Electronic Supplementary Material (ESI) for Environmental Science: Atmospheres.

An unexpectedly feasible route for the formation of organosulfates by the gas phase reaction of sulfuric acid with acetaldehyde catalyzed by dimethylamine in the atmosphere

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Calculated details for kinetics

For the $CH_3CHO + H_2SO_4 + (CH_3)_2NH \rightarrow CH_3HC(OH)OSO_3H + (CH_3)_2NH$ reaction, we only consider the reaction mechanism can be written in detail as the following expression.

$(CH_3)_2NH + H_2SO_4 \leftrightarrow H_2SO_4\cdots(CH_3)_2NH$ (R2)

$H_2SO_4\cdots(CH_3)_2NH + CH_3CHO \rightarrow CH_3HC(OH)OSO_3H + (CH_3)_2NH$ (R3)

As the result, the total rate constant $k = K_{eq1}k_1$,

$$K_{eq1} = \sigma\frac{Q_{H_2SO_4\cdots(CH_3)_2NH}}{Q_{H_2SO_4}Q_{(CH_3)_2NH}}exp(\frac{E_{H_2SO_4\cdots(CH_3)_2NH} - E_{H_2SO_4} - E_{(CH_3)_2NH}}{RT}) \quad (5)$$

where K_{eq1} is the equilibrium constant of $H_2SO_4\cdots(CH_3)_2NH$ with respect to H_2SO_4 and $(CH_3)_2NH$, which is computed by using equation (5). k_1 is the bimolecular rate constant of the $H_2SO_4\cdots(CH_3)_2NH + CH_3CHO$ reaction.

With regard to R3, we consider the following reaction mechanism in reactions (R4) and (R5).

$H_2SO_4\cdots(CH_3)_2NH + CH_3CHO \rightarrow H_2SO_4\cdots(CH_3)_2NH\cdots CH_3CHO$ (R4)

$H_2SO_4\cdots(CH_3)_2NH\cdots CH_3CHO \rightarrow CH_3HC(OH)OSO_3H + (CH_3)_2NH$ (R5)

The bimolecular rate constant (k_1) of the reaction R3 is equal to $K_{eq2}k_u$, where K_{eq2} is the equilibrium constant of $H_2SO_4\cdots(CH_3)_2NH\cdots CH_3CHO$ with respect to $H_2SO_4\cdots(CH_3)_2NH$ and CH_3CHO and k_u is the unimolecular reaction rate constant of the reaction R5. K_{eq2} and k_u are calculated by using the formulas in equations (6) and (7.)

$$K_{eq2} = \sigma\frac{Q_{H_2SO_4\cdots(CH_3)_2NH\cdots CH_3CHO}}{Q_{H_2SO_4\cdots(CH_3)_2NH}Q_{CH_3CHO}}exp(\frac{E_{H_2SO_4\cdots(CH_3)_2NH\cdots CH_3CHO} - E_{H_2SO_4\cdots(CH_3)_2N}}{RT}) \quad (6)$$

$$k_u = \kappa \frac{k_B T\, Q_{TS}}{h Q_{H_2SO_4\cdots(CH_3)_2NH\cdots CH_3CHO}} exp(-\frac{E_{TS} - E_{H_2SO_4\cdots(CH_3)_2NH\cdots CH_3CHO}}{RT}) \quad (7)$$

In the equations (5)-(7), σ is the reaction symmetry number, κ is the tunneling coefficient obtained by Eckart correction, $Q_{H_2SO_4\cdots(CH_3)_2NH\cdots CH_3CHO}$, $Q_{H_2SO_4\cdots(CH_3)_2NH}$, $Q_{H_2SO_4}$, Q_{CH_3CHO}, $Q_{(CH_3)_2NH}$, and Q_{TS} are the partition functions of $H_2SO_4\cdots(CH_3)_2NH\cdots CH_3CHO$, $H_2SO_4\cdots(CH_3)_2NH$, H_2SO_4, CH_3CHO, $(CH_3)_2NH$, and the transition states . The $E_{H_2SO_4\cdots(CH_3)_2NH\cdots CH_3CHO}$, $E_{H_2SO_4\cdots(CH_3)_2NH}$, E_{CH_3CHO} $E_{H_2SO_4}$, $E_{(CH_3)_2NH}$, and E_{TS} are the total energies with zero-point vibrational energies of $H_2SO_4\cdots(CH_3)_2NH\cdots CH_3CHO$, $H_2SO_4\cdots(CH_3)_2NH$, CH_3CHO, H_2SO_4, $(CH_3)_2NH$, and the transition states calculated by CCSD(T)-F12a/jun-cc-pV(T+d)Z//M06-2X/MG3S. k_B and h are the Boltzmann and Planck constants, respectively.

Thus, the total rate of the $CH_3CHO + H_2SO_4 + (CH_3)_2NH$ reaction can be written as the eq7.

$$v_1 = \frac{d[CH_3HC(OH)OSO_3H]}{dt} = K_{eq1}k_1[CH_3CHO][H_2SO_4][(CH_3)_2NH] \quad (7)$$

Besides, the following rate ratios can be expressed as equations (8)-(10).

$$\frac{v_1}{v_2} = \frac{K_{eq1}k_1[CH_3CHO][H_2SO_4][(CH_3)_2NH]}{k_2[CH_3CHO][H_2SO_4]} = \frac{K_{eq1}k_1[(CH_3)_2NH]}{k_2} \quad (8)$$

$$\frac{v_1}{v_{CH_3CHO+OH}} = \frac{K_{eq1}k_1[CH_3CHO][H_2SO_4][(CH_3)_2NH]}{k_{CH_3CHO+OH}[CH_3CHO][OH]} = \frac{K_{eq1}k_1[H_2SO_4][(CH_3)_2NH]}{k_{CH_3CHO+OH}[OH]} \quad (9)$$

$$\frac{v_1}{v_{H_2SO_4+OH}} = \frac{K_{eq1}k_1[CH_3CHO][H_2SO_4][(CH_3)_2NH]}{k_{H_2SO_4+OH}[H_2SO_4][OH]} = \frac{K_{eq1}k_1[CH_3CHO][(CH_3)_2NH]}{k_{H_2SO_4+OH}[OH]} \quad (10)$$

Table S1. T1 diagnostic values for all the species at the CCSD(T)-F12a/jun-cc-pV(T+d)Z //M06-2X/MG3S level.

species	CH_3CHO	H_2SO_4	$(CH_3)_2NH$	C1A	TS1A	C1B
T_1	0.014	0.015	0.009	0.014	0.014	0.014
species	TS1B	C1C	TS1C	C1D	TS1D	C1E
T_1	0.014	0.014	0.014	0.014	0.014	0.014
species	TS1E	C1F	TS1F	CP1	P1	
T_1	0.014	0.014	0.014	0.013	0.014	

Table S2. The calculated binding energies of the $H_2SO_4\cdots(CH_3)_2NH$, $H_2SO_4\cdots CH_3CHO$ and $CH_3CHO\cdots(CH_3)_2NH$ complexes at the CCSD(T)-F12a/jun-cc-pV(T+d)Z//M06-2X/MG3S level. (kcal /mol)

Method	△E		
	$H_2SO_4\cdots(CH_3)_2NH$ (M1A)	$H_2SO_4\cdots CH_3CHO$	$CH_3CHO\cdots(CH_3)_2NH$
CCSD(T)-F12a/jun-cc-pV(T+d)Z //M06-2X/MG3S	-22.18	-11.91	-3.43

Table S3. The calculated equilibrium constants (K_{eq}, cm^3 $molecules^{-1}$) and the concentrations of the dimer complexes when the $[(CH_3)_2NH] = 3.2 \times 10^9$, $[H_2SO_4] = 4 \times 10^8$, $[CH_3CHO] = 1.12 \times 10^{12}$ molecule cm^{-3} for the $H_2SO_4 + (CH_3)_2NH + CH_3CHO$ in the temperature range of 200 - 298 K.

T(K)	K_{eq1}[a]	K_{eq2}[b]	K_{eq3}[c]	$[H_2SO_4\cdots(CH_3)_2NH]$[d]	$[H_2SO_4\cdots CH_3CHO]$[e]	$[CH_3CHO\cdots(CH_3)_2NH]$[f]
200	2.33×10^{-3}	1.64×10^{-14}	5.83×10^{-23}	2.98×10^{15}	7.34×10^{6}	2.09×10^{-1}
220	1.56×10^{-5}	1.14×10^{-15}	3.06×10^{-23}	1.99×10^{13}	5.12×10^{5}	1.10×10^{-1}
240	2.43×10^{-7}	1.26×10^{-16}	1.82×10^{-23}	3.11×10^{11}	5.65×10^{4}	6.53×10^{-2}
260	7.27×10^{-9}	1.98×10^{-17}	1.20×10^{-23}	9.31×10^{9}	8.85×10^{3}	4.29×10^{-2}
280	3.63×10^{-10}	4.08×10^{-18}	8.47×10^{-24}	4.64×10^{8}	1.83×10^{3}	3.04×10^{-2}
298	3.47×10^{-11}	1.19×10^{-18}	6.54×10^{-24}	4.44×10^{7}	5.34×10^{2}	2.34×10^{-2}
320	2.84×10^{-12}	3.23×10^{-19}	5.02×10^{-24}	3.63×10^{6}	1.44×10^{2}	1.80×10^{-2}
340	3.88×10^{-13}	1.15×10^{-19}	4.11×10^{-24}	4.97×10^{5}	5.14×10^{1}	1.47×10^{-2}

[a]The equilibrium constants of the $H_2SO_4\cdots(CH_3)_2NH$ complex with respect to H_2SO_4 and $(CH_3)_2NH$.

[b]The equilibrium constants of the $H_2SO_4\cdots CH_3CHO$ complex with respect to H_2SO_4 and CH_3CHO.

[c]The equilibrium constants of the $CH_3CHO\cdots(CH_3)_2NH$ complex with respect to CH_3CHO

and $(CH_3)_2NH$.
[d]$[H_2SO_4\cdots(CH_3)_2NH] = K_{eq1}[H_2SO_4][(CH_3)_2NH]$.
[e]$[H_2SO_4\cdots CH_3CHO] = K_{eq2}[H_2SO_4][CH_3CHO]$.
[f]$[CH_3CHO\cdots(CH_3)_2NH] = K_{eq3}[CH_3CHO][(CH_3)_2NH]$.

Table S4. The calculated bimolecular rate constants k_2 cm^3 $molecules^{-1}$ s^{-1} for the individual reaction pathways over the temperature range 200 - 298 K.

