



*Supplement of*

**Atmospheric fate of organosulfates through gas-phase and aqueous-phase reactions with hydroxyl radicals: implications for inorganic sulfate formation**

**Narcisse Tsona Tchinda et al.**

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## S1 Calculation of the Gibbs free energy in aqueous phase

For a given species, the Gibbs free energy in aqueous phase is calculated as:

$$G = E^{\text{CCSD(T)}} + E_{\text{SMD}}^{\text{M06-2X}} - E_{\text{Gas}}^{\text{M06-2X}} + G_{\text{corr}}^{\text{M06-2X}} + \Delta G_{\text{latm} \rightarrow \text{1M}} \quad (\text{S1})$$

where  $E^{\text{CCSD(T)}}$  is the electronic energy obtained from DLPNO-CCSD(T)/aug-cc-pVTZ,  $E_{\text{SMD}}^{\text{M06-2X}}$  and  $E_{\text{Gas}}^{\text{M06-2X}}$  are electronic energies obtained from  $\omega\text{B97XD}/6\text{-31++G(d,p)}$  calculations in aqueous-phase and in gas-phase, respectively,  $G_{\text{corr}}^{\text{M06-2X}}$  is the thermal correction to Gibbs free energy obtained from M06-2X/6-311+g(2df,2pd) calculations at 298.15 K and 1 atm, and  $\Delta G_{\text{latm} \rightarrow \text{1M}}$  is the term that converts the standard pressure of 1 atm in the gas-phase to the standard concentration of 1 M in aqueous-phase. The numerical value of this term is 1.89 kcal mol<sup>-1</sup> (Marenich et al., 2009).

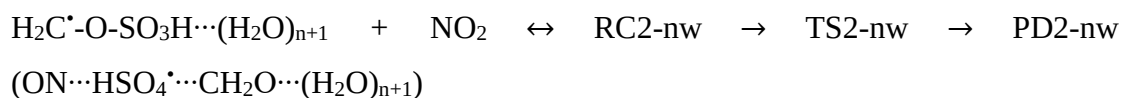
**Table S1: Numerical values of radii and diffusion coefficients (calculated with Eq. (6) in the main article) of reactants in the aqueous-phase.**

| Reactants                                                        | Radius (m)             | Diffusion coefficient (m <sup>2</sup> s <sup>-1</sup> ) |
|------------------------------------------------------------------|------------------------|---------------------------------------------------------|
| HO•                                                              | 1.82×10 <sup>-10</sup> | 1.30×10 <sup>-9</sup>                                   |
| O <sub>3</sub>                                                   | 2.21×10 <sup>-10</sup> | 1.10×10 <sup>-9</sup>                                   |
| CH <sub>3</sub> -O-SO <sub>3</sub> <sup>-</sup> (methyl sulfate) | 2.27×10 <sup>-10</sup> | 8.20×10 <sup>-10</sup>                                  |
| H <sub>2</sub> C•-O-SO <sub>3</sub> <sup>-</sup>                 | 3.18×10 <sup>-10</sup> | 7.70×10 <sup>-10</sup>                                  |
| HOOC-CH•-O-SO <sub>3</sub> <sup>-</sup> (glycolic acid sulfate)  | 3.26×10 <sup>-10</sup> | 7.50×10 <sup>-10</sup>                                  |
| HOOC-CH(O)•-O-SO <sub>3</sub> <sup>-</sup>                       | 3.24×10 <sup>-10</sup> | 7.60×10 <sup>-10</sup>                                  |

**Table S2: Steady-state Smoluchowski rate constants (calculated with Eq. (5) in the main article) for the reactions in the aqueous-phase.**

| Reaction                                              | Smoluchowski rate constant ( $k_D$ , M <sup>-1</sup> s <sup>-1</sup> ) |
|-------------------------------------------------------|------------------------------------------------------------------------|
| CH <sub>3</sub> -O-SO <sub>3</sub> <sup>-</sup> + HO• | 7.88×10 <sup>9</sup>                                                   |
| HOOC-CH(O)•-O-SO <sub>3</sub> <sup>-</sup> + HO•      | 8.07×10 <sup>9</sup>                                                   |

**Table S3: Electronic energy changes ( $\Delta E$ ) and Gibbs free energy changes ( $\Delta G$ ) for all intermediate species in the reaction of H<sub>2</sub>C•-O-SO<sub>3</sub>H... (H<sub>2</sub>O)<sub>n+1</sub> with NO<sub>2</sub>. Energy units are kcal mol<sup>-1</sup>. “RC” stands for intermediate reactant complex, “TS” stands for transition state, “PD” stands for product, “w” stands for water.**



| Species | $\Delta G$ | $\Delta E$ |
|---------|------------|------------|
| n = 1   |            |            |
| RC2-1w  | -54.85     | -63.59     |
| TS2-1w  | 18.55      | 11.94      |
| PD2-1w  | -52.45     | -55.63     |
| n = 2   |            |            |
| RC2-2w  | -53.57     | -63.48     |
| TS2-2w  | 20.90      | 17.20      |
| PD2-2w  | -52.45     | -54.56     |

**Table S4: Electronic energy changes ( $\Delta E$ ) and Gibbs free energy changes ( $\Delta G$  at 298.15 K and 1 atm) for intermediate species in the reaction of methyl sulfate with  $\text{HO}^\bullet$  radicals. Energy units are  $\text{kcal mol}^{-1}$ . “RC” stands for intermediate reactant complex, “TS” stands for transition state, “PD” stands for product, “nw” stands for the number of added water molecules to the reaction of methyl sulfate with  $\text{HO}^\bullet$  radicals.**

| Reaction                                                                                                                                                                                                                                                                                                                                                  | $\Delta G$ | $\Delta E$ |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------|------------|
| $\text{H}_2\text{C}^\bullet\text{-O-SO}_3\text{H}\cdots(\text{H}_2\text{O})_n + \text{O}_3 \leftrightarrow \text{RC3-nw} \rightarrow \text{TS3-nw} \rightarrow \text{PD3-nw}$<br>$(\text{O}_2 + \bullet\text{O-H}_2\text{C-O-SO}_3\text{H}\cdots(\text{H}_2\text{O})_n) \rightarrow \text{RC3b-nw} \rightarrow \text{TS3b-nw} \rightarrow \text{PD3b-nw}$ |            |            |
| n = 1                                                                                                                                                                                                                                                                                                                                                     |            |            |
| RC3-1w                                                                                                                                                                                                                                                                                                                                                    | -19.60     | -41.12     |
| TS3-1w                                                                                                                                                                                                                                                                                                                                                    | -28.49     | -46.67     |
| PD3-1w                                                                                                                                                                                                                                                                                                                                                    | -23.40     | -38.32     |
| RC3b-1w                                                                                                                                                                                                                                                                                                                                                   | -6.51      | 4.65       |
| TS3b-1w                                                                                                                                                                                                                                                                                                                                                   | 9.32       | 26.08      |
| PD3b-1w                                                                                                                                                                                                                                                                                                                                                   | -24.52     | -6.85      |
| n = 2                                                                                                                                                                                                                                                                                                                                                     |            |            |
| RC3-2w                                                                                                                                                                                                                                                                                                                                                    | -12.46     | -30.92     |
| TS3-2w                                                                                                                                                                                                                                                                                                                                                    | -19.70     | -35.50     |
| PD3-2w                                                                                                                                                                                                                                                                                                                                                    | -18.35     | -29.87     |
| RC3b-2w                                                                                                                                                                                                                                                                                                                                                   | -5.05      | 6.28       |
| TS3b-2w                                                                                                                                                                                                                                                                                                                                                   | 1.53       | 15.33      |

|         |        |        |
|---------|--------|--------|
| PD3b-2w | -25.88 | -10.68 |
|---------|--------|--------|

**Table S5:** Electronic energy changes ( $\Delta E$ ) and Gibbs free energy changes ( $\Delta G$  at 298.15 K and 1 atm) for all intermediate species in the reaction of glycolic acid sulfate with HO• radicals proceeding through hydrogen abstraction from the -CH<sub>2</sub>- group. Energy units are kcal mol<sup>-1</sup>. “RC” stands for intermediate reactant complex, “TS” stands for transition state, “PD” stands for product, “nw” stands for the number of added water molecules to the reaction of methyl sulfate with HO• radicals.

| Reaction                                                                                              | $\Delta G$ | $\Delta E$ |
|-------------------------------------------------------------------------------------------------------|------------|------------|
| HOOC-CH <sub>2</sub> -O-SO <sub>3</sub> H + •OH ↔ RC11 → TS11 → PD11 (HOOC-CH•-O-SO <sub>3</sub> H)   |            |            |
| RC11                                                                                                  | 2.09       | -8.16      |
| TS11                                                                                                  | 4.03       | -3.92      |
| PD11                                                                                                  | -27.03     | -38.09     |
| HOOC-CH•-O-SO <sub>3</sub> H + O <sub>2</sub> ↔ RC12 → TS12 → PD12 (HOOC-CH•(OO)-O-SO <sub>3</sub> H) |            |            |
| RC12                                                                                                  | -30.83     | -40.72     |
| TS12                                                                                                  | -23.13     | -35.28     |
| PD12                                                                                                  | -45.13     | -63.18     |
| HOOC-CH•(OO)-O-SO <sub>3</sub> H + HOOC-CH•(OO)-O-SO <sub>3</sub> H ↔ RC13 → TS13 → PD13              |            |            |
| RC13                                                                                                  | -93.12     | -149.43    |
| TS13                                                                                                  | -53.38     | -102.96    |
| PD13                                                                                                  | -156.16    | -207.04    |

\* Geometry optimizations were at the M06-2X/6-31++G(d,p) level of theory.

**Table S6:** Electronic energy changes ( $\Delta E$ ) and Gibbs free energy changes ( $\Delta G$  at 298.15 K and 1 atm) for all intermediate species in the reaction of glycolic acid sulfate with HO• radicals proceeding through hydrogen abstraction from the -COOH group. Energy units are kcal mol<sup>-1</sup>. “RC” stands for intermediate reactant complex, “TS” stands for transition state, “PD” stands for product, “nw” stands for the number of added water molecules to the reaction of methyl sulfate with HO• radicals.

| Reaction                                                                                                                               | $\Delta G$ | $\Delta E$ |
|----------------------------------------------------------------------------------------------------------------------------------------|------------|------------|
| HOOC-CH <sub>2</sub> -O-SO <sub>3</sub> H + •OH ↔ RC11' → TS11' → PD11' (H <sub>2</sub> O...•OOC-CH <sub>2</sub> -O-SO <sub>3</sub> H) |            |            |
| RC11'                                                                                                                                  | 1.26       | -7.92      |

|                                                                                                                                                     |        |        |
|-----------------------------------------------------------------------------------------------------------------------------------------------------|--------|--------|
| TS11'                                                                                                                                               | 9.29   | 4.98   |
| PD11'                                                                                                                                               | -3.44  | -12.55 |
| $\bullet\text{OOC-CH}_2\text{-O-SO}_3\text{H} \rightarrow \text{TS12} \rightarrow \text{PD12} (\text{CO}_2\cdots\text{CH}_2\text{-O-SO}_3\text{H})$ |        |        |
| RC12'                                                                                                                                               | -5.46  | 6.43   |
| TS12'                                                                                                                                               | -7.06  | 6.51   |
| PD12'                                                                                                                                               | -32.62 | -15.54 |

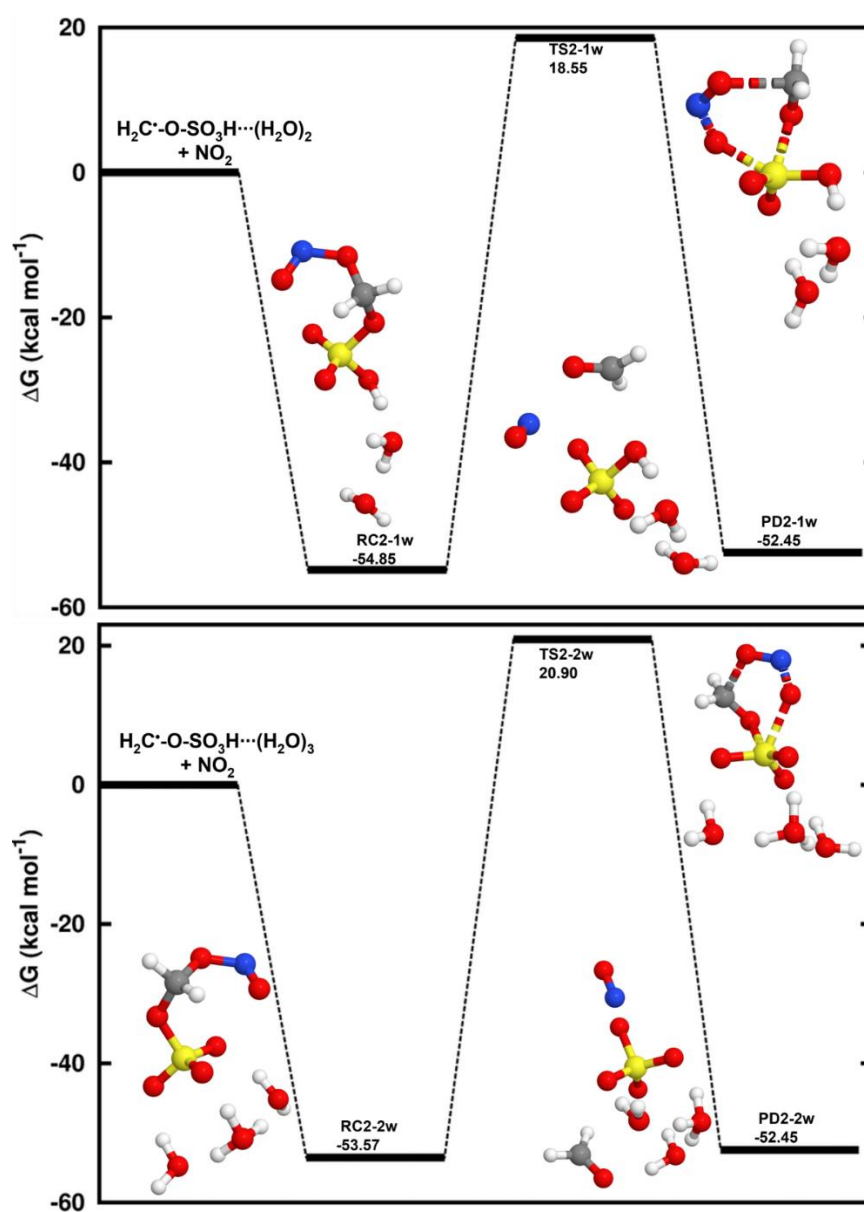


Figure S1: Gibbs free energy changes (in  $\text{kcal mol}^{-1}$ ) and optimized structures of all stationary states in the reaction of  $\text{H}_2\text{C}^\bullet\text{-O-SO}_3\text{H}\cdots(\text{H}_2\text{O})_{2-3}$  with  $\text{NO}_2$ . The sulfur atom is in yellow, the oxygen atom is in red, the nitrogen atom is in blue, the carbon atom is in gray, and the hydrogen atom is

in white. “RC” stands for intermediate reactant complex, “TS” stands for transition state, “PD” stands for product, “nw” stands for the number of added water molecules to the reaction of methyl sulfate with HO<sup>•</sup> radicals.

