668

Compound: sCI 4 + HCHO TS_c reaction profile
IRC 

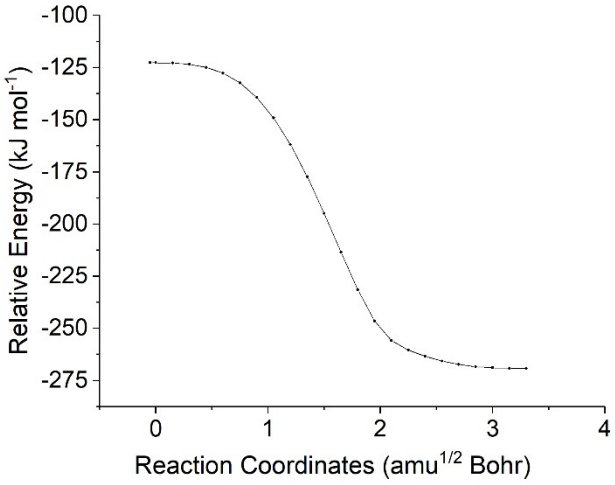
Compound: sCI 4 + HCHO HOZ 1	**Energy (kJ mol^{-1}):** -739.880971561098
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.203229 -0.230964 0.058463 6 0.191425 0.440783 -0.055823 9 -0.018442 1.768072 -0.284796 8 0.923264 -0.051022 -1.159256 8 2.011888 -0.814233 -0.568390 9 -1.873473 0.255806 1.109021 9 -1.065362 -1.550484 0.213301 9 -1.918007 -0.002321 -1.047544 8 0.930952 0.217053 1.072410 6 2.246328 -0.074884 0.601161 1 2.755836 -0.715948 1.315224 1 2.785743 0.852302 0.394021	62.9168, 82.3412, 181.5539, 225.3051, 306.3116, 333.8341, 372.3751, 383.1249, 472.7730, 537.6227, 578.2342, 616.4528, 733.4968, 748.0603, 840.5352, 900.2599, 961.3323, 1051.7447, 1075.2302, 1084.3749, 1160.0607, 1174.0468, 1194.6284, 1204.5660, 1240.5871, 1353.3296, 1400.3061, 1519.3524, 3039.2896, 3147.1681

Compound: sCI 5 + HCHO PRC	**Energy (kJ mol^{-1}):** -739.777926184174
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.414853 0.141074 -0.112497 6 -0.050978 -0.450704 0.236511 9 0.273257 -0.457980 1.482950 8 0.616211 -1.031007 -0.636363 8 1.855522 -1.524854 -0.274925 9 -1.545297 1.342529 0.441524 9 -2.373565 -0.660000 0.384471 9 -1.564546 0.229935 -1.426569	34.8048, 60.5055, 70.4194, 101.2900, 143.9768, 186.7900, 200.3901, 237.6640, 298.5269, 339.1001, 362.6188, 384.0722, 406.9206, 514.5633, 577.3863, 663.2692, 730.6738, 857.5480, 900.9980, 1138.3690, 1178.3830, 1181.7442, 1238.6573, 1260.7686,

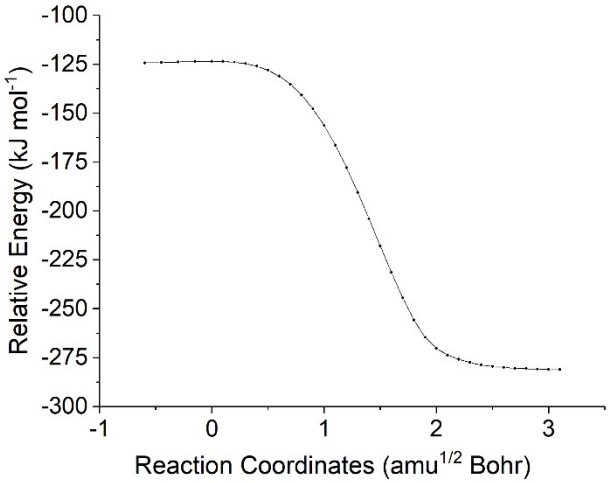
6 2.716861 0.890240 -0.070701 8 1.640783 1.447690 -0.108533 1 3.315311 0.728201 -0.979729 1 3.169732 0.563154 0.877031	1402.6054, 1526.8058, 1612.0198, 1752.6652, 2940.4081, 3008.9838

Compound: sCI 5 + HCHO TS_c	**Energy (kJ mol^{-1}):** -739.778430516598
Reaction Coordinates: 6 -1.380202 0.101938 -0.105985 6 0.026431 -0.396275 0.231970 9 0.339614 -0.408275 1.484467 8 0.674169 -1.022580 -0.631521 8 1.973753 -1.364286 -0.283260 9 -1.617791 1.251789 0.515572 9 -2.273681 -0.806175 0.325723 9 -1.521302 0.255771 -1.414694 6 2.529514 0.925062 -0.042405 8 1.408494 1.394738 -0.179406 1 3.221657 0.854342 -0.891297 1 2.931003 0.660345 0.943705	**Frequencies (cm^{-1}):** -118.4252, 38.2811, 89.8377, 110.0542, 181.1767, 201.7179, 229.7311, 297.2903, 325.3079, 373.7338, 408.0919, 414.9295, 476.0417, 518.7753, 577.7736, 650.4742, 730.7338, 849.8975, 909.3393, 1133.4831, 1156.2947, 1183.8163, 1241.0371, 1252.0155, 1396.4643, 1511.2865, 1586.8143, 1697.9348, 2967.7444, 3042.2769
IRC  	

Compound: sCI 1 + CF_3CFO PRC 3	**Energy (kJ mol^{-1}):** -739.813259682201
Reaction Coordinates: 6 1.276276 -0.317441 0.042768 6 0.199237 0.765686 0.278781 9 0.332320 1.754487 -0.609756 8 -0.466774 0.863601 1.257424 9 1.452943 -0.610239 -1.240654 9 2.442962 0.159259 0.528183 9 0.975427 -1.429876 0.713343 6 -2.711550 -0.451865 0.655072 1 -2.030034 -1.117147 1.167434 1 -3.638928 -0.080588 1.070988 8 -2.468023 -0.081048 -0.512669 8 -1.283662 -0.487955 -1.072029	**Frequencies (cm^{-1}):** 42.13, 63.96, 88.06, 113.40, 161.90, 192.84, 220.11, 240.50, 279.50, 379.83, 428.50, 513.34, 528.59, 586.64, 680.60, 693.20, 716.22, 802.10, 885.19, 1024.72, 1084.45, 1147.22, 1223.53, 1243.79, 1311.45, 1417.81, 1571.35, 1851.85, 3127.16, 3272.45

Compound: sCI 1 + HCHO TS_c 3	**Energy (kJ mol^{-1}):** -739.811613027458
Reaction Coordinates: 6 1.245988 -0.265523 -0.092261 6 0.041332 0.700989 -0.145855 9 0.189726 1.675069 0.774721 8 -0.632687 0.863682 -1.129472 9 0.969226 -1.399460 -0.736156 9 2.281569 0.329362 -0.721769 9 1.631765 -0.547889 1.150351 6 -2.741525 0.035486 -0.376479 1 -2.703817 1.033485 0.033747 1 -3.404323 -0.266334 -1.177649 8 -2.081522 -0.894047 0.143083 8 -1.137941 -0.482961 1.064781	**Frequencies (cm^{-1}):** -109.92, 56.94, 80.14, 142.31, 211.44, 220.36, 269.82, 308.99, 347.33, 383.64, 438.27, 518.42, 539.95, 587.75, 681.43, 700.45, 719.16, 802.82, 898.27, 1048.01, 1067.15, 1146.40, 1218.82, 1236.65, 1296.61, 1415.35, 1570.32, 1749.53, 3135.01, 3279.84
IRC  	

Compound: sCI 1 + CF_3CFO PRC 4	**Energy (kJ mol^{-1}):** -739.812611750193
Reaction Coordinates: 6 1.260836 -0.292596 -0.100143 6 0.149504 0.780864 -0.149444 9 0.297955 1.652770 0.857863 8 -0.528324 1.011186 -1.101148 9 0.919770 -1.358554 -0.820669 9 2.367461 0.250369 -0.655394 9 1.568501 -0.670948 1.136250 6 -2.843813 0.077420 -0.381769 1 -2.757537 1.070839 0.035688 1 -3.523078 -0.196672 -1.178448 8 -2.165570 -0.862809 0.084248 8 -1.243822 -0.539755 1.050455	**Frequencies (cm^{-1}):** 47.51, 65.26, 85.39, 118.69, 174.40, 200.92, 245.37, 260.90, 295.89, 379.05, 431.01, 513.18, 531.84, 586.90, 683.81, 689.53, 708.55, 800.11, 888.72, 1029.39, 1075.49, 1142.75, 1227.75, 1241.45, 1305.29, 1418.19, 1572.94, 1830.56, 3129.42, 3274.44

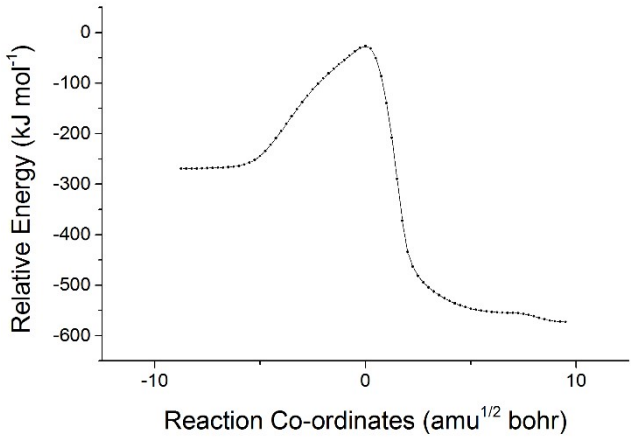
Compound: sCI 5 + HCHO TS_c 4	**Energy (kJ mol^{-1}):** -739.810121917775
Reaction Coordinates: 6 -1.248348 -0.270044 0.006638 6 -0.008169 0.583650 -0.339239 9 -0.144618 1.819566 0.181718 8 0.652411 0.405323 -1.339539 9 -1.571793 -0.215886 1.298125 9 -2.295289 0.186594 -0.706355 9 -1.043079 -1.547385 -0.334192 6 2.510833 -0.639402 -0.503616 1 1.860205 -1.459838 -0.765152 1 3.419149 -0.395132 -1.040673 8 2.340293 0.000196 0.562465 8 1.093266 -0.202550 1.135756	**Frequencies (cm^{-1}):** -183.41, 56.54, 69.23, 156.11, 217.15, 232.18, 267.46, 317.85, 359.89, 391.03, 438.72, 523.41, 544.08, 588.04, 680.37, 717.37, 735.62, 813.89, 897.93, 1063.92, 1073.84, 1155.76, 1205.38, 1234.21, 1299.76, 1411.54, 1567.26, 1700.60, 3135.05, 3279.77
IRC  	

Compound: sCI 4 + HCHO HOZ 2	**Energy (kJ mol^{-1}):** -739.882612577417
Reaction Coordinates: 6 1.226910 -0.202398 -0.060082 6 -0.201622 0.381734 0.127609 9 -0.062041 1.673083 0.536046 8 -0.874081 0.296507 -1.089563 8 -2.266214 0.162553 -0.664667 9 1.914395 -0.099267 1.079534 9 1.884341 0.455130 -1.019776 9 1.155217 -1.494768 -0.399219 6 -2.112229 -0.756332 0.387029 8 -0.929811 -0.323497 1.059019 1 -1.972248 -1.775555 0.020385 1 -2.972454 -0.654571 1.044696	**Frequencies (cm^{-1}):** 64.4536, 102.3338, 183.0668, 231.2002, 294.0750, 331.7999, 368.8521, 380.9341, 498.1395, 541.8807, 578.3703, 614.4270, 736.4144, 747.4253, 853.1992, 888.9747, 962.5108, 1062.4176, 1072.9408, 1103.2970, 1140.8250, 1158.2995, 1199.1282, 1201.9356, 1230.5616, 1346.8978, 1405.6107, 1520.8092, 3040.2533, 3134.6001

Compound: sCI 4 + HCHO TS_{HOZ}	**Energy (kJ mol^{-1}):** -739.875860313659
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.265369 -0.175561 0.037602 6 -0.208538 0.310764 -0.045038 9 -0.184141 1.676299 -0.198393 8 -0.829394 -0.290458 -1.120223 8 -2.230537 -0.415601 -0.725606 9 1.884369 0.424204 1.057845 9 1.910458 0.124204 -1.093056 9 1.313647 -1.495448 0.223619 8 -0.898614 -0.037440 1.082003 6 -2.251377 -0.184335 0.692050 1 -2.668140 -1.050180 1.204313 1 -2.815225 0.729644 0.888491	-189.6719, 62.0184, 109.2801, 182.8716, 230.0115, 331.1898, 348.7338, 374.9499, 499.8881, 542.7314, 582.2789, 610.0967, 746.4942, 754.1945, 869.7451, 901.9045, 968.8900, 1048.1702, 1086.4867, 1121.6619, 1139.7391, 1146.8914, 1196.4040, 1206.6516, 1208.5915, 1362.0792, 1415.8068, 1546.9949, 3037.1675, 3106.9218

Compound: sCI 4 + HCHO TS_d	**Energy (kJ mol^{-1}):** -739.782964789564
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.132888 -0.348496 0.049909 6 0.088137 0.601384 -0.200781 9 -0.351809 1.880118 0.009060 8 0.692141 0.446831 -1.329195 8 2.166824 -1.086986 -0.341132 9 -1.665464 -0.132582 1.258465 9 -2.068538 -0.112927 -0.873457 9 -0.765110 -1.629932 -0.029165 8 1.040273 0.404491 0.955358 6 2.194450 -0.076899 0.433864 1 3.083877 0.021690 1.088126 1 2.482319 0.765599 -0.350458	-1092.6757, 10.7391, 58.7066, 102.7274, 208.6094, 221.0911, 289.6020, 325.9773, 353.6172, 364.6832, 462.4753, 511.2091, 536.9760, 584.6930, 630.5246, 690.8930, 747.1988, 814.9985, 891.8665, 954.1079, 1052.8209, 1130.4231, 1189.0187, 1191.1713, 1196.9907, 1221.1659, 1306.7988, 1394.4501, 2143.4453, 2907.5597

IRC



Compound: sCI 4 + HCHO HAE Con 1	**Energy (kJ mol^{-1}):** -739.996820249036
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.027344 0.687582 0.061851 9 0.541121 1.825651 -0.379093 6 1.069431 -0.424089 -0.008015 9 1.545648 -0.560058 -1.249390 9 0.546169 -1.601185 0.374737 9 2.079687 -0.122821 0.807936 8 -0.492323 0.894840 1.311132 1 -1.196959 0.244012 1.495796 8 -1.029442 0.369800 -0.917077 6 -2.150050 -0.303772 -0.587385 1 -2.754555 -0.439892 -1.488583 8 -2.455027 -0.694230 0.506741	57.1808, 70.9230, 175.4045, 217.9644, 261.4777, 273.1843, 344.6606, 348.2922, 389.4253, 465.3067, 496.8327, 576.1035, 582.0878, 591.6309, 692.0873, 767.3125, 831.8341, 957.2695, 1041.7683, 1089.3072, 1164.7213, 1187.9694, 1210.3953, 1227.3088, 1340.8463, 1404.0025, 1408.7922, 1775.9420, 3078.0550, 3558.3955

Compound: sCI 4 + HCHO TS_{ISO}	**Energy (kJ mol^{-1}):** -739.995345880234
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.180838 -0.342869 -0.047973 6 0.073704 0.584064 0.009736 9 -0.311472 1.726564 0.635169 8 0.533091 0.864102 -1.223076 8 2.708270 -0.408426 -0.546306 9 -0.834243 -1.531697 -0.567266 9 -2.119928 0.203241 -0.820694 9 -1.692200 -0.548962 1.169557 8 0.994616 -0.042609 0.911524 6 2.210140 -0.487251 0.545545 1 2.693131 -0.941839 1.415039 1 1.421598 0.471337 -1.346912	-65.3287, 65.3295, 166.1356, 213.5199, 249.6288, 294.2800, 334.9333, 360.6191, 367.4474, 473.8145, 495.1819, 570.1397, 578.3899, 600.4688, 687.7175, 766.2511, 829.2022, 951.9805, 1042.0443, 1086.6002, 1174.1938, 1187.2994, 1210.9436, 1233.8137, 1329.3611, 1409.5539, 1441.6080, 1769.3460, 3080.5580, 3478.084

Compound: sCI 4 + HCHO HAE Con 2	**Energy (kJ mol^{-1}):** -740.000308948885
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.321852 -0.149789 -0.076490 6 -0.155453 0.309802 0.082835 9 -0.271021 0.919507 1.304423 8 -0.467139 1.141710 -0.926994 8 -2.894484 0.204685 -0.202411 9 1.670431 -0.952740 0.933231 9 2.129042 0.912548 -0.076403 9 1.484130 -0.813728 -1.225184 8 -0.932051 -0.884704 0.150989 6 -2.272728 -0.797419 0.017660 1 -2.706482 -1.794969 0.133869 1 -1.419383 1.335588 -0.875184	62.9145, 78.9746, 159.2883, 218.4675, 240.9289, 261.5800, 319.6150, 363.1625, 387.2717, 494.0228, 520.8418, 570.2369, 584.1607, 606.8505, 657.1655, 769.9403, 843.4823, 972.8608, 1041.0624, 1049.4737, 1157.4872, 1199.4818, 1205.8249, 1227.3689, 1264.5355, 1400.2948, 1476.3678, 1784.9247, 3074.5473, 3642.2040

Compound: sCI 4 + HCHO $TS_{HAE}1$	**Energy (kJ mol^{-1}):** -739.973401978791
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.270961 0.225027 -0.120025 6 0.067462 -0.548936 0.046984 9 -0.045608 -1.375286 1.118974 8 0.616065 -1.007043 -0.985121 8 2.721721 -0.011133 -0.566773 9 -1.706195 0.736593 1.034153 9 -2.198727 -0.617761 -0.589049 9 -1.119164 1.223240 -0.997924 8 1.021045 0.649180 0.745659 6 2.215773 0.724389 0.322488 1 2.840018 1.495011 0.779358 1 1.842939 -0.646990 -0.921553	-949.5685, 39.2733, 64.5013, 169.6876, 218.9110, 259.7737, 315.1775, 356.2053, 360.5612, 421.2820, 485.2187, 541.0347, 583.6573, 625.6704, 695.3956, 773.3250, 878.5740, 885.8521, 1061.8765, 1064.7041, 1178.3447, 1184.4422, 1203.2622, 1306.9569, 1376.1017, 1392.3137, 1618.0324, 1702.9903, 1832.9846, 3099.3367

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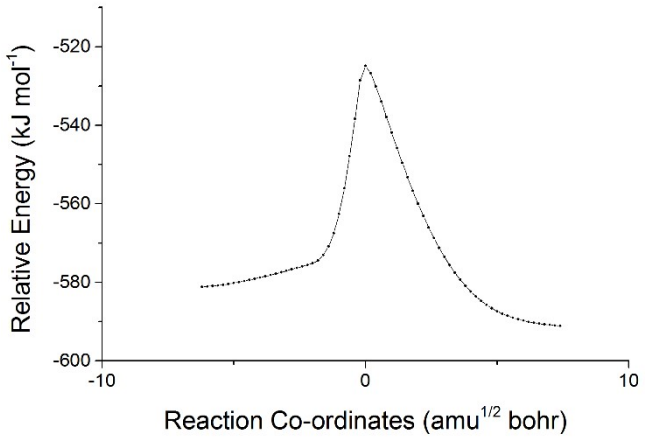

Compound: sCI 4 + HCHO $C_{FAc}3$	**Energy (kJ mol^{-1}):** -739.998047248532
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.303574 -0.423757 -0.134810 6 -0.542531 0.923451 -0.061129 9 -0.880671 1.585261 1.039484 8 0.177014 1.361022 -0.887458 9 -1.346035 -1.037976 1.041452 9 -0.738419 -1.221730 -1.034678 9 -2.564929 -0.160186 -0.526656 8 1.707875 -0.538008 0.986448 6 2.746001 -0.483644 0.380256 8 2.938640 0.151744 -0.778891 1 2.105506 0.574602 -1.052806 1 3.677370 -0.957283 0.709707	19.1597, 41.5247, 46.2241, 60.3739, 103.4226, 115.2644, 137.3165, 232.0005, 242.2931, 378.9404, 421.5547, 511.4081, 586.5512, 650.9862, 693.5929, 730.3301, 759.1088, 805.5547, 1060.7112, 1102.4056, 1154.7082, 1162.0222, 1234.4325, 1313.3144, 1332.7441, 1412.3901, 1787.5158, 1911.7446, 3053.1846, 3652.1981

Compound: sCI 4 + HCHO $TS_{FAc}1$	**Energy (kJ mol^{-1}):** -739.806907643778
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.249403 -0.207960 -0.071445 6 -0.136173 0.515847 -0.043915 9 -0.036599 1.614349 0.743981 8 -0.722589 0.624809 -1.149411 8 -2.550474 0.172171 -0.451244 9 1.736422 -0.392010 1.156046 9 2.116045 0.545375 -0.758823 9 1.144722 -1.394462 -0.677279 8 -0.973738 -0.526973 0.935336 6 -2.022844 -0.827505 0.223626 1 -3.122417 -0.555871 0.681826 1 -2.090814 -1.845743 -0.184181	-1180.7629, 71.5676, 94.3298, 177.0207, 221.5961, 286.7658, 296.2595, 310.7880, 364.2419, 418.3103, 467.9715, 471.7714, 541.7660, 587.4465, 665.9389, 704.6313, 756.7313, 833.3443, 888.0859, 1062.5610, 1150.5311, 1182.8067, 1202.5667, 1226.2364, 1259.7834, 1305.1679, 1394.7117, 1473.7019, 2271.2614, 2992.2183
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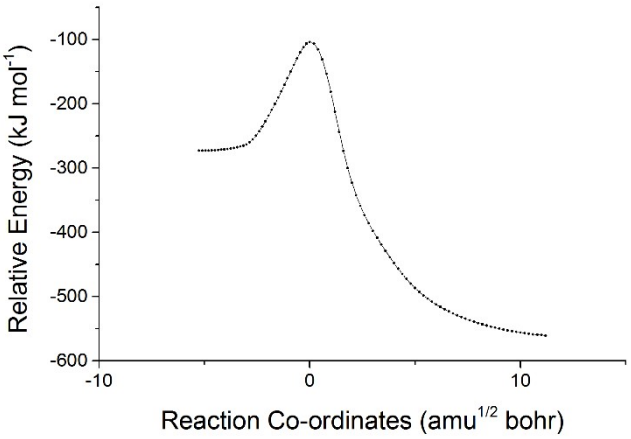
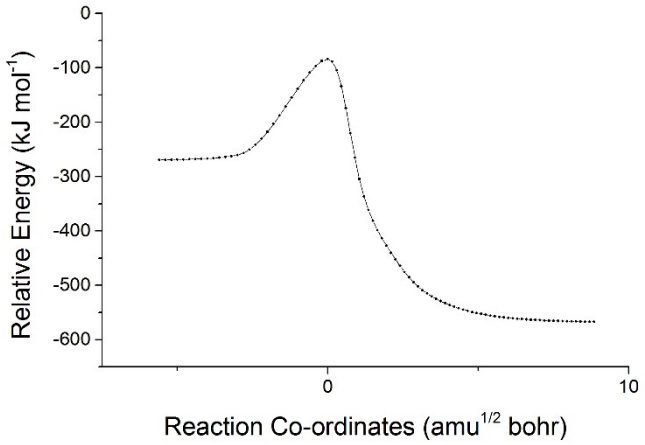


Compound: sCI 4 + HCHO $C_{FAc}1$	**Energy (kJ mol^{-1}):** -739.988628614865
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.483755 -0.338849 -0.052076 6 -0.609282 0.901099 0.255281 9 -0.273207 1.517624 -0.882979 8 -0.344831 1.310813 1.324133 9 -1.077788 -0.992867 -1.137908 9 -2.745012 0.090180 -0.267307 9 -1.493370 -1.169297 0.984494 8 1.652661 -0.858738 0.114745 6 2.838184 -0.717960 0.124003 8 3.429826 0.431611 -0.250386 1 4.389305 0.358859 -0.171998 1 3.542958 -1.504848 0.434112	12.2529, 20.2627, 35.6667, 44.4359, 61.7051, 76.2215, 106.1653, 231.3434, 242.0643, 378.2535, 420.8184, 511.7076, 538.9062, 585.0890, 663.4870, 689.6856, 755.8780, 800.1773, 1037.2738, 1083.9196, 1119.7911, 1149.5036, 1229.3486, 1271.2585, 1311.0063, 1415.9550, 1846.2374, 1934.9597, 2981.0252, 3779.8872

Compound: sCI 2 + HCHO $TS_{FAc}2$	**Energy (kJ mol^{-1}):** -739.799988971889
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.263159 -0.231854 0.043601 6 0.102664 0.427301 -0.293785 9 0.021464 1.768105 -0.050184 8 0.710354 0.068060 -1.326239 8 2.392624 -0.674104 -0.554776 9 -1.708869 0.127474 1.248179 9 -1.156407 -1.558841 -0.000709 9 -2.163586 0.156430 -0.871899 8 1.020614 -0.082642 1.079098 6 2.216518 -0.013896 0.573236 1 2.952503 -0.932840 0.826383 1 2.789200 0.914505 0.722162	-1104.2800, 62.1223, 68.0935, 171.2913, 216.9350, 272.6382, 279.8117, 307.6771, 350.9695, 387.9892, 427.3649, 484.5099, 540.8308, 585.7682, 660.9810, 703.0031, 750.5784, 812.8046, 884.6414, 1047.5704, 1160.2951, 1176.9495, 1212.6657, 1233.5197, 1260.8937, 1309.0540, 1400.2571, 1491.3314, 2343.7280, 2968.5175
IRC  	

Compound: sCI 4 + HCHO $C_{FAc}2$	**Energy (kJ mol^{-1}):** -739.988569845236
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.210441 -0.586106 -0.060428 6 0.951717 0.878761 0.367628 9 1.170879 1.701187 -0.662919 8 0.687562 1.243968 1.452601 9 0.766535 -0.844231 -1.288894 9 0.643623 -1.427640 0.797277 9 2.543536 -0.792621 -0.043619 8 -3.160120 -0.849352 0.341988 6 -2.883208 0.325688 -0.253731 8 -1.765750 0.680545 -0.478184 1 -3.774505 0.918577 -0.511101 1 -4.113886 -0.960173 0.442444	9.2098, 19.1505, 33.4684, 43.5209, 59.6264, 74.8819, 104.5050, 231.1540, 242.2426, 378.5483, 420.8136, 511.9706, 538.9994, 585.0978, 662.8509, 689.9521, 757.8900, 800.6257, 1037.2046, 1085.4595, 1119.5570, 1150.2551, 1227.3961, 1271.4277, 1311.4866, 1416.1844, 1846.9631, 1934.9215, 2980.6069, 3779.7123

Compound: sCI 4 + HCHO $TS_{ester}1$	**Energy (kJ mol^{-1}):** -739.781535601567
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.422805 -0.213581 0.086132 6 0.359595 0.380720 -0.081407 9 0.191519 1.620006 -0.668748 8 0.538537 -0.583618 -0.907970 8 2.469527 -0.856868 -0.466226 9 -1.926600 0.722605 0.853416 9 -1.399451 -1.367685 0.681583 9 -2.034024 -0.242012 -1.065347 8 0.871900 0.395574 1.076719 6 2.664197 0.007717 0.427705 1 3.007473 -0.336057 1.408659 1 2.863899 1.049987 0.168430	-588.2564, 60.7916, 99.0798, 108.1427, 164.7614, 193.2517, 230.6891, 255.7045, 306.6388, 317.2887, 487.2591, 534.9642, 554.2207, 567.5308, 621.5868, 676.4830, 756.5990, 807.2190, 898.5517, 976.0160, 1150.8830, 1197.0207, 1251.1035, 1261.5896, 1330.9552, 1395.3279, 1473.9622, 1554.1570, 2995.2314, 3082.5091

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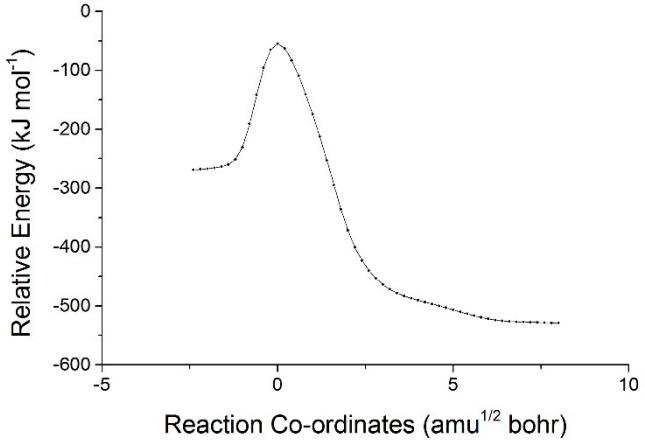

Compound: sCI 4 + HCHO $C_{ester}1$	**Energy (kJ mol^{-1}):** -739.977318615772
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.438091 -0.328538 -0.053297 9 -2.123748 0.239571 0.936736 9 -2.280767 -0.693219 -1.009719 9 -0.817177 -1.406218 0.414875 8 -0.556511 0.567248 -0.640931 6 0.433924 1.093616 0.117396 9 1.086785 1.935488 -0.663881 8 0.673618 0.909472 1.257292 8 2.281535 -0.867481 -0.682601 6 2.928435 -1.225038 0.266485 1 3.752697 -1.952181 0.162579 1 2.726723 -0.842568 1.281745	31.7264, 43.5110, 60.0890, 78.1354, 102.3299, 117.0928, 149.9059, 165.4967, 179.4153, 378.1240, 403.6030, 427.4693, 550.9837, 609.0345, 669.9364, 737.6815, 757.5186, 879.5778, 1023.6817, 1149.5186, 1207.6212, 1215.8080, 1240.9116, 1267.7803, 1278.8360, 1527.3657, 1803.0161, 1911.4485, 2906.0910, 2974.0356

Compound: sCI 4 + HCHO $TS_{ester}2$	**Energy (kJ mol^{-1}):** -739.786202678286
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.396175 -0.267274 0.002936 6 -0.388780 0.495260 0.047108 9 -0.090167 1.814698 -0.114078 8 -0.540319 -0.195561 -1.022155 8 -2.553430 -0.185580 -0.752387 9 1.934085 0.381624 1.010036 9 1.284892 -1.539686 0.259211 9 2.044179 -0.022649 -1.101464 6 -2.469377 -0.623178 0.426331 8 -0.970239 0.192826 1.133098 1 -2.121480 -1.639456 0.624488 1 -3.151636 -0.188761 1.165464	-594.8467, 54.8487, 91.2012, 121.2305, 171.7936, 201.1541, 241.4115, 246.9698, 297.8808, 328.8755, 519.5294, 529.9244, 550.6988, 593.3187, 627.0561, 672.7171, 743.0208, 879.0350, 937.2457, 970.3107, 1143.5766, 1189.1849, 1256.0499, 1280.3139, 1328.2734, 1378.7216, 1490.3402, 1533.3773, 2992.9535, 3075.6329
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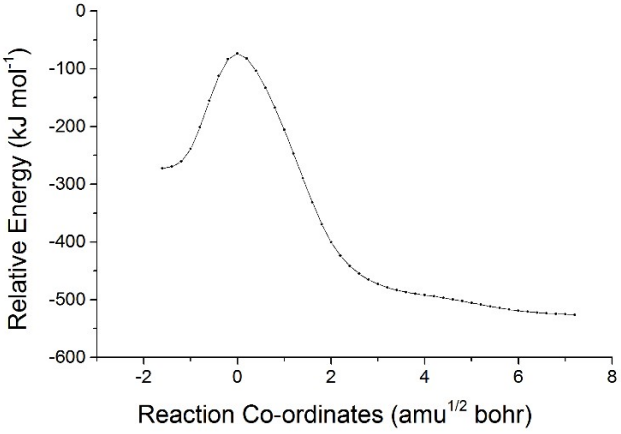
	

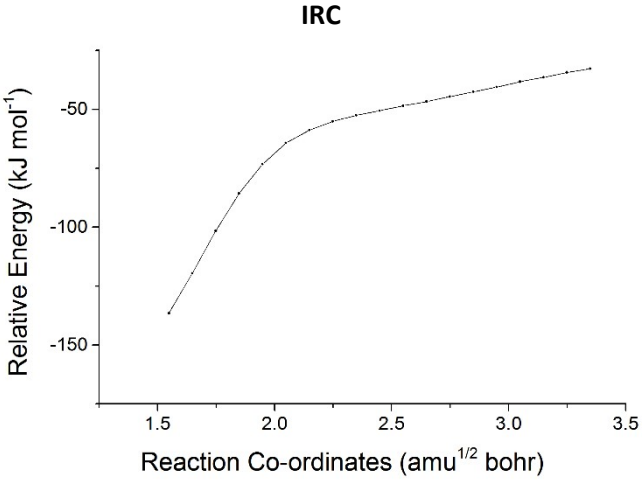
Compound: CF_3CFO	**Energy (kJ mol^{-1}):** -451.199957828211
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.590884 0.016760 -0.000000 6 0.950258 0.161191 -0.000000 8 1.560686 1.164510 0.000000 9 1.511346 -1.053957 -0.000000 9 -0.986585 -0.656718 1.087722 9 -1.165035 1.213645 -0.000003 9 -0.986585 -0.656723 -1.087719	43.7845, 226.0109, 238.7949, 378.7825, 419.3861,1. 512.0808, 584.7772, 688.3344, 765.2522, 800.0823, 1086.2930, 1167.3575, 1222.6180, ,1305.3726, 1935.9581

Compound: CF_3OCFO	**Energy (kJ mol^{-1}):** -526.392169685219
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.985021 -0.064022 0.000000 9 1.142265 0.688671 1.083247 9 1.895578 -1.026215 -0.000000 9 1.142264 0.688671 -1.083247 8 -0.249812 -0.707922 0.000001 6 -1.372203 0.051286 0.000000 9 -2.386217 -0.800803 -0.000000 8 -1.477929 1.223361 -0.000000	75.3080, 177.0143, 376.9655, 401.4174, 427.2777, 550.7688, 610.1072, 668.4452, 737.8881, 774.4134, 880.1638, 1021.3954, 1141.4172, 1225.8672, 1237.8952, 1275.4731, 1923.5619

S8.3 Reactions with SO_2

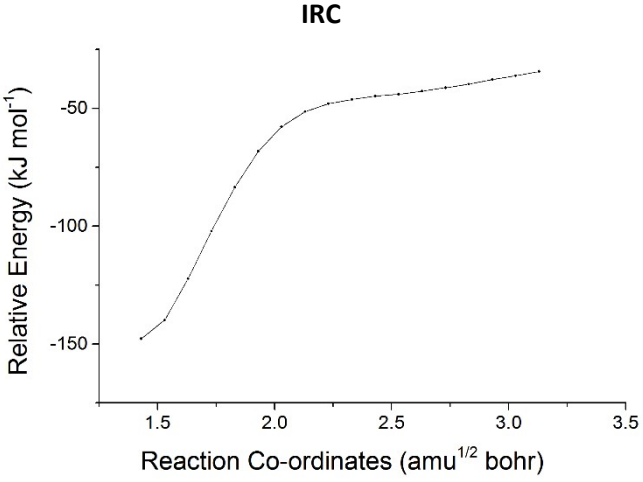
Compound: SO_2	**Energy (kJ mol^{-1}):** -548.08584429715
Reaction Coordinates: 16 0.000000 0.000000 0.372669 8 0.000000 1.245290 -0.372669 8 -0.000000 -1.245290 -0.372669	**Frequencies (cm^{-1}):** 513.3417, 1156.5416, 1337.5576

Compound: sCI 1 + SO_2 $TS_{Cyc}1$ reaction profile



Compound: sCI 1 + SO_2 SOZ 1	**Energy (kJ mol^{-1}):** -737.54758505440
Reaction Coordinates: 6 1.382069 -0.646247 0.414243 1 1.138310 -0.656463 1.477779 8 1.589137 0.652527 -0.058367 8 0.269739 1.234086 0.029932 16 -0.903903 0.016549 -0.430359 8 0.274519 -1.149994 -0.346833 8 -1.787516 -0.049041 0.719351 1 2.264694 -1.231458 0.169849	**Frequencies (cm^{-1}):** 122.2352, 300.3218, 365.2906, 429.7004, 512.9059, 611.8820, 691.2164, 714.2195, 868.9158, 923.9394, 1046.7403, 1148.9215, 1243.2803, 1247.7933, 1377.9775, 1505.9329, 3052.1770, 3146.1962

Compound: sCI 1 + SO_2 $TS_{Cyc}2$ reaction profile



Compound: sCI 1 + SO_2 SOZ 2	**Energy (kJ mol^{-1}):** -737.54937458407
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.556878 -0.547909 0.071274 1 -2.103692 -0.542148 -0.874056 8 -1.293568 0.748906 0.523130 8 -0.267816 1.181102 -0.421646 16 0.909912 -0.063250 -0.409928 8 -0.292974 -1.188917 -0.119714 8 1.727057 -0.003975 0.785128 1 -2.095215 -1.055326 0.870085	132.0686, 287.7793, 374.3085, 447.0565, 519.4221, 630.6105, 667.5639, 714.3830, 835.9980, 947.7173, 1040.2338, 1133.8437, 1234.1709, 1258.4403, 1386.7702, 1504.2540, 3036.7579, 3124.0647

Compound: sCI 1 + SO_2 TS_{hoz}	**Energy (kJ mol^{-1}):** -737.54937458407
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.386780 -0.692255 0.278605 1 1.274693 -1.092237 1.287451 8 1.397845 0.745999 0.369330 8 0.212787 1.242656 -0.331163 16 -0.931332 0.018255 -0.381583 8 0.303256 -1.082345 -0.546129 8 -1.538487 -0.158847 0.927095 1 2.302725 -1.026016 -0.206819	-179.8160, 159.1954, 353.4794, 451.0161, 572.8258, 671.8872, 697.3124, 723.2182, 833.2018, 938.3023, 1040.7095, 1126.7846, 1197.2006, 1241.8372, 1393.0334, 1531.9412, 3041.7383, 3108.8411

Compound: sCI 1 + SO_2 $TS_{SO_3}1$	**Energy (kJ mol^{-1}):** -737.51404208200
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.501312 -0.650356 0.305770 1 1.174843 -1.145000 1.224048 8 1.700162 0.635117 0.346011 8 -0.052180 1.317998 -0.225692 16 -0.881951 0.066084 -0.304427 8 0.227311 -0.967082 -0.711171 8 -1.665008 -0.337595 0.852781 1 2.246226 -1.197717 -0.283267	-559.6034, 124.6928, 185.5359, 320.2554, 418.0848, 482.2966, 535.8077, 616.2304, 804.3402, 960.9313, 1009.8710, 1160.8091, 1224.0481, 1249.8633, 1310.5436, 1506.3998, 2983.3701, 3065.2443

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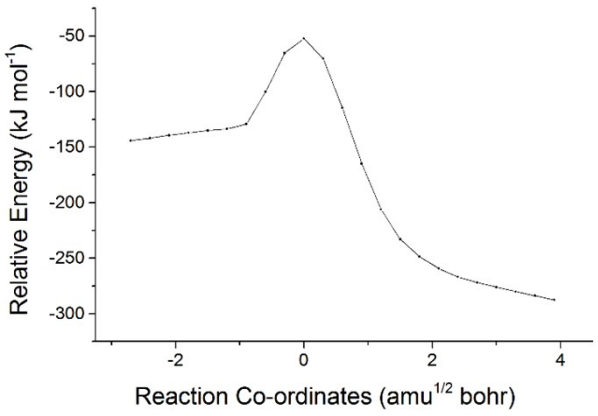
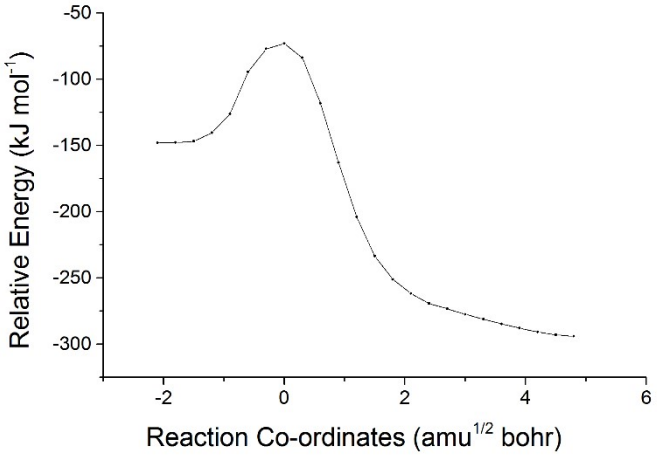
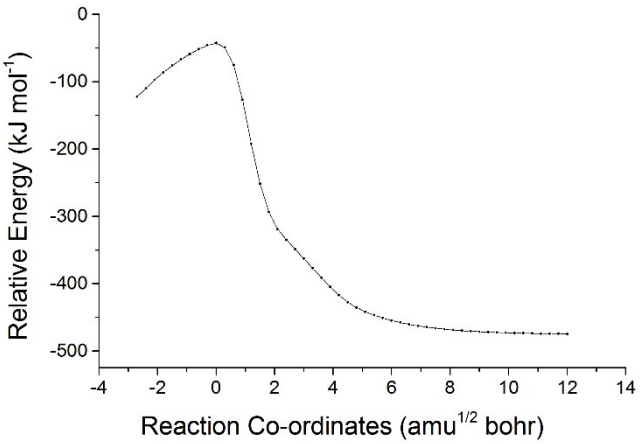
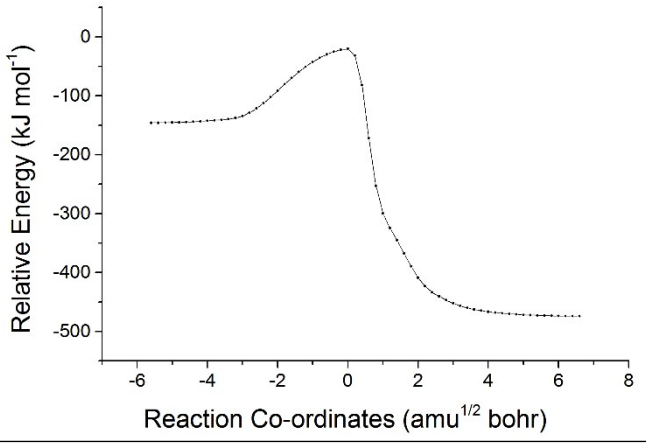


Compound: sCl 1 + SO_2 $Cso_3$1	**Energy (kJ mol^{-1}):** -737.62562027792
Reaction Coordinates: 6 2.341652 0.110229 -0.000001 1 3.391734 -0.210515 0.000002 1 2.117654 1.185058 -0.000005 8 1.456406 -0.714452 0.000001 8 -1.068999 -0.553788 1.247214 16 -0.728472 0.078182 0.000000 8 -0.306356 1.461227 -0.000032 8 -1.069019 -0.553840 -1.247182	**Frequencies (cm^{-1}):** 57.7179, 151.3388, 177.0498, 181.1805, 298.8735, 366.7314, 474.7464, 514.5355, 515.9279, 1039.7032, 1215.7655, 1262.8801, 1342.6023, 1367.2268, 1508.6567, 1769.9047, 2969.2137, 3063.1764

Compound: sCl 1 + SO_2 $TSso_3$2	**Energy (kJ mol^{-1}):** -737.52348576070
Reaction Coordinates: 6 1.675324 -0.427293 0.002391 1 2.138285 -0.364549 -0.986984 8 1.512196 0.659717 0.679127 8 -0.065910 1.221055 -0.501149 16 -0.865776 -0.027908 -0.316199 8 -1.784157 -0.175642 0.798381 8 0.285073 -1.128409 -0.300800 1 2.084584 -1.238935 0.627351	**Frequencies (cm^{-1}):** -443.3199, 143.9413, 241.7856, 303.0127, 428.7202, 491.0293, 511.7264, 656.5097, 759.3473, 969.7000, 1000.6678, 1124.3188, 1249.0727, 1270.1735, 1322.2826, 1438.5225, 2937.7277, 3037.1136

IRC

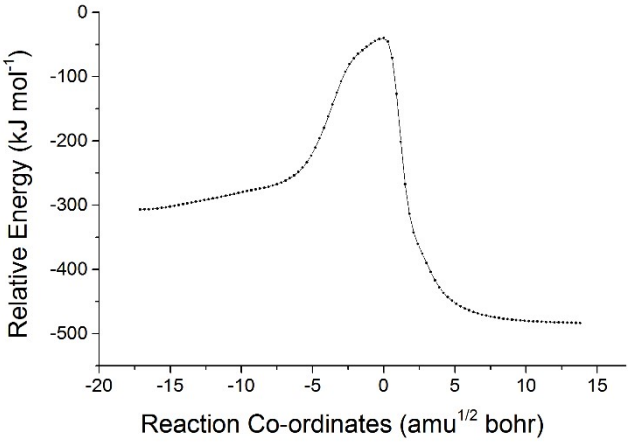


Compound: sCl 1 + SO_2 $TS_{acid}1$	**Energy (kJ mol^{-1}):** -737.49389238926
Reaction Coordinates: 6 1.629372 -0.345072 -0.136515 1 2.240069 -0.218982 -1.044043 8 1.512066 0.699746 0.661067 8 -0.200944 1.243956 -0.386806 16 -0.992011 -0.032259 -0.373489 8 0.632019 -1.195266 -0.210455 8 -1.755655 -0.317004 0.823119 1 2.355981 -0.645892 0.743562	**Frequencies (cm^{-1}):** -832.8318, 133.5888, 195.8912, 247.3174, 358.5430, 385.4304, 432.5792, 505.1556, 704.0409, 802.4629, 986.7936, 1136.3870, 1204.3920, 1276.1307, 1298.1726, 1376.3094, 2452.6451, 2962.2799
IRC  	
Compound: sCl 1 + SO_2 $TS_{acid}2$	**Energy (kJ mol^{-1}):** -737.50143644919
Reaction Coordinates: 6 1.405536 -0.555411 0.316090 1 1.245825 -0.987224 1.317976 8 1.705258 0.735066 0.276800 8 -0.214092 1.312346 -0.104809 16 -1.027584 0.071542 -0.362876 8 0.694356 -1.055207 -0.664845 8 -1.658572 -0.514248 0.807833 1 2.546705 -0.648638 0.071658	**Frequencies (cm^{-1}):** -731.4789, 123.8317, 184.0541, 234.6166, 338.4323, 409.5670, 426.8130, 509.2331, 691.9101, 790.8737, 971.3345, 1128.3870, 1220.4001, 1255.4461, 1285.1249, 1375.6071, 2501.8042, 2945.3882
IRC  	

Compound: sCl 1 + SO_2 $C_{acid}1$	**Energy (kJ mol^{-1}):** -737.67576753941
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.324179 -0.010590 -0.355769 1 -3.146885 0.039791 1.368678 8 -1.344757 -0.030178 -1.041439 8 1.571462 -1.228815 0.473015 16 1.508648 -0.009039 -0.313940 8 -2.260866 0.029061 0.985361 8 1.571843 1.253882 0.401687 1 -3.347860 -0.023224 -0.760015	21.5880, 28.3617, 29.0618, 78.5591, 96.3446, 133.8663, 517.6701, 540.0397, 665.5994, 1037.9677, 1126.1208, 1156.9469, 1270.4993, 1328.5625, 1414.4276, 1835.1316, 2984.2698, 3780.5005

Compound: sCl 1 + SO_2 $TS_{acid}3$	**Energy (kJ mol^{-1}):** -737.50120403903
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.709591 0.242649 -0.179014 1 2.146751 1.259339 0.231095 8 1.783991 -0.584592 0.760050 8 -0.399436 -1.312706 -0.358881 16 -1.001669 0.023142 -0.323319 8 0.603396 1.091388 -0.319156 8 -1.810743 0.415679 0.812871 1 2.204744 0.036341 -1.142972	-678.6198, 109.1496, 138.7703, 218.4693, 272.9500, 341.8787, 378.3924, 500.2041, 662.2154, 704.1694, 924.9739, 1094.5164, 1142.6219, 1294.3151, 1318.3949, 1468.5642, 2392.1632, 2938.2548

IRC



Compound: sCl 1 + SO_2 $C_{acid}2$	**Energy (kJ mol^{-1}):** -737.68599404256
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.153108 0.466614 -0.030781 8 1.189385 1.145996 0.230713 8 2.145949 -0.843591 -0.256551 1 1.232434 -1.183415 -0.184780 1 3.169916 0.865614 -0.112439 8 -2.084303 0.668245 -0.679832 16 -1.347910 -0.002589 0.371589 8 -0.720335 -1.275707 0.022731	31.4878, 68.9111, 113.5839, 137.3046, 162.6219, 182.6245, 519.2643, 661.9957, 774.6861, 1064.2063, 1148.5395, 1178.5391, 1313.9712, 1351.0209, 1416.0962, 1763.6747, 3056.0992, 3574.5704

Compound: SO_3	**Energy (kJ mol^{-1}):** -623.22229804288
Reaction Coordinates:	**Frequencies (cm^{-1}):**
16 0.000000 -0.000000 0.000000 8 0.246828 -1.418352 0.000000 8 -1.351743 0.495417 0.000000	475.6389, 507.9530, 507.9566, 1044.8229, 1363.4683, 1363.4939

8 1.104915 0.922936 -0.000000	

Compound: sCl 2 + SO_2 PRC1	**Energy (kJ mol^{-1}):** -1074.30049656118
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.680849 -0.330936 0.008724 6 -1.137494 0.933439 0.662474 8 -0.286665 1.695181 0.151214 8 0.351463 1.317116 -0.987851 1 -1.567548 1.282222 1.592022 9 -2.292584 -0.014933 -1.139885 9 -0.764980 -1.257811 -0.222516 9 -2.603039 -0.837675 0.848126 16 2.325088 0.008750 0.066354 8 1.581156 -0.072555 1.323138 8 2.381748 -1.195175 -0.743052	29.2239, 48.4725, 62.4815, 91.7570, 100.6754, 174.7347, 180.0268, 226.5884, 268.6855, 328.0287, 471.8117, 505.2088, 516.6429, 535.2394, 580.3347, 756.1669, 830.0680, 877.0832, 910.6656, 1135.9560, 1154.7572, 1181.4849, 1253.8791, 1308.2990, 1367.8966, 1568.4158, 3206.0587

