

**Supporting material for:**

**Atmospheric oxidation of fluoroalcohols initiated by  $\cdot\text{OH}$  radical in the presence of water and mineral dusts: Mechanism, kinetics, and risk assessment**

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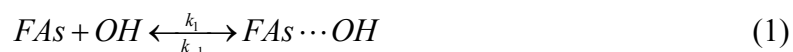
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## S1. Calculation details of the rate constant

In fact, for the reactions between  $\text{CF}_3\text{CF}_2\text{CF}_2\text{CH}_2\text{OH}/\text{CF}_3\text{CHFCH}_2\text{CH}_2\text{OH}$  (FAs) and OH without catalyst (water or mineral dusts), it can occur according to the two-step mechanism proposed in eq. 1 and 2:



If  $k_1$  and  $k_{-1}$  are the forward and reverse rate constants for the first step, respectively, and  $k_2$  corresponds to the second step, the rate constant for this process is shown by eq. 3 according to the steady-state conditions.<sup>1</sup>

$$k = \frac{k_1 k_2}{k_{-1} + k_2} \quad (3)$$

Due to the very loose transition state, the entropy change in  $k_{-1}$  is much larger than in the formation of products. Therefore,  $k_{-1}$  is considerably larger than  $k_2$ ,<sup>1,2</sup> and a pseudo equilibrium assumption can be used in the formation of the reactant complex.

Hence, eq. 3 can be represented as

$$k = \frac{k_1}{k_{-1} + k_2} k_2 = k_{eq} k_2 \quad (4)$$

where  $K_{eq}$  and  $k_2$  are the equilibrium constant of the first step and the rate constant of the second step in the reactions, and they can be displayed by eq. 5 and 6, respectively.

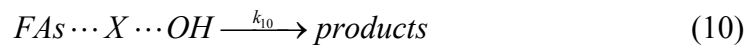
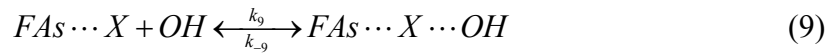
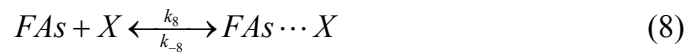
$$k_{eq} = \frac{\sigma Q_{FAs \cdots OH}}{Q_{FAs} Q_{OH}} \exp\left(\frac{E_{FAs+OH} - E_{FAs \cdots OH}}{RT}\right) \quad (5)$$

$$k_2 = \frac{\kappa \sigma}{\beta h} \frac{Q_{TS}}{Q_{FAs \cdots OH}} \exp\left(-\frac{E_{TS} - E_{FAs \cdots OH}}{RT}\right) \quad (6)$$

The total rate constant  $k$  can be obtained as

$$k = k_2 \frac{\sigma Q_{FAs \cdots OH}}{Q_{FAs} Q_{OH}} \exp\left(\frac{E_{FAs+OH} - E_{FAs \cdots OH}}{RT}\right) \quad (7)$$

For the multi-molecular reaction (when the number of reactants  $\geq 3$ ), the reaction is inclined to begin when the collision of two reactants forms two-body complex, then the third reactant combines with the formed two-body complex to start reaction and produce the corresponding products. In this work, the effects of combination order for the two-body and three-body complexes on the  $H_2O$ -assisted rate constants were considered (see Table 1). The following three steps have been taken into account in the reaction assisted by catalysts (X),:



According to Sinha<sup>3</sup> and Fliegl,<sup>4</sup> the above reaction sequence is typically regarded as one involving the formation of the three-body complex prereactive collision

complex, which then undergoes unimolecular reaction. From the energy information, it can be concluded that reaction 10 is the rate-determining step, and the rate can be expressed as

$$\frac{d[p]}{dt} = k_{10}[FAs \cdots X \cdots OH] \quad (11)$$

Applying a steady-state theory to  $FAs \cdots X \cdots OH$  and assuming that it is in equilibrium with the reactants and by assuming that the equilibrium of reaction 6 is not inferred by reaction 9, then

$$[FAs \cdots X \cdots OH] = \frac{k_9[FAs \cdots X][OH]}{k_{-9} + k_{10}} \quad (12)$$

where  $[FAs \cdots X] = K_{eq8}[FAs][X]$ . Because  $k_{-9}$  is larger than  $k_{10}$ , eq. 12 can be represented as

$$[FAs + X \cdots OH] = \frac{k_9 K_{eq8}[FAs][X][OH]}{k_{-9}} \quad (13)$$

$$[FAs + X \cdots OH] = K_{eq8} K_{eq9}[FAs][X][OH] \quad (14)$$

Consequently, eq. 11 can be given as

$$\frac{d[p]}{dt} = k_{10} K_{eq8} K_{eq9}[FAs][X][OH] \quad (15)$$

In the end, the rate constant  $k$  for the total reaction is obtained by eq. 16

$$k = k_{10} K_{eq8} K_{eq9}[X] \quad (16)$$

where  $K_{eq8}$  and  $K_{eq9}$  are the equilibrium constants for reactions 8 and 9, respectively,  $k_{10}$  is the rate constant of reaction 10, and  $[X]$  is the atmospheric concentration of

catalyst.

If reaction 8 is not taken into account, the rate constants for the title reaction assisted by catalyst can be represented as

$$k' = K_{eq9} k_{10} \quad (17)$$

## **S2. Materials and methods for the toxicity of PBFA**

### **Acute toxicity of PBFA to HepG2 and zebrafish embryos**

Acute toxicity of PBFA in HepG2 cells and zebrafish embryos were assessed with survival rate over 48 hours and 96 hours, respectively. HepG2 cells were cultured in DMEM medium containing 10% fetal bovine serum (FBS) and 1% antibiotics (10 mg/mL streptomycin and 10 U/mL penicillin) at 37 °C with 5% CO<sub>2</sub>. Cells in the logarithmic phase were collected and seeded in 96-well plates with 6000 cells per well. After 24 hours incubation, cells were exposed to cell culture medium containing PBFA at different concentrations (0, 50, 100, 250, 750 and 1000 mg/L) for 48 hours. Cell viability was determined using a CellTiter-Lumi™ Luminescent Cell Viability Assay Kit according to the manufacturer's protocol (Beyotime Institute of Biotechnology, Shanghai, China). Toxicity of PBFA in zebrafish embryos was assessed with survival rate over 96 hours. Ninety-six embryos at ~6 hours post fertilized (hpf) were transferred into 96-well plates for exposure. In experiments, embryos were treated with 0, 25, 50, 100, 250 and 500 mg/L at 28±1°C. The chemical

was prepared as per above and renewed daily at the same time of the day. Development and survival rate of zebrafish embryos were recorded every 24 hours until 96 hours exposure using stereomicroscope (Leica Microsystems, S9 series, US).

### **S3. Kinetic properties analysis.**

Based on the energy information obtained from the CCSD(T)//M06-2X/6-311+G(d,p) level, the rate constants were computed under the aegis of the TST, CVT, and CVT/SCT methods, which were adopted to analyze the role of variational and small-curvature tunneling effects in the reaction processes. The curves of  $V_{MEP}$ , ZPE, and  $V_a^G$  versus  $s$  (amu)<sup>1/2</sup> bohr at the CCSD(T)//M06-2X/6-311+G(d,p) level for all the five pathways presented in Figures S4–S5 suggested that the variational effects could be omitted because the tendency and zenith between  $V_{MEP}$  and  $V_a^G$  were similar. The curves of TST and CVT rate coefficients for the five channels displayed in the Figures S6–S7 were close and even overlap, showing that the variational effect was negligible.

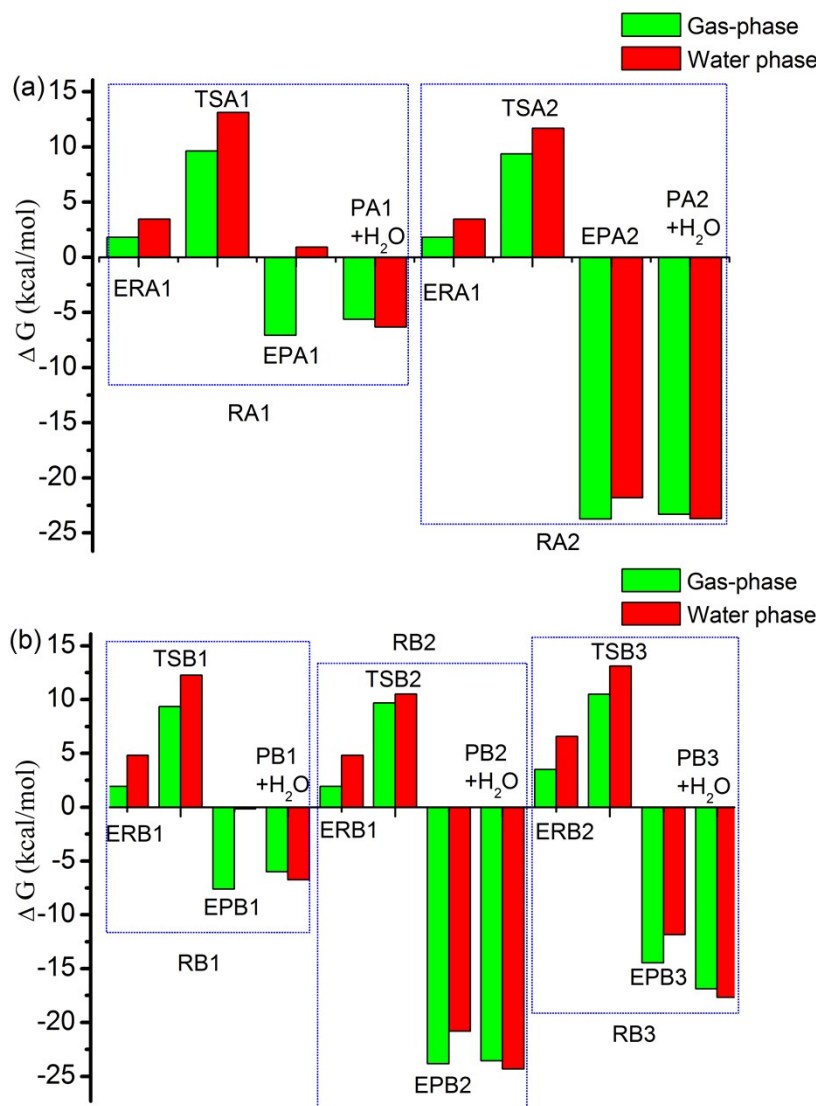
Atoms tunneling acted a significant role in many chemical transformations, which changed reaction paths and branching ratios and enabled chemical reactions in an astrochemical environment.<sup>5</sup> Recently, Schreiner<sup>6</sup> proposed that tunneling could be served as the third reactivity paradigm in control of chemical reactions. Thus, the influence of tunneling on the reaction rates must be simulated directly by computational studies so as to provide useful information for the further experimental