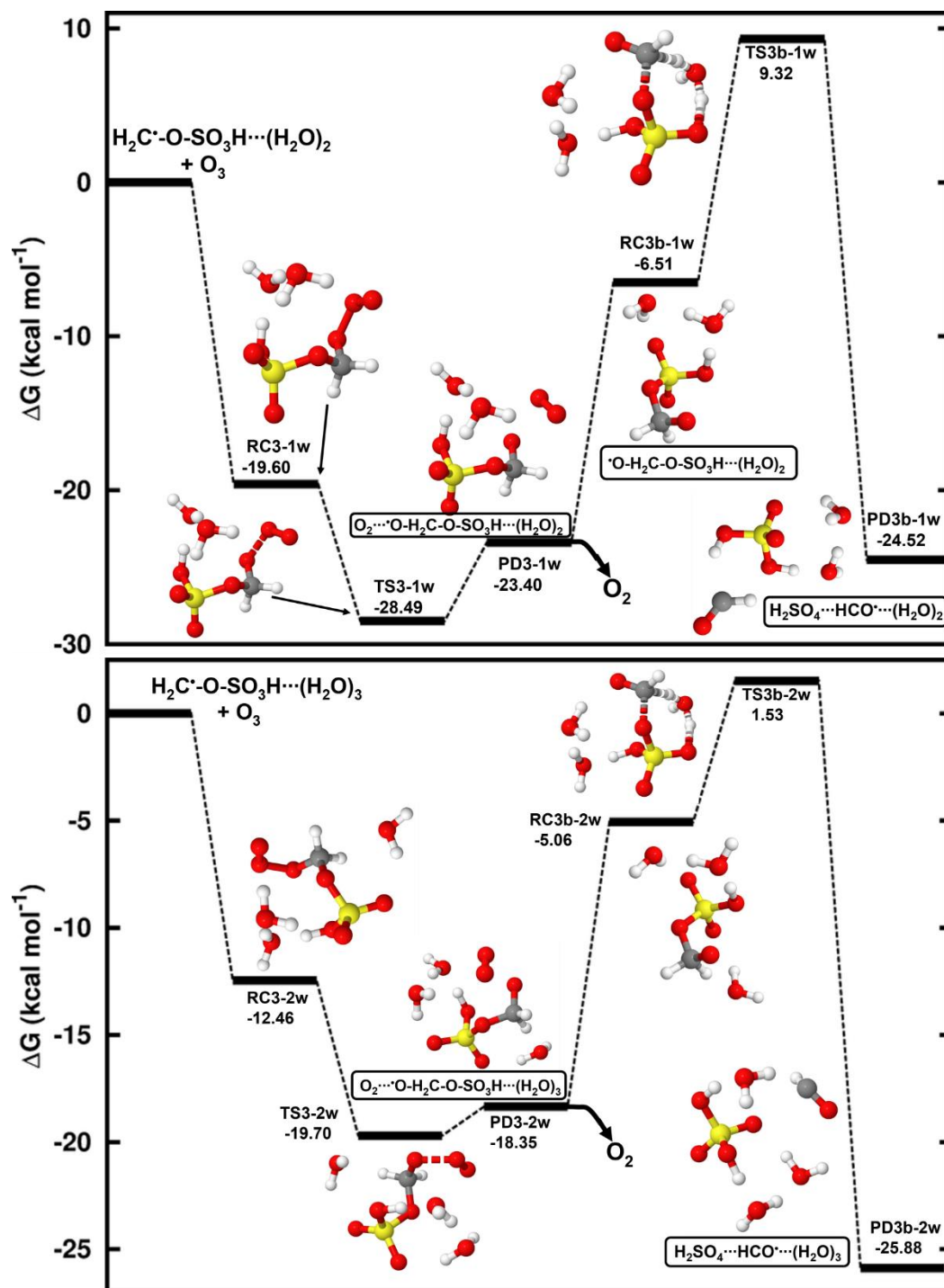


Figure S2: Gibbs free energy changes (in kcal mol<sup>-1</sup>) and optimized structures for all intermediates in the reaction of  $\text{O}_3$  with  $\text{H}_2\text{C}^\bullet\text{-O-SO}_3\text{H}\cdots(\text{H}_2\text{O})_2$  (top) and  $\text{H}_2\text{C}^\bullet\text{-O-SO}_3\text{H}\cdots(\text{H}_2\text{O})_3$  (bottom). The sulfur atom is in yellow, the oxygen atom is in red, the carbon atom is in gray, and the hydrogen atom is in white.

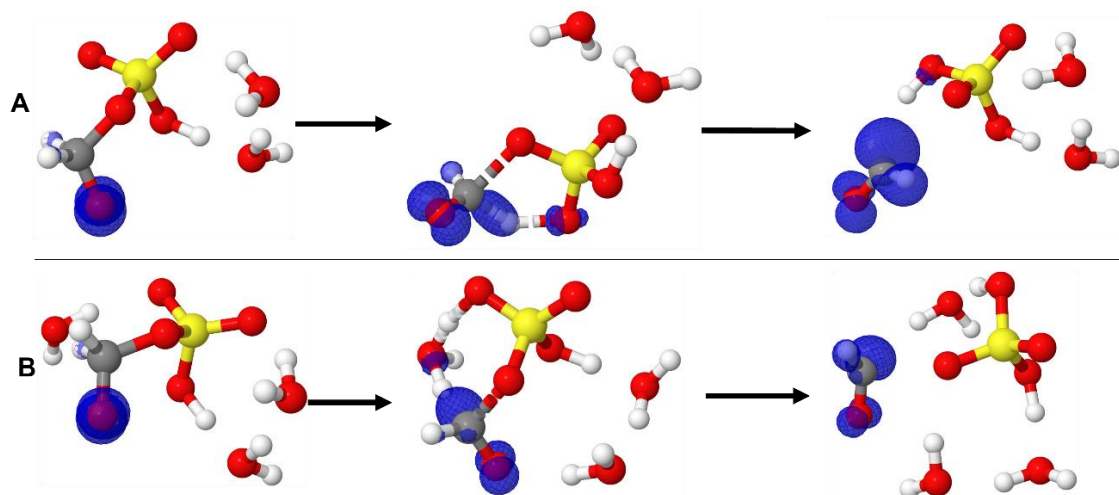


Figure S3: Representation of the spin density (blue color) on the electronic states of the decomposition of (A)  $\bullet\text{O-H}_2\text{C-O-SO}_3\text{H}\cdots(\text{H}_2\text{O})_2$  and (B)  $\bullet\text{O-H}_2\text{C-O-SO}_3\text{H}\cdots(\text{H}_2\text{O})_3$ . From left to right are the reactant, transition state and the product complex, respectively. The sulfur atom is yellow, the oxygen atom is red, the carbon atom is grey and the hydrogen atom is white.

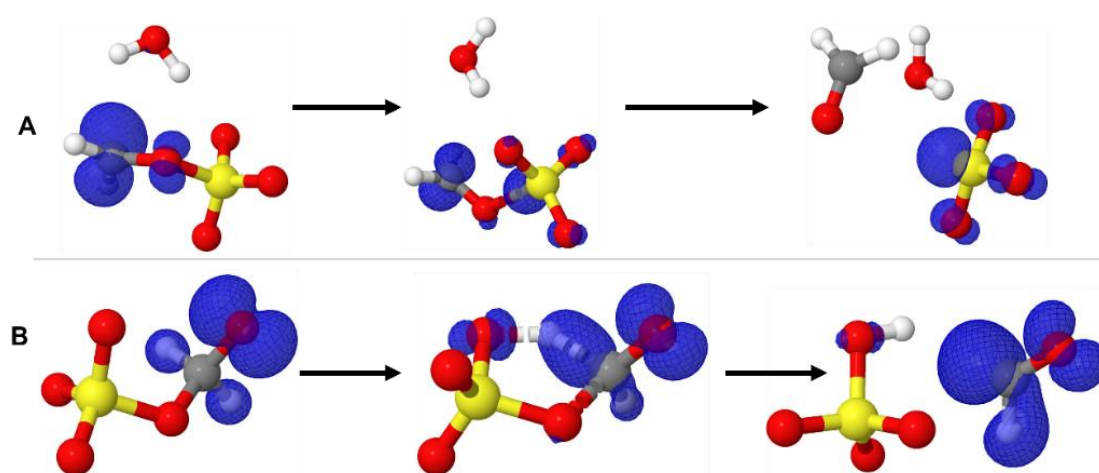


Figure S4: Representation of the spin density (blue color) on the electronic states of the decomposition of (A)  $\text{H}_2\text{C}^\bullet\text{-O-SO}_3^-$  and (B)  $^\bullet\text{O-H}_2\text{C-O-SO}_3^-$ . From left to right are the reactant, transition state and product complex, respectively. The sulfur atom is in yellow, the oxygen atom is in red, the carbon atom is in gray, and the hydrogen atom is in white.

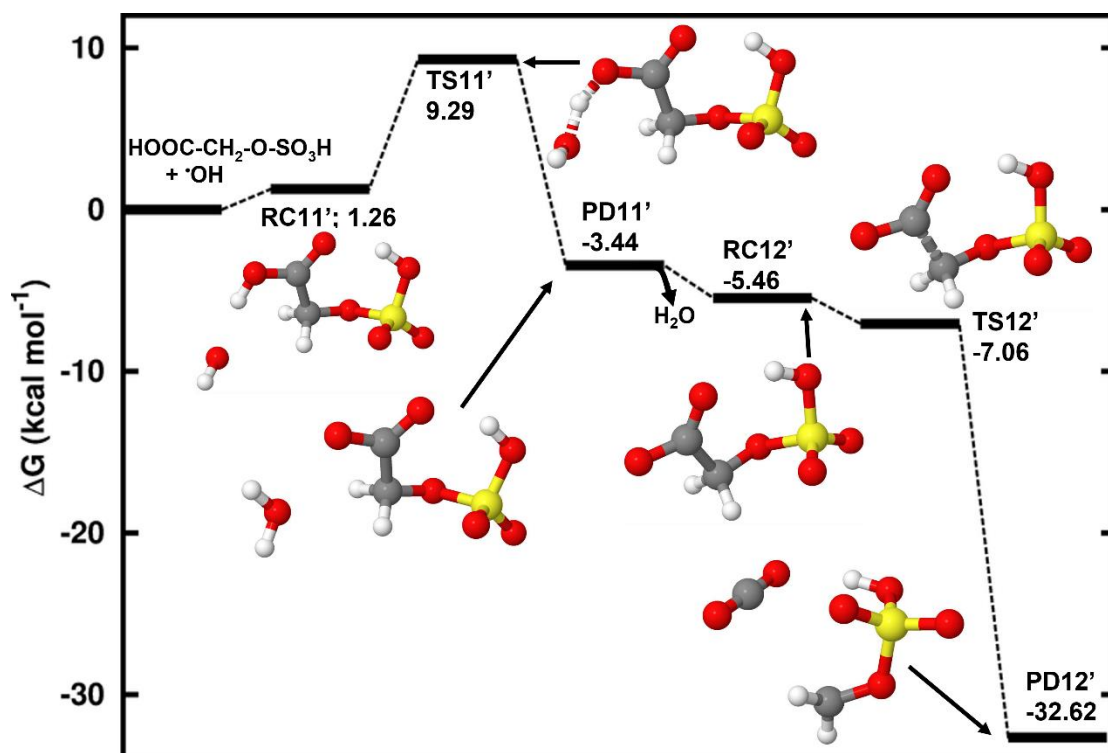


Figure S5: Gibbs free energy changes (in  $\text{kcal mol}^{-1}$ ) and optimized structures for all intermediates in the reaction of  $\text{HOOC-CH}_2\text{-O-SO}_3\text{H}$  reaction with  $\text{HO}\cdot$  radicals proceeding through hydrogen abstraction from the  $-\text{COOH}-$  group. The sulfur atom is yellow, the oxygen atom is red, the carbon atom is grey and the hydrogen atom is white.

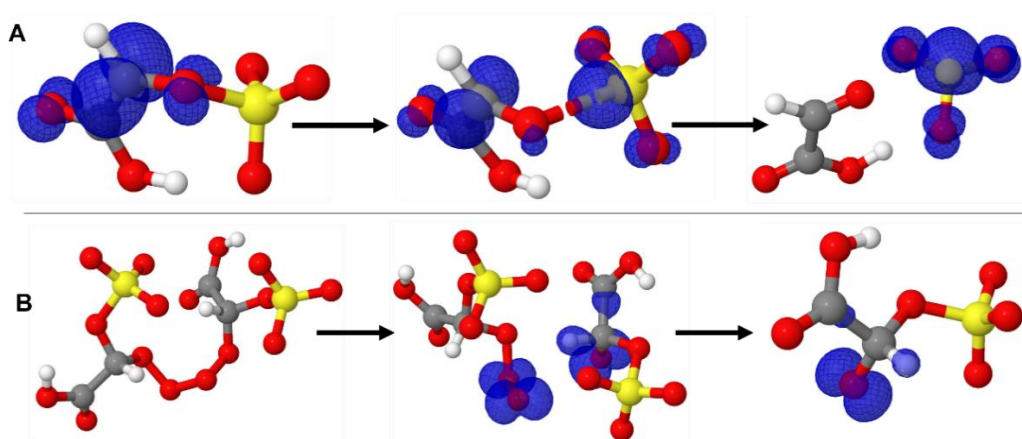


Figure S6: Representation of the spin density (blue color) on the electronic states of the decomposition of (A)  $\text{HOOC-CH}\cdot\text{-O-SO}_3^-$  (where from left to right are the reactant, transition state and the product complex, respectively) and (B)  $\text{O}_3\text{S-O-CH(COOH)-OOOO-CH(COOH)-O-SO}_3^-$  (where from left to right are the singlet state, triplet state and the decomposition product, respectively). The sulfur atom is in yellow, the oxygen atom is in red, the carbon atom is in gray, and the hydrogen atom is in white.