Compound: sCl 2 + SO_2 $TS_{Cyc}1$	**Energy (kJ mol^{-1}):** -1074.29932649603
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.567535 -0.331819 -0.021801 6 -0.988288 0.893200 0.685292 8 -0.211136 1.738966 0.185226 8 0.497696 1.392847 -0.932081 1 -1.437201 1.192710 1.623913 9 -2.387958 0.121866 -0.988788 9 -0.705693 -1.173798 -0.552521 9 -2.314631 -0.984971 0.884328 16 2.173682 -0.031753 0.130690 8 1.283290 -0.181356 1.294872 8 2.263619 -1.165560 -0.770900	-44.3238, 45.4533, 84.8741, 109.5867, 127.1715, 192.3251, 213.1513, 285.4045, 305.8816, 334.5709, 462.8314, 505.3981, 515.4080, 535.7839, 572.3408, 754.0951, 843.8360, 874.8355, 916.4321, 1106.9795, 1146.0291, 1161.5810, 1276.1099, 1295.7925, 1367.9148, 1566.9924, 3200.2906

Compound: sCl 2 + SO_2 SOZ 1	**Energy (kJ mol^{-1}):** -1074.35461788075
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.509783 -0.211551 0.070085 6 0.472691 0.607230 -0.732729 8 -0.097190 1.667245 -0.006489 8 -1.133556 1.051570 0.784769 1 0.991158 1.063821 -1.576545 9 2.487991 0.611495 0.483098 9 1.000662 -0.831871 1.132375 9 2.057394 -1.134082 -0.739936 16 -1.965027 -0.084757 -0.232373 8 -0.582831 -0.198334 -1.205133 8 -2.106424 -1.256938 0.600670	44.2404, 70.6265, 157.2900, 209.8630, 255.8569, 303.1416, 343.8475, 400.9612, 422.9259, 510.4862, 527.3151, 561.9128, 628.6370, 670.6377, 673.0996, 794.4516, 871.0570, 895.9295, 1002.9074, 1065.5800, 1165.6786, 1168.0381, 1268.0762, 1290.8391, 1306.0599, 1396.4551, 3091.8167

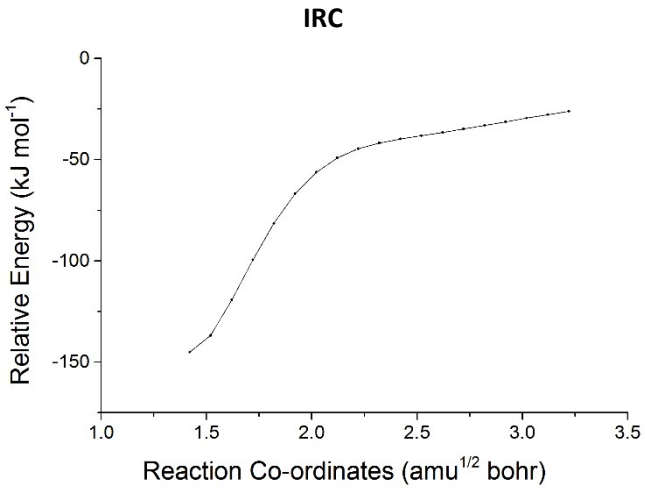
Compound: sCl 2 + SO_2 PRC2	**Energy (kJ mol^{-1}):** -1074.29958900339
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.884175 -0.194669 -0.056099 6 -1.045646 0.530654 0.987311 8 -0.092184 1.297137 0.725886 8 0.348291 1.408367 -0.552527 1 -1.314868 0.467760 2.033230	24.6678, 6.0920, 55.9841, 81.8352, 103.1086, 146.9604, 190.9617, 214.3366, 264.9684, 327.1424, 474.3552, 505.0058, 518.9497, 534.9524, 582.8485, 756.8278,

9 -2.513437 0.695230 -0.833304 9 -1.191282 -1.028633 -0.819448 9 -2.815482 -0.900882 0.610603 16 2.275655 -0.411951 -0.361018 8 1.470431 -1.130483 0.624267 8 3.419101 0.326993 0.144266	825.7794, 877.5626, 913.2445, 1139.9864, 1156.8720, 1179.9236, 1250.4563, 1309.9265, 1368.0173, 1568.8053, 3207.4250

Compound: sCI 2 + SO_2 $TS_{Cyc}2$	**Energy (kJ mol^{-1}):** -1074.29940211685
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.767970 -0.200627 -0.050972 6 -0.892727 0.535501 0.961344 8 -0.010909 1.378492 0.685315 8 0.437785 1.465943 -0.599539 1 -1.147977 0.467376 2.011078 9 -2.588927 0.704888 -0.612708 9 -1.135920 -0.854988 -1.007771 9 -2.520183 -1.071524 0.642652 16 2.118402 -0.439758 -0.360278 8 1.208848 -1.095346 0.588120 8 3.292152 0.195178 0.212553	-31.0837, 46.6099, 55.9795, 106.4244, 127.9574, 150.6068, 212.6447, 267.3147, 290.7125, 327.6061, 469.3283, 504.8931, 519.0325, 534.8190, 577.3396, 755.5527, 838.7640, 874.0912, 912.2329, 1120.7541, 1149.9620, 1164.0053, 1271.7624, 1294.7358, 1367.7513, 1573.1131, 3202.7905

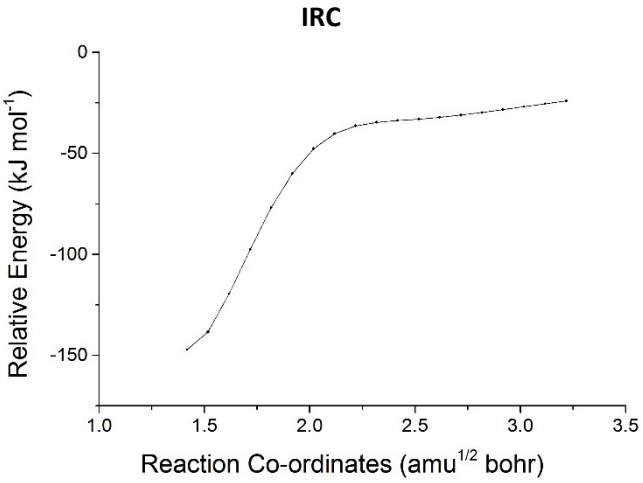
Compound: sCI 2 + SO_2 SOZ 2	**Energy (kJ mol^{-1}):** -1074.36037274421
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.660626 -0.102587 0.034820 6 0.359614 0.028112 -0.791388 8 -0.261150 1.276678 -0.666093 8 -1.040876 1.153037 0.563436 1 0.609532 -0.077818 -1.848446 9 2.505897 0.881224 -0.304427 9 1.452955 -0.048177 1.353799 9 2.248145 -1.276966 -0.250026 16 -1.869280 -0.327151 0.446264 8 -0.560881 -0.969187 -0.405574 8 -2.972776 -0.241233 -0.485078	48.0706, 78.6188, 141.0420, 202.3361, 257.8851, 294.1922, 383.5957, 399.3418, 467.0707, 518.5585, 545.0363, 578.2684, 638.3053, 663.9512, 690.5619, 788.0789, 833.9486, 863.3242, 1009.0424, 1064.5929, 1159.6992, 1175.8721, 1265.5730, 1282.5502, 1289.6916, 1391.5748, 3085.6763

Compound: sCI 3 + SO_2 $TS_{Cyc}1$ reaction profile



Compound: sCl 2 + SO_2 SOZ3	**Energy (kJ mol^{-1}):** -1074.35773058988
Reaction Coordinates: 6 1.702452 -0.118431 0.047577 6 0.387703 0.424608 -0.543796 8 -0.198834 1.268729 0.409836 8 -1.564676 1.367343 -0.075039 16 -2.078769 -0.251684 -0.317001 8 -0.511096 -0.644797 -0.784013 8 -2.332760 -0.913456 0.942857 1 0.594851 0.949559 -1.480180 9 2.537742 0.903356 0.291605 9 2.283775 -0.929409 -0.847908 9 1.509979 -0.794193 1.176345	**Frequencies (cm^{-1}):** 51.6628, 66.2206, 165.4099, 188.0028, 271.1719, 303.6911, 367.9778, 380.8930, 444.9106, 520.1523, 532.6612, 559.3600, 636.8891, 685.6619, 705.9521, 715.0671, 872.6268, 881.7316, , 1019.6375, 1089.4928, 1170.7546, 1177.1922, 1265.7594, 1283.3818, 1342.3435, 1410.2857, 3050.3375

Compound: sCl 3 + SO_2 $TS_{Cyc}2$ reaction profile



Compound: sCl 2 + SO_2 SOZ4	**Energy (kJ mol^{-1}):** -1074.35489019767
Reaction Coordinates: 6 1.779444 -0.130676 -0.041084 6 0.306102 0.102417 -0.412299 8 -0.074918 1.371532 0.041590 8 -1.506844 1.335170 -0.093337 16 -2.072519 -0.245121 0.411857 8 -0.508107 -0.825571 0.290510 8 -2.873972 -0.681963 -0.712054 1 0.169485 -0.002257 -1.491093 9 1.987951 -0.045424 1.272100 9 2.154784 -1.347066 -0.458012 9 2.544850 0.781422 -0.657643	**Frequencies (cm^{-1}):** 51.7553, 81.6765, 142.5523, 164.0122, 266.7253, 320.0954, 323.3741, 385.3553, 427.9052, 524.1165, 526.5158, 558.0106, 610.8184, 685.2486, 717.4421, 729.0240, 887.8522, 932.4643, 996.8673, 1088.8626, 1172.7260, 1183.7142, 1259.5769, 1278.4975, 1332.3607, 1420.1472, 3063.9397

Compound: sCl 2 + SO_2 $TS_{SOZ\,1}$	**Energy (kJ mol^{-1}):** -1074.35121769837
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.525315 -0.164536 -0.056157 6 -0.430735 0.665276 0.657307 8 0.145384 1.597292 -0.246252 8 1.535307 1.215057 -0.487627 1 -0.910361 1.222606 1.465011 9 -2.054881 -1.045162 0.807896 9 -2.503007 0.669459 -0.452593 9 -1.076416 -0.825045 -1.120134 16 1.940963 -0.260886 0.233548 8 0.581371 -0.131710 1.211230 8 1.775436 -1.336408 -0.718004	-144.3866, 50.6273, 105.2007, 181.7474, 205.0582, 309.4378, 330.6954, 397.4601, 417.8668, 517.0891, 558.6261, 567.8528, 652.0541, 679.3330, 685.5999, 785.9350, 842.6908, 854.7400, 1010.1829, 1080.4706, 1162.5741, 1171.6860, 1266.5673, 1295.1893, 1303.7839, 1404.6539, 3062.0777

Compound: sCl 2 + SO_2 $TS_{SOZ\,2}$	**Energy (kJ mol^{-1}):** -1074.35365432423
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.748937 -0.114434 -0.024259 6 0.274018 -0.031580 -0.460387 8 -0.153842 1.321783 -0.344886 8 -1.482972 1.313361 0.269186 1 0.176216 -0.373303 -1.494543 9 2.486196 0.699763 -0.793583 9 1.915846 0.233503 1.250191 9 2.194913 -1.368014 -0.190779 16 -2.072430 -0.261113 0.390273 8 -0.498174 -0.817146 0.413770 8 -2.680969 -0.650508 -0.867371	-101.5726, 62.6211, 99.9642, 155.2252, 220.0687, 319.4128, 339.1073, 379.8420, 449.1546, 518.6561, 554.8601, 588.8998, 669.4501, 686.7225, 717.7112, 738.3950, 859.8401, 869.9778, 1010.8214, 1073.4618, 1171.8732, 1176.4586, 1252.2470, 1280.7008, 1331.7885, 1416.1239, 3048.0420

Compound: sCl 2 + SO_2 $TS_{SO_3}1$	**Energy (kJ mol^{-1}):** -1074.33512300027
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.681073 0.106352 0.052263 6 -0.432132 -0.144608 -0.832003 8 0.079204 -1.329812 -0.848233 8 1.230573 -1.027724 0.793877 1 -0.614523 0.241506 -1.849452 9 -2.117836 1.366947 -0.108056 9 -1.449414 -0.096900 1.350768 9 -2.655367 -0.725443 -0.342431 16 1.847120 0.256751 0.351536 8 0.609315 0.938962 -0.387725 8 3.048831 0.290896 -0.457819	-441.1456, 46.9288, 90.8543, 126.8517, 191.0219, 253.8848, 286.2551, 330.2239, 420.2077, 443.1656, 502.5533, 517.3251, 538.3314, 574.7456, 694.5466, 749.8890, 789.9627, 844.1961, 994.5220, 1091.1145, 1149.2041, 1185.0667, 1223.4300, 1266.6729, 1269.7930, 1382.1165, 2946.7385
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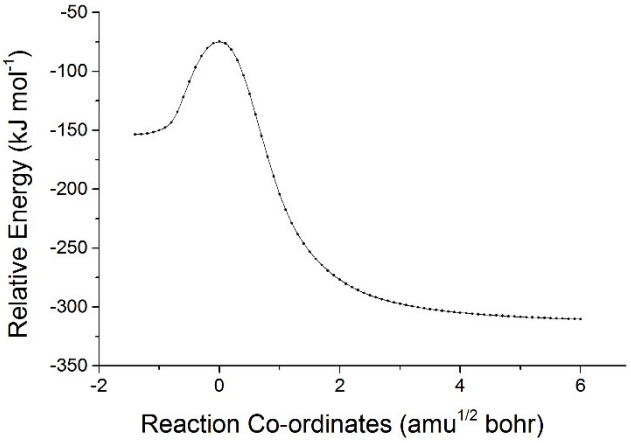
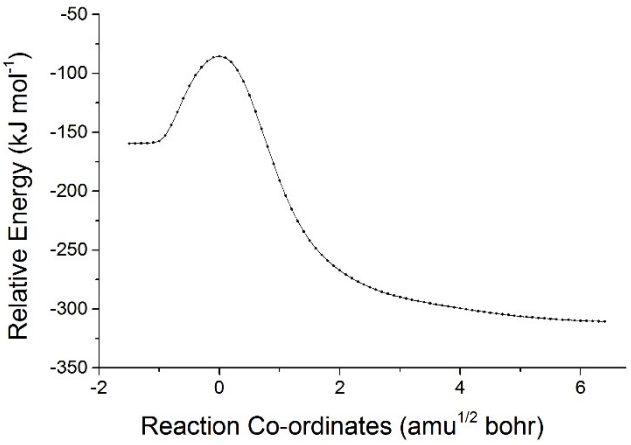


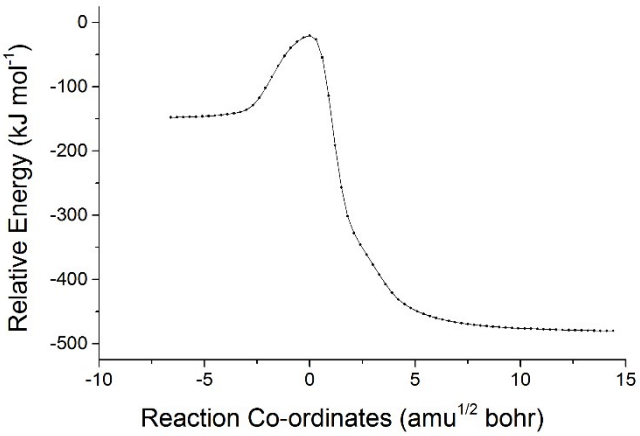
Compound: sCl 2 + SO_2 $CsO_3$1	**Energy (kJ mol^{-1}):** -1074.43431110038
Reaction Coordinates: 6 -2.359197 0.002975 -0.000000 6 -0.844225 -0.282288 -0.000001 8 -0.032595 0.601469 -0.000001 8 2.641537 0.592391 -1.247684 1 -0.574830 -1.348409 -0.000002 9 -2.904523 -0.565307 1.089032 9 -2.636321 1.298767 -0.000005 9 -2.904526 -0.565316 -1.089025 16 2.370290 -0.068647 0.000000 8 1.984410 -1.460059 -0.000014 8 2.641529 0.592367 1.247698	**Frequencies (cm^{-1}):** 20.1907, 42.5260, 69.5071, 81.9062, 83.0338, 166.6485, 171.1706, 294.3903, 329.2156, 434.3420, 463.1476, 509.8777, 511.3396, 527.5328, 529.7630, 706.9608, 846.3766, 999.3410, 1043.9802, 1163.3722, 1181.5146, 1289.2590, 1351.4924, 1373.8588, 1399.6574, 1819.7549, 3013.7213

Compound: sCl 2 + SO_2 $TSsO_3$2	**Energy (kJ mol^{-1}):** -1074.32997089072
Reaction Coordinates: 6 1.728009 -0.125183 0.034650 6 0.441912 0.660406 -0.396289 8 -0.050099 1.358879 0.576907 8 -1.915066 1.267761 -0.144913 1 0.611404 1.151115 -1.360112 9 2.138415 -0.915789 -0.963504 9 1.529476 -0.858648 1.121655 9 2.695958 0.767152 0.278919 16 -1.992157 -0.223075 -0.273980 8 -0.517223 -0.532291 -0.772050 8 -2.396494 -1.060311 0.837555	**Frequencies (cm^{-1}):** -441.5083, 56.4485, 72.5008, 161.8351, 186.0835, 266.6349, 292.1361, 317.1228, 403.2586, 441.0609, 507.0897, 515.8940, 530.1940, 567.2088, 679.8117, 737.2216, 794.7079, 840.8249, 975.2500, 1151.3726, 1175.2529, 1210.0695, 1257.0745, 1277.7910, 1303.9932, 1360.3222, 3030.9695
IRC	


-50
-100
-150
-200
-250
-300
-350
-2
0
2
4
6
Relative Energy (kJ mol-1)
Reaction Co-ordinates (amu1/2 bohr)

Compound: sCl 2 + SO_2 $TS_{acid}1$	**Energy (kJ mol^{-1}):** -1074.30007800359
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.505222 -0.239235 -0.072830 6 -0.468416 0.779170 0.532436 8 -0.117868 1.770499 -0.267234 8 1.675590 0.954167 -0.770812 1 -1.112337 1.616668 1.033243 9 -2.586837 0.431945 -0.501419 9 -0.984302 -0.900871 -1.104109 9 -1.892435 -1.114031 0.857215 16 2.020959 -0.176837 0.163869 8 0.396458 0.320788 1.397348 8 1.769694 -1.517986 -0.319049	-688.6455, 34.5698, 102.7656, 106.7723, 153.6091, 184.0275, 240.9328, 282.9228, 334.7932, 384.6055, 428.8683, 438.7417, 490.1544, 522.3457, 589.2997, 694.3193, 792.1899, 813.5240, 883.2912, 961.6328, 1139.4703, 1187.9310, 1206.3680, 1248.5025, 1281.7435, 1340.6893, 2496.1816

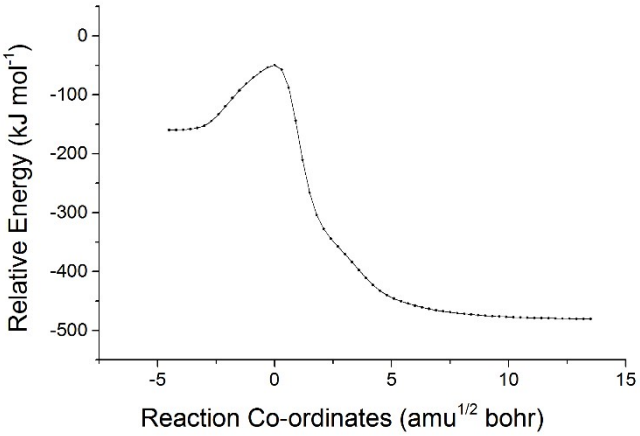
IRC



Compound: sCl 2 + SO_2 $C_{acid}1$	**Energy (kJ mol^{-1}):** -1074.48261883124
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.244544 -0.262546 -0.114768 6 0.894474 0.357660 0.356378 8 0.884820 1.682848 0.496233 1 1.738515 2.069558 0.254068 8 -0.046837 -0.341178 0.576054 9 2.072883 -0.954956 -1.237657 9 3.167254 0.703181 -0.353907 9 2.733065 -1.071123 0.825914 8 -2.852061 0.915641 -0.944483 16 -3.036633 0.092495 0.238408 8 -3.454086 -1.284071 0.043772	10.4592, 11.1773, 14.8872, 26.3993, 43.1879, 67.6075, 108.1088, 252.6177, 259.5524, 385.2853, 426.5345, 505.0798, 516.9555, 571.0955, 584.3263, 688.8721, 776.4952, 793.7122, 1118.9072, 1157.7687, 1179.0938, 1197.1657, 1239.8601, 1332.5658, 1372.3901, 1868.7735, 3746.5623

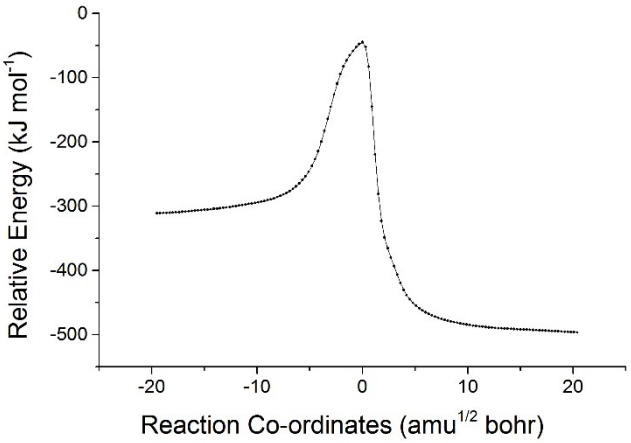
Compound: sCI 2 + SO_2 $TS_{acid}2$	**Energy (kJ mol^{-1}):** -1074.31032548775
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.719219 -0.101523 0.094679 6 0.407056 0.052457 -0.744778 8 -0.078855 1.275075 -0.892810 8 -1.295967 1.040241 0.709241 1 0.733771 0.348845 -1.848093 9 2.545062 0.924515 -0.130028 9 1.435752 -0.149389 1.398708 9 2.343233 -1.234436 -0.248524 16 -1.963491 -0.284174 0.456166 8 -0.410283 -0.954650 -0.706844 8 -3.088894 -0.282400 -0.451010	-887.2658, 41.0240, 81.3727, 118.9355, 184.5431, 234.3204, 260.7966, 266.7216, 358.3049, 388.3995, 428.5897, 449.4796, 503.2875, 521.6048, 590.2512, 700.7906, 797.3061, 818.5908, 886.7907, 979.8302, 1149.4563, 1190.2700, 1204.9755, 1265.7669, 1286.7673, 1378.7296, 2403.5005

IRC

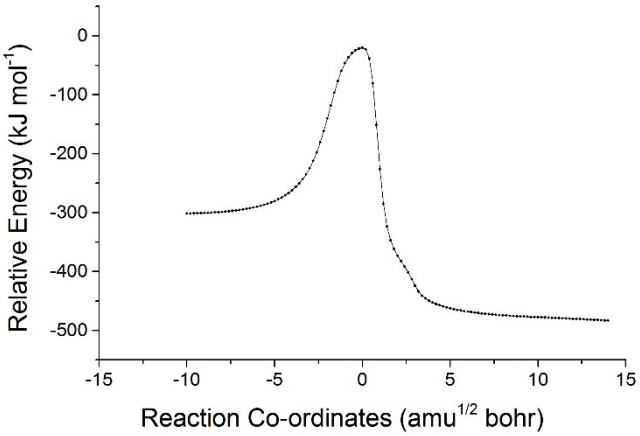


Compound: sCI 2 + SO_2 $C_{acid}2$	**Energy (kJ mol^{-1}):** -1074.48289929713
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.331526 -0.166516 0.000018 6 -0.825440 0.234423 -0.000032 8 -0.574098 1.541614 -0.000171 1 -1.391387 2.060194 -0.000217 8 0.021437 -0.606313 0.000049 9 -3.128764 0.930676 -0.000075 9 -2.620147 -0.883912 -1.084761 9 -2.620128 -0.883715 1.084931 8 3.209723 0.291203 -1.242572 16 3.045037 -0.442475 0.000064 8 3.209681 0.291561 1.242495	7.9403, 13.7672, 18.1848, 27.8477, 46.3445, 67.3022, 109.4827, 252.8838, 259.5677, 385.3358, 427.0890, 505.0127, 517.1221, 570.0799, 584.6192, 689.1895, 776.5047, 793.8786, 1121.8089, 1157.6692, 1181.6738, 1193.8914, 1238.5964, 1331.6294, 1373.0344, 1866.6247, 3747.6477

Compound: sCI 2 + SO_2 $TS_{acid}3$	**Energy (kJ mol^{-1}):** -1074.30934048683
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.728380 -0.129799 0.105668 6 0.489885 0.281918 -0.767563 8 0.192326 1.481797 -0.897550 8 -1.440532 0.892288 0.995355 1 0.630922 -0.217479 -1.837251 9 2.700575 0.766552 -0.040366 9 1.387182 -0.198364 1.394931 9 2.192927 -1.331188 -0.272209 16 -1.958439 -0.308316 0.343069 8 -0.484910 -0.738650 -0.812091 8 -3.158338 -0.247332 -0.463424	-761.9918, 33.0059, 71.7498, 91.8382, 131.5788, 187.0189, 244.1248, 277.6319, 321.4680, 337.8402, 400.8382, 428.6618, 502.3980, 517.5784, 579.7048, 670.5444, 751.5279, 779.8846, 845.4066, 977.9521, 1103.1089, 1170.8089, 1210.1752, 1223.9501, 1306.7573, 1516.0627, 2325.4651
IRC	

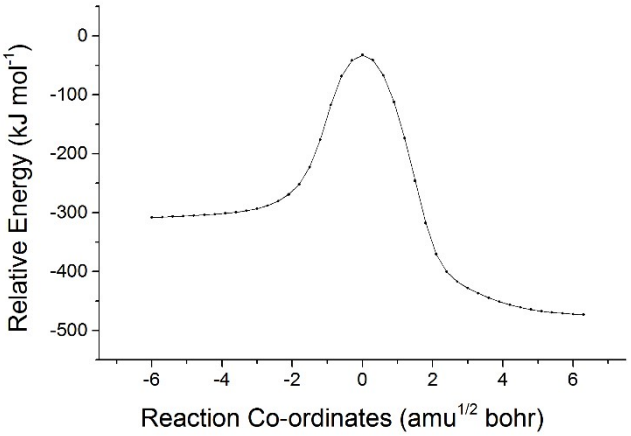


Compound: sCI 2 + SO_2 $C_{acid}3$	**Energy (kJ mol^{-1}):** -1074.49220772753
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.428819 -0.098941 0.012849 6 -0.878113 -0.026969 0.000391 8 -0.182944 -1.004912 0.003846 8 -0.475453 1.235062 -0.015518 1 0.504113 1.254826 -0.019547 9 -2.838189 -1.364577 0.029163 9 -2.919259 0.521800 1.097360 9 -2.934592 0.498452 -1.078159 8 4.423124 -0.352641 0.234115 16 3.030917 -0.280874 -0.155708 8 2.369168 1.009183 0.027076	10.4595, 19.9218, 36.7816, 47.8233, 71.4015, 92.8783, 126.1916, 252.5346, 254.4247, 391.1867, 425.0695, 513.8513, 528.8470, 586.4652, 685.4860, 746.0666, 799.0625, 820.6465, 1146.8988, 1155.9481, 1162.3236, 1204.1614, 1278.1810, 1321.4712, 1436.3382, 1826.7385, 3524.3309

Compound: sCl 2 + SO_2 $TS_{acid}4$	**Energy (kJ mol^{-1}):** -1074.30138997618
Reaction Coordinates: 6 -1.497821 -0.271097 -0.082599 6 -0.562574 0.861364 0.490426 8 -0.446143 1.902397 -0.203525 8 1.828179 -1.522474 -0.221845 1 -1.022648 1.154923 1.518209 9 -2.676354 0.257539 -0.419533 9 -0.945041 -0.819783 -1.166104 9 -1.704821 -1.230321 0.826601 16 1.970706 -0.132616 0.164348 8 0.481865 0.391824 1.297929 8 1.859808 0.923056 -0.842985	**Frequencies (cm^{-1}):** -441.0022, 40.1146, 58.8253, 78.2172, 101.2594, 185.7786, 238.6275, 279.3428, 340.8934, 369.1801, 377.0582, 423.5238, 486.6397, 521.1562, 576.1011, 669.4742, 749.4600, 776.2415, 832.2168, 969.7756, 1090.0897, 1173.6587, 1199.9138, 1221.0713, 1289.3918, 1448.7891, 2476.7645
IRC  	

Compound: sCl 2 + SO_2 $TS_{ester}1$	**Energy (kJ mol^{-1}):** -1074.29521365977
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.907634 -0.201494 0.010597 6 0.319341 0.835769 -0.322223 8 0.148875 1.494348 0.703135 8 -2.502454 -1.154144 0.790211 1 0.629705 1.306123 -1.270803 9 2.172713 -0.929108 -1.038725 9 1.743607 -0.892227 1.092480 9 2.793668 0.748959 0.157964 16 -2.141148 -0.275051 -0.307714 8 -0.302258 -0.389701 -0.530099 8 -2.359547 1.167052 -0.193433	-376.2534, 55.8878, 58.7232, 88.2166, 111.0868, 182.5976, 209.2988, 250.7035, 260.5697, 343.0394, 358.6689, 446.6899, 496.5903, 539.0026, 555.7381, 669.7221, 704.3805, 880.2197, 1005.9261, 1070.1386, 1094.6664, 1279.1533, 1284.1591, 1334.0598, 1347.3691, 1524.3376, 2933.3175

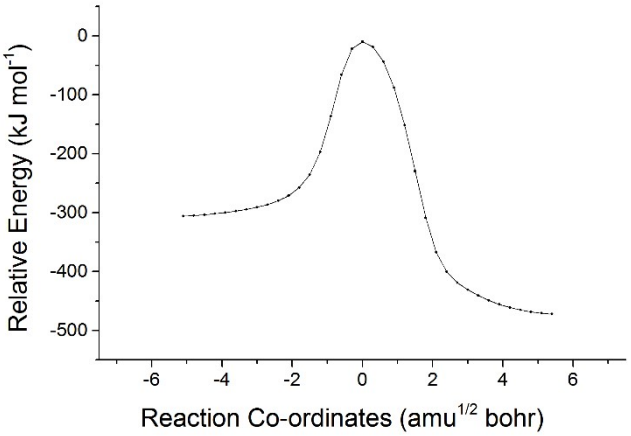
IRC



Compound: sCl 2 + SO_2 $C_{ester}1$	**Energy (kJ mol^{-1}):** -1074.48491076640
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.489750 0.054945 0.021225 9 3.664742 -0.422508 0.415892 9 2.317397 1.265565 0.546732 9 2.488990 0.153804 -1.306848 8 1.530686 -0.840754 0.468921 6 0.204279 -0.610540 0.208814 8 -0.236492 0.320211 -0.389198 1 -0.374555 -1.429350 0.644969 8 -3.528716 1.114411 0.585437 16 -3.176166 0.069126 -0.356488 8 -2.916869 -1.258222 0.181918	22.5722, 27.3868, 43.6691, 55.6613, 78.4418, 103.8095, 131.6737, 206.5524, 230.6056, 377.5828, 442.6376, 518.2029, 551.5669, 581.7440, 619.2136, 823.7137, 847.0023, 1047.8936, 1116.4729, 1154.9553, 1161.2201, 1215.7607, 1246.9872, 1327.6292, 1404.2327, 1818.7131, 3085.7404

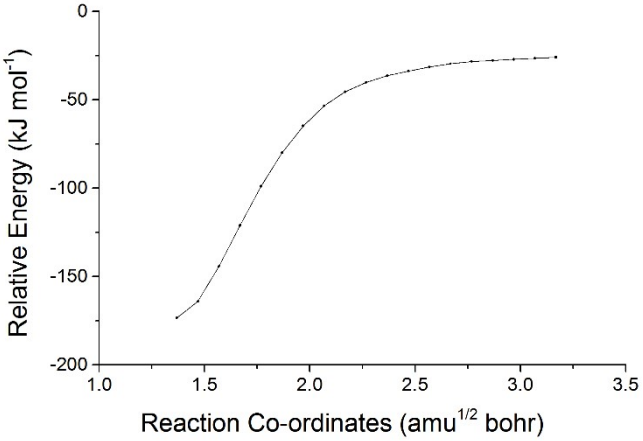
Compound: sCI 2 + SO_2 $TS_{ester}2$	**Energy (kJ mol^{-1}):** -1074.28858393056
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.927643 -0.162049 0.052578 6 0.254333 0.308269 -0.576751 8 0.244085 1.551032 -0.533290 8 -2.324640 1.192076 0.341498 1 0.269447 -0.211321 -1.550195 9 2.037732 -1.464759 0.024301 9 2.091976 0.333440 1.240500 9 2.728281 0.388857 -0.827102 16 -2.169287 -0.261877 0.335354 8 -0.324575 -0.456447 0.437230 8 -2.641696 -1.010886 -0.821653	-370.1730, 16.1198, 59.0942, 67.3353, 109.0338, 167.2670, 226.5308, 246.5961, 279.0198, 325.4507, 365.6545, 468.5518, 508.7152, 543.8417, 559.1264, 664.1420, 698.8355, 866.9331, 984.6277, 1087.8560, 1112.9125, 1263.7941, 1268.3799, 1320.8891, 1351.4615, 1470.4502, 2929.3623

IRC



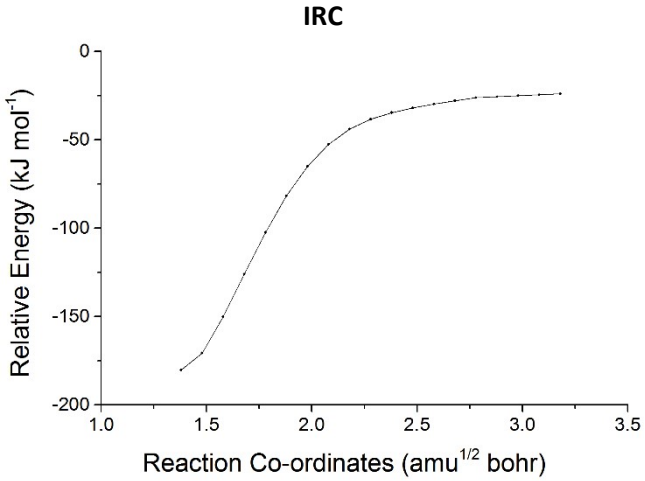
Compound: sCI 4 + SO_2 $TS_{Cyc}1$ reaction profile

IRC



Compound: sCI 4 + SO_2 SOZ 1	**Energy (kJ mol^{-1}):** -1173.53663043677
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.554889 -0.444082 0.043971 6 0.418853 0.592260 -0.202881 8 -0.143415 1.061194 1.019003 8 -1.305516 0.258857 1.272495 9 0.975223 1.683375 -0.767063 9 2.520008 0.104416 0.786549 9 1.071205 -1.509809 0.684478 9 2.079728 -0.839043 -1.119604 16 -2.122305 0.153740 -0.233675 8 -0.568098 0.060591 -0.987590 8 -2.695603 -1.168061 -0.249779	45.0068, 58.5952, 129.6858, 213.5561, 224.3170, 262.4941, 314.9923, 344.4554, 355.5024, 424.7648, 458.8257, 504.6762, 546.0177, 566.3235, 595.6943, 678.9116, 700.9905, 741.4844, 823.3340, 959.3827, 1049.1246, 1089.6695, 1186.4706, 1198.4167, 1209.5305, 1289.7024, 1326.0809

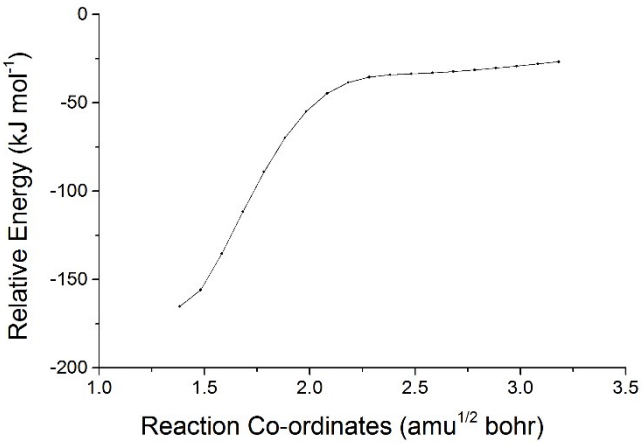
Compound: sCI 4 + SO_2 $TS_{Cyc}2$ reaction profile



Compound: sCI 4 + SO_2 SOZ 2	**Energy (kJ mol^{-1}):** -1173.54107480780
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.700331 -0.154031 -0.148664 6 0.290126 0.421615 0.178222 8 -0.275947 -0.212825 1.306963 8 -1.295685 -1.117905 0.824562 16 -2.064144 -0.354469 -0.480549 8 -0.540673 0.263838 -0.911824 8 -2.887610 0.744374 -0.032400 9 0.443800 1.719711 0.510316 9 2.513062 0.005565 0.897738 9 1.602657 -1.457920 -0.424287 9 2.227468 0.471104 -1.204541	52.0720, 62.2597, 115.6779, 186.1203, 220.2380, 287.1115, 337.0379, 366.2857, 370.7109, 444.9691, 462.2021, 513.7914, 556.2475, 589.4587, 603.7358, 673.9915, 707.4480, 739.9283, 823.3987, 922.4626, 1057.9091, 1076.2351, 1166.6656, 1200.6382, 1206.7401, 1278.0201, 1326.4546

Compound: sCI 5 + SO_2 $TS_{Cyc}1$ reaction profile

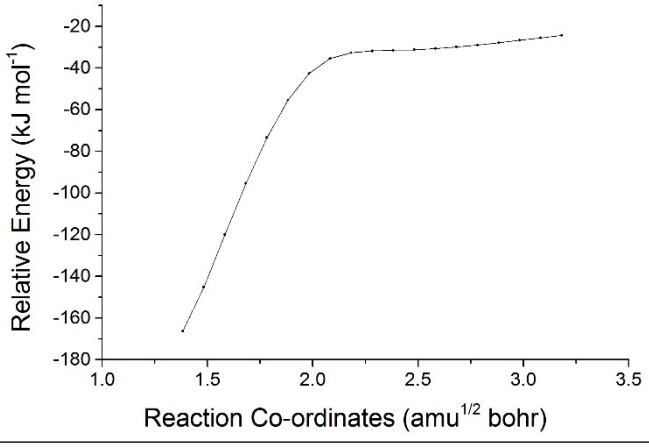
IRC



Compound: sCI 4 + SO_2 SOZ3	**Energy (kJ mol^{-1}):** -1173.53937137970
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.624021 -0.369006 -0.066746 6 0.353772 0.513907 0.141124 8 -0.226344 0.719616 -1.101301 8 -1.613861 1.041606 -0.800585 9 0.743711 1.684853 0.707724 9 2.468636 0.238292 -0.904194 9 2.233981 -0.549345 1.105701 9 1.290437 -1.554870 -0.569920 16 -2.139784 -0.085078 0.360085 8 -0.552474 -0.117628 0.973985 8 -2.389958 -1.378411 -0.229779	53.3878, 68.0440, 151.6147, 187.7091, 228.6704, 288.5831, 322.0043, 349.3383, 381.0432, 412.5424, 495.2303, 532.1745, 559.7927, 593.1859, 611.7228, 650.3890, 708.1821, 748.7677, 862.8946, 872.8553, 1070.9764, 1093.4081, 1121.3912, 1203.8397, 1217.8460, 1280.2051, 1321.1927

Compound: sCI 5 + SO_2 $TS_{Cyc}2$ reaction profile

IRC



Compound: sCl 4 + SO_2 SOZ4	**Energy (kJ mol^{-1}):** -1173.54521761536
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.778298 -0.133786 0.148059 6 -0.307417 0.102434 -0.310864 8 0.091734 1.343827 0.168329 8 1.533488 1.319434 0.113336 9 -0.271368 0.056396 -1.665292 9 -2.562575 0.837897 -0.323002 9 -2.209507 -1.304759 -0.320778 9 -1.855159 -0.145465 1.479357 16 2.090638 -0.266878 0.539013 8 0.523530 -0.863798 0.224799 8 2.995195 -0.616770 -0.528957	46.1589, 65.1210, 128.8650, 147.8182, 225.6994, 278.1023, 308.3286, 360.6921, 370.7065, 423.8983, 479.7653, 525.5699, 543.1417, 567.8888, 613.8405, 640.0293, 691.9122, 750.1205, 872.2915, 924.5181, 1078.2136, 1091.8311, 1117.2803, 1207.6709, 1212.2055, 1282.2160, 1335.4386

Compound: sCl 4 + SO_2 $TS_{HOZ\,1}$	**Energy (kJ mol^{-1}):** -1173.53388111950
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.605497 0.411392 -0.090610 6 -0.406323 -0.535798 0.221133 8 0.108691 -1.057032 -0.980044 8 1.495851 -0.681514 -1.126061 9 -0.891300 -1.580363 0.940705 9 -2.141387 0.867559 1.044041 9 -1.185318 1.446912 -0.818228 9 -2.543014 -0.248470 -0.774978 16 2.149123 -0.051263 0.324664 8 0.557708 0.130605 0.922345 8 2.654514 1.257428 -0.003943	-159.4294, 20.7987, 61.5444, 186.1793, 208.8163, 252.6619, 309.6699, 337.1985, 356.3283, 412.3298, 461.4061, 513.1769, 554.4058, 572.6469, 597.5426, 650.9426, 700.4405, 744.3853, 849.4978, 939.8015, 1061.2802, 1087.6116, 1158.9090, 1201.5767, 1212.2239, 1288.0152, 1318.8162

Compound: sCl 4 + SO_2 $TS_{HOZ\,2}$	**Energy (kJ mol^{-1}):** -1173.53931994965
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.762539 -0.012924 -0.172343 6 -0.279093 0.160238 0.279076 8 0.134175 -1.014808 0.898621 8 1.502083 -1.304033 0.481358 9 -0.233441 1.196656 1.158317 9 -2.208773 1.122235 -0.711780 9 -1.857571 -0.987962 -1.076651 9 -2.522903 -0.320903 0.880330 16 2.110800 -0.109799 -0.563686 8 0.517626 0.412641 -0.816737 8 2.831265 0.879033 0.202589	-73.1102, 60.9569, 89.3910, 152.7468, 210.2652, 280.6427, 305.0765, 360.0640, 369.2964, 423.3978, 478.9291, 527.1686, 549.7716, 587.5226, 604.3232, 669.3209, 698.7581, 748.6942, 858.8646, 895.0221, 1069.7381, 1085.3498, 1119.4200, 1206.0798, 1212.6063, 1280.9879, 1324.0728

Compound: sCl 4 + SO_2 $TS_{SO_3}1$	**Energy (kJ mol^{-1}):** -1173.50370754569
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.668664 -0.237000 -0.168337 6 -0.413921 0.543417 0.338601 8 0.072233 0.141382 1.476579 8 3.097138 0.560455 -0.262500 9 -0.662681 1.866634 0.289683 9 -1.413638 -1.547102 -0.141910 9 -2.696874 0.019967 0.647230 9 -2.010279 0.093547 -1.420071 16 1.984108 -0.352264 -0.343062 8 0.640213 0.337422 -0.821845 8 1.415545 -1.051721 0.869394	-607.2684, 31.0897, 62.5197, 107.9680, 179.7528, 222.9153, 286.2726, 331.5185, 356.5920, 359.3231, 416.2636, 459.0275, 516.0829, 524.9626, 555.8419, 589.5866, 657.4417, 730.7599, 799.7264, 891.7564, 939.3861, 1099.1259, 1187.0108, 1199.5459, 1221.4319, 1289.6165, 1338.8248

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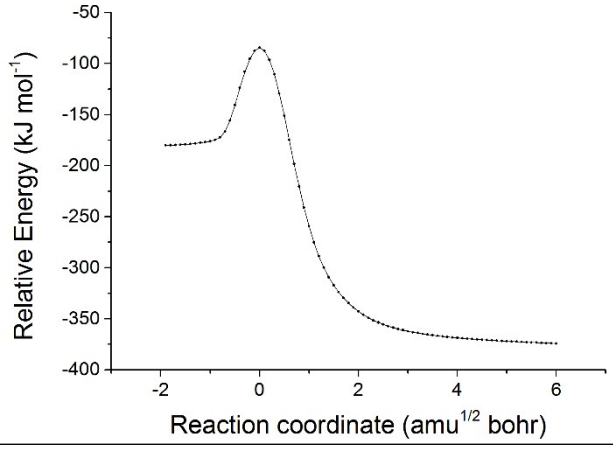

Compound: sC4 + SO_2 $C_{SO_3}1$	**Energy (kJ mol^{-1}):** -1173.62784782028
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.480382 -0.197438 -0.000000 6 0.990324 0.225637 0.000003 8 0.063167 -0.503181 0.000008 8 -2.590732 0.669827 -1.245757 9 0.890156 1.550175 0.000000 9 3.086529 0.290825 1.087804 9 2.581707 -1.519403 0.000001 9 3.086524 0.290823 -1.087808 16 -2.691450 -0.044144 -0.000001 8 -2.590737 0.669888 1.245720 8 -2.952357 -1.458369 0.000033	10.6507, 20.4972, 25.4670, 42.7300, 56.9356, 89.3577, 107.8055, 231.8421, 243.1069, 383.0292, 423.8821, 467.4804, 509.3791, 509.7174, 513.3808, 586.9497, 694.4524, 769.1260, 806.4467, 1047.9805, 1106.0690, 1173.2322, 1229.7700, 1312.0304, 1364.8420, 1369.6582, 1912.9001

Compound: sCl 4 + SO_2 $TSso_32$	**Energy (kJ mol^{-1}):** -1173.51911565224
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.641991 -0.377135 0.066413 6 0.404346 0.615056 0.020625 8 -0.092071 0.826587 1.179483 8 -1.946170 1.079105 0.567999 9 0.765621 1.706244 -0.698967 9 2.081261 -0.628174 -1.164642 9 2.621593 0.200698 0.760119 9 1.298166 -1.516645 0.654253 16 -2.052978 -0.132169 -0.311558 8 -0.570151 -0.129146 -0.905302 8 -2.432874 -1.423038 0.221049	-454.1605, 58.6418, 74.9140, 139.1367, 193.4154, 225.2846, 294.4132, 309.7366, 334.7464, 376.4847, 434.5312, 460.9770, 527.9330, 545.8351, 554.8277, 580.4535, 666.8636, 739.8676, 800.0289, 902.6551, 974.8452, 1057.3650, 1180.4144, 1203.0018, 1225.8099, 1268.3720, 1310.7709

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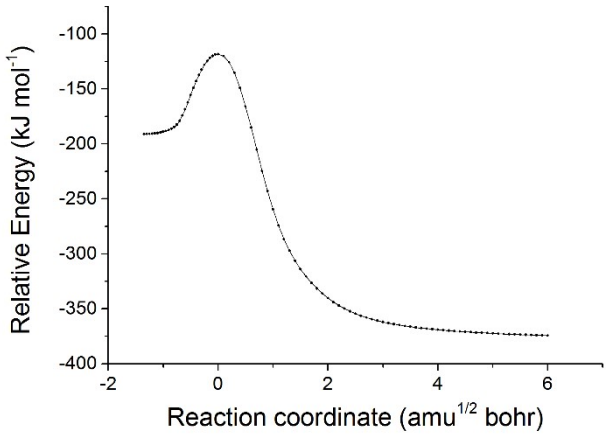

Compound: sCl 4 + SO_2 $TSso_3$3	**Energy (kJ mol^{-1}):** -1173.51026243837
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.780248 -0.026481 -0.181348 6 -0.330964 0.078455 0.433961 8 0.018791 -0.951516 1.110358 8 1.770743 -1.335123 0.367013 9 -0.228904 1.275837 1.075993 9 -2.059986 1.043211 -0.922984 9 -1.873485 -1.118473 -0.933310 9 -2.663251 -0.100650 0.814656 16 2.057744 -0.116000 -0.470885 8 0.547504 0.247348 -0.835633 8 2.809712 0.994895 0.071922	-517.8014, 60.7850, 75.0296, 117.7628, 168.3618, 223.2707, 288.8933, 321.0568, 357.7665, 401.9041, 413.9117, 439.8401, 510.8812, 541.3957, 552.9248, 588.5194, 646.5623, 741.3055, 796.7976, 905.0981, 950.8611, 1049.9909, 1201.1346, 1203.7136, 1221.8266, 1267.7164, 1289.7390

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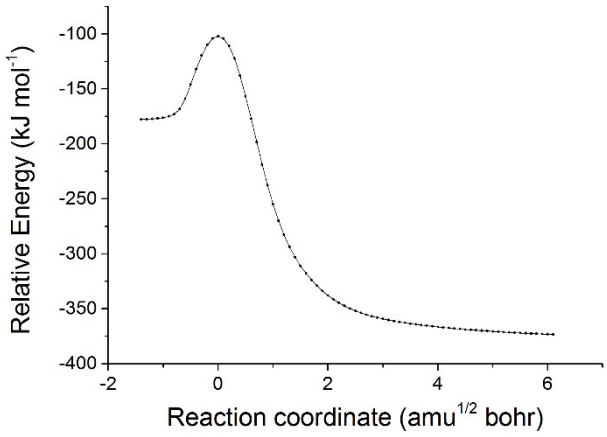