studies. From Figures S4–S5, it could be found that the small-curvature tunneling for all the five reaction channels were outstanding on improving the performance of the individual rate coefficients when the temperature was lower than about 500 K. Taking the main reaction pathway of  $\text{CF}_3\text{CF}_2\text{CF}_2\text{CH}_2\text{OH}$  with OH radical as an example, the small-curvature tunneling factor was 14.84 at 200 K, 4.40 at 273 K, 3.40 at 298 K, and 1.31 at 500 K. The obvious small-curvature tunneling effects have been also reported in the OH radical degradation of congeneric FAs.<sup>7–9</sup>

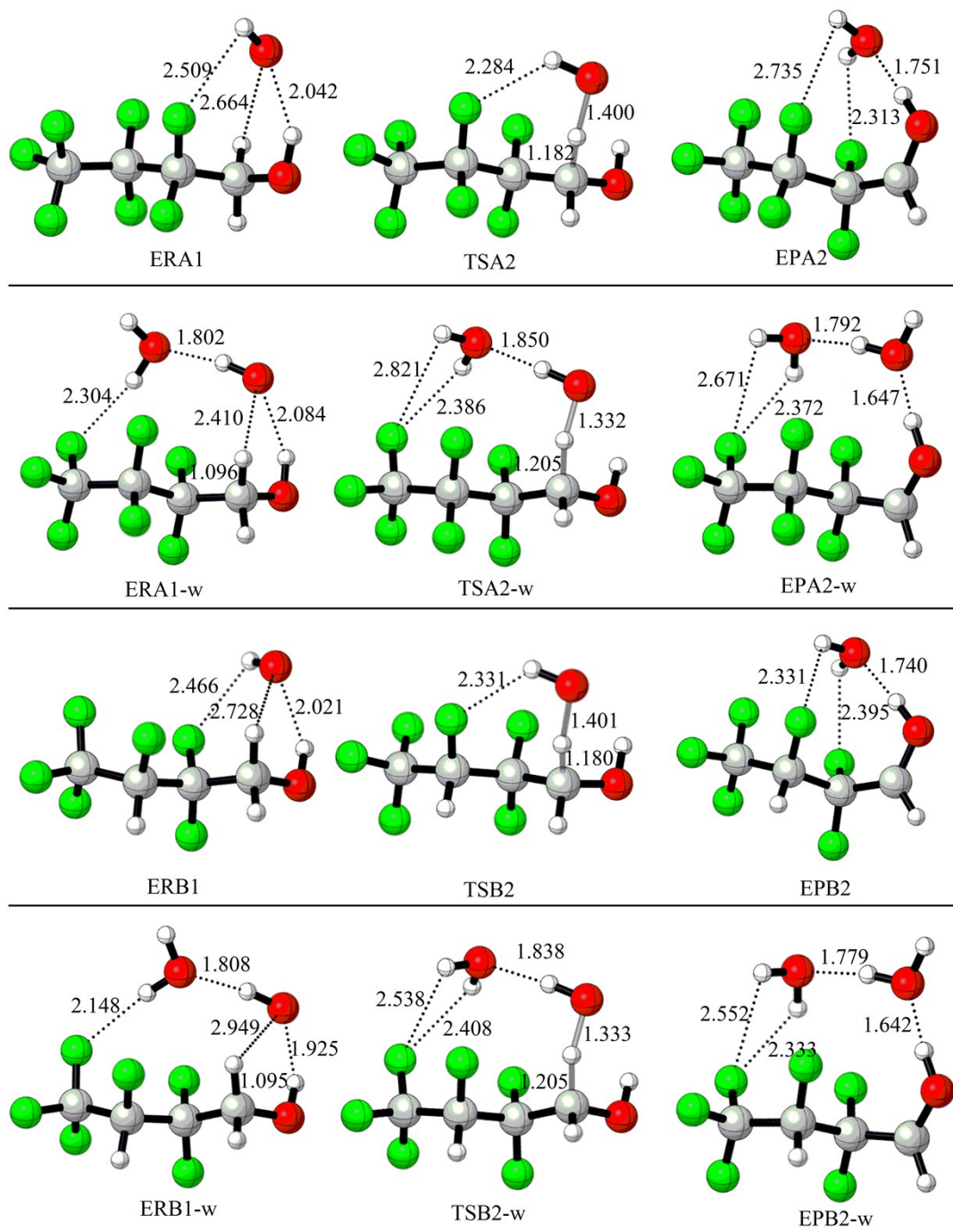
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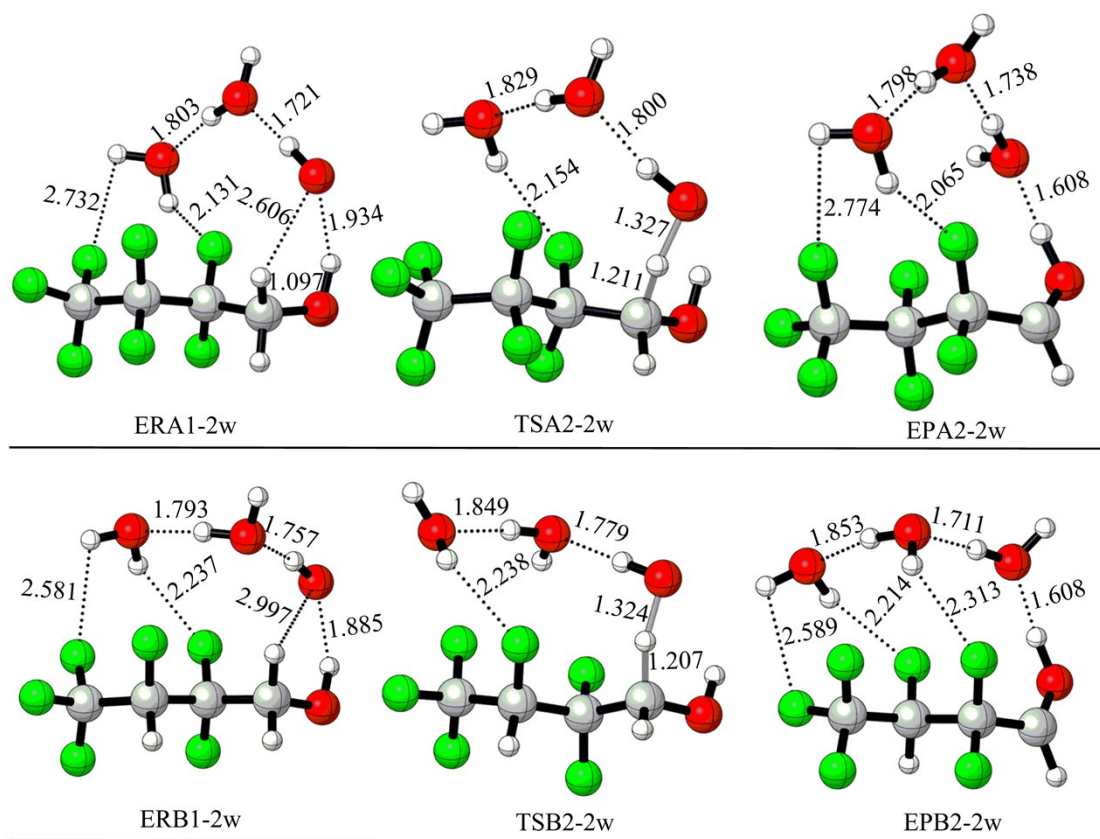


**Figure S1.** Gas-phase (g) and water-phase (w) free energies of reaction intermediates, products, and transition states for the reactions of  $\text{CF}_3\text{CF}_2\text{CF}_2\text{CH}_2\text{OH}$ / $\text{CF}_3\text{CHFCH}_2\text{CH}_2\text{OH}$  with OH radical at the M06-2X/6-311+G(d,p) and M06-2X/(PCM)6-311+G(d,p) levels, respectively.