	200 K	220 K	240 K	260 K	280 K	298 K
k_2[a]	3.88×10^{-16}	4.23×10^{-16}	4.61×10^{-16}	4.99×10^{-16}	5.39×10^{-16}	5.77×10^{-16}

[a]k_2 is the he bimolecular rate constants of the $H_2SO_4 + CH_3CHO$ reaction.

Table S5. The rate ratio of each reaction path when the $[(CH_3)_2NH] = 3.2 \times 10^9$, $[H_2SO_4] = 4 \times 10^8$, $[CH_3CHO] = 1.12 \times 10^{12}$ molecule cm^{-3} of each reaction channel in the temperature range of 200 - 298 K.[a]

Reaction	200 K	220 K	240 K	260 K	280 K	298 K
v_1/v_2	2.98×10^6	2.00×10^4	3.21×10^2	9.95×10^0	5.17×10^{-1}	5.15×10^{-2}

[a] $\frac{v_1}{v_2} = \frac{K_{eq1}k_1[CH_3CHO][H_2SO_4][(CH_3)_2NH]}{k_2[CH_3CHO][H_2SO_4]} = \frac{K_{eq1}k_1[(CH_3)_2NH]}{k_2}$

Table S6. The rate ratio of the $v_1/v_{CH_3CHO+OH}$ in the temperature range of 200 - 298 K ([$(CH_3)_2NH$] = 3.2 × 10^9, [H_2SO_4] = 1.0 × 10^6 molecule cm^{-3}).

Reaction	200 K	220 K	240 K	260 K	280 K	298 K
$CH_3CHO + H_2SO_4 + (CH_3)_2NH \rightarrow CH_3HC(OH)OSO_3H + (CH_3)_2NH$						
$CH_3CHO + OH \rightarrow CH_3CO + H_2O$ [OH]=1 × 10^6 molecule cm^{-3}						
$v_1/v_{CH_3CHO+OH}$	4.23 × 10^1	3.67 × 10^{-1}	7.34 × 10^{-3}	2.77 × 10^{-4}	1.72 × 10^{-5}	1.98 × 10^{-6}
$CH_3CHO + OH \rightarrow CH_3CO + H_2O$ [OH]=1 × 10^5 molecule cm^{-3}						
$v_1/v_{CH_3CHO+OH}$	4.23 × 10^2	3.67 × 10^0	7.34 × 10^{-2}	2.77 × 10^{-3}	1.72 × 10^{-4}	1.98 × 10^{-5}
$CH_3CHO + OH \rightarrow CH_3CO + H_2O$ [OH]=1 × 10^4 molecule cm^{-3}						
$v_1/v_{CH_3CHO+OH}$	4.23 × 10^3	3.67 × 10^1	7.34 × 10^{-1}	2.77 × 10^{-2}	1.72 × 10^{-3}	1.98× 10^{-4}
$CH_3CHO + OH \rightarrow CH_3CO + H_2O$ [OH]=1 × 10^3 molecule cm^{-3}						

$v_1/v_{CH_3CHO+OH}$	4.23 × 10^4	3.67 × 10^2	7.34 × 10^0	2.77 × 10^{-1}	1.72 × 10^{-2}	1.98 × 10^{-3}

Table S7. The rate ratio of the $v_1/v_{CH_3CHO+OH}$ in the temperature range of 200 - 298 K ([$(CH_3)_2NH$] = 3.2 × 10^9, [H_2SO_4] = 1.0 × 10^7 molecule cm^{-3}).

Reaction	200 K	220 K	240 K	260 K	280 K	298 K
$CH_3CHO + H_2SO_4 + (CH_3)_2NH \rightarrow CH_3HC(OH)OSO_3H + (CH_3)_2NH$						
$CH_3CHO + OH \rightarrow CH_3CO + H_2O$ [OH]=1 × 10^6 molecule cm^{-3}						
$v_1/v_{CH_3CHO+OH}$	4.23 × 10^2	3.67 × 10^0	7.34 × 10^{-2}	2.77 × 10^{-3}	1.72 × 10^{-4}	1.98 × 10^{-5}
$CH_3CHO + OH \rightarrow CH_3CO + H_2O$ [OH]=1 × 10^5 molecule cm^{-3}						
$v_1/v_{CH_3CHO+OH}$	4.23 × 10^3	3.67 × 10^1	7.34 × 10^{-1}	2.77 × 10^{-2}	1.72 × 10^{-3}	1.98 × 10^{-4}
$CH_3CHO + OH \rightarrow CH_3CO + H_2O$ [OH]=1 × 10^4 molecule cm^{-3}						
$v_1/v_{CH_3CHO+OH}$	4.23 × 10^4	3.67 × 10^2	7.34 × 10^0	2.77 × 10^{-1}	1.72 × 10^{-2}	1.98 × 10^{-3}
$CH_3CHO + OH \rightarrow CH_3CO + H_2O$ [OH]=1 × 10^3 molecule cm^{-3}						

$v_1/v_{CH_3CHO+OH}$	4.23 × 10^5	3.67 × 10^3	7.34 × 10^1	2.77 × 10^0	1.72 × 10^{-1}	1.98 × 10^{-2}

Table S8. The rate ratio of the $v_1/v_{CH_3CHO+OH}$ in the temperature range of 200 - 298 K ([$(CH_3)_2NH$] = 3.2 × 10^9, [H_2SO_4] = 4.0 × 10^8 molecule cm^{-3}).

Reaction	200 K	220 K	240 K	260 K	280 K	298 K
$CH_3CHO + H_2SO_4 + (CH_3)_2NH \rightarrow CH_3HC(OH)OSO_3H + (CH_3)_2NH$						
$CH_3CHO + OH \rightarrow CH_3CO + H_2O$ [OH]=1 × 10^6 molecule cm^{-3}						
$v_1/v_{CH_3CHO+OH}$	1.69 × 10^4	1.47 × 10^2	2.94 × 10^0	1.11 × 10^{-1}	6.89 × 10^{-3}	7.93 × 10^{-4}
$CH_3CHO + OH \rightarrow CH_3CO + H_2O$ [OH]=1 × 10^5 molecule cm^{-3}						
$v_1/v_{CH_3CHO+OH}$	1.69 × 10^5	1.47 × 10^3	2.94 × 10^1	1.11 × 10^0	6.89 × 10^{-2}	7.93 × 10^{-3}
$CH_3CHO + OH \rightarrow CH_3CO + H_2O$ [OH]=1 × 10^4 molecule cm^{-3}						
$v_1/v_{CH_3CHO+OH}$	1.69 × 10^6	1.47 × 10^4	2.94 × 10^2	1.11 × 10^1	6.89 × 10^{-1}	7.93× 10^{-2}
$CH_3CHO + OH \rightarrow CH_3CO + H_2O$ [OH]=1 × 10^3 molecule cm^{-3}						

$v_1/v_{CH_3CHO+OH}$	1.69 × 10^7	1.47 × 10^5	2.94 × 10^3	1.11 × 10^2	6.89 × 10^0	7.93 × 10^{-1}

Table S9. The rate ratio of the $v_1/v_{CH_3CHO+OH}$ in the temperature range of 200 - 298 K ([$(CH_3)_2NH$] = 3.2 × 10^9, [H_2SO_4] = 5.1 × 10^9 molecule cm^{-3}).

Reaction	200 K	220 K	240 K	260 K	280 K	298 K
$CH_3CHO + H_2SO_4 + (CH_3)_2NH \rightarrow CH_3HC(OH)OSO_3H + (CH_3)_2NH$						
$CH_3CHO + OH \rightarrow CH_3CO + H_2O$ [OH]=1 × 10^6 molecule cm^{-3}						
$v_1/v_{CH_3CHO+OH}$	2.16 × 10^5	1.87 × 10^3	3.74 × 10^1	1.41 × 10^0	8.78 × 10^{-2}	1.01 × 10^{-2}
$CH_3CHO + OH \rightarrow CH_3CO + H_2O$ [OH]=1 × 10^5 molecule cm^{-3}						
$v_1/v_{CH_3CHO+OH}$	2.16 × 10^6	1.87 × 10^4	3.74 × 10^2	1.41 × 10^1	8.78 × 10^{-1}	1.01 × 10^{-1}
$CH_3CHO + OH \rightarrow CH_3CO + H_2O$ [OH]=1 × 10^4 molecule cm^{-3}						
$v_1/v_{CH_3CHO+OH}$	2.16 × 10^7	1.87 × 10^5	3.74 × 10^3	1.41 × 10^2	8.78 × 10^0	1.01× 10^0
$CH_3CHO + OH \rightarrow CH_3CO + H_2O$ [OH]=1 × 10^3 molecule cm^{-3}						

$v_1/v_{CH_3CHO+OH}$	2.16 × 10^8	1.87 × 10^6	3.74 × 10^4	1.41 × 10^3	8.78× 10^1	1.01 × 10^1

Table S10. The rate ratio of the $v_1/v_{H_2SO_4+OH}$ in the temperature range of 200 - 298 K ([$(CH_3)_2NH$] = 3.2 × 10^9, [CH_3CHO] = 1.12 × 10^{12} molecule cm^{-3}).

Reaction	200 K	220 K	240 K	260 K	280 K	298 K
$CH_3CHO + H_2SO_4 + (CH_3)_2NH \rightarrow CH_3HC(OH)OSO_3H + (CH_3)_2NH$						
$H_2SO_4 + OH \rightarrow HSO_4 + H_2O$ [OH]=1 × 10^6 molecule cm^{-3}						
$v_1/v_{H_2SO_4+OH}$	1.10 × 10^{12}	8.07 × 10^9	1.41 × 10^8	4.73 × 10^6	2.66 × 10^5	2.83 × 10^4
$H_2SO_4 + OH \rightarrow HSO_4 + H_2O$ [OH]=1 × 10^5 molecule cm^{-3}						
$v_1/v_{H_2SO_4+OH}$	1.10 × 10^{13}	8.07 × 10^{10}	1.41 × 10^9	4.73 × 10^7	2.66 × 10^6	2.83 × 10^5
$H_2SO_4 + OH \rightarrow HSO_4 + H_2O$ [OH]=1 × 10^4 molecule cm^{-3}						
$v_1/v_{H_2SO_4+OH}$	1.10 × 10^{14}	8.07 × 10^{11}	1.41 × 10^{10}	4.73 × 10^8	2.66 × 10^7	2.83 × 10^6
$H_2SO_4 + OH \rightarrow HSO_4 + H_2O$ [OH]=1 × 10^3 molecule cm^{-3}						

$v_1/v_{H_2SO_4+OH}$	1.10 × 10^{15}	8.07 × 10^{12}	1.41 × 10^{11}	4.73 × 10^{9}	2.66 × 10^{8}	2.83 × 10^{7}

Table S11. The atmospheric lifetime of H_2SO_4 calculated for the reaction of CH_3CHO and H_2SO_4 catalyzed by $(CH_3)_2NH$ at the $(CH_3)_2NH$ concentration of 3.2 × 10^9 molecules cm^{-3}, the CH_3CHO concentration of 2.46 × 10^9 molecules cm^{-3} and the temperature range of 200 - 298 K.