Compound: sCl 4 + SO_2 $TS_{ester}1$	**Energy (kJ mol^{-1}):** -1173.49144000029
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.813541 -0.425632 0.042717 6 0.274173 0.730620 0.067894 8 0.066864 0.917325 1.254961 8 -2.497059 -1.481374 0.252421 9 0.702671 1.753524 -0.724793 9 2.118193 -0.700091 -1.194231 9 1.518967 -1.476391 0.744034 9 2.726344 0.316466 0.605889 16 -2.171217 -0.197071 -0.337911 8 -0.408018 -0.192280 -0.697802 8 -2.334586 1.041535 0.423522	-432.3408, 52.1672, 65.8122, 74.4737, 101.0197, 173.4216, 204.0668, 237.4051, 246.1582, 261.4374, 324.8358, 399.0983, 480.5209, 522.8040, 543.1451, 550.5618, 617.6896, 642.3351, 750.8306, 865.2657, 965.8175, 1056.6910, 1092.7159, 1283.7314, 1295.9325, 1334.5393, 1561.5094
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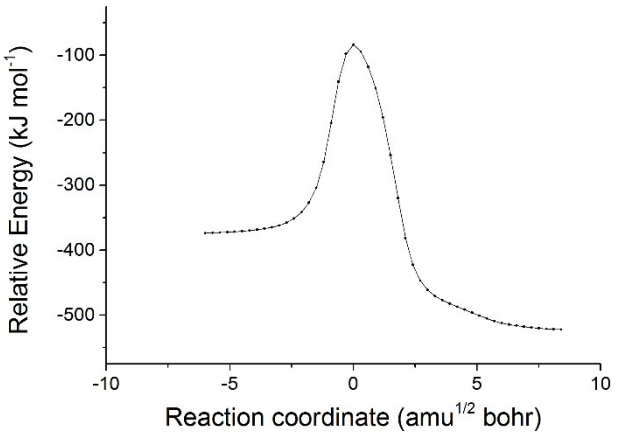

Compound: sCl 4 + SO_2 $C_{ester}1$	**Energy (kJ mol^{-1}):** -1173.67282156150
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.246873 -0.570136 0.101837 8 1.940832 0.791280 0.167279 6 0.721378 1.198058 -0.243863 8 -0.171463 0.557311 -0.672656 9 0.693301 2.509378 -0.080159 9 1.426723 -1.287616 0.858143 9 2.198158 -1.015942 -1.147950 9 3.482804 -0.683183 0.560926 16 -3.222589 -0.092447 -0.196467 8 -3.110889 0.436899 1.151248 8 -3.215600 -1.534503 -0.361245	4.0162, 9.3991, 10.7021, 33.6407, 46.7280, 80.6640, 87.7644, 108.0431, 178.9699, 377.6690, 401.8068, 427.2020, 516.1418, 551.9297, 609.9868, 669.3564, 739.3163, 777.5055, 882.0199, 1027.4147, 1136.8106, 1158.2408, 1231.0917, 1248.0268, 1282.9061, 1335.0611, 1909.4847

Compound: sCl 4 + SO_2 $TS_{ester}2$	**Energy (kJ mol^{-1}):** -1173.48550327144
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.928820 -0.043969 -0.274499 9 -2.756202 0.164973 0.713137 9 -2.017816 0.864366 -1.198659 9 -2.036458 -1.257296 -0.737470 6 -0.230013 0.172164 0.564537 8 -0.217642 1.305626 1.000133 9 -0.229429 -0.888169 1.431347 8 0.377679 -0.215843 -0.633797 16 2.166005 -0.028066 -0.515698 8 2.322683 1.308562 0.047720 8 2.724287 -1.182719 0.165411	-484.6874, 18.2260, 52.9006, 73.6833, 96.9497, 157.9094, 184.7185, 237.6844, 242.4637, 268.2822, 319.2501, 401.4810, 492.4707, 513.6895, 538.3604, 550.0115, 599.3580, 656.1937, 759.4240, 827.2184, 963.3271, 1011.3589, 1097.8469, 1282.8564, 1293.6220, 1328.5142, 1574.4308

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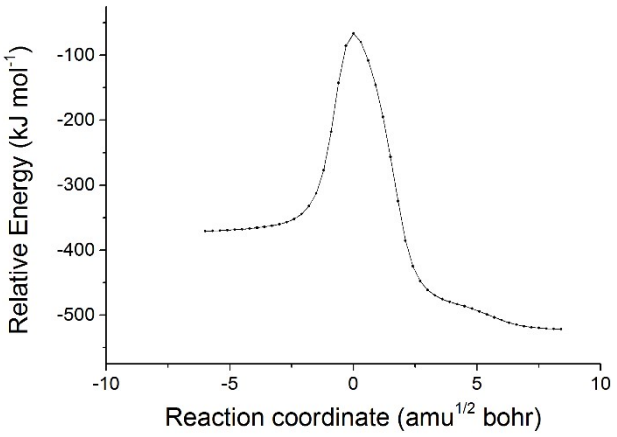


Compound: sCl 4 + SO_2 $C_{ester}2$	**Energy (kJ mol^{-1}):** -1173.67290696018
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.575150 -0.328946 0.000001 9 2.302730 -1.047093 -1.083133 9 3.857326 -0.002343 -0.000075 9 2.302824 -1.046954 1.083252 8 1.874870 0.878202 -0.000047 6 0.524808 0.841279 0.000013 9 0.119153 2.097405 -0.000051 8 -0.191560 -0.096475 0.000103 8 -3.554650 0.056304 -1.243433 16 -3.276802 -0.639925 0.000012 8 -3.554811 0.056426 1.243351	5.3901, 13.1636, 13.2084, 35.5690, 48.4244, 83.3192, 87.0781, 108.4973, 181.3048, 378.5363, 402.3076, 427.2285, 516.3645, 552.1696, 609.9813, 670.0603, 739.8784, 777.3801, 881.6767, 1029.0054, 1139.0554, 1158.2309, 1228.1209, 1248.4840, 1284.6130, 1334.6173, 1907.1417

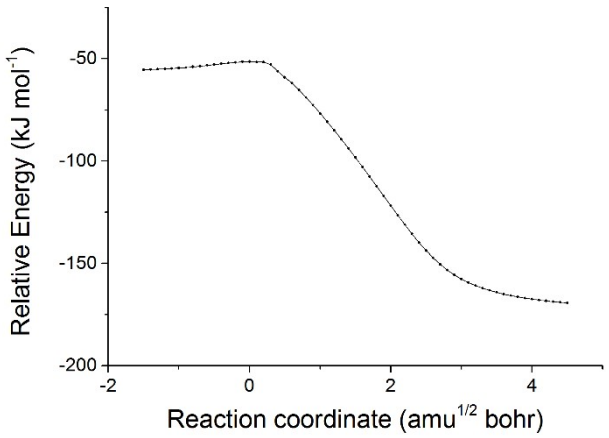
S8.4 Reactions with HNO_3

Compound: HNO_3	**Energy (kJ mol^{-1}):** -280.649387120256
Reaction Coordinates:	**Frequencies (cm^{-1}):**
7 0.152578 0.031983 0.000001 8 -1.152277 -0.512972 -0.000001 1 -1.719886 0.275568 0.000002 8 0.214973 1.237996 -0.000000 8 1.018784 -0.787456 -0.000000	479.4853, 584.8104, 646.7663, 783.1012, 896.0178, 1315.3030, 1341.5904, 1744.4127, 3711.8876

Compound: sCI 1 + HNO_3 PRC	**Energy (kJ mol^{-1}):** -470.072694506353
Reaction Coordinates:	**Frequencies (cm^{-1}):**
7 1.496892 -0.134866 -0.004943 8 0.667020 -1.033235 0.097948 8 2.688425 -0.260005 -0.068599 8 1.033607 1.141055 -0.058826 1 0.017702 1.095134 0.053631 6 -2.072567 -1.012782 0.120554 1 -2.498385 -1.822306 -0.459681 1 -1.658928 -1.120610 1.114625 8 -2.091056 0.101544 -0.429116 8 -1.535900 1.159208 0.283930	52.2249, 78.8218, 102.2949, 138.9453, 196.7530, 265.7980, 511.6154, 649.6811, 676.6982, 698.8865, 799.8732, 841.0081, 972.2831, 981.5672, 1060.8488, 1235.4845, 1308.1266, 1425.6956, 1481.8275, 1597.1874, 1708.0574, 2730.1492, 3121.7345, 3266.4971

Compound: sCI 1 + HNO_3 TS	**Energy (kJ mol^{-1}):** -470.068648204036
Reaction Coordinates:	**Frequencies (cm^{-1}):**
7 1.382578 -0.063861 -0.008349 8 0.628369 -1.058966 0.034369 8 2.580436 -0.135427 -0.065503 8 0.846896 1.149168 0.004906 1 -0.251112 1.114260 0.091169 6 -1.671765 -1.057011 0.209054 1 -1.838608 -2.006498 -0.286142 1 -1.395054 -0.967906 1.249688 8 -1.962928 -0.044666 -0.454559 8 -1.613108 1.171046 0.199461	-248.9265, 39.6720, 92.4916, 198.5650, 324.0410, 328.8518, 500.7085, 660.3195, 702.1595, 736.2226, 801.4920, 819.3851, 1019.9294, 1047.0691, 1133.6644, 1160.2011, 1235.8102, 1425.0247, 1489.9202, 1598.7784, 1614.2350, 1818.4260, 3129.3696, 3269.8948

IRC



Compound: sCI 1 + HNO_3 Pr	**Energy (kJ mol^{-1}):** -470.123652687780
Reaction Coordinates:	**Frequencies (cm^{-1}):**
7 1.319520 0.088216 0.023524 8 0.339308 -0.963575 -0.181566 8 2.203213 0.022791 -0.773304 8 1.153464 0.838501 0.944072 1 -2.557702 1.413878 -0.088671 6 -0.881066 -0.827107 0.545024 1 -1.176279 -1.846124 0.792990 1 -0.722852 -0.212452 1.427306 8 -1.915046 -0.352282 -0.253432 8 -1.717616 1.078293 -0.431574	59.4191, 85.4098, 119.9476, 176.7737, 319.2844, 409.9451, 490.4761, 609.3846, 649.9965, 762.5552, 827.8298, 879.8808, 967.8881, 1053.3829, 1314.9395, 1324.3246, 1376.4783, 1413.3481, 1450.9690, 1729.9552, 3075.3309, 3143.0899, 3755.3317

Compound: sCI 2 + HNO_3 PRC	**Energy (kJ mol^{-1}):** -806.869427684078
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.515030 -0.052204 -0.107496 6 1.389569 -0.745025 0.644316 1 1.560507 -1.689924 1.142933 8 0.227784 -0.294611 0.738235 8 -0.080258 0.887326 0.149683 9 2.227109 0.088467 -1.399867 9 3.605581 -0.830507 0.003357 9 2.793296 1.139411 0.420540 7 -3.324819 -0.165770 -0.101840 8 -2.563876 -1.114006 -0.129467 8 -4.520237 -0.167655 -0.204149 8 -2.760562 1.079774 0.072769 1 -1.771052 0.930738 0.116199	10.6140, 29.7830, 41.8008, 71.7241, 87.0513, 112.6532, 156.6378, 230.4114, 250.4582, 346.9186, 480.9087, 511.7626, 534.9130, 590.1757, 637.4624, 683.9769, 759.8603, 795.8386, 829.4514, 880.5639, 898.0185, 915.0071, 944.1144, 1161.7325, 1192.1409, 1241.8657, 1328.2504, 1371.8255, 1456.0238, 1578.6816, 1718.6016, 3124.6857, 3206.9984

Compound: sCI 2 + HNO_3 TS	**Energy (kJ mol^{-1}):** -806.865419736050
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.457042 -0.475653 -0.141690 6 0.852838 0.357702 1.001659 1 1.011599 -0.015041 2.007643 8 0.497497 1.549201 0.927013 8 0.160563 1.992571 -0.376021 9 2.631826 0.100273 -0.447165 9 0.735781 -0.596154 -1.240535 9 1.705108 -1.697626 0.349632 7 -2.096267 -0.333890 0.053274 8 -1.146941 -0.657051 0.801488 8 -3.113098 -0.960538 -0.038094 8 -1.997430 0.768090 -0.684379 1 -1.056180 1.263359 -0.537811	-203.8987, 49.4921, 52.7535, 87.1304, 156.0214, 182.5010, 225.3687, 278.4959, 313.8332, 331.5867, 435.8589, 494.9747, 533.3277, 566.1095, 672.6409, 713.0831, 749.8274, 795.0142, 821.6187, 871.5104, 928.1138, 1012.3118, 1072.1094, 1156.5460, 1157.5824, 1203.4557, 1278.5401, 1364.2600, 1517.8599, 1612.8964, 1678.5251, 1999.6916, 3181.7398

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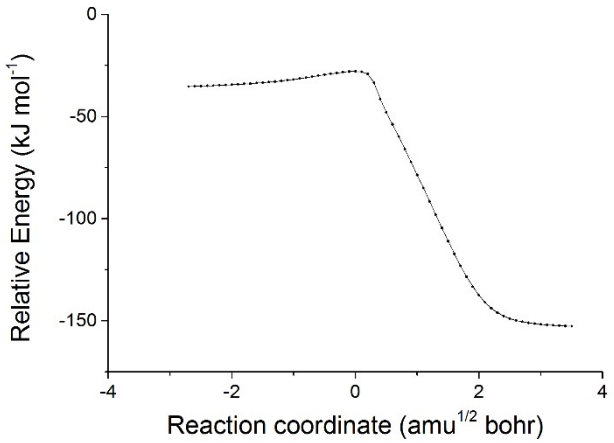
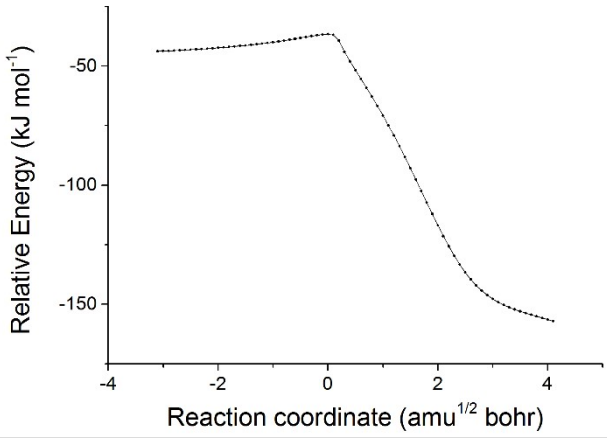


Compound: sCI 2 + HNO_3 Pr	**Energy (kJ mol^{-1}):** -806.932710531538
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.234029 -0.565793 0.129147 6 -0.349089 0.145478 -0.926576 1 -0.712055 -0.170001 -1.906167 8 -0.403111 1.520637 -0.953015 8 -0.576378 2.097828 0.361211 1 0.337481 2.085119 0.692904 8 0.970650 -0.458847 -0.960221 7 1.946953 -0.186099 0.064084 8 2.831375 -0.979569 0.047569 8 1.800977 0.790017 0.754362 9 -2.448500 -0.017571 0.164558 9 -0.709971 -0.557213 1.359726 9 -1.368583 -1.853111 -0.240951	44.3668, 69.3809, 93.2717, 165.4610, 193.4546, 225.3272, 240.7962, 311.0701, 340.0379, 373.9625, 427.2332, 497.8110, 521.5399, 571.7072, 598.0567, 692.9346, 751.7581, 791.1962, 835.0732, 879.9702, 908.8883, 950.6032, 1108.0501, 1146.4447, 1199.1320, 1261.5324, 1325.5211, 1370.8742, 1383.7320, 1426.0054, 1726.0957, 3084.8214, 3675.8920

Compound: sCI 3 + HNO_3 PRC	**Energy (kJ mol^{-1}):** -806.873300576158
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.112628 -0.328139 0.028361 6 0.908402 0.441619 -0.483405 1 0.465875 0.214030 -1.445228 8 0.470057 1.364109 0.223449 8 -0.606103 2.078684 -0.261243 9 1.843444 -1.636496 -0.000813 9 2.452909 0.025482 1.261816 9 3.148127 -0.092228 -0.796140 7 -2.653927 -0.536448 -0.005582 8 -1.512598 -0.885133 -0.284588 8 -3.621877 -1.233995 0.095295 8 -2.859805 0.794106 0.223427 1 -1.972286 1.247236 0.060069	21.4603, 39.8574, 42.1601, 82.6932, 121.6740, 130.1110, 185.7289, 193.1965, 279.0018, 384.2481, 408.0808, 414.2012, 549.8226, 560.8570, 642.0486, 692.4597, 699.3590, 796.8093, 883.5112, 893.9237, 921.1985, 934.1911, 964.5752, 1152.1060, 1186.0423, 1272.6374, 1309.2140, 1361.4585, 1467.2626, 1597.6705, 1714.9508, 2962.3969, 3199.0004

Compound: sCI 3 + HNO_3 TS	**Energy (kJ mol^{-1}):** -806.868520205216
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.818613 -0.336853 0.015696 6 0.680377 0.567369 -0.455800 1 0.360756 0.545037 -1.488749 8 0.341153 1.489782 0.307661 8 -0.741762 2.259824 -0.211481 9 1.744065 -1.513427 -0.599055 9 1.807029 -0.513721 1.330099 9 2.975078 0.255896 -0.335374 7 -2.227662 -0.599860 -0.008985 8 -1.026866 -0.871200 -0.254858 8 -3.079524 -1.435682 0.103724 8 -2.586961 0.664416 0.137561 1 -1.744927 1.355041 -0.029616	-260.2949, 27.4937, 40.4603, 88.1780, 105.7760, 179.0839, 203.4849, 275.8988, 319.4801, 377.8967, 409.7391, 454.2256, 548.0832, 575.2912, 655.4133, 700.2323, 714.5006, 798.0752, 842.4628, 879.2374, 953.5183, 1023.6301, 1113.2491, 1146.1651, 1152.6934, 1201.8256, 1269.3687, 1355.5625, 1491.3837, 1604.5822, 1620.3004, 1807.0887, 3208.5505

IRC

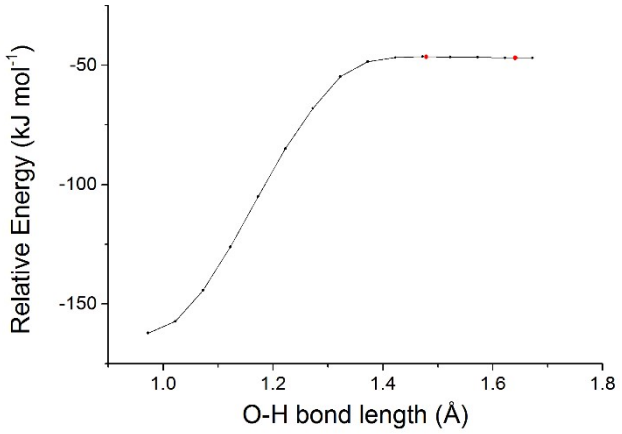


Compound: sCl 3 + HNO_3 Pr	**Energy (kJ mol^{-1}):** -806.931663308635
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.554013 -0.423933 -0.077892 6 0.164526 0.246695 -0.151113 1 -0.026945 0.562928 -1.173348 8 0.130797 1.346934 0.710919 8 -0.158323 2.541173 -0.049835 1 -1.116845 2.619476 0.077256 8 -0.738620 -0.763913 0.274806 7 -2.123510 -0.506101 -0.059810 8 -2.841991 -1.374969 0.312222 8 -2.360662 0.517636 -0.645814 9 1.603211 -1.485321 -0.897005 9 1.854320 -0.826693 1.159300 9 2.481083 0.455219 -0.476695	49.4586, 57.3126, 79.0791, 84.2792, 143.7444, 200.6062, 254.1429, 293.8911, 327.8966, 346.1094, 396.5055, 460.3064, 534.3509, 564.3218, 632.4380, 686.2828, 735.0960, 768.6991, 831.3235, 896.1398, 956.4319, 1034.0722, 1083.2847, 1165.6245, 1186.5185, 1265.2167, 1315.8773, 1363.6233, 1367.2948, 1402.3144, 1735.4845, 3121.9660, 3715.7873

Compound: sCl 4 + HNO_3 PRC	**Energy (kJ mol^{-1}):** -906.045603878535
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.658334 0.372214 0.473504 6 1.097655 -0.333428 -0.787865 9 1.505255 0.115087 -1.928174 8 0.375536 -1.332887 -0.814800 8 -0.098135 -1.807086 0.428713 9 0.703171 0.787599 1.281294 9 2.381676 1.417913 0.071727 9 2.455978 -0.487057 1.107298 7 -2.601910 0.376304 -0.044351 8 -1.580861 0.753597 -0.602810 8 -3.656535 0.942884 0.004730 8 -2.555480 -0.829958 0.598602 1 -1.613484 -1.181122 0.491835	16.2163, 36.9939, 57.1225, 63.5689, 97.7905, 148.4175, 177.8060, 206.6922, 232.4838, 295.4329, 326.5404, 364.4840, 479.4276, 504.9650, 581.2690, 625.4322, 646.2131, 689.5643, 693.3045, 778.4011, 796.2974, 908.9884, 915.6068, 960.0898, 1154.7636, 1195.1805, 1236.8306, 1317.4677, 1410.4083, 1478.1360, 1633.9975, 1716.9084, 2949.9386

Compound: sCI 4 + HNO_3 TS	**Energy (kJ mol^{-1}):** -906.045088871693
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.398496 -0.436428 -0.468817 6 0.867915 0.352803 0.765201 9 1.204294 -0.149419 1.903834 8 0.443344 1.516117 0.791631 8 -0.032299 1.992907 -0.477231 9 1.702773 -1.669054 -0.072328 9 2.524212 0.191170 -0.837436 9 0.572753 -0.496022 -1.489867 7 -2.249696 -0.361885 0.046000 8 -1.207449 -0.703022 0.633327 8 -3.263342 -0.998166 0.032105 8 -2.260915 0.801357 -0.617246 1 -1.321586 1.271330 -0.538819	-59.3438, 41.5877, 45.9090, 81.3198, 146.6454, 182.1514, 202.5032, 222.6189, 271.4277, 289.0449, 340.0328, 368.7527, 476.7036, 511.9915, 584.5135, 618.8684, 662.2343, 671.8021, 717.1168, 778.5606, 796.8572, 913.2326, 1001.6289, 1052.8716, 1137.9920, 1188.2205, 1246.8738, 1258.8145, 1399.1859, 1525.1097, 1626.9631, 1707.7546, 2259.7416

IRC

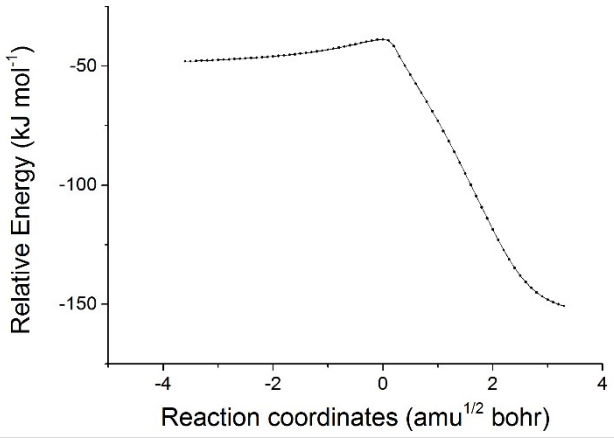


Compound: sCI 4 + HNO_3 Pr	**Energy (kJ mol^{-1}):** -906.106548786604
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.227307 -0.388855 -0.480905 6 0.286623 -0.045093 0.725794 9 0.807811 -0.639351 1.815327 8 0.136881 1.282818 1.051278 8 0.468229 2.163071 -0.038453 1 -0.399261 2.247293 -0.469648 8 -0.957084 -0.760446 0.587626 7 -2.061352 -0.183353 -0.162301 8 -3.001400 -0.904766 -0.146699 8 -1.908607 0.888922 -0.681185 9 2.401415 0.221046 -0.353700 9 0.674689 -0.061869 -1.653575 9 1.431750 -1.710595 -0.479619	44.8465, 68.6884, 90.0800, 170.5517, 192.8878, 215.5921, 220.9380, 292.2829, 303.6735, 329.7248, 378.8194, 385.4820, 439.3492, 486.2138, 534.3046, 589.1877, 605.8283, 733.3051, 735.8503, 759.7463, 794.2091, 817.1514, 973.8141, 1002.2183, 1112.1058, 1174.8338, 1190.1717, 1216.3470, 1324.8542, 1344.1334, 1428.7677, 1744.5606, 3684.7511

Compound: sCI 5 + HNO_3 PRC	**Energy (kJ mol^{-1}):** -906.050679111630
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.024036 -0.408554 -0.156972 6 -0.898435 0.547176 0.259645 9 -0.631948 0.608199 1.510031 8 -0.341672 1.256494 -0.586459 8 0.674143 2.112512 -0.136549 9 -1.770253 -1.623626 0.317061 9 -2.134048 -0.448742 -1.475439 9 -3.171585 0.032730 0.373663 7 2.638426 -0.592217 -0.022548 8 1.462692 -0.892302 0.143819 8 3.584626 -1.326169 -0.000491 8 2.919907 0.722010 -0.265209 1 2.038779 1.216373 -0.226934	-342.4923, 28.9714, 49.3276, 82.5971, 111.5724, 174.9899, 207.6669, 232.6207, 279.7650, 309.1249, 355.8683, 366.6454, 409.2298, 501.2836, 577.5929, 604.5163, 676.6835, 720.4099, 732.5958, 797.3823, 829.3727, 869.4917, 1027.6151, 1063.0087, 1141.1869, 1163.0930, 1198.8878, 1257.3653, 1389.4405, 1472.1235, 1595.3393, 1632.8779, 1786.9313

Compound: sCI 5 + HNO_3 TS	**Energy (kJ mol^{-1}):** -906.046705839706
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.742183 -0.435894 -0.157683 6 -0.650973 0.584244 0.238844 9 -0.525944 0.808845 1.494184 8 -0.237295 1.366965 -0.637231 8 0.816568 2.232361 -0.169389 9 -1.731318 -1.463165 0.675897 9 -1.565256 -0.847937 -1.401863 9 -2.924779 0.191290 -0.062463 7 2.212431 -0.656382 0.002688 8 1.005196 -0.854236 0.295766 8 3.032763 -1.530154 0.004117 8 2.608305 0.559055 -0.321911 1 1.793287 1.311347 -0.228389	-342.4923, 28.9714, 49.3276, 82.5971, 111.5724, 174.9899, 207.6669, 232.6207, 279.7650, 309.1249, 355.8683, 366.6454, 409.2298, 501.2836, 577.5929, 604.5163, 676.6835, 720.4099, 732.5958, 797.3823, 829.3727, 869.4917, 1027.6151, 1063.0087, 1141.1869, 1163.0930, 1198.8878, 1257.3653, 1389.4405, 1472.1235, 1595.3393, 1632.8779, 1786.9313

IRC



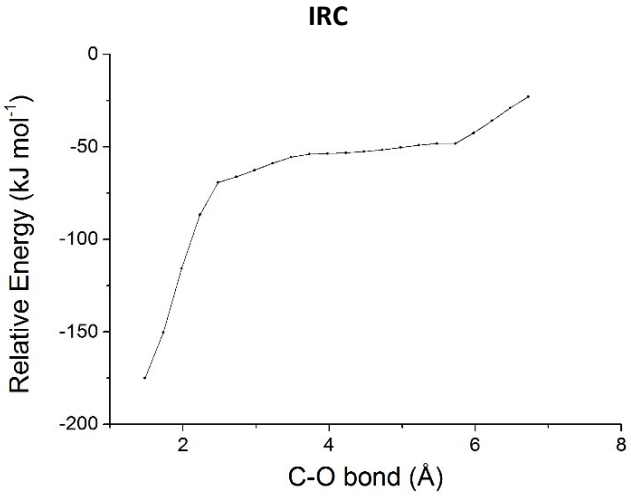
Compound: sCI 5 + HNO_3 Pr	**Energy (kJ mol^{-1}):** -906.107641820181
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.465714 -0.616502 -0.018853 6 -0.115197 0.174139 0.129909 9 -0.052168 0.626231 1.411907 8 0.029375 1.215056 -0.779855 8 -0.915161 2.264455 -0.484275 1 -0.365195 2.867713 0.039005 8 0.871098 -0.747902 -0.156537 7 2.324097 -0.279474 -0.042045 8 3.035235 -1.130435 -0.445880 8 2.511379 0.791426 0.427935 9 -1.437120 -1.713019 0.746717 9 -1.643942 -0.981473 -1.289204 9 -2.497153 0.135148 0.363674	35.8609, 48.3223, 97.7733, 106.6229, 136.6438, 216.4055, 218.5739, 253.9864, 277.4184, 303.7563, 362.2100, 388.0438, 420.9834, 486.3317, 532.0771, 574.0953, 591.9207, 684.5924, 740.6256, 752.6333, 787.4242, 825.9496, 976.3362, 1070.5744, 1118.2801, 1131.5996, 1199.1168, 1211.7936, 1299.2723, 1364.2598, 1411.7186, 1805.9040, 3725.8754

S8.5 Reactions with TFA

Compound: TFA (CF_3COOH) conformer 1	**Energy (kJ mol^{-1}):** -526.396690747069
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.600232 -0.000700 0.000001 6 -0.943150 0.162408 0.000002 8 -1.495890 1.220466 0.000000 8 -1.526983 -1.040018 0.000002 1 -2.487822 -0.910329 -0.000003 9 0.999822 -0.678016 -1.087812 9 1.192393 1.189052 0.000043 9 0.999820 -0.678091 1.087766	30.3904, 237.0884, 242.9524, 384.3951, ,420.8035, 503.5971, 582.5530, 595.2069, 666.0224, 787.6331, 791.1373, 1135.0381, 1156.4050, 1192.2434, 1246.2417, 1400.8344, 1853.8568, 3732.4833

Compound: sCI 1 + TFA PRC	**Energy (kJ mol^{-1}):** -715.814752163838
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.117654 -0.201348 -0.000023 6 -0.740521 0.519046 0.000004 8 -0.649473 1.715143 -0.000182 8 0.232966 -0.368608 0.000253 1 1.134260 0.077798 0.000265 9 -2.248565 -0.983360 1.087847 9 -3.118080 0.678690 -0.000299 9 -2.248314 -0.983755 -1.087640 6 4.708687 -0.314834 -0.000181 1 5.296134 -1.223034 -0.000511 1 5.113259 0.690859 0.000074 8 3.472618 -0.479587 -0.000102 8 2.679877 0.637179 0.000306	15.3101, 29.2792, 36.3834, 50.1211, 77.4504, 101.5880, 169.1057, 257.8198, 279.2418, 395.5788, 433.3071, 515.8541, 550.4847, 591.1333, 681.1988, 706.1226, 780.6440, 807.7600, 880.7623, 972.0749, 1018.4284, 1141.8677, 1169.1472, 1202.8182, 1242.1331, 1335.0572, 1418.3576, 1486.5195, 1576.3894, 1824.8056, 3021.8298, 3114.8857, 3264.5288

Compound:	sCI 1 + TFA TS reaction profile

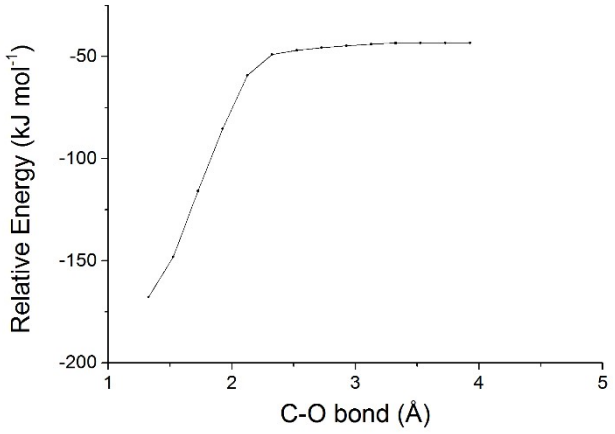


Compound: sCI 1 + TFA Pr	**Energy (kJ mol^{-1}):** -715.871685168671
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.697881 0.022687 0.042552 6 0.163468 0.215542 -0.116231 8 -0.437279 -0.958119 -0.095178 8 -0.330901 1.305557 -0.235475 1 -2.196182 1.415419 -0.011856 9 2.182883 -0.686901 -0.989582 9 2.314212 1.200094 0.072752 9 1.976930 -0.636459 1.175780 6 -1.892893 -1.058709 -0.328960 1 -2.076150 -2.112990 -0.142555 1 -2.090489 -0.767998 -1.358185 8 -2.652048 -0.337966 0.557765 8 -3.044039 0.927759 -0.027376	26.1591, 61.2351, 109.7878, 146.1666, 202.8784, 235.0052, 284.5678, 340.3942, 425.7682, 460.6063, 515.6973, 550.8166, 556.4842, 587.4142, 741.1113, 785.3393, 817.4884, 856.4786, 912.6225, 1084.6461, 1146.4313, 1157.7037, 1164.2388, 1217.5341, 1304.1561, 1338.5859, 1429.5640, 1470.8223, 1479.9155, 1804.5397, 3083.1395, 3158.9283, 3560.1146

Compound: sCI 2 + TFA PRC	**Energy (kJ mol^{-1}):** -1052.601700422370
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -3.799697 -0.091409 -0.000002 6 -2.347221 0.459861 -0.000005 8 -2.108307 1.633985 -0.000084 8 -1.484502 -0.540871 0.000090 1 -0.547214 -0.201783 0.000087 9 -4.020862 -0.851857 1.087808 9 -4.685788 0.902500 -0.000097 9 -4.020806 -0.852015 -1.087714 6 2.986750 -1.120937 -0.000139 1 3.407058 -2.117903 -0.000289 6 3.892144 0.100749 0.000001 9 5.160273 -0.346119 -0.000099 9 3.707438 0.844929 1.088662 9 3.707372 0.845228 -1.088443 8 1.736864 -1.066737 -0.000094 8 1.120900 0.141888 0.000090	7.4879, 14.3532, 20.6102, 31.1970, 55.4650, 76.5639, 94.0482, 96.9370, 212.7209, 246.4799, 256.8046, 272.6323, 344.7727, 397.8334, 434.7728, 480.6449, 513.6752, 515.4363, 534.8743, 588.9227, 589.4324, 700.5560, 761.7026, 777.5234, 804.9535, 826.1389, 882.6705, 910.8651, 921.5577, 1144.3144, 1159.2873, 1167.2045, 1194.3575, 1203.5754, 1241.3283, 1319.8137, 1369.8098, 1464.7495, 1574.1753, 1831.1291, 3185.8483, 3207.3049

Compound: sCI 2 + TFA TS reaction profile

IRC

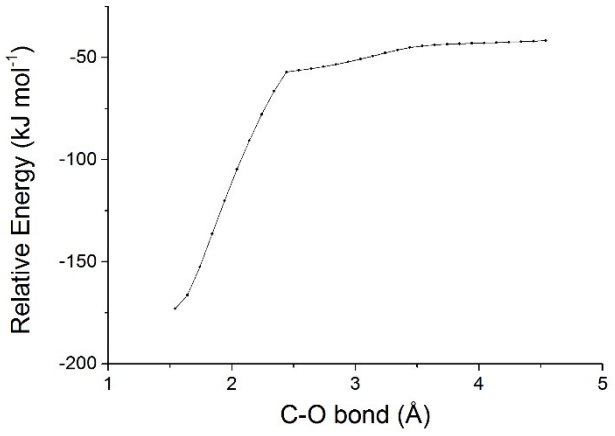


Compound: sCI 2 + TFA Pr	**Energy (kJ mol^{-1}):** -1052.676223405220
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.466755 -0.218822 -0.010253 6 1.077154 0.480250 -0.048466 8 0.223035 -0.229661 0.676838 8 0.898034 1.503630 -0.647334 1 -0.795315 2.179440 -0.631200 9 2.920504 -0.276317 1.250781 9 2.376110 -1.467759 -0.486261 9 3.341071 0.457006 -0.747324 6 -1.184517 0.121186 0.891958 1 -1.378609 -0.275710 1.886916 6 -2.012724 -0.706613 -0.124124 9 -1.906052 -2.007793 0.205177 9 -1.584011 -0.572463 -1.382367 9 -3.299166 -0.365633 -0.056782 8 -1.472670 1.453093 0.975477 8 -1.716172 2.040048 -0.324908	20.9216, 46.4107, 59.5233, 66.9627, 140.9286, 180.6824, 208.0201, 222.3190, 241.0757, 274.9078, 308.1438, 334.1048, 362.8241, 433.7150, 463.3602, 517.3656, 523.8811, 555.0554, 587.9584, 609.8561, 615.5457, 729.8126, 772.5619, 776.2809, 802.3635, 872.2091, 915.3374, 953.1669, 1107.5102, 1140.5180, 1162.3852, 1165.8355, 1202.4495, 1221.0011, 1267.8230, 1322.9942, 1382.6886, 1408.0581, 1477.9667, 1816.0211, 3111.6009, 3521.6190

Compound: sCI 3 + TFA PRC	**Energy (kJ mol^{-1}):** -1052.615934886960
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -3.826946 -0.368024 -0.000004 6 -2.584060 0.564096 -0.000003 8 -2.680549 1.758804 -0.000038 8 -1.477753 -0.157249 0.000039 1 -0.672574 0.431164 0.000037 9 -3.828923 -1.159749 1.087783 9 -4.953816 0.341783 -0.000036 9 -3.828888 -1.159792 -1.087759 6 2.969286 0.773171 0.000006 1 3.182798 1.836550 0.000002 6 4.078973 -0.256742 -0.000008 9 4.845283 -0.070606 1.085930 9 4.845246 -0.070616 -1.085974 9 3.615989 -1.499861 0.000006 8 1.792081 0.363588 0.000023 8 0.792750 1.288215 0.000034	8.0185, 13.9625, 17.7010, 31.4483, 52.0818, 71.8914, 86.6937, 120.1090, 190.2986, 210.7532, 256.8293, 275.0837, 386.6084, 394.2236, 396.0285, 421.2855, 451.0603, 515.4830, 554.8464, 559.4263, 589.1000, 698.3424, 705.4141, 777.8235, 805.1851, 889.5173, 920.3806, 930.2730, 947.7599, 1144.8606, 1151.5780, 1165.9538, 1177.1230, 1203.4499, 1274.2055, 1321.6529, 1361.6588, 1469.0207, 1581.1019, 1829.5164, 3173.9935, 3180.2493

Compound: sCI 3 + TFA TS reaction profile

IRC

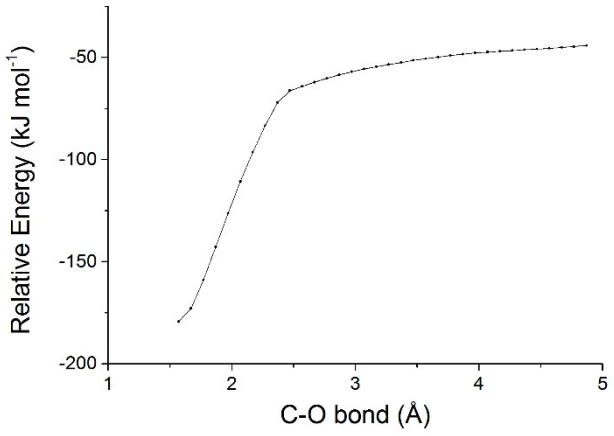


Compound: sCI 3 + TFA Pr	**Energy (kJ mol^{-1}):** -1052.680470535266
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.483742 -0.372757 0.043442 6 1.223571 0.514359 -0.157311 8 0.130443 -0.232202 -0.054291 8 1.287584 1.692255 -0.374094 1 -0.321270 2.775251 -0.088311 9 3.581760 0.373543 -0.007121 9 2.436718 -0.993124 1.228581 9 2.548991 -1.301029 -0.922371 6 -1.164747 0.389585 -0.277037 1 -1.228744 0.736793 -1.306612 6 -2.179111 -0.747309 -0.045264 9 -2.159505 -1.183022 1.216602 9 -1.911159 -1.779682 -0.857902 9 -3.407912 -0.300273 -0.326609 8 -1.428419 1.408876 0.610965 8 -1.293451 2.685692 -0.053664	17.8491, 45.2659, 57.3567, 85.9303, 91.0158, 151.4031, 198.4283, 211.4683, 224.0042, 267.5022, 321.0179, 347.0376, 363.7984, 417.9770, 437.2892, 506.6700, 519.4156, 526.9220, 556.0132, 568.8105, 623.4046, 705.7929, 743.5205, 783.8159, 844.5009, 924.0822, 935.2929, 966.8157, 1099.5354, 1155.7595, 1167.5156, 1170.7616, 1193.8652, 1221.3136, 1272.0266, 1319.1611, 1369.9295, 1392.6546, 1461.7710, 1815.8484, , 3107.3684, 3594.7285

Compound: sCI 4 + TFA PRC	**Energy (kJ mol^{-1}):** -1151.785667585767
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -4.026188 0.115087 -0.000003 6 -2.590419 -0.478626 0.000010 8 -2.387789 -1.660124 0.000042 8 -1.698604 0.494542 -0.000019 1 -0.769777 0.125201 -0.000013 9 -4.225296 0.881788 -1.087785 9 -4.941674 -0.852194 0.000027 9 -4.225289 0.881850 1.087737 6 2.783742 0.841986 0.000010 9 3.411589 1.974591 0.000026 6 3.639321 -0.443219 -0.000005 9 4.924581 -0.087026 0.000003 9 3.385389 -1.156257 -1.088876 9 3.385383 -1.156287 1.088843 8 1.548119 0.894821 0.000007 8 0.850635 -0.318584 -0.000011	7.5674, 12.4297, 19.3225, 31.2593, 50.4704, 72.6003, 74.4628, 94.2524, 216.1131, 223.6194, 256.7145, 267.3417, 268.5318, 320.3421, 365.0210, 398.2187, 434.9504, 492.4184, 502.1436, 515.5134, 583.1883, 588.9652, 634.5484, 681.7848, 703.3383, 778.2821, 779.5247, 806.1318, 916.0536, 931.0692, 1144.0082, 1159.5167, 1167.1897, 1203.5568, 1210.5858, 1215.0487, 1326.4277, 1409.5507, 1475.7611, 1612.9563, 1828.5912, 3134.7645

Compound: sCI 4 + TFA TS reaction profile

IRC

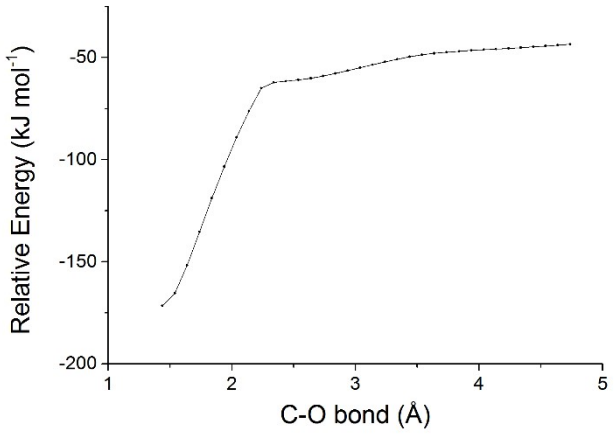


Compound: sCI 4 + TFA Pr	**Energy (kJ mol^{-1}):** -1052.676223405220
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.570852 -0.220706 -0.048599 6 1.190871 0.497624 -0.075921 8 0.283900 -0.301589 0.489465 8 1.044352 1.588401 -0.545206 1 -0.664295 2.301576 -0.536636 9 3.492197 0.545148 -0.621273 9 2.937107 -0.467545 1.215532 9 2.502004 -1.383092 -0.709593 6 -1.101065 0.050357 0.709143 9 -1.402883 -0.578986 1.851964 6 -1.936484 -0.600185 -0.449206 9 -1.876419 -1.929874 -0.319117 9 -1.443070 -0.281041 -1.649312 9 -3.207065 -0.219797 -0.371946 8 -1.331892 1.376630 0.958426 8 -1.583557 2.108129 -0.257954	20.2362, 43.7482, 55.1268, 71.0110, 130.8120, 182.2072, 200.8834, 216.0355, 230.5157, 259.6638, 289.3327, 312.5332, 347.1908, 356.0338, 399.2152, 434.5129, 490.6210, 515.8851, 523.0897, 560.4187, 596.1424, 614.6958, 622.2812, 679.8581, 747.6963, 769.5610, 778.4174, 874.1228, 952.1876, 996.2569, 1112.7478, 1154.2816, 1169.0466, 1189.6280, 1209.4820, 1220.9972, 1226.1166, 1321.2883, 1351.3150, 1478.4904, 1827.5146, 3538.5897

Compound: sCI 5 + TFA PRC	**Energy (kJ mol^{-1}):** -1151.790445383220
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 4.041057 -0.371401 -0.006528 6 2.784865 0.542457 -0.033261 8 2.860138 1.727432 -0.196890 8 1.695334 -0.181267 0.147064 1 0.879129 0.394538 0.130234 9 3.966641 -1.314052 -0.963965 9 5.150320 0.337787 -0.206780 9 4.150014 -0.995914 1.180402 6 -2.746033 0.517700 0.030689 9 -3.121296 1.746140 0.046299 6 -3.846116 -0.543715 -0.034636 9 -4.564366 -0.357332 -1.144769 9 -4.648539 -0.404246 1.023560 9 -3.319784 -1.757664 -0.040486 8 -1.552125 0.186312 0.064841 8 -0.603184 1.197866 0.120465	10.8869, 16.0276, 18.2924, 33.1220, 39.6677, 68.5474, 72.3076, 109.6280, 158.5230, 203.3723, 257.2177, 263.1301, 323.1912, 339.7670, 376.5955, 402.9848, 407.9736, 441.1388, 515.5822, 519.6200, 576.9508, 589.1252, 690.4387, 700.7299, 732.6585, 778.2141, 805.1062, 866.9637, 878.4136, 931.1100, 1143.9517, 1159.9433, 1166.6482, 1175.0592, 1203.4005, 1242.0594, 1324.6173, 1404.8743, 1470.9930, 1632.4361, 1829.4762, 3145.9245

Compound: sCI 5 + TFA TS reaction profile

IRC



Compound: sCl 5 + TFA Pr	**Energy (kJ mol^{-1}):** -1151.857358431300
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.478273 -0.365041 0.052667 6 -1.231413 0.534401 -0.189079 8 -0.195732 0.002265 0.469856 8 -1.274726 1.527937 -0.851783 1 0.139962 2.699595 -0.432420 9 -3.536735 0.153442 -0.559265 9 -2.258822 -1.595347 -0.428923 9 -2.738447 -0.458172 1.362722 6 1.185449 0.380691 0.339739 9 1.599361 0.605801 1.597192 6 1.928243 -0.878655 -0.221274 9 1.470194 -1.176197 -1.441770 9 1.716059 -1.919260 0.583947 9 3.236846 -0.646728 -0.291123 8 1.475822 1.397572 -0.509050 8 0.999621 2.647248 0.032861	16.5182, 35.7526, 42.6654, 58.4852, 128.4627, 176.2977, 193.2411, 204.6366, 231.9707, 261.3122, 277.9253, 325.7491, 342.7255, 366.9216, 381.0447, 427.6308, 485.9296, 514.6093, 529.4620, 555.3729, 562.0244, 587.2120, 642.9921, 722.2777, 750.2701, 769.7615, 816.3052, 860.7169, 949.7770, 1006.6998, 1096.7814, 1147.6885, 1168.4412, 1201.0525, 1210.1647, 1225.0795, 1225.6274, 1317.1342, 1334.0822, 1463.8412, 1831.1421, 3559.6296

S8.6 Reactions with HF

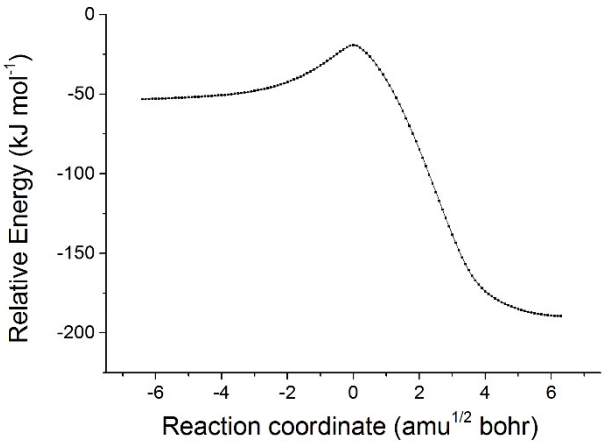
sCI 1 + HF

Compound: HF	**Energy (kJ mol^{-1}):** -100.388736810254
Reaction Coordinates:	**Frequencies (cm^{-1}):**
9 0.000000 0.000000 0.092410 1 0.000000 0.000000 -0.831689	4072.1142

Compound: sCI 1 + HF PRC	**Energy (kJ mol^{-1}):** -289.808532547218
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.968789 -0.977363 -0.000007 1 1.860439 -1.590782 0.000013 1 -0.050820 -1.352498 -0.000039 8 1.192344 0.252290 0.000012 8 0.149073 1.146514 -0.000009 1 -1.194974 0.358284 -0.000001 9 -1.906524 -0.304584 0.000005	79.1803, 152.0807, 307.7401, 557.6608, 691.8667, 864.2225, 887.5397, 1046.3924, 1095.0887, 1278.6763, 1433.0717, 1562.9479, 3045.8930, 3102.0931, 3246.6880

Compound: sCI 1 + HF TS	**Energy (kJ mol^{-1}):** -289.791769474177
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.304787 1.051637 0.223711 1 -0.360805 2.020957 -0.260655 1 0.124674 0.914501 1.204044 8 -0.967644 0.141252 -0.333197 8 -0.540291 -1.132555 0.180239 1 0.624123 -0.809496 0.047753 9 1.500468 -0.056152 -0.123305	-829.2644, 336.8971, 483.6272, 530.5988, 696.5045, 765.8268, 835.9935, 1117.4420, 1197.3750, 1234.8638, 1420.0552, 1580.7735, 1822.9523, 3125.6008, 3268.4885

IRC

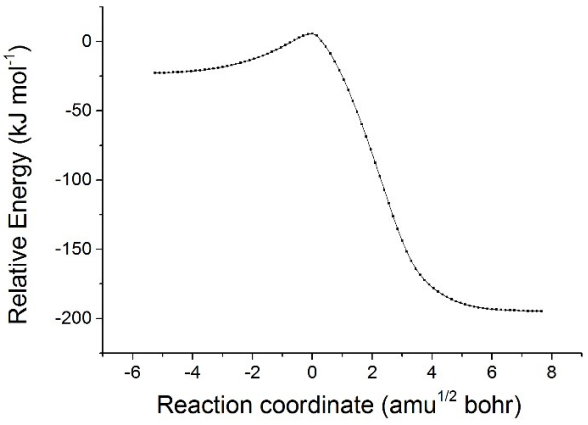


Compound: sCI 1 + HF Pr	**Energy (kJ mol^{-1}):** -289.865197002865
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.631649 0.519902 0.269119 1 1.175202 1.409728 -0.049661 1 0.499281 0.459144 1.348441 8 -0.574863 0.581176 -0.391641 8 -1.469572 -0.389753 0.211664 1 -1.362095 -1.142101 -0.388781 9 1.361467 -0.597507 -0.120544	168.4645, 277.9778, 421.6778, 595.9358, 882.7828, 995.6691, 1077.0262, 1160.2288, 1287.4215, 1383.4539, 1415.0926, 1480.2425, 3056.8428, 3125.4267, 3737.5366