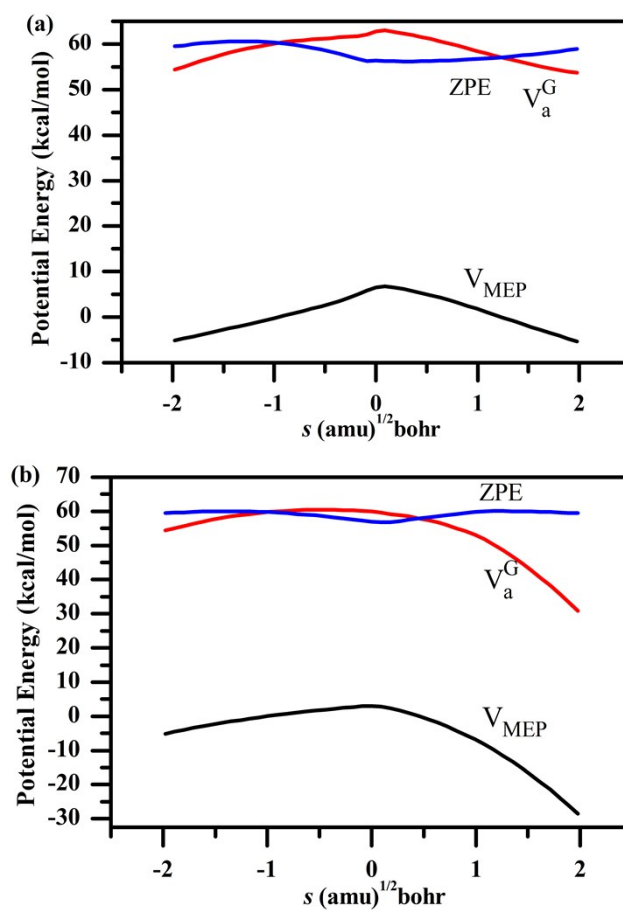


**Figure S2.** The geometries for the reaction processes of ERA1→TSA2→EPA2 and

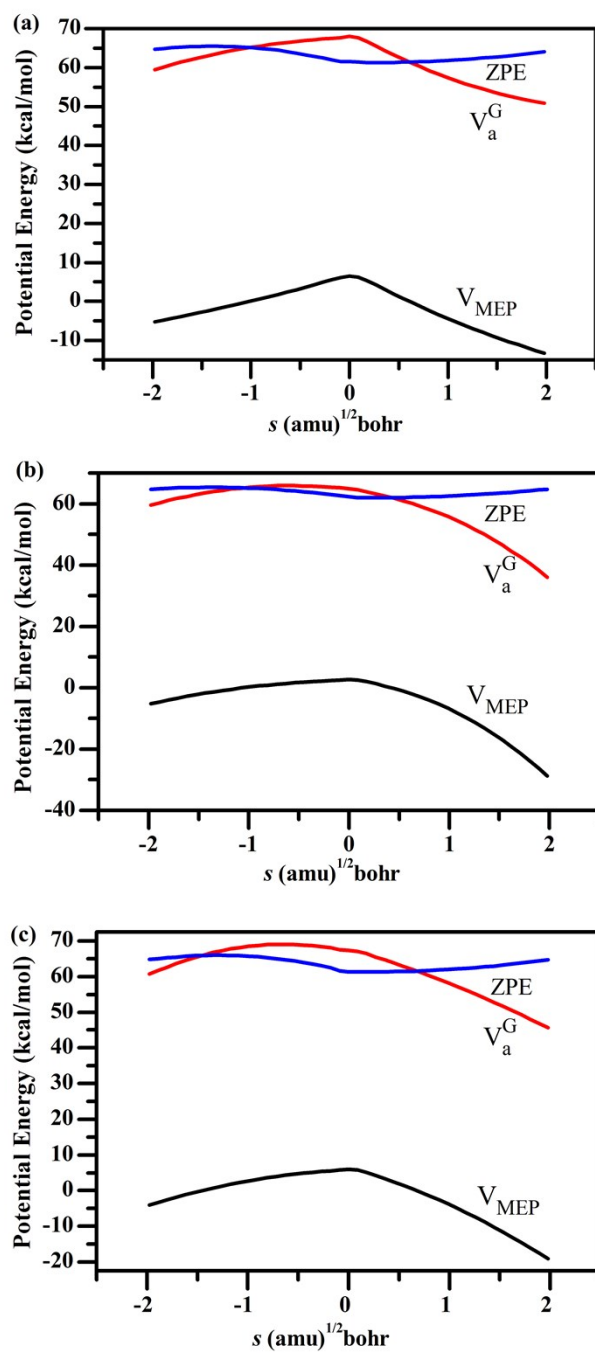
ERB1→TSB2→EPB2 in the absence and presence of H<sub>2</sub>O molecule in the gas-phase optimized at the M06-2X/6-311+G(d,p) level.



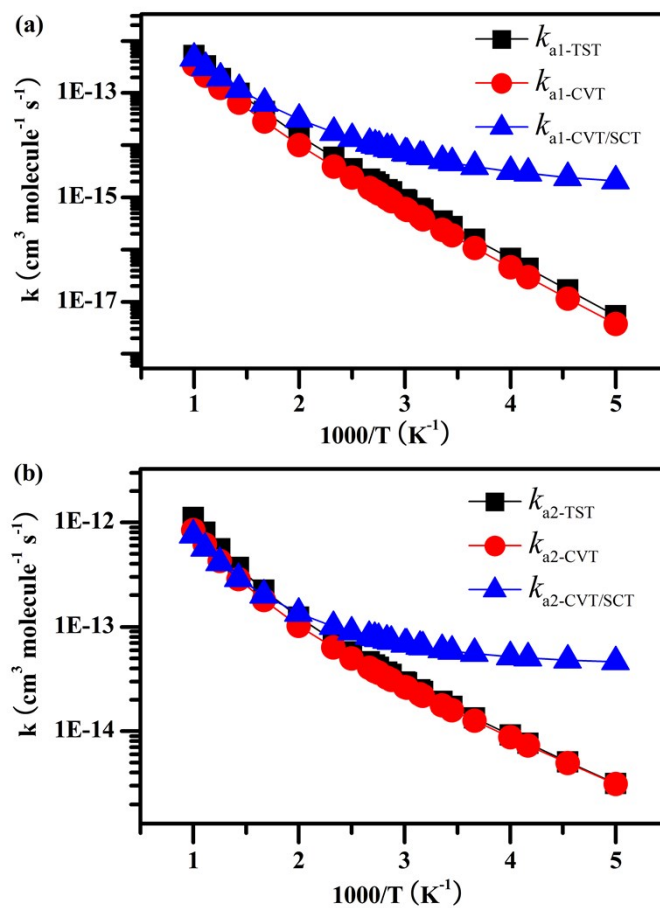
**Figure S3.** The geometries for the reaction processes of ERA1→TSA2→EPA2 and ERB1→TSB2→EPB2 in the presence of two water molecules in the gas-phase optimized at the M06-2X/6-311+G(d,p) level.



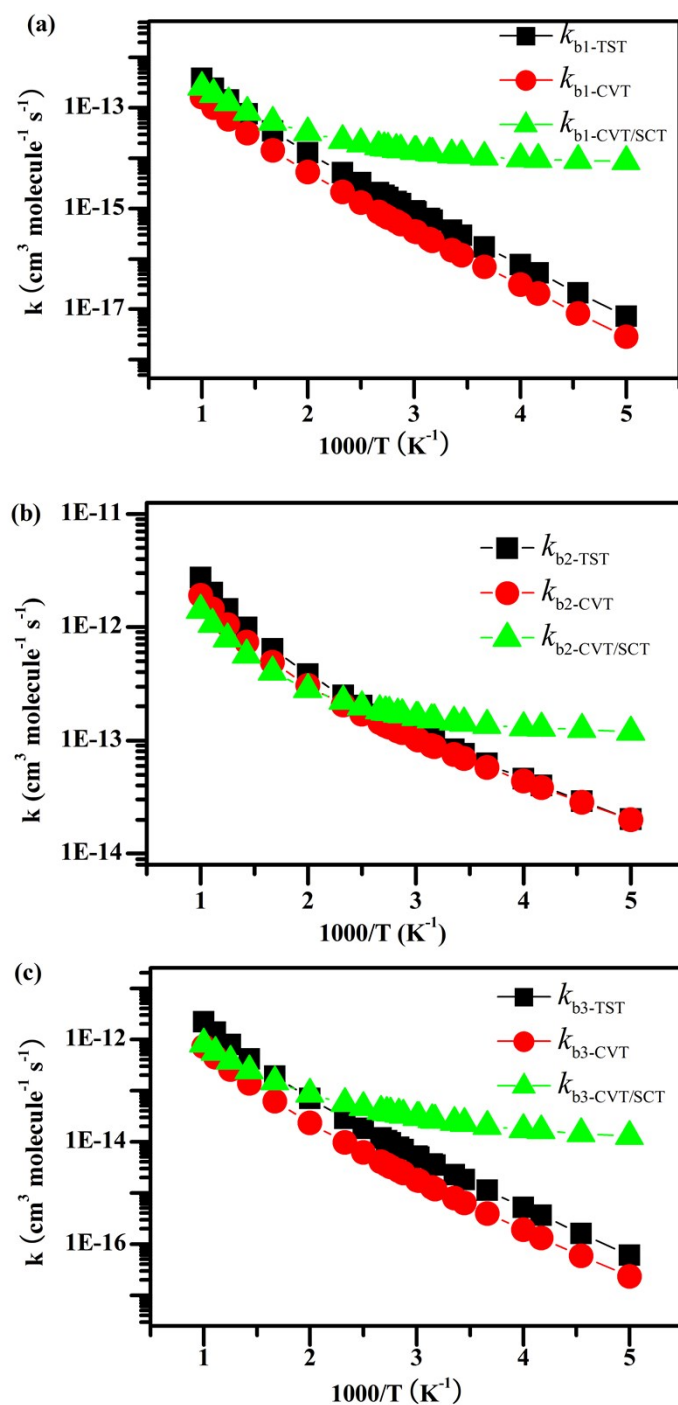
**Figure S4.** Curves of  $V_{MEP}$ , ZPE, and  $V_a^G$  versus  $s \text{ (amu)}^{1/2} \text{ bohr}$  for the reaction channels of RA1 (a) and RA2 (b) obtained at the CCSD(T)//M06-2X/6-311+G(d,p) level.