T(K)	k_3 (cm^6 $molecule^{-2}$ s^{-1})	τ^a (s)
200	3.60 × 10^{-19}	3.52 × 10^{-1}
220	2.65 × 10^{-21}	4.79 × 10^{1}
240	4.62 × 10^{-23}	2.75 × 10^{3}
260	1.55 × 10^{-24}	8.18 × 10^{4}
280	8.72 × 10^{-26}	1.46 × 10^{6}
298	9.27 × 10^{-27}	1.37 × 10^{7}

$^a\tau = \frac{1}{k_3[CH_3CHO][(CH_3)_2NH]}$, $k_3 = K_{eq1}k_1$.

Table S12. The atmospheric lifetime of H_2SO_4 calculated for the reaction of CH_3CHO and H_2SO_4 catalyzed by $(CH_3)_2NH$ at the $(CH_3)_2NH$ concentration of 3.2×10^9 molecules cm^{-3}, the CH_3CHO concentration of 1.12×10^{12} molecules cm^{-3} and the temperature range of 200 - 298 K.

T(K)	k_3 (cm^6 $molecule^{-2}$ s^{-1})	τ^a (s)
200	3.60×10^{-19}	7.74×10^{-4}
220	2.65×10^{-21}	1.05×10^{-1}
240	4.62×10^{-23}	6.04×10^{0}
260	1.55×10^{-24}	1.80×10^{2}
280	8.72×10^{-26}	3.20×10^{3}
298	9.27×10^{-27}	3.01×10^{4}

[a] $\tau = \frac{1}{k_3[CH_3CHO][(CH_3)_2NH]}$, $k_3 = K_{eq1}k_1$.

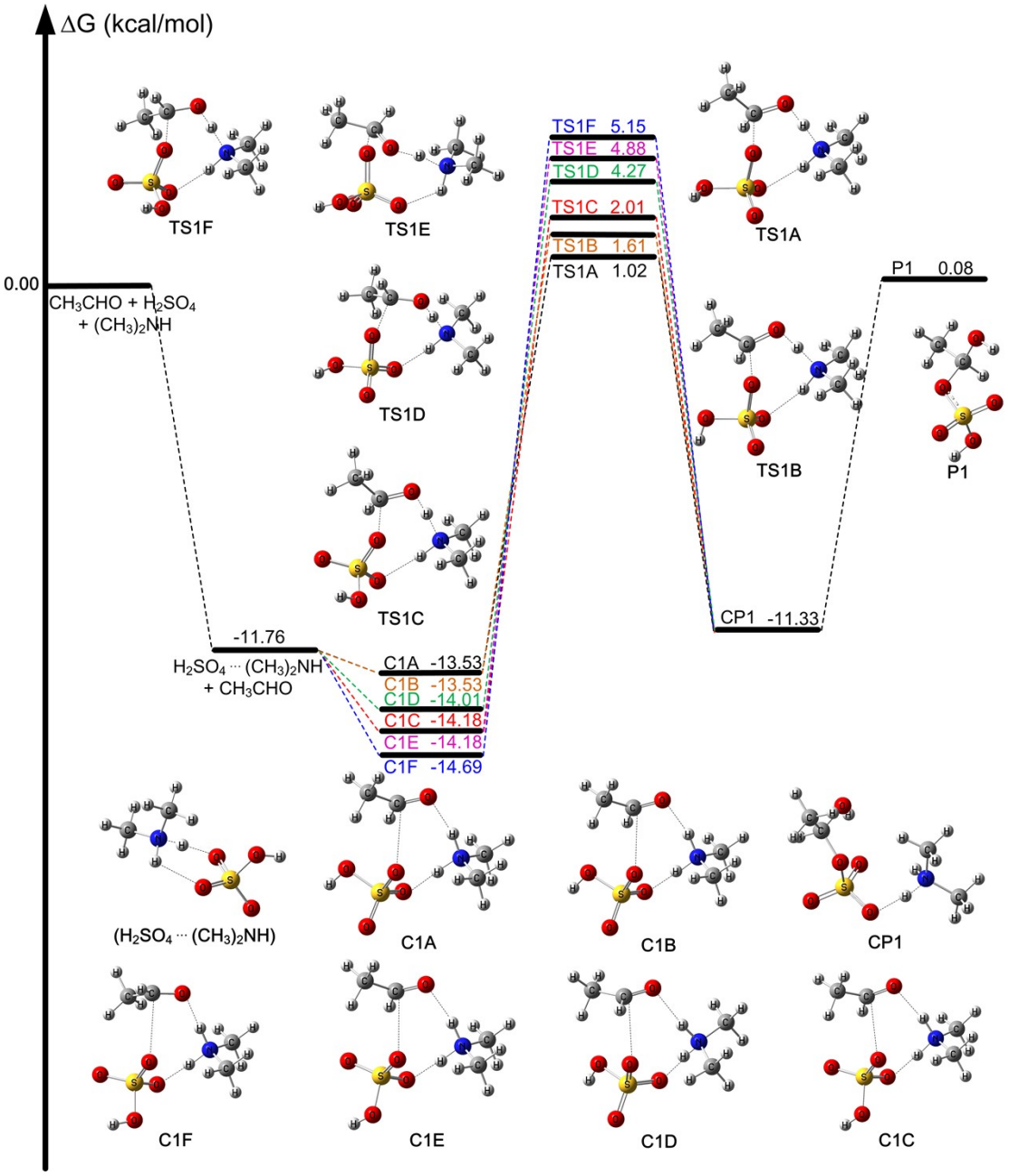

Figure S1. The free energy potential profile for the CH_3CHO + H_2SO_4 + $(CH_3)_2NH$ reaction at 1 atmospheric pressure at the CCSD(T)-F12a/jun-cc-pV(T+d)Z//M06-2X/MG3S level (kcal/mol) .

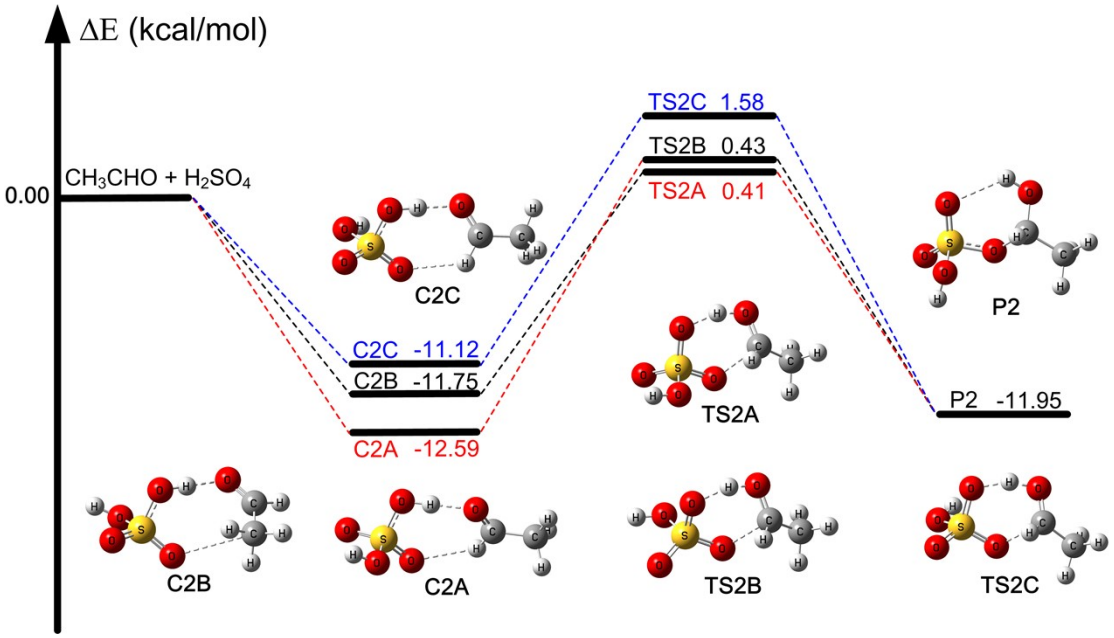

Figure S2. Calculated relative energies with zero-point vibrational correction for the CH_3CHO + H_2SO_4 reaction at the CCSD(T)-F12a/cc-pVTZ-F12//M06-2X/MG3S level. (kcal /mol)