Compound: sCI 2 + HF PRC	**Energy (kJ mol^{-1}):** -626.606991675634
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.371755 0.052827 0.000001 6 -0.311811 -1.035991 -0.000000 1 -0.594705 -2.080061 0.000002 8 0.919805 -0.815171 -0.000003 8 1.370679 0.461411 -0.000005 9 -2.569662 -0.558544 0.000006 9 -1.289552 0.816787 -1.088349 9 -1.289546 0.816792 1.088347 1 3.031578 0.273012 -0.000001 9 3.964389 0.095644 0.000003	26.9508, 54.9483, 84.1009, 132.1838, 246.9818, 247.4661, 354.7131, 480.7731, 510.2538, 534.0738, 590.3146, 749.8774, 756.3514, 821.6079, 866.9841, 896.0442, 918.1111, 1161.0342, 1191.3784, 1242.0397, 1370.7088, 1572.2553, 3208.6780, 3509.336

Compound: sCI 2 + HF TS	**Energy (kJ mol^{-1}):** -626.586057924863
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.889086 -0.029145 0.056776 6 0.302863 -0.341538 -0.860655 1 0.039340 -0.360371 -1.915298 8 1.376077 -0.931380 -0.588680 8 1.887292 -0.545928 0.692138 9 -1.656484 -1.145380 -0.046981 9 -1.575119 0.987143 -0.465474 9 -0.652471 0.193255 1.329209 1 1.652604 0.682188 0.400681 9 1.186123 1.489509 -0.204506	-744.6703, 64.3780, 155.9795, 218.8689, 290.9263, 305.9879, 388.0168, 478.4261, 514.3063, 536.6919, 562.2071, 731.4878, 809.2587, 838.2783, 880.0394, 1017.9591, 1097.0831, 1182.4137, 1196.0533, 1309.7201, 1372.5351, 1594.9569, 1789.9811, 3154.0510

IRC

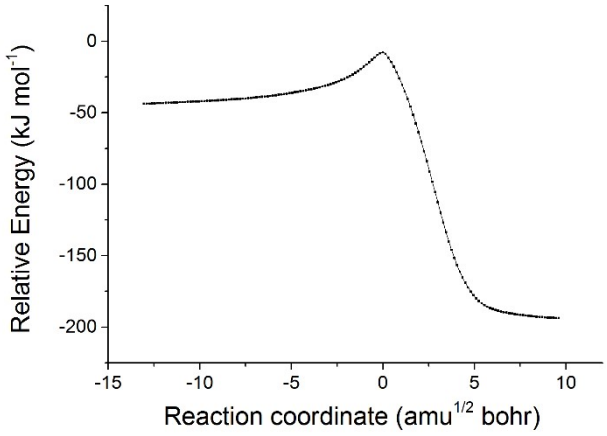


Compound: sCI 2 + HF Pr	**Energy (kJ mol^{-1}):** -626.673546284392
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.834570 -0.148326 0.006261 6 0.403604 0.587437 -0.563339 1 0.154218 0.966869 -1.556157 8 1.519250 -0.186749 -0.771280 8 1.871523 -0.876548 0.454931 9 -1.921667 0.615688 -0.223556 9 -0.766233 -0.375379 1.316841 9 -1.007864 -1.313996 -0.628918 1 2.545035 -0.281518 0.817457 9 0.669137 1.649949 0.270295	56.8425, 135.9833, 203.5157, 232.7615, 265.9833, 305.1939, 368.6668, 433.8158, 523.9364, 580.0369, 619.4572, 762.1754, 860.2378, 911.8567, 1057.9257, 1104.4746, 1150.6938, 1188.4176, 1283.4743, 1344.2761, 1394.2047, 1408.6765, 3084.3933, 3733.0817

Compound: sCI 3 + HF PRC	**Energy (kJ mol^{-1}):** -626.610016871772
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.276051 0.122225 0.000000 6 0.238154 0.075338 0.000006 1 0.838781 0.982707 0.000012 8 0.768267 -1.055007 -0.000001 8 2.128693 -1.184191 0.000001 9 -1.691044 0.792038 -1.086257 9 -1.691051 0.792061 1.086241 9 -1.825166 -1.087203 0.000011 1 2.778804 0.267521 -0.000000 9 2.922163 1.222879 -0.000001	25.8279, 77.5369, 107.2193, 170.3821, 207.5782, 288.9583, 383.9496, 395.5151, 441.0878, 557.4098, 560.1105, 699.9805, 843.3993, 888.2642, 940.8348, 962.1647, 1046.2065, 1153.2153, 1187.3539, 1277.1579, 1388.8897, 1567.4454, 3116.9891, 3196.4029

Compound: sCI 3 + HF TS	**Energy (kJ mol^{-1}):** -626.592526379491
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.096361 -0.003094 -0.004462 6 -0.359680 -0.155275 -0.438103 1 -0.663416 0.236291 -1.398539 8 -1.066073 -0.963183 0.210641 8 -2.446944 -0.742017 -0.123188 9 1.292227 -0.377960 1.252167 9 1.472246 1.263687 -0.159861 9 1.844629 -0.776019 -0.813585 1 -2.284641 0.482190 0.001683 9 -1.649980 1.431772 0.093791	-850.5241, 34.8760, 114.4545, 182.7985, 287.3622, 336.1011, 376.2820, 453.9894, 513.0961, 549.5780, 621.8010, 675.8334, 751.4147, 869.5333, 909.5337, 990.2752, 1150.4901, 1190.6701, 1203.7874, 1284.1834, 1363.3160, 1575.9778, 1814.8849, 3212.0268

IRC

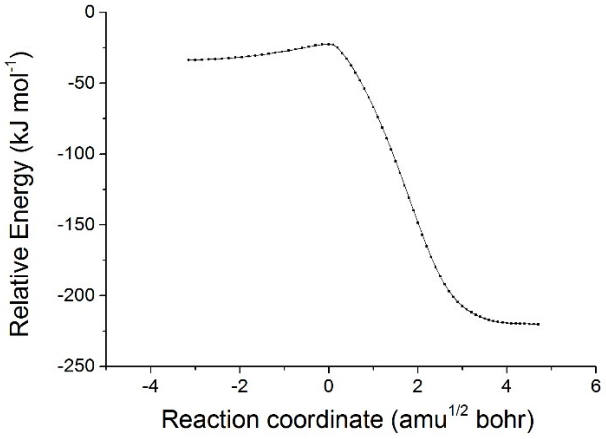


Compound: sCI 3 + HF Pr	**Energy (kJ mol^{-1}):** -626.675135107360
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.969274 -0.137135 -0.021241 6 -0.481096 0.279164 -0.340046 1 -0.659604 0.233344 -1.414282 8 -1.307314 -0.572338 0.355007 8 -2.626661 -0.476319 -0.234610 9 1.816862 0.714657 -0.615447 9 1.209603 -1.366423 -0.497401 9 1.215729 -0.131085 1.291727 1 -3.077769 0.085638 0.413486 9 -0.655516 1.584862 0.066159	65.4287, 108.2183, 184.1493, 231.2871, 271.0036, 350.3917, 357.5479, 394.4965, 522.2061, 565.1454, 617.2866, 716.1753, 879.1933, 954.1929, 1050.5288, 1128.3522, 1171.5778, 1185.5722, 1272.5277, 1359.8608, 1390.0408, 1400.2829, 3095.2578, 3732.6363

Compound: sCl 4 + HF PRC	**Energy (kJ mol^{-1}):** -725.776277323618
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.869815 -0.421998 -0.153846 6 -0.057258 0.866122 0.122023 9 -0.705444 1.716305 0.859512 8 1.041347 1.252070 -0.287829 8 1.874968 0.393522 -1.032891 9 -1.160303 -0.995607 1.009684 9 -0.271405 -1.272555 -0.951345 9 -2.015111 -0.010512 -0.727888 1 2.114898 -0.665378 0.158952 9 1.943042 -1.122532 0.987564	39.0244, 59.7387, 76.7172, 200.0033, 227.3232, 252.6997, 259.1565, 334.3436, 367.7980, 483.1061, 505.5070, 571.4816, 615.5282, 690.0793, 772.8026, 790.5163, 904.4336, 1008.4787, 1127.7364, 1176.1445, 1275.3385, 1391.3018, 1613.3843, 3263.4439

Compound: sCl 4 + HF TS	**Energy (kJ mol^{-1}):** -725.769990619824
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.911285 -0.279396 -0.087736 6 0.299622 0.697087 -0.086988 9 -0.032873 1.863438 0.356311 8 1.359429 0.666224 -0.746314 8 1.914009 -0.673218 -0.801520 9 -1.555553 -0.185057 1.066053 9 -0.621937 -1.530199 -0.352728 9 -1.709117 0.200215 -1.066745 1 1.697315 -0.807733 0.510584 9 1.228942 -0.530892 1.432714	-380.2160, 57.5077, 139.3986, 207.0471, 239.1676, 263.7697, 320.3367, 363.6198, 390.7479, 486.7055, 527.9314, 592.5551, 610.0036, 681.7931, 781.8620, 904.2735, 1094.1675, 1117.9363, 1172.3312, 1246.5506, 1283.4670, 1385.0778, 1607.1290, 1837.8803

IRC

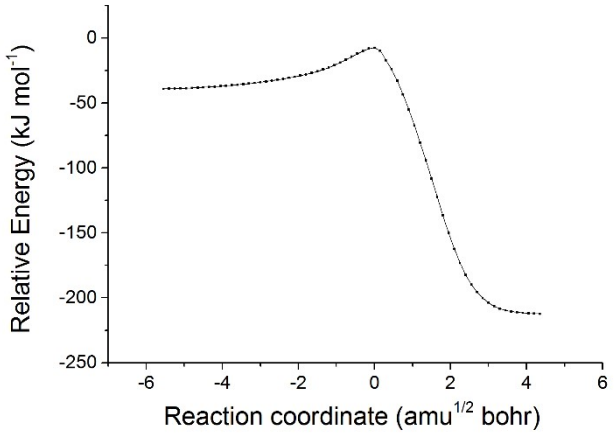


Compound: sCl 4 + HF Pr	**Energy (kJ mol^{-1}):** -725.857806332430
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.889167 -0.292627 -0.009267 6 0.415104 0.571256 0.005386 9 0.164758 1.722671 -0.629602 8 1.490616 0.038298 -0.679680 8 1.861000 -1.213187 -0.064101 9 -1.914062 0.459599 0.411129 9 -0.792497 -1.353455 0.790426 9 -1.142632 -0.705041 -1.253049 1 2.609374 -0.935161 0.485985 9 0.731328 0.838726 1.290825	39.7363, 126.2403, 202.0897, 225.5792, 249.4652, 288.7103, 343.6012, 376.3539, 399.9664, 489.8662, 531.6127, 590.5430, 653.5497, 687.2684, 782.6821, 980.2959, 1090.2120, 1155.7713, 1192.3813, 1201.6568, 1214.8916, 1350.7749, 1413.8516, 3727.6606

Compound: sCl 5 + HF PRC	**Energy (kJ mol^{-1}):** -725.783185514069
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.346110 0.061678 -0.133186 6 0.098792 -0.185894 0.312407 9 0.521788 0.510871 1.301754 8 0.788018 -1.043836 -0.255240 8 2.103466 -1.228631 0.181675 9 -1.485883 1.341631 -0.475855 9 -2.163912 -0.201940 0.891456 9 -1.655856 -0.715041 -1.159465 1 2.712299 0.234128 -0.283211 9 2.743833 1.141245 -0.580512	30.4167, 43.0085, 72.9994, 156.8884, 180.1979, 258.9762, 302.7274, 353.6017, 371.6271, 405.6737, 519.5743, 576.0599, 697.7263, 726.7195, 729.3323, 852.1026, 862.2567, 943.3627, 1160.6948, 1179.4724, 1241.3002, 1404.9745, 1636.1444, 3393.8484

Compound: sCl 5 + HF TS	**Energy (kJ mol^{-1}):** -725.770085507023
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.160862 -0.032260 -0.105695 6 0.320445 -0.209963 0.292269 9 0.608204 0.190085 1.479794 8 1.027540 -1.005634 -0.363899 8 2.432868 -0.685533 -0.155085 9 -1.328521 -0.276154 -1.394517 9 -1.554072 1.199715 0.183001 9 -1.888106 -0.903457 0.609456 1 2.131169 0.574495 -0.392815 9 1.410058 1.390720 -0.497152	-665.3587, 34.4507, 114.8127, 178.8817, 256.6845, 300.9149, 309.4190, 360.2051, 402.1590, 431.0590, 525.5625, 578.3785, 668.3228, 719.8528, 823.8600, 842.9141, 1036.0573, 1142.1647, 1151.2266, 1195.4510, 1254.3528, 1400.3879, 1606.9244, 1817.2889

IRC

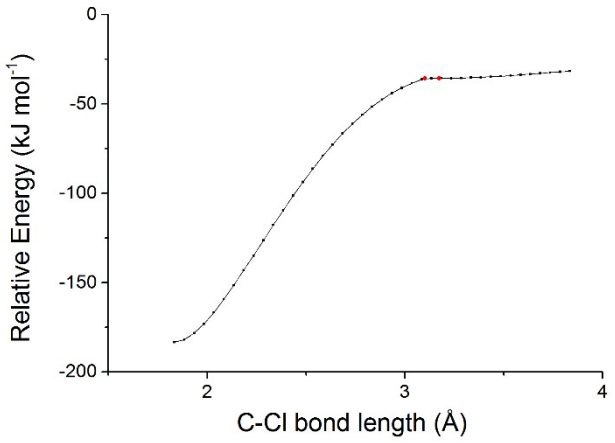


Compound: sCl 5 + HF Pr	**Energy (kJ mol^{-1}):** -725.860158374757
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.071132 -0.164947 -0.001594 6 -0.426713 0.274719 -0.004529 9 -0.640177 1.108402 -1.036237 8 -1.174458 -0.867810 -0.087232 8 -2.571414 -0.496277 -0.117625 9 1.845035 0.918898 0.084820 9 1.369026 -0.819623 -1.124342 9 1.322689 -0.957224 1.043687 1 -2.829982 -0.688425 0.797048 9 -0.682080 0.965379 1.129688	60.1460, 121.4786, 168.5796, 220.2847, 255.1560, 295.0352, 336.5640, 374.0731, 376.8953, 523.2280, 529.6868, 594.5260, 606.2032, 738.2555, 833.3664, 943.2474, 1094.1752, 1144.8046, 1184.4607, 1206.5191, 1211.8461, 1345.0714, 1411.1882, 3726.8452

S8.7 Reactions with HCl

Compound: HCl	**Energy (kJ mol^{-1}):** -460.373228449128
Reaction Coordinates: 17 0.000000 0.000000 0.071311 1 0.000000 0.000000 -1.212290	**Frequencies (cm^{-1}):** 2935.7855

Compound: sCI 1 + HCL PRC	**Energy (kJ mol^{-1}):** -649.786096409260
Reaction Coordinates: 6 -1.336144 1.008146 0.177187 1 -1.868220 1.826217 -0.292080 1 -0.680692 1.112214 1.032231 8 -1.535125 -0.111981 -0.335374 8 -0.828331 -1.180579 0.194099 1 0.554522 -0.654641 0.096022 17 1.701112 0.118107 -0.045241	**Frequencies (cm^{-1}):** 60.4557, 176.4811, 230.4019, 509.8882, 663.3721, 754.8100, 850.5504, 1022.5705, 1035.4059, 1244.4996, 1423.1906, 1578.1814, 11.5544:13, 1619.2991, 1528.6350, 3120.4571, 3265.3577

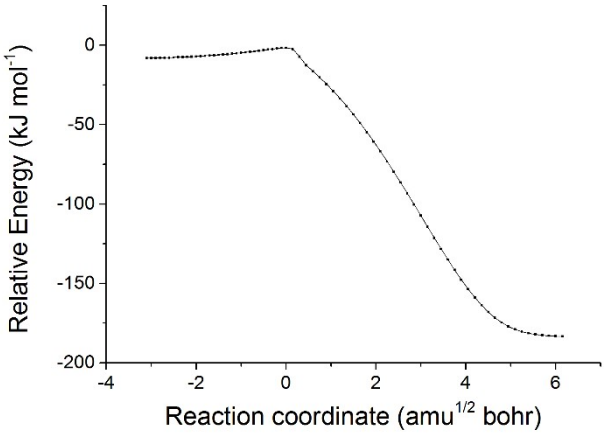
Compound: sCI 1 + HCL TS	**Energy (kJ mol^{-1}):** -649.785673633254
Reaction Coordinates: 6 -1.290274 1.012234 0.181602 1 -1.794768 1.846515 -0.290202 1 -0.647019 1.095745 1.047673 8 -1.515281 -0.099860 -0.338189 8 -0.822644 -1.182523 0.193323 1 0.504896 -0.678863 0.099185 17 1.669526 0.113074 -0.046314	**Frequencies (cm^{-1}):** -93.7733, 179.6707, 237.6760, 498.5803, 659.3270, 803.9659, 842.1572, 1033.4816, 1060.7591, 1247.6658, 1385.9919, 1428.7903, 1579.5775, 3122.0712, 3266.8750
IRC	
	

Compound: sCI 1 + HCL Pr	**Energy (kJ mol^{-1}):** -649.851301605594
Reaction Coordinates: 6 0.003850 0.838496 0.263509 1 0.297621 1.812033 -0.116982 1 -0.155121 0.828835 1.337016 8 -1.125194 0.483448 -0.438558 8 -1.737316 -0.651057 0.217450 1 -1.350257 -1.388632 -0.279390 17 1.416749 -0.290726 -0.044285	**Frequencies (cm^{-1}):** 143.1167, 260.0739, 365.5883, 494.0492, 664.4717, 877.6148, 996.3526, 1078.6954, 1267.3400, 1322.2118, 1390.8227, 1456.2616, 3091.0927, 3169.7044, 3717.0894

Compound: sCl 2 + HCL PRC	**Energy (kJ mol^{-1}):** -986.587116795699
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.914503 -0.050458 0.000001 6 -0.847721 1.030051 -0.000000 1 -1.123123 2.075925 0.000001 8 0.383224 0.799262 -0.000004 8 0.828024 -0.476783 -0.000006 9 -3.108809 0.568984 0.000006 9 -1.839190 -0.816240 1.088202 9 -1.839196 -0.816235 -1.088204 1 2.617586 -0.277000 -0.000004 17 3.910215 -0.040288 0.000002	18.7102, 37.3389, 83.0612, 92.6607, 213.5202, 246.5783, 337.0294, 479.6058, 504.7996, 533.0463, 534.5479, 590.3170, 642.5689, 762.8747, 814.3955, 883.6309, 920.2579, 1159.4939, 1188.9489, 1241.8058, 1369.4349, 1565.8153, 2527.4977, 3209.9424

Compound: sCl 2 + HCL TS	**Energy (kJ mol^{-1}):** -986.576964395944
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.137573 -0.246816 -0.047542 6 -0.290786 0.621775 0.888296 1 -0.577372 0.576857 1.933905 8 0.466574 1.578942 0.609843 8 1.039573 1.594156 -0.656418 9 -1.287606 -1.449642 0.511022 9 -0.741805 -0.374196 -1.292953 9 -2.349561 0.364692 -0.044438 1 1.696166 0.354117 -0.489858 17 2.047819 -0.907835 0.077726	-358.2410, 48.0071, 105.4872, 151.4765, 218.8015, 291.2973, 302.2909, 431.4392, 491.8270, 528.5665, 560.3076, 734.0336, 813.2396, 820.9045, 858.0104, 896.8840, 1023.7636, 1096.4000, 1188.0244, 1307.9946, 1370.7250, 1398.7693, 1581.5061, 3174.8648

IRC

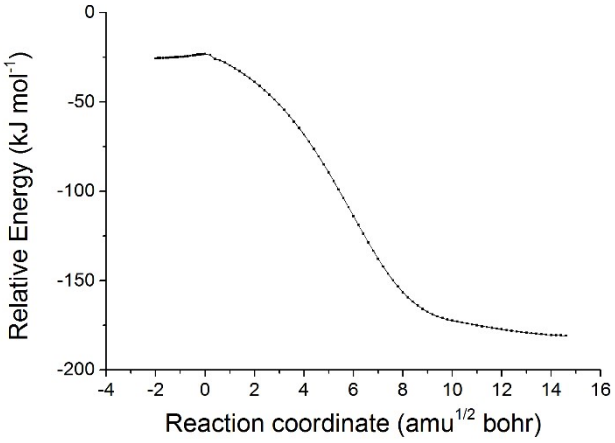


Compound: sCl 2 + HCL Pr	**Energy (kJ mol^{-1}):** -986.659667626854
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.016093 -0.086265 0.021645 6 -0.362052 -0.043383 -0.679606 1 -0.215083 -0.351869 -1.712506 8 -0.930566 1.207428 -0.779110 8 -1.082098 1.795492 0.533299 9 1.623303 -1.247388 -0.288003 9 0.963234 0.009638 1.348314 9 1.778337 0.913227 -0.447178 1 -1.999280 1.557641 0.741066 17 -1.464261 -1.266502 0.080441	59.1331, 127.2325, 176.6045, 208.4503, 234.4071, 305.8910, 328.7563, 382.3320, 505.5717, 524.4360, 577.9461, 715.5376, 806.8403, 845.2028, 905.7538, 1083.8250, 1135.3758, 1167.9676, 1262.5845, 1268.2043, 1380.2082, 1398.1375, 3116.5427, 3717.2765

Compound: sCI 3 + HCL PRC	**Energy (kJ mol^{-1}):** -986.588821076460
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.582120 -0.230508 0.004148 6 0.216761 0.291935 0.403795 1 -0.350700 -0.175656 1.199747 8 -0.219477 1.289563 -0.205145 8 -1.454922 1.771203 0.136133 9 1.479664 -1.523676 -0.327477 9 2.406751 -0.134788 1.061239 9 2.105067 0.442975 -1.013836 1 -2.403940 0.424704 0.044861 17 -2.856870 -0.833197 -0.036442	21.7466, 41.5599, 106.4836, 157.8438, 195.5869, 236.1469, 381.4594, 399.6774, 414.5187, 550.3914, 559.1233, 605.1213, 699.8698, 797.7048, 886.7464, 909.3514, 939.2583, 1151.0214, 1182.2896, 1273.7220, 1365.0410, 1572.7375, 2192.8173, 3188.7321

Compound: sCI 3 + HCL TS	**Energy (kJ mol^{-1}):** -986.585206698211
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.475079 0.187092 -0.003645 6 0.113282 -0.345669 -0.423827 1 -0.380015 0.037238 -1.307222 8 -0.350271 -1.303630 0.229611 8 -1.634527 -1.704090 -0.136852 9 1.424826 1.518227 0.057538 9 2.368854 -0.162839 -0.945122 9 1.869014 -0.298242 1.166832 1 -2.230512 -0.494197 -0.058986 17 -2.470912 0.938580 0.039749	-400.1643, 26.3909, 67.7722, 177.8239, 199.7647, 266.5886, 373.9922, 399.3114, 423.0809, 539.4095, 564.3907, 685.5681, 723.5873, 842.5092, 873.5717, 899.9578, 1006.9712, 1152.7589, 1193.0976, 1275.6814, 1348.0393, 1369.7483, 1576.1347, 3208.3909

IRC

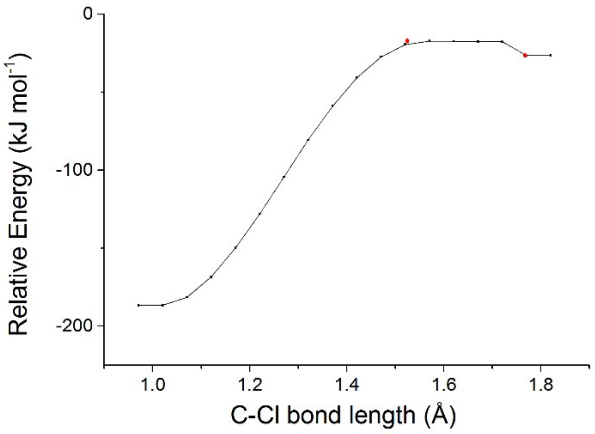


Compound: sCI 3 + HCL Pr	**Energy (kJ mol^{-1}):** -986.660655427993
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.117713 -0.163739 -0.020203 6 -0.382956 -0.078604 -0.356523 1 -0.522871 -0.220769 -1.424751 8 -1.013282 -1.059037 0.380371 8 -2.293145 -1.322743 -0.231825 9 1.796699 0.773587 -0.693662 9 1.589405 -1.363303 -0.395803 9 1.356619 -0.008933 1.284400 1 -2.885091 -0.816900 0.346833 17 -1.013745 1.584342 0.023264	62.6223, 105.0812, 183.4353, 187.3409, 251.3766, 322.8491, 339.7521, 364.9799, 461.5709, 534.4284, 562.4427, 700.6468, 762.1871, 878.4267, 954.3954, 1100.9976, 1141.3416, 1180.7016, 1259.3337, 1285.8863, 1358.3179, 1399.9080, 3119.8932, 3717.5641

Compound: sCI 4 + HCL PRC	**Energy (kJ mol^{-1}):** -1085.756886776330
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.788499 -0.376521 -0.000005 6 0.756492 0.768406 0.000006 9 1.213983 1.981969 -0.000002 8 -0.473795 0.640091 0.000021 8 -0.994569 -0.653408 0.000031 9 3.009876 0.160989 -0.000023 9 1.643236 -1.121713 -1.088590 9 1.643265 -1.121708 1.088587 1 -2.736778 -0.349696 0.000010 17 -4.022323 -0.058289 -0.000011	14.4742, 35.2968, 60.1189, 94.2784, 219.7336, 222.6743, 266.1698, 304.8624, 364.6273, 483.8170, 500.3309, 549.8405, 578.5807, 631.2857, 675.8252, 683.1820, 780.3017, 920.0740, 1160.6457, 1207.0769, 1210.1306, 1406.4075, 1607.6839, 2477.0829

Compound: sCI 4 + HCL TS	**Energy (kJ mol^{-1}):** -1085.755515324460
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.061675 -0.485134 0.206104 6 0.379040 0.780930 -0.373687 9 0.884630 1.135589 -1.513276 8 -0.374195 1.615144 0.150847 8 -1.098287 1.227245 1.298940 9 1.142806 -1.405621 -0.747312 9 0.490864 -0.980490 1.275721 9 2.309365 -0.081099 0.520230 1 -1.903232 0.158409 0.567437 17 -2.259423 -0.746336 -0.410500	-80.0949, .7463, 83.4905, 155.8752, 212.6513, 252.4910, 265.0050, 288.4477, 368.3748, 478.8249, 506.8511, 578.2229, 615.7454, 668.1614, 732.7236, 777.3729, 902.0691, 1007.4100, 1112.4128, 1181.8976, 1278.3178, 1385.3241, 1592.9476, 1757.0919

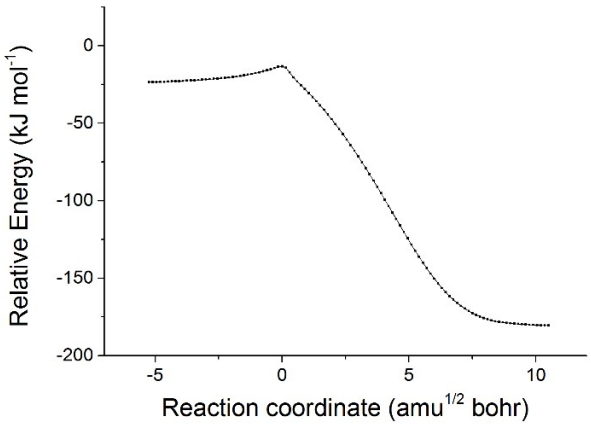
IRC



Compound: sCI 4 + HCL Pr	**Energy (kJ mol^{-1}):** -1085.834620970350
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.060856 -0.008297 -0.189123 6 0.355338 -0.108230 0.475200 9 0.197689 -0.699204 1.669813 8 0.927380 1.111898 0.791717 8 1.101114 1.895565 -0.401700 9 -1.647677 -1.209971 -0.157015 9 -1.008596 0.402535 -1.453358 9 -1.808957 0.848469 0.512907 1 2.027791 1.705099 -0.618622 17 1.434426 -1.126006 -0.551124	50.2033, 121.4143, 171.8280, 217.7511, 223.4230, 278.6540, 312.2242, 345.4722, 366.0803, 405.1581, 506.9394, 538.8667, 590.2412, 624.2460, 743.7466, 909.3164, 980.1865, 1102.6952, 1157.4600, 1191.4081, 1211.5291, 1295.0756, 1416.7299, 3710.0443

Compound: sCI 5 + HCL PRC	**Energy (kJ mol^{-1}):** -1085.762584407700
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.652214 -0.266535 -0.132727 6 0.351559 0.434522 0.266554 9 -0.039641 0.277222 1.479483 8 -0.252232 1.146365 -0.549289 8 -1.429760 1.763605 -0.136867 9 1.529614 -1.576698 0.079388 9 2.646860 0.200300 0.630556 9 1.929256 -0.041822 -1.407761 1 -2.492164 0.382844 -0.129858 17 -2.980549 -0.847149 -0.130520	26.6352, 29.6193, 55.4301, 131.9833, 181.2789, 204.0811, 294.9425, 344.6381, 364.5925, 405.7232, 517.2215, 526.6510, 576.2596, 686.3177, 706.9846, 728.9803, 860.5920, 873.3529, 1157.9005, 1176.9629, 1240.1319, 1399.6990, 1626.7741, 2402.4687

Compound: sCI 5 + HCL TS	**Energy (kJ mol^{-1}):** -1085.758646350020
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.444993 -0.202352 -0.117201 6 0.113833 0.485166 0.242495 9 -0.193524 0.488128 1.486587 8 -0.439482 1.208925 -0.609714 8 -1.744542 1.629281 -0.252622 9 1.461858 -1.426052 0.392147 9 2.440338 0.511295 0.427362 9 1.603459 -0.248916 -1.429169 1 -2.214678 0.368181 -0.166095 17 -2.204428 -1.099459 -0.092902	-581.3091, 32.0565, 70.2436, 158.4864, 182.2178, 211.7313, 297.6019, 335.8299, 359.1080, 405.1791, 496.9126, 577.5197, 610.7858, 727.0141, 760.3198, 856.8177, 858.9326, 929.6950, 1145.8207, 1192.6900, 1252.5531, 1387.6973, 1411.2767, 1610.8001
IRC	



Compound: sCI 5 + HCL Pr	**Energy (kJ mol^{-1}):** -1085.837345614150
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.194899 -0.120815 -0.111015 6 0.331124 -0.083210 0.229355 9 0.474675 -0.305365 1.551533 8 0.899285 -1.074209 -0.524802 8 2.303812 -1.172668 -0.216102 9 -1.841384 0.800655 0.603411 9 -1.693257 -1.321710 0.195276 9 -1.401636 0.111274 -1.408265 1 2.690449 -0.706358 -0.974330 17 1.001285 1.549519 -0.134476	64.4258, 128.1095, 167.6467, 186.4425, 223.1601, 270.7713, 308.4509, 349.4830, 369.6766, 425.8388, 452.6172, 546.5202, 575.5520, 706.3830, 742.8602, 932.2223, 962.3080, 1078.0033, 1146.1876, 1198.7855, 1211.6191, 1288.9764, 1413.0046, 3714.6669

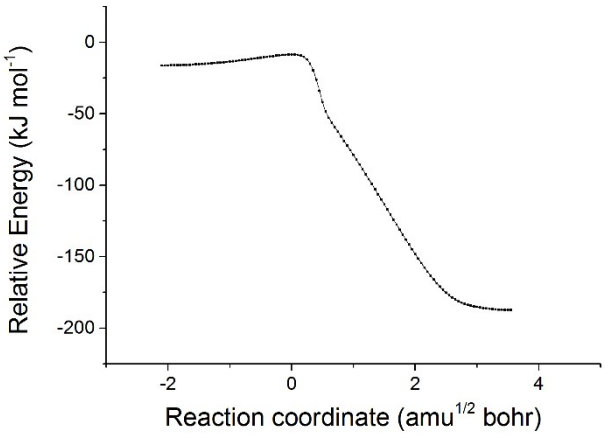
S8.8 Reactions with H_2S

Compound: H_2S	**Energy (kJ mol^{-1}):** -398.964896610182
Reaction Coordinates:	**Frequencies (cm^{-1}):**
16 0.000000 -0.000000 0.103242 1 -0.000000 0.971861 -0.825934 1 -0.000000 -0.971861 -0.825934	1206.0101, 2682.8315, 2695.9979

Compound: sCI 1 + H_2S PRC1	**Energy (kJ mol^{-1}):** -588.373411489393
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.383147 1.052216 -0.190803 1 0.857402 1.062232 -1.135927 1 1.750328 1.932456 0.319036 8 1.620589 -0.035140 0.381047 8 1.154027 -1.183091 -0.196698 16 -1.894674 0.073705 -0.044649 1 -0.816788 -0.757434 -0.095069 1 -1.971973 0.016017 1.296363	63.4000, 131.8291, 149.4863, 162.3626, 233.3899, 476.4641, 530.3435, 672.4471, 883.9619, 975.7551, 1211.1926, 1238.8171, 1410.6771, 1558.3845, 2475.3799, 2689.0854, 3126.9057, 3271.963

Compound: sCI 1 + H_2S TS1	**Energy (kJ mol^{-1}):** -588.366724078241
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.850344 1.071250 -0.227889 1 0.603134 0.952593 -1.271614 1 0.880621 2.037578 0.259668 8 1.403926 0.127025 0.404241 8 1.163723 -1.125721 -0.183869 16 -1.571014 -0.031723 -0.035438 1 -0.410264 -0.882903 -0.126424 1 -1.580531 -0.037629 1.309724	-287.4348, 192.8922, 266.6416, 346.5469, 470.9489, 503.0721, 727.6948, 853.5293, 903.8597, 1013.4027, 1212.6890, 1229.2910, 1385.7411, 1535.5675, 1640.5057, 2683.0310, 3132.3039, 3269.0933

IRC



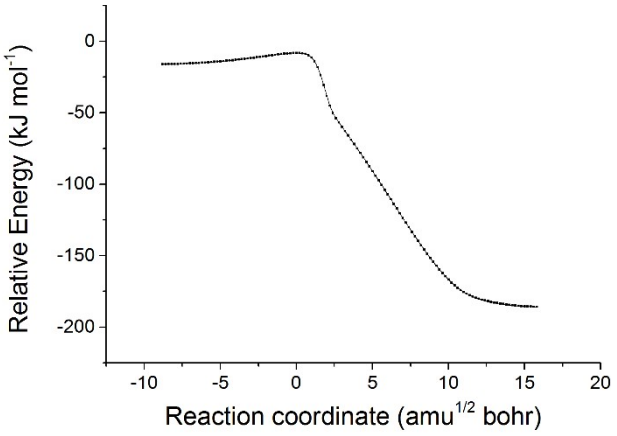
Compound: sCI 1 + H_2S Pr1	**Energy (kJ mol^{-1}):** -588.446035792738
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.001168 0.835726 0.290620 1 -0.181880 0.839497 1.364179 1 0.259165 1.833670 -0.056535 8 -1.165429 0.503394 -0.417719 8 -1.733621 -0.684680 0.175653 16 1.415014 -0.309297 0.024241 1 -1.234849 -1.384014 -0.276466	141.7941, 250.1772, 306.7244, 361.7041, 504.1382, 667.7742, 797.3210, 884.0190, 1004.4493, 1070.2357, 1270.4039, 1327.6749, 1388.0540, 1442.1300, 2670.1919, 3063.0127, 3131.2502, 3694.8508

1 1.702732 0.095537 -1.226224	

Compound: sCI 1 + H_2S PRC2	**Energy (kJ mol^{-1}):** -588.373317449885
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.374106 1.051493 0.211173 1 0.855371 1.043508 1.160152 1 1.727983 1.941423 -0.291192 8 1.615258 -0.026559 -0.376434 8 1.163584 -1.185240 0.192467 16 -1.875235 0.076608 -0.116169 1 -0.812930 -0.764087 0.024453 1 -2.242037 -0.061138 1.169987	63.0680, 130.1110, 145.4168, 162.6574, 245.2900, 464.0536, 527.5536, 671.0392, 883.0327, 974.9178, 1215.9064, 1239.3125, 1410.1846, 1558.0192, 2476.9496, 2688.8034, 3126.9908, 3272.3093

Compound: sCI 1 + H_2S TS2	**Energy (kJ mol^{-1}):** -588.366581083392
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.849619 1.069515 0.237062 1 0.578535 0.941856 1.273377 1 0.890091 2.038022 -0.245086 8 1.413656 0.127668 -0.389692 8 1.159069 -1.127293 0.188155 16 -1.550820 -0.025704 -0.128931 1 -0.404959 -0.883882 0.065341 1 -1.930063 -0.104826 1.159185	-295.7329, 192.3838, 268.3680, 346.2326, 491.6914, 513.1666, 715.6320, 853.2832, 888.9700, 1003.2864, 1205.4724, 1243.2746, 1385.4237, 1534.7258, 1629.1815, 2683.1069, 3135.1386, 3273.1921

IRC



Compound: sCI 1 + H_2S Pr2	**Energy (kJ mol^{-1}):** -588.445571445584
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.012289 0.836673 0.292041 1 0.137899 0.843930 1.369473 1 -0.261437 1.835409 -0.062595 8 1.182629 0.525484 -0.380415 8 1.707413 -0.699298 0.182137 16 -1.445103 -0.237773 -0.114264 1 1.423595 -1.344209 -0.482939 1 -1.225017 -1.160284 0.838262	138.0723, 205.9238, 297.5899, 356.7590, 494.4525, 686.5323, 780.5804, 886.2457, 1009.5045, 1062.2832, 1278.9894, 1319.8557, 1377.8454, 1439.6650, 2680.0174, 3066.0637, 3129.7951, 3725.2061

Compound: sCl 2 + H_2S PRC1	**Energy (kJ mol^{-1}):** -925.175112004368
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.484229 -0.344913 -0.006771 6 -0.855916 0.661362 0.935858 8 0.009345 1.502272 0.588972 8 0.449903 1.536780 -0.681884 1 -1.150956 0.698319 1.974948 9 -2.154044 0.255184 -0.994064 9 -0.584013 -1.177125 -0.531100 9 -2.361052 -1.072857 0.711674 16 3.190953 -0.600746 0.031241 1 4.010342 0.349054 0.514893 1 2.344237 0.306641 -0.499502	9.9024, 23.7127, 61.6911, 106.0087, 107.9417, 135.5994, 181.9940, 245.6847, 314.0242, 327.5125, 477.9915, 506.4081, 535.5159, 589.4703, 757.9055, 792.8041, 883.2286, 931.3426, 1155.0768, 1180.1698, 1209.2232, 1242.6978, 1366.4837, 1550.9099, , 2626.7917, 2690.7441, 3215.4330

Compound: sCl 2 + H_2S TS1	**Energy (kJ mol^{-1}):** -925.168836880090
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.079377 -0.272562 0.017459 6 0.062519 0.407790 -0.903023 8 -0.458449 1.540497 -0.680542 8 -0.719497 1.804417 0.660310 1 0.145936 0.148250 -1.951564 9 2.137961 0.548220 0.135183 9 0.674673 -0.606080 1.237017 9 1.493402 -1.393073 -0.605044 16 -1.985813 -0.912407 0.044771 1 -2.799656 -0.366896 -0.878246 1 -1.755408 0.304882 0.684309	-186.5290, 50.4707, 126.9609, 154.6013, 210.6029, 314.1125, 322.1871, 331.7323, 435.1666, 465.2846, 510.9986, 542.6879, 571.0339, 731.1105, 763.7064, 845.8696, 865.8312, 913.6169, 1145.9236, 1154.6731, 1216.9637, 1258.5030, 1344.6574, 1524.9039, 2125.4049, 2679.8543, 3182.1468

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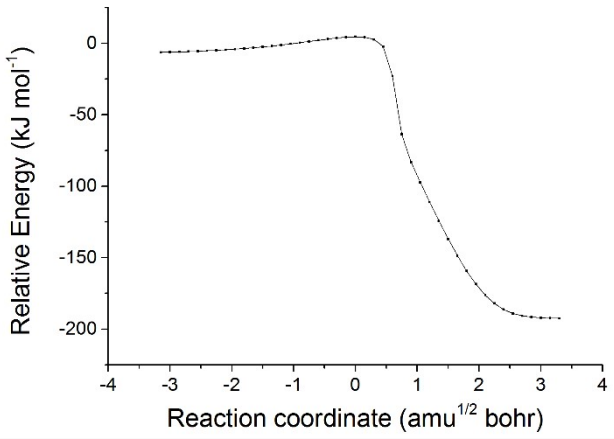

Compound: sCl 2 + H_2S Pr1	**Energy (kJ mol^{-1}):** -925.256025297439
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.023936 -0.130202 0.007316 6 -0.359856 -0.030549 -0.670201 8 -0.837859 1.281713 -0.779296 8 -1.004095 1.851805 0.537383 1 -0.222963 -0.334569 -1.706347 9 1.801492 0.896816 -0.354922 9 0.959825 -0.154651 1.346215 9 1.632480 -1.266220 -0.389625 16 -1.524866 -1.200782 0.148899	60.8407, 124.4968, 176.2385, 192.0415, 221.4286, 285.4577, 327.4123, 332.3845, 379.4655, 502.9899, 524.0442, 568.9290, 712.1710, 780.1388, 832.6499, 895.8157, 966.2179, 1039.8374, 1122.2301, 1175.2785, 1249.6693, 1260.7064, 1364.3021, 1394.9375, 2680.3929, 3106.7373, 3692.8576

1 -2.278442 -1.380984 -0.949920 1 -1.893773 1.540930 0.771481	

Compound: sCl 2 + H_2S PRC2	**Energy (kJ mol^{-1}):** -925.174429805702
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.021718 -0.038630 0.002520 6 -0.932518 1.013408 0.041877 8 0.295322 0.750975 0.020220 8 0.714242 -0.524723 -0.042152 1 -1.182713 2.063680 0.091864 9 -1.978894 -0.759165 -1.119635 9 -1.960687 -0.858685 1.053557 9 -3.203548 0.606804 0.042095 16 4.235132 0.005906 -0.070083 1 4.435857 -0.406631 1.193404 1 2.921818 -0.310813 -0.039009	9.7858, 20.5426, 55.3474, 63.8132, 84.8668, 177.3682, 191.4593, 247.0686, 328.2667, 354.2698, 479.2267, 508.8930, 536.1159, 591.1425, 758.8193, 791.7027, 884.2323, 934.7058, 1155.4684, 1181.4413, 1216.3689, 1242.5905, 1366.8974, 1550.6684, 2608.8873, 2691.3503, 3215.2254

Compound: sCl 2 + H_2S TS2	**Energy (kJ mol^{-1}):** -925.167972073153
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.084640 -0.267962 0.020490 6 0.061333 0.409724 -0.893056 8 -0.466565 1.540319 -0.671974 8 -0.744439 1.796104 0.668712 1 0.150330 0.153688 -1.942151 9 2.171907 0.524589 0.062317 9 0.721390 -0.535782 1.268061 9 1.442690 -1.426479 -0.567284 16 -2.059113 -0.840429 -0.076063 1 -1.625042 -1.640531 0.913255 1 -1.791177 0.330804 0.639548	-200.4295, 46.0578, 134.0311, 158.5604, 213.1732, 290.9336, 312.7965, 319.5703, 408.7537, 472.4336, 517.6245, 550.6113, 573.3513, 731.3071, 761.6964, 844.7599, 865.9906, 916.4786, 1140.3623, 1152.3552, 1224.1910, 1264.0710, 1345.3041, 1524.3551, 2085.2288, 2694.0451, 3181.0752

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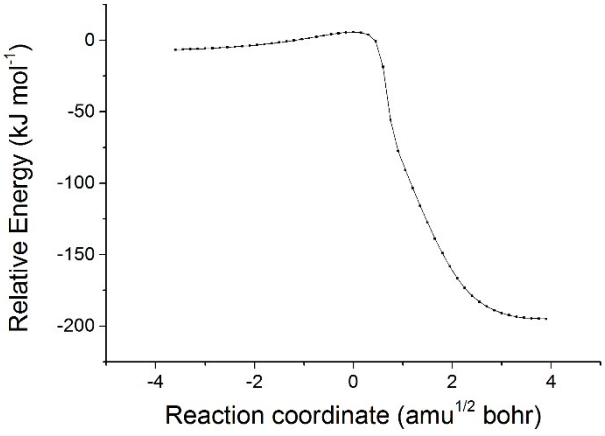

Compound: sCl 2 + H_2S Pr2	**Energy (kJ mol^{-1}):** -925.257286575136
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.038101 -0.073681 0.017437 6 -0.345508 -0.051413 -0.667474 8 -0.874309 1.246164 -0.774009 8 -1.218307 1.740515 0.541365 1 -0.172466 -0.327747 -1.708250 9 1.795556 0.938754 -0.429649 9 0.976078 0.020668 1.354219 9 1.674062 -1.222024 -0.282036 16 -1.485535 -1.318144 -0.007489	57.7190, 119.0022, 183.5200, 191.0234, 220.5122, 285.8439, 322.5651, 331.8899, 379.7520, 507.0559, 523.3513, 575.9561, 710.5756, 730.3250, 850.4188, 893.4750, 976.3478, 1031.4681, 1131.8965, 1166.8457, 1247.6794, 1285.3044, 1356.0743, 1388.4082, 2684.6621, 3088.2825, 3730.1768

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1 -1.301491 -1.020792 1.290740
1 -2.183383 1.659403 0.515897
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Compound: sCl 3 + H_2S PRC1	**Energy (kJ mol^{-1}):** -925.175112004368
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.505791 -0.283359 -0.011193 6 0.260325 0.445841 -0.455155 1 -0.241765 0.189576 -1.378153 8 -0.136738 1.398076 0.254026 8 -1.246501 2.074357 -0.133452 9 2.508066 -0.023426 -0.873639 9 1.895522 0.071654 1.210826 9 1.286545 -1.606577 -0.032310 16 -2.822560 -0.892838 -0.052930 1 -2.655982 0.447927 0.043415 1 -2.683283 -1.081307 1.271215	16.7560, 35.6648, 94.9104, 129.5199, 144.0315, 187.5120, 195.2086, 226.6565, 356.3090, 388.4219, 406.5327, 422.0334, 552.0897, 561.1364, 699.6543, 868.5870, 888.1502, 960.6589, 1135.9140, 1176.5214, 1209.5645, 1267.4663, 1356.5936, 1553.5525, 2574.0746, 2688.7827, 3207.5983

Compound: sCl 3 + H2S TS1	**Energy (kJ mol^{-1}):** -925.172857190441
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.310051 -0.131310 -0.019387 6 0.013684 0.470188 -0.452503 8 0.483121 1.387908 0.280974 8 1.747748 1.813111 -0.134919 1 0.324899 0.372530 -1.482418 9 -1.370451 -0.327937 1.299070 9 -1.499155 -1.299640 -0.643653 9 -2.318385 0.691074 -0.367375 16 2.010557 -1.162230 -0.043231 1 2.319981 0.217673 -0.042042 1 1.809374 -1.207415 1.286670	-211.4560, 36.1197, 92.0602, 175.9207, 196.7871, 283.0048, 313.1884, 378.3885, 411.0245, 418.9613, 486.3471, 552.6049, 586.6452, 698.7495, 805.2558, 876.8659, 919.3305, 933.5828, 1139.9428, 1182.4716, 1216.9751, 1254.8214, 1338.8958, 1515.4506, 1912.7856, 2681.5459, 3207.0263

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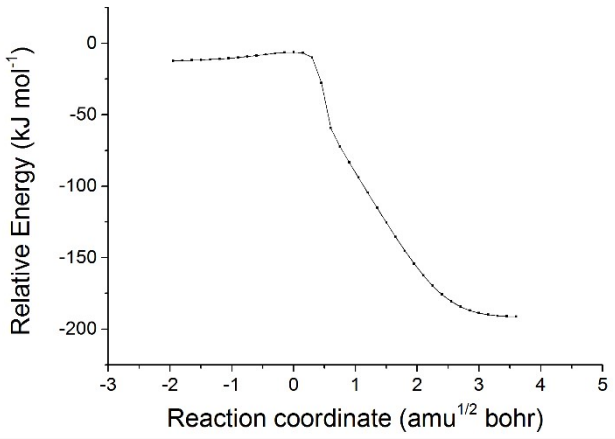

Compound: sCl 3 + H_2S Pr1	**Energy (kJ mol^{-1}):** -925.257735936140
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.126290 -0.140551 -0.031638 6 -0.374715 -0.078433 -0.357479 8 -0.970615 -1.118009 0.379968 8 -2.255017 -1.394028 -0.209024 1 -0.488446 -0.255832 -1.427000 9 1.372263 0.107002 1.266689 9 1.623239 -1.352756 -0.318668 9 1.801010 0.759696 -0.761611 16 -1.116036 1.571429 -0.048806	63.8128, 102.0609, 186.4836, 187.1548, 245.7465, 301.4951, 321.9712, 351.3219, 365.2552, 454.8641, 534.7094, 561.6093, 685.2206, 715.5061, 873.8865, 932.6839, 970.9561, 1059.7406, 1138.6731, 1177.0163, 1243.1934, 1311.3835, 1339.9383, 1399.0168, 2671.5249, 3082.4983, 3694.2213