## Cartesian coordinates of optimized structures

Gas-phase species

•OH

|   |            |            |             |
|---|------------|------------|-------------|
| O | 0.00000000 | 0.00000000 | 0.10788700  |
| H | 0.00000000 | 0.00000000 | -0.86309800 |

CH<sub>3</sub>-O-SO<sub>3</sub>H

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 0.51112200  | 1.17269300  | -0.89108900 |
| O | 1.47111400  | -1.00074300 | -0.29656000 |
| O | 0.36409900  | 0.43170700  | 1.41276100  |
| O | -0.89307800 | -0.72121100 | -0.35811300 |
| S | 0.46526600  | -0.08327100 | 0.08432600  |
| H | -2.11968200 | 0.94380400  | -0.52607800 |
| C | -2.09649900 | -0.01708100 | -0.01502700 |
| H | -2.90549900 | -0.64720000 | -0.36695700 |
| H | -2.15392400 | 0.11691400  | 1.06202800  |
| H | 0.68778700  | 1.96173700  | -0.36405200 |

HOOC-CH<sub>2</sub>-O-SO<sub>3</sub>H

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.21640000  | 1.43678200  | -0.32553800 |
| O | 2.58953400  | -0.52029200 | -0.23165300 |
| O | 0.78306200  | -0.20274300 | 1.45005300  |
| O | 0.25473700  | -0.74356500 | -0.86456500 |
| S | 1.30889600  | -0.04790500 | 0.13218800  |
| C | -1.87301500 | 0.14588800  | -0.08440700 |
| C | -1.01637800 | -1.07802100 | -0.36202600 |
| H | -1.49335500 | -1.68011800 | -1.13592800 |
| H | -0.93755600 | -1.66577000 | 0.55501700  |
| H | 0.27578800  | 1.71251600  | -0.27482000 |
| O | -1.49159300 | 1.27448000  | -0.19872800 |
| H | -3.29456500 | -1.05816100 | 0.37213400  |
| O | -3.12167800 | -0.11331200 | 0.30133100  |

CH<sub>3</sub>-O-SO<sub>3</sub>H⋯(H<sub>2</sub>O)<sub>n=0-2</sub> + •OH ↔ RC1-nw → TS1-nw → PD1-nw (H<sub>2</sub>C•-O-SO<sub>3</sub>H⋯(H<sub>2</sub>O)<sub>n+1</sub>)

RC1-0w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.29726500 | 0.20207200  | 1.34111400  |
| O | -0.84578500 | -1.66293200 | -0.17673500 |
| O | -1.54161500 | 0.56773400  | -1.04381600 |
| O | 0.67525000  | 0.15881700  | -0.06089400 |
| S | -0.83873100 | -0.25047300 | -0.10984300 |
| H | 0.61482700  | 2.01745800  | 0.85888600  |
| C | 0.99376500  | 1.56435700  | -0.05508200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.07730600  | 1.60370900  | -0.07787600 |
| H | 0.56499600  | 2.03919800  | -0.93342200 |
| H | -2.06077000 | 0.78652100  | 1.25417200  |
| O | 3.47274700  | -0.62637900 | 0.06509000  |
| H | 2.55408700  | -0.93996400 | -0.01184900 |

#### TS1-0w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.32916700 | -0.74081100 | -1.16039200 |
| O | -1.50569200 | 1.45494000  | -0.09780700 |
| O | -1.23266900 | -0.61832400 | 1.25880100  |
| O | 0.58508800  | 0.31276000  | -0.11317600 |
| S | -0.97051900 | 0.16216500  | 0.09380000  |
| H | 1.29812900  | -1.52513900 | -0.77126400 |
| C | 1.39270100  | -0.83685900 | 0.06565200  |
| H | 2.51907200  | -0.41521100 | 0.03447400  |
| H | 1.24800100  | -1.28759400 | 1.04359300  |
| H | -1.77668800 | -1.53741700 | -0.84836800 |
| O | 3.57633200  | 0.34057500  | -0.04042800 |
| H | 3.13244300  | 1.19875000  | -0.12912600 |

#### PD1-0w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 0.45484100  | -0.30370700 | -1.17070600 |
| O | -1.35875600 | -1.55322100 | -0.12961400 |
| O | 0.33434100  | -0.36537600 | 1.24992600  |
| O | -1.38446800 | 0.82940900  | -0.04058200 |
| S | -0.46993900 | -0.47369400 | 0.06802300  |
| H | -1.48942400 | 2.86271600  | 0.12660500  |
| C | -0.78108100 | 2.05801200  | 0.03987100  |
| H | 3.36433900  | 0.81482200  | -0.04626700 |
| H | 0.18232000  | 2.17429700  | -0.43345600 |
| H | 1.39262300  | -0.12227600 | -0.86930700 |
| O | 2.75151200  | 0.07754600  | -0.02956500 |
| H | 2.37588300  | 0.02426100  | 0.85915700  |

#### RC1-1w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 0.98389900  | -0.28741200 | -1.19841500 |
| O | -0.25804300 | -2.01688000 | -0.02725000 |
| O | 1.05106100  | -0.31136800 | 1.22403300  |
| O | -1.03508800 | 0.23060700  | 0.06663500  |
| S | 0.23887200  | -0.69934400 | 0.10419300  |
| H | -0.16569900 | 2.01510800  | -0.54550200 |
| C | -0.82701900 | 1.64356000  | 0.23602700  |
| H | -1.81251700 | 2.08723000  | 0.14042800  |
| H | -0.40693800 | 1.83489400  | 1.22019700  |
| H | 1.79060000  | 0.25886300  | -0.96654100 |
| O | 2.94139700  | 1.10880300  | -0.21794900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.87389400  | 0.96895700  | -0.39671100 |
| H | 2.76422700  | 0.77489700  | 0.67187100  |
| O | -3.90824900 | 0.46054100  | -0.22572700 |
| H | -3.10321800 | -0.08612700 | -0.17761800 |

#### TS1-1w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.18306100 | 0.11469300  | -1.15624500 |
| O | -0.54654500 | 2.18907000  | -0.06299700 |
| O | -0.99100000 | 0.13067400  | 1.26000300  |
| O | 1.01314200  | 0.38376100  | -0.12469100 |
| S | -0.50698300 | 0.78363200  | 0.07516100  |
| H | 1.03521600  | -1.53741600 | -0.91850900 |
| C | 1.34470700  | -0.98718000 | -0.03207100 |
| H | 2.54384400  | -1.00347400 | -0.01999400 |
| H | 1.01521400  | -1.42460500 | 0.90699500  |
| H | -1.65976900 | -0.71628200 | -0.86570200 |
| O | -2.25501100 | -1.96503800 | -0.02969200 |
| H | -3.15941600 | -2.27458100 | -0.11403500 |
| H | -2.16223700 | -1.57317400 | 0.84911400  |
| O | 3.80642200  | -0.65248100 | 0.00935300  |
| H | 3.67906300  | 0.30907000  | -0.01387200 |

#### PD1-1w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -0.11581600 | -0.83468800 | -0.91318700 |
| O | -2.38163500 | -0.01554400 | -0.89568900 |
| O | -1.25985300 | -0.68200400 | 1.22799700  |
| O | -0.65076400 | 1.36854200  | 0.01997700  |
| S | -1.22639200 | -0.14268000 | -0.09101000 |
| H | 0.54306200  | 0.90217300  | 1.67729300  |
| C | 0.40563200  | 1.58758500  | 0.85293700  |
| H | 2.38704100  | 1.16886500  | -0.34387100 |
| H | 0.66177900  | 2.63281200  | 0.92390000  |
| H | 0.63276300  | -1.17704100 | -0.31720000 |
| O | 1.87201300  | -1.48395900 | 0.52625800  |
| H | 2.58458600  | -0.93301800 | 0.15412700  |
| H | 2.20020900  | -2.37309000 | 0.67041700  |
| O | 3.15004400  | 0.62363700  | -0.57800200 |
| H | 3.26713900  | 0.72880500  | -1.52495300 |

#### RC1-2w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -0.48382500 | -0.62164800 | -1.07105300 |
| O | -0.22710500 | 1.40009600  | 0.29223900  |
| O | -0.36590500 | -0.82649600 | 1.34589700  |
| O | 1.58635400  | -0.11642900 | 0.02141500  |
| S | 0.03687700  | -0.00632700 | 0.24484800  |
| H | 1.72241000  | -2.02250000 | -0.78775500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.16011400  | -1.44004300 | 0.01969400  |
| H | 3.22017300  | -1.28286300 | -0.14831000 |
| H | 1.98172900  | -1.91299800 | 0.98172600  |
| H | -1.46859500 | -0.91302500 | -0.92451000 |
| O | -2.87552800 | -1.14238800 | -0.51363200 |
| H | -3.17651600 | -0.22672900 | -0.33509700 |
| H | -2.85288900 | -1.58358200 | 0.34109400  |
| O | -3.05052400 | 1.51025200  | -0.08657100 |
| H | -3.60560500 | 2.14457300  | 0.36851300  |
| H | -2.13056300 | 1.75163300  | 0.09724000  |
| O | 4.11716600  | 1.23720900  | -0.40877400 |
| H | 3.15407300  | 1.26221600  | -0.26478000 |

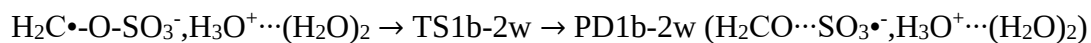
#### TS1-2w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -0.43024000 | 0.27462100  | 1.26492600  |
| O | -0.74649900 | -1.41057900 | -0.48705200 |
| O | 0.46255900  | 0.68275300  | -0.95822400 |
| O | 1.39664500  | -1.06563300 | 0.50428100  |
| S | 0.10461100  | -0.35364600 | -0.03499200 |
| H | 3.19812100  | -0.90813800 | 1.40062100  |
| C | 2.45668100  | -0.24839100 | 0.96439100  |
| H | 2.99119400  | 0.28499900  | 0.03314100  |
| H | 2.10922500  | 0.52697800  | 1.64292600  |
| H | -1.23141500 | 0.90222100  | 1.03525000  |
| O | -2.41031500 | 1.62616700  | 0.57004100  |
| H | -2.93603200 | 0.93782400  | 0.09821200  |
| H | -2.20300300 | 2.31172300  | -0.07045400 |
| O | -3.41594600 | -0.49037900 | -0.68084200 |
| H | -4.11434500 | -1.06488100 | -0.36254600 |
| H | -2.61047700 | -1.02770800 | -0.73289600 |
| O | 3.38046800  | 0.89861800  | -1.06906300 |
| H | 2.48949900  | 1.06112400  | -1.42325500 |

#### PD1-2w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 0.31032300  | 0.01677100  | 1.21274200  |
| O | 0.26791000  | -1.51761600 | -0.68605900 |
| O | 0.49515100  | 0.89176200  | -1.04160000 |
| O | 2.31450000  | -0.44726700 | -0.09087500 |
| S | 0.73170700  | -0.24966200 | -0.17763200 |
| H | 4.10822300  | 0.39908400  | 0.39742200  |
| C | 3.04811600  | 0.55950900  | 0.48483300  |
| H | -1.78167800 | 3.09011200  | -0.42644400 |
| H | 2.59546200  | 1.09565600  | 1.30437300  |
| H | -1.12531300 | 0.23135500  | 1.31537700  |
| O | -2.14892200 | 0.36506500  | 1.15050200  |
| H | -2.41080400 | -0.48328700 | 0.64918000  |
| H | -2.16982900 | 1.14246000  | 0.49033800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -2.38082300 | -1.81449100 | -0.12613500 |
| H | -2.92460800 | -1.95986900 | -0.90274700 |
| H | -1.44615700 | -1.89735700 | -0.40938900 |
| O | -1.84408100 | 2.15214100  | -0.61669400 |
| H | -0.95375800 | 1.84845500  | -0.90003800 |

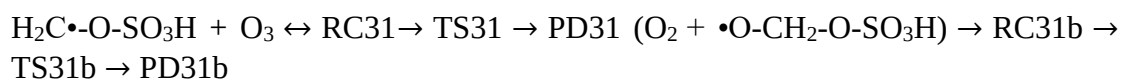


#### TS1b-2w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -0.36486700 | -0.05073100 | 1.11765100  |
| O | -0.36067200 | 1.24301500  | -0.96306700 |
| O | -0.15895100 | -1.21025100 | -1.04031100 |
| O | -2.70083200 | -0.24863200 | -0.27198100 |
| S | -0.67380500 | -0.03974000 | -0.33758100 |
| H | -3.23232400 | -0.57541900 | 1.66725200  |
| C | -3.24094800 | 0.09458800  | 0.80869900  |
| H | 2.42969500  | -2.82424100 | 0.03866300  |
| H | -3.66786200 | 1.09193100  | 0.91551400  |
| H | 1.07044100  | 0.03244100  | 1.37280800  |
| O | 2.11192600  | 0.07276600  | 1.30176400  |
| H | 2.27237900  | 0.89286900  | 0.71486900  |
| H | 2.33410200  | -0.75580400 | 0.74977600  |
| O | 2.10881500  | 2.09179700  | -0.22733800 |
| H | 2.70071600  | 2.23027400  | -0.96951200 |
| H | 1.20911200  | 1.96271500  | -0.59763100 |
| O | 2.32449400  | -1.91651300 | -0.25296000 |
| H | 1.43101400  | -1.83806500 | -0.65270400 |

#### PD1b-2w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -0.31564200 | -0.46259700 | 0.96129800  |
| O | -0.82062400 | 0.91469300  | -1.00729600 |
| O | 0.73008400  | -0.99243100 | -1.19820400 |
| O | -3.32606900 | -0.72781700 | 0.09888600  |
| S | -0.45722100 | -0.42768300 | -0.53065500 |
| H | -4.43636500 | 0.57510000  | 1.14179500  |
| C | -3.45729300 | 0.28404400  | 0.72523500  |
| H | 3.30787900  | -2.19481300 | 0.45683600  |
| H | -2.61006900 | 0.96259900  | 0.90909000  |
| H | 0.94333400  | 0.07931500  | 1.36296900  |
| O | 1.91074000  | 0.49764800  | 1.43173700  |
| H | 1.86150100  | 1.27946400  | 0.78308000  |
| H | 2.50100700  | -0.21310600 | 1.00987600  |
| O | 1.44859300  | 2.31436500  | -0.30583000 |
| H | 2.03233000  | 2.43252100  | -1.05879400 |
| H | 0.59332200  | 2.00637100  | -0.66909900 |
| O | 3.06957800  | -1.33507900 | 0.10452700  |
| H | 2.29306900  | -1.45905200 | -0.47763200 |