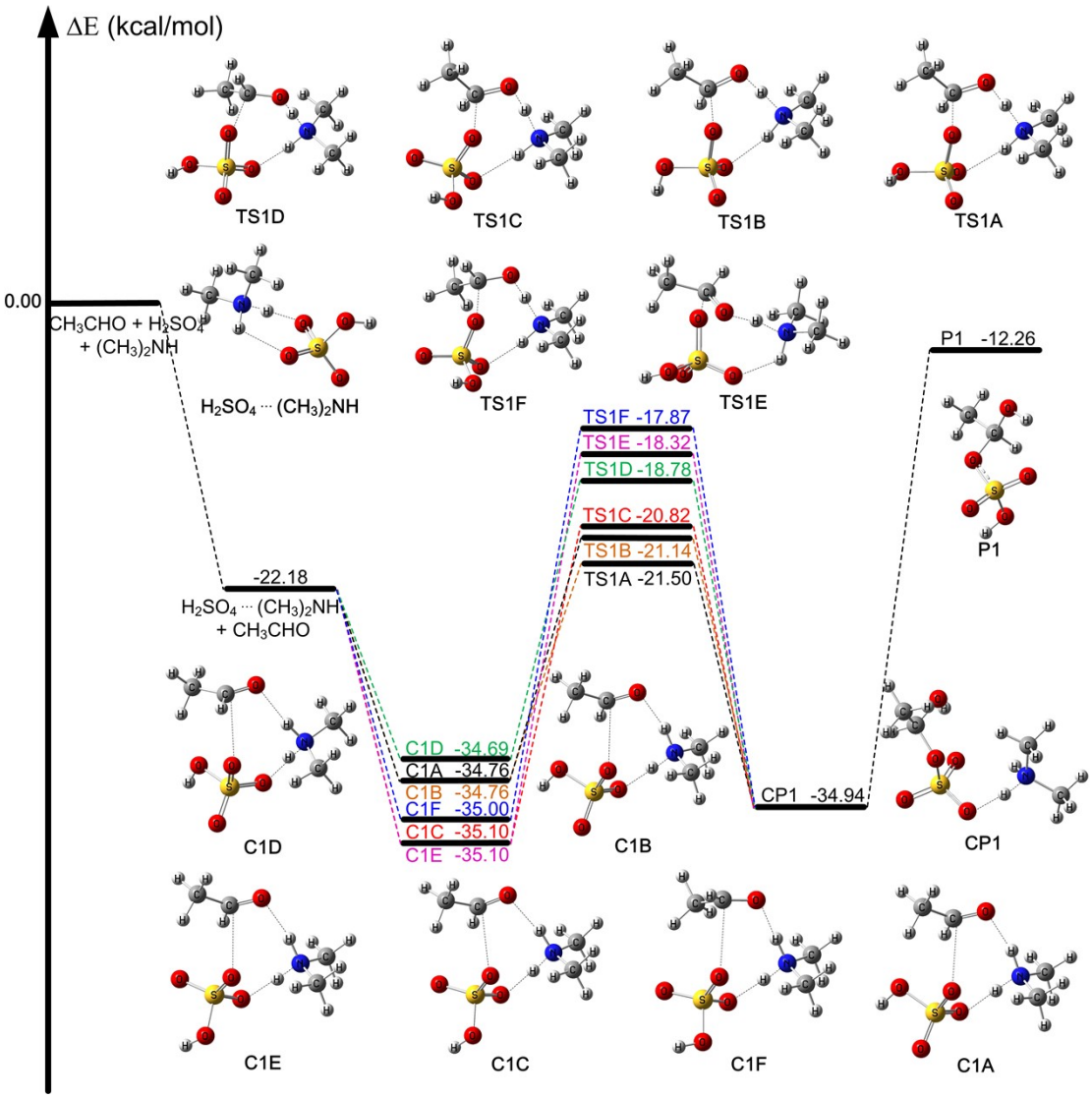

Figure S3. Calculated relative energies with zero-point vibrational correction for the $CH_3CHO + H_2SO_4 + (CH_3)_2NH$ reaction at the CCSD(T)-F12a/jun-cc-pV(T+d)Z//M06-2X/MG3S level. (kcal /mol)

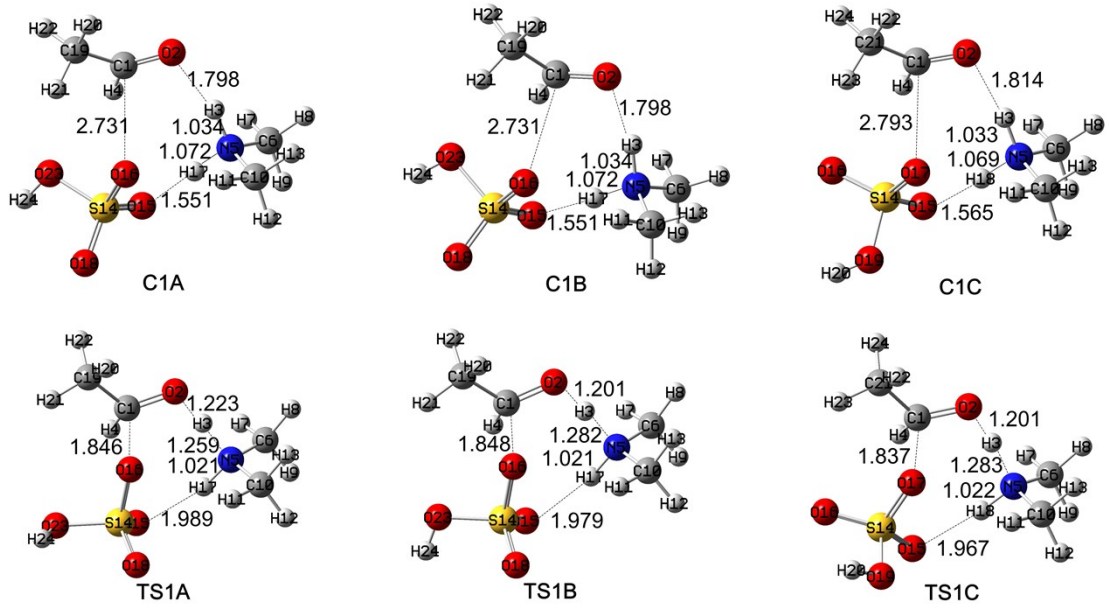

Figure S4. Selected geometrical parameters of the optimized transition states and complexes at the M06-2X/MG3S level of theory.

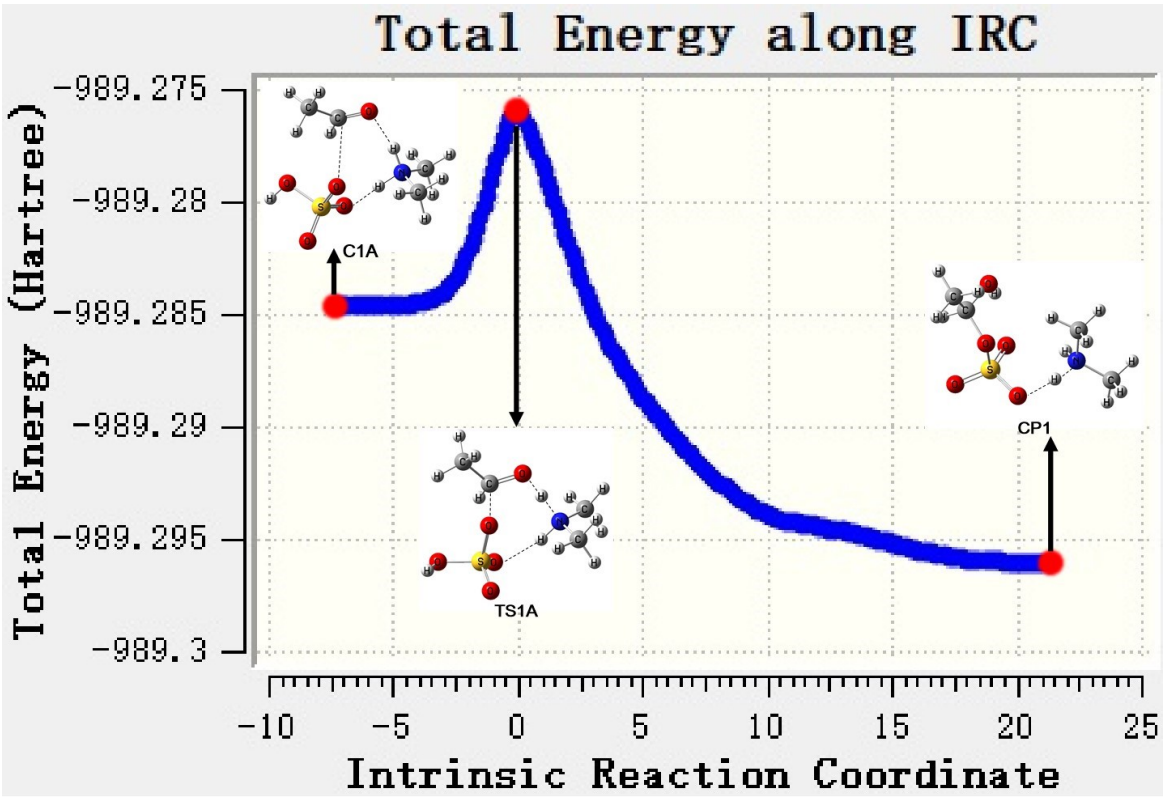

Figure S5. Intrinsic reaction coordinate results of TS1A.

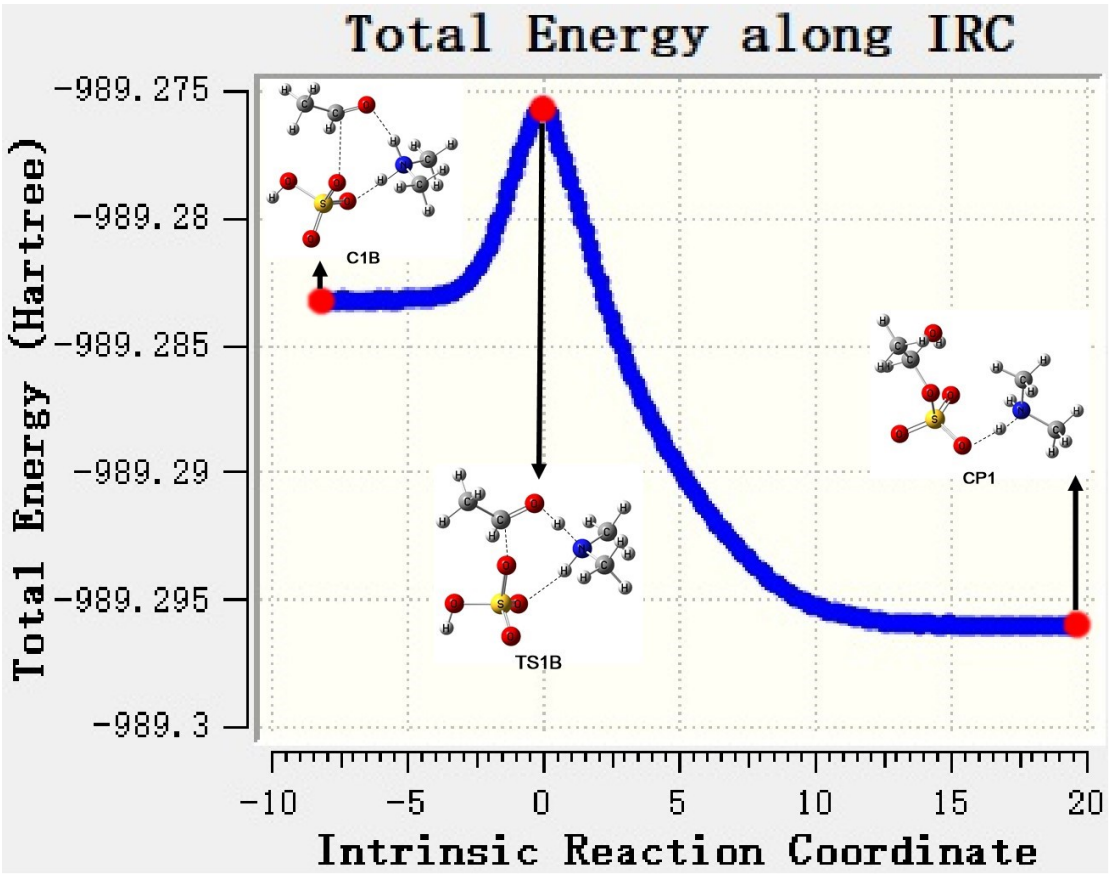

Figure S6. Intrinsic reaction coordinate results of TS1B.