1 -0.702156 1.668348 1.228465 1 -2.825833 -0.770645 0.268896	

Compound: sCl 3 + H_2S PRC2	**Energy (kJ mol^{-1}):** -925.174429805702
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.503567 -0.284485 -0.011828 6 0.262393 0.449685 -0.460027 1 -0.232363 0.202682 -1.389467 8 -0.140290 1.396906 0.252344 8 -1.244397 2.078583 -0.143226 9 2.521171 0.007486 -0.846631 9 1.866725 0.037533 1.226876 9 1.293556 -1.607184 -0.077163 16 -2.780476 -0.902092 0.105562 1 -2.645184 0.445483 0.070505 1 -3.286178 -0.950318 -1.139579	16.8693, 36.2707, 93.7280, 127.5679, 142.8341, 192.0942, 193.9604, 235.7731, 350.9350, 388.0237, 405.4637, 420.8305, 552.1704, 560.7231, 699.7189, 868.7005, 887.7995, 959.2261, 1134.4405, 1177.7167, 1212.8077, 1267.9318, 1356.3589, 1554.0258, 2572.1811, 2688.1979, 3207.6933

Compound: sCl 3 + H_2S TS2	**Energy (kJ mol^{-1}):** -925.172354744837
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.313290 -0.136608 -0.016959 6 0.012714 0.461428 -0.447671 8 0.472921 1.396341 0.269616 8 1.739945 1.815318 -0.146902 1 0.338165 0.341324 -1.470376 9 -1.399575 -0.286104 1.303791 9 -1.479678 -1.327746 -0.605359 9 -2.320475 0.664428 -0.417352 16 1.993002 -1.140977 0.118183 1 2.311340 0.234651 0.001975 1 2.360541 -1.417753 -1.146189	-217.3443, 37.4007, 92.6508, 175.1327, 197.5688, 276.0734, 313.8069, 377.8487, 409.8519, 428.7319, 504.0821, 553.3237, 586.0863, 698.2452, 797.9012, 875.7437, 913.3066, 924.9756, 1137.9528, 1181.1166, 1221.2218, 1260.3439, 1339.4354, 1516.3591, 1892.3908, 2682.5789, 3211.9961

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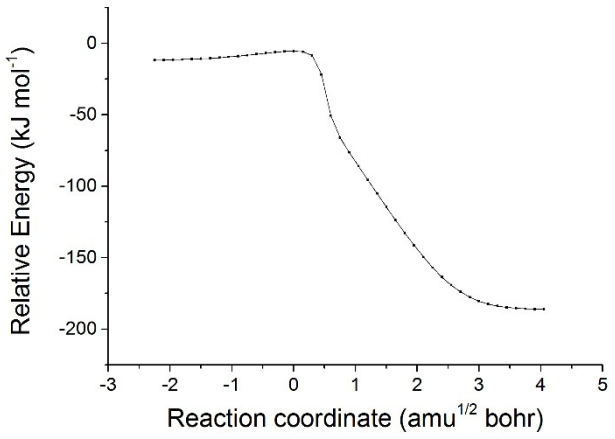

Compound: sCl 3 + H_2S Pr2	**Energy (kJ mol^{-1}):** -925.255754732320
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.134988 -0.125424 -0.029628 6 -0.364644 -0.085999 -0.364057 8 -0.934831 -1.167480 0.329847 8 -2.255123 -1.380183 -0.204046 1 -0.472188 -0.217740 -1.438933 9 1.367666 0.136530 1.266332 9 1.653715 -1.330722 -0.307283 9 1.796972 0.781311 -0.764700 16 -1.089668 1.545198 0.104755	60.8375, 103.4306, 134.5855, 184.9709, 193.2162, 286.4429, 316.1939, 345.9497, 365.6998, 459.7549, 532.6234, 561.6597, 689.6998, 743.5890, 858.3025, 935.5761, 969.8389, 1060.0747, 1133.8875, 1176.0136, 1248.1780, 1284.2039, 1341.6047, 1396.1450, 2689.6046, 3097.4785, 3703.1385

1 -1.766818 1.718580 -1.042276 1 -2.793900 -0.858226 0.411706	

Compound: sCI 4 + H_2S PRC1	**Energy (kJ mol^{-1}):** -1024.345549005980
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.255536 -0.535628 0.094499 6 0.626941 0.785770 -0.380958 8 -0.126808 1.515607 0.276098 8 -0.522536 1.094310 1.539803 9 0.962643 1.208923 -1.564048 9 2.026957 -0.306980 1.155540 9 0.326616 -1.431341 0.398410 9 2.015402 -1.018278 -0.892853 16 -3.000013 -0.564130 -0.301112 1 -3.719085 0.534199 -0.591370 1 -2.365378 0.040780 0.727263	13.8664, 36.9070, 53.5079, 92.9337, 136.2438, 162.2992, 185.3213, 221.2522, 268.6021, 293.8398, 361.4009, 365.2395, 483.2266, 495.6568, 581.6967, 629.1721, 660.3300, 779.6001, 920.3828, 1158.5904, 1193.0932, 1207.0404, 1213.5979, 1399.6569, 1594.5146, 2610.1312, 2690.0168

Compound: sCI 4 + H_2S TS1	**Energy (kJ mol^{-1}):** -1024.344013062570
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.068099 -0.371050 -0.242756 6 -0.149806 0.520690 0.627818 8 0.372002 1.604912 0.291859 8 0.697364 1.725914 -1.073496 9 -0.348033 0.376851 1.912128 9 -2.176887 0.344798 -0.489359 9 -0.545925 -0.760632 -1.390633 9 -1.409574 -1.449026 0.466501 16 2.142449 -0.885776 -0.036405 1 2.851505 -0.192450 0.873466 1 1.945591 0.212507 -0.835992	-91.8475, 37.6949, 103.0268, 109.1560, 196.2418, 251.7585, 272.1509, 290.8062, 306.5540, 368.1350, 388.3813, 476.4108, 503.3478, 581.3188, 599.5715, 622.8849, 636.5919, 779.7094, 918.7570, 1129.6648, 1176.7367, 1214.0730, 1236.0744, 1354.9605, 1549.5736, 2369.6784, 2681.9410

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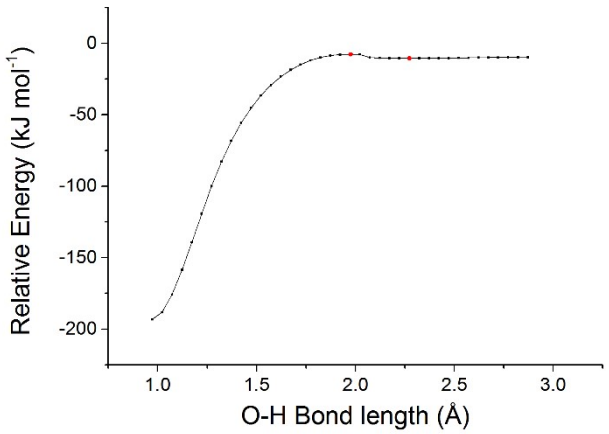

Compound: sCI 4 + H_2S Pr1	**Energy (kJ mol^{-1}):** -1024.429431015390
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.063006 -0.096610 -0.176165 6 0.364858 -0.080465 0.466586 8 0.807099 1.210387 0.789287 8 0.864917 2.002775 -0.408568 9 0.265422 -0.664548 1.686821 9 -1.843260 0.815874 0.402587 9 -1.015127 0.146435 -1.491994 9 -1.618803 -1.302127 -0.000355 16 1.534813 -1.013646 -0.610945	54.3934, 121.0861, 167.5154, 207.0012, 213.8160, 266.5950, 294.2510, 326.0987, 341.1989, 365.7182, 402.0517, 504.0054, 533.5151, 570.6240, 619.2433, 741.0527, 848.8025, 965.6506, 986.2968, 1073.9629, 1140.1976, 1183.4904, 1203.7794, 1296.0267, 1415.5088, 2674.3831, 3673.9102

1 2.431715 -1.133411 0.385610 1 1.729943 1.748193 -0.772298	

Compound: sCl 4 + H_2S PRC2	**Energy (kJ mol^{-1}):** -1024.345353229650
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.290490 -0.529706 0.062238 6 0.625134 0.799092 -0.334777 8 -0.151494 1.465079 0.362419 8 -0.534378 0.958574 1.598056 9 0.948948 1.301501 -1.489789 9 2.048350 -0.347356 1.141503 9 0.386033 -1.469738 0.301393 9 2.070049 -0.927379 -0.947657 16 -3.108159 -0.396842 -0.360503 1 -2.936307 -1.694105 -0.052990 1 -2.420334 0.024770 0.723423	12.1242, 35.9569, 52.7329, 92.3689, 131.0919, 163.6602, 185.7154, 220.6224, 268.9694, 293.8148, 352.6309, 364.3246, 483.3067, 495.7094, 581.7737, 629.2548, 660.4071, 779.5938, 920.6439, 1159.0171, 1193.5348, 1206.2207, 1213.6770, 1399.8534, 1594.0341, 2612.4339, 2691.7932

Compound: sCl 4 + H_2S TS2	**Energy (kJ mol^{-1}):** -1024.343079346060
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.071211 -0.363698 -0.245937 6 -0.143560 0.530370 0.609849 8 0.395490 1.605527 0.265975 8 0.765781 1.693599 -1.091961 9 -0.369535 0.414344 1.892212 9 -2.212221 0.326010 -0.415284 9 -0.596972 -0.699277 -1.430353 9 -1.348295 -1.474452 0.441689 16 2.182199 -0.810150 0.100843 1 1.863614 -1.755094 -0.800983 1 1.962861 0.224832 -0.782456	-106.4507, 34.4170, 112.2563, 116.6783, 198.6133, 249.1393, 270.2184, 276.6378, 290.3873, 369.0565, 394.2326, 476.6437, 508.8478, 581.8044, 606.0935, 631.4851, 641.8063, 780.1505, 918.8704, 1125.8058, 1174.7524, 1218.2103, 1239.2021, 1353.1718, 1543.8164, 2316.0817, 2695.1504

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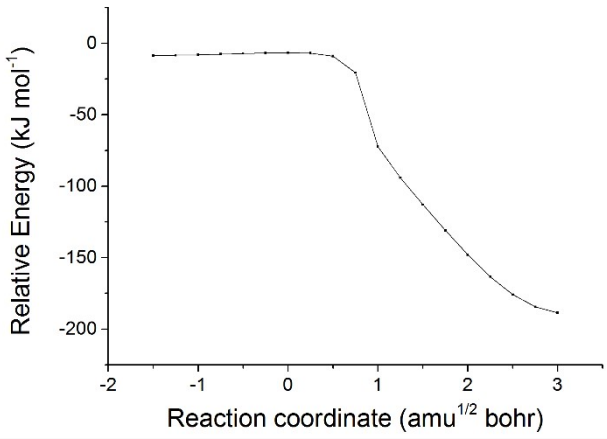

Compound: sCl 4 + H_2S Pr2	**Energy (kJ mol^{-1}):** -1024.428919132390
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.106304 0.072990 -0.218224 6 0.285982 -0.089087 0.463772 8 0.862223 1.170956 0.686912 8 1.642238 1.563219 -0.463465 1 2.518795 1.636667 -0.056694 9 0.033549 -0.561191 1.715421 16 1.413265 -1.206650 -0.455943 1 0.747460 -2.301924 -0.046329 9 -1.901340 0.848771 0.527851	57.2635, 70.9939, 175.7844, 201.2701, 214.0455, 240.9941, 300.2199, 308.2382, 339.6347, 369.4160, 400.5555, 502.7278, 530.9276, 585.2028, 602.8116, 736.3936, 886.0484, 946.5138, 983.6877, 1100.7233, 1134.3376, 1177.3711, 1198.8231, 1281.0401, 1405.6513, 2679.1684, 3732.9729

9 -0.982485 0.632823 -1.423831 9 -1.704417 -1.120976 -0.359747	

Compound: sCl 5 + H_2S PRC1	**Energy (kJ mol^{-1}):** -1024.352019623190
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.497901 -0.354035 0.113257 6 0.326787 0.557329 -0.235223 9 -0.019078 0.609081 -1.476740 8 -0.193080 1.273361 0.636115 8 -1.239250 2.096406 0.275803 9 2.611061 0.116300 -0.469978 9 1.680445 -0.398850 1.426610 9 1.270769 -1.583402 -0.350508 16 -2.739843 -0.999585 -0.011305 1 -2.696080 0.342916 0.141142 1 -2.844680 -1.215609 1.311733	24.1450, 33.1121, 65.0647, 98.5150, 140.2987, 166.9719, 185.3141, 197.8389, 294.3611, 326.7809, 360.0382, 382.8149, 406.7516, 511.8452, 576.5956, 655.5405, 728.7778, 856.9027, 892.9799, 1146.7193, 1172.6328, 1209.1424, 1230.9405, 1399.6934, 1611.3284, 2609.0297, 2689.4607

Compound: sCl 5 + H_2S TS1	**Energy (kJ mol^{-1}):** -1024.345922619310
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.336779 -0.162720 -0.101569 6 -0.019006 0.479715 0.216224 8 -0.515172 1.245306 -0.649683 8 -1.802057 1.722392 -0.318134 9 -0.263186 0.631311 1.489973 9 1.395870 -0.518762 -1.382031 9 1.531605 -1.232089 0.666795 9 2.316371 0.720581 0.146452 16 -1.882243 -1.286634 0.014244 1 -2.329438 0.029629 -0.155333 1 -1.749424 -1.496399 -1.308676	-212.8655, 41.9183, 92.7584, 169.9711, 177.8020, 214.1780, 286.9091, 319.6417, 355.8809, 364.4907, 404.7532, 463.5875, 507.2484, 576.2040, 629.5656, 721.3812, 762.2249, 829.4224, 881.0242, 1129.7304, 1178.1249, 1207.3719, 1225.3137, 1358.6645, 1530.2690, 2071.9114, 2682.1682

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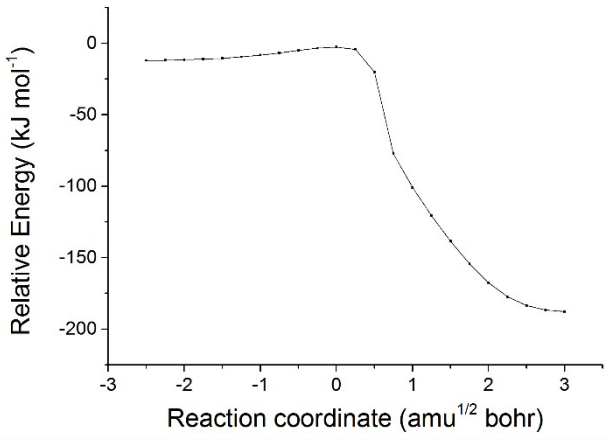

Compound: sCl 5 + H_2S Pr1	**Energy (kJ mol^{-1}):** -1024.433159728430
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.200903 -0.095266 -0.099958 6 0.326675 -0.089049 0.223901 8 0.843690 -1.117581 -0.540345 8 2.245704 -1.284167 -0.257708 9 0.464397 -0.342426 1.555653 9 -1.413293 0.221313 -1.387446 9 -1.725040 -1.300860 0.129524 9 -1.837661 0.792828 0.664830 16 1.114990 1.556337 -0.055220	66.2156, 137.0343, 156.8050, 176.9816, 200.0302, 245.6916, 278.2893, 295.7701, 347.7871, 367.4199, 411.0122, 439.2158, 545.3320, 571.0266, 694.6552, 738.6398, 887.3473, 938.7696, 993.2027, 1069.6573, 1123.6025, 1182.6165, 1203.6161, 1282.2079, 1414.9629, 2679.6380, 3680.8781

1 0.651037 1.684950 -1.311783 1 2.643713 -0.604157 -0.826976	

Compound: sCI 3 + H_2S PRC2	**Energy (kJ mol^{-1}):** -1024.352020666000
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.489163 -0.357160 -0.112118 6 -0.325648 0.564108 0.235950 9 0.005099 0.635842 1.480987 8 0.200272 1.270865 -0.639145 8 1.238752 2.103600 -0.278495 9 -2.612149 0.122593 0.444942 9 -1.651870 -0.429464 -1.426202 9 -1.266596 -1.575910 0.381370 16 2.710350 -1.019175 -0.143759 1 2.696623 0.331667 -0.190098 1 3.044108 -1.039826 1.158502	24.7913, 33.7033, 65.0276, 97.7672, 141.4668, 166.3063, 186.3025, 196.5192, 293.6860, 323.5083, 358.0252, 379.9072, 406.7070, 511.7565, 576.6243, 655.0017, 728.6802, 856.4586, 892.6362, 1145.3146, 1172.1473, 1210.5034, 1232.6576, 1399.1867, 1611.2523, 2611.1316, 2690.4468

Compound: sCI 5 + H_2S TS2	**Energy (kJ mol^{-1}):** -1024.345712139260
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.337645 -0.163068 -0.103782 6 -0.018713 0.475773 0.220019 8 -0.507990 1.263483 -0.629415 8 -1.797439 1.732071 -0.294004 9 -0.268582 0.597141 1.496683 9 1.413666 -0.473263 -1.392902 9 1.515718 -1.259729 0.631286 9 2.317632 0.705926 0.191884 16 -1.859989 -1.285882 -0.160405 1 -2.322831 0.034760 -0.220607 1 -2.193410 -1.431987 1.134461	-214.3248, 43.9396, 94.7246, 172.0993, 177.1296, 218.7101, 287.8239, 316.2546, 346.1578, 363.8654, 405.7866, 461.7908, 513.6250, 576.1385, 630.2736, 720.9692, 758.5877, 828.0010, 879.3764, 1128.0337, 1176.9447, 1213.5395, 1228.9550, 1357.9335, 1531.4213, 2070.7635, 2687.8493

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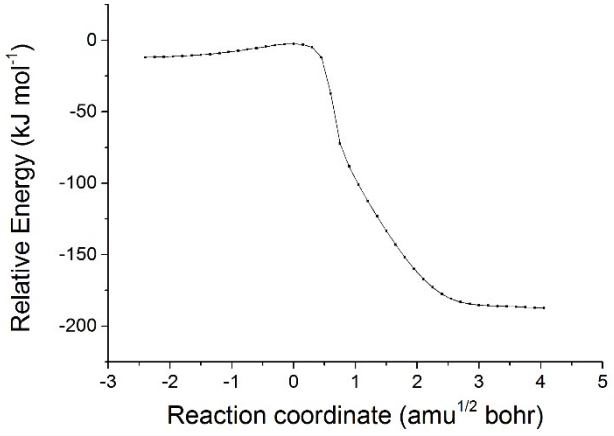

Compound: sCI 5 + H_2S Pr2	**Energy (kJ mol^{-1}):** -1024.433112228060
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.202362 -0.089113 -0.109268 6 0.318048 -0.089101 0.243524 8 0.827351 -1.177761 -0.442171 8 2.255224 -1.241345 -0.260519 9 0.431335 -0.281065 1.592046 9 -1.379704 0.255548 -1.393450 9 -1.735591 -1.297017 0.084936 9 -1.853762 0.786093 0.658312 16 1.058272 1.538292 -0.208423	60.9853, 112.5120, 142.6837, 171.9181, 186.3778, 257.8669, 279.9189, 301.2905, 349.5684, 369.4286, 417.1116, 449.7881, 543.9532, 571.0201, 686.0786, 737.2994, 855.3090, 942.0929, 999.5997, 1067.2588, 1100.2573, 1187.4977, 1204.3373, 1292.5349, 1408.4410, 2689.6565, 3708.1167

1 1.989300 1.468211 0.758434 1 2.563125 -0.830796 -1.084279	

S8.9 Reactions with H_2O

Compound: H_2O	**Energy (kJ mol^{-1}):** -76.372669648641
Reaction Coordinates:	**Frequencies (cm^{-1}):**
8 -0.000000 -0.000000 0.116992 1 -0.000000 0.763520 -0.467967 1 -0.000000 -0.763520 -0.467967	1626.9293, 3796.3639, 3899.0961

Compound: sCI 1 + H_2O PRC	**Energy (kJ mol^{-1}):** -265.786257491251
Reaction Coordinates:	**Frequencies (cm^{-1}):**
8 0.357047 -1.171861 -0.000014 8 1.289920 -0.173564 0.000019 6 0.924903 1.024191 -0.000004 1 -0.129754 1.281859 -0.000044 1 1.739280 1.736480 0.000025 8 -2.012469 0.273086 -0.000021 1 -1.353128 -0.449947 -0.000007 1 -2.881795 -0.134832 0.000186	21.8780, 75.7289, 148.6369, 209.9306, 493.6039, 549.1761, 629.7151, 691.8102, 881.1881, 1017.5999, 1272.0176, 1429.7599, 1558.0952, 1645.6134, 3091.7849, 3248.5013, 3499.8200, 3871.1216

Compound: sCI 1 + H_2O TS1	**Energy (kJ mol^{-1}):** -265.772122072372
Reaction Coordinates:	**Frequencies (cm^{-1}):**
8 -0.950605 -0.946963 0.167769 8 -0.886084 0.399108 -0.376202 6 0.046206 0.999114 0.246331 1 0.186984 0.820730 1.304039 1 0.394195 1.921099 -0.209200 8 1.446354 -0.374579 -0.005867 1 0.557419 -0.948603 0.076115 1 1.706835 -0.408441 -0.934541	-433.3116, 326.5769, 426.8495, 531.9388, 597.5414, 656.1524, 809.2086, 899.0486, 1157.5178, 1211.4121, 1251.2657, 1392.4448, 1546.5882, 1605.7472, 2196.2030, 3103.8784, 3225.5749, 3798.4004
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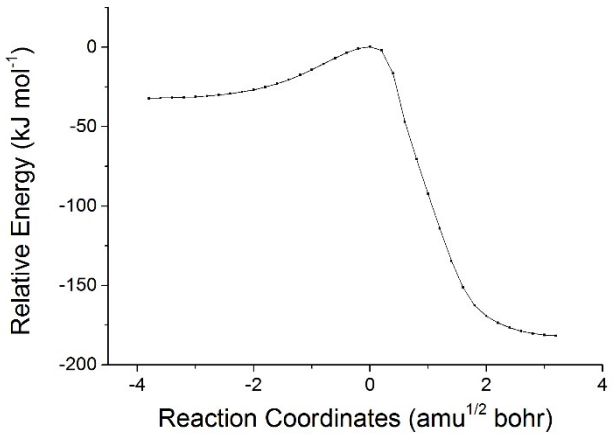	

Compound:	sCl 1 + H_2O Pr1	**Energy (kJ mol^{-1}):**	-265.849083661745
Reaction Coordinates:		**Frequencies (cm^{-1}):**	
6 0.613216 0.542122 0.285606 8 1.381072 -0.594495 -0.014848 8 -0.614068 0.578422 -0.401400 8 -1.485958 -0.421022 0.182400 1 0.443979 0.526639 1.360537 1 1.100746 1.469391 -0.028131 1 -1.183095 -1.228893 -0.258159 1 1.710703 -0.523108 -0.917100		159.0267, 283.2184, 374.4906, 424.9952, 616.1269, 877.8835, 1010.2947, 1032.0533, 1068.5203, 1276.8372, 1369.8581, 1382.2124, 1414.7043, 1484.3437, 3030.0864, 3111.6326, 3728.0279, 3798.4265	

Compound:	sCl 1 + H_2O TS2	**Energy (kJ mol^{-1}):**	-265.770736044301
Reaction Coordinates:		**Frequencies (cm^{-1}):**	
8 0.934736 -0.958068 0.182645 8 0.902650 0.394968 -0.348596 6 -0.043467 0.997720 0.247728 1 -0.205224 0.815507 1.302611 1 -0.372999 1.921901 -0.214833 8 -1.412711 -0.344459 -0.213952 1 -0.543987 -0.941192 -0.052972 1 -2.014398 -0.522066 0.518046		-455.6181, 348.7363, 410.1920, 526.9050, 613.2280, 689.4603, 815.0326, 880.2699, 1126.8327, 1206.7266, 1219.8467, 1386.7034, 1527.2808, 1634.3676, 2149.3718, 3103.4468, 3222.4555, 3813.0408	

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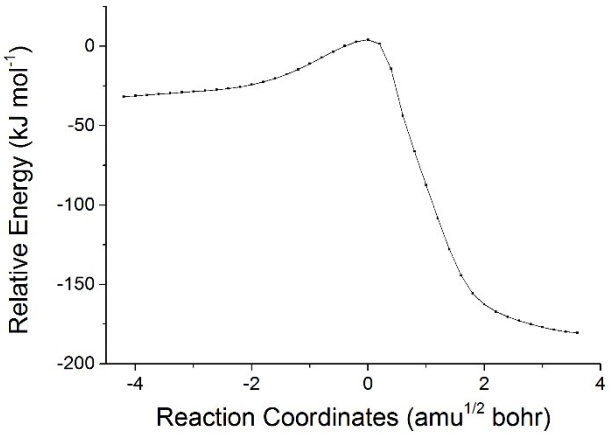

Compound:	sCl 1 + H_2O Pr2	**Energy (kJ mol^{-1}):**	-265.848846609638
Reaction Coordinates:		**Frequencies (cm^{-1}):**	
6 -0.647196 0.538648 0.261567 8 0.625293 0.629426 -0.338740 8 1.425464 -0.454794 0.213290 1 1.601714 -0.966752 -0.587818 1 -0.529616 0.517625 1.347966 1 -1.138554 1.456034 -0.061035 8 -1.414034 -0.537971 -0.192946 1 -1.144148 -1.332081 0.278647		167.4320, 205.9488, 363.0291, 433.1822, 606.0638, 871.9321, 998.8296, 1044.5819, 1074.2590, 1272.8836, 1372.2326, 1384.1981, 1412.5021, 1484.6978, 3025.6587, 3107.6286, 3758.6628, 3815.8683	

Compound: sCI 2 + H_2O PRC	**Energy (kJ mol^{-1}):** -602.585302654489
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.418122 -0.035776 -0.000003 6 0.319563 1.008948 -0.000001 8 -0.904792 0.737430 0.000011 8 -1.312365 -0.546032 0.000023 1 0.561195 2.062640 -0.000010 9 1.370649 -0.806322 1.087881 9 1.370633 -0.806333 -1.087879 9 2.594145 0.620050 -0.000015 8 -4.162630 0.061529 -0.000005 1 -4.718098 -0.722268 -0.000085 1 -3.249743 -0.269386 0.000006	12.9685, 28.0322, 34.6398, 84.0523, 109.5999, 211.6467, 247.2163, 334.3561, 375.5031, 479.5982, 510.8715, 534.4531, 536.6024, 591.4602, 759.7032, 800.6129, 884.1656, 931.3447, 1157.2991, 1183.4831, 1242.5624, 1368.6752, 1557.3767, 1658.4346, 3213.8618, 3648.1189, 3869.8220

Compound: sCI 2 + H_2O TS1	**Energy (kJ mol^{-1}):** -602.571519549324
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.880942 -0.040291 0.035680 6 0.374737 -0.063934 -0.855948 8 1.370730 -0.828340 -0.705354 8 1.782336 -0.820106 0.676516 1 0.161124 0.207677 -1.886552 9 -1.469403 -1.243069 -0.117446 9 -0.724983 0.193086 1.324767 9 -1.712041 0.890310 -0.469775 8 1.168700 1.545355 0.045488 1 1.846465 1.896020 -0.545448 1 1.613361 0.783438 0.582497	-335.6905, 48.6609, 176.1151, 213.7137, 280.4627, 322.3603, 348.6340, 448.8651, 514.6696, 537.3357, 550.1125, 572.5144, 667.5975, 744.2436, 808.1946, 872.6150, 993.2852, 1139.3767, 1148.0772, 1195.9793, 1292.0680, 1346.8227, 1554.7138, 1616.4176, 2586.7975, 3144.4219, 3801.2117

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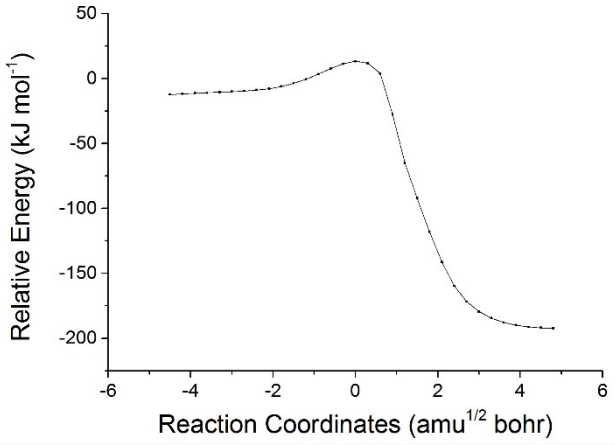

Compound: sCI 2 + H_2O Pr1	**Energy (kJ mol^{-1}):** -602.660056059595
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.840616 -0.134696 0.006007 6 0.411407 0.581582 -0.551944 8 1.505490 -0.266093 -0.775674 8 1.864918 -0.931170 0.458894 1 0.162315 0.911744 -1.564471 9 -1.020367 -1.310094 -0.610249 9 -0.798843 -0.344692 1.322507 9 -1.922869 0.632033 -0.251339 8 0.694373 1.640349 0.310457	64.6652, 135.2115, 205.5945, 222.1310, 272.2757, 294.3622, 343.4660, 378.4008, 436.4043, 525.6920, 583.1678, 617.3587, 763.2320, 842.4769, 902.3706, 1043.7056, 1097.6907, 1131.6755, 1170.8830, 1236.4595, 1291.7286, 1366.8442, 1389.1393, 1442.1396, 3049.9342, 3723.7563, 3812.8925

1 1.185863 2.316989 -0.166310 1 2.387533 -0.249960 0.908728	

Compound: sCl 2 + H_2O TS2	**Energy (kJ mol^{-1}):** -602.571987979725
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.872000 -0.055866 0.026501 6 0.388125 -0.059725 -0.862867 8 1.376054 -0.829330 -0.693386 8 1.752043 -0.797944 0.701867 1 0.188509 0.212024 -1.895001 9 -1.361524 -1.300237 0.049360 9 -0.744726 0.376239 1.278093 9 -1.777175 0.740324 -0.583722 8 1.278925 1.534698 -0.102153 1 0.727023 2.081282 0.470334 1 1.682365 0.793917 0.498653	-353.5599, 32.7498, 178.7265, 213.7614, 289.5076, 323.6146, 366.4348, 447.5482, 507.7217, 533.8073, 567.4192, 588.3382, 709.5027, 739.4606, 811.9352, 864.6585, 1000.0724, 1111.6344, 1160.0164, 1190.1058, 1257.9738, 1345.9494, 1542.6598, 1655.3576, 2544.8281, 3157.6649, 3805.1193

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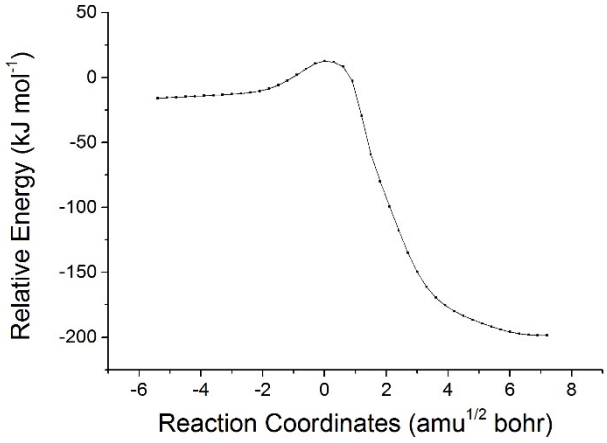

Compound: sCl 2 + H_2O Pr2	**Energy (kJ mol^{-1}):** -602.658023397310
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.841050 -0.157441 0.010445 6 0.405739 0.532657 -0.593230 8 1.494897 -0.309691 -0.777127 8 1.946041 -0.824612 0.499873 1 0.139028 0.801180 -1.622219 9 -1.170039 -1.245554 -0.691500 9 -0.722055 -0.493929 1.295152 9 -1.878208 0.721576 -0.076130 8 0.792725 1.643641 0.164788 1 0.020802 2.136425 0.465070 1 2.515462 -0.102443 0.805901	45.8073, 137.2188, 149.7556, 211.4607, 231.3373, 267.9918, 313.5215, 368.2515, 437.2812, 520.0905, 583.4169, 618.8499, 755.5434, 854.2256, 905.1872, 1039.2504, 1097.6375, 1127.1441, 1192.6499, 1236.5467, 1296.0157, 1351.6378, 1398.2769, 1425.9067, 3020.2585, 3727.7188, 3803.4861

Compound: sCl 3 + H_2O PRC	**Energy (kJ mol^{-1}):** -602.589934294451
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.265134 0.155609 -0.000000 6 -0.238467 0.008675 0.000003 8 -0.691074 -1.158101 -0.000001 8 -2.031785 -1.370658 0.000001 1 -0.897012 0.874551 0.000007 9 1.644005 0.852596 1.085581 9 1.897770 -1.014649 -0.000008 9 1.644000 0.852607 -1.085576 8 -2.920854 1.280203 0.000006	18.9310, 29.3495, 78.1991, 106.2923, 155.7969, 203.6063, 225.9814, 381.2152, 394.8102, 416.6995, 467.3076, 556.2957, 557.9028, 579.8286, 700.0094, 892.9234, 942.1189, 959.7400, 1141.7667, 1183.2773, 1280.4930, 1388.8948, 1556.7441, 1626.8972, 3124.7371, 3577.8101, 3872.5923

1 -3.823997 1.606901 -0.000046 1 -2.961273 0.306298 -0.000000	

Compound: sCl 3 + H_2O TS1	**Energy (kJ mol^{-1}):** -602.577917489654
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.039070 -0.051694 -0.022089 6 -0.419427 -0.182932 -0.448222 8 -1.146757 -0.949377 0.249124 8 -2.521237 -0.668508 -0.120692 1 -0.665573 0.023250 -1.482782 9 1.617879 0.945434 -0.698388 9 1.153163 0.194419 1.287084 9 1.694390 -1.188659 -0.300101 8 -1.326421 1.520273 -0.024545 1 -1.163554 1.758943 0.897664 1 -2.122302 0.845713 -0.021481	-344.2658, 39.3846, 140.2218, 175.5019, 268.4806, 340.7036, 381.7182, 433.9197, 491.8150, 551.9982, 564.2127, 603.5697, 674.9171, 717.4654, 848.3778, 884.9556, 1079.4615, 1171.3551, 1184.0130, 1221.8795, 1258.0253, 1343.7326, 1536.7055, 1608.3451, 2435.5100, 3172.2175, 3783.6617

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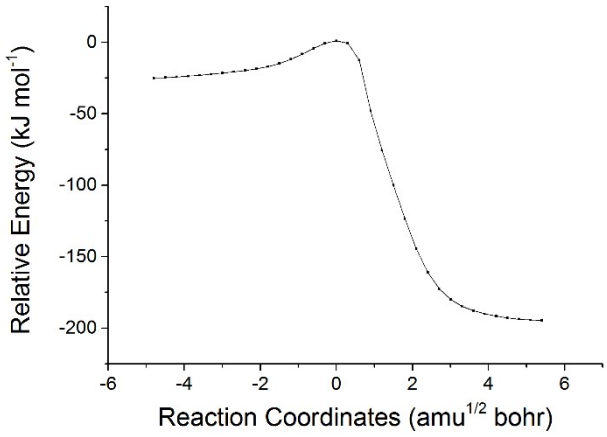

Compound: sCl 3 + H_2O Pr1	**Energy (kJ mol^{-1}):** -602.662813970698
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.963295 -0.146555 -0.034177 6 0.480869 0.288837 -0.359532 8 1.306945 -0.586625 0.368263 8 2.626042 -0.522137 -0.216993 1 0.654164 0.172304 -1.428349 9 -1.168282 -1.440472 -0.294445 9 -1.249598 0.074900 1.266542 9 -1.829589 0.568705 -0.767756 8 0.691587 1.629400 -0.052602 1 0.435506 1.791110 0.864764 1 3.035510 0.189595 0.297415	66.6299, 105.1886, 185.4932, 233.3104, 264.2291, 352.9867, 355.6744, 385.5909, 428.9955, 519.5011, 563.7230, 626.6447, 712.4712, 857.8522, 949.6848, 1040.3403, 1088.3219, 1151.0923, 1194.1080, 1250.6670, 1293.5017, 1361.2445, 1390.1415, 1437.9011, 3102.6609, 3728.9304, 3764.5581

Compound: sCI 3 + H_2O TS2	**Energy (kJ mol^{-1}):** -602.576912007240
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.039856 -0.049677 -0.010843 6 0.419539 -0.170430 -0.434149 8 1.150764 -0.956828 0.233990 8 2.523335 -0.666412 -0.143361 1 0.657816 0.049055 -1.468419 9 -1.552721 1.085282 -0.508187 9 -1.729827 -1.080080 -0.533333 9 -1.194383 -0.057248 1.306915 8 1.306977 1.471994 0.180893 1 1.388018 2.132416 -0.517541 1 2.119841 0.817564 0.095175	-364.8804, 52.2464, 143.0267, 175.9772, 274.1325, 343.0331, 381.2444, 435.7241, 478.2902, 553.8646, 583.4874, 590.5433, 694.4015, 732.1931, 850.8644, 881.0498, 1063.1370, 1153.9872, 1161.0462, 1190.5992, 1280.3717, 1337.8593, 1529.0559, 1631.0497, 2387.3409, 3161.7624, 3808.2251

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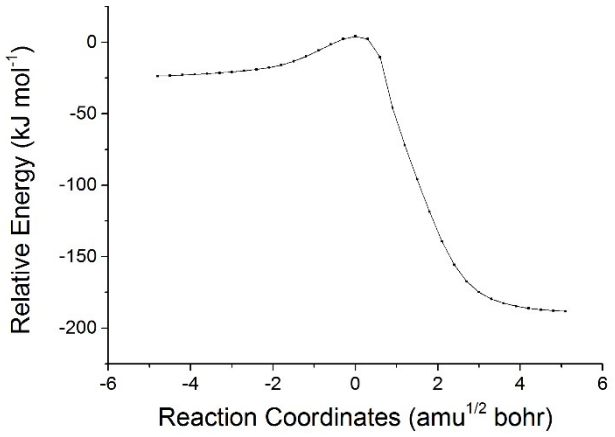

Compound: sCI 3 + H_2O Pr2	**Energy (kJ mol^{-1}):** -602.660922289812
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.977653 -0.122020 -0.020540 6 0.472388 0.292316 -0.339887 8 1.280676 -0.678073 0.280541 8 2.623938 -0.461809 -0.218113 1 0.609833 0.242347 -1.422859 9 -1.229129 -1.358117 -0.477948 9 -1.232482 -0.098538 1.291950 9 -1.828074 0.720918 -0.628725 8 0.676183 1.576208 0.153493 1 1.316213 2.032740 -0.399749 1 3.066331 -0.165837 0.590302	67.1172, 105.0116, 130.0950, 184.4267, 243.6539, 324.8792, 345.4993, 359.5577, 404.8713, 522.4187, 565.5794, 632.5000, 706.2299, 854.7571, 950.9452, 1050.2587, 1103.0362, 1142.7893, 1177.1310, 1242.9134, 1283.6311, 1354.4268, 1388.8170, 1458.0452, 3049.1963, 3747.1703, 3833.6975

Compound: sCI 4 + H_2O PRC1	**Energy (kJ mol^{-1}):** -701.757032802282
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.967467 -0.448045 -0.009361 6 0.154124 0.861668 -0.039692 8 -0.853476 1.115458 0.628635 8 -1.371797 0.108216 1.448886 9 0.598175 1.811820 -0.805522 9 1.460108 -0.630382 1.215244 9 0.228312 -1.484773 -0.360912 9 1.985779 -0.325431 -0.866525 8 -2.659392 -0.685120 -0.979841	8.9142, 50.9829, 56.8709, 125.1006, 160.5746, 181.1844, 225.8585, 279.1395, 292.2263, 336.4398, 363.7598, 481.9951, 500.3346, 573.4040, 583.7145, 626.9831, 674.6696, 778.6339, 914.2553, 1156.3613, 1190.7739, 1224.5363, 1401.3945, 1608.7930, 1641.3966, 3642.7446, 3869.6071

1 -3.601914 -0.543870 -1.101342 1 -2.501686 -0.587409 -0.026351	

Compound: sCl 4 + H_2O TS1	**Energy (kJ mol^{-1}):** -701.754722973199
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.922876 -0.252529 0.014628 6 0.362255 0.565884 -0.294872 8 1.349650 0.211899 -0.976788 8 1.789010 -1.121052 -0.588485 9 0.114206 1.848404 -0.318084 9 -1.590196 -0.321598 -1.153003 9 -0.722079 -1.470293 0.466790 9 -1.669098 0.426961 0.885625 8 1.193811 0.106194 1.564075 1 1.851343 0.781472 1.770174 1 1.657121 -0.589197 0.988920	-182.9477, 43.9809, 165.4231, 198.8283, 243.5936, 262.9655, 302.4476, 351.3823, 371.3221, 477.0843, 499.7850, 525.3643, 565.6404, 605.5389, 625.5149, 679.1056, 780.3852, 887.6970, 1089.4681, 1123.5063, 1179.4890, 1256.3551, 1357.2587, 1570.7234, 1615.7012, 2887.0314, 3807.7211

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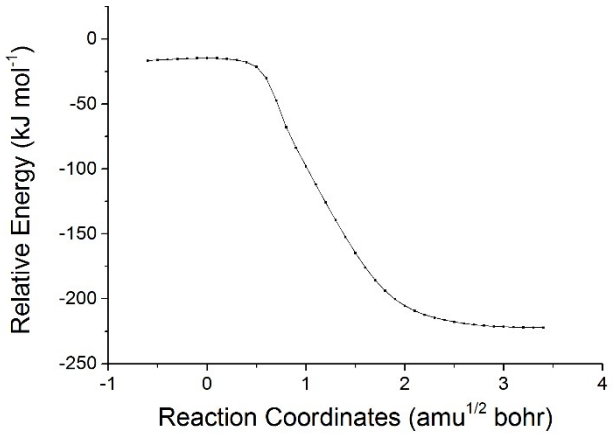

Compound: sCl 4 + H_2O Pr1	**Energy (kJ mol^{-1}):** -701.845677031827
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.889789 -0.270159 -0.010129 6 -0.431897 0.565724 -0.011041 8 -1.498264 -0.049484 0.670262 8 -1.771437 -1.321015 0.048761 9 -0.220327 1.671207 0.757854 9 1.087753 -0.810191 1.194456 9 0.872008 -1.241878 -0.923082 9 1.921381 0.540493 -0.285449 8 -0.714328 0.904974 -1.300334 1 -1.390579 1.595805 -1.297851 1 -2.431879 -1.081688 -0.618650	51.9068, 129.7086, 196.6813, 208.7458, 233.2065, 285.1346, 323.0522, 346.4562, 381.7148, 419.7601, 492.7066, 538.4071, 588.2672, 653.1779, 672.0489, 781.1123, 972.7409, 1033.4888, 1094.4151, 1182.9092, 1202.5091, 1207.0919, 1232.2767, 1402.9368, 1432.4007, 3728.7382, 3765.6990

Compound: sCl 4 + H_2O PRC2	**Energy (kJ mol^{-1}):** -701.757770997730
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.977575 -0.375535 -0.047959 6 0.014302 0.825274 0.048720 8 -0.967734 0.922922 0.791449 8 -1.354925 -0.209247 1.516763 9 0.320286 1.874211 -0.652500 9 1.562304 -0.551250 1.138425 9 0.366719 -1.487941 -0.415148 9 1.920185 -0.080620 -0.948960 8 -2.458473 -0.520975 -1.109929	22.4289, 55.7258, 71.6779, 148.8436, 161.0054, 182.5709, 232.8751, 282.2735, 294.0666, 364.2100, 373.9421, 478.9771, 500.5261, 510.9374, 581.3517, 626.6840, , 671.8741, 778.5441, 913.6810, 1155.7015, 1186.0906, 1223.3890, 1399.8811, 1611.1781, 1643.5507, 3661.4245, 3872.2454

1 -2.795570 -1.317291 -1.528523 1 -2.432075 -0.712349 -0.158653	

Compound: sCl 4 + H_2O TS2	**Energy (kJ mol^{-1}):** -701.754639690128
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.917298 -0.252424 -0.015764 6 0.371649 0.577981 -0.264789 8 1.364908 0.247768 -0.952222 8 1.799098 -1.098137 -0.590989 9 0.113971 1.855245 -0.249161 9 -1.583242 -0.275303 -1.178912 9 -0.722470 -1.491868 0.394882 9 -1.667441 0.384204 0.892193 8 1.278018 0.176684 1.517952 1 0.761571 -0.259947 2.205324 1 1.708783 -0.554405 0.949053	-224.4680, 28.2180, 165.0634, 199.2546, 254.2594, 262.0571, 307.3955, 357.3279, 373.8725, 477.9454, 515.0983, 551.0126, 567.1130, 602.8137, 611.6785, 727.2799, 786.6461, 895.3756, 1061.2898, 1139.5150, 1176.2030, 1240.2368, 1354.8576, 1556.1705, 1650.3191, 2770.0033, 3814.6039

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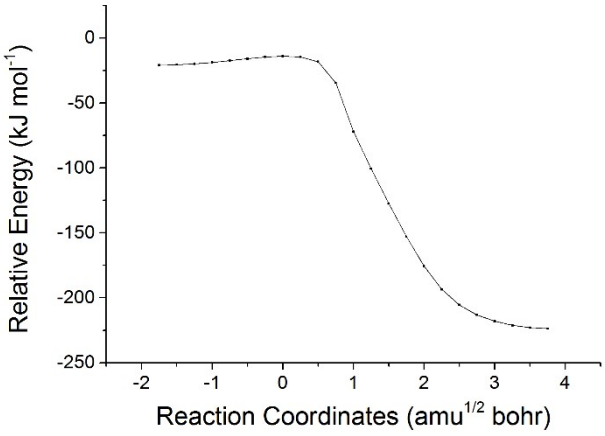

Compound: sCl 4 + H_2O Pr2	**Energy (kJ mol^{-1}):** -701.845674474457
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.888438 -0.308532 -0.010458 6 0.410990 0.559492 0.002560 8 1.463801 0.006090 -0.725260 8 1.980769 -1.149354 -0.036166 9 0.109977 1.683447 -0.712380 9 -1.317669 -0.516289 -1.252096 9 -0.715606 -1.485877 0.590294 9 -1.851494 0.359527 0.669975 8 0.819587 0.863153 1.266749 1 0.065762 1.113776 1.815604 1 2.658803 -0.745908 0.527062	46.9670, 131.6299, 205.9108, 226.8588, 245.4856, 290.8668, 306.3950, 347.6743, 377.9855, 414.5608, 484.6199, 529.2277, 590.4181, 642.2163, 692.5148, 784.1847, 968.1183, 1044.0527, 1092.7799, 1158.1546, 1195.9693, 1221.8558, 1289.7655, 1378.5484, 1419.4410, 3725.9129, 3782.9088

Compound: sCI 5 + H_2O PRC1	**Energy (kJ mol^{-1}):** -701.764103446066
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.253199 0.089592 0.115211 6 -0.153286 -0.368008 -0.261044 8 -0.872970 -0.931109 0.575069 8 -2.156873 -1.298958 0.195285 9 -0.507050 -0.188673 -1.485279 9 1.402006 1.379556 -0.186073 9 1.477454 -0.097338 1.407847 9 2.147090 -0.615696 -0.594844 8 -2.203577 1.547561 0.297113 1 -2.753188 2.142143 -0.220012 1 -2.654432 0.687754 0.280419	32.7360, 46.8598, 92.4712, 157.7812, 179.9572, 181.7624, 189.5062, 294.9945, 332.2552, 361.8550, 371.8605, 406.9222, 515.8260, 532.4507, 576.6471, 676.3573, 728.5135, 858.4915, 876.1783, 1149.8613, 1173.9584, 1235.9757, 1403.0899, 1628.8278, 1641.2467, 3658.9141, 3871.8932

Compound: sCI 5 + H_2O TS1	**Energy (kJ mol^{-1}):** -701.756908629529
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.126733 -0.047615 -0.093143 6 0.367795 -0.221556 0.235940 8 1.063441 -0.897170 -0.559318 8 2.478562 -0.642997 -0.295352 9 0.643596 -0.130985 1.504069 9 -1.657265 0.907431 0.663875 9 -1.279619 0.274686 -1.378264 9 -1.769314 -1.197000 0.143966 8 1.217696 1.555346 -0.143389 1 1.005306 1.861075 -1.034714 1 2.034135 0.945334 -0.240420	-292.2117, 38.7233, 137.0646, 175.9347, 252.9241, 290.7045, 310.8719, 365.5904, 388.1022, 418.6521, 507.5719, 527.4436, 574.7313, 656.1128, 696.2299, 726.4874, 809.6219, 845.9113, 1123.2579, 1160.3658, 1191.9307, 1222.6289, 1369.5290, 1563.9859, 1622.8314, 2744.9152, 3792.4031

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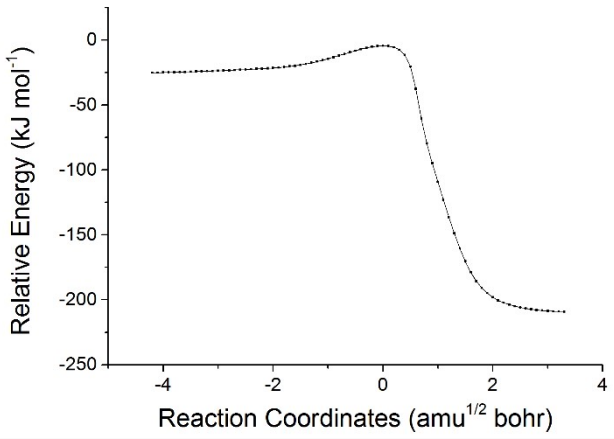

Compound: sCI 5 + H_2O Pr1	**Energy (kJ mol^{-1}):** -701.845741873404
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.062154 -0.164450 0.008092 6 0.430105 0.300164 -0.048891 8 1.168471 -0.873619 0.086297 8 2.569482 -0.553850 -0.039440 9 0.649193 0.876050 -1.249055 9 -1.314131 -1.157639 -0.839044 9 -1.351761 -0.581518 1.259980 9 -1.864993 0.861751 -0.279192 8 0.705758 1.255653 0.899749	62.5858, 126.1553, 156.3520, 187.5452, 228.7942, 295.2365, 316.7880, 342.0580, 377.0116, 393.9381, 521.8175, 530.1352, 587.2667, 609.4954, 733.9792, 831.8169, 943.4958, 1051.7784, 1091.0788, 1157.7878, 1177.4707, 1219.1982, 1284.5333, 1384.6587, 1403.4261, 3729.2527, 3786.2786