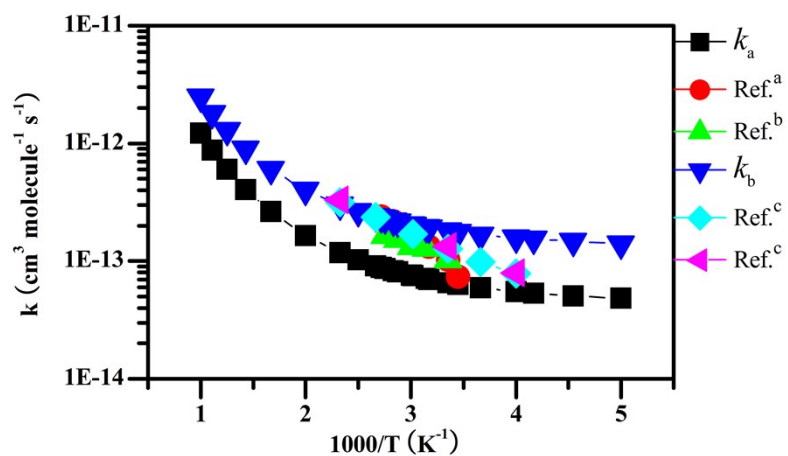
**Figure S5.** Curves of  $V_{MEP}$ , ZPE, and  $V_a^G$  versus  $s \text{ (amu)}^{1/2} \text{ bohr}$  for the reaction channels of RB1 (a), RB2 (b), and RB3 (c) obtained at the CCSD(T)//M06-2X/6-311+G(d,p) level..



**Figure S6.** Calculated TST, CVT, and CVT/SCT rate constants as a function of  $1000/T$  for the reaction channels RA1 (a) and RA2 (b) in the temperature range of 200–1000 K at the CCSD(T)//M06-2X/6-311+G(d,p) level.

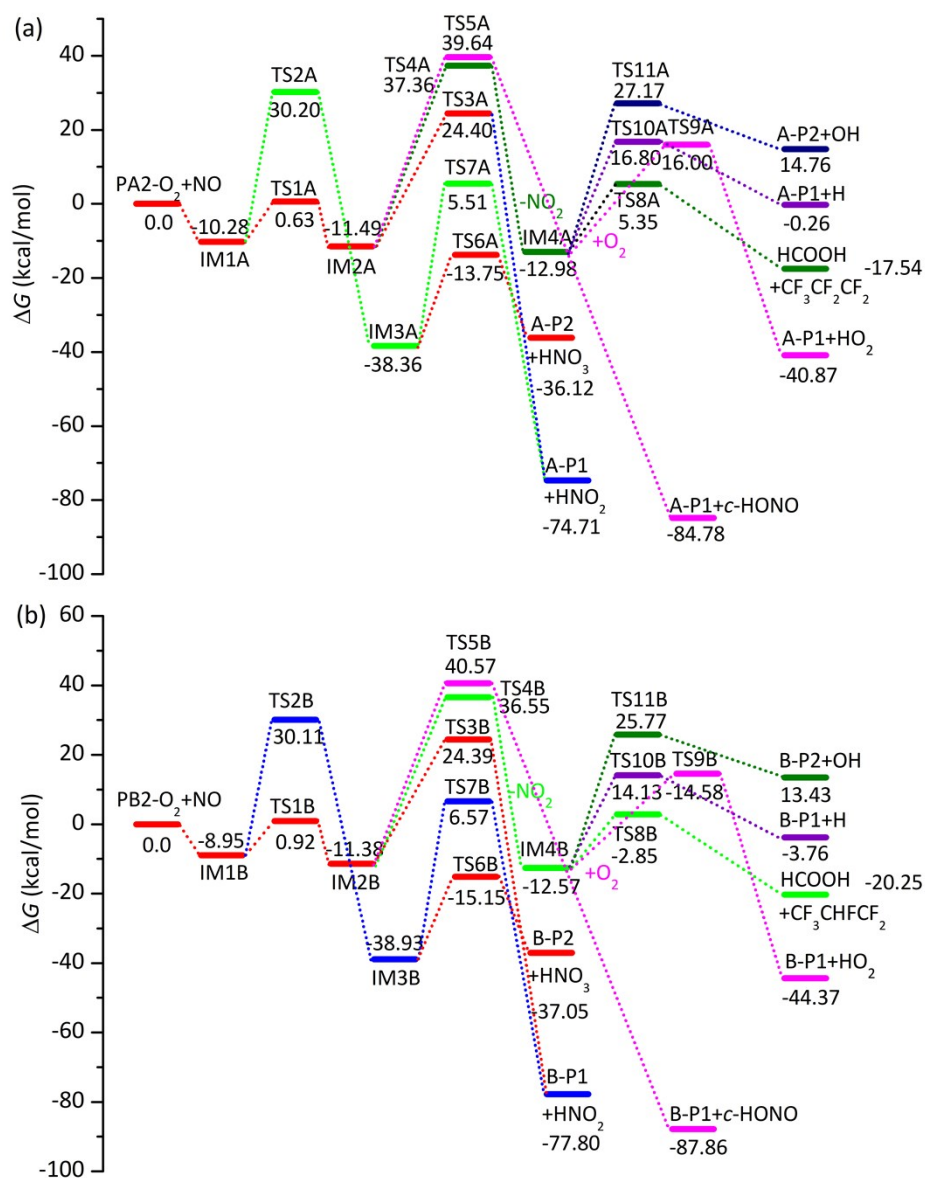


**Figure S7.** Calculated TST, CVT, and CVT/SCT rate constants as a function of  $1000/T$  for the reaction channels RB1 (a), RB2 (b), and RB3 (c) in the temperature range of 200–1000 K at the CCSD(T)//M06-2X/6-311+G(d,p) level.

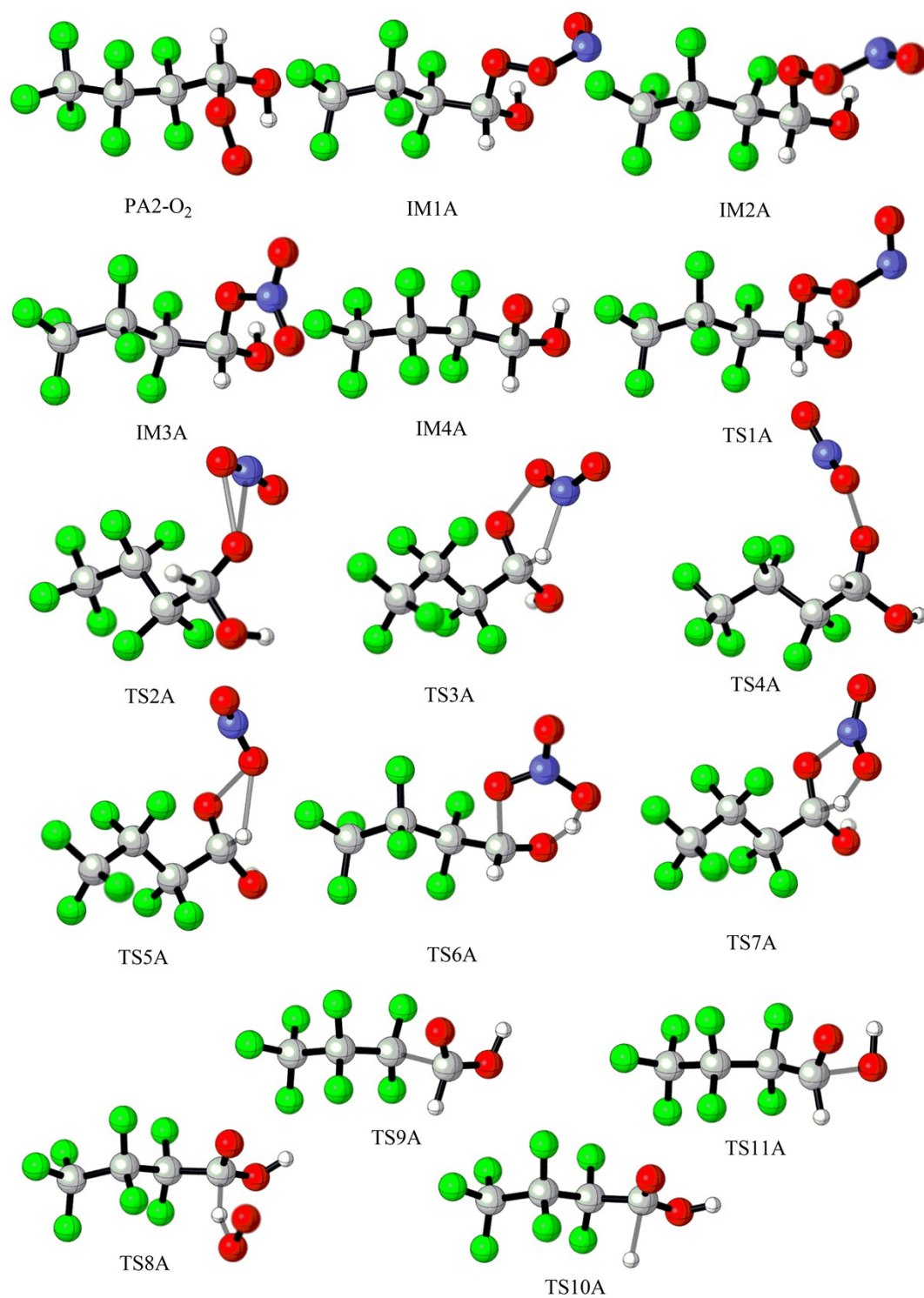


**Figure S8.** Computed total CVT/SCT rate constants along with the experimental data as a function of  $1000/T$  for the reactions of  $\text{CF}_3\text{CF}_2\text{CF}_2\text{CH}_2\text{OH} + \text{OH}$  ( $k_a$ ) and  $\text{CF}_3\text{CHFCH}_2\text{CH}_2\text{OH} + \text{OH}$  ( $k_b$ ) in the temperature range of 200–1000 K at the CCSD(T)//M06-2X/6-311+G(d,p) level.