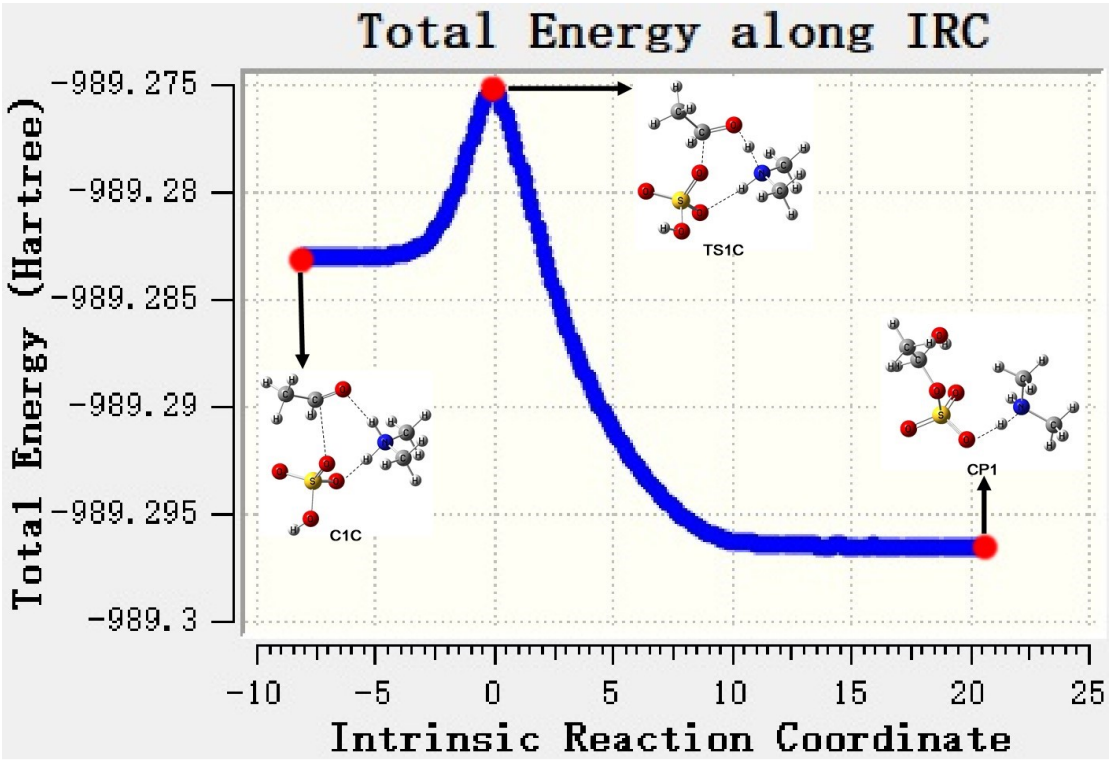

Figure S7. Intrinsic reaction coordinate result of TS1C.

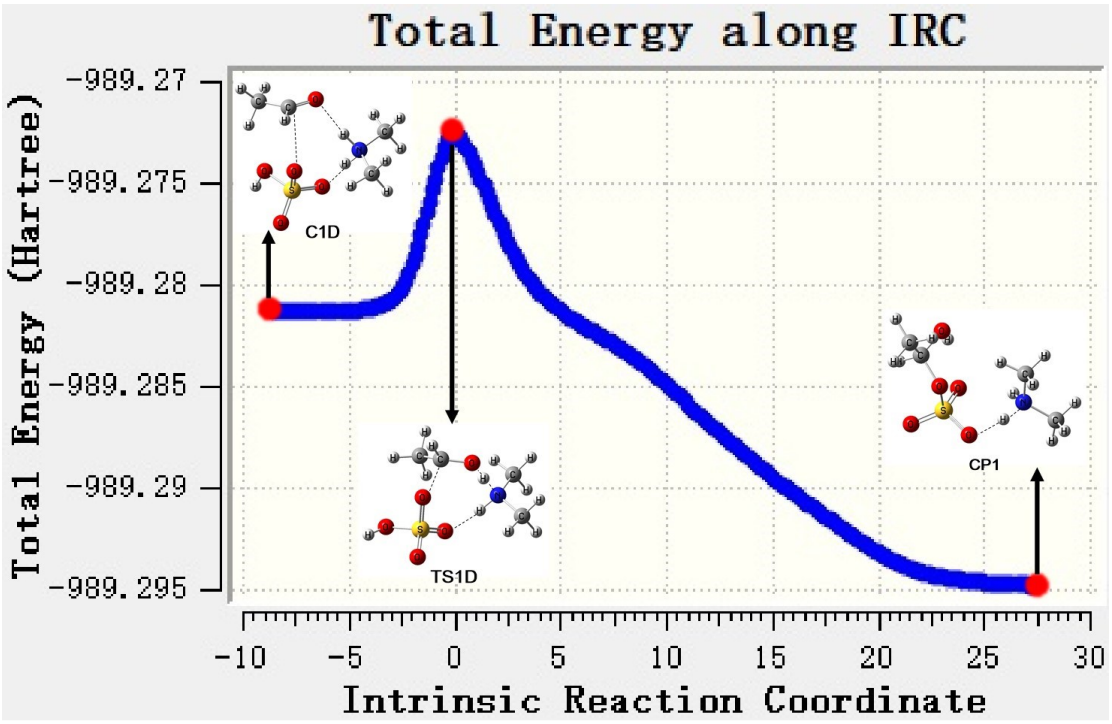

Figure S8. Intrinsic reaction coordinate result of TS1D.

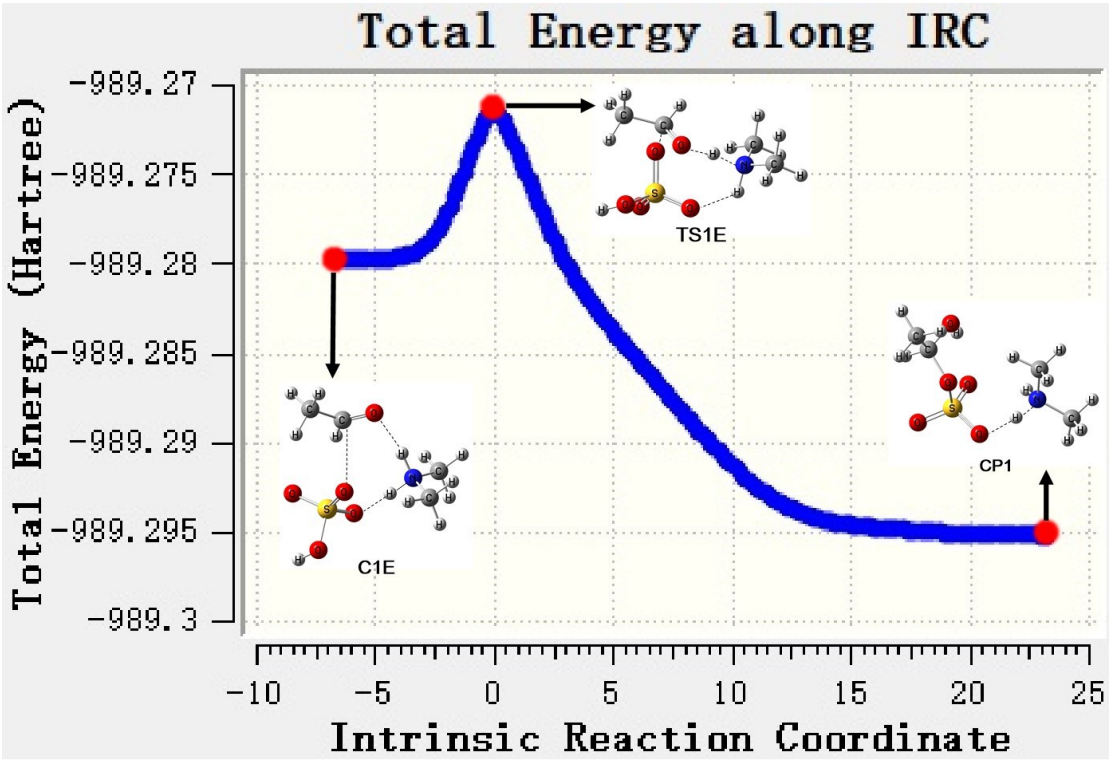

Figure S9. Intrinsic reaction coordinate result of TS1E.

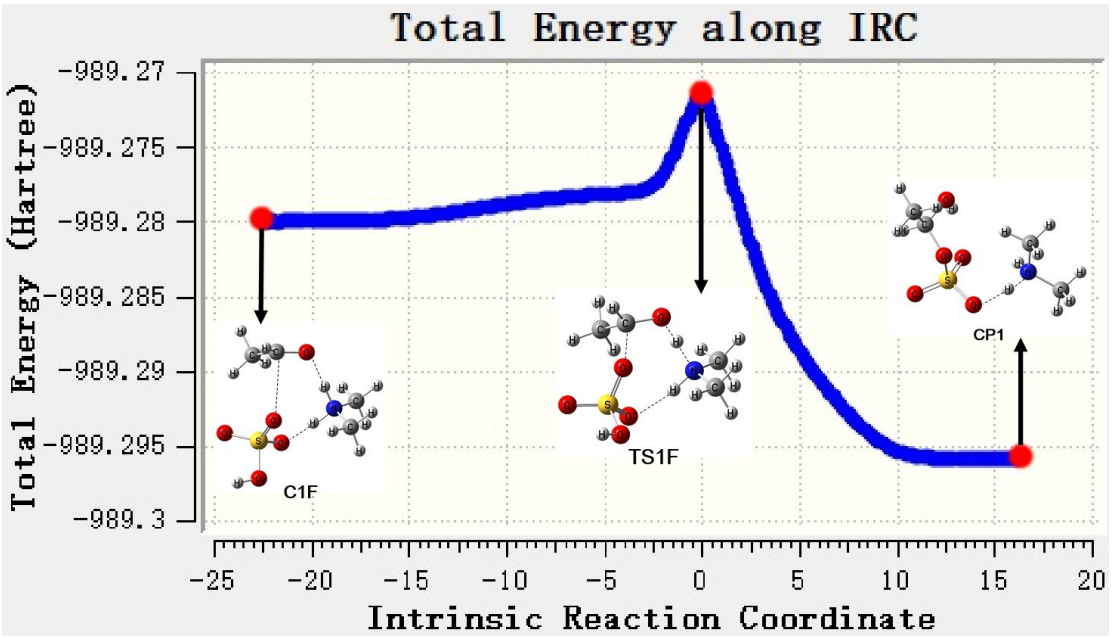

Figure S10. Intrinsic reaction coordinate result of TS1F.