1 0.356738 0.972335 1.754092 1 2.821091 -0.399880 0.883653	

Compound: sCl 5 + H_2O TS2	**Energy (kJ mol^{-1}):** -701.757550624596
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.127586 -0.061446 -0.098574 6 -0.368149 -0.185799 0.245111 8 -1.066102 -0.970698 -0.432758 8 -2.481840 -0.695167 -0.198366 9 -0.636159 0.097016 1.495767 9 1.600071 1.101582 0.352276 9 1.794427 -1.054918 0.506831 9 1.320420 -0.142869 -1.406306 8 -1.193324 1.473055 -0.506932 1 -1.313450 2.140834 0.178902 1 -2.021883 0.877816 -0.490794	-294.5242, 49.7277, 138.2138, 175.5823, 256.1652, 276.7056, 308.7521, 363.4740, 390.8796, 419.0342, 512.6498, 542.4217, 576.1978, 644.9694, 692.3609, 722.8270, 805.8408, 845.4312, 1078.8819, 1142.1180.9943, 1236.9997, 1357.9910, A, 1561.3891, 1646.0271, 2797.5934, 3809.6964

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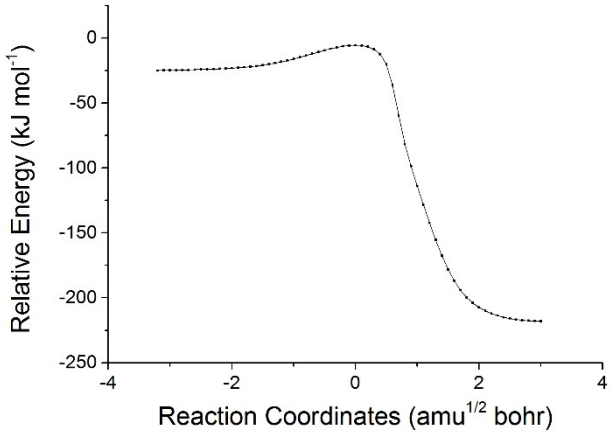

Compound: sCl 5 + H_2O Pr2	**Energy (kJ mol^{-1}):** -701.848967983056
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.061640 -0.178518 0.026237 6 0.433844 0.274899 -0.021704 8 1.170177 -0.885298 -0.006673 8 2.574014 -0.556023 -0.067483 9 0.594253 0.968979 -1.194790 9 -1.393384 -0.902540 -1.041940 9 -1.309837 -0.892268 1.126667 9 -1.837660 0.920355 0.053817 8 0.763942 1.076495 1.038769 1 0.429834 1.968970 0.887611 1 2.791526 -0.479383 0.874497	67.4708, 125.8551, 166.0025, 224.1819, 237.1201, 253.3577, 306.5786, 340.7011, 375.3352, 389.2286, 520.6247, 526.0073, 586.7124, 605.7663, 733.6858, 829.3280, 939.0000, 1044.0602, 1068.6489, 1176.7477, 1183.4267, 1211.4081, 1330.7134, 1346.9850, 1414.6427, 3722.6833, 3796.5626

S8.10 Reactions with $(H_2O)_2$

Compound: $(H_2O)_2$	**Energy (kJ mol^{-1}):** -152.753039538317
Reaction Coordinates:	**Frequencies (cm^{-1}):**
8 -1.516947 0.000002 -0.121143 1 -1.926876 -0.000012 0.747807 1 -0.561489 -0.000002 0.044554 8 1.391185 -0.000002 0.109911 1 1.747231 -0.766159 -0.351264 1 1.747228 0.766171 -0.351242	136.9386, 159.6379, 161.0494, 190.5114, 364.4335, 626.4275, 1628.1114, ,1647.2164, 3675.9138, 3791.8236, 3871.0307, 3890.8064

Compound: sCI 1 + $(H_2O)_2$ PRC1	**Energy (kJ mol^{-1}):** -342.172906791257
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.941512 -1.103855 0.343798 8 -1.411547 -0.220247 -0.397069 8 -1.297519 1.104921 0.041057 1 -0.528363 -0.842561 1.308425 1 -1.044879 -2.119710 -0.010485 8 1.374142 1.413463 0.128117 1 0.383318 1.436018 0.084927 1 1.688347 2.087966 -0.479194 8 1.534375 -1.298054 -0.030337 1 1.664081 -0.321597 -0.036516 1 1.890960 -1.617648 -0.864079	34.7620, 92.3912, 128.1685, 229.3716, 245.7725, 251.4917, 264.5672, 292.4871, 435.7695, 509.2517, 527.9532, 708.4598, 757.5050, 820.9549, 928.0187, 1050.4965, 1233.0677, 1420.8772, 1585.0220, 1657.2334, 1667.4210, 3135.5422, 3229.4431, 3276.7943, 3402.4775, 3852.3723, 3864.9663

Compound: sCI 1 + $(H_2O)_2$ TS1	**Energy (kJ mol^{-1}):** -342.168010859089
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.192422 0.529632 0.316311 8 1.160920 -0.499868 -0.434508 8 0.318766 -1.553240 0.115411 1 0.932868 0.410061 1.360688 1 1.931337 1.267746 0.027052 8 -1.845919 -0.326514 0.101626 1 -0.993520 -0.964941 0.078703 1 -2.433201 -0.575827 -0.616514 8 -0.296944 1.611904 -0.010087 1 -1.070723 0.887825 -0.013058 1 -0.215877 1.939076 -0.914276	-331.9075, 71.9222, 194.6061, 351.7547, 414.3802, 422.4307, 475.2839, 500.9594, 542.9366, 635.6221, 785.6676, 811.7532, 997.0156, 1174.5653, 1210.7296, 1231.3393, 1340.8124, 1379.1202, 1510.8264, 1574.8904, 1701.3286, 1933.9475, 2324.7193, 3111.8165, 3225.2142, 3799.8888, 3856.3891

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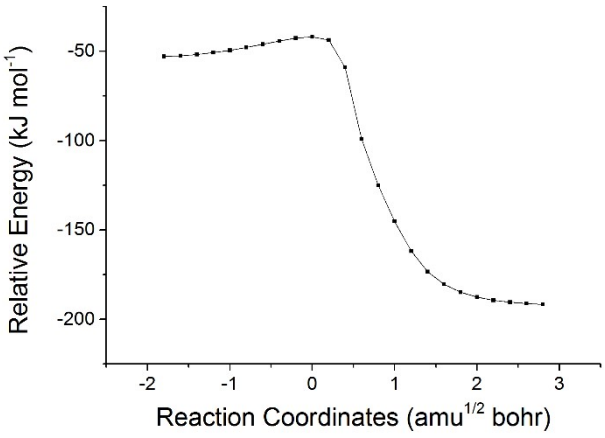

Compound: sCI 1 + $(H_2O)_2$ Pr1	**Energy (kJ mol^{-1}):** -342.233729892064
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.310155 -0.387971 0.211196 8 -0.951903 0.746125 -0.518256 8 -0.007548 1.526793 0.257320 1 0.849294 1.100333 0.040465 1 -1.377092 -0.153293 1.270671 1 -2.278477 -0.684059 -0.197767 8 -0.375966 -1.458639 0.095441 1 -0.493571 -1.871459 -0.766643 8 2.199355 -0.167618 0.041687 1 2.736653 -0.384393 -0.725326 1 1.512619 -0.852597 0.101887	80.2143, 135.1051, 177.1882, 218.1612, , 245.4740, 311.2889, 418.3506, 430.3680, , 548.4011, 606.7308, 762.0375, 878.9051, 985.8147, 1044.7150, 1057.6103, 1281.4671, 1376.6100, 1409.4124, 1477.9090, 1487.4796, 1643.2095, 3043.3769, 3125.9909, 3485.3233, 3647.4380, 3800.8669, 3864.6927

Compound: sCI 1 + $(H_2O)_2$ PRC2	**Energy (kJ mol^{-1}):** -342.172820831981
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.183018 1.034344 0.165699 8 1.329699 -0.039021 -0.445103 8 1.120434 -1.214004 0.287038 1 0.963648 1.023652 1.224482 1 1.336764 1.932257 -0.416177 8 -1.553924 -1.256559 -0.144544 1 -0.591428 -1.418379 0.018269 1 -2.032764 -1.857041 0.431979 8 -1.306680 1.470287 -0.041135 1 -1.570090 0.522258 -0.059751 1 -1.920468 1.905555 0.556951	44.7709, 92.2913, 121.6969, 190.2055, 221.7461, 229.2992, 252.4455, 269.8093, 454.4412, 508.4079, 558.2405, 679.0943, 700.7851, 820.4844, 849.8782, 1042.4600, 1234.4812, 1421.5825, 1590.4005, 1666.4577, 1681.3650, 3134.9513, 3276.2042, 3280.1314, 3422.0270, 3856.0097, 3867.7459

Compound: sCI 1 + $(H_2O)_2$ TS2	**Energy (kJ mol^{-1}):** -342.166034138439
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.320571 0.408091 0.121837 8 0.985248 -0.661014 -0.484936 8 0.151751 -1.508354 0.360187 1 1.343904 0.381680 1.205155 1 2.027564 1.018985 -0.425759 8 -1.846984 -0.152850 -0.195992 1 -1.096225 -0.874018 0.055889 1 -2.570960 -0.233348 0.430105 8 -0.101441 1.596433 -0.018511 1 -0.949800 0.944191 -0.069664 1 -0.186498 2.120247 0.787262	-390.4521, 77.4610, 199.6630, 350.7358, 398.6994, 428.1677, 472.3849, 496.8026, 547.9891, 695.6734, 814.1253, 819.6207, 974.9830, 1065.5883, 1190.1939, 1237.5317, 1311.3755, 1373.6134, 1500.2665, 1605.5800, 1703.6058, 1871.0365, 2225.0288, 3105.5587, 3220.4414, 3799.7280, 3857.9859
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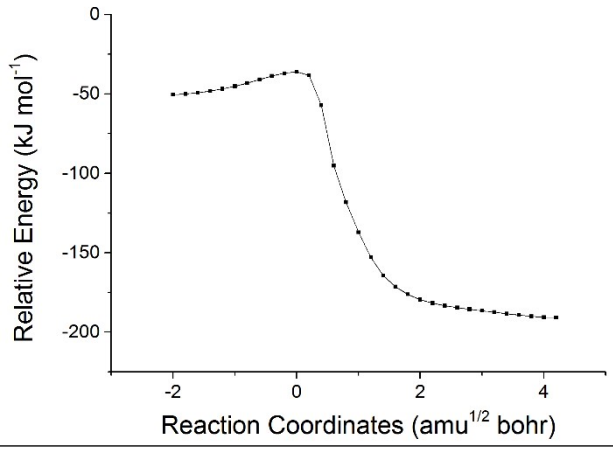

Compound: sCI 1 + $(H_2O)_2$ Pr2	**Energy (kJ mol^{-1}):** -342.234765929815
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.379368 -0.331531 -0.143936 8 -0.679769 0.790306 -0.597330 8 -0.021638 1.388099 0.551088 1 0.893352 1.074027 0.403685 1 -2.043645 -0.057252 0.678174 1 -1.943257 -0.656645 -1.017525 8 -0.533159 -1.399710 0.242642 1 -0.346092 -1.309180 1.182284 8 2.153792 -0.217292 -0.222703 1 2.906674 -0.673391 0.162826 1 1.455373 -0.879593 -0.335403	109.1770, 119.5232, 156.5756, 175.0228, 220.1963, 279.2470, 378.5575, 410.0549, 490.8357, 612.7953, 691.0145, 881.9182, 1015.8576, 1037.4611, 1059.6915, 1284.5684, 1380.9111, 1410.5284, 1482.8420, 1487.0272, 1630.3323, 3034.4784, 3109.8974, 3543.4798, 3698.6881, 3813.3170, 3873.2790

Compound: sCI 1 + $(H_2O)_2$ PRC3	**Energy (kJ mol^{-1}):** -342.173701402131
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.112307 1.068481 0.203569 8 1.344169 0.032511 -0.444929 8 1.171224 -1.184469 0.230492 1 0.857189 0.999313 1.252239 1 1.242551 1.998643 -0.331254 8 -1.514347 -1.304856 0.053226 1 -0.531564 -1.416493 0.119399 1 -1.799220 -1.866540 -0.672457 8 -1.363138 1.408770 -0.093024 1 -1.572574 0.445034 -0.085667 1 -1.973493 1.813512 0.530199	53.1327, 101.9900, 132.7817, 216.3090, 243.7112, 262.3092, 281.8423, 301.6424, 438.3076, 477.5225, 510.9797, , 696.7678, 816.7400, 821.8222, 950.4880, 1046.3538, 1235.4963, 1422.2397, 1589.6123, 1640.0256, 1668.4226, , 3134.9327, 3239.5935, 3277.1102, 3384.2768, 3849.1270, 3859.6874

Compound: sCI 1 + $(H_2O)_2$ TS3	**Energy (kJ mol^{-1}):** -342.168160410100
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.307862 0.444852 0.124825 8 1.010389 -0.627475 -0.492431 8 0.206552 -1.515403 0.339739 1 1.306652 0.417002 1.208064 1 1.999163 1.084525 -0.409325 8 -1.868295 -0.197275 -0.001163 1 -1.074048 -0.895604 0.133812 1 -2.336835 -0.426090 -0.808385	-357.3390, 83.2044, 206.4492, 353.9082, 392.4595, 425.2889, 475.5641, 507.1320, 550.1419, 625.3160, 800.6382, 818.4120, 964.7382, 1192.1193, 1215.3899, 1240.6843, 1362.3744, 1421.4184, 1509.2727, 1574.1521, 1652.4906, 1867.5595, 2284.4761, 3108.9557,

8 -0.159866 1.602317 -0.040412 1 -0.977060 0.917827 -0.074545 1 -0.275279 2.135912 0.755561	3225.1613, 3795.7823, 3851.9574

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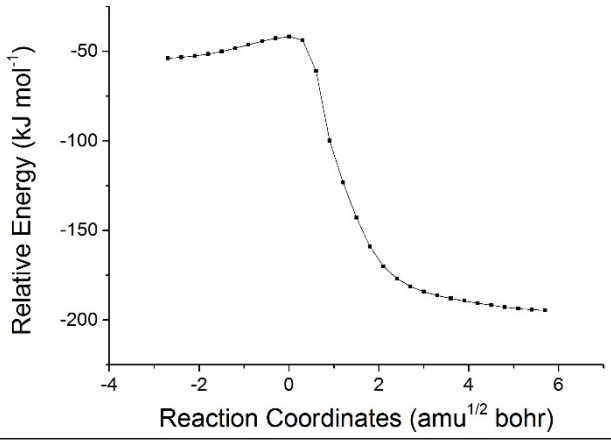

Compound: sCI 1 + $(H_2O)_2$ Pr3	**Energy (kJ mol^{-1}):** -342.236055056007
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.379185 -0.321230 0.130494 8 0.687283 0.800439 0.597518 8 -0.001863 1.393427 -0.534429 1 -0.902001 1.029461 -0.396438 1 2.012555 -0.049944 -0.716190 1 1.974993 -0.634252 0.987427 8 0.525348 -1.397117 -0.215878 1 0.333934 -1.347236 -1.157888 8 -2.159058 -0.297409 0.068324 1 -2.681414 -0.178741 0.866979 1 -1.426865 -0.886630 0.308862	102.8232, 138.8594, 161.2587, 217.9648, 234.9476, 270.5088, 401.6741, 440.9790, 540.4841, 624.9479, 753.4956, 882.5366, 1015.2832, 1038.1739, 1058.5376, 1284.3506, 1377.0341, 1410.5592, 1482.3422, 1486.2977, 1632.4035, 3037.2242, 3108.2353, 3498.1506, 3681.9869, 3811.6239, 3862.6764

Compound: sCI 1 + $(H_2O)_2$ PRC4	**Energy (kJ mol^{-1}):** -342.173268681123
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.035941 1.088804 0.263467 8 1.393543 0.111275 -0.419126 8 1.227174 -1.156101 0.155147 1 0.679362 0.944771 1.273830 1 1.175061 2.058545 -0.193582 8 -1.453888 -1.351848 -0.097799 1 -0.469779 -1.435667 -0.012495 1 -1.834915 -1.938947 0.560283 8 -1.452168 1.361236 0.051517 1 -1.617832 0.390095 0.007285 1 -1.864840 1.731884 -0.734030	50.1715, 95.4727, 125.9329, 230.6779, 244.3856, 258.3228, 278.3355, 306.0719, 455.3526, 497.6357, 520.4366, 705.8264, 768.2027, 821.0998, 923.8951, 1049.5097, 1230.3444, 1419.6329, 1586.9402, 1653.3753, 1680.2783, 3136.0331, 3239.6046, 3277.0653, 3385.2974, 3850.4666, 3861.9778

Compound: sCI 1 + $(H_2O)_2$ TS4	**Energy (kJ mol^{-1}):** -342.168384007199
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.218398 0.517405 0.297770 8 1.143425 -0.519292 -0.438134 8 0.301105 -1.548507 0.154723 1 1.002418 0.412531 1.353308 1 1.951131 1.244668 -0.032246	-323.4815, 80.5480, 190.8851, 346.9591, 381.6466, 419.4027, 479.1782, 508.9306, 558.1013, 663.7923, 772.5704, 815.4304, 1002.2355, 1105.5810, 1208.6211,

8 -1.851952 -0.311351 -0.103947 1 -1.017154 -0.960857 -0.003975 1 -2.470054 -0.505205 0.605649 8 -0.279622 1.609468 0.030322 1 -1.055363 0.888764 0.009180 1 -0.225014 1.973128 -0.862245	1227.3572, 1350.2545, 1391.6604, 1512.9992, 1651.4838, 1666.7662, 1957.8254, 2347.4213, 3111.9292, 3225.4165, 3795.6111, 3855.2238

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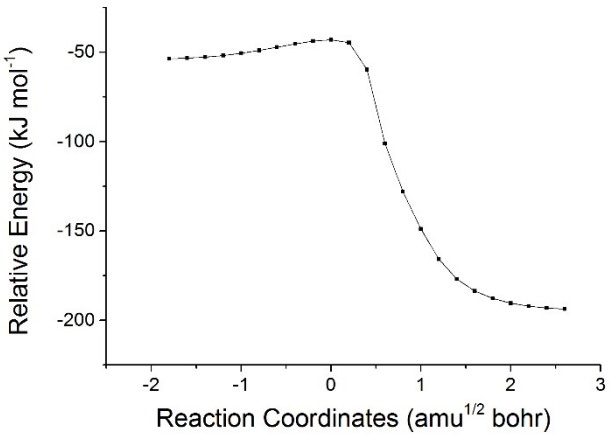

Compound: sCl 1 + $(H_2O)_2$ Pr4	**Energy (kJ mol^{-1}):** -342.234605099278
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.304886 -0.428786 0.217856 8 -1.000200 0.731096 -0.495025 8 -0.047719 1.514145 0.267961 1 0.809870 1.123777 -0.003827 1 -1.389838 -0.214913 1.280822 1 -2.256525 -0.761623 -0.202357 8 -0.320406 -1.449584 0.094944 1 -0.369645 -1.814832 -0.795559 8 2.196659 -0.145098 -0.146881 1 2.878349 -0.161457 0.530961 1 1.530433 -0.802702 0.114842	90.9279, 136.5893, 170.6335, 225.5069, 258.9680, 329.8411, 426.2758, 439.7446, 528.9552, 608.3053, 766.9180, 880.2249, 992.4407, 1045.1451, 1060.6803, 1281.0766, 1375.5973, 1412.5202, 1479.2496, 1496.9437, 1626.5333, 3042.1788, 3121.4472, 3499.4066, 3641.3869, 3792.6196, 3861.7379

Compound: sCl 2 + $(H_2O)_2$ PRC1	**Energy (kJ mol^{-1}):** -678.974835113330
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.226886 0.069658 -0.173860 6 -0.327629 -0.153120 1.036917 8 0.548333 -1.036039 1.112313 8 0.877813 -1.749719 -0.030010 1 -0.543624 0.376619 1.953269 9 -2.014559 1.127672 0.099043 9 -0.591222 0.307883 -1.313380 9 -2.019818 -1.000758 -0.332959 8 2.879487 0.074156 -0.588399 1 2.302773 -0.717172 -0.511804 1 3.224136 0.073448 -1.485108 8 1.106164 1.829012 0.588222 1 1.819692 1.348332 0.111352 1 0.860129 2.567097 0.022605	37.4045, 57.1535, 91.4813, 107.9226, 134.2558, 193.0122, 218.4290, 225.2269, 231.9446, 276.5813, 295.5504, 320.5879, 430.4866, 480.3114, 500.0589, 526.4522, 539.5277, 591.2657, 652.9329, 753.0271, 816.7426, 846.1514, 855.7267, 885.9751, 1150.1725, 1170.1522, 1262.1541, 1371.4928, 1593.0624, 1662.6313, 1668.8617, 3222.1025, 3389.2633, 3463.1346, 3847.8267, 3865.5964

Compound: sCl 2 + $(H_2O)_2$ TS1	**Energy (kJ mol^{-1}):** -678.970889225415
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.173357 -0.023374 0.164242 6 -0.151008 0.080429 -0.982054 8 0.689286 1.025230 -1.064898 8 1.119634 1.538355 0.223773 1 -0.541650 -0.236571 -1.942191 9 -2.015736 -1.041562 -0.149138 9 -0.676530 -0.288170 1.368967 9 -1.889874 1.098391 0.215695 8 2.710861 -0.401175 0.533202 1 2.185805 0.495286 0.505416 1 2.922854 -0.588301 1.451650 8 0.810773 -1.490775 -0.664878 1 1.644758 -1.159895 -0.104261 1 0.329264 -2.143876 -0.141050	-290.0059, 46.3837, 64.5511, 168.5922, 182.7072, 230.3468, 301.4527, 314.3332, 372.6685, 395.7978, 408.1420, 473.8506, 507.6275, 518.0961, 554.1721, 598.6566, 675.9497, 744.7321, 805.4973, 824.7409, 879.3618, 1008.2971, 1075.2479, 1122.4730, 1206.1978, 1262.7319, 1277.8725, 1351.6705, 1530.8641, 1673.7946, 1713.3045, 2078.5849, 2543.4807, 3168.9662, 3787.2140, 3854.6140

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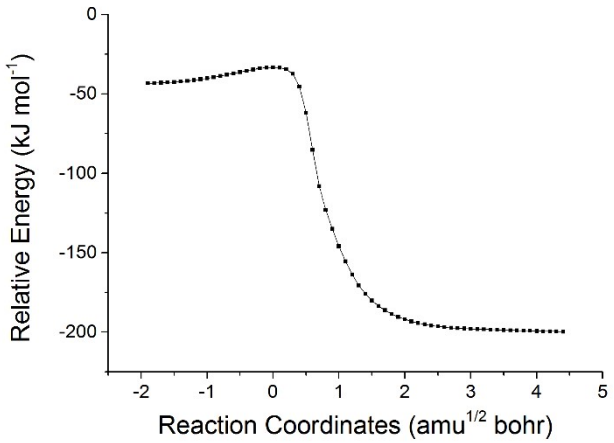

Compound: sCl 2 + $(H_2O)_2$ Pr1	**Energy (kJ mol^{-1}):** -679.043932127222
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.319171 -0.025832 0.129707 6 -0.099793 -0.222029 -0.803922 8 0.688475 0.894559 -0.978112 8 1.172711 1.381058 0.299920 1 2.046883 0.932451 0.348848 1 -0.505125 -0.398751 -1.805744 8 0.677895 -1.319844 -0.364164 1 0.115687 -2.093579 -0.242853 9 -2.120810 -1.120416 -0.019587 9 -1.024117 0.063500 1.425112 9 -2.028327 1.047038 -0.229328 8 3.336058 -0.357324 0.286854 1 3.755770 -0.629253 1.108307 1 2.658744 -1.022384 0.094960	36.4715, 56.0671, 125.3481, 135.0123, 185.8482, 211.5810, 235.6883, 243.2222, 254.3634, 298.8896, 330.1348, 376.5204, 437.9258, 469.2699, 520.0383, 582.8195, 611.9422, 744.2850, 754.9017, 852.2004, 908.7220, 1033.2727, 1092.9097, 1112.6719, 1195.4946, 1247.0912, 1300.8185, 1359.0143, 1425.1312, 1528.9667, 1632.6548, 3033.4111, 3443.2887, 3715.3179, 3798.3722, 3865.9905

Compound: sCl 2 + $(H_2O)_2$ PRC2	**Energy (kJ mol^{-1}):** -678.975412531634
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.214882 0.071350 -0.175366 6 -0.325793 -0.161017 1.042058 8 0.545657 -1.048070 1.121063 8 0.887838 -1.752056 -0.026755 1 -0.554234 0.358827 1.961138 9 -2.001088 1.130774 0.097863 9 -0.570514 0.311513 -1.307792 9 -2.010442 -0.996175 -0.342068 8 2.774490 0.122967 -0.749245 1 2.224618 -0.679219 -0.605514 1 3.666755 -0.111412 -0.480022 8 1.103865 1.811852 0.619107 1 1.806175 1.330267 0.123785 1 0.844351 2.546984 0.055074	41.8023, 58.0072, 98.6309, 113.1135, 134.6924, 193.3712, 224.3711, 238.4057, 254.7038, 282.1835, 319.6521, 335.3226, 404.7950, 467.5258, 481.0277, 507.0066, 536.9264, 591.7953, 747.8361, 759.8966, 829.6064, 858.2697, 886.5529, 908.8787, 1149.1735, 1170.7208, 1265.3439, 1371.2946, 1593.6215, 1637.7621, 1663.6177, 3221.0408, 3359.0331, 3445.1478, 3842.8330, 3860.0165

Compound: sCl 2 + $(H_2O)_2$ TS2	**Energy (kJ mol^{-1}):** -678.972203381997
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.178354 0.022029 0.158851 6 0.147978 -0.071725 -0.980800 8 -0.697411 -1.010264 -1.065886 8 -1.114160 -1.543374 0.218888 1 0.525561 0.262066 -1.940232 9 2.018163 1.042347 -0.152675 9 0.690659 0.271855 1.367738 9 1.895185 -1.101577 0.189445 8 -2.649322 0.416120 0.673704 1 -2.152135 -0.487113 0.573358 1 -3.524230 0.315367 0.288595 8 -0.818695 1.511442 -0.634519 1 -1.653999 1.160100 -0.097130 1 -0.352551 2.142745 -0.070962	-269.7946, 50.1764, 63.9495, 173.4678, 183.5984, 229.1705, 302.2534, 313.6691, 372.7622, 379.2671, 408.0386, 477.1009, 511.5748, 517.6791, 549.2021, 595.0579, 610.6639, 742.1387, 800.8068, 814.9207, 879.3384, 1064.6348, 1124.1278, 1139.8038, 1205.8730, 1270.9158, 1347.7219, 1368.6629, 1535.3773, 1606.6560, 1661.9980, 2136.0068, 2593.0390, 3171.4988, 3783.4700, 3851.0261

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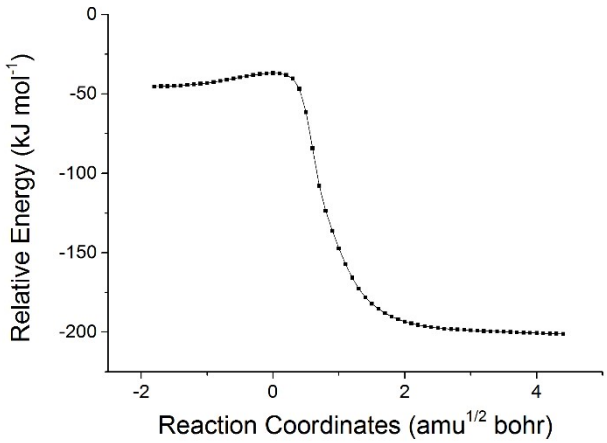

Compound: sCl 2 + $(H_2O)_2$ Pr2	**Energy (kJ mol^{-1}):** -679.044522555901
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.322906 -0.020520 0.112406 6 -0.084043 -0.241045 -0.789019 8 0.716228 0.869099 -0.963624 8 1.167558 1.378038 0.317840 1 2.031053 0.914065 0.408348 1 -0.467995 -0.429444 -1.797286 8 0.679699 -1.335631 -0.321104 1 0.102371 -2.044888 -0.015769 9 -2.130590 -1.110357 -0.037283 9 -1.055727 0.085110 1.412809 9 -2.012187 1.052759 -0.279522 8 3.301497 -0.378920 0.431258 1 3.995376 -0.356724 -0.234385 1 2.647576 -1.021918 0.119768	38.5690, 54.0929, 129.2809, 136.0169, 157.2516, 214.1037, 237.6501, 255.5837, 260.4528, 282.1900, 301.5859, 369.7651, 436.3490, 518.4205, 527.5382, 584.3273, 621.5032, 752.7175, 793.5276, 854.1331, 908.7737, 1041.4784, 1090.5830, 1113.8186, 1199.1434, 1244.6945, 1302.0778, 1353.1822, 1431.0382, 1512.5730, 1626.9675, 3031.5325, 3431.1048, 3713.0756, 3796.4734, 3864.3227

Compound: sCI 2 + $(H_2O)_2$ PRC3	**Energy (kJ mol^{-1}):** -678.973863351660
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.190559 0.094535 -0.196108 6 -0.369816 -0.172653 1.062611 8 0.480011 -1.077431 1.176344 8 0.862903 -1.784611 0.048000 1 -0.634506 0.341912 1.974995 9 -1.984786 1.148371 0.055349 9 -0.480784 0.343171 -1.283526 9 -1.981592 -0.969140 -0.421792 8 2.702079 0.091542 -0.818995 1 2.159514 -0.701130 -0.614895 1 3.616997 -0.164226 -0.676270 8 1.073424 1.846982 0.551227 1 1.771615 1.367837 0.052656 1 1.525750 2.310843 1.261611	43.5999, 60.5434, 98.9220, 102.2304, 122.5014, 186.2915, 219.4830, 223.4351, 231.6112, 247.9051, 277.4087, 319.6655, 395.1912, 476.6845, 496.7676, 505.7365, 536.0064, 588.8097, 688.7703, 754.5842, 820.2495, 852.0429, 862.4511, 887.8182, 1150.9682, 1170.0254, 1268.7329, 1368.4085, 1591.2971, 1644.9660, 1665.7561, 3219.0326, 3402.1416, 3471.6488, 3853.1968, 3865.0665

Compound: sCI 2 + $(H_2O)_2$ TS3	**Energy (kJ mol^{-1}):** -678.970261942381
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.151495 -0.045174 -0.184872 6 0.170938 0.072243 0.998151 8 -0.653792 1.026446 1.122183 8 -1.115610 1.577872 -0.136639 1 0.591290 -0.262956 1.940555 9 2.030092 -1.024962 0.114831 9 0.607304 -0.324768 -1.358357 9 1.837879 1.100638 -0.273055 8 -2.529554 -0.422462 -0.791602 1 -2.072740 0.486607 -0.603370 1 -3.451191 -0.349556 -0.529791 8 -0.772075 -1.527413 0.614835 1 -1.582115 -1.188548 0.037894 1 -1.129066 -1.841687 1.454050	-255.0687, 55.2659, 77.0544, 168.0979, 178.5946, 222.8289, 303.1951, 315.0054, 370.2693, 390.8977, 403.1160, 468.3366, 482.4316, 519.7345, 552.4007, 603.8288, 621.6264, 742.8942, 784.0733, 809.4791, 898.8488, 1058.3895, 1108.0793, 1143.1440, 1188.6024, 1271.7654, 1305.2514, 1345.2191, 1534.5795, 1613.5212, 1707.5809, 2181.4832, 2610.1198, 3155.3420, 3805.6386, 3855.2006

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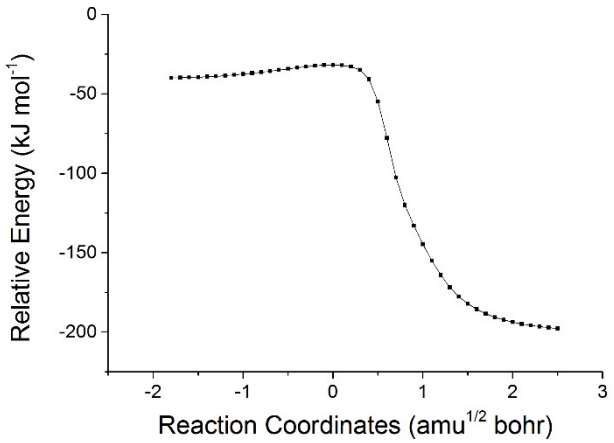
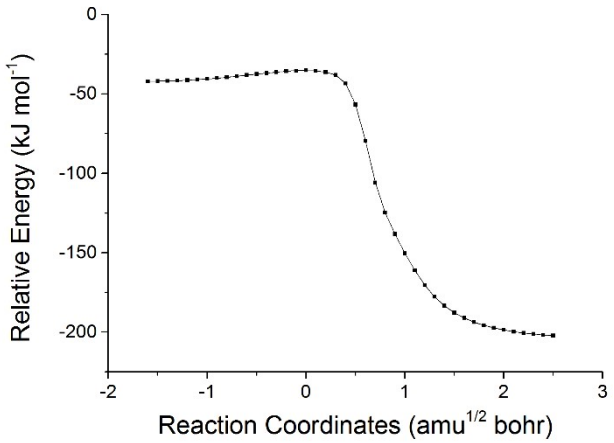


Compound: sCl 2 + $(H_2O)_2$ Pr3	**Energy (kJ mol^{-1}):** -679.044046393108
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.235036 -0.074225 -0.201158 6 0.180498 -0.131186 0.928825 8 -0.576023 1.025870 1.082329 8 -1.115760 1.449222 -0.193629 1 -1.945106 0.927595 -0.260668 1 0.729962 -0.193591 1.871195 8 -0.585846 -1.296230 0.707444 1 -0.893072 -1.622913 1.558947 9 2.181647 -1.006601 0.055252 9 0.739031 -0.332562 -1.412406 9 1.839106 1.118160 -0.225203 8 -3.084291 -0.441560 -0.675776 1 -3.903200 -0.686352 -0.235492 1 -2.424486 -1.101660 -0.421706	38.0835, 64.6328, 96.1394, 135.5457, 197.8564, 201.4051, 234.9116, 243.3833, 261.0024, 303.1512, 331.9013, 371.1792, 436.1274, 449.1955, 525.3000, 582.6400, 609.0144, 750.8165, 767.7665, 844.1162, 907.7243, 1051.8707, 1076.2109, 1126.7896, 1177.7901, 1246.2906, 1291.8476, 1373.1354, 1437.7390, 1483.7264, 1632.1168, 3059.6863, 3479.9112, 3732.3887, 3815.2581, 3872.7493

Compound: sCl 2 + $(H_2O)_2$ PRC4	**Energy (kJ mol^{-1}):** -678.974423926339
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.195272 0.096888 -0.192917 6 -0.363456 -0.174980 1.057263 8 0.485322 -1.082150 1.161247 8 0.865860 -1.777624 0.024545 1 -0.627595 0.330073 1.975107 9 -1.987364 1.149471 0.068122 9 -0.497726 0.350479 -1.289404 9 -1.987331 -0.966137 -0.416690 8 2.796504 0.076841 -0.680249 1 2.233024 -0.714988 -0.535574 1 2.968365 0.113539 -1.625230 8 1.069922 1.825415 0.546226 1 1.765743 1.329712 0.056432 1 1.523766 2.266039 1.270788	44.5943, 61.0444, 104.8336, 125.3744, 189.9980, 221.1578, 232.1002, 241.0143, 280.2124, 303.1346, 320.0261, 427.4818, 469.8666, 496.1996, 500.6470, 536.0040, 590.0928, 694.7367, 754.2804, 834.5125, 857.8793, 885.0821, 896.8702, 1151.3690, 1169.9219, 1265.2790, 1368.1246, 1590.6157, 1649.7949, 1669.9483, 3218.8672, 3367.2346, 3453.9721, 3847.7674, 3858.5145

Compound: sCl 2 + $(H_2O)_2$ TS4	**Energy (kJ mol^{-1}):** -678.971433697789
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.148516 -0.052598 -0.185936 6 0.180719 0.099865 1.002687 8 -0.638403 1.059164 1.109814 8 -1.110604 1.582452 -0.154346 1 0.603794 -0.220212 1.948898 9 2.026834 -1.026730 0.127879 9 0.590992 -0.363862 -1.349187 9 1.836346 1.087250 -0.317239 8 -2.611693 -0.414783 -0.662662 1 -2.124068 0.486864 -0.549865 1 -2.687895 -0.585007 -1.605794 8 -0.778960 -1.510779 0.657020 1 -1.572380 -1.177308 0.057052 1 -1.165135 -1.786280 1.497513	-242.4381, 56.9560, 77.5768, 163.9943, 178.3123, 224.0854, 302.7484, 314.3336, 362.0054, 378.2726, 389.8786, 472.0494, 518.6113, 520.7586, 551.5244, 606.7181, 632.0949, 734.4464, 779.3153, 813.3456, 899.3494, 1014.0479, 1074.2958, 1146.1441, 1188.0078, 1269.7607, 1330.6011, 1355.1327, 1539.8493, 1652.5416, 1695.9196, 2208.5205, 2657.1975, 3158.3164, 3799.5431, 3850.0937
IRC  	

Compound: sCl 2 + $(H_2O)_2$ Pr4	**Energy (kJ mol^{-1}):** -679.045781275488
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.229414 -0.104076 -0.197877 6 0.186925 -0.032536 0.942221 8 -0.541302 1.152571 0.996142 8 -1.125871 1.444229 -0.296751 1 -1.949458 0.909925 -0.286233 1 0.744590 -0.018329 1.882382 8 -0.605649 -1.191117 0.830119 1 -1.027534 -1.354289 1.680771 9 2.160525 -1.027778 0.129379 9 0.710813 -0.462019 -1.376728 9 1.854483 1.068510 -0.341170 8 -3.100430 -0.541605 -0.489931 1 -3.472311 -0.705733 -1.361849 1 -2.339708 -1.132937 -0.401095	42.2630, 62.8676, 110.5466, 138.7273, 184.2194, 196.6160, 232.1943, 261.7272, 299.5725, 324.8941, 355.9719, 403.2916, 436.8545, 455.0373, 525.8731, 582.1368, 611.4955, 738.4935, 765.3435, 848.2237, 906.3519, 1060.1520, 1075.5174, 1128.1962, 1175.7514, 1244.6938, 1288.3378, 1370.2384, 1443.8454, 1497.8364, 1615.5190, 3054.8039, 3485.5656, 3726.2780, 3802.1332, 3865.2728

Compound: sCl 3 + $(H_2O)_2$ PRC1	**Energy (kJ mol^{-1}):** -678.976463310368
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.499637 0.034189 0.029921 9 -2.421756 -0.917529 -0.234744 9 -1.481601 0.246835 1.339166 9 -1.879268 1.149648 -0.601056 6 -0.161123 -0.437563 -0.509120 8 0.528005 -1.160758 0.229694 8 1.703726 -1.674615 -0.315970 1 0.107263 -0.285593 -1.545557 8 3.323108 0.443097 0.301092 1 2.903426 -0.428271 0.114598 1 4.143665 0.463451 -0.197932 8 0.947209 1.699816 -0.129811 1 1.885003 1.425164 -0.007395 1 0.952445 2.474579 -0.698853	30.2311, 48.3526, 78.3380, 121.2136, 129.1577, 183.8853, 210.7690, 233.2283, 237.6079, 250.3556, 291.0299, 378.0381, 406.7864, 419.5053, 447.6724, 548.6580, 556.0472, 567.2963, 661.5093, 697.1129, 828.2620, 881.3964, 901.0656, 932.5150, 1129.1888, 1190.4575, 1271.2460, 1360.2601, , 1593.5489, 1654.6893, 1672.7892, 3208.8953, 3342.6622, 3427.3235, 3855.6257, 3865.3133

Compound: sCl 3 + $(H_2O)_2$ TS1	**Energy (kJ mol^{-1}):** -678.974181399714
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.433893 -0.010821 0.025018 6 0.000721 0.275629 -0.421110 8 -0.642633 1.080587 0.312812 8 -1.879165 1.511302 -0.325547 1 -0.181859 0.294659 -1.490112 9 1.919606 -1.067259 -0.651454 9 2.194354 1.053299 -0.281898 9 1.536228 -0.247488 1.326860 8 -3.054122 -0.636397 0.296387 1 -2.742309 0.326894 0.061902 1 -3.810052 -0.849239 -0.256998 8 -0.720537 -1.425674 -0.112831 1 -1.747372 -1.231075 0.021585 1 -0.606141 -2.015594 -0.867951	-263.1970, 41.2328, 75.5833, 147.1956, 171.5294, 195.8320, 313.2451, 347.0769, 363.3666, 390.1600, 411.0510, 428.8565, 468.8022, 522.5049, 557.4381, 588.2506, 669.5502, 698.9099, 812.9743, 859.6684, 893.5243, 996.8146, 1104.8172, 1159.1604, 1187.8663, 1254.9663, 1279.0990, 1335.4104, 1518.4628, 1670.5092, 1710.7505, 2130.1417, 2552.0395, 3156.0023, 3798.9059, 3858.0062

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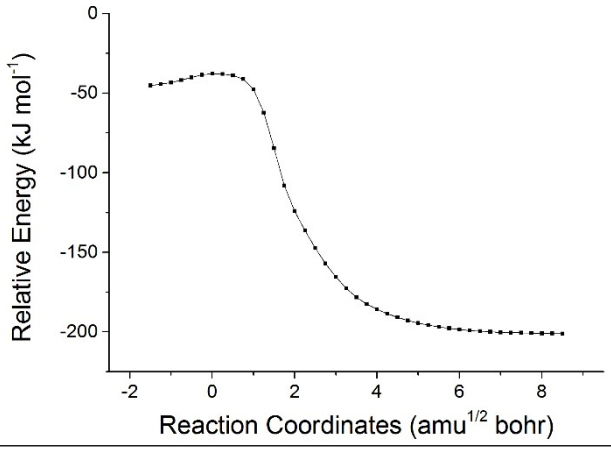
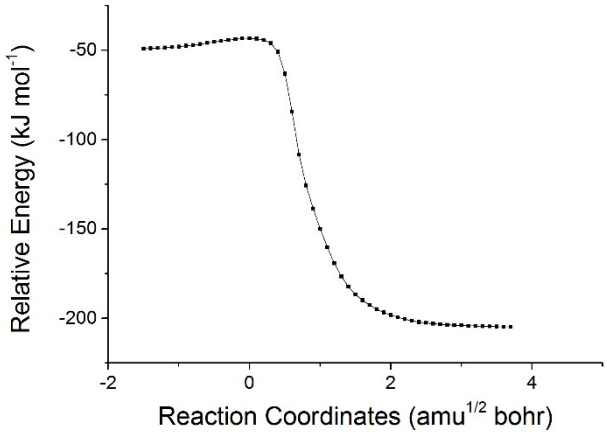


Compound: sCl 3 + $(H_2O)_2$ Pr1	**Energy (kJ mol^{-1}):** -679.046695526630
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.449107 −0.036898 0.087914 6 0.037661 0.090957 −0.522040 8 −0.658996 0.963041 0.289197 8 −1.798886 1.451237 −0.458160 1 −2.502768 0.852493 −0.119323 1 0.137230 0.491542 −1.534270 8 −0.601361 −1.173366 −0.536544 1 −0.323123 −1.670114 −1.313281 9 2.147732 −0.948405 −0.627237 9 2.110176 1.125660 0.018976 9 1.428296 −0.441198 1.359734 8 −3.294813 −0.659336 0.509863 1 −4.052965 −1.078680 0.093172 1 −2.522371 −1.196702 0.280354	39.4378, 67.9434, 112.9031, 127.4279, 182.7777, 199.1615, 225.0892, 240.7713, 252.2604, 330.8000, 355.9574, 366.0785, 403.1514, 467.2147, 520.1325, 565.5773, 620.0285, 711.2871, 732.5789, 872.7445, 951.3378, 1036.5657, 1089.3071, 1145.6563, 1177.6616, 1276.8225, 1278.9342, 1379.7424, 1401.6927, 1531.8141, 1634.1229, 3045.2327, 3438.3881, 3713.2347, 3811.0091, 3869.9623

Compound: sCl 3 + $(H_2O)_2$ PRC2	**Energy (kJ mol^{-1}):** -678.977263064497
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 −1.489581 0.032561 0.017263 6 −0.130363 −0.424195 −0.483405 8 0.528723 −1.168690 0.262489 8 1.721301 −1.679972 −0.259762 1 0.165924 −0.264696 −1.511268 9 −1.863219 1.146325 −0.620301 9 −2.392537 −0.928016 −0.277285 9 −1.512613 0.240448 1.327654 8 3.328823 0.482446 0.065681 1 2.893099 −0.399289 −0.020606 1 3.863618 0.443308 0.863291 8 0.915829 1.691448 −0.041072 1 1.859539 1.407848 0.030886 1 0.895401 2.431960 −0.654738	30.6497, 52.9885, 88.3887, 126.1346, 131.7672, 188.4279, ,227.6577, 257.3088, 270.5375, 298.3777, 326.5543, 377.5462, 406.6573, 419.9501, 426.6031, 504.1159, 551.6708, 565.5651, 696.6782, 801.3020, 868.7779, 896.7671, 932.7880, 956.1836, 1130.7885, 1190.6128, 1270.0021, 1360.0737, 1591.7576, 1632.3812, 1658.9014, 3206.3576, 3280.1552, 3382.2637, 3846.1059, 3857.7617

Compound: sCl 3 + $(H_2O)_2$ TS2	**Energy (kJ mol^{-1}):** -678.976125632750
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.435077 -0.010533 0.024264 6 0.002922 0.283163 -0.418283 8 -0.638892 1.083167 0.318663 8 -1.874687 1.523888 -0.310848 1 -0.193354 0.288870 -1.484716 9 1.916127 -1.067784 -0.651339 9 2.198962 1.051509 -0.282868 9 1.537638 -0.246161 1.327155 8 -3.093194 -0.653611 0.111027 1 -2.754194 0.314963 -0.024240 1 -3.541326 -0.693970 0.960482 8 -0.723810 -1.442665 -0.094417 1 -1.744088 -1.234536 0.030523 1 -0.624922 -2.035418 -0.849864	-237.6757, 42.6112, 75.8600, 147.3213, 171.3151, 201.4235, 313.1240, 346.9833, 365.9511, 381.3066, 410.6057, 432.7579, 477.7047, 524.5486, 553.7698, 575.2125, 603.5414, 699.2346, 790.1670, 857.8705, 890.3554, 1092.8087, 1134.3888, 1160.1992, 1186.3775, 1275.9931, 1337.7155, 1346.5485, 1525.6492, 1604.5939, 1661.5278, 2196.6905, ,2613.5636, 3161.3782, 3795.8025, 3850.4897
IRC  	

Compound: sCl 3 + $(H_2O)_2$ Pr2	**Energy (kJ mol^{-1}):** -679.048259309215
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.439730 -0.040130 0.094282 6 0.041573 0.113367 -0.539534 8 -0.664860 0.966737 0.289088 8 -1.811918 1.448383 -0.451212 1 -2.503211 0.821351 -0.135658 1 0.160701 0.545794 -1.535594 8 -0.589337 -1.151117 -0.607078 1 -0.516255 -1.508389 -1.497434 9 2.166630 -0.898248 -0.650811 9 2.089350 1.131291 0.116479 9 1.385711 -0.519510 1.341232 8 -3.287949 -0.726004 0.392427 1 -3.520615 -0.824360 1.320614 1 -2.451151 -1.199605 0.271668	29.1021, 68.3708, 114.9367, 133.5549, 142.3315, 197.9780, 232.6122, 258.8916, 279.9146, 298.2524, 352.5085, 360.8069, 402.4199, 511.5738, 552.9532, 565.9581, 640.1037, 711.7799, 793.0365, 869.3275, 951.3602, 1042.2727, 1083.7799, 1149.1644, 1176.6648, 1269.7387, 1286.4346, 1366.9773, 1414.0520, 1516.4983, 1627.6177, 3054.0939, 3419.5323, 3703.4480, 3823.5165, 3861.4461

Compound: sCl 3 + $(H_2O)_2$ PRC3	**Energy (kJ mol^{-1}):** -678.976758543801
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.485381 0.029360 0.008310 6 -0.118211 -0.417021 -0.481879 8 0.508388 -1.199324 0.254757 8 1.716295 -1.697852 -0.234009 1 0.213743 -0.202963 -1.488591 9 -1.903593 1.082738 -0.695441 9 -2.367865 -0.971427 -0.177248 9 -1.480214 0.342995 1.305648 8 3.317663 0.478742 0.072711 1 2.881421 -0.402415 -0.003996 1 3.910307 0.425006 0.826937 8 0.936741 1.748319 -0.204451 1 1.862031 1.456501 -0.027708 1 0.686411 2.322011 0.526067	22.7981, 33.1705, 84.6555, 116.8194, 135.7398, 183.9906, 226.2528, 250.2507, 260.1566, 277.5607, 297.0635, 378.3309, 404.9927, 413.8918, 425.4943, 540.8087, 552.1992, 568.2039, 696.2535, 731.1253, 865.8081, 891.1302, 921.7357, 942.0771, 1143.3441, 1195.7403, 1250.2764, 1360.4244, 1586.1495, 1639.6708, 1665.4309, 3208.9233, 3314.2435, 3405.6402, 3846.2551, 3863.2852

Compound: sCl 3 + $(H_2O)_2$ TS3	**Energy (kJ mol^{-1}):** -678.975252603565
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.431618 -0.011054 -0.034022 6 -0.034263 0.263996 -0.375191 8 -0.606445 1.103863 0.379333 8 -1.881019 1.551034 -0.156779 1 -0.317238 0.214681 -1.420450 9 1.934015 -0.944984 -0.846552 9 2.143596 1.110552 -0.191312 9 1.577245 -0.428714 1.234683 8 -3.089048 -0.671805 -0.096550 1 -2.739105 0.303517 -0.088996 1 -3.714809 -0.772452 0.625598 8 -0.713585 -1.470124 -0.036222 1 -1.741506 -1.277314 -0.007735 1 -0.444395 -1.721504 0.857244	-234.0953, 40.5246, 63.1378, 148.1200, 169.9852, 188.6379, 317.5559, 337.1536, 365.4847, 395.3353, 407.4014, 434.1385, 485.7447, 516.9718, 555.8605, 592.6492, 628.4843, 696.8288, 787.2052, 853.9549, 900.9870, 1084.2440, 1123.9700, 1185.4779, 1191.7999, 1247.1847, 1307.6331, 1338.5639, 1518.0518, 1617.4855, 1696.5678, 2227.8831, 2604.6378, 3168.8170, 3781.6508, 3855.6553