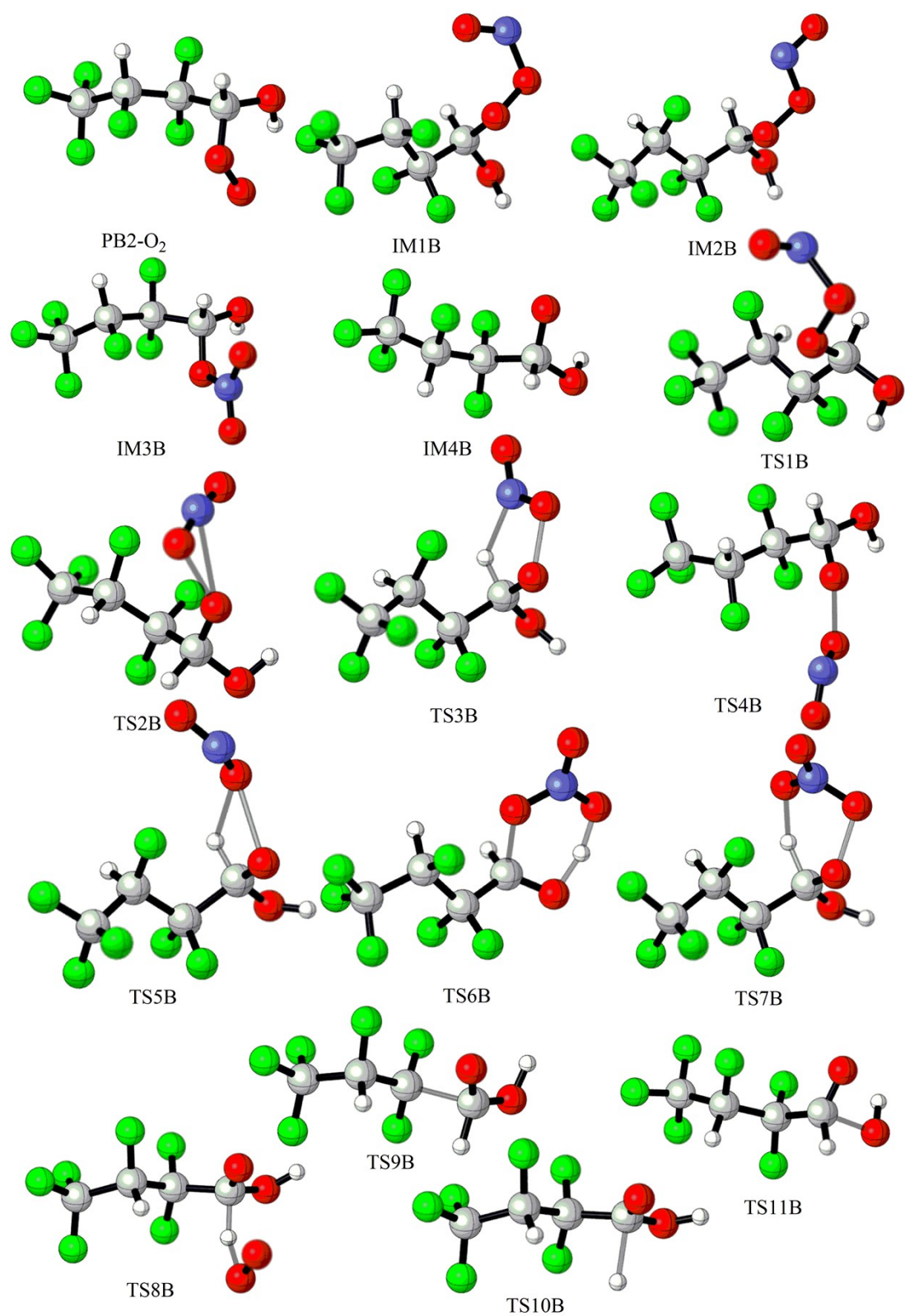




**Figure S9.** Complete free energy surfaces (298 K) for the reactions of  $\text{CF}_3\text{CF}_2\text{CF}_2\text{CH}(\text{OO}\cdot)\text{OH}$  (PA2- $\text{O}_2$ )/ $\text{CF}_3\text{CHF}_2\text{CF}_2\text{CH}(\text{OO}\cdot)\text{OH}$  (PB2- $\text{O}_2$ ) with NO.

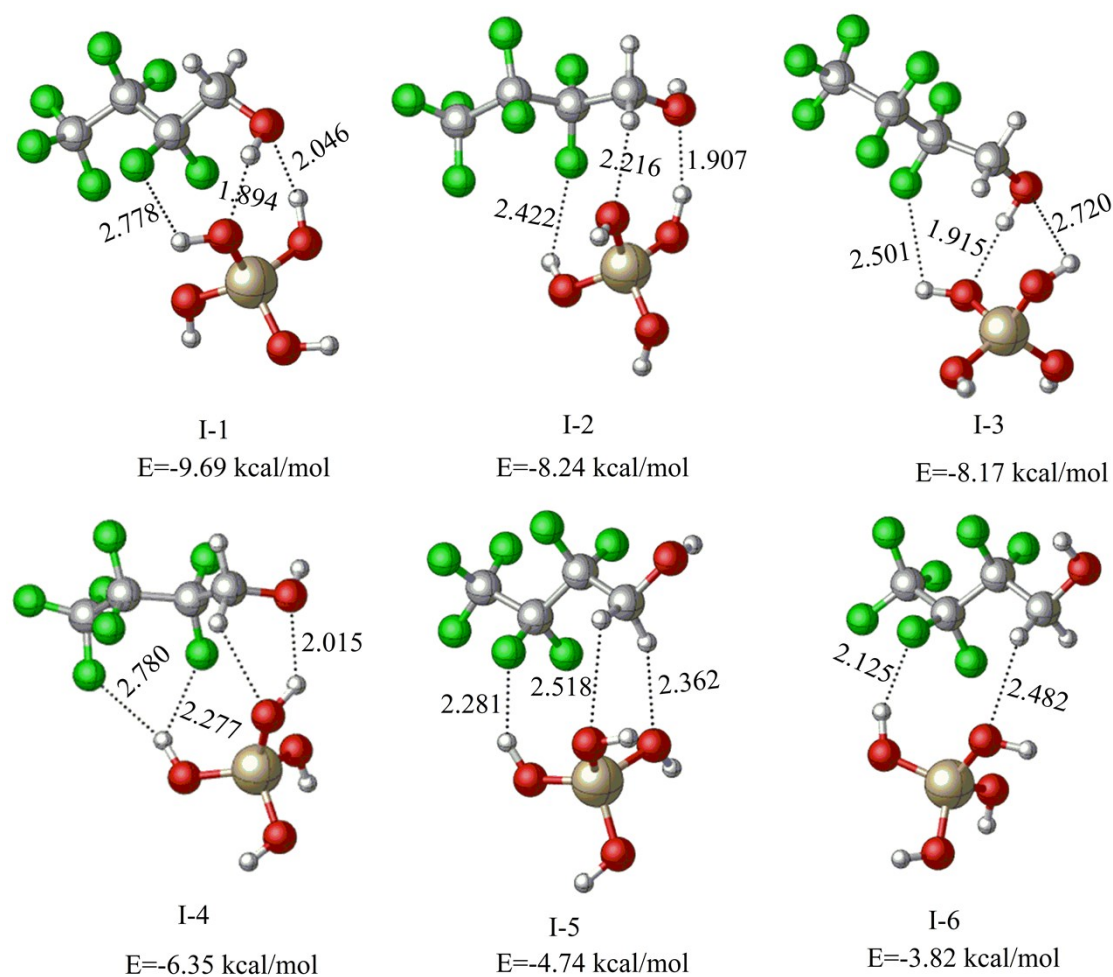


**Figure S10.** The geometries for the stationary points and transition states involving in the reactions of PA2-O<sub>2</sub> with NO in the existence of O<sub>2</sub>.