Table S13. Molecular coordinates and frequency information.

Species	Coordinate M06-2X/MG3S	Frequencies cm^{-1}
CH_3CHO	0 1 C 1.162693 -0.147293 0.000002 H 1.696008 0.223717 0.876878 H 1.695975 0.223681 -0.876913 H 1.148366 -1.233453 0.000016 C -0.234181 0.398094 0.000004 H -0.316141 1.502330 -0.000008 O -1.224410 -0.277635 0.000000	162.39 514.01 776.21 900.22 1138.03 1144.93 1383.51 1431.76 1468.44 1476.87 1870.55 2942.70 3064.20 3127.03 3180.27
H_2SO_4	0 1 S 0.000000 0.000000 -0.154206 O 0.640138 1.069468 -0.819825 O -0.640138 -1.069465 -0.819830 O -1.029703 0.662496 0.836377 H -1.692984 0.011484 1.101263 O 1.029702 -0.662499 0.836375 H 1.692986 -0.011490 1.101261	261.79 340.84 384.43 446.59 509.63 560.23 571.28 876.01 923.29 1156.80 1177.34 1263.05 1508.99 3831.24 3835.90
$(CH_3)_2NH$	0 1 N 0.026533 0.585047 0.000000 H -0.770809 1.206498 0.000000 C 0.026533 -0.223084 -1.205668 H -0.028182 0.418519 -2.083382 H 0.960967 -0.783611 -1.258995 H -0.799442 -0.947316 -1.248017 C 0.026533 -0.223084 1.205668 H 0.960967 -0.783611 1.258995 H -0.028182 0.418519 2.083382 H -0.799442 -0.947316 1.248017	221.71 270.49 390.73 770.54 963.20 1038.76 1108.10 1192.51 1200.97 1271.47 1444.61 1473.18 1479.59 1494.19 1505.27 1521.60 1524.37 2983.19 2983.83 3086.51 3088.44 3137.56 3137.73 3575.49
C1A	0 1 C 0.116118 2.212395 -0.307388 O 1.265532 2.258130 0.075369 H 1.900915 0.578377 -0.018875 H -0.172770 1.504621 -1.101508 N 2.023749 -0.447535 -0.059449 C 3.095693 -0.799434 -1.007017 H 2.857406 -0.383981 -1.981928 H 4.043416 -0.398662 -0.655290 H 3.158039 -1.882278 -1.079605 C 2.237860 -0.969659 1.306791 H 1.399551 -0.654573 1.920180 H 2.274247 -2.055447 1.260397 H 3.175680 -0.582854 1.698905 S -1.304463 -0.909386 0.042232 O -0.278527 -1.374911 -0.906206 O -0.723448 -0.019985 1.023071 H 1.090883 -0.829627 -0.424304 O -2.169736 -1.944760 0.511327	31.17 44.96 61.91 77.59 99.47 101.96 114.98 123.15 130.59 147.54 180.01 188.09 193.70 229.05 264.57 321.32 400.11 408.92 448.10 527.27 583.75 592.52 596.43 814.49 825.96 916.51 940.46 964.47 1058.69 1073.48 1080.18 1148.96 1153.76 1160.11 1162.45 1220.65 1262.20 1293.27

	C -0.980653 3.063430 0.224504 H -0.609104 3.751331 0.978328 H -1.730706 2.391705 0.646078 H -1.454517 3.604360 -0.595957 O -2.233587 0.086455 -0.824099 H -2.923859 -0.439891 -1.243018	1379.20 1385.63 1444.77 1447.58 1463.52 1471.30 1472.90 1477.34 1495.55 1512.67 1517.50 1522.71 1590.55 1703.72 1816.12 2548.24 3010.18 3067.21 3088.56 3090.44 3133.62 3170.52 3173.65 3182.84 3183.79 3194.92 3211.02 3864.86
TS1A	0 1 C -0.034886 1.775263 -0.179658 O 1.140293 1.766095 0.297385 H 1.713967 0.725874 0.007072 H -0.192632 1.322113 -1.162485 N 2.201401 -0.418996 -0.185616 C 3.546557 -0.361000 -0.763828 H 3.507757 0.148305 -1.723485 H 4.195526 0.199630 -0.093556 H 3.958584 -1.361197 -0.901335 C 2.150472 -1.122965 1.105636 H 1.121078 -1.146022 1.455721 H 2.528238 -2.140736 1.008624 H 2.757907 -0.577487 1.825517 S -1.342746 -0.799281 -0.036403 O -0.416039 -1.102941 -1.093792 O -0.928628 0.426502 0.709104 H 1.539861 -0.869118 -0.819434 O -1.706366 -1.843197 0.864898 C -0.935454 2.910676 0.182272 H -0.889745 3.082302 1.254734 H -1.957638 2.709071 -0.125348 H -0.572171 3.801256 -0.333077 O -2.661788 -0.362047 -0.821250 H -3.416505 -0.459664 -0.228474	-571.11 22.01 52.10 64.69 77.36 111.32 122.27 147.72 179.12 188.97 207.87 219.15 247.76 271.44 326.23 399.00 421.52 444.53 488.24 531.17 578.97 598.63 633.23 667.30 858.90 923.38 954.63 997.91 1023.22 1044.62 1052.96 1090.56 1154.83 1162.48 1164.87 1201.82 1266.40 1273.69 1287.78 1384.76 1397.89 1406.35 1451.22 1467.15 1471.79 1486.06 1491.33 1497.89 1512.33 1516.44 1520.49 1575.52 1623.36 1744.26 3069.14 3071.64 3076.26 3080.29 3141.96 3147.34 3154.47 3166.29 3172.57 3186.53 3459.54 3854.79
C1B	0 1 C 0.116042 2.212385 -0.307420 O 1.265461 2.258125 0.075320 H 1.900877 0.578398 -0.018952 H -0.172850 1.504624 -1.101550	31.17 44.96 61.91 77.58 99.47 101.96 114.98 123.15 130.59 147.54

	N 2.023769 -0.447511 -0.059460 C 3.095732 -0.799409 -1.007006 H 2.857405 -0.384057 -1.981951 H 4.043426 -0.398536 -0.655319 H 3.158160 -1.882255 -1.079503 C 2.237916 -0.969518 1.306819 H 1.399586 -0.654442 1.920185 H 2.274380 -2.055308 1.260508 H 3.175711 -0.582618 1.698902 S -1.304443 -0.909410 0.042235 O -0.278515 -1.374908 -0.906223 O -0.723433 -0.019992 1.023062 H 1.090924 -0.829672 -0.424289 O -2.169679 -1.944807 0.511351 C -0.980728 3.063395 0.224514 H -0.609171 3.751283 0.978345 H -1.730764 2.391651 0.646090 H -1.454617 3.604338 -0.595924 O -2.233613 0.086404 -0.824078 H -2.923885 -0.439960 -1.242974	180.01 188.09 193.70 229.05 264.57 321.32 400.11 408.92 448.10 527.27 583.75 592.52 596.43 814.49 825.95 916.51 940.46 964.47 1058.69 1073.48 1080.18 1148.96 1153.76 1160.11 1162.45 1220.65 1262.20 1293.27 1379.20 1385.63 1444.77 1447.58 1463.52 1471.30 1472.90 1477.34 1495.55 1512.67 1517.50 1522.71 1590.55 1703.72 1816.12 2548.23 3010.18 3067.21 3088.56 3090.44 3133.62 3170.53 3173.65 3182.84 3183.79 3194.92 3211.03 3864.86
TS1B	0 1 C -0.041972 1.747773 -0.173552 O 1.136571 1.782238 0.296832 H 1.716102 0.768894 0.013116 H -0.189120 1.268748 -1.146080 N 2.209241 -0.398175 -0.181960 C 3.527621 -0.359500 -0.818996 H 3.449262 0.125403 -1.788966 H 4.207281 0.215591 -0.192595 H 3.932614 -1.363869 -0.949444 C 2.213764 -1.072619 1.125157 H 1.200900 -1.078849 1.520980 H 2.580179 -2.095512 1.035850 H 2.856635 -0.516457 1.805259 S -1.355372 -0.806170 -0.007303 O -0.411560 -1.203110 -1.027576 O -0.882814 0.383421 0.746772 H 1.521890 -0.865409 -0.775365 O -1.839222 -1.838928 0.844804 C -0.977631 2.857883 0.170806 H -0.917538 3.065308 1.236130 H -1.996341 2.604530 -0.108402 H -0.659133 3.744352 -0.380401 O -2.600123 -0.169602 -0.785750	-588.74 28.26 55.62 74.07 80.87 107.32 119.92 148.57 175.93 191.05 201.75 215.60 250.17 271.08 325.11 399.54 430.83 446.56 477.92 523.10 578.84 586.80 624.99 695.21 850.57 922.41 957.68 1008.13 1028.21 1052.03 1052.93 1091.95 1153.43 1158.81 1167.90 1210.11 1265.03 1281.57 1294.48 1378.33 1383.98 1408.03 1450.23 1469.24 1471.73 1486.86 1489.99 1497.80