#### RC31

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 0.95254500  | 1.24742400  | 0.84096200  |
| O | 2.35385800  | 0.46319000  | -0.98840700 |
| O | 1.62104200  | -1.05940600 | 0.85509700  |
| O | 0.07981300  | -0.28332100 | -0.87595200 |
| S | 1.39718200  | 0.01756000  | -0.04050700 |
| H | -0.50309100 | -2.00739100 | 0.12934500  |
| C | -0.92962800 | -1.09092600 | -0.27577400 |
| H | -1.63790000 | -1.29027500 | -1.07701800 |
| H | 1.10933500  | 2.06447500  | 0.34874800  |
| O | -2.36775500 | 0.67030200  | 0.34062200  |
| O | -3.08796600 | 0.37701200  | -0.61553800 |
| O | -1.51972400 | -0.47797700 | 0.80592700  |

#### TS31

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.29032900  | -0.72882600 | 1.27118400  |
| O | 2.16468300  | 1.33662900  | 0.27948600  |
| O | 1.95459800  | -0.78653500 | -1.01706500 |
| O | 0.00808500  | 0.55759200  | -0.38855300 |
| S | 1.49014300  | 0.13094000  | -0.03851900 |
| H | -0.38988900 | -1.29551500 | -1.26823600 |
| C | -0.91980400 | -0.47640800 | -0.77316800 |
| H | -1.58796100 | 0.01443900  | -1.49091800 |
| H | 1.10539100  | -0.14858300 | 2.02187000  |
| O | -2.87943300 | 0.06596100  | 0.61237300  |
| O | -3.13455300 | 0.81276700  | -0.28410200 |
| O | -1.58508500 | -0.98345400 | 0.27575100  |

#### PD31

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.44026400 | 0.51866500  | 1.33430500  |
| O | -1.91303900 | -1.56403300 | 0.12309600  |
| O | -2.10659500 | 0.68381600  | -0.94708600 |
| O | 0.05838500  | -0.32625600 | -0.41762100 |
| S | -1.47833400 | -0.22730900 | -0.05737100 |
| H | 0.09191700  | 1.63980100  | -1.11885000 |
| C | 0.77038900  | 0.90462700  | -0.65782600 |
| H | 1.54409700  | 0.64057600  | -1.39101900 |
| H | -1.11563500 | -0.07789100 | 2.02265700  |
| O | 3.14009100  | -0.37403900 | 0.60845200  |
| O | 3.26579400  | -0.86685800 | -0.46421200 |
| O | 1.30945700  | 1.42954100  | 0.43207900  |

## RC31b

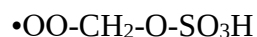
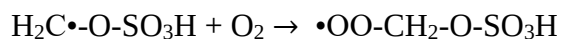
|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 0.45654500  | 1.40518400  | 0.46105400  |
| O | 1.83512600  | -0.07522600 | -0.92964100 |
| O | 0.83051200  | -0.81844800 | 1.23196000  |
| O | -0.51726400 | -0.47375500 | -0.78135600 |
| S | 0.78571000  | -0.07593000 | 0.02257200  |
| H | -1.54659700 | -0.91377300 | 0.97694700  |
| C | -1.75356700 | -0.56279300 | -0.04646900 |
| H | -2.33692400 | -1.33486600 | -0.56574000 |
| H | 0.51712000  | 1.99686500  | -0.30148000 |
| O | -2.44036400 | 0.56767200  | -0.00602400 |

## TS31b

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.11943300  | 1.43354300  | 0.12493300  |
| O | 1.91240600  | -0.79243400 | -0.44252500 |
| O | 0.20763200  | -0.44232100 | 1.32600100  |
| O | -0.40572500 | -0.15321000 | -0.95297900 |
| S | 0.75059100  | -0.09818800 | -0.00602900 |
| H | -1.17264800 | -0.49407800 | 0.97756500  |
| C | -1.94458000 | -0.41978400 | -0.00439000 |
| H | -2.13695000 | -1.41610900 | -0.42593200 |
| H | 1.92628400  | 1.60572900  | -0.37693500 |
| O | -2.70358000 | 0.50369400  | -0.06191600 |

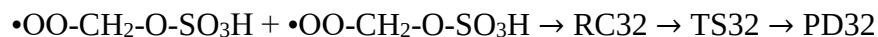
## PD31b

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -0.34737500 | 1.41993600  | -0.19657900 |
| O | -2.25247400 | 0.02748400  | 0.21041700  |
| O | -0.51568300 | -0.80513800 | -1.22930900 |
| O | -0.02208100 | -0.59362900 | 1.14348800  |
| S | -0.84668800 | -0.04067400 | 0.11125900  |
| H | 0.39471200  | -1.13925700 | -1.19217500 |
| C | 2.40215400  | -0.57900300 | 0.00463700  |
| H | 2.81004600  | -1.22582500 | 0.81181000  |
| H | 0.61509800  | 1.47923400  | -0.09250300 |
| O | 2.55189100  | 0.57767800  | -0.09490400 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 0.61365300  | -0.60708600 | 1.33097600  |
| O | 2.27316300  | 0.51369900  | -0.02273200 |
| O | 0.65321300  | -1.06311100 | -1.06422200 |
| O | -0.02452100 | 1.15880900  | -0.26757800 |
| S | 0.99378500  | -0.07599600 | -0.10267400 |
| H | -1.77293800 | 2.07299200  | 0.00986300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.31895300 | 1.11686000  | 0.24886500  |
| H | -1.32073400 | 0.90005200  | 1.31497800  |
| H | -0.12554000 | -1.23217900 | 1.24040600  |
| O | -1.97973900 | -1.04111400 | 0.12527200  |
| O | -2.13172200 | 0.13554200  | -0.40367300 |



#### RC32

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.37504500 | -0.75181600 | -1.28772500 |
| O | -3.17225800 | -1.90351800 | -0.08774200 |
| O | -1.14447700 | -1.19431300 | 1.09043700  |
| O | -2.81914400 | 0.43151300  | 0.27932000  |
| S | -2.11746000 | -0.97555900 | 0.04663900  |
| H | -3.26067900 | 2.29888100  | -0.32731600 |
| C | -2.39586400 | 1.64227700  | -0.31403900 |
| H | -2.00507600 | 1.45599000  | -1.31126300 |
| H | -0.37718700 | -0.90015200 | -1.20996000 |
| O | -0.34740500 | 1.46806200  | 0.60000700  |
| O | -1.45444200 | 2.31447500  | 0.47527300  |
| O | 1.37446300  | -0.75270400 | 1.28766000  |
| O | 3.17140100  | -1.90445500 | 0.08755300  |
| O | 1.14381700  | -1.19445800 | -1.09050600 |
| O | 2.81902600  | 0.43067300  | -0.27911700 |
| S | 2.11689100  | -0.97614100 | -0.04668500 |
| H | 3.26179400  | 2.29760700  | 0.32834800  |
| C | 2.39656600  | 1.64150100  | 0.31457900  |
| H | 2.00554800  | 1.45510700  | 1.31170800  |
| H | 0.37644200  | -0.90000800 | 1.20970700  |
| O | 0.34853000  | 1.46893800  | -0.60101900 |
| O | 1.45604200  | 2.31474200  | -0.47460900 |

#### TS32

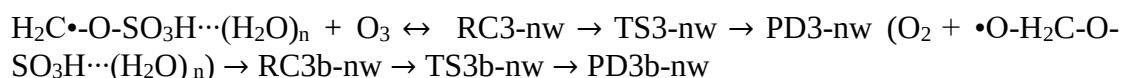
|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 3.09339600  | -1.26513400 | 1.10087100  |
| O | 5.11354100  | -0.52606700 | -0.04291800 |
| O | 2.96327900  | -0.79093700 | -1.27421400 |
| O | 3.35526400  | 1.03547300  | 0.32839900  |
| S | 3.70669100  | -0.44719000 | -0.10909900 |
| H | 2.08910600  | 2.39365200  | 1.07126700  |
| C | 2.01323400  | 1.41802600  | 0.59195700  |
| H | 1.53341800  | 0.70647600  | 1.27140800  |
| H | 2.32477800  | -1.75796700 | 0.78137200  |
| O | 0.44733200  | 0.32468100  | -0.90439900 |
| O | 1.26014700  | 1.61977100  | -0.52921100 |
| O | -3.26554500 | -1.59913400 | 0.38267400  |
| O | -4.91795100 | -0.54285600 | -1.00032400 |
| O | -4.22402900 | 0.51441800  | 1.15198300  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -2.75577100 | 0.50064600  | -0.79797900 |
| S | -3.94847800 | -0.24309500 | -0.02086100 |
| H | -1.82532100 | 2.12225300  | 0.14121900  |
| C | -1.71782400 | 1.03933600  | -0.00022400 |
| H | -0.75744300 | 1.04065300  | -0.81658900 |
| H | -2.59078000 | -1.42221800 | 1.05767200  |
| O | 0.33789500  | -0.46447900 | 0.03140500  |
| O | -1.24226400 | 0.34581000  | 0.93153900  |

#### PD32

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.05435300 | -1.03867700 | -1.35272400 |
| O | -3.30819600 | -1.49874700 | -0.68269300 |
| O | -1.45925500 | -1.66798700 | 0.97429700  |
| O | -2.16157900 | 0.48083200  | 0.21678400  |
| S | -2.05603100 | -1.07357000 | -0.17989600 |
| H | -3.28248600 | 0.86574100  | -1.49202400 |
| C | -2.77719700 | 1.36524900  | -0.65935600 |
| H | -0.23901900 | -0.81728200 | 1.93991900  |
| H | -0.10370800 | -1.05335000 | -1.04238000 |
| O | -0.24872700 | 0.99882800  | 2.55520600  |
| O | -2.72667200 | 2.52196600  | -0.44972700 |
| O | 2.57059200  | 0.08200500  | 1.12530800  |
| O | 3.86228800  | -0.83802200 | -0.70625200 |
| O | 1.42170400  | -1.18250200 | -0.59496600 |
| O | 2.40464800  | 1.01832800  | -1.14510400 |
| S | 2.58847200  | -0.38800600 | -0.31065000 |
| H | 1.36775300  | 2.67471000  | -1.57057900 |
| C | 1.31137000  | 1.78205900  | -0.94263100 |
| H | -0.37185800 | 1.37224700  | 1.66756400  |
| H | 1.62271900  | -0.02530800 | 1.60365800  |
| O | 0.43792200  | -0.20701300 | 2.29979400  |
| O | 0.42194100  | 1.51656600  | -0.19561000 |



#### RC3-1w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.15079800  | -0.03431500 | 1.39293100  |
| O | 1.89480900  | 1.06734000  | -0.66814500 |
| O | 2.39390700  | -1.32112700 | -0.19805000 |
| O | 0.13839000  | -0.51913300 | -0.78408700 |
| S | 1.54500000  | -0.18885300 | -0.08062700 |
| H | 0.09498600  | -2.44216300 | 0.01107800  |
| C | -0.57778500 | -1.66024300 | -0.34512800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.15377800 | -1.99518800 | -1.20443300 |
| H | 0.43200400  | 0.70540000  | 1.50620800  |
| O | -0.66779600 | 2.35348900  | -1.07457800 |
| H | -1.20206300 | 1.71414000  | -1.55461000 |
| H | 0.24902000  | 2.09311700  | -1.24685400 |
| O | -0.64585800 | 1.71106500  | 1.49390400  |
| H | -0.53883000 | 2.47458700  | 2.06521700  |
| H | -0.74230600 | 2.04345500  | 0.56568900  |
| O | -2.54834300 | -0.52763800 | 0.35311200  |
| O | -2.63715400 | -0.30465900 | -0.85645400 |
| O | -1.37779400 | -1.37630100 | 0.74368100  |

#### TS3-1w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.14712000  | -0.22119700 | 1.40008200  |
| O | 2.11230800  | 0.66199700  | -0.67257900 |
| O | 2.05039100  | -1.76880500 | -0.19048000 |
| O | 0.03163400  | -0.47941900 | -0.76234500 |
| S | 1.47438500  | -0.47483700 | -0.07871300 |
| H | -0.35308200 | -2.44576500 | -0.17524700 |
| C | -0.88763300 | -1.50816300 | -0.36252000 |
| H | -1.54822200 | -1.62970000 | -1.22863000 |
| H | 0.57667300  | 0.63117800  | 1.50360200  |
| O | 0.18378200  | 2.69206300  | -1.00959100 |
| H | -0.43618500 | 2.43920500  | -1.69685100 |
| H | 0.95585800  | 2.11692600  | -1.13105500 |
| O | -0.29096400 | 1.85224500  | 1.47091600  |
| H | -0.08695000 | 2.53992300  | 2.10837400  |
| H | -0.21161000 | 2.25453400  | 0.57270300  |
| O | -2.80864900 | -0.11458800 | 0.30907700  |
| O | -3.00930900 | -0.08011500 | -0.86810800 |
| O | -1.56141900 | -1.19967200 | 0.75823200  |

PD3-1w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.31449600  | 0.19015400  | 1.32691300  |
| O | 1.52661800  | 1.35694200  | -0.81674100 |
| O | 2.59933100  | -0.84396700 | -0.41087700 |
| O | 0.16858000  | -0.58897900 | -0.68768100 |
| S | 1.53517900  | 0.07104300  | -0.18648500 |
| H | 0.80134800  | -2.52356800 | -0.24712500 |
| C | -0.12269400 | -1.92297600 | -0.24270700 |
| H | -0.80395500 | -2.32830100 | -1.00236100 |
| H | 0.47207900  | 0.75805000  | 1.52938000  |
| O | -1.17996100 | 2.20506100  | -0.88967300 |
| H | -1.67111800 | 1.59093600  | -1.44057500 |
| H | -0.24947700 | 2.07388700  | -1.12916400 |
| O | -0.78068300 | 1.53829700  | 1.66377200  |
| H | -0.72468500 | 2.33250300  | 2.19992000  |
| H | -1.06076600 | 1.81808100  | 0.75966900  |
| O | -2.73178700 | -0.51478500 | 0.25362500  |
| O | -2.81766000 | -0.51723800 | -0.93143700 |
| O | -0.67269900 | -1.99053600 | 0.96338000  |