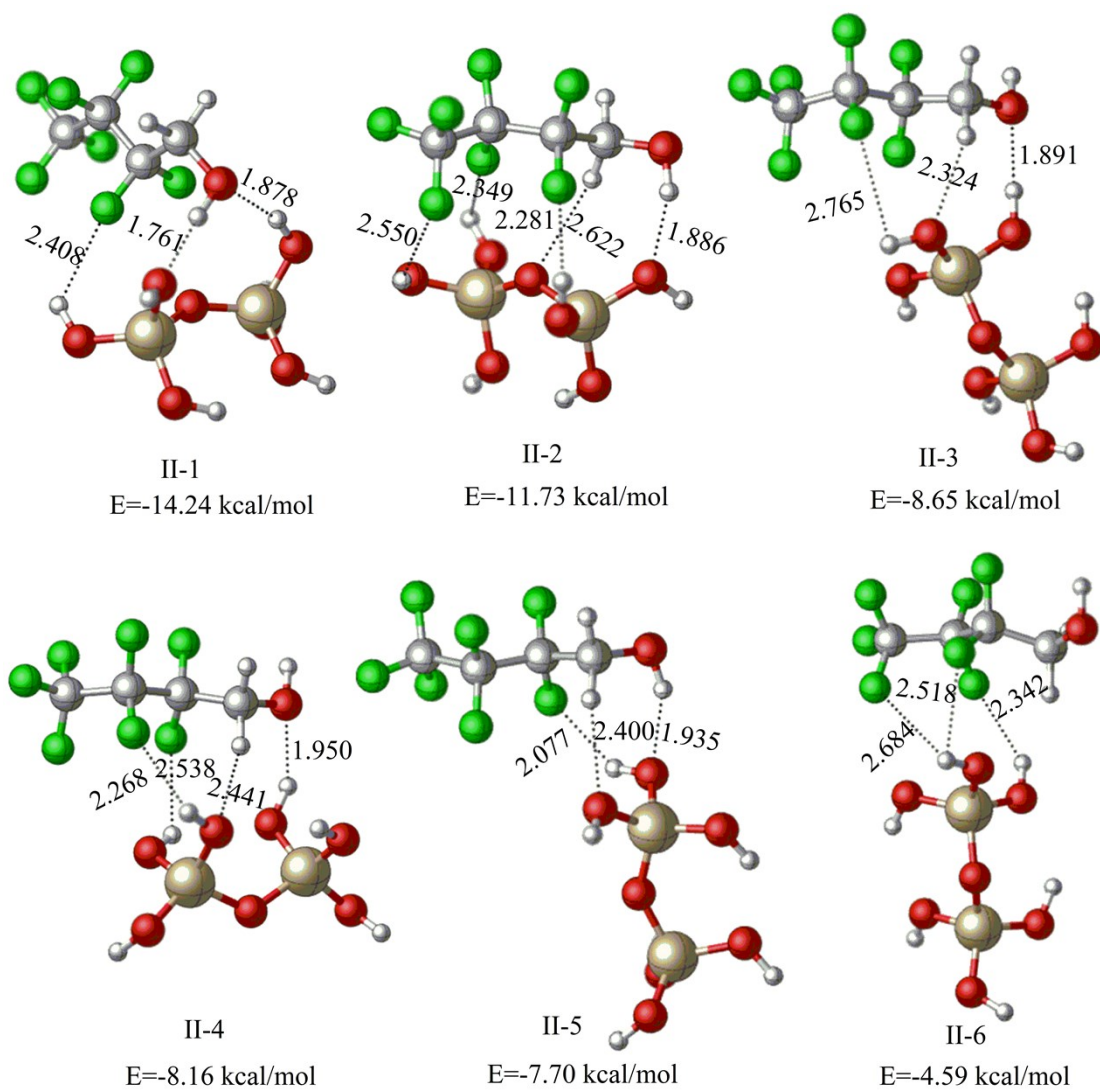
**Figure S11.** The geometries for the stationary points and transition states involving in the

reactions of PB2-O<sub>2</sub> with NO in the existence of O<sub>2</sub>.

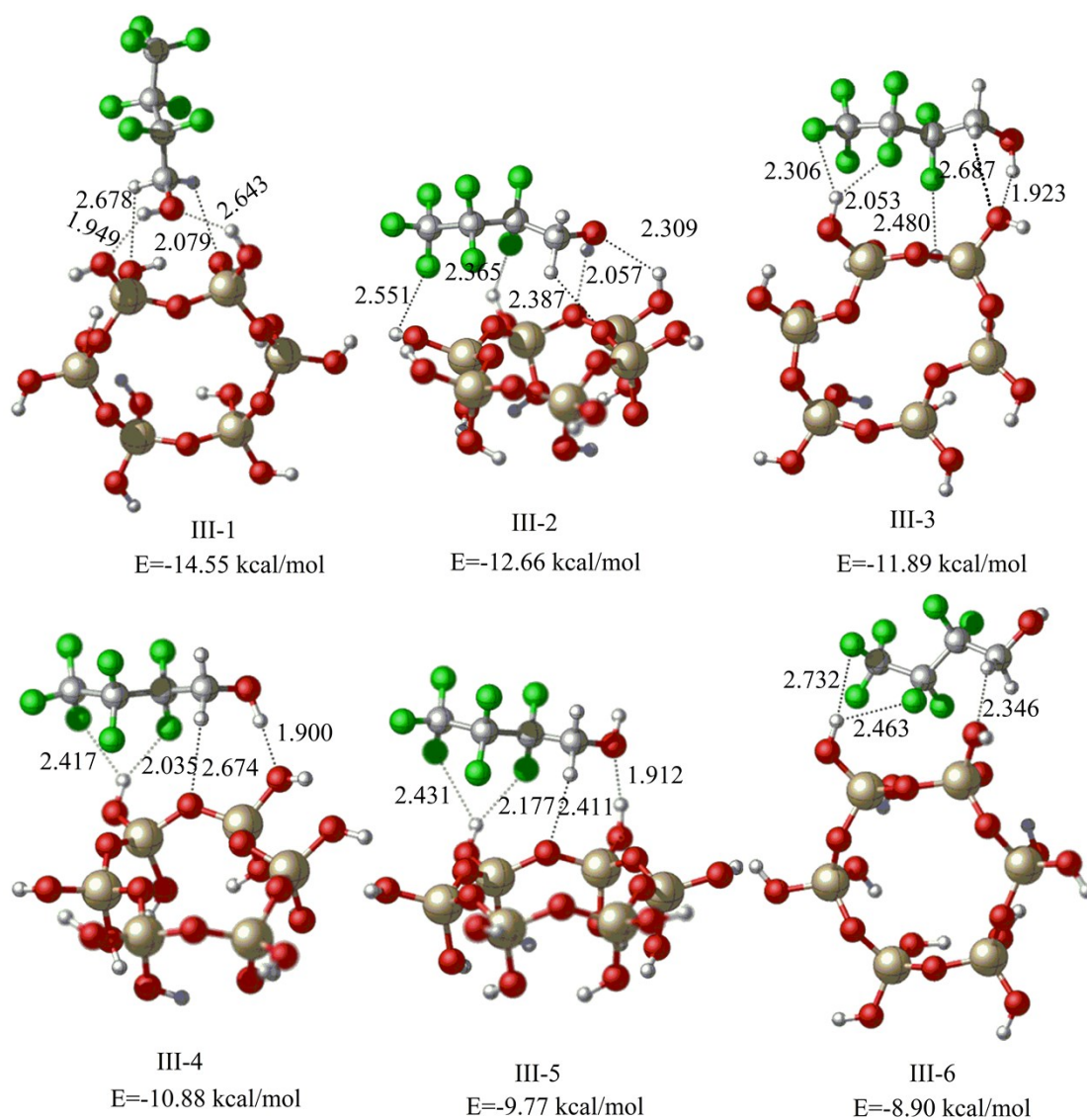


**Figure S12.** Adsorption complexes of CF<sub>3</sub>CF<sub>2</sub>CF<sub>2</sub>CH<sub>2</sub>OH on the silicate monomer (H<sub>4</sub>SiO<sub>4</sub>) surface optimized at the M06-2X/6-311+G(d,p) level. (Distances are given in Å).





**Figure S13.** Adsorption complexes of  $\text{CF}_3\text{CF}_2\text{CF}_2\text{CH}_2\text{OH}$  on the dimer model ( $\text{H}_6\text{Si}_2\text{O}_7$ ) surface optimized at the M06-2X/6-311+G(d,p) level. (Distances are given in Å).



**Figure S14.** Adsorption complexes of  $\text{CF}_3\text{CF}_2\text{CF}_2\text{CH}_2\text{OH}$  on the hexamer model ( $\text{H}_{12}\text{Si}_6\text{O}_{18}$ ) surface optimized at the M06-2X/6-311+G(d,p) level. (Distances are given in Å).