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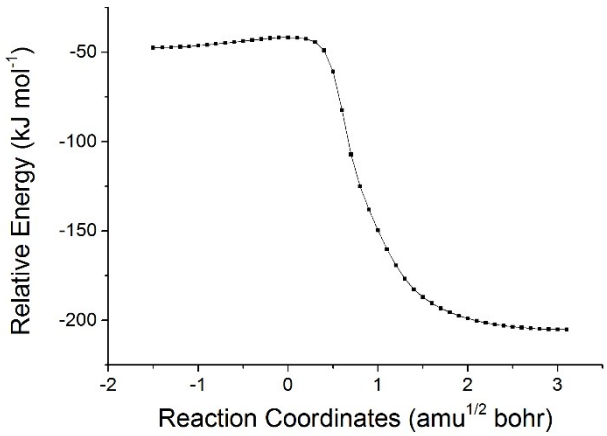

Compound: sCl 3 + $(H_2O)_2$ Pr3	**Energy (kJ mol^{-1}):** -679.047730845463
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.471334 -0.037790 -0.013291 6 -0.025816 -0.002631 -0.378566 8 -0.609598 0.972687 0.429755 8 -1.751106 1.522386 -0.268795 1 -2.465622 0.891842 -0.025845 1 -0.131809 0.259331 -1.429368 8 -0.595147 -1.281875 -0.211757 1 -0.359250 -1.609005 0.666398 9 2.123837 -0.889429 -0.820830 9 2.040916 1.162355 -0.128133 9 1.642956 -0.470542 1.256125 8 -3.462714 -0.631195 0.014372 1 -3.945142 -0.971691 0.773244 1 -2.692139 -1.205440 -0.106349	42.3450, 68.1372, 93.4777, 108.7143, 196.3265, 225.6205, 232.9114, 251.4983, 300.4113, 355.5126, 363.0538, 395.7893, 417.7649, 498.8204, 529.5849, 566.0577, 617.7195, 712.3798, 766.2066, 860.6738, 952.0996, 1039.1784, 1072.2515, 1145.9665, 1198.6877, 1249.1969, 1289.4075, 1358.5433, 1439.6431, 1502.5135, 1634.4066, 3112.1802, 3454.4926, 3707.6218, 3759.0631, 3867.6327

Compound: sCl 3 + $(H_2O)_2$ PRC4	**Energy (kJ mol^{-1}):** -678.977086514110
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.488498 0.031281 0.024393 6 -0.139236 -0.422659 -0.505341 8 0.517339 -1.188274 0.222487 8 1.710186 -1.685984 -0.301775 1 0.155884 -0.226073 -1.526722 9 -1.911345 1.099923 -0.654924 9 -2.386673 -0.956767 -0.156662 9 -1.449487 0.325814 1.324340 8 3.279493 0.457583 0.323859 1 2.878271 -0.422784 0.134575 1 4.085206 0.508678 -0.197337 8 0.967077 1.729600 -0.302147 1 1.874419 1.418739 -0.068966 1 0.707409 2.345586 0.389960	29.7774, 35.1066, ,82.1077, 119.2790, 134.9192, 186.3092, 224.0826, 246.1701, 255.0849, 291.8496, 316.9709, 378.1117, 405.2150, 423.9155, 457.8222, 503.7150, 551.7795, 567.5064, 697.2139, 721.0081, 871.9403, 897.5611, 925.5407, 938.4995, 1142.2460, 1193.3356, 1253.5596, 1359.8805, 1587.0451, 1645.5366, 1672.1439, 3211.2763, 3307.8078, 3403.5872, 3843.0633, 3860.4701

Compound: sCl 3 + $(H_2O)_2$ TS4	**Energy (kJ mol^{-1}):** -678.975564636070
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.434044 -0.011313 -0.024390 6 -0.022466 0.274629 -0.394792 8 -0.611372 1.101933 0.359427 8 -1.877562 1.547582 -0.196765 1 -0.280451 0.243820 -1.446862 9 1.949462 -0.936385 -0.840424 9 2.154234 1.109008 -0.151706 9 1.551251 -0.447853 1.239679 8 -3.086228 -0.660807 0.136398 1 -2.750726 0.310568 0.018441 1 -3.759521 -0.826499 -0.528976 8 -0.722771 -1.464038 -0.109070 1 -1.746568 -1.259910 -0.040437 1 -0.443264 -1.768169 0.765066	-230.2011, 45.3686, 61.9067, 147.4104, 167.3891, 189.3980, 315.2304, 335.2181, 359.4677, 372.5325, 407.4650, 429.6039, 499.3162, 532.1970, 555.8467, 597.6203, 643.8656, 692.1889, 782.8539, 855.6845, 904.1119, 1019.4664, 1117.2722, 1185.2994, 1189.6672, 1247.6992, 1333.1465, 1337.8353, 1522.8713, 1650.7437, 1691.7606, 2234.3606, 2625.9690, 3171.1611, 3776.7366, 3854.5783

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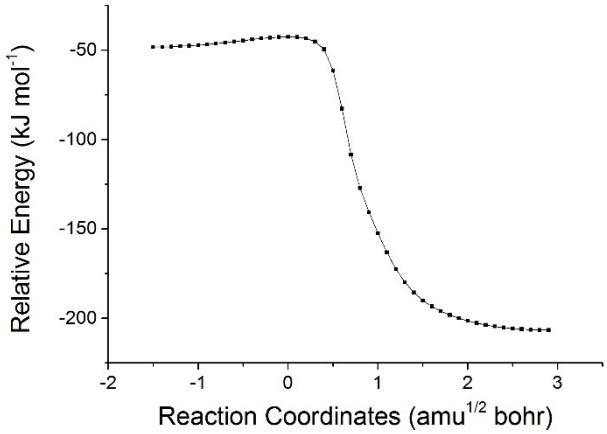

Compound: sCl 3 + $(H_2O)_2$ Pr4	**Energy (kJ mol^{-1}):** -679.048442818014
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.473365 -0.048274 -0.009183 6 -0.017733 0.015656 -0.396791 8 -0.588033 1.008271 0.399375 8 -1.756684 1.519684 -0.282462 1 -2.456069 0.894736 0.011096 1 -0.100937 0.272677 -1.451227 8 -0.618388 -1.247903 -0.233660 1 -0.451590 -1.552115 0.668792 9 2.116547 -0.920993 -0.801862 9 2.070281 1.138954 -0.129843 9 1.620238 -0.471046 1.264785 8 -3.423651 -0.667016 0.204786 1 -4.198421 -0.854948 -0.333091 1 -2.696323 -1.191175 -0.161751	45.4830, 68.1509, 96.2361, 111.7822, 200.6320, 212.3986, 224.1042, 255.2367, 326.9426, 357.3304, 359.0549, 397.2458, 448.0537, 491.5462, 526.1644, 565.7096, 622.7980, 709.8585, 744.2916, 863.3097, 952.3372, 1042.3365, 1074.2045, 1148.1966, 1196.2764, 1251.1962, 1293.0989, 1358.9790, 1438.9013, 1514.9716, 1617.2477, 3107.5602, 3467.5822, 3706.4459, 3753.9161, 3865.9236

Compound: sCl 4 + $(H_2O)_2$ PRC1	**Energy (kJ mol^{-1}):** -778.151182680016
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.111046 -0.242350 -0.451022 6 -0.319261 0.204891 0.799848 8 0.575408 -0.431904 1.369785 8 1.120026 -1.545860 0.653615 9 -0.884438 1.141948 1.494932 9 -1.929498 0.753446 -0.810346 9 -0.360874 -0.568707 -1.485809 9 -1.858617 -1.293633 -0.091832 8 3.018649 -0.020536 -0.530220 1 2.469097 -0.728816 -0.111137 1 3.419388 -0.408470 -1.312330 8 0.971763 1.712560 -0.356346 1 1.791707 1.193541 -0.556293 1 0.715716 2.156936 -1.170372	40.0825, 56.3618, 104.6947, 124.7390, 139.3793, 203.2420, 215.3984, 255.4641, 258.4817, 270.6400, 290.8050, 315.0485, 329.4540, 367.7848, 474.7718, 484.1919, 516.7047, 573.4577, 595.0829, 616.8202, 678.6174, 729.7337, 775.5858, 897.1599, 919.6383, 1148.1800, 1174.6125, 1237.1290, 1396.7823, 1618.5332, 1663.0453, 1680.6735, 3236.0138, 3341.1214, 3843.7417,81.5127:36,A,3864.2392

Compound: sCl 4 + $(H_2O)_2$ TS1	**Energy (kJ mol^{-1}):** -778.151865721165
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.071336 -0.436984 -0.252730 6 -0.195585 0.603494 0.504754 8 0.644406 0.301050 1.388751 8 1.223716 -1.028274 1.197705 9 -0.852254 1.710937 0.754235 9 -1.930356 0.240110 -1.038544 9 -0.390157 -1.267841 -1.028562 9 -1.773384 -1.127291 0.642186 8 2.865226 -0.188927 -0.587322 1 2.360559 -0.647889 0.173793 1 3.166402 -0.874471 -1.189704 8 0.827583 1.247575 -0.958306 1 1.697315 0.678420 -0.962383 1 0.405161 1.190257 -1.824314	-198.8784, 46.7101, 59.4403, 154.1929, 180.3588, 225.9582, 267.3994, 284.3814, 305.0015, 352.9306, 366.8464, 375.1442, 413.2466, 466.3781, 489.4181, 524.0339, 590.5112, 604.9577, 620.5837, 681.7673, 768.9943, 815.7543, 922.5824, 949.7419, 1141.7483, 1172.0635, 1196.5290, 1236.0527, 1347.4144, 1540.3012, 1669.2159, 1713.3148, 2389.5730, 2791.1720, 3797.1962, 3855.6133

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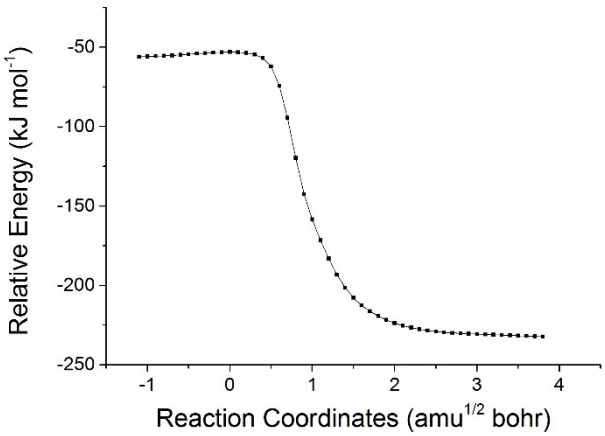

Compound: sCl 4 + $(H_2O)_2$ Pr1	**Energy (kJ mol^{-1}):** -778.232205653240
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.331732 -0.259160 -0.190820 6 -0.039214 0.512746 0.233494 8 0.764673 -0.162432 1.133093 8 1.312123 -1.347541 0.514380 1 2.182508 -1.003043 0.204879 9 -0.474965 1.589770 0.953448 8 0.685330 0.923230 -0.860574 1 0.094400 1.270164 -1.541213 9 -2.075203 0.566046 -0.970916 9 -1.068394 -1.350754 -0.905759 9 -2.056443 -0.598624 0.871114 8 3.488053 -0.006943 -0.504972 1 4.126455 0.403140 0.086804 1 2.895931 0.699771 -0.792911	32.3377, 52.9666, 94.2196, 128.8150, 195.0532, 218.4669, 228.6420, 249.4912, 273.3105, 290.7010, 313.4979, 346.1309, 373.3548, 414.6536, 455.3092, 489.2980, 530.6004, 591.5891, 641.9204, 688.4057, 780.1559, 801.9113, 973.3600, 1055.2043, 1096.2389, 1155.3190, 1174.3793, 1225.3692, 1284.0680, 1391.8185, 1531.8581, 1625.7848, 3408.2526, 3757.6239, 3776.9067, 3869.8559

Compound: sCl 4 + $(H_2O)_2$ PRC2	**Energy (kJ mol^{-1}):** -778.152030386117
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.102056 -0.246402 -0.448061 6 -0.309488 0.215351 0.798177 8 0.581044 -0.419529 1.378511 8 1.132067 -1.536629 0.665104 9 -0.883620 1.150068 1.490200 9 -1.922500 0.745436 -0.815800 9 -0.352326 -0.581202 -1.478943 9 -1.847989 -1.294069 -0.075748 8 2.932636 -0.065549 -0.689559 1 2.410849 -0.746220 -0.192153 1 3.788217 -0.003687 -0.256363 8 0.961724 1.705387 -0.353570 1 1.779495 1.176094 -0.549424 1 0.688847 2.108570 -1.184028	44.2525, 56.9310, 108.9406, 127.2046, 144.0984, 205.2413, 220.0133, 259.9402, 278.6197, 289.1779, 291.1197, 327.8403, 367.6214, 373.9608, 453.8346, 477.7278, 511.0120, 544.8312, 583.1474, 616.4050, 680.1004, 775.2032, 854.8557, 905.2343, 1010.7203, 1147.5637, 1173.6930, 1240.8031, 1394.5360, 1614.3180, 1634.0857, 1665.3915, 3182.2936, 3305.4328, 3836.1632, 3858.2832

Compound: sCl 4 + $(H_2O)_2$ TS2	**Energy (kJ mol^{-1}):** -778.153124563473
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.084712 -0.399692 -0.287877 6 -0.191557 0.546852 0.565262 8 0.658260 0.151351 1.399623 8 1.215031 -1.162107 1.079200 9 -0.822179 1.637356 0.924134 9 -1.940502 0.364194 -0.992171 9 -0.419363 -1.156160 -1.144925 9 -1.789585 -1.166016 0.542485 8 2.818351 -0.243774 -0.704543 1 2.332416 -0.728241 0.049174 1 3.660685 0.063565 -0.357981 8 0.841237 1.328127 -0.860702 1 1.709802 0.766160 -0.892860 1 0.436348 1.312415 -1.736981	-177.7862, 49.0472, 59.1808, 160.8012, 178.1110, 225.5547, 265.3601, 284.9991, 302.9429, 350.7331, 365.3687, 371.9797, 411.7477, 478.0180, 488.3767, 524.4662, 554.8934, 590.9387, 610.9689, 658.8232, 762.7452, 799.4225, 918.3369, 1066.2885, 1143.3405, 1176.7433, 1228.7899, 1283.7771, 1353.1035, 1546.1413, 1614.5921, 1666.4543, 2456.5473, 2835.4191, 3795.4097, 3851.4800
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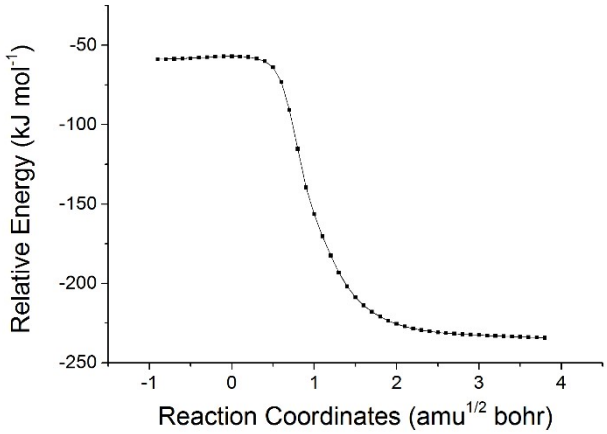
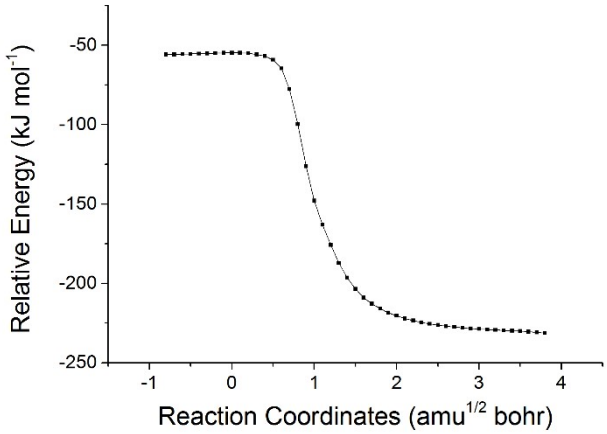
	

Compound: sCl 4 + $(H_2O)_2$ PRC3	**Energy (kJ mol^{-1}):** -778.150954513382
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.080992 -0.293421 -0.439963 6 -0.309977 0.296432 0.768099 8 0.558811 -0.280279 1.437111 8 1.142219 -1.451989 0.846038 9 -0.903730 1.292366 1.361635 9 -1.932577 0.628095 -0.892785 9 -0.309351 -0.698009 -1.425552 9 -1.793038 -1.329614 0.028997 8 2.895030 -0.122247 -0.698902 1 2.389433 -0.744109 -0.114572 1 3.785256 -0.065695 -0.342575 8 0.878281 1.626475 -0.616822 1 1.728462 1.123576 -0.720068 1 1.096196 2.456950 -0.181662	44.4745, 66.9528, 96.0815, 125.4516, 153.5415, 200.0214, 219.7523, 260.3854, 275.8252, 281.7944, 289.4425, 326.5408, 354.4326, 368.4141, 467.1720, 478.9558, 512.2091, 570.8623, 586.5908, 615.7412, 664.1888, 775.7265, 811.7557, 899.0429, 990.4887, 1138.0675, 1179.2284, 1248.4219, 1385.5339, 1609.8626, 1639.6982, 1667.4722, 3188.2346, 3302.8218, 3837.7311, 3863.9650

Compound: sCl 4 + $(H_2O)_2$ TS3	**Energy (kJ mol^{-1}):** -778.152472459163
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.082084 -0.407518 -0.299218 6 -0.198345 0.551416 0.551826 8 0.634511 0.174899 1.410128 8 1.208951 -1.137901 1.126727 9 -0.818533 1.666468 0.875847 9 -1.970688 0.327254 -0.978632 9 -0.403180 -1.149068 -1.152950 9 -1.751044 -1.192463 0.551658 8 2.804368 -0.280419 -0.710283 1 2.322994 -0.734257 0.060595 1 3.676598 -0.023686 -0.399645 8 0.791809 1.255863 -0.967272 1 1.683872 0.744202 -0.952463 1 0.973014 2.181102 -0.761853	-146.3251, 49.3026, 72.0586, 154.6811, 178.9292, 219.8028, 260.3543, 284.4433, 301.4294, 346.7877, 360.6724, 366.8654, 398.8429, 455.9246, 480.5366, 524.7640, 572.1872, 592.4314, 615.8183, 681.7242, 751.1917, 778.9990, 909.6363, 1006.4112, 1144.1584, 1178.5495, 1208.3181, 1237.4715, 1352.2406, 1550.9475, 1624.7314, 1689.1680, 2567.1970, 2888.7471, 3804.3213, 3857.4399
IRC  	

Compound: sCl 4 + $(H_2O)_2$ Pr3	**Energy (kJ mol^{-1}):** -778.234111047535
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.404526 -0.102729 -0.158678 6 0.034254 0.408306 0.152328 8 0.766080 -0.465395 0.988045 8 1.165242 -1.636982 0.246539 1 2.053615 -1.369750 -0.045347 9 -0.113531 1.494110 0.982194 8 0.644104 0.732125 -1.004260 1 1.605443 0.791571 -0.855854 9 -2.113371 0.863791 -0.760818 9 -1.386305 -1.169082 -0.962133 9 -2.029860 -0.437116 0.975584 8 3.370981 0.253816 -0.332380 1 3.626690 0.591064 0.533536 1 4.152231 0.319812 -0.891232	33.9279, 48.3442, 76.1769, 116.7370, 164.3800, 207.5971, 232.5643, 262.9793, 278.8395, 285.3071, 314.5749, 352.1083, 377.7050, 397.3941, 479.3980, 491.5629, 531.8580, 585.8175, 631.6467, 656.0214, 687.7963, 785.5537, 965.8965, 1034.0498, 1076.4672, 1180.9327, 1200.5000, 1231.8247, 1279.5941, 1450.8232, 1474.8038, 1626.3847, 3592.4584, 3661.4694, 3782.2367, 3879.5888

Compound: sCl 4 + $(H_2O)_2$ PRC4	**Energy (kJ mol^{-1}):** -778.151343097919
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.087243 -0.309769 -0.423180 6 -0.300324 0.336446 0.745069 8 0.562981 -0.217347 1.441526 8 1.141377 -1.414420 0.896658 9 -0.890442 1.359501 1.296098 9 -1.936840 0.592432 -0.916534 9 -0.328843 -0.770648 -1.397152 9 -1.800836 -1.316349 0.102686 8 2.962826 -0.076017 -0.560233 1 2.434468 -0.715318 -0.014219 1 3.301488 -0.567780 -1.313216 8 0.878739 1.568034 -0.692410 1 1.724342 1.046292 -0.767222 1 1.110375 2.410320 -0.286886	46.2907, 67.0974, 91.8090, 125.6174, 157.8162, 203.5801, 221.3492, 264.0061, 277.3274, 288.9341, 289.9045, 328.7980, 367.2176, 400.7399, 478.6531, 506.1075, 512.5963, 568.4710, 590.0375, 619.6265, 663.8341, 776.0588, 796.5534, 902.5942, 1034.2265, 1140.0628, 1180.1310, 1242.4727, 1383.1677, 1606.5946, 1647.5553, 1678.8281, 3134.9621, 3275.3006, 3830.4288, 3858.6479

Compound: sCl 4 + $(H_2O)_2$ TS4	**Energy (kJ mol^{-1}):** -778.153113870118
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.077057 -0.423552 -0.289992 6 -0.213471 0.573107 0.536270 8 0.614289 0.237747 1.414317 8 1.202688 -1.077550 1.192543 9 -0.841564 1.697007 0.803171 9 -1.964096 0.275233 -1.006670 9 -0.380214 -1.189805 -1.110522 9 -1.747493 -1.187118 0.578433 8 2.873625 -0.201596 -0.590203 1 2.368533 -0.672630 0.151143 1 3.159081 -0.873792 -1.215226 8 0.800188 1.222752 -1.014849 1 1.679394 0.693746 -0.977376 1 1.010146 2.146665 -0.830371	-131.8994, 49.7399, 71.5302, 148.2910, 178.8931, 220.1116, 257.5315, 284.2300, 299.6407, 338.1935, 345.6464, 363.6927, 394.7051, 479.8384, 488.8758, 522.9158, 585.5910, 593.2244, 608.6505, 679.4158, 739.0556, 778.5179, 910.2331, 935.9471, 1146.0830, 1180.7008, 1227.9638, 1243.4577, 1355.2067, 1557.3275, 1644.1015, 1693.0530, 2597.1393, 2930.6112, 3800.2592, 3853.4549

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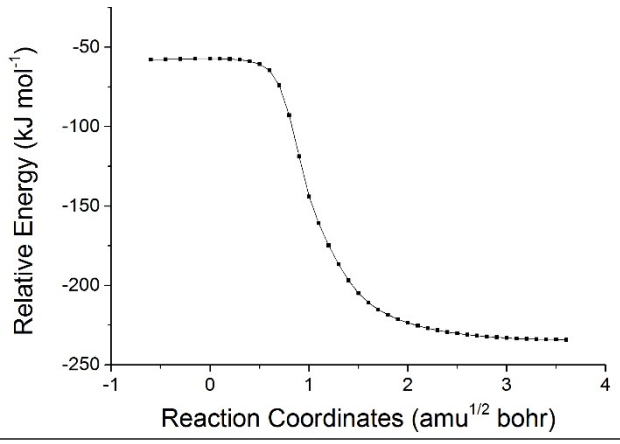

Compound: sCI 5 + $(H_2O)_2$ PRC1	**Energy (kJ mol^{-1}):** -778.155321450549
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.504971 0.099406 0.193399 6 -0.160033 -0.476306 -0.265725 8 0.586751 -1.004163 0.567732 8 1.752981 -1.640438 0.080858 9 -0.001255 -0.619282 -1.534660 9 -2.417557 -0.889230 0.123292 9 -1.438786 0.532881 1.440451 9 -1.895849 1.079132 -0.615166 8 3.287219 0.603792 0.401354 1 2.917263 -0.305750 0.320743 1 4.114254 0.608406 -0.087241 8 0.878010 1.700375 -0.234065 1 1.818974 1.471403 -0.050230 1 0.880874 2.279305 -1.001596	29.4729, 57.0746, 90.7417, 110.8940, 132.9723, 165.3457, 188.1994, 242.3211, 245.6618, 251.7649, 285.3981, 302.2243, 350.6313, 361.6697, 408.5250, 456.8954, 521.4813, 556.2997, 576.4187, 668.3638, 675.6645, 726.7701, 836.6869, 853.3457, 875.4031, 1128.9044, 1186.8392, 1249.0461, 1403.4828, 1632.9929, 1660.5967, 1674.8863, 3334.9174, 3419.1514, 3854.0781, 3865.4630

Compound: sCI 5 + $(H_2O)_2$ TS1	**Energy (kJ mol^{-1}):** -778.154483796209
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.452057 -0.094944 -0.202984 6 -0.035845 0.328312 0.244444 8 0.643489 0.940770 -0.616381 8 1.899689 1.481311 -0.106517 9 0.026824 0.653674 1.514325 9 -1.969470 -0.968997 0.665102 9 -2.234068 0.992813 -0.218975 9 -1.432751 -0.632623 -1.414317 8 3.030580 -0.790958 -0.439314 1 2.771664 0.195011 -0.357470 1 3.841343 -0.926600 0.058152 8 0.723371 -1.395286 0.379901 1 1.717345 -1.268679 0.095196 1 0.705207 -1.690439 1.298636	-231.7521, 36.0051, 70.1748, 146.3315, 159.4260, 185.6379, 275.1852, 297.2816, 324.5751, 352.2152, 376.7297, 388.5598, 399.7561, 415.8618, 503.1695, 530.5402, 577.9666, 635.6021, 680.1667, 720.5649, 786.4159, 823.5539, 862.7035, 937.3476, 1137.6409, 1181.8605, 1230.4427, 1238.2808, 1358.6367, 1535.1706, 1670.4773, 1707.3520, 2352.8141, 2779.8576, 3800.1789, 3857.8733

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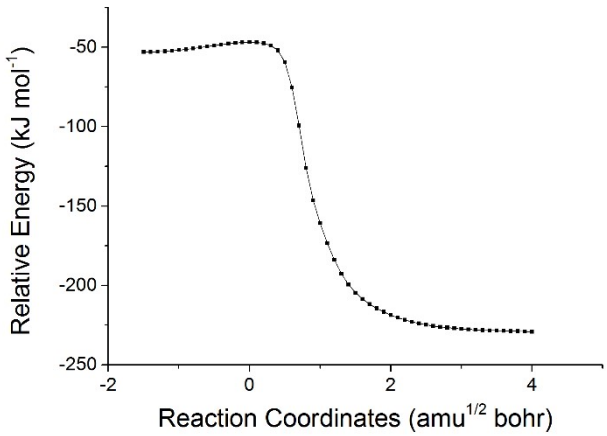

Compound: sCl 5 + $(H_2O)_2$ Pr1	**Energy (kJ mol^{-1}):** -778.234695133756
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.391502 -0.324803 -0.183500 6 -0.060577 0.360168 0.265844 8 0.650426 0.577335 -0.877070 8 1.877358 1.273273 -0.560158 1 2.503994 0.515564 -0.497802 9 -0.415662 1.527793 0.894584 8 0.634214 -0.433231 1.158979 1 0.212620 -0.376145 2.025158 9 -2.119291 -0.605465 0.915204 9 -2.113200 0.467005 -0.974187 9 -1.148361 -1.471151 -0.823439 8 3.269025 -1.063971 -0.100132 1 4.117224 -1.122038 0.349666 1 2.599077 -1.320459 0.546508	41.1071, 60.7539, 94.4583, 129.5898, 168.0954, 191.6362, 221.2917, 237.0399, 249.2516, 304.8284, 316.2066, 339.9198, 370.2838, 386.2925, 400.1450, 519.9118, 527.7303, 588.4687, 604.3415, 728.9488, 739.0615, 825.2194, 938.9418, 1052.5637, 1076.7670, 1161.1253, 1179.2310, 1212.3881, 1326.7694, 1362.8227, 1545.5041, 1626.3435, 3424.4355, 3759.2232, 3792.0834, 3875.4461

Compound: sCl 5 + $(H_2O)_2$ PRC2	**Energy (kJ mol^{-1}):** -778.156341672640
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.505495 0.091967 -0.182594 6 0.145724 -0.463043 0.259704 8 -0.580325 -1.013433 -0.578212 8 -1.759359 -1.639526 -0.100613 9 -0.039231 -0.580917 1.527508 9 1.890669 1.082516 0.615014 9 2.406149 -0.904017 -0.077432 9 1.467986 0.503414 -1.438943 8 -3.304652 0.601187 -0.208372 1 -2.912148 -0.303888 -0.208056 1 -3.817922 0.675253 -1.017456 8 -0.861293 1.702999 0.161215 1 -1.805294 1.458593 0.002872 1 -0.857080 2.277717 0.932501	32.9450, 59.2730, 96.3828, 114.5765, 135.1450, 169.7028, 194.0592, 250.8541, 258.7338, 273.8438, 300.7887, 335.5543, 356.6988, 361.4179, 408.9676, 419.6888, 511.1819, 524.4003, 576.1856, 673.9396, 726.6771, 793.2353, 838.3362, 858.1026, 953.6168, 1129.8197, 1187.6602, 1247.7782, 1403.7621, 1627.8877, 1637.1693, 1664.8016, 3293.5011, 3392.0249, 3847.2631, 3859.1687

Compound: sCl 5 + $(H_2O)_2$ TS2	**Energy (kJ mol^{-1}):** -778.155935062267
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.456606 0.088286 -0.198395 6 0.036941 -0.328311 0.242080 8 -0.639985 -0.946054 -0.615417 8 -1.893626 -1.493088 -0.108280 9 -0.046269 -0.623819 1.514582 9 1.965682 0.978723 0.656214 9 2.238800 -0.999666 -0.186658 9 1.448326 0.601553 -1.421252 8 -3.088705 0.769786 -0.261179 1 -2.789827 -0.205953 -0.262939 1 -3.460061 0.964938 -1.126053 8 -0.721292 1.424044 0.330129 1 -1.713908 1.278347 0.061623 1 -0.707471 1.754189 1.237248	-216.7111, 40.3464, 71.3754, 145.7554, 159.8329, 190.0347, 275.2563, 296.7082, 321.7700, 352.9757, 365.4023, 383.5055, 400.9371, 423.6081, 502.0856, 530.9374, 569.4630, 584.9973, 673.1975, 718.6764, 776.5858, 821.7894, 865.7069, 1058.9036, 1140.9912, 1183.5082, 1229.8557, 1306.4008, 1365.6796, 1541.4011, 1613.3738, 1666.1703, 2396.9997, 2814.5238, 3796.9692, 3852.1032

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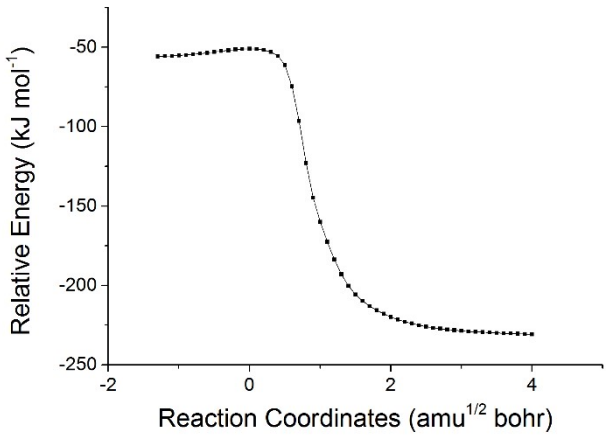

Compound: sCl 5 + $(H_2O)_2$ Pr2	**Energy (kJ mol^{-1}):** -778.235686023368
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.378531 -0.337083 -0.171891 6 -0.058616 0.384232 0.252293 8 0.667177 0.532385 -0.893775 8 1.888164 1.250847 -0.604039 1 2.512185 0.498809 -0.471100 9 -0.426818 1.585788 0.801457 8 0.627112 -0.349190 1.201680 1 0.251341 -0.172849 2.072726 9 -2.128952 -0.542988 0.925578 9 -2.085203 0.390208 -1.035037 9 -1.114776 -1.526471 -0.723517 8 3.280512 -1.025707 0.066205 1 3.427652 -1.733253 -0.569030 1 2.529728 -1.301115 0.608085	41.8459, 61.8886, 97.8940, 133.9444, 167.1742, 202.7544, 221.7193, 235.2008, 248.8184, 282.3243, 309.0498, 340.7138, 373.9820, 385.3118, 448.2935, 521.3360, 531.7991, 588.4637, 605.8464, 732.5280, 796.7416, 827.2153, 939.3215, 1050.6581, 1079.8613, 1161.1824, 1181.5318, 1208.9991, 1327.8406, 1357.9245, 1528.8648, 1624.7530, 3406.4916, 3756.1722, 3794.7283, 3870.0375

Compound: sCI 5 + $(H_2O)_2$ PRC3	**Energy (kJ mol^{-1}):** -778.155292325029
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.520553 0.077431 -0.133529 6 0.135438 -0.454670 0.253545 8 -0.530569 -1.060240 -0.597416 8 -1.735393 -1.666024 -0.170800 9 -0.147230 -0.479485 1.505653 9 1.895351 1.053734 0.681438 9 2.401742 -0.932279 -0.020323 9 1.526387 0.507772 -1.390230 8 -3.298053 0.579879 -0.278807 1 -2.896847 -0.320345 -0.267278 1 -4.002248 0.571976 0.375149 8 -0.886250 1.748320 0.139381 1 -1.826386 1.476250 0.011460 1 -0.694596 2.372397 -0.567128	25.7960, 41.9021, 91.7538, 116.0609, 131.6452, 166.6911, 189.2848, 241.5052, 249.2321, 261.3399, 299.9707, 321.0976, 349.3877, 361.8052, 406.4638, 446.2832, 509.0366, 524.6695, 575.3292, 678.4179, 726.8862, 730.8695, 844.2676, 858.9722, 933.6184, 1136.4634, 1190.4264, 1239.2175, 1407.6330, 1630.3118, 1650.7443, 1673.1293, 3312.5611, 3406.4417, 3846.2994, 3859.1966

Compound: sCI 5 + $(H_2O)_2$ TS3	**Energy (kJ mol^{-1}):** -778.154047110573
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.483665 0.044071 -0.083684 6 -0.005044 -0.255421 0.204566 8 -0.553413 -1.049839 -0.607125 8 -1.871996 -1.524924 -0.202453 9 -0.296320 -0.294613 1.477390 9 1.953513 0.959049 0.758604 9 2.193963 -1.077157 0.059407 9 1.630507 0.489838 -1.337807 8 -3.080035 0.726521 -0.184941 1 -2.743969 -0.245753 -0.204133 1 -3.659142 0.821790 0.576606 8 -0.694641 1.469487 -0.086641 1 -1.730137 1.287986 -0.079072 1 -0.472765 1.740066 -0.987767	-250.6799, 39.0414, 60.9470, 136.9924, 161.6331, 177.9353, 287.5360, 301.9577, 318.5255, 354.5256, 369.5178, 392.4984, 414.7727, 425.6464, 528.2966, 539.3143, 574.3108, 635.7136, 679.6143, 720.4778, 805.9932, 841.1296, 876.5957, 1023.1045, 1148.2582, 1189.5948, 1216.7132, 1332.4466, 1385.5696, 1517.5508, 1651.9311, 1680.8426, 2199.0066, 2688.3510, 3780.5289, 3849.5355

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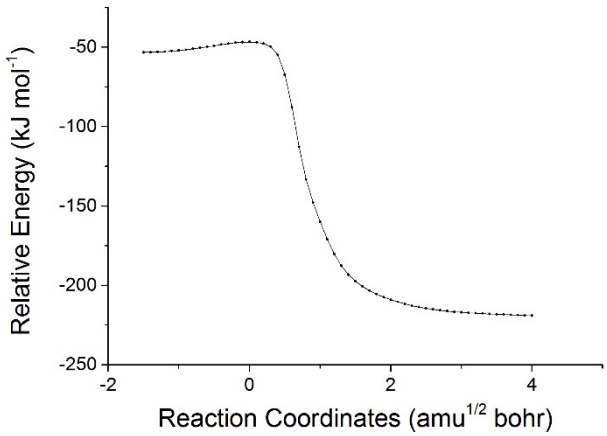

Compound: sCl 5 + $(H_2O)_2$ Pr3	**Energy (kJ mol^{-1}):** -778.234941477938
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.281619 -0.396869 -0.141349 6 -0.073615 0.502297 0.285331 8 0.679689 0.627928 -0.880580 8 1.863158 1.410381 -0.608218 1 2.514029 0.701364 -0.464738 9 -0.587670 1.698848 0.673107 8 0.589165 -0.024461 1.352062 1 1.313173 -0.592262 1.036499 9 -2.127289 -0.534924 0.882116 9 -1.949836 0.114088 -1.178433 9 -0.840746 -1.623148 -0.487456 8 2.827771 -1.274646 0.090297 1 2.584162 -1.895382 -0.605510 1 3.591648 -1.653679 0.537359	30.8261, 58.0992, 91.0942, 125.3530, 168.5796, 188.2988, 222.2970, 239.3348, 272.1691, 295.7873, 313.8342, 340.1174, 378.3839, 379.9574, 466.4912, 514.4522, 531.0048, 583.5516, 603.2174, 630.9793, 732.1940, 829.7446, 939.0117, 1048.7712, 1086.3898, 1165.0852, 1200.8282, 1208.3361, 1331.2638, 1405.5919, 1457.5082, 1627.6146, 3614.9543, 3656.6230, 3783.3352, 3879.9193

Compound: sCl 5 + $(H_2O)_2$ PRC4	**Energy (kJ mol^{-1}):** -778.154802564593
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.523631 0.070204 -0.117940 6 0.126545 -0.448086 0.244963 8 -0.517977 -1.072454 -0.609207 8 -1.734406 -1.668085 -0.200888 9 -0.192591 -0.438451 1.487670 9 1.887208 1.054233 0.691694 9 2.395072 -0.943889 0.026528 9 1.559768 0.483838 -1.380501 8 -3.302494 0.564233 -0.063406 1 -2.884949 -0.325637 -0.137135 1 -3.976892 0.606944 -0.746286 8 -0.867860 1.766934 0.050317 1 -1.815934 1.508925 -0.029492 1 -0.686495 2.350457 -0.692268	19.4727, 41.9568, 92.4435, 115.0151, 131.1127, 166.1585, 185.4852, 246.9869, 255.5549, 255.9820, 280.3702, 300.0568, 350.8270, 362.2080, 405.1394, 421.3097, 521.6741, 535.5956, 575.1269, 678.9162, 718.8823, 730.9504, 840.7204, 858.5765, 910.2685, 1136.8887, 1190.2595, 1239.3736, 1409.2583, 1630.3548, 1644.9207, 1672.4348, 3327.8774, 3413.8679, 3850.3844, 3863.5024

Compound: sCI 5 + $(H_2O)_2$ TS4	**Energy (kJ mol^{-1}):** -778.153225068607
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.482042 -0.041610 -0.082930 6 0.010444 0.247204 0.200130 8 0.556018 1.044842 -0.614002 8 1.877025 1.518238 -0.210042 9 0.304275 0.288980 1.471268 9 -1.956400 -0.952454 0.760697 9 -2.184337 1.084144 0.058772 9 -1.634812 -0.489053 -1.337317 8 3.062989 -0.717905 0.000049 1 2.725841 0.253057 -0.108109 1 3.703589 -0.893273 -0.694674 8 0.686397 -1.465941 -0.099859 1 1.728012 -1.293563 -0.087031 1 0.454186 -1.718206 -1.003343	-269.4438, 38.7369, 61.8805, 137.6329, 165.4533, 177.4985, 287.8044, 300.9685, 321.0749, 355.1282, 391.5197, 406.9766, 418.2621, 429.1966, 509.3777, 536.6606, 573.7250, 630.1877, 682.9775, 721.9018, 812.5196, 845.7557, 873.0997, 1071.2964, 1151.0672, 1187.7224, 1217.4694, 1320.0152, 1376.8772, 1507.2047, 1621.9928, 1698.8260, 2132.0505, 2622.0161, 3783.7703, 3852.4844

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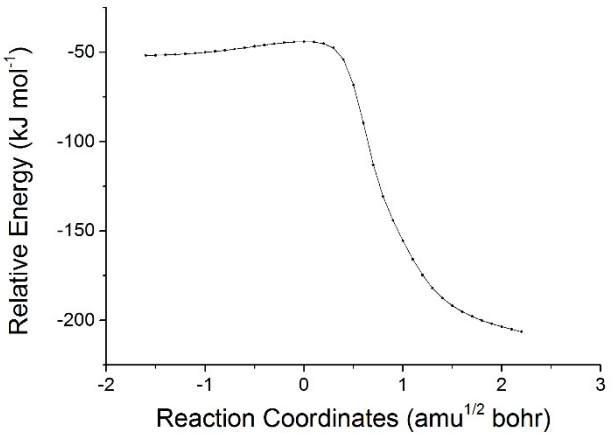

S8.11 Reactions with MeOH

Compound: MeOH	**Energy (kJ mol^{-1}):** -115.607115778238
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.667408 -0.020462 0.000000 8 0.748822 0.122098 0.000000 1 1.151097 -0.750378 -0.000000 1 -1.026778 -0.544214 -0.890795 1 -1.026779 -0.544207 0.890799 1 -1.083670 0.984791 -0.000004	290.6856, 1039.0192, 1076.1201, 1170.5975, 1365.7526, 1477.3714, 1498.2111, 1508.8548, 2994.1556, 3039.5029, 3108.4416, 3828.6843

Compound: sCI 1 + MeOH PRC	**Energy (kJ mol^{-1}):** -305.020987250893
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 2.662111 -0.046788 0.000044 8 1.315288 0.399727 -0.000067 1 0.698704 -0.357599 -0.000052 1 2.893216 -0.640865 -0.889276 1 3.300954 0.835093 0.000016 1 2.893113 -0.640734 0.889478 6 -1.635466 0.998502 0.000005 8 -1.950142 -0.213639 0.000033 8 -0.974471 -1.171188 -0.000023 1 -0.591507 1.299365 -0.000058 1 -2.479754 1.675256 0.000055	24.8880, 82.1748, 110.6320, 111.6029, 135.5092, 259.5276, 549.7940, 665.8058, 696.6622, 879.6470, 1019.2042, 1061.0776, 1138.6918, 1172.9739, 1273.0125, 1420.9590, 1449.4821, 1477.4975, 1497.7786, 1512.0957, 1560.2724, 2992.6031, 3037.4403, 3082.1700, 3095.0315, 3243.6738, 3517.8399

Compound: sCI 1 + MeOH TS1	**Energy (kJ mol^{-1}):** -305.012539571568
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.863745 -0.172056 0.389771 8 0.934811 0.041282 -0.675937 1 0.218702 -0.701416 -0.634231 1 2.400052 -1.106997 0.222573 1 2.571438 0.654242 0.391134 1 1.353139 -0.227500 1.353711 6 -0.701900 1.051055 -0.161035 8 -1.199505 0.166901 0.601952 8 -1.260499 -1.070358 -0.153254 1 -0.936660 1.041876 -1.217190 1 -0.376203 1.963201 0.329508	-303.3420, 135.4580, 151.7227, 188.5069, 331.0013, 453.7042, 543.7435, 799.9595, 865.9194, 1006.5269, 1112.0219, 1165.7576, 1181.7513, 1211.1356, 1251.4969, ,1381.3223, 1464.5139, 1490.1175, 1494.0108, 1518.0904, 1546.2798, 2568.4657, 3021.4453, 3082.0592, 3100.9807, 3116.4553, 3224.8375

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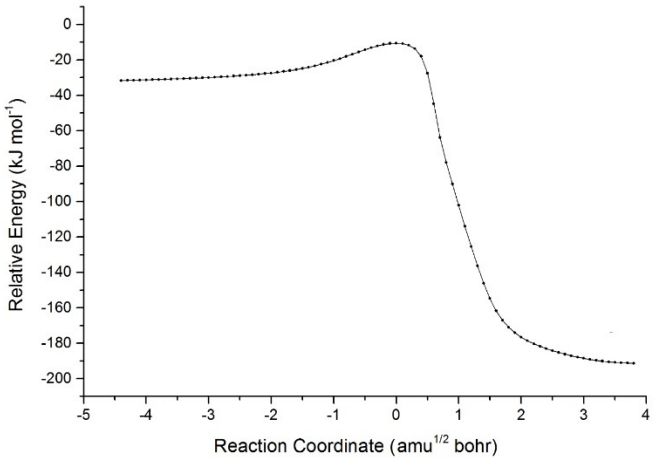

Compound: sCI 1 + MeOH Pr1	**Energy (kJ mol^{-1}):** -305.089754793660
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.866681 -0.450981 0.277009 8 0.921620 0.046899 -0.666119 1 -1.363992 -1.344923 -0.391532 1 1.387002 -1.064896 1.042174 1 2.576523 -1.057064 -0.280043 1 2.399568 0.372679 0.762678 6 -0.055601 0.877798 -0.117095 8 -1.003092 0.190929 0.670639 8 -1.879360 -0.542945 -0.220829 1 -0.552119 1.373600 -0.949241 1 0.373190 1.600643 0.586949	106.8116, ,132.8786, 193.1857, 247.0967, 336.7449, 481.1437, 625.3832, 875.9852, 931.0861, 997.2289, 1089.2781, 1166.6214, 1175.0153, 1227.8307, 1319.6211, 1377.1010, 1404.1314, 1465.0513, 1483.3431, 1491.0236, 1509.4422, 2998.4938, 3004.6735, 3060.3119, 3105.6338, 3124.8533, 3730.9399

Compound: sCI 1 + MeOH TS2	**Energy (kJ mol^{-1}):** -305.010689091126
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.062272 -0.126803 0.198882 8 -0.873223 0.024855 -0.569815 1 -0.214440 -0.747176 -0.352060 1 -1.847455 -0.183951 1.270177 1 -2.707715 0.727406 0.003845 1 -2.578012 -1.040668 -0.100269 6 0.640245 1.001204 0.262268 8 1.540533 0.241828 -0.206971 8 1.213700 -1.115998 0.192501 1 0.218716 0.788854 1.237825 1 0.612990 2.003651 -0.152141	-314.5301, 101.6876, 161.3604, 201.5254, 339.3872, 430.7475, 527.8844, 805.4684, 867.5779, 1023.6465, 1084.8305, 1162.9890, 1178.4686, 1211.8856, 1228.6814, 1382.1058, 1466.4546, 1494.9678, 1496.1083, 1518.4641, 1588.9879, 2483.6260, 3006.1591, 3068.6532, 3092.7445, 3110.5584, 3214.1642

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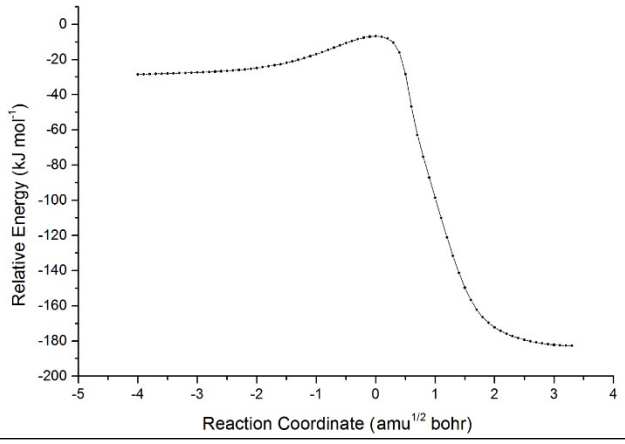

Compound: sCI 1 + MeOH Pr2	**Energy (kJ mol^{-1}):** -305.086315844733
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -2.116714 -0.273591 0.130007 8 -0.830169 -0.175072 -0.456215 1 1.492242 -1.320331 -0.436822 1 -2.675006 -1.004118 -0.449884 1 -2.647746 0.684065 0.098946 1 -2.055814 -0.610559 1.170591 6 0.028141 0.707631 0.225843 8 1.324359 0.556662 -0.254477 8 1.836333 -0.710029 0.232219	60.9145, 147.5248, 209.1549, 293.1227, 338.1013, 403.9749, 592.9671, 884.4403, 980.1253, 1063.0713, 1112.7765, 1149.6046, 1181.9207, 1223.0636, 1284.8284, 1380.7824, 1419.0086, 1472.8164, 1492.5940, 1494.2584, 1510.0321, 2973.2882, 2985.8560, 3021.2134, 3028.7648, 3121.4429, 3730.7851

1 -0.011022 0.520149 1.305723 1 -0.215404 1.754062 0.004136	

Compound: sCI 2 + MeOH PRC	**Energy (kJ mol^{-1}):** -641.819794756621
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.976708 -0.101676 -0.000009 6 0.996614 1.054995 -0.000301 8 -0.249822 0.916410 -0.000190 8 -0.792449 -0.316205 0.000213 1 1.349980 2.076669 -0.000628 9 1.846753 -0.862233 1.088123 9 1.846623 -0.862894 -1.087664 9 3.216292 0.424173 -0.000243 8 -3.584966 0.541108 0.000387 6 -4.538112 -0.507407 -0.000285 1 -4.454459 -1.141356 -0.889827 1 -5.526454 -0.049380 -0.000250 1 -4.454787 -1.142196 0.888688 1 -2.694655 0.158864 0.000358	7.8778, 13.7557, 25.1694, 81.2882, 84.6164, 111.2334, 128.0235, 216.1099, 246.9664, 334.8528, 479.5373, 509.5491, 535.8498, 587.6098, 593.6590, 759.4478, 800.7172, 884.0324, 930.6324, 1060.9119, 1120.5796, 1157.2830, 1171.8072, 1183.6161, 1242.3480, 1368.3585, 1435.6089, 1476.2118, 1497.0762, 1511.4617, 1558.0757, 2979.1708, 3018.1652, 3089.2369, 3213.6535, 3666.0389