RC3b-1w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -0.16212100 | -0.21271900 | 1.41659300  |
| O | 0.65578000  | -1.60160200 | -0.43006900 |
| O | -1.73816400 | -1.55886100 | 0.22097200  |
| O | -0.65251700 | 0.32769800  | -0.91604600 |
| S | -0.48402800 | -0.90374400 | 0.08516400  |
| H | -2.53327800 | 0.72745900  | -0.11555700 |
| C | -1.70583100 | 1.25716800  | -0.61347500 |
| H | -2.06920700 | 1.61527400  | -1.58629900 |
| H | 0.76596600  | 0.25558200  | 1.39205500  |
| O | 2.67659700  | 0.18806400  | -1.22402200 |
| H | 2.39120100  | 0.75159500  | -1.94615400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.06368500  | -0.56342100 | -1.21484300 |
| O | 2.06923800  | 0.91308900  | 1.25831500  |
| H | 2.75020400  | 0.61491600  | 1.86530700  |
| H | 2.39962100  | 0.74391500  | 0.34298700  |
| O | -1.32240700 | 2.29077800  | 0.12184800  |

#### TS3b-1w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 0.41913500  | -0.96165800 | 1.13068400  |
| O | 0.85767600  | -0.87574500 | -1.26340400 |
| O | -1.36360200 | -1.50790500 | -0.37303200 |
| O | -0.63829200 | 0.76368000  | -0.25668000 |
| S | -0.14791700 | -0.66800700 | -0.26342700 |
| H | -2.31461200 | -0.49998800 | -0.18180000 |
| C | -2.43914800 | 0.75552500  | -0.08104400 |
| H | -2.63830700 | 1.19183000  | -1.06953000 |
| H | 1.37133700  | -0.56758900 | 1.23821600  |
| O | 2.24485300  | 1.60882900  | -0.86816800 |
| H | 1.47100100  | 2.14879600  | -0.68071200 |
| H | 1.89601500  | 0.87530900  | -1.39379200 |
| O | 2.68819000  | 0.10351800  | 1.30370800  |
| H | 3.45164500  | -0.46749600 | 1.19381900  |
| H | 2.68213900  | 0.73301900  | 0.54483700  |
| O | -2.82266700 | 1.21191800  | 0.95814900  |

#### PD3b-1w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 0.07231200  | 0.38493700  | -1.14761900 |
| O | -1.32823000 | -1.50265200 | -0.42832800 |
| O | 1.07067700  | -1.66206900 | -0.44161800 |
| O | -0.02692300 | -0.21006800 | 1.20665000  |
| S | -0.15495800 | -0.74993100 | -0.12059900 |
| H | 1.89118300  | -1.18413900 | -0.20537200 |
| C | 2.86998300  | 0.66203900  | 0.43536100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.06260400  | 1.22438700  | 0.96127900  |
| H | -0.68831400 | 1.07672300  | -1.05802900 |
| O | -2.91552900 | 0.41413100  | 1.14495000  |
| H | -2.16902500 | 0.36264800  | 1.75385400  |
| H | -2.90344700 | -0.44731400 | 0.70929700  |
| O | -1.84838300 | 1.96879300  | -0.74762600 |
| H | -2.45031400 | 2.18544300  | -1.46259100 |
| H | -2.36817300 | 1.49692000  | -0.05201700 |
| O | 3.96169100  | 1.02092800  | 0.24746500  |

#### RC3-2w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 0.25368100  | -1.24831900 | -1.39310000 |
| O | 0.50664900  | -2.01659800 | 0.92393300  |
| O | 2.35219100  | -0.90708500 | -0.30119800 |
| O | 0.36404800  | 0.30939900  | 0.49321900  |
| S | 0.95751800  | -1.06841600 | -0.04649000 |
| H | 1.22988800  | 1.43174900  | -1.04586300 |
| C | 0.38470200  | 1.45100100  | -0.35852200 |
| H | 0.45403900  | 2.30815900  | 0.30377500  |
| H | 3.96616800  | 2.04352200  | 0.77809300  |
| H | -0.78204500 | -1.29909600 | -1.26714600 |
| O | -2.09115300 | -0.95940200 | 1.67010000  |
| H | -1.95675400 | -0.03797900 | 1.91156600  |
| H | -1.22637200 | -1.37926200 | 1.78551400  |
| O | -2.20369200 | -1.28929000 | -0.95271000 |
| H | -2.69130800 | -2.08438600 | -1.18005000 |
| H | -2.29158100 | -1.15834400 | 0.02584500  |
| O | 3.09980600  | 1.73426200  | 0.51069500  |
| H | 3.19233500  | 0.78780100  | 0.34896100  |
| O | -1.96709000 | 1.80382600  | -0.40660900 |
| O | -1.77548800 | 2.06656100  | 0.78510300  |
| O | -0.72931200 | 1.47870700  | -1.17514800 |

TS3-2w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -0.99773300 | -0.55249600 | 1.17876700  |
| O | -0.55107700 | -2.25988400 | -0.52588900 |
| O | -2.35671400 | -0.58636300 | -0.78924700 |
| O | 0.03478300  | -0.00713800 | -0.97305300 |
| S | -1.06334800 | -0.94168400 | -0.30825900 |
| H | -1.12090000 | 1.74799800  | -0.81690500 |
| C | -0.07359000 | 1.42460400  | -0.79945400 |
| H | 0.47186600  | 1.83069000  | -1.65742400 |
| H | -2.38521100 | 1.69443300  | 1.44757700  |
| H | -0.03652300 | -0.68512400 | 1.54521200  |
| O | 2.28153400  | -2.00679200 | -0.33357800 |
| H | 2.56650500  | -1.39303700 | -1.01493600 |
| H | 1.40700100  | -2.31337600 | -0.61860000 |
| O | 1.38505000  | -0.88370100 | 1.90366700  |
| H | 1.56239200  | -1.44250600 | 2.66367300  |
| H | 1.83970300  | -1.29219100 | 1.12661700  |
| O | -2.83708000 | 1.94535500  | 0.63835700  |
| H | -3.13824900 | 1.10910500  | 0.26740300  |
| O | 2.13322600  | 1.78197400  | 0.24660400  |
| O | 2.51973600  | 1.64614300  | -0.87677200 |
| O | 0.42434100  | 1.83081900  | 0.37942600  |

PD3-2w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -0.54865500 | -1.09239200 | 1.33183100  |
| O | -0.07127900 | -2.06657100 | -0.86816000 |
| O | -2.24616300 | -1.01781300 | -0.35042400 |
| O | -0.17826800 | 0.29416000  | -0.64419100 |
| S | -0.83140100 | -1.07135800 | -0.17434900 |
| H | -1.73829100 | 1.52079200  | 0.07306000  |
| C | -0.63695800 | 1.53012100  | -0.03579900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.38244600 | 2.29896400  | -0.77758600 |
| H | -4.58388100 | 1.42929200  | 0.37733400  |
| H | 0.47236200  | -1.03688600 | 1.51314600  |
| O | 2.61094400  | -1.17433700 | -0.95336000 |
| H | 2.70711300  | -0.40208700 | -1.51516200 |
| H | 1.76242600  | -1.57386900 | -1.20002400 |
| O | 1.93893700  | -0.91851700 | 1.61641700  |
| H | 2.38163300  | -1.59404300 | 2.13505600  |
| H | 2.31607000  | -0.95799700 | 0.70539200  |
| O | -3.81761300 | 1.34741100  | -0.19222800 |
| H | -3.63508800 | 0.40291500  | -0.26260900 |
| O | 2.33751600  | 1.82893600  | 0.17154300  |
| O | 2.28968400  | 1.99964000  | -1.00340700 |
| O | -0.08706900 | 1.78372300  | 1.13645000  |

#### RC3b-2w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -0.12188700 | -0.30011300 | 1.23847900  |
| O | 1.02072000  | -1.67713100 | -0.44268700 |
| O | -1.44429700 | -1.52916000 | -0.32945300 |
| O | -0.04841100 | 0.33638900  | -1.11912200 |
| S | -0.16322100 | -0.92272500 | -0.16279000 |
| H | -1.85970800 | 1.13012600  | -0.37262100 |
| C | -0.92572200 | 1.46429700  | -0.86525400 |
| H | -1.18936200 | 1.84936000  | -1.85961600 |
| H | -3.68389600 | 0.28606400  | 1.49506500  |
| H | 0.83042700  | 0.06846600  | 1.47474200  |
| O | 3.10742000  | 0.23089900  | -0.74512600 |
| H | 2.83971400  | 0.90434600  | -1.37476100 |
| H | 2.54239200  | -0.53473800 | -0.92927200 |
| O | 2.15973300  | 0.57912500  | 1.70674000  |
| H | 2.68795100  | 0.07211200  | 2.32769200  |
| H | 2.62239800  | 0.54329600  | 0.83298100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -3.51137200 | 0.23776000  | 0.55333300  |
| H | -3.06502400 | -0.60589000 | 0.41163300  |
| O | -0.35678500 | 2.40531600  | -0.13837400 |

#### TS3b-2w

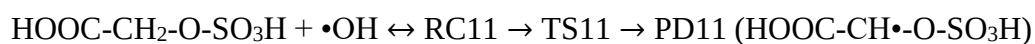
|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -0.05481900 | -0.66433200 | 1.09758700  |
| O | 0.26380800  | -1.99994500 | -0.93994200 |
| O | -1.93290500 | -1.08860900 | -0.28739500 |
| O | -0.15351000 | 0.36357600  | -1.11641800 |
| S | -0.47374400 | -0.93025400 | -0.36081200 |
| H | -1.79771500 | 1.41388400  | 0.45359400  |
| C | -0.59708400 | 1.79581100  | -0.51173600 |
| H | -1.08697400 | 2.22699300  | -1.39457700 |
| H | -2.23767900 | 0.75996000  | 1.91141300  |
| H | 0.99611000  | -0.78671800 | 1.21714300  |
| O | 2.74542100  | 1.08121900  | -0.38561500 |
| H | 1.99626600  | 1.64789800  | -0.12632800 |
| H | 2.51917500  | 0.79143000  | -1.27399300 |
| O | 2.38935400  | -0.91240300 | 1.26449700  |
| H | 2.65778800  | -1.74877400 | 0.87391100  |
| H | 2.68098900  | -0.18881500 | 0.64436200  |
| O | -2.57700100 | 0.87217700  | 1.01237500  |
| H | -2.45053200 | -0.06646800 | 0.50552900  |
| O | 0.30527300  | 2.35579300  | 0.10895500  |

#### PD3b-2w

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.11908000  | 0.10445100  | 1.08892900  |
| O | 2.19742700  | 0.42159600  | -1.09660800 |
| O | 1.48340100  | -1.76431600 | -0.34170500 |
| O | -0.19681200 | -0.10612200 | -0.94589500 |
| S | 1.14797100  | -0.25843900 | -0.42175200 |
| H | -1.26339400 | -2.28043700 | 0.84727500  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.61612300 | -1.04121000 | -0.45374100 |
| H | -2.40827900 | -1.23619000 | -1.52892000 |
| H | -0.27100400 | -1.96752500 | 1.97685800  |
| H | 0.97304900  | 1.12178700  | 1.19695300  |
| O | -1.43514200 | 2.38134600  | -0.39005500 |
| H | -2.31729800 | 2.20011000  | -0.05688200 |
| H | -1.12727800 | 1.54387500  | -0.77104500 |
| O | 0.66504800  | 2.57543700  | 1.22909300  |
| H | 1.34678800  | 3.11506000  | 0.82094800  |
| H | -0.15062700 | 2.67607200  | 0.68415600  |
| O | -0.42258000 | -2.56333200 | 1.23557600  |
| H | 0.77755300  | -2.21537800 | 0.21334200  |
| O | -3.18921000 | -0.12094700 | -0.01836200 |



#### RC11

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 0.52651900  | -0.38134800 | 1.47798600  |
| O | 2.45664300  | -0.31517600 | -0.13970600 |
| O | 0.70741900  | -1.96794700 | -0.43102400 |
| O | 0.22503200  | 0.41049200  | -0.84988200 |
| S | 1.06923100  | -0.55100900 | 0.15303000  |
| C | -0.92276400 | 1.04963800  | -0.32183400 |
| H | -1.21872300 | 1.77729700  | -1.08308400 |
| H | -0.68083700 | 1.57721400  | 0.60781400  |
| C | -2.04561000 | 0.04611500  | -0.09210500 |
| H | -0.27389600 | -2.05166100 | -0.41387100 |
| O | -1.92853600 | -1.14029700 | -0.26790700 |
| H | -3.15924600 | 1.51891300  | 0.45294500  |
| O | -3.20720900 | 0.56261200  | 0.31520900  |
| O | 1.67208700  | 2.52278700  | -0.03519900 |
| H | 2.41961600  | 1.89088600  | -0.08446700 |

#### TS11

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -0.53435400 | 0.70064100  | -1.16099100 |
| O | -2.62328500 | 0.79594000  | 0.24881500  |
| O | -1.69177900 | -1.35549200 | -0.37094600 |
| O | -0.46798000 | 0.08553800  | 1.22491100  |
| S | -1.39741500 | 0.16745800  | -0.12490200 |
| C | 0.91294100  | 0.19173500  | 1.05989700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.36316800  | 0.13190900  | 2.05470200  |
| H | 1.22374700  | 1.25873200  | 0.64607200  |
| C | 1.51955700  | -0.84376600 | 0.11799500  |
| H | -0.83079800 | -1.84186900 | -0.40591900 |
| O | 0.95389000  | -1.87933800 | -0.15054300 |
| H | 2.90115000  | 0.40066800  | -0.27484000 |
| O | 2.72576900  | -0.55915000 | -0.33797200 |
| O | 1.87718900  | 2.10933800  | -0.22394000 |
| H | 1.19079000  | 2.10360700  | -0.92360900 |

#### PD11

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -0.56999300 | 0.96804400  | -0.98458000 |
| O | -2.69121200 | 0.73527500  | 0.35464200  |
| O | -1.62901500 | -1.24215400 | -0.60190100 |
| O | -0.53219200 | -0.04238200 | 1.27963200  |
| S | -1.44209900 | 0.21788800  | -0.10247600 |
| C | 0.80944400  | -0.10930200 | 1.16475300  |
| H | 1.36572800  | 0.43244000  | 1.91839000  |
| C | 1.44301100  | -0.92554100 | 0.14033400  |
| H | -0.69572000 | -1.65868600 | -0.64791600 |
| O | 0.84294300  | -1.79829100 | -0.48569100 |
| H | 2.92968800  | 0.23581200  | 0.07196400  |
| O | 2.73742000  | -0.71328900 | -0.06407500 |
| O | 2.11591300  | 1.97258600  | -0.27613500 |
| H | 1.24186300  | 1.90074400  | -0.69302800 |
| H | 2.52639200  | 2.77423900  | -0.61544400 |