**Table S1.** The imaginary frequency (IF) (in  $\text{cm}^{-1}$ ) and the Wigner tunneling factors ( $\kappa$ ) at 298 K for the transition states involving the reactions of  $\text{CF}_3\text{CF}_2\text{CF}_2\text{CH}_2\text{OH}/\text{CF}_3\text{CHFCF}_2\text{CH}_2\text{OH}$  with OH radical in gaseous (g) and aqueous (aq) phases obtained by M06-2X/6-311+G(d,p) and M06-2X(PCM)/6-311+G(d,p) levels, respectively.

|      | IF <sub>g</sub>  | $\kappa_g$ | IF <sub>aq</sub> | $\kappa_{aq}$ |
|------|------------------|------------|------------------|---------------|
| TSA1 | 1632.01 <i>i</i> | 3.588      | 1856.14 <i>i</i> | 4.348         |
| TSA2 | 1152.45 <i>i</i> | 2.290      | 1126.61 <i>i</i> | 2.233         |
| TSB1 | 1630.09 <i>i</i> | 3.582      | 1811.82 <i>i</i> | 4.190         |
| TSB2 | 1112.52 <i>i</i> | 2.203      | 1084.92 <i>i</i> | 2.144         |
| TSB3 | 1496.49 <i>i</i> | 3.176      | 1707.20 <i>i</i> | 3.832         |



**Table S2.** The energies including the ZPE corrections ( $\Delta E$ ) and Gibbs free energies ( $\Delta G$ ) for the complexes and transition states involving one (1w) and two water (2w) molecules on the reaction of  $\text{CF}_3\text{CF}_2\text{CF}_2\text{CH}_2\text{OH}$  (A) and  $\text{CF}_3\text{CHFCH}_2\text{CH}_2\text{OH}$  (B) with OH radical at the M06-2X/6-311+G(d,p) level of theory.

|                     | $\Delta E$ | $\Delta G$ |
|---------------------|------------|------------|
| A + OH              | 0.0        | 0.0        |
| ERA1                | -5.55      | 1.80       |
| TSA2                | 0.89       | 9.36       |
| EPA2                | -32.05     | -23.75     |
| P2+H <sub>2</sub> O | -22.40     | -23.31     |
| ERA1-w              | -13.69     | 3.29       |
| TSA2-w              | -6.25      | 11.35      |
| EPA2-w              | -40.63     | -23.99     |
| ERA1-2w             | -21.66     | 4.32       |
| TSA2-2w             | -13.38     | 12.68      |
| EPA2-2w             | -48.19     | -23.06     |
| B + OH              | 0.0        | 0.0        |
| ERB1                | -5.63      | 1.92       |
| TSB2                | 1.59       | 9.68       |
| EPB2                | -32.49     | -23.83     |
| P2+H <sub>2</sub> O | -22.39     | -23.57     |
| ERB1-w              | -14.63     | 2.34       |
| TSB2-w              | -6.92      | 10.87      |

|         |        |        |
|---------|--------|--------|
| EPB2-w  | -40.16 | -23.61 |
| ERB1-2w | -22.13 | 3.97   |
| TSB2-2w | -13.88 | 12.51  |
| EPB2-2w | -48.12 | -21.83 |

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**Table S3.** The CVT/SCT rate constants along with the experimental values for the hydrogen abstraction reactions of  $\text{CF}_3\text{CF}_2\text{CF}_2\text{CH}_2\text{OH}$  (A) by OH radical within 200–1000 K calculated at the CCSD(T)//M06-2X/6-311+G(d,p) level.

| $T$ (K) | $k_{a1}$ | $k_{a2}$ | $k_a$    | $k_{\text{Exp.}}$ (Bravo et al) | $k_{\text{Exp.}}$ (Indulkar et al) |
|---------|----------|----------|----------|---------------------------------|------------------------------------|
| 200     | 2.06E-15 | 4.63E-14 | 4.84E-14 |                                 |                                    |

|      |          |          |          |                                |                                |
|------|----------|----------|----------|--------------------------------|--------------------------------|
| 220  | 2.42E-15 | 4.79E-14 | 5.03E-14 |                                |                                |
| 240  | 2.89E-15 | 5.03E-14 | 5.32E-14 |                                |                                |
| 250  | 3.16E-15 | 5.17E-14 | 5.49E-14 |                                |                                |
| 273  | 3.94E-15 | 5.54E-14 | 5.93E-14 |                                |                                |
| 290  | 4.65E-15 | 5.86E-14 | 6.33E-14 | $(9.12 \pm 1.71)\text{E-14}^a$ |                                |
| 298  | 5.04E-15 | 6.02E-14 | 6.52E-14 | $(1.07 \pm 0.05)\text{E-13}^a$ | $(1.15 \pm 0.12)\text{E-13}^b$ |
| 315  | 5.96E-15 | 6.40E-14 | 7.00E-14 | $(1.51 \pm 0.18)\text{E-13}^a$ |                                |
| 318  | 6.14E-15 | 6.47E-14 | 7.08E-14 |                                | $(1.47 \pm 0.18)\text{E-13}^b$ |
| 331  | 6.98E-15 | 6.80E-14 | 7.50E-14 |                                |                                |
| 333  | 7.11E-15 | 6.85E-14 | 7.56E-14 | $(1.72 \pm 0.14)\text{E-13}^a$ | $(1.50 \pm 0.17)\text{E-13}^b$ |
| 348  | 8.23E-15 | 7.26E-14 | 8.08E-14 |                                | $(1.70 \pm 0.18)\text{E-13}^b$ |
| 353  | 8.64E-15 | 7.40E-14 | 8.26E-14 | $(2.35 \pm 0.18)\text{E-13}^a$ |                                |
| 363  | 9.51E-15 | 7.70E-14 | 8.65E-14 |                                | $(1.86 \pm 0.22)\text{E-13}^b$ |
| 368  | 9.97E-15 | 7.85E-14 | 8.85E-14 | $(2.67 \pm 0.28)\text{E-13}^a$ |                                |
| 375  | 1.07E-14 | 8.07E-14 | 9.14E-14 |                                |                                |
| 400  | 1.34E-14 | 8.93E-14 | 1.03E-13 |                                |                                |
| 430  | 1.75E-14 | 1.01E-13 | 1.19E-13 |                                |                                |
| 500  | 3.11E-14 | 1.34E-13 | 1.65E-13 |                                |                                |
| 600  | 6.31E-14 | 2.00E-13 | 2.63E-13 |                                |                                |
| 700  | 1.16E-13 | 2.90E-13 | 4.06E-13 |                                |                                |
| 800  | 1.95E-13 | 4.10E-13 | 6.05E-13 |                                |                                |
| 900  | 3.08E-13 | 5.65E-13 | 8.73E-13 |                                |                                |
| 1000 | 4.62E-13 | 7.59E-13 | 1.22E-12 |                                |                                |

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<sup>a</sup> Obtained by discharge flow technique with mass-spectrometric detection technique.

<sup>b</sup> Obtained by laser photolysis laser induced fluorescence (LP-LIF) technique.

**Table S4.** The CVT/SCT rate constants along with the experimental values for the hydrogen abstraction reactions of CF<sub>3</sub>CHFCF<sub>2</sub>CH<sub>2</sub>OH (B) by OH radical within 200–1000 K calculated at the CCSD(T)/M06-2X/6-311+G(d,p) level.

| <i>T</i> (K) | <i>k</i> <sub>b1</sub> | <i>k</i> <sub>b2</sub> | <i>k</i> <sub>b3</sub> | <i>k</i> <sub>b</sub> | <i>k</i> <sub>Exp.</sub> (Chen et al) | <i>k</i> <sub>Exp.</sub> (Chen et al) |
|--------------|------------------------|------------------------|------------------------|-----------------------|---------------------------------------|---------------------------------------|
| 200          | 8.60E-15               | 1.19E-13               | 1.27E-14               | 1.40E-13              |                                       |                                       |
| 220          | 8.95E-15               | 1.25E-13               | 1.43E-14               | 1.48E-13              |                                       |                                       |
| 240          | 9.46E-15               | 1.28E-13               | 1.62E-14               | 1.54E-13              |                                       |                                       |
| 250          | 9.76E-15               | 1.30E-13               | 1.73E-14               | 1.57E-13              | (7.84 ± 0.69)E-14 <sup>a</sup>        | (7.90 ± 0.58)E-14 <sup>b</sup>        |
| 273          | 1.06E-14               | 1.36E-13               | 2.01E-14               | 1.67E-13              | (9.82 ± 0.77)E-14 <sup>a</sup>        |                                       |
| 290          | 1.13E-14               | 1.42E-13               | 2.26E-14               | 1.76E-13              |                                       |                                       |
| 298          | 1.17E-14               | 1.45E-13               | 2.38E-14               | 1.81E-13              | (1.27 ± 0.08)E-13 <sup>a</sup>        | (1.33 ± 0.07)E-13 <sup>b</sup>        |

|      |          |          |          |          |                                |                                |
|------|----------|----------|----------|----------|--------------------------------|--------------------------------|
| 315  | 1.26E-14 | 1.52E-13 | 2.66E-14 | 1.91E-13 |                                |                                |
| 318  | 1.28E-14 | 1.53E-13 | 2.72E-14 | 1.93E-13 |                                |                                |
| 331  | 1.36E-14 | 1.59E-13 | 2.96E-14 | 2.02E-13 | (1.69 ± 0.09)E-13 <sup>a</sup> |                                |
| 333  | 1.37E-14 | 1.60E-13 | 3.00E-14 | 2.04E-13 |                                |                                |
| 348  | 1.48E-14 | 1.68E-13 | 3.31E-14 | 2.16E-13 |                                |                                |
| 353  | 1.51E-14 | 1.70E-13 | 3.42E-14 | 2.19E-13 |                                |                                |
| 363  | 1.59E-14 | 1.76E-13 | 3.65E-14 | 2.28E-13 |                                |                                |
| 368  | 1.63E-14 | 1.79E-13 | 3.77E-14 | 2.33E-13 |                                |                                |
| 375  | 1.69E-14 | 1.83E-13 | 3.95E-14 | 2.39E-13 | (2.36 ± 0.09)E-13 <sup>a</sup> |                                |
| 400  | 1.91E-14 | 1.99E-13 | 4.63E-14 | 2.64E-13 |                                |                                |
| 430  | 2.23E-14 | 2.21E-13 | 5.59E-14 | 2.99E-13 | (3.15 ± 0.12)E-13 <sup>a</sup> | (3.29 ± 0.15)E-13 <sup>b</sup> |
| 500  | 3.19E-14 | 2.83E-13 | 8.49E-14 | 4.00E-13 |                                |                                |
| 600  | 5.22E-14 | 4.04E-13 | 1.47E-13 | 6.03E-13 |                                |                                |
| 700  | 8.24E-14 | 5.68E-13 | 2.41E-13 | 8.91E-13 |                                |                                |
| 800  | 1.25E-13 | 7.85E-13 | 3.76E-13 | 1.29E-12 |                                |                                |
| 900  | 1.84E-13 | 1.06E-12 | 5.63E-13 | 1.81E-12 |                                |                                |
| 1000 | 2.60E-13 | 1.41E-12 | 8.15E-13 | 2.49E-12 |                                |                                |

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<sup>a</sup> Obtained by flash photolysis laser induced fluorescence (FP-LIF) technique.