	H -3.034981 -0.860157 -1.300670	1513.50 1516.47 1520.67 1565.38 1621.70 1746.94 3066.48 3069.32 3074.40 3077.93 3138.58 3144.08 3155.41 3164.10 3171.46 3189.08 3453.59 3850.74
C1C	0 1 C -0.060274 2.237836 0.292284 O -1.200191 2.254861 -0.120111 H -1.822827 0.551259 -0.100193 H 0.208764 1.590772 1.144343 N -2.017004 -0.455648 0.027316 C -3.111493 -0.629682 0.998375 H -2.839519 -0.136674 1.927259 H -4.025397 -0.193590 0.602158 H -3.257712 -1.691685 1.178309 C -2.268703 -1.087616 -1.284031 H -1.401230 -0.908260 -1.911296 H -2.406179 -2.155661 -1.133537 H -3.164759 -0.658194 -1.726199 S 1.294591 -0.745577 0.094515 O 0.276612 -1.309603 0.995644 O 2.296539 0.019949 0.782831 O 0.672888 -0.104254 -1.042004 H -1.111267 -0.853232 0.433322 O 2.046067 -2.005879 -0.538065 H 2.764356 -2.255552 0.054103 C 1.055518 3.038212 -0.274767 H 0.715232 3.651171 -1.104124 H 1.823548 2.331400 -0.595709 H 1.496958 3.653916 0.510583	27.37 48.97 52.89 68.36 94.20 106.02 113.51 118.25 127.79 142.74 153.36 186.58 191.20 222.12 256.44 315.00 402.43 408.36 447.19 524.42 584.27 593.59 598.61 815.08 855.88 915.38 942.12 959.86 1057.43 1071.22 1086.46 1148.75 1155.87 1158.61 1166.58 1218.85 1262.80 1293.03 1355.00 1383.54 1439.14 1446.14 1462.48 1467.21 1467.67 1474.99 1495.51 1511.76 1515.71 1522.75 1581.90 1707.21 1816.07 2592.34 2999.76 3065.13 3089.28 3091.37 3130.03 3171.44 3174.68 3184.32 3184.48 3195.97 3234.30 3866.40
TS1C	0 1 C -0.010209 1.747186 0.173552 O -1.183659 1.796034 -0.312447 H -1.745162 0.770055 -0.037693 H 0.109884 1.296441 1.165400 N -2.193841 -0.417725 0.145211 C -3.480072 -0.442659 0.845794 H -3.367397 0.005275 1.830033 H -4.205425 0.136484 0.276965 H -3.850114 -1.462927 0.954724	-616.70 31.11 52.83 71.91 87.76 104.68 116.16 150.60 178.79 193.40 221.76 226.82 251.28 265.06 330.67 398.67 420.95 444.97 478.68 523.44

	C -2.241790 -1.042653 -1.185029 H -1.245376 -1.004204 -1.617980 H -2.577041 -2.077959 -1.117956 H -2.929233 -0.480114 -1.814603 S 1.411974 -0.681180 0.179388 O 0.408690 -1.456280 0.855050 O 2.462182 -0.121135 0.972053 O 0.787754 0.349701 -0.712384 H -1.469542 -0.896934 0.684041 O 2.059443 -1.696217 -0.852760 H 2.908715 -1.343957 -1.145385 C 0.954706 2.834670 -0.160345 H 0.921392 3.033551 -1.228579 H 1.959459 2.558685 0.147675 H 0.644048 3.732463 0.376746	565.91 604.96 624.89 691.93 879.41 919.71 958.20 1019.99 1027.09 1048.59 1052.23 1092.14 1158.11 1162.58 1169.55 1205.84 1265.36 1282.75 1297.87 1369.73 1389.06 1407.22 1447.94 1468.27 1471.93 1485.60 1488.15 1496.80 1514.59 1516.48 1520.19 1560.86 1618.87 1757.46 3049.23 3066.35 3068.50 3075.71 3138.35 3142.53 3153.68 3163.86 3173.42 3187.13 3436.62 3852.22
C1D	0 1 C -0.514656 2.468597 -0.559799 O -1.534265 2.067653 -0.042865 H -1.749280 0.244768 -0.187037 N -1.877216 -0.738215 0.084953 C -2.963486 -0.833546 1.074573 H -2.739246 -0.168175 1.902946 H -3.904036 -0.541258 0.613549 H -3.029180 -1.858806 1.429844 C -2.074458 -1.569130 -1.119121 H -1.217287 -1.421220 -1.769650 H -2.134624 -2.611530 -0.816609 H -2.993047 -1.273543 -1.620800 S 1.409314 -0.769711 -0.029167 O 0.498508 -1.484482 0.877500 O 0.666308 0.090029 -0.927698 H -0.939793 -1.028550 0.515573 O 2.419554 -1.601090 -0.604454 O 2.183523 0.285346 0.908424 H 2.950064 -0.161008 1.285577 C 0.589145 3.138600 0.179151 H 1.473931 2.505161 0.087211 H 0.816125 4.097640 -0.288807 H 0.332322 3.270315 1.226362 H -0.362748 2.342315 -1.642241	22.44 40.74 45.94 75.23 86.12 99.20 105.82 122.51 139.28 154.16 179.70 185.78 191.76 224.58 241.29 309.60 399.95 407.10 449.91 522.22 583.86 592.64 598.21 792.42 832.36 915.28 938.12 942.82 1053.42 1071.74 1083.56 1146.81 1151.34 1155.71 1162.80 1214.95 1262.64 1292.58 1374.92 1386.82 1442.63 1445.92 1457.36 1465.62 1472.32 1474.95 1492.50 1509.43 1514.28 1521.13 1568.02 1697.48 1818.40 2563.98 3020.79 3064.97 3089.36 3091.95

		3132.48 3173.65 3173.90 3180.97 3188.03 3190.50 3339.47 3863.43
TS1D	0 1 C -0.069796 1.733802 -0.782206 O -1.090697 1.100936 -1.172752 H -1.666730 0.347720 -0.368947 N -2.276550 -0.506789 0.287372 C -3.529975 0.012476 0.838613 H -3.315582 0.847288 1.501990 H -4.153725 0.365279 0.019468 H -4.069146 -0.758853 1.389027 C -2.454220 -1.652860 -0.617426 H -1.470584 -1.990142 -0.931623 H -2.986017 -2.463855 -0.119832 H -3.022238 -1.325067 -1.485906 S 1.616525 -0.531369 0.011658 O 0.378687 -0.988160 0.584138 O 1.403888 0.616888 -0.910619 H -1.616883 -0.770566 1.015448 O 2.496737 -1.499994 -0.552773 O 2.379628 0.106622 1.269009 H 3.325107 0.099043 1.079806 C 0.042324 2.189056 0.645717 H 1.043386 2.547882 0.865712 H -0.670223 3.005005 0.781668 H -0.204350 1.380838 1.332302 H 0.402489 2.379683 -1.521457	-506.50 29.48 58.92 78.65 91.28 110.96 137.44 146.63 169.63 197.61 203.47 247.33 253.29 289.75 361.01 395.01 417.57 457.53 465.78 565.37 582.45 590.32 612.97 630.94 843.20 910.53 948.02 961.74 996.96 1032.11 1048.81 1089.74 1145.82 1164.67 1166.81 1200.52 1266.83 1272.30 1281.29 1390.01 1404.38 1409.23 1445.00 1456.04 1471.02 1484.91 1492.05 1496.92 1512.39 1517.35 1520.33 1581.46 1622.43 1715.35 3069.67 3070.65 3072.97 3118.83 3143.54 3146.71 3148.74 3163.60 3183.16 3183.92 3517.82 3859.18
C1E	0 1 C -0.060281 2.237817 0.292310 O -1.200199 2.254864 -0.120081 H -1.822881 0.551299 -0.100074 H 0.208758 1.590718 1.144342 N -2.017012 -0.455632 0.027330 C -3.111467 -0.629831 0.998396 H -2.839483 -0.136939 1.927339 H -4.025399 -0.193721 0.602263 H -3.257643 -1.691863 1.178195 C -2.268719 -1.087451 -1.284087 H -1.401270 -0.907984 -1.911354 H -2.406141 -2.155522 -1.133718 H -3.164807 -0.658018 -1.726178 S 1.294595 -0.745579 0.094500	27.37 48.97 52.89 68.36 94.20 106.02 113.51 118.25 127.78 142.73 153.33 186.59 191.20 222.12 256.44 315.00 402.43 408.37 447.19 524.43 584.27 593.59 598.61 815.09 855.89 915.38 942.12 959.86 1057.43 1071.22

	O 0.276600 -1.309613 0.995609 O 2.296531 0.01993 0.782844 O 0.672915 -0.104240 -1.042020 H -1.111248 -0.853227 0.433275 O 2.046073 -2.005874 -0.538090 H 2.764312 -2.255603 0.054114 C 1.055514 3.038210 -0.274712 H 0.715227 3.651206 -1.104042 H 1.823538 2.331407 -0.595689 H 1.496961 3.653877 0.510662	1086.46 1148.75 1155.87 1158.61 1166.58 1218.86 1262.81 1293.03 1355.00 1383.54 1439.14 1446.14 1462.48 1467.22 1467.67 1474.99 1495.51 1511.76 1515.72 1522.75 1581.90 1707.21 1816.08 2592.29 2999.76 3065.13 3089.28 3091.36 3130.03 3171.44 3174.68 3184.32 3184.48 3195.96 3234.26 3866.39
TS1E	0 1 C -0.015788 1.729291 0.391771 O -0.725819 1.415532 -0.608980 H -1.557749 0.556358 -0.385085 H -0.478219 1.709818 1.381867 N -2.316929 -0.429063 -0.167440 C -2.333804 -0.697148 1.277193 H -1.307831 -0.816168 1.618555 H -2.795510 0.147063 1.787772 H -2.901892 -1.600283 1.502180 C -3.649978 -0.273942 -0.752977 H -3.556773 -0.100363 -1.821961 H -4.261814 -1.160358 -0.580991 H -4.139674 0.585361 -0.298226 S 1.382540 -0.821366 0.000555 O 0.211022 -1.467730 -0.517784 O 2.412217 -1.639306 0.553962 O 1.024612 0.291505 0.930384 H -1.785008 -1.169747 -0.622075 O 2.020130 -0.078441 -1.264770 H 2.979069 -0.121794 -1.174694 C 1.069042 2.736695 0.188558 H 1.612883 2.495545 -0.721343 H 1.741761 2.765840 1.040228 H 0.594489 3.712175 0.067197	-541.34 40.07 65.59 85.04 89.30 110.12 128.35 156.92 165.05 188.75 212.67 217.61 260.97 269.11 326.20 385.87 417.06 430.40 488.78 540.52 570.70 608.62 612.57 669.26 850.97 926.89 951.54 961.95 985.38 1038.30 1048.62 1092.89 1152.18 1161.85 1174.50 1200.91 1267.71 1273.00 1277.99 1377.42 1401.09 1404.65 1446.77 1463.02 1469.83 1485.76 1490.01 1499.32 1515.51 1519.29 1523.29 1595.60 1624.06 1714.79 3065.22 3068.00 3073.28 3077.74 3136.23 3139.73 3154.63 3167.29 3168.92 3192.14 3496.69 3862.01
C1F	0 1	21.32 38.65