#### RC12

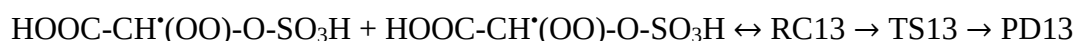
|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.58492400 | -1.55928000 | 0.14364200  |
| O | -2.71606800 | 0.58284000  | -0.58082900 |
| O | -1.15228500 | 0.60656200  | 1.28088000  |
| O | -0.32358700 | 0.22492500  | -1.04985700 |
| S | -1.61597400 | -0.13000100 | -0.01535500 |
| C | 0.76637500  | -0.54957300 | -1.08277300 |
| H | 1.16974700  | -0.71558600 | -2.07569500 |
| C | 1.45024700  | -0.96724500 | 0.13057800  |
| H | -0.26264300 | 0.20859800  | 1.53252600  |
| O | 1.12453400  | -0.60822600 | 1.25323700  |
| H | 2.65432900  | -2.03173400 | -0.93440100 |
| O | 2.51731500  | -1.76087400 | -0.01717000 |
| O | 1.21393100  | 2.30502700  | 0.33672300  |
| O | 2.04538700  | 1.92398100  | -0.43707400 |

#### TS12

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.50160600 | -1.49098900 | -0.44643000 |
| O | -2.70900500 | 0.72831000  | -0.50928700 |
| O | -1.38788500 | 0.12991900  | 1.43722700  |
| O | -0.26310800 | 0.64336500  | -0.74661200 |
| S | -1.62684500 | -0.10234000 | -0.09155300 |
| C | 0.89550000  | 0.00252900  | -0.92012300 |
| H | 1.28044600  | 0.01261800  | -1.93598200 |
| C | 1.41636400  | -0.93127100 | 0.09480900  |
| H | -0.53493600 | -0.32795300 | 1.67395500  |
| O | 0.96317500  | -1.01917000 | 1.21908000  |
| H | 2.76036400  | -1.49766200 | -1.16581000 |
| O | 2.50668800  | -1.62320700 | -0.24190600 |
| O | 1.38784900  | 2.23467500  | 0.48174900  |
| O | 2.08544900  | 1.52495900  | -0.21325000 |

#### PD12

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.55832700 | 0.42026000  | 1.42298000  |
| O | -2.67847300 | -1.10034000 | -0.25197800 |
| O | -1.82188000 | 1.04891500  | -0.96858600 |
| O | -0.23981100 | -0.73162000 | -0.32010900 |
| S | -1.70982200 | -0.10923800 | 0.08910900  |
| C | 0.85390800  | -0.40411100 | 0.48004100  |
| H | 0.58546100  | -0.35906000 | 1.54094600  |
| C | 1.46432300  | 0.94191100  | 0.03892000  |
| H | -1.03121600 | 1.62999300  | -0.88155000 |
| O | 0.76741600  | 1.80495400  | -0.42858500 |
| H | 3.19882300  | 0.32898300  | 0.58308800  |
| O | 2.74999000  | 1.13599300  | 0.28981400  |
| O | 2.31688900  | -1.49994500 | -0.83775100 |
| O | 1.80103100  | -1.46308100 | 0.37146500  |



#### RC13

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -3.77418100 | 0.02422500  | 0.98563800  |
| O | -4.33408400 | 0.74957100  | -1.35665300 |
| O | -2.52374900 | 1.84334100  | -0.20058900 |
| O | -2.25731700 | -0.51116900 | -0.87641900 |
| S | -3.38656400 | 0.54053200  | -0.30772800 |
| C | -1.85429500 | -1.54354600 | -0.02161100 |
| H | -2.70251800 | -2.16595900 | 0.29071200  |
| C | -1.11023000 | -1.00840100 | 1.22246200  |
| H | -1.69757900 | 1.69869800  | 0.31601600  |
| O | -0.83457100 | 0.14947700  | 1.38057800  |
| H | -0.97916300 | -2.83256100 | 1.80537200  |
| O | -0.79489200 | -1.93677500 | 2.12310800  |
| O | 0.01001800  | -1.65169800 | -1.33130200 |
| O | -1.04891400 | -2.42576300 | -0.76332900 |

|   |            |             |             |
|---|------------|-------------|-------------|
| O | 2.09978500 | 1.95287000  | 1.52043100  |
| O | 0.17806600 | 2.55645700  | 0.00024400  |
| O | 2.43793300 | 2.58397800  | -0.86160300 |
| O | 1.39648800 | 0.43465500  | -0.30517500 |
| S | 1.47103200 | 1.98185200  | 0.22380700  |
| C | 2.14073100 | -0.53476100 | 0.37684700  |
| H | 2.27025400 | -0.27139900 | 1.43553800  |
| C | 3.52372500 | -0.65960400 | -0.29032900 |
| H | 3.23909600 | 2.01256100  | -0.91905400 |
| O | 4.06280600 | 0.30821500  | -0.76385300 |
| H | 3.51733900 | -2.51659400 | 0.14459500  |
| O | 4.10576600 | -1.84718800 | -0.23808200 |
| O | 1.18738300 | -2.20711500 | -0.91230300 |
| O | 1.43964900 | -1.74870800 | 0.41747400  |

### TS13

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 4.25935800  | -1.13697000 | 0.49319200  |
| O | 5.16594000  | 0.44428800  | -1.25553100 |
| O | 3.25608200  | -0.93920800 | -1.77575100 |
| O | 3.02224600  | 0.90218300  | -0.13531200 |
| S | 4.08326600  | -0.24141100 | -0.62719700 |
| C | 2.38260300  | 0.75260700  | 1.09717900  |
| H | 2.90733500  | 0.08010500  | 1.79813600  |
| C | 1.05148900  | -0.51515200 | 0.90131200  |
| H | 2.46542900  | -1.37217300 | -1.39210500 |
| O | 1.18301100  | -1.31963500 | 0.04559100  |
| H | 0.31406600  | 0.32165400  | 2.39716000  |
| O | 0.35947500  | -0.57030200 | 2.00514400  |
| O | 0.32268500  | 1.48202100  | 0.39642000  |
| O | 1.84284600  | 1.78996500  | 1.56397300  |
| O | -3.93452200 | -1.45551700 | 0.78499500  |
| O | -1.70857000 | -2.64270700 | 0.66280600  |
| O | -2.81406500 | -1.94991900 | -1.37997700 |
| O | -1.88151000 | -0.24550800 | 0.14716500  |
| S | -2.65407700 | -1.69673300 | 0.16392500  |
| C | -2.63123700 | 0.92140400  | 0.37104500  |
| H | -3.43525800 | 0.75001600  | 1.09870200  |
| C | -3.25239400 | 1.41015700  | -0.95430300 |
| H | -3.26752100 | -1.16930300 | -1.77884800 |
| O | -3.60632700 | 0.63332400  | -1.80520100 |
| H | -3.05306600 | 3.19285800  | -0.31267200 |
| O | -3.44384400 | 2.71470000  | -1.06150000 |
| O | -0.72488200 | 2.13001900  | -0.00200000 |
| O | -1.81051800 | 1.88739700  | 0.95481000  |

### PD13

|   |            |            |            |
|---|------------|------------|------------|
| O | 3.53749600 | 0.48611200 | 1.02456700 |
|---|------------|------------|------------|

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 4.70501800  | 0.03448500  | -1.17353100 |
| O | 2.99157800  | -1.48291100 | -0.36657800 |
| O | 2.38477600  | 0.79279300  | -1.16344000 |
| S | 3.55766700  | -0.01461600 | -0.32635800 |
| C | 1.39627500  | 1.46075300  | -0.48707100 |
| H | 1.41381600  | 1.33155400  | 0.60289300  |
| C | -1.10273900 | 2.87339600  | 0.80952000  |
| H | 2.34670300  | -1.62152200 | 0.36672600  |
| O | -0.67350200 | 1.99776400  | 1.48326400  |
| H | -1.16691600 | 4.65210100  | 0.14375400  |
| O | -0.82849900 | 4.16252800  | 0.90857700  |
| O | -2.08333000 | 2.72255700  | -0.18177200 |
| O | 0.60738600  | 2.11684200  | -1.10010200 |
| O | -1.32601700 | -2.63169800 | 1.82915900  |
| O | 0.93940300  | -1.58849300 | 1.46000300  |
| O | -0.05318400 | -2.89413300 | -0.30010900 |
| O | -1.01829100 | -0.70167300 | 0.31402800  |
| S | -0.34641600 | -2.02271700 | 0.97027700  |
| C | -2.42483100 | -0.62665200 | 0.21499800  |
| H | -2.91244200 | -1.16909900 | 1.03534100  |
| C | -2.86213000 | -1.25471500 | -1.12729300 |
| H | -0.86485100 | -2.91985100 | -0.87359500 |
| O | -2.34289700 | -2.26835000 | -1.53131700 |
| H | -4.12479200 | 0.15061100  | -1.31449200 |
| O | -3.87142800 | -0.68047700 | -1.74916200 |
| O | -2.12458100 | 1.43235900  | -0.64923300 |
| O | -2.85780000 | 0.68440300  | 0.35511300  |



RC11'

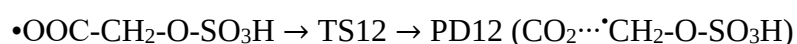
|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 2.04951600  | 1.14419400  | -0.03413200 |
| O | 2.69493500  | -1.14864600 | -0.28553400 |
| O | 0.96088700  | -0.53609700 | 1.38710500  |
| O | 0.47797900  | -0.45292400 | -0.99852200 |
| S | 1.61358300  | -0.33968900 | 0.13196600  |
| C | -1.28492800 | 0.98208200  | -0.11188200 |
| C | -0.87071600 | -0.40052400 | -0.59360100 |
| H | -1.45972800 | -0.66712300 | -1.47065300 |
| H | -1.06999800 | -1.12436800 | 0.19923800  |
| H | 1.23797900  | 1.69908900  | 0.01488900  |
| O | -0.53154000 | 1.91317600  | -0.03007300 |
| H | -3.03465700 | 0.25560600  | 0.13606400  |
| O | -2.56283000 | 1.10025000  | 0.21313600  |
| O | -3.65410100 | -1.54862700 | 0.04955200  |
| H | -4.03582500 | -1.98812600 | 0.82964900  |

TS11'

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.98091300  | 1.24699800  | -0.12204300 |
| O | 2.78494200  | -1.00237100 | -0.25228500 |
| O | 1.03088800  | -0.41899000 | 1.41183300  |
| O | 0.51431300  | -0.51056800 | -0.96796500 |
| S | 1.65122300  | -0.25412700 | 0.13683300  |
| C | -1.36954100 | 0.75037300  | -0.12661600 |
| C | -0.82667100 | -0.60572300 | -0.54389200 |
| H | -1.39211300 | -0.98078800 | -1.39499300 |
| H | -0.93830800 | -1.30419800 | 0.28416600  |
| H | 1.14747000  | 1.75627900  | -0.04878900 |
| O | -0.70612000 | 1.75009300  | -0.06087700 |
| H | -3.29387800 | -0.10976900 | -0.06775600 |
| O | -2.66075300 | 0.81741000  | 0.17298500  |
| O | -3.56578500 | -1.23777500 | 0.07425100  |
| H | -3.79265700 | -1.32177200 | 1.01389400  |

#### PD11'

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 2.08660000  | 1.12842000  | -0.25491600 |
| O | 2.68905400  | -1.18539300 | -0.25321900 |
| O | 1.07577600  | -0.33489300 | 1.43899600  |
| O | 0.43450100  | -0.54683300 | -0.90326600 |
| S | 1.64296100  | -0.31555000 | 0.12931800  |
| C | -1.28414100 | 0.92430000  | -0.08461800 |
| C | -0.88794700 | -0.51161400 | -0.41552900 |
| H | -1.53104000 | -0.89491100 | -1.20236700 |
| H | -1.01410600 | -1.12210400 | 0.47618700  |
| H | 1.30595700  | 1.71424400  | -0.18090300 |
| O | -0.54862700 | 1.87925600  | -0.12777200 |
| H | -4.40521900 | -0.70603900 | 0.15784200  |
| O | -2.53777600 | 1.06594400  | 0.26602400  |
| O | -3.66550600 | -1.29439300 | -0.01035300 |
| H | -3.88260700 | -2.11538100 | 0.43708600  |



#### RC12'

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.16687000  | 1.43224600  | -0.38414300 |
| O | 2.53298400  | -0.52926400 | -0.31628000 |
| O | 0.82977100  | -0.15176400 | 1.46081600  |
| O | 0.16692300  | -0.75951900 | -0.80788400 |
| S | 1.27984900  | -0.03905300 | 0.11210800  |
| C | -1.94155800 | 0.12556200  | -0.04897200 |
| C | -1.05734400 | -1.12300300 | -0.22651000 |
| H | -1.53327900 | -1.82727600 | -0.90426200 |
| H | -0.92556900 | -1.57996300 | 0.75389800  |
| H | 0.24237600  | 1.72896000  | -0.25918400 |
| O | -1.55506900 | 1.26210300  | -0.11520600 |
| O | -3.17494100 | -0.21783000 | 0.19628600  |

TS12'

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.15907700  | 1.42849000  | -0.39030500 |
| O | 2.52183300  | -0.53745200 | -0.36591300 |
| O | 0.87782600  | -0.15436600 | 1.46458800  |
| O | 0.14163600  | -0.76018300 | -0.78596000 |
| S | 1.28635100  | -0.04037800 | 0.10349900  |
| C | -1.96915800 | 0.15456200  | -0.03606000 |
| C | -1.06313100 | -1.12148500 | -0.17865100 |
| H | -1.54071600 | -1.85776400 | -0.81733600 |
| H | -0.92072300 | -1.51454200 | 0.82722100  |
| H | 0.23563200  | 1.72176000  | -0.24242600 |
| O | -1.54250000 | 1.27765600  | -0.07539900 |
| O | -3.17813300 | -0.24187800 | 0.13609100  |

PD12'

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 0.83040700  | -1.14573900 | 0.98767100  |
| O | 2.51569800  | -0.43619900 | -0.57218600 |
| O | 0.09351900  | -0.25589500 | -1.15616400 |
| O | 1.14818600  | 1.23131400  | 0.47976500  |
| S | 1.17036800  | -0.20560300 | -0.21840700 |
| C | -2.45733900 | -0.29308600 | -0.01249200 |
| C | -0.05732800 | 1.88127500  | 0.59220700  |
| H | -0.02283000 | 2.68092300  | 1.31217500  |
| H | -0.68122300 | 1.90734700  | -0.28845800 |
| H | -0.13356100 | -1.25062900 | 1.06472100  |
| O | -2.03172100 | -1.01362200 | 0.79214500  |
| O | -2.90612500 | 0.42300000  | -0.79025900 |