Compound: sCI 2 + MeOH TS1	**Energy (kJ mol^{-1}):** -641.812455653684
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.150706 -0.248514 0.005650 6 -0.071605 0.205229 -0.809726 8 -0.611723 1.344246 -0.747619 8 -0.733833 1.770494 0.616132 1 -0.154234 -0.288556 -1.773672 9 2.171590 0.555970 -0.346428 9 1.053301 -0.254276 1.323237 9 1.454370 -1.497428 -0.400749 6 -2.690554 -0.860532 -0.159831 8 -1.391399 -0.737195 0.430712 1 -1.334405 0.156953 0.889988 1 -2.897122 -0.031950 -0.840073 1 -2.719147 -1.804051 -0.699014 1 -3.444072 -0.868249 0.627885	-238.8203, 43.8051, 115.7554, 142.3150, 155.5798, 189.5276, 207.0024, ,276.0069, 319.3805, 350.2625, 450.7578, 518.3362, 556.3651, 567.6475, 740.0036, 808.7216, 866.5284, 964.4575, 1019.1294, 1049.3368, 1140.5097, 1153.8883, 1176.3217, 1185.9025, 1284.6473, 1345.3465, 1461.2570, 1472.4469, 1494.5943, 1512.0143, 1557.6297, 2991.1165, 3032.5103, 3091.3535, 3130.1032, 3152.3093

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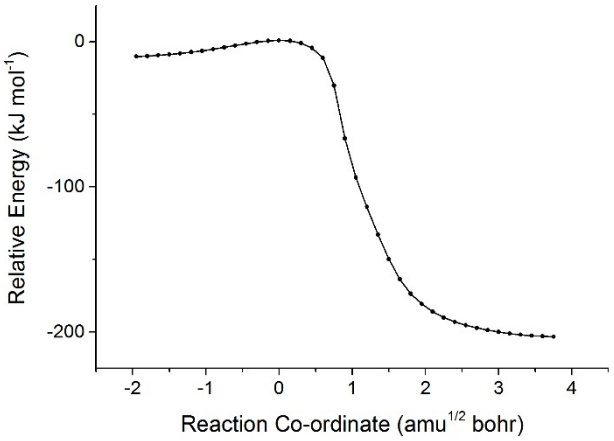

Compound: sCl 2 + MeOH Pr	**Energy (kJ mol^{-1}):** -641.901373422778
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.056705 -0.301665 -0.003500 6 -0.397832 -0.082695 -0.480375 8 -0.714080 1.258866 -0.757921 8 -0.472266 2.067993 0.418501 1 -0.482679 -0.547118 -1.470054 9 1.903483 0.451576 -0.718120 9 1.246603 -0.043594 1.291534 9 1.385379 -1.595895 -0.213342 6 -2.521234 -1.032375 -0.044004 8 -1.230634 -0.673220 0.454765 1 -1.272492 1.909798 0.941578 1 -2.430630 -1.768178 -0.847228 1 -3.059988 -1.473098 0.789745 1 -3.063378 -0.158881 -0.410168	60.3433, 90.3684, 124.3320, 151.2099, 188.2054, 212.0435, 237.2391, 305.6409, 340.8455, 363.2585, 422.9918, 528.8540, 570.8971, 655.1884, 754.2538, 868.8478, 912.9361, 1005.4468, 1038.2480, 1119.0917, 1138.1004, 1176.0669, 1184.7505, 1222.8966, 1280.1943, 1359.9493, 1384.1052, 1403.7418, 1478.3985, 1493.7604, 1507.6477, 3013.0098, 3019.4411, 3075.1426, 3138.0241, 3726.2609

Compound: sCl 2 + MeOH TS2	**Energy (kJ mol^{-1}):** -641.809840895326
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.960039 -0.367008 0.033781 6 0.122443 0.567493 -0.851126 8 -0.143691 1.775553 -0.591170 8 -0.619507 1.888320 0.773109 1 0.227665 0.343139 -1.908782 9 2.222760 0.096404 -0.002129 9 0.603569 -0.516218 1.299182 9 0.954865 -1.586276 -0.548416 6 -2.133213 -1.321958 0.136887 8 -1.682887 -0.076672 -0.411040 1 -1.606554 0.652054 0.300384 1 -2.003882 -2.088661 -0.622590 1 -1.581375 -1.594839 1.034505 1 -3.193516 -1.225657 0.374309	-277.7025, 52.5164, 87.4164, 135.7958, 147.4743, 219.8415, 244.7700, 290.8680, 320.4487, 370.4519, 440.5767, 514.9018, 547.2127, 570.6901, 736.4417, 796.0657, 859.8538, 956.7795, 1013.0329, 1054.6223, 1134.6948, 1157.8251, 1176.4975, 1200.3395, 1281.7528, 1349.0475, 1456.1694, 1477.7089, 1495.4363, ,1506.8177, 1574.5134, 2755.9507, 3037.8079, 3105.9950, 3134.6294, 3150.9265

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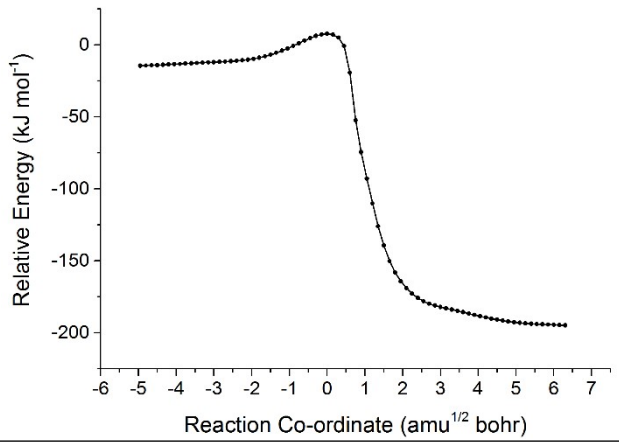

Compound: sCI 3 + MeOH PRC1	**Energy (kJ mol^{-1}):** -641.824942996462
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.702464 -0.317385 0.000001 6 -0.267270 0.153707 -0.000011 8 -0.081319 1.391538 0.000007 8 1.182001 1.890171 -0.000002 1 0.567221 -0.546139 -0.000033 9 -1.920794 -1.080498 -1.085601 9 -2.575951 0.686259 0.000039 9 -1.920758 -1.080548 1.085575 6 3.987682 -0.820759 0.000021 8 2.596940 -0.526234 -0.000035 1 2.443182 0.434526 -0.000022 1 4.483773 -0.424164 0.890025 1 4.483852 -0.424129 -0.889923 1 4.090831 -1.904185 0.000005	18.1908, 34.4140, 66.9668, 84.2489, 109.7187, 124.1555, 174.7514, 207.8882, 243.9959, 388.4638, 395.5289, 429.3178, 556.4368, 560.2631, 620.7028, 699.2395, 891.0590, 945.0049, 957.2409, 1056.3515, 1128.5630, 1140.7914, 1173.1779, 1183.4579, 1280.8269, 1379.4922, 1421.3731, 1477.8260, 1498.3830, 1510.6159, 1557.8223, 3000.7618, 3049.0279, 3103.5151, 3105.0225, 3595.1865

Compound: sCI 3 + MeOH TS1	**Energy (kJ mol^{-1}):** -641.819503461060
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.228989 0.036844 -0.016691 6 -0.081692 -0.623835 -0.423002 8 -0.677064 -1.303157 0.463605 8 -1.989265 -1.630824 -0.052192 1 -0.219375 -0.847004 -1.473984 9 2.226195 -0.857648 -0.132697 9 1.206699 0.483418 1.240251 9 1.494590 1.062726 -0.834186 6 -1.732897 1.659385 0.402170 8 -1.479661 0.761487 -0.688621 1 -2.046041 -0.080869 -0.548528 1 -1.570998 1.168913 1.362818 1 -2.766982 1.999803 0.343730 1 -1.062445 2.508280 0.298454	-243.0166, 36.9354, 105.3890, 136.5967, 150.0916, 183.1191, 202.5561, 273.7948, 356.5155, 382.0647, 434.5178, 510.9263, 556.1704, 626.3829, 699.0313, 842.7075, 874.2598, 972.1449, 1093.6682, 1098.0531, 1156.7695, 1179.4347, 1180.7510, 1231.7325, 1265.7809, 1339.2162, 1464.9060, 1477.8580, 1495.2058, 1509.6940, 1543.6809, 2693.1227, 3032.9744, 3096.4649, 3134.2897, 3170.8923

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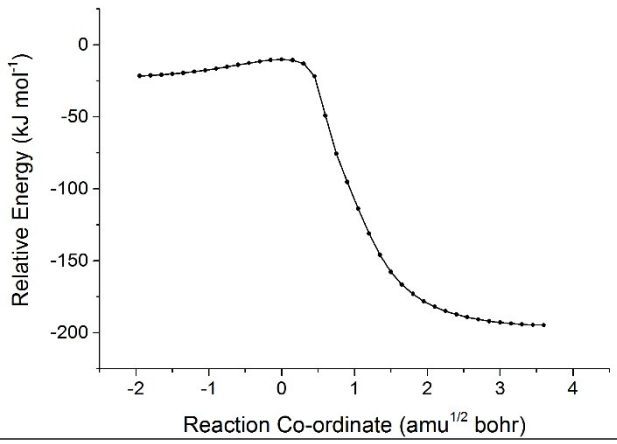

Compound: sCl 3 + MeOH Pr1	**Energy (kJ mol^{-1}):** -641.900575600613
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.077346 -0.234150 -0.016420 6 0.397023 -0.161881 -0.487208 8 1.120044 -0.864566 0.498306 8 2.346263 -1.329349 -0.110191 1 0.458794 -0.690367 -1.437924 9 -1.840623 0.563469 -0.781733 9 -1.541369 -1.486609 -0.135968 9 -1.241862 0.145906 1.262837 6 0.843658 2.057974 0.355278 8 0.867172 1.118444 -0.729322 1 2.958803 -0.610424 0.104143 1 -0.166490 2.428275 0.531427 1 1.236148 1.617870 1.271989 1 1.479588 2.881851 0.043896	61.1974, 99.9853, 120.8446, 175.3253, 192.0609, 226.6944, 232.3815, 305.6868, 353.7993, 357.0616, 405.5817, 529.1777, 562.7402, 651.7204, 731.2299, 869.2845, 929.3750, 956.3906, 1042.2889, 1126.8783, 1165.2849, 1170.3066, 1178.5134, 1221.2817, 1262.6593, 1355.1356, 1386.0573, 1406.5670, 1476.3858, 1500.9000, 1509.1502, 3034.6652, 3094.0915, 3100.0399, 3134.7282, 3734.0248

Compound: sCl 3 + MeOH TS2	**Energy (kJ mol^{-1}):** -641.817837970547
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.246729 -0.152999 -0.014850 6 -0.087939 0.463953 -0.409750 8 -0.388112 1.568790 0.119735 8 -1.780107 1.835183 -0.174680 1 -0.512401 0.177832 -1.365617 9 1.218922 -1.471246 -0.265562 9 2.222144 0.388616 -0.768270 9 1.542659 0.038787 1.265197 6 -2.160149 -1.627810 -0.199932 8 -1.501347 -0.588883 0.526825 1 -1.989149 0.295222 0.387213 1 -1.571607 -2.535336 -0.094325 1 -3.153390 -1.786818 0.221191 1 -2.262298 -1.375899 -1.258594	-225.5585, 40.1970, 100.8561, 103.6552, 163.1262, 184.2740, 200.7893, 274.4572, 346.5777, 380.2987, 428.4281, 494.4856, 553.9362, 609.1866, 696.1118, 844.6004, 876.1550, 1000.2079, 1049.8813, 1073.6859, 1149.3181, 1173.9607, 1179.1282, 1204.5798, 1277.1445, 1335.9007, 1468.1314, 1485.2395, 1496.1987, 1511.5663, 1570.4721, 2775.1052, 3017.4396, 3080.9557, 3130.7253, 3154.6612

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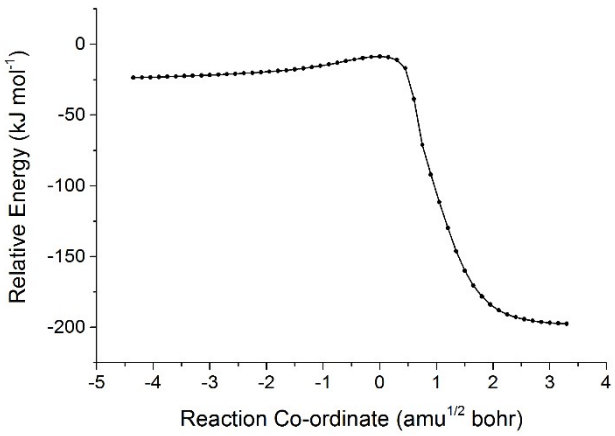

Compound: sCl 3 + MeOH Pr2	**Energy (kJ mol^{-1}):** -641.900995173475
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.140921 -0.070875 -0.025442 6 0.390369 -0.091534 -0.230218 8 0.795574 -1.359801 0.194497 8 2.159133 -1.540207 -0.248752 1 0.593059 0.037779 -1.298686 9 -1.746540 -0.979668 -0.804939 9 -1.491807 -0.301256 1.242750 9 -1.613723 1.144187 -0.373417 6 1.430951 2.061296 -0.178662 8 1.007046 0.896056 0.530933 1 2.647360 -1.258947 0.539414 1 2.015439 2.648362 0.524422 1 2.056613 1.789365 -1.032606 1 0.579747 2.652358 -0.519588	57.8629, 68.4967, 113.4587, 145.8866, 174.8856, 236.2027, .0564, 318.4633, 344.6182, 369.3135, 416.0334, 523.7378, 563.2944, 600.2046, 710.5586, 874.5574, 953.2717, 1005.4349, 1096.5989, 1118.0767, 1151.8004, 1169.1534, 1177.0464, 1226.9317, 1272.1301, 1359.1766, 1388.8027, 1401.1096, 1480.1900, 1494.4337, 1510.4290, 3013.4252, 3022.8458, 3078.2457, 3132.4287, 3731.7653

Compound: sCl 4 + MeOH PRC1	**Energy (kJ mol^{-1}):** -740.991754000359
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.345909 -0.507442 -0.044013 6 0.625157 0.851684 -0.146677 8 -0.223135 1.293586 0.635300 8 -0.649103 0.469357 1.681353 9 0.980931 1.633422 -1.120889 9 2.043850 -0.548257 1.090717 9 0.492606 -1.514647 -0.088400 9 2.194596 -0.607178 -1.072000 8 -2.380149 -0.513216 -0.386899 6 -3.780639 -0.285373 -0.442830 1 -4.331255 -0.968623 0.211071 1 -4.097218 -0.463621 -1.469291 1 -4.040672 0.743369 -0.173975 1 -2.062164 -0.332229 0.510432	13.4464, 24.6617, 45.5949, 55.0213, 91.4055, 120.5258, 153.4675, 186.3622, 223.7360, 286.8126, 294.2847, 363.6197, 481.8579, 499.8008, 579.4303, 601.6396, 627.1066, 673.1296, 778.5503, 913.7607, 1056.2770, 1114.3121, 1156.3328, 1172.9210, 1189.8948, 1224.7012, 1395.9169, 1416.2135, 1477.3762, 1497.2475, 1511.3971, 1608.5151, 2989.7309, 3033.1589, 3096.4651, 3665.396

Compound: sCI 4 + MeOH TS1	**Energy (kJ mol^{-1}):** N/A
Reaction Coordinates: N/A	**Frequencies (cm^{-1}):** N/A

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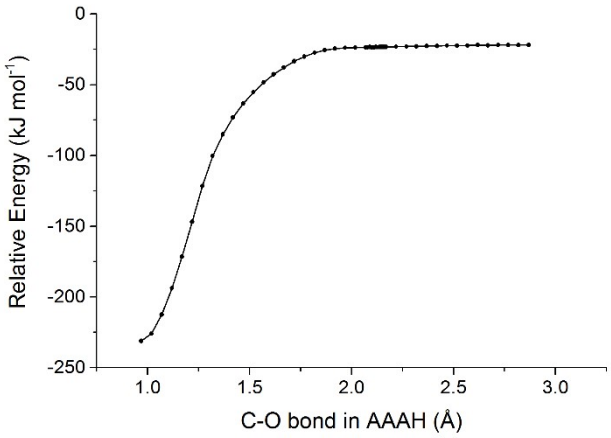

Compound: sCI 4 + MeOH Pr1	**Energy (kJ mol^{-1}):** -741.086414234267
Reaction Coordinates: 6 -1.143419 -0.203351 -0.157986 6 0.355218 -0.121118 0.283497 8 0.716882 1.129692 0.829131 8 0.469736 2.151148 -0.157813 9 0.498577 -0.935162 1.372468 9 -1.922991 0.388266 0.751186 9 -1.356176 0.367116 -1.344599 9 -1.504495 -1.492389 -0.247342 6 2.503829 -0.784249 -0.483154 8 1.114227 -0.524834 -0.762691 1 1.325266 2.209555 -0.608262 1 2.606413 -1.691707 0.108214 1 2.972764 -0.916680 -1.452615 1 2.960785 0.052604 0.044084	**Frequencies (cm^{-1}):** 50.7280, 91.7135, 115.4661, 143.9077, 175.5203, 189.7637, 228.0648, 279.0368, 301.0774, 343.7678, 377.1871, 404.5267, 490.8650, 534.0094, 578.3152, 651.8784, 719.7240, 780.8109, 976.3218, 985.8803, 1069.1732, 1120.5552, 1156.4130, 1178.4296, 1186.2852, 1208.0363, 1225.0568, 1353.0381, 1398.3361, 1478.0025, 1493.4508, 1511.1965, 3047.7620, 3118.8728, 3154.7933, 3731.0958

Compound: sCI 4 + MeOH PRC2	**Energy (kJ mol^{-1}):** -740.993837410730
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.929081 -0.620812 -0.234927 6 -0.496165 0.618695 0.577499 8 -0.182377 1.733354 0.147822 8 0.153174 1.822995 -1.219691 9 -0.703493 0.531270 1.857480 9 -2.153690 -0.360273 -0.719156 9 -0.130295 -0.942005 -1.232427 9 -1.017064 -1.660041 0.600950 8 1.994666 0.171217 0.315203 6 2.917818 -0.871055 0.009075 1 1.882285 0.743176 -0.459932 1 2.565636 -1.494846 -0.815822 1 3.014127 -1.486422 0.900852 1 3.899690 -0.463959 -0.243262	8.7072, 46.5863, 71.4762, 97.4421, 106.1329, 151.1997, 166.6269, 198.8084, 241.5571, 290.2502, 301.1464, 367.8671, 479.2797, 504.8591, 573.9102, 587.2462, 621.5557, 661.9547, 776.3573, 904.1488, 1047.7881, 1118.3302, 1138.6682, 1173.3138, 1174.2899, 1238.6741, 1384.8004, 1408.7191, 1477.5542, 1498.1583, 1510.5444, 1615.5861, 3010.9504, 3063.2416, 3114.2077, 3671.1396

Compound: sCI 4 + MeOH TS2	**Energy (kJ mol^{-1}):** -740.993170960665
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 0.912032 -0.498276 -0.251751 6 0.224113 0.640651 0.542940 8 -0.042847 1.794029 0.143502 8 -0.657774 1.759785 -1.178840 9 0.482013 0.543914 1.818389 9 0.836580 -1.628139 0.462242 9 0.429997 -0.723657 -1.457506 9 2.206117 -0.152187 -0.357672 6 -2.312308 -1.258884 0.017758 8 -1.725805 0.002627 0.354061 1 -2.151755 -1.932718 0.855253 1 -3.384317 -1.121322 -0.131474 1 -1.872395 -1.683438 -0.884327 1 -1.715513 0.625624 -0.431989	-139.5049, 45.0230, 110.9201, 124.5856, 127.9697, 211.7240, 234.6986, 259.1681, 269.3948, 299.0881, 353.7192, 373.6648, 477.4372, 520.0065, 591.1868, 608.4627, 656.8282, 774.8334, 887.3562, 919.3007, 1037.4115, 1130.0942, 1166.9577, 1176.9158, 1178.2235, 1243.7823, 1350.6568, 1454.6869, 1476.6927, 1497.6563, 1508.5865, 1591.4098, 3027.0633, 3066.5636, 3095.9547, 3132.7609

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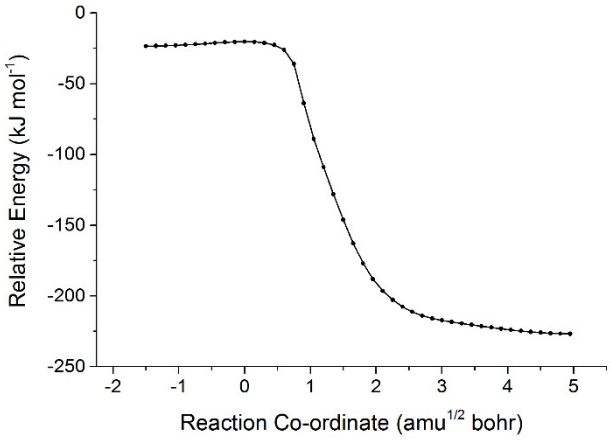

Compound: sCI 4 + MeOH Pr2	**Energy (kJ mol^{-1}):** -741.084841781096
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -0.344807 -0.941573 -0.121459 6 0.112414 0.462115 0.425148 8 -0.961502 1.339061 0.593550 8 -1.542744 1.619546 -0.695240 9 0.530358 0.245318 1.708747 9 -1.503957 -1.307551 0.423963 9 -0.478617 -0.930906 -1.452747 9 0.574092 -1.877788 0.186432 6 2.314643 0.392960 -0.558851 8 1.067317 1.074188 -0.322164 1 -0.984830 2.351446 -1.000773 1 2.185348 -0.422482 -1.268434 1 2.731827 0.020531 0.374593 1 2.972709 1.145487 -0.981134	53.5293, 94.1894, 117.9877, 172.1974, 184.4551, 227.5704, 251.8725, 293.5800, 311.8578, 346.8714, 385.0132, 404.2358, 495.8009, 535.1331, 590.8703, 649.2973, 667.2216, 763.0140, 973.6865, 1021.0925, 1090.3159, 1116.6744, 1163.8665, 1176.1525, 1190.3010, 1201.4369, 1229.9396, 1320.1716, 1407.5733, 1485.8850, 1500.9230, 1505.6670, 3051.1521, 3125.5750, 3152.1045, 3720.6253

Compound: sCI 5 + MeOH PRC1	**Energy (kJ mol^{-1}):** -740.999159807260
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.490530 -0.385650 -0.110808 6 0.352908 0.588183 0.182951 8 -0.223060 1.173232 -0.746175 8 -1.277295 2.020177 -0.431860 9 0.090667 0.808213 1.421679 9 2.631497 0.105665 0.394281 9 1.631711 -0.559880 -1.418454 9 1.242669 -1.558110 0.473031 6 -3.154391 -1.296185 -0.266739 8 -2.245899 -0.501111 0.485391 1 -2.363558 0.431126 0.246002 1 -3.008124 -1.176368 -1.344319 1 -4.193753 -1.058374 -0.023763 1 -2.967710 -2.335846 -0.004026	23.4150, 30.2598, 55.7144, 93.4399, 96.9298, 128.3982, 163.7270, 180.7896, 193.8496, 298.6344, 348.4901, 371.8411, 406.8468, 513.5737, 576.3078, 606.4957, 668.9614, 728.7800, 858.6425, 879.7724, 1052.8820, 1112.2481, 1153.0375, 1174.2597, 1175.2901, 1231.5187, 1405.4956, 1405.7647, 1477.6171, 1497.5943, 1511.8428, 1627.0351, 2996.8581, 3043.5378, 3102.7127, 3663.0055

Compound: sCI 5 + MeOH TS1	**Energy (kJ mol^{-1}):** -740.997867488158
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 -1.259490 0.148992 -0.102836 6 0.059196 -0.610304 0.115493 8 0.678664 -1.019101 -0.894231 8 2.007574 -1.470926 -0.516689 9 0.126921 -1.208161 1.270269 9 -2.261522 -0.733491 -0.215233 9 -1.202728 0.879234 -1.214396 9 -1.509496 0.945964 0.934208 6 1.711322 1.877478 -0.137315 8 1.459590 0.746031 0.708515 1 2.061477 -0.003075 0.413809 1 1.599694 1.616308 -1.190411 1 2.726097 2.234749 0.039112 1 1.001370 2.655080 0.131037	-205.1661, 38.2984, 102.6548, 121.0210, 144.8702, 183.0251, 193.0694, 249.3440, 283.4880, 313.9283, 365.6897, 394.5012, 438.0071, 518.7592, 577.9844, 655.4661, 716.1101, 804.1347, 841.3071, 1005.0264, 1037.8971, 1137.6091, 1170.9206, 1179.4643, 1192.0744, 1221.4657, 1363.3945, 1464.4646, 1474.2037, 1496.0565, 1509.8960, 1567.7328, 3017.9730, 3045.0308, 3096.6112, 3135.6940
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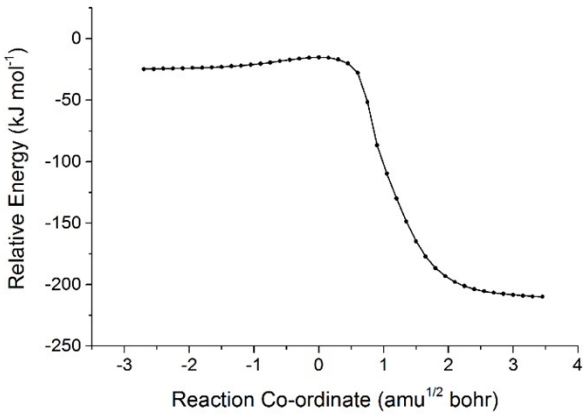	

Compound: sCI 5 + MeOH Pr1	**Energy (kJ mol^{-1}):** -741.083786682520
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.162766 -0.094593 -0.145678 6 -0.336932 -0.199013 0.310960 8 -0.989709 -0.731512 -0.802437 8 -2.349799 -1.046730 -0.429102 9 -0.363652 -1.069577 1.347633 9 1.874669 0.510363 0.811497 9 1.684982 -1.300826 -0.366239 9 1.282160 0.628147 -1.273515 6 -0.966001 2.093138 -0.078952 8 -0.862075 0.962079 0.798518 1 -2.836987 -0.340649 -0.878001 1 -0.005667 2.597393 -0.179178 1 -1.327022 1.802088 -1.065158 1 -1.680096 2.760303 0.394142	49.3012, 91.7056, 126.2046, 156.2736, 168.1687, 187.3095, 219.5661, 279.4858, 298.1538, 340.6490, 375.8051, 386.4420, 506.4326, 535.9658, 569.5700, 631.1461, 731.8482, 792.7966, 939.1143, 1040.9147, 1064.8271, 1121.6918, 1172.9430, 1174.9616, 1188.9573, 1201.2160, 1226.1309, 1319.3342, 1396.8534, 1481.1796, 1499.2622, 1511.3160, 3040.3468, 3106.9472, 3143.4978, 3740.4493

Compound: sCI 5 + MeOH PRC2	**Energy (kJ mol^{-1}):** -740.999519026160
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.478552 -0.363963 -0.107978 6 0.302930 0.526805 0.282388 8 -0.096395 1.409091 -0.489724 8 -1.199076 2.162088 -0.104616 9 -0.174435 0.358706 1.466674 9 1.147628 -1.644957 0.055155 9 1.832907 -0.149597 -1.366851 9 2.519460 -0.092485 0.695326 8 -2.108488 -0.523532 -0.567881 6 -3.143139 -1.265147 0.067307 1 -3.232368 -1.014743 1.128483 1 -4.109511 -1.101912 -0.417281 1 -2.885668 -2.318824 -0.021184 1 -2.300880 0.423135 -0.495280	27.2164, 29.1571, 44.1111, 98.3915, 112.5842, 130.8381, 155.6303, 186.9520, 189.4560, 296.7684, 352.8434, 370.3431, 406.8896, 513.4863, 563.0249, 576.8378, 667.3351, 727.7428, 855.7292, 873.3712, 1053.6440, 1116.0326, 1147.1925, 1173.5514, 1174.1936, 1235.5851, 1392.7941, 1416.8320, 1478.0135, 1498.0017, 1511.2876, 1628.5936, 2998.5418, 3046.4055, 3105.3834, 3683.5289

Compound: sCI 5 + MeOH TS2	**Energy (kJ mol^{-1}):** -740.997917500017
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.307922 0.174914 -0.088889 6 -0.030787 -0.497853 0.252216 8 -0.350067 -1.530668 -0.371599 8 -1.745683 -1.865783 -0.135037 9 -0.452090 -0.240559 1.461252 9 1.258492 1.470852 0.227443 9 2.282346 -0.398716 0.633781 9 1.590182 0.043528 -1.376615 8 -1.427798 0.665981 -0.686305 6 -2.123589 1.697954 0.021513 1 -1.953859 -0.183444 -0.649350 1 -3.062137 1.912886 -0.490910 1 -2.331973 1.403900 1.050571 1 -1.495299 2.584383 0.011431	-197.6026, 42.9807, 90.8632, 104.7350, 158.1694, 177.4376, 189.3850, 254.1702, 291.5018, 322.0428, 363.0570, 384.2663, 427.2196, 511.8214, 577.6791, 650.3933, 714.1091, 800.7403, 839.3112, 931.2749, 1039.6013, 1135.8987, 1168.9848, 1175.3687, 1181.7913, 1234.0324, 1363.7070, 1458.9705, 1475.8815, 1496.5038, 1509.9165, 1590.7369, 3030.0270, 3094.6498, 3118.1393, 3138.0592

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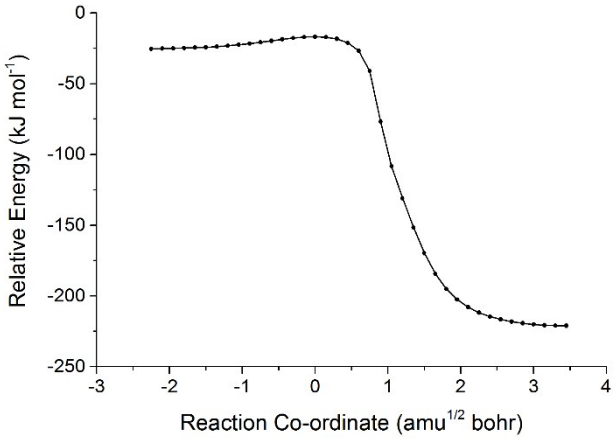

Compound: sCl 5 + MeOH Pr2	**Energy (kJ mol^{-1}):** -741.087346378048
Reaction Coordinates:	**Frequencies (cm^{-1}):**
6 1.193125 -0.130966 -0.075831 6 -0.360430 -0.102593 0.125412 8 -0.775470 -1.369380 -0.236340 8 -2.208064 -1.455681 -0.094286 9 -0.581278 0.131016 1.458852 9 1.767040 -1.081280 0.664166 9 1.500076 -0.340829 -1.358925 9 1.711964 1.054975 0.288796 6 -1.137958 2.174483 -0.141075 8 -0.976074 0.836339 -0.650734 1 -2.502510 -1.133336 -0.960161 1 -1.617729 2.721975 -0.946229 1 -1.775055 2.172851 0.740006 1 -0.176486 2.627805 0.090227	44.9757, 73.5984, 126.1443, 143.4334, 171.5709, 224.3379, 239.8204, 283.2250, 310.2977, 332.6826, 377.7186, 389.2323, 504.7051, 544.3302, 584.7558, 623.1479, 729.8109, 784.1960, 941.3039, 1035.3797, 1067.2085, 1104.9170, 1170.5624, 1179.6748, 1184.6668, 1202.5637, 1226.4720, 1325.3801, 1408.3648, 1484.1721, 1496.9524, 1509.2122, 3057.9428, 3133.2275, 3152.2286, 3722.1372

S9. Example of a Mesmer file

sCI 1 + HNO_3

```
<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema"
xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
 <me:title>HCHOO+HNO3</me:title>
 <moleculeList convention="">
  <molecule id="N2">
   <atomArray>
    <atom id="a1" elementType="N" />
    <atom id="a2" elementType="N" />
   </atomArray>
   <bondArray>
    <bond atomRefs2="a2 a1" order="3" />
   </bondArray>
   <propertyList>
    <property dictRef="me:epsilon">
     <scalar>48.0</scalar>
    </property>
    <property dictRef="me:sigma">
     <scalar>3.90</scalar>
    </property>
    <property dictRef="me:MW">
     <scalar units="amu">28.0</scalar>
    </property>
```

```
    </propertyList>
    <metadata name="copiedFrom" content="C:\Mesmer-5.2/librarymols.xml"
timestamp="20190405_164436" />
  </molecule>
  <molecule id="Cl 1" spinMultiplicity="1" default="true">
    <atomArray>
      <atom id="a1" elementType="C" spinMultiplicity="2" x3="-1.068412" y3="0.202194" z3="-
0.000000" />
      <atom id="a2" elementType="O" x3="-0.003231" y3="-0.459294" z3="-0.000000" />
      <atom id="a3" elementType="O" spinMultiplicity="2" x3="1.179333" y3="0.194958"
z3="0.000000" />
      <atom id="a4" elementType="H" x3="-1.021445" y3="1.284352" z3="-0.000000" />
      <atom id="a5" elementType="H" x3="-1.976903" y3="-0.382830" z3="0.000002" />
    </atomArray>
    <bondArray>
      <bond atomRefs2="a1 a2" order="1" />
      <bond atomRefs2="a1 a4" order="1" />
      <bond atomRefs2="a1 a5" order="1" />
      <bond atomRefs2="a2 a3" order="1" />
    </bondArray>
    <propertyList>
      <property title="program">
        <scalar>Gaussian 09, Revision D.01</scalar>
      </property>
      <property title="basis">
        <scalar>Aug-CC-pVTZ (5D, 7F)</scalar>
      </property>
      <property title="method">
        <scalar>B3LYP</scalar>
      </property>
```

<property title="File Format">

<scalar>g03</scalar>

</property>

<property title="Energy" dictRef="me:ZPE">

<scalar units="kJ/mol" convention="computational" zeroPointVibEnergyAdded="true">0.00</scalar>

</property>

<property title="Vibrational Frequencies" dictRef="me:vibFreqs">

<array units="cm-1">527.76 673.76 912.85 951.07 1242.06 1402.00 1543.54 3118.17 3267.96</array>

</property>

<property title="Rotational Constants" dictRef="me:rotConsts">

<array units="cm-1">2.693 0.413 0.358</array>

</property>

<property title="Symmetry Number" dictRef="me:symmetryNumber">

<scalar>1</scalar>

</property>

<property dictRef="me:frequenciesScaleFactor" default="true">

<scalar>1</scalar>

</property>

</propertyList>

<me:DOSCMethod xsi:type="QMRotors" />

</molecule>

<molecule id="HNO3" spinMultiplicity="1" default="true">

<atomArray>

<atom id="a1" elementType="N" x3="-0.152562" y3="0.032028" z3="-0.000002" />

<atom id="a2" elementType="O" x3="1.152087" y3="-0.513293" z3="0.000000" />

<atom id="a3" elementType="H" x3="1.719946" y3="0.275046" z3="0.000002" />

<atom id="a4" elementType="O" x3="-0.214564" y3="1.238054" z3="0.000001" />

<atom id="a5" elementType="O" x3="-1.019025" y3="-0.787166" z3="0.000001" />

```
    </atomArray>
    <bondArray>
     <bond atomRefs2="a1 a2" order="1" />
     <bond atomRefs2="a1 a4" order="2" />
     <bond atomRefs2="a1 a5" order="2" />
     <bond atomRefs2="a2 a3" order="1" />
    </bondArray>
    <propertyList>
     <property title="program">
      <scalar>Gaussian 09, Revision D.01</scalar>
     </property>
     <property title="basis">
      <scalar>Aug-CC-pVTZ (5D, 7F)</scalar>
     </property>
     <property title="method">
      <scalar>B3LYP</scalar>
     </property>
     <property title="File Format">
      <scalar>g03</scalar>
     </property>
     <property title="Energy" dictRef="me:ZPE">
      <scalar units="kJ/mol" convention="computational"
zeroPointVibEnergyAdded="true">0.00</scalar>
     </property>
     <property title="Vibrational Frequencies" dictRef="me:vibFreqs">
      <array units="cm-1">479.28 584.84 646.82 783.11 896.08 1315.31 1341.55 1744.38
3712.10</array>
     </property>
     <property title="Rotational Constants" dictRef="me:rotConsts">
      <array units="cm-1">0.436 0.402 0.209</array>
```

```
      </property>
      <property title="Symmetry Number" dictRef="me:symmetryNumber">
       <scalar>1</scalar>
      </property>
      <property dictRef="me:frequenciesScaleFactor" default="true">
       <scalar>1</scalar>
      </property>
     </propertyList>
     <me:DOSCMethod xsi:type=“QMRotors” />
   </molecule>
   <molecule id="PRC" spinMultiplicity="1" default="true">
    <atomArray>
     <atom id="a1" elementType="N" x3="1.496914" y3="-0.134725" z3="-0.004950" />
     <atom id="a2" elementType="O" x3="0.667866" y3="-1.033940" z3="0.097505" />
     <atom id="a3" elementType="O" x3="2.688525" y3="-0.258885" z3="-0.068858" />
     <atom id="a4" elementType="O" x3="1.032740" y3="1.140905" z3="-0.058034" />
     <atom id="a5" elementType="H" x3="0.016643" y3="1.094684" z3="0.054113" />
     <atom id="a6" elementType="C" spinMultiplicity="2" x3="-2.071887" y3="-1.012931"
z3="0.121133" />
     <atom id="a7" elementType="H" x3="-2.497662" y3="-1.823013" z3="-0.458347" />
     <atom id="a8" elementType="H" x3="-1.657407" y3="-1.119954" z3="1.114924" />
     <atom id="a9" elementType="O" x3="-2.091387" y3="0.101106" z3="-0.429087" />
     <atom id="a10" elementType="O" spinMultiplicity="2" x3="-1.536325" y3="1.159431"
z3="0.283118" />
    </atomArray>
    <bondArray>
     <bond atomRefs2="a7 a6" order="1" />
     <bond atomRefs2="a9 a6" order="1" />
     <bond atomRefs2="a9 a10" order="1" />
     <bond atomRefs2="a3 a1" order="2" />
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<bond atomRefs2="a4 a1" order="1" />

<bond atomRefs2="a4 a5" order="1" />

<bond atomRefs2="a1 a2" order="2" />

<bond atomRefs2="a6 a8" order="1" />

</bondArray>

<propertyList>

<property title="program">

<scalar>Gaussian 09, Revision D.01</scalar>

</property>

<property title="basis">

<scalar>Aug-CC-pVTZ (5D, 7F)</scalar>

</property>

<property title="method">

<scalar>B3LYP</scalar>

</property>

<property title="File Format">

<scalar>g03</scalar>

</property>

<property title="Energy" dictRef="me:ZPE">

<scalar units="kJ/mol" convention="computational" zeroPointVibEnergyAdded="true">-54.38</scalar>

</property>

<property title="Vibrational Frequencies" dictRef="me:vibFreqs">

<array units="cm-1">51.88 79.16 103.33 140.18 197.95 266.46 512.02 650.00 676.78 699.25 799.76 841.22 972.46 981.87 1060.98 1235.72 1307.83 1425.90 1483.69 1597.68 1708.48 2730.22 3121.31 3266.04</array>

</property>

<property title="Rotational Constants" dictRef="me:rotConsts">

<array units="cm-1">0.198 0.049 0.040</array>

</property>

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    <property title="Symmetry Number" dictRef="me:symmetryNumber">
     <scalar>1</scalar>
    </property>
    <property dictRef="me:sigma" default="true">
     <scalar>5.0</scalar>
    </property>
    <property dictRef="me:epsilon" default="true">
     <scalar>50.0</scalar>
    </property>
    <property dictRef="me:frequenciesScaleFactor" default="true">
     <scalar>1</scalar>
    </property>
   </propertyList>
   <me:DOSCMethod xsi:type="QMRotors" />
   <me:DistributionCalcMethod default="true" name="Boltzmann" />
   <me:energyTransferModel name="ExponentialDown" default="true" />
   <me:deltaEDown units="cm-1">300.0</me:deltaEDown>
  </molecule>
  <molecule id="Pr">
   <atomArray>
    <atom id="a1" elementType="C" x3="0.811606" y3="0.963884" z3="0.434921" />
    <atom id="a2" elementType="O" x3="-0.557612" y3="1.030658" z3="-0.030897" />
    <atom id="a3" elementType="N" x3="-1.293667" y3="-0.183308" z3="0.009949" />
    <atom id="a4" elementType="O" x3="-2.436401" y3="-0.043762" z3="-0.299483" />
    <atom id="a5" elementType="O" x3="-0.701594" y3="-1.186614" z3="0.335941" />
    <atom id="a6" elementType="H" x3="1.046451" y3="2.024122" z3="0.518457" />
    <atom id="a7" elementType="H" x3="0.872854" y3="0.446444" z3="1.388182" />
    <atom id="a8" elementType="O" x3="1.680810" y3="0.406987" z3="-0.493329" />
    <atom id="a9" elementType="O" x3="2.126689" y3="-0.896290" z3="-0.049719" />
```

```
    <atom id="a10" elementType="H" x3="1.371600" y3="-1.458544" z3="-0.285911" />
   </atomArray>
   <bondArray>
    <bond atomRefs2="a8 a9" order="1" />
    <bond atomRefs2="a8 a1" order="1" />
    <bond atomRefs2="a4 a3" order="2" />
    <bond atomRefs2="a10 a9" order="1" />
    <bond atomRefs2="a2 a3" order="1" />
    <bond atomRefs2="a2 a1" order="1" />
    <bond atomRefs2="a3 a5" order="2" />
    <bond atomRefs2="a1 a6" order="1" />
    <bond atomRefs2="a1 a7" order="1" />
   </bondArray>
   <propertyList>
    <property title="program">
     <scalar>Gaussian 09, Revision C.01</scalar>
    </property>
    <property title="basis">
     <scalar>Aug-CC-pVTZ (5D, 7F)</scalar>
    </property>
    <property title="method">
     <scalar>B3LYP</scalar>
    </property>
    <property title="File Format">
     <scalar>g03</scalar>
    </property>
    <property title="Energy" dictRef="me:ZPE">
     <scalar units="kJ/mol" convention="computational" zeroPointVibEnergyAdded="true">-
179.86</scalar>
    </property>
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<property title="Vibrational Frequencies" dictRef="me:vibFreqs">

<array units="cm-1">76.14 109.04 149.89 274.39 331.02 399.04 504.07 596.45 671.09 778.42 848.25 892.71 929.91 1066.43 1143.07 1299.64 1322.74 1400.83 1417.85 1455.02 1703.96 3076.26 3148.97 3703.26</array>

</property>

<property title="Rotational Constants" dictRef="me:rotConsts">

<array units="cm-1">0.199 0.062 0.051</array>

</property>

<property title="Symmetry Number" dictRef="me:symmetryNumber">

<scalar>1</scalar>

</property>

</propertyList>

</molecule>

<molecule id="TS" spinMultiplicity="1" default="true">

<atomArray>

<atom id="a1" elementType="N" x3="1.382578" y3="-0.063861" z3="-0.008349" />

<atom id="a2" elementType="O" x3="0.628369" y3="-1.058966" z3="0.034369" />

<atom id="a3" elementType="O" x3="2.580436" y3="-0.135427" z3="-0.065503" />

<atom id="a4" elementType="O" x3="0.846896" y3="1.149168" z3="0.004906" />

<atom id="a5" elementType="H" x3="-0.251112" y3="1.114260" z3="0.091169" />

<atom id="a6" elementType="C" spinMultiplicity="2" x3="-1.671765" y3="-1.057011" z3="0.209054" />

<atom id="a7" elementType="H" x3="-1.838608" y3="-2.006498" z3="-0.286142" />

<atom id="a8" elementType="H" x3="-1.395054" y3="-0.967906" z3="1.249688" />

<atom id="a9" elementType="O" x3="-1.962928" y3="-0.044666" z3="-0.454559" />

<atom id="a10" elementType="O" spinMultiplicity="2" x3="-1.613108" y3="1.171046" z3="0.199461" />

</atomArray>

<bondArray>

<bond atomRefs2="a9 a10" order="1" />

<bond atomRefs2="a9 a6" order="1" />

<bond atomRefs2="a7 a6" order="1" />

<bond atomRefs2="a3 a1" order="2" />

<bond atomRefs2="a1 a4" order="1" />

<bond atomRefs2="a1 a2" order="2" />

<bond atomRefs2="a4 a5" order="1" />

<bond atomRefs2="a6 a8" order="1" />

</bondArray>

<propertyList>

<property title="program">

<scalar>Gaussian 09, Revision D.01</scalar>

</property>

<property title="basis">

<scalar>Aug-CC-pVTZ (5D, 7F)</scalar>

</property>

<property title="method">

<scalar>B3LYP</scalar>

</property>

<property title="File Format">

<scalar>g03</scalar>

</property>

<property title="Energy" dictRef="me:ZPE">

<scalar units="kJ/mol" convention="computational" zeroPointVibEnergyAdded="true">-48.32</scalar>

</property>

<property title="Vibrational Frequencies" dictRef="me:vibFreqs">

<array units="cm-1">39.67 92.49 198.57 324.04 328.85 500.71 660.32 702.16 736.22 801.49 819.39 1019.93 1047.07 1133.66 1160.20 1235.81 1425.02 1489.92 1598.78 1614.23 1818.43 3129.37 3269.89</array>

</property>

<property title="ImaginaryFrequency" dictRef="me:imFreqs">

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      <scalar units="cm-1">248.93</scalar>
     </property>
     <property title="Rotational Constants" dictRef="me:rotConsts">
      <array units="cm-1">0.193 0.056 0.045</array>
     </property>
     <property title="Symmetry Number" dictRef="me:symmetryNumber">
      <scalar>1</scalar>
     </property>
     <property dictRef="me:frequenciesScaleFactor" default="true">
      <scalar>1</scalar>
     </property>
    </propertyList>
    <me:DOSCMethod xsi:type=“QMRotors” />
   </molecule>
  </moleculeList>
  <reactionList>
   <reaction id="R1" reversible="true">
    <reactantList>
     <reactant>
      <molecule ref="CI 1" role="deficientReactant" />
     </reactant>
     <reactant>
      <molecule ref="HNO3" role="excessReactant" />
     </reactant>
    </reactantList>
    <productList>
     <product>
      <molecule ref="PRC" role="modelled" />
     </product>
```

```
    </productList>
    <rateParameters reactionType="arrhenius" reversible="true">
     <A>1.000e-010</A>
     <n>0</n>
     <E>0</E>
    </rateParameters>
    <me:MCRCMethod default="CanonicalRateCoefficient, DefinedSumOfStates,
LandauZenerCrossing, MesmerILT, SimpleBimolecularSink, SimpleILT, MesmerILT, WKBCrossing,
ZhuNakamuraCrossing" name="MesmerILT" />
    <me:excessReactantConc default="true">1.0E16</me:excessReactantConc>
    <me:TInfinity default="true">298</me:TInfinity>
   </reaction>
   <reaction id="R2">
    <reactantList>
     <reactant>
      <molecule ref="PRC" role="modelled" />
     </reactant>
    </reactantList>
    <productList>
     <product>
      <molecule ref="Pr" role="sink" />
     </product>
    </productList>
    <me:transitionState>
     <molecule ref="TS" role="transitionState" />
    </me:transitionState>
    <me:MCRCMethod name="SimpleRRKM" />
    <me:tunneling>Eckart</me:tunneling>
   </reaction>
  </reactionList>
```

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<me:conditions>
 <me:bathGas>N2</me:bathGas>
 <me:PTs>
  <me:PTpair units="Torr" P="27" T="295." precision="d" default="true" bathGas="N2" />
  <me:PTpair units="Torr" P="31" T="295." precision="d" default="true" bathGas="N2" />
  <me:PTpair units="Torr" P="35" T="295." precision="d" default="true" bathGas="N2" />
  <me:PTpair units="Torr" P="760" T="295." precision="d" default="true" bathGas="N2" />
  <me:PTpair units="Torr" P="760" T="200." precision="d" default="true" bathGas="N2" />
  <me:PTpair units="Torr" P="760" T="275." precision="d" default="true" bathGas="N2" />
  <me:PTpair units="Torr" P="760" T="298." precision="d" default="true" bathGas="N2" />
  <me:PTpair units="Torr" P="760" T="325." precision="d" default="true" bathGas="N2" />
  <me:PTpair units="Torr" P="760" T="400." precision="d" default="true" bathGas="N2" />
 </me:PTs>
</me:conditions>
<me:modelParameters>
 <me:grainSize units="cm-1">10</me:grainSize>
 <me:energyAboveTheTopHill>30.0</me:energyAboveTheTopHill>
</me:modelParameters>
<me:control>
 <!--<me:calcMethod xsi:type="me:marquardt">
 <me:MarquardtIterations>50</me:MarquardtIterations>
 <me:MarquardtTolerance>0.1</me:MarquardtTolerance>
 <me:testMicroRates Tstep="25" default="true" Tmin="200" Tmax="400" />
 </me:calcMethod>-->
 <me:printSpeciesProfile />
 <me:testRateConstants />
 <!--<me:printGrainBoltzmann />-->
 <me:printGrainedSpeciesProfile />
 <me:eigenvalues>3</me:eigenvalues>
```

```
    <!-- <me:hideInactive/>  Molecules and reactions with attribute active="false" are not shown-->
    <me:diagramEnergyOffset>0</me:diagramEnergyOffset>
    <!--Adjusts displayed energies to this values for the lowest species. -->
    <me:calcMethod default="true" name="simpleCalc" />
    <me:ForceMacroDetailedBalance default="true">true</me:ForceMacroDetailedBalance>
  </me:control>
  <metadataList xmlns:dc="http://purl.org/dc/elements/1.1/">
    <dc:title>HCHOO+HNO3</dc:title>
    <dc:source>sCI 1_HNO3.xml</dc:source>
    <dc:creator>Mesmer v5.2</dc:creator>
    <dc:date>20190405_183821</dc:date>
    <dc:contributor>c1675612</dc:contributor>
  </metadataList>
</me:mesmer>
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