	C -1.021090 2.405262 -0.540354 O -1.998875 1.700080 -0.649441 H -1.840515 0.011118 -0.051234 N -1.687926 -0.989051 0.150255 C -2.663886 -1.464657 1.145279 H -2.569445 -0.867663 2.047830 H -3.670518 -1.372236 0.744429 H -2.453314 -2.506002 1.375367 C -1.715374 -1.736606 -1.124145 H -0.964835 -1.302427 -1.777383 H -1.478557 -2.778254 -0.921305 H -2.705514 -1.658439 -1.567201 S 1.546642 -0.263668 0.069488 O 0.779903 -1.059715 1.032704 O 2.453211 0.685575 0.648572 O 0.675707 0.268611 -0.962599 H -0.697112 -1.047245 0.550754 O 2.460449 -1.373967 -0.636733 H 3.283922 -0.951838 -0.904747 C -0.255432 2.604898 0.720587 H -0.442101 3.621841 1.075917 H -0.559720 1.890521 1.483167 H 0.812542 2.506185 0.527512 H -0.674082 2.978434 -1.414902	47.08 63.97 78.31 98.87 107.30 113.53 122.99 129.57 148.55 180.48 202.19 217.01 237.96 313.32 400.42 408.08 451.52 527.04 576.05 588.24 612.33 781.21 847.59 917.51 941.51 951.88 1056.70 1072.96 1088.77 1138.32 1150.96 1153.63 1156.68 1228.45 1262.26 1294.67 1351.39 1394.03 1435.80 1445.58 1460.15 1468.80 1473.76 1477.19 1493.69 1511.31 1515.09 1522.08 1584.72 1698.32 1821.25 2577.34 3007.73 3056.38 3089.42 3091.12 3130.44 3166.51 3172.37 3174.17 3183.08 3196.51 3261.23 3872.52
TS1F	0 1 C 0.148470 1.827597 0.700369 O 1.321852 1.450988 1.030763 H 1.738241 0.576530 0.342040 N 2.100090 -0.520372 -0.241957 C 3.424056 -0.424837 -0.858644 H 3.412558 0.343839 -1.627954 H 4.150622 -0.146980 -0.096946 H 3.724751 -1.374667 -1.303245 C 2.007196 -1.561171 0.791649 H 0.988776 -1.578571 1.172555 H 2.267090 -2.540444 0.388285 H 2.687501 -1.311190 1.604016 S -1.547697 -0.395032 -0.170716 O -0.583860 -0.891548 -1.112441 O -2.696278 0.277485 -0.688550 O -0.889661 0.374897 0.936904 H 1.374440 -0.706724 -0.933887 O -2.049781 -1.695996 0.589621 H -2.886773 -1.497424 1.026643	-638.81 36.26 46.35 74.73 78.96 107.10 120.54 152.85 183.22 195.80 227.87 250.56 262.66 307.00 362.86 392.49 420.24 457.09 484.37 503.54 557.55 600.70 621.86 677.38 872.69 908.30 955.38 991.69 1004.16 1028.71 1051.11 1092.25 1146.38 1164.32 1170.33 1206.12 1262.59 1266.23 1286.16 1381.47

	C -0.127214 2.251894 -0.714147 H 0.359479 3.219537 -0.845730 H 0.298352 1.548589 -1.428002 H -1.192655 2.358212 -0.901170 H -0.393082 2.384918 1.462812	1392.71 1410.95 1448.58 1461.27 1474.30 1487.16 1490.05 1496.73 1509.86 1514.59 1519.86 1538.13 1598.06 1709.81 3064.12 3067.08 3074.35 3127.16 3136.16 3142.23 3149.27 3161.09 3171.06 3179.83 3472.46 3851.90
CP1	0 1 C -0.344326 1.587868 -0.109146 O 0.881150 1.850104 0.384552 H 1.507814 1.109341 0.115167 H -0.326005 1.245105 -1.147071 N 2.387109 -0.285666 -0.235318 C 3.754211 -0.060208 -0.690067 H 3.744873 0.470525 -1.639903 H 4.276293 0.557510 0.040663 H 4.315366 -0.993087 -0.810533 C 2.332026 -1.053022 1.007220 H 1.294817 -1.241587 1.278493 H 2.857167 -2.010443 0.930141 H 2.791633 -0.469622 1.805189 S -1.297889 -0.878875 -0.053893 O -0.347365 -1.179724 -1.066706 O -0.924104 0.429774 0.670834 H 1.851689 -0.773847 -0.944595 O -1.635569 -1.823750 0.946405 C -1.285870 2.739763 0.109112 H -1.318609 2.978821 1.170252 H -2.284435 2.491147 -0.244165 H -0.915766 3.604817 -0.437295 O -2.612123 -0.483332 -0.842904 H -3.370538 -0.538000 -0.246989	36.01 51.80 56.00 72.40 96.52 108.78 129.28 180.11 203.05 211.20 247.23 274.95 298.41 333.47 378.14 414.17 423.49 468.94 505.42 547.44 575.00 616.52 767.76 884.00 897.65 923.53 963.43 977.08 1040.41 1059.73 1071.35 1111.09 1151.44 1166.45 1194.05 1218.68 1233.04 1271.10 1273.32 1389.21 1420.64 1426.93 1449.55 1462.28 1476.55 1480.43 1489.53 1494.97 1495.98 1508.00 1521.27 1524.58 1597.55 2936.66 3027.67 3035.32 3076.36 3083.77 3105.81 3109.62 3147.82 3152.27 3167.02 3169.18 3554.86 3837.04
P1	0 1 C -1.497256 0.018815 0.252084 O -1.846748 -1.259818 -0.091260 H -1.155115 -1.864728 0.202046 H -1.194247 0.097894 1.299414 S 1.064025 -0.058849 -0.089161	71.17 107.20 197.64 235.05 282.70 328.90 376.92 396.33 477.37 489.10 529.05 558.98

	O 0.925032 -1.362003 0.458753 O -0.332901 0.458158 -0.541907 O 1.973809 0.239780 -1.128355 C -2.609423 0.963728 -0.102911 H -2.824743 0.876470 -1.165960 H -2.328131 1.987555 0.129958 H -3.496998 0.692001 0.463654 O 1.385627 0.868961 1.148317 H 1.776359 1.696510 0.838047	613.42 638.05 812.71 895.59 928.56 963.12 1069.02 1125.44 1165.06 1211.96 1261.15 1320.55 1408.17 1410.05 1471.79 1488.71 1495.48 1501.70 3074.65 3089.79 3173.26 3177.70 3834.04 3834.63
$(CH_3)_2NH$ $\ldots H_2SO_4$	0 1 H -1.023840 -0.027709 -0.543349 O 0.329679 -0.108074 -1.109677 S 1.281861 -0.124493 0.023401 O 1.985489 1.312959 -0.021673 O 0.563097 -0.107867 1.279915 O 2.326346 -1.086250 -0.129002 H -1.409476 -0.010820 1.019634 N -1.900374 0.007193 0.118546 H 2.797320 1.228488 -0.533845 C -2.627985 1.274081 -0.056969 H -1.930420 2.095381 0.082141 H -3.034381 1.308724 -1.064679 H -3.436993 1.344489 0.666928 C -2.717386 -1.204571 -0.055736 H -3.124208 -1.211372 -1.063835 H -2.080172 -2.073236 0.084656 H -3.529656 -1.215604 0.667827	-42.92 36.60 75.81 101.47 159.84 195.29 196.28 229.04 327.91 393.62 406.03 459.41 582.18 595.69 610.15 846.68 874.78 947.19 1053.08 1060.01 1073.84 1154.92 1161.75 1174.61 1262.84 1269.19 1382.08 1449.35 1462.73 1472.73 1497.77 1512.14 1513.78 1517.62 1586.73 1681.73 2256.63 3087.29 3088.54 3169.81 3170.64 3182.60 3183.64 3398.06 3869.29
CH_3CHO … $(CH_3)_2NH$	0 1 N -1.383071 -0.138174 0.129751 H -0.926589 -0.703575 -0.575893 C -2.725199 -0.627112 0.387071 H -2.693325 -1.684400 0.645062 H -3.148620 -0.087425 1.235767 H -3.407663 -0.495681 -0.464410 C -1.377460 1.250558 -0.295272 H -1.713471 1.882424 0.528826 H -0.365781 1.548869 -0.566842 H -2.034516 1.444748 -1.154489 C 2.831689 0.359204 0.594999 H 3.523463 -0.263833 1.164181 H 2.447194 1.115383 1.282246 H 3.345716 0.832507 -0.236825	36.60 55.51 75.89 84.17 118.93 133.01 166.85 221.48 275.69 398.48 520.07 791.30 842.32 905.53 970.90 1042.00 1107.82 1138.61 1159.21 1194.77 1203.07 1272.66 1384.13 1441.02 1442.49 1467.82 1471.28 1476.73 1484.41 1494.49

	C 1.688933 -0.477569 0.106542 H 1.105958 -1.001469 0.883289 O 1.380169 -0.581352 -1.051151	1505.06 1523.60 1525.39 1849.34 2979.82 2984.59 2986.95 3063.88 3080.17 3083.76 3126.30 3132.93 3134.76 3179.21 3558.49
CH_3CHO … H_2SO_4	0 1 S 1.183922 -0.207178 -0.043669 O 2.467173 -0.644161 -0.444342 O 0.116848 -1.110912 0.199906 O 0.742607 0.873493 -1.070020 H -0.193018 1.130959 -0.914830 O 1.318010 0.622025 1.293970 H 2.148650 1.115674 1.289759 C -3.022290 -0.857964 -0.134797 H -4.004323 -0.921664 0.336558 H -2.471916 -1.762593 0.130043 H -3.118463 -0.778548 -1.213634 C -2.277143 0.305170 0.419754 H -2.151266 0.327068 1.515236 O -1.814114 1.199644 -0.248784	31.53 64.71 90.76 128.12 171.12 201.92 224.25 262.21 397.05 438.62 531.93 536.68 566.13 576.92 782.44 880.73 916.33 940.14 971.64 1150.58 1161.28 1166.74 1252.27 1362.42 1391.91 1439.50 1455.32 1473.57 1491.11 1823.96 2966.58 3020.81 3067.55 3131.84 3186.06 3840.96