**Aqueous-phase**

•OH

|   |            |            |             |
|---|------------|------------|-------------|
| O | 0.00000000 | 0.00000000 | 0.10818600  |
| H | 0.00000000 | 0.00000000 | -0.86549100 |

CH<sub>3</sub>-O-SO<sub>3</sub><sup>-</sup>

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -0.46236800 | -0.84419100 | -1.21513000 |
| O | -1.47664900 | 1.01784700  | -0.00012600 |
| O | -0.46255600 | -0.84407200 | 1.21520100  |
| O | 0.89194200  | 0.79614700  | 0.00005700  |
| S | -0.48147400 | -0.04041500 | -0.00000400 |
| H | 2.14641000  | -0.60090400 | -0.89392800 |
| C | 2.09578500  | 0.01837600  | 0.00000700  |
| H | 2.91338100  | 0.73290500  | 0.00036600  |
| H | 2.14613600  | -0.60146100 | 0.89357300  |

HOOC-CH<sub>2</sub>-O-SO<sub>3</sub><sup>-</sup>

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 0.80433900  | 1.26935500  | 0.60528200  |
| O | 2.31339100  | 0.26574500  | -1.03616600 |
| O | 1.78451900  | -0.90995700 | 1.04352100  |
| O | 0.12656500  | -0.63467800 | -0.75181200 |
| S | 1.36892600  | 0.04089600  | 0.03250400  |
| C | -2.11931200 | -0.00465600 | -0.01356900 |
| C | -1.00656400 | -1.03595000 | 0.01118400  |
| H | -1.38562100 | -1.95375200 | -0.42737800 |
| H | -0.73985500 | -1.22990800 | 1.05299900  |
| O | -3.28098700 | -0.33874800 | -0.02699200 |
| H | -0.80358300 | 1.38586900  | 0.16290600  |
| O | -1.77514000 | 1.27166900  | 0.00438100  |

CH<sub>3</sub>-O-SO<sub>3</sub><sup>-</sup> + •OH ↔ RC4 → TS4 → PD4 (H<sub>2</sub>C•-O-SO<sub>3</sub><sup>-</sup>⋯H<sub>2</sub>O)

H<sub>2</sub>C•-O-SO<sub>3</sub><sup>-</sup>⋯H<sub>2</sub>O → TS4-b → PD4-b (H<sub>2</sub>CO⋯SO<sub>3</sub><sup>-</sup>⋯H<sub>2</sub>O)

RC4

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.61403100 | 0.32674000  | -0.98297500 |
| O | -1.32836800 | -1.09589600 | 0.99810300  |
| O | 0.43096600  | -0.95072000 | -0.69654100 |
| O | -0.04427800 | 0.91651300  | 0.81037400  |
| S | -0.71529900 | -0.30821600 | -0.04056500 |
| H | -0.09766800 | 2.33901700  | -0.68794700 |
| C | 0.60160300  | 1.89850800  | 0.02460000  |
| H | 0.95808500  | 2.66162200  | 0.71466600  |
| H | 1.45198600  | 1.47065200  | -0.50936300 |
| O | 2.99312300  | -0.70919200 | 0.01725300  |
| H | 2.02346400  | -0.83043300 | -0.18562200 |

TS4

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.22568100  | 0.47216400  | 1.28282400  |
| O | 1.87769200  | -0.31568700 | -0.93779500 |
| O | -0.00106600 | -1.34489400 | 0.23477600  |
| O | -0.14683300 | 0.91523300  | -0.70338800 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| S | 0.82046300  | -0.15453300 | 0.03709000  |
| H | -1.07414300 | 1.57816700  | 1.04138800  |
| C | -1.29081000 | 1.33559800  | 0.00254900  |
| H | -1.72531000 | 2.17165100  | -0.53772700 |
| H | -2.08955400 | 0.49760700  | -0.00224600 |
| O | -2.77588200 | -0.79149800 | -0.02494000 |
| H | -1.93028000 | -1.27104300 | 0.07802800  |

#### PD4

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.58334500  | 0.50246200  | 1.02838200  |
| O | 1.57756800  | -0.80318300 | -1.03971100 |
| O | -0.18554400 | -1.11402400 | 0.62327700  |
| O | -0.05746400 | 0.91188700  | -0.75469500 |
| S | 0.80975900  | -0.22322200 | 0.03939300  |
| H | -0.66192100 | 1.84099200  | 1.04071900  |
| C | -0.90517400 | 1.68982300  | -0.00074800 |
| H | -1.43399700 | 2.42325400  | -0.58710600 |
| H | -3.05326900 | 0.19629300  | -0.02347000 |
| O | -2.96148200 | -0.76253500 | -0.01457700 |
| H | -2.02729600 | -0.90477400 | 0.20264500  |

#### TS4-b

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 0.63495700  | -0.84493400 | 1.33207100  |
| O | 2.21952700  | -0.18882500 | -0.44109000 |
| O | -0.09990300 | -0.80625200 | -1.00666600 |
| O | 0.17846400  | 1.71448600  | 0.14072800  |
| S | 0.83054700  | -0.27544600 | -0.00046200 |
| H | -1.70910900 | 1.87928700  | 0.89742300  |
| C | -1.06759500 | 1.87218500  | 0.01709100  |
| H | -1.51642700 | 1.95553600  | -0.97219100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.96112100 | -1.76145400 | 0.30409800  |
| O | -2.78544300 | -0.87338000 | -0.02071900 |
| H | -1.87733300 | -0.90810900 | -0.35906700 |

#### PD4-b

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.39442900 | -0.06401200 | 1.42641000  |
| O | -2.42109600 | -0.32260000 | -0.80457000 |
| O | -0.44501700 | 1.11562400  | -0.51880000 |
| O | 1.68008500  | -1.70428100 | 0.33709600  |
| S | -1.19133800 | -0.06951100 | -0.03262400 |
| H | 3.28397000  | -0.86671400 | -0.54089900 |
| C | 2.19940400  | -1.03822200 | -0.52438100 |
| H | 1.61203400  | -0.59269100 | -1.33982000 |
| H | 2.68538700  | 1.77817900  | -0.51373600 |
| O | 2.20486900  | 1.66647600  | 0.31234900  |
| H | 1.28830700  | 1.49308400  | 0.04284600  |



#### RC5

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -0.51832300 | -1.27837000 | -0.72704100 |
| O | -2.60037300 | -0.05044700 | -0.41653600 |
| O | -1.04340400 | -0.32784900 | 1.45150600  |
| O | -0.54271200 | 1.15994700  | -0.43730000 |
| S | -1.23093800 | -0.25101900 | 0.01253400  |
| H | 0.66689800  | 1.41009800  | 1.22404700  |
| C | 0.68233700  | 1.53632200  | 0.14250600  |
| H | 0.84274400  | 2.57537100  | -0.13353400 |
| O | 1.98122000  | -0.34453200 | 0.43068100  |
| O | 2.70890300  | -1.14846700 | -0.16563800 |

|   |            |            |             |
|---|------------|------------|-------------|
| O | 1.77610600 | 0.84133000 | -0.40393400 |
|---|------------|------------|-------------|

#### TS5

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -0.68021200 | -1.24758500 | 0.74090600  |
| O | -2.16490100 | -0.70189900 | -1.12365900 |
| O | -2.14569200 | 0.68334100  | 0.89131200  |
| O | -0.28578100 | 0.69903400  | -0.69940400 |
| S | -1.41202300 | -0.21952100 | 0.01704800  |
| H | 0.53317400  | 1.03012400  | 1.18655800  |
| C | 0.67421900  | 1.32697300  | 0.14407300  |
| H | 0.56025700  | 2.41037500  | 0.04913400  |
| O | 2.29897300  | -0.48164600 | 0.37902000  |
| O | 3.21059000  | -0.98668500 | -0.19803800 |
| O | 1.94872500  | 1.04918900  | -0.28675000 |

#### PD5

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -0.11471400 | -0.98554900 | -0.81669200 |
| O | -2.51899300 | -0.63106800 | -0.54592500 |
| O | -1.05199100 | -0.71447900 | 1.40814200  |
| O | -1.03092300 | 1.18780600  | -0.13534300 |
| S | -1.18803900 | -0.42516400 | -0.01131000 |
| H | 0.52612600  | 1.23040800  | 1.24974800  |
| C | 0.18867400  | 1.74165000  | 0.33449200  |
| H | -0.03005600 | 2.78476400  | 0.60791100  |
| O | 2.64086600  | -0.39366100 | 0.49384700  |
| O | 3.06657200  | -1.16813200 | -0.29909300 |
| O | 1.18174500  | 1.74727600  | -0.56539200 |

#### RC5-b

|   |            |            |            |
|---|------------|------------|------------|
| O | 0.39609200 | 1.36609400 | 0.54306500 |
|---|------------|------------|------------|

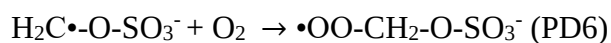
|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.77585800  | 0.07471000  | -1.01198000 |
| O | 1.02869600  | -0.91274600 | 1.09542500  |
| O | -0.52572300 | -0.50153500 | -0.75241200 |
| S | 0.77931200  | 0.05604100  | 0.03957500  |
| H | -1.52942500 | -0.84670400 | 1.04378400  |
| C | -1.72826500 | -0.56427300 | -0.00235300 |
| H | -2.33316200 | -1.37087600 | -0.44413000 |
| O | -2.45452300 | 0.56179600  | -0.02644000 |

#### TS5-b

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.17762000  | 1.43171700  | -0.03426500 |
| O | 1.78113900  | -0.88892500 | -0.47742500 |
| O | 0.25864100  | -0.35304300 | 1.36854400  |
| O | -0.51081200 | -0.13702400 | -0.87809700 |
| S | 0.78972800  | 0.04354500  | -0.00398300 |
| H | -0.92346600 | -0.51674500 | 1.08592700  |
| C | -1.74861800 | -0.45138400 | -0.05727700 |
| H | -1.99661900 | -1.49648100 | -0.27625800 |
| O | -2.60957000 | 0.45037700  | -0.02904200 |

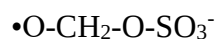
#### PD5-b

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 2.29084000  | 0.26260100  | -0.34979300 |
| O | 0.72719800  | -1.23219700 | 0.79046300  |
| O | 0.41894500  | 1.19663500  | 0.79339300  |
| O | 0.04876000  | -0.10422400 | -1.24915700 |
| S | 0.90651400  | -0.07043900 | -0.07020700 |
| H | -0.51660600 | 1.07207800  | 1.02874100  |
| C | -2.32175300 | -0.27186600 | 0.29048900  |
| H | -2.08944700 | -1.35871900 | 0.26243500  |
| O | -3.23169800 | 0.25779200  | -0.22375600 |

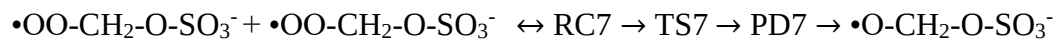


PD6

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.50539500 | -0.77311000 | 1.16719300  |
| O | -2.16344900 | 0.17347100  | -0.98840100 |
| O | -0.60791200 | 1.37606900  | 0.47036600  |
| O | 0.05613100  | -0.66978100 | -0.72509800 |
| S | -1.17023600 | 0.10269400  | 0.05978300  |
| H | 1.10926000  | -0.81890300 | 1.05983900  |
| C | 1.24049100  | -0.81234000 | -0.02096000 |
| H | 1.76595200  | -1.69246700 | -0.38073000 |
| O | 3.20750200  | 0.26893900  | 0.24016200  |
| O | 2.06382500  | 0.34219900  | -0.35295600 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.03183200 | -0.91685600 | 1.09089600  |
| O | -1.77443100 | 0.08112200  | -1.01319700 |
| O | -0.39400600 | 1.36303000  | 0.54938800  |
| O | 0.52557100  | -0.50046300 | -0.75275500 |
| S | -0.77935200 | 0.05606700  | 0.03963700  |
| H | 1.52937900  | -0.84805300 | 1.04287200  |
| C | 1.72793500  | -0.56426200 | -0.00294000 |
| H | 2.33295000  | -1.37038600 | -0.44557700 |
| O | 2.45465900  | 0.56153500  | -0.02606300 |



RC7

|   |            |             |             |
|---|------------|-------------|-------------|
| O | 4.76986300 | -0.01394300 | 1.04026900  |
| O | 4.74745000 | -0.78108800 | -1.27968000 |
| O | 3.08800100 | -1.61293400 | 0.31748900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 3.02715800  | 0.69537800  | -0.53501500 |
| S | 3.99362500  | -0.54488100 | -0.06659100 |
| H | 2.29760700  | 0.83928300  | 1.40368500  |
| C | 2.04885000  | 1.09823200  | 0.37494700  |
| H | 1.89129500  | 2.16753400  | 0.25533300  |
| O | -0.17295200 | 0.86141200  | 0.80546200  |
| O | 0.85586500  | 0.39982000  | -0.01604000 |
| O | -4.74997600 | -0.65728500 | -0.76945500 |
| O | -3.73199800 | -1.69094000 | 1.19825600  |
| O | -2.41203200 | -1.31882000 | -0.82589000 |
| O | -3.12352600 | 0.54059500  | 0.62243800  |
| S | -3.53840700 | -0.90835400 | -0.00564500 |
| H | -3.52217100 | 1.51685700  | -1.16685100 |
| C | -2.89125400 | 1.59187800  | -0.28162600 |
| H | -3.07164100 | 2.51555700  | 0.26167900  |
| O | -0.69783500 | 2.00012300  | 0.21752500  |
| O | -1.57803700 | 1.58666500  | -0.79511000 |

TS7

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 4.47205300  | -0.13469600 | -0.05715200 |
| O | 3.26915300  | -2.24580100 | -0.33851700 |
| O | 2.68915100  | -0.74314300 | 1.48865000  |
| O | 2.15483900  | -0.20323300 | -0.85826800 |
| S | 3.24398700  | -0.88264700 | 0.15502400  |
| H | 2.39671600  | 1.56447900  | -1.92119000 |
| C | 2.08289300  | 1.20606000  | -0.93097600 |
| H | 0.85414700  | 1.39601200  | -1.06471500 |
| O | 0.48692800  | 2.30454300  | 0.77654500  |
| O | 2.33160900  | 1.91282500  | 0.07783600  |
| O | -3.80964400 | -1.76014100 | -0.44821300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -4.87296700 | 0.42159200  | -0.16004000 |
| O | -3.23367400 | -0.38180900 | 1.46896200  |
| O | -2.57389300 | 0.32800900  | -0.79268800 |
| S | -3.72259400 | -0.41775400 | 0.10149700  |
| H | -1.26634400 | -1.26252600 | -0.46912200 |
| C | -1.27361500 | -0.19866000 | -0.70977900 |
| H | -0.79070900 | -0.01780000 | -1.66967100 |
| O | -0.17914300 | 1.75026400  | -0.12784500 |
| O | -0.53338200 | 0.38682200  | 0.32884200  |

#### PD7

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 3.84994400  | -1.50257000 | 0.99117300  |
| O | 5.77551000  | -0.09250800 | 0.44663700  |
| O | 4.34532700  | -0.97011700 | -1.33511800 |
| O | 3.55444100  | 0.82423300  | 0.18307100  |
| S | 4.49773500  | -0.61910000 | 0.05461100  |
| H | 1.87960500  | -0.23944200 | -0.35939600 |
| C | 2.28276600  | 0.73607700  | -0.07726900 |
| H | 0.31868100  | 1.58809300  | -0.27588400 |
| O | -1.35347900 | 2.46988300  | 0.35982500  |
| O | 1.58072400  | 1.73575400  | -0.00137900 |
| O | -4.39967400 | -1.93406500 | -0.22849700 |
| O | -5.40237900 | 0.28825900  | -0.05516300 |
| O | -3.64397700 | -0.40200500 | 1.49885500  |
| O | -3.16836800 | 0.08603600  | -0.86660100 |
| S | -4.24437800 | -0.54832200 | 0.18449000  |
| H | -1.86683500 | -1.50500700 | -0.54101900 |
| C | -1.87228000 | -0.46193300 | -0.85798500 |
| H | -1.47638500 | -0.35243700 | -1.86410400 |
| O | -0.77540600 | 1.50667500  | -0.45632300 |

|   |             |            |            |
|---|-------------|------------|------------|
| O | -1.03412500 | 0.18326100 | 0.06680900 |
|---|-------------|------------|------------|

HOOC-CH<sub>2</sub>-O-SO<sub>3</sub><sup>-</sup> + •OH ↔ RC8 → TS8 → PD8 (HOOC-CH•-O-SO<sub>3</sub><sup>-</sup>···H<sub>2</sub>O)

HOOC-CH•-O-SO<sub>3</sub><sup>-</sup> (RC9) → TS9 → PD9 (HOOC-CHO··· SO<sub>3</sub>•<sup>-</sup>)

RC8

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.62420300  | 1.13853800  | 0.56416300  |
| O | 2.75809000  | -0.34602300 | -1.01071300 |
| O | 1.84197600  | -1.22601600 | 1.08120400  |
| O | 0.39134700  | -0.48775900 | -0.76159600 |
| S | 1.77338000  | -0.22500100 | 0.03720900  |
| C | -1.53716300 | 0.82262500  | -0.01647200 |
| C | -0.81862400 | -0.51351500 | -0.01535100 |
| H | -1.46862100 | -1.25045700 | -0.48041900 |
| H | -0.64553700 | -0.80776500 | 1.02297800  |
| O | -2.74976900 | 0.87898100  | -0.00397300 |
| H | 0.15168800  | 1.72355600  | 0.13873700  |
| O | -0.81322100 | 1.91929200  | -0.00649900 |
| O | -4.12529600 | -1.53599700 | 0.00178200  |
| H | -3.69552700 | -0.64811000 | -0.00063400 |

TS8

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.51310800 | -1.31201500 | 0.29015500  |
| O | -2.51873100 | 0.43927200  | -1.09021000 |
| O | -1.85355600 | 0.90973800  | 1.21856400  |
| O | -0.18999000 | 0.54133100  | -0.56397400 |
| S | -1.65800100 | 0.12054000  | 0.02181100  |
| C | 1.72318700  | -0.84185500 | 0.05496000  |
| C | 0.90892100  | 0.41442500  | 0.29520100  |
| H | 1.62969600  | 1.31384700  | 0.06269700  |
| H | 0.64897500  | 0.51647300  | 1.35117600  |



|   |            |             |             |
|---|------------|-------------|-------------|
| O | 2.92788200 | -0.83870200 | 0.13525600  |
| H | 0.07675900 | -1.81494500 | -0.13090900 |
| O | 1.05132800 | -1.94315100 | -0.22907800 |
| O | 2.72185000 | 2.10786300  | -0.20759200 |
| H | 3.37454600 | 1.38587000  | -0.15786600 |

#### PD8

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.97153000  | 1.10538400  | -0.40650100 |
| O | 2.77287200  | -1.19343100 | -0.30768300 |
| O | 1.36660100  | -0.29215100 | 1.49260900  |
| O | 0.44050500  | -0.79050200 | -0.73295000 |
| S | 1.77540900  | -0.24551500 | 0.10907000  |
| C | -1.33408900 | 0.83300700  | -0.07841100 |
| C | -0.81835400 | -0.48154300 | -0.37769600 |
| H | -3.83395400 | -1.96315500 | -0.25433600 |
| H | -1.52204600 | -1.29907900 | -0.43956700 |
| O | -2.52232800 | 0.96257900  | 0.20129100  |
| H | 0.38818100  | 1.71536400  | -0.32148300 |
| O | -0.55559000 | 1.90988300  | -0.11537800 |
| O | -4.32822900 | -1.21955000 | 0.10245600  |
| H | -3.68695300 | -0.49135600 | 0.13615000  |

#### RC9

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.01648000  | 1.35455500  | -0.51540000 |
| O | 2.55933100  | -0.51739600 | -0.28804000 |
| O | 0.94129100  | -0.02111600 | 1.49149300  |
| O | 0.22688300  | -0.96774400 | -0.66455400 |
| S | 1.29889400  | 0.05966400  | 0.09484200  |
| C | -1.99688000 | -0.02252100 | -0.03776400 |
| C | -1.05638500 | -1.09235600 | -0.27751500 |

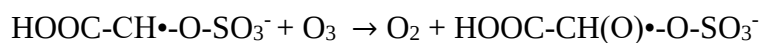
|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.43099700 | -2.10451600 | -0.26362400 |
| O | -3.14626400 | -0.29744700 | 0.28022900  |
| H | -0.69192800 | 1.38512300  | -0.40290500 |
| O | -1.64019500 | 1.25590200  | -0.17363500 |

#### TS9

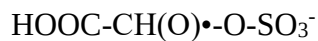
|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.50404200  | 1.40778500  | -0.39629500 |
| O | 2.66369000  | -0.73823900 | -0.01389500 |
| O | 0.74857600  | -0.09011900 | 1.40772000  |
| O | -0.21567000 | -0.81621800 | -1.15693600 |
| S | 1.44057700  | 0.04485800  | 0.12850300  |
| C | -2.09213900 | 0.01433500  | 0.02010800  |
| C | -1.20391500 | -1.08239200 | -0.45787500 |
| H | -1.44770400 | -2.09247900 | -0.12787300 |
| O | -3.07561400 | -0.19061300 | 0.69325600  |
| H | -0.93394000 | 1.22634400  | -0.88433400 |
| O | -1.73643300 | 1.24699800  | -0.33600300 |

#### PD9

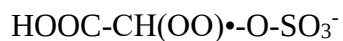
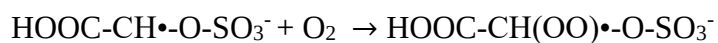
|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.05320400 | -0.85264200 | -0.78693700 |
| O | -3.31829500 | -0.15974300 | -0.12719700 |
| O | -1.39387800 | 0.29506200  | 1.36146700  |
| O | 0.89731900  | 1.46872100  | -0.58314000 |
| S | -1.87801500 | 0.11745000  | -0.01701300 |
| C | 2.36927600  | -0.29636400 | 0.06816800  |
| C | 1.98473400  | 1.16292000  | -0.18635500 |
| H | 2.78697300  | 1.88305900  | 0.01815800  |
| O | 3.49677000  | -0.55863000 | 0.41113300  |
| H | 0.54570500  | -0.86200100 | -0.37719500 |
| O | 1.44522400  | -1.20521800 | -0.10778000 |



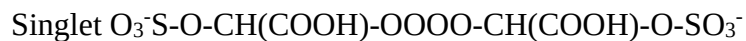
|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.55397300 | -0.05188200 | 1.19000100  |
| O | -0.75809200 | -2.26426900 | 0.54970100  |
| O | -2.58096300 | -1.23626400 | -0.69272400 |
| O | -0.35206400 | -0.34668400 | -0.92714400 |
| S | -1.40637200 | -1.03726700 | 0.13069400  |
| C | -0.28064000 | 1.97884800  | -0.18688000 |
| C | 0.49995200  | 0.64370500  | -0.41510100 |
| H | 1.20929800  | 0.89220200  | -1.22600000 |
| O | -1.25962800 | 2.24414400  | -0.81884400 |
| H | 1.03040200  | 2.41086200  | 1.11967500  |
| O | 0.25911400  | 2.80868500  | 0.68553100  |
| O | 3.20237600  | -0.86562000 | -0.54100800 |
| O | 4.20296300  | -0.90488200 | 0.09490400  |
| O | 1.20856500  | 0.31150800  | 0.66297200  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.47694800 | -0.57274700 | 1.43282800  |
| O | -2.36437200 | -0.93855900 | -0.81757100 |
| O | -1.92731200 | 1.33063000  | -0.00993600 |
| O | -0.09984600 | -0.21073300 | -0.56289800 |
| S | -1.61454300 | -0.08318400 | 0.07316900  |
| C | 2.23511900  | -0.26395400 | 0.06653400  |
| C | 0.90338700  | 0.55241100  | 0.06588600  |
| H | 0.68124100  | 0.70216700  | 1.14113600  |
| O | 3.26326200  | 0.24115400  | 0.40949700  |
| H | 1.22022800  | -1.73885500 | -0.55504200 |
| O | 2.13268500  | -1.52412100 | -0.29847600 |
| O | 1.11005400  | 1.75398700  | -0.47235900 |



|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.80963800 | -0.67154200 | 1.35748200  |
| O | -2.61265800 | -0.66833800 | -0.95288200 |
| O | -1.79657200 | 1.39834400  | 0.07984700  |
| O | -0.26416300 | -0.43046000 | -0.53973900 |
| S | -1.78103500 | -0.04934700 | 0.05020000  |
| C | 2.02852700  | -0.77764000 | 0.03212100  |
| C | 0.80095800  | 0.13971000  | 0.11875400  |
| H | 0.60532100  | 0.37443300  | 1.16783800  |
| O | 3.14277000  | -0.33862400 | 0.08604600  |
| H | 0.82931100  | -2.24817700 | -0.14986000 |
| O | 1.77858700  | -2.07107600 | -0.05345800 |
| O | 1.12433100  | 1.37342800  | -0.55510600 |
| O | 1.69797100  | 2.21962900  | 0.23700400  |



|   |            |             |             |
|---|------------|-------------|-------------|
| O | 0.50147400 | 1.62905700  | -1.04972400 |
| O | 1.86070900 | 3.24776100  | 0.19219600  |
| O | 0.50704900 | 1.60729700  | 1.38311500  |
| O | 2.53491500 | 0.94418300  | 0.15429100  |
| S | 1.21673800 | 1.95569600  | 0.16865800  |
| C | 3.79544300 | -0.89337800 | -0.61970900 |
| C | 2.39416100 | -0.30612700 | -0.42609600 |
| H | 1.88275100 | -0.26428200 | -1.39077000 |
| O | 4.04081800 | -2.04655400 | -0.39828000 |
| H | 4.37202700 | 0.84451000  | -1.16652500 |
| O | 4.71005800 | -0.06131400 | -1.09463500 |
| O | 1.64435900 | -1.11267900 | 0.47235200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.17747600  | -2.23649300 | -0.22280900 |
| O | -2.81304900 | 1.54830800  | -0.82048300 |
| O | -4.60724300 | -0.07937500 | -1.14587900 |
| O | -2.37892900 | -0.49062800 | -2.07693400 |
| O | -2.80441400 | -0.60562400 | 0.34088500  |
| S | -3.18603700 | 0.16895200  | -1.06845100 |
| C | -1.22817000 | -0.59720100 | 2.12062500  |
| C | -1.43832600 | -0.74580700 | 0.60791900  |
| H | -0.83836000 | 0.01720900  | 0.10612400  |
| O | -0.42589200 | -1.24733800 | 2.72986600  |
| H | -2.58995500 | 0.74036100  | 2.08496500  |
| O | -1.96809400 | 0.33133400  | 2.70690800  |
| O | -1.00502900 | -2.02598100 | 0.20829800  |
| O | -0.03124900 | -1.91159300 | -0.79586000 |

Triplet  $\text{O}_3\text{-S-O-CH(COOH)-OOOO-CH(COOH)-O-SO}_3^-$

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.23305700  | 1.46771800  | -1.89423600 |
| O | 2.16797900  | 3.11166800  | -0.33653700 |
| O | 0.23554100  | 1.77757600  | 0.30769900  |
| O | 2.47886000  | 0.77953300  | 0.11758900  |
| S | 1.41815700  | 1.89027700  | -0.52109000 |
| C | 3.77993600  | -1.19516700 | -0.01860200 |
| C | 2.44176600  | -0.52485900 | -0.34492700 |
| H | 2.27592900  | -0.57336700 | -1.42430300 |
| O | 3.85503400  | -2.37971700 | 0.15972000  |
| H | 4.59306200  | 0.52208400  | -0.10308500 |
| O | 4.84344000  | -0.40971500 | -0.00025300 |
| O | 1.39188000  | -1.20312100 | 0.32850700  |
| O | 0.91120700  | -2.28364200 | -0.52399800 |
| O | -2.32015300 | 0.67197600  | -1.53275900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -4.65085200 | 0.44759700  | -0.82055700 |
| O | -3.28654500 | -1.53859700 | -1.24211600 |
| O | -2.90748500 | -0.10808300 | 0.71840500  |
| S | -3.32940300 | -0.13655200 | -0.87289000 |
| C | -1.07137700 | 0.25569000  | 2.24682500  |
| C | -1.60076200 | -0.54804600 | 1.01888600  |
| H | -0.89894900 | -0.26004600 | 0.20942200  |
| O | -0.08304900 | -0.08219300 | 2.82915600  |
| H | -2.54980800 | 1.41028100  | 1.99337900  |
| O | -1.77321000 | 1.32256800  | 2.57080700  |
| O | -1.47607300 | -1.85294300 | 1.22453400  |
| O | 0.11315700  | -1.85615900 | -1.37906400 |