<sup>b</sup> Obtained by laser photolysis laser induced fluorescence (LP-LIF) technique.

**Table S5.** The frequencies, IR intensities, and radiative forcing of CF<sub>3</sub>CF<sub>2</sub>CF<sub>2</sub>CH<sub>2</sub>OH obtained at the M06-2X/6-311+G(d,p) level in the calculation of GWP.

| Frequencies<br>(cm <sup>-1</sup> ) | Ak (IR<br>intensities)<br>(km/mol) | Ak (IR<br>intensities)<br>(cm/molecule) | Radiative forcing<br>per Unit Cross<br>Section 10 <sup>15</sup> W<br>m <sup>-2</sup> (cm <sup>-1</sup> ) <sup>-1</sup> (cm <sup>2</sup><br>molecule <sup>-1</sup> ) <sup>-1</sup> | Radiative<br>forcing 10 <sup>15</sup><br>(W/m <sup>2</sup> ppbv<br>) | Total<br>Radiative<br>forcing<br>(W/m <sup>2</sup> ppb<br>v) |
|------------------------------------|------------------------------------|-----------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------|--------------------------------------------------------------|
| 35.6725                            | 0.595                              | 9.88E-20                                | 0.0363                                                                                                                                                                            | 3.59E-21                                                             |                                                              |
| 67.8335                            | 0.1743                             | 2.90E-20                                | 0.0724                                                                                                                                                                            | 2.10E-21                                                             |                                                              |
| 105.6563                           | 3.1956                             | 5.31E-19                                | 0.191                                                                                                                                                                             | 1.01E-19                                                             |                                                              |
| 125.9299                           | 2.7007                             | 4.49E-19                                | 0.202                                                                                                                                                                             | 9.06E-20                                                             |                                                              |
| 206.7708                           | 1.3814                             | 2.29E-19                                | 0.484                                                                                                                                                                             | 1.11E-19                                                             |                                                              |
| 220.9867                           | 1.6089                             | 2.67E-19                                | 0.42                                                                                                                                                                              | 1.12E-19                                                             | 3.12E-01                                                     |
| 235.5341                           | 0.079                              | 1.31E-20                                | 0.514                                                                                                                                                                             | 6.75E-21                                                             |                                                              |
| 292.4289                           | 8.5401                             | 1.42E-18                                | 0.776                                                                                                                                                                             | 1.10E-18                                                             |                                                              |
| 315.7822                           | 30.2394                            | 5.02E-18                                | 0.732                                                                                                                                                                             | 3.68E-18                                                             |                                                              |
| 327.3867                           | 9.4522                             | 1.57E-18                                | 0.856                                                                                                                                                                             | 1.34E-18                                                             |                                                              |
| 340.1812                           | 0.0866                             | 1.44E-20                                | 0.862                                                                                                                                                                             | 1.24E-20                                                             |                                                              |

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|           |          |          |       |          |
|-----------|----------|----------|-------|----------|
| 373.8656  | 70.0056  | 1.16E-17 | 0.99  | 1.15E-17 |
| 387.0334  | 1.8574   | 3.09E-19 | 1     | 3.09E-19 |
| 420.0524  | 38.6063  | 6.41E-18 | 1.33  | 8.53E-18 |
| 520.6421  | 2.457    | 4.08E-19 | 1.97  | 8.04E-19 |
| 543.7158  | 15.8474  | 2.63E-18 | 1.96  | 5.16E-18 |
| 551.6554  | 17.2695  | 2.87E-18 | 2.21  | 6.34E-18 |
| 615.5029  | 0.9256   | 1.54E-19 | 2.01  | 3.09E-19 |
| 668.8897  | 2.0684   | 3.44E-19 | 2.13  | 7.32E-19 |
| 753.5698  | 78.0032  | 1.30E-17 | 2.37  | 3.07E-17 |
| 804.7279  | 11.2868  | 1.87E-18 | 3.09  | 5.79E-18 |
| 938.1568  | 114.7289 | 1.91E-17 | 2.81  | 5.36E-17 |
| 961.1997  | 61.7842  | 1.03E-17 | 2.81  | 2.88E-17 |
| 1143.4767 | 82.8398  | 1.38E-17 | 1.88  | 2.59E-17 |
| 1164.1314 | 165.1141 | 2.74E-17 | 1.72  | 4.72E-17 |
| 1176.0377 | 25.3608  | 4.21E-18 | 1.52  | 6.40E-18 |
| 1233.3518 | 121.2055 | 2.01E-17 | 1.26  | 2.54E-17 |
| 1242.7379 | 21.9849  | 3.65E-18 | 0.906 | 3.31E-18 |
| 1268.4349 | 164.729  | 2.74E-17 | 0.455 | 1.25E-17 |
| 1285.2621 | 242.1863 | 4.02E-17 | 0.359 | 1.44E-17 |
| 1303.6599 | 337.6616 | 5.61E-17 | 0.207 | 1.16E-17 |
| 1349.9713 | 55.3016  | 9.19E-18 | 0.28  | 2.57E-18 |
| 1401.6607 | 82.2133  | 1.37E-17 | 0.182 | 2.49E-18 |
| 1409.6758 | 39.2639  | 6.52E-18 | 0.098 | 6.39E-19 |
| 1443.3142 | 17.8319  | 2.96E-18 | 0.122 | 3.61E-19 |

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|           |        |          |        |          |
|-----------|--------|----------|--------|----------|
| 1499.3399 | 2.8204 | 4.69E-19 | 0.0372 | 1.74E-20 |
|-----------|--------|----------|--------|----------|

**Table S6.** The frequencies, IR intensities, and radiative forcing of CF<sub>3</sub>CHFCF<sub>2</sub>CH<sub>2</sub>OH obtained at the M06-2X/6-311+G(d,p) level in the calculation of GWP.

| Frequencies<br>(cm <sup>-1</sup> ) | Ak (IR<br>intensities)<br>(km/mol) | Ak (IR<br>intensities)<br>(cm/molecule) | Radiative forcing<br>per Unit Cross<br>Section 10 <sup>15</sup> W<br>m <sup>-2</sup> (cm <sup>-1</sup> ) <sup>-1</sup> (cm <sup>2</sup><br>molecule <sup>-1</sup> ) <sup>-1</sup> | Radiative<br>forcing 10 <sup>15</sup><br>(W/m <sup>2</sup> ppbv<br>) | Total<br>Radiative<br>forcing<br>(W/m <sup>2</sup> ppb<br>v) |
|------------------------------------|------------------------------------|-----------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------|--------------------------------------------------------------|
| 47.1557                            | 0.7199                             | 1.20E-19                                | 0.0421                                                                                                                                                                            | 5.03E-21                                                             |                                                              |
| 69.815                             | 0.6401                             | 1.06E-19                                | 0.0724                                                                                                                                                                            | 7.70E-21                                                             |                                                              |
| 102.0598                           | 5.7201                             | 9.50E-19                                | 0.131                                                                                                                                                                             | 1.24E-19                                                             |                                                              |
| 135.5697                           | 0.8423                             | 1.40E-19                                | 0.255                                                                                                                                                                             | 3.57E-20                                                             |                                                              |
| 215.3239                           | 0.2747                             | 4.56E-20                                | 0.42                                                                                                                                                                              | 1.92E-20                                                             |                                                              |
| 231.2396                           | 2.8221                             | 4.69E-19                                | 0.584                                                                                                                                                                             | 2.74E-19                                                             |                                                              |
| 266.6353                           | 3.4325                             | 5.70E-19                                | 0.611                                                                                                                                                                             | 3.48E-19                                                             |                                                              |
| 302.8813                           | 5.2116                             | 8.66E-19                                | 0.678                                                                                                                                                                             | 5.87E-19                                                             |                                                              |
| 325.6                              | 15.7451                            | 2.62E-18                                | 0.856                                                                                                                                                                             | 2.24E-18                                                             | 2.74E-01                                                     |
| 340.2732                           | 1.3803                             | 2.29E-19                                | 0.862                                                                                                                                                                             | 1.98E-19                                                             |                                                              |
| 383.186                            | 47.9734                            | 7.97E-18                                | 1.06                                                                                                                                                                              | 8.45E-18                                                             |                                                              |
| 428.9574                           | 68.9157                            | 1.14E-17                                | 1.41                                                                                                                                                                              | 1.61E-17                                                             |                                                              |
| 479.04                             | 22.0367                            | 3.66E-18                                | 1.68                                                                                                                                                                              | 6.15E-18                                                             |                                                              |
| 535.8701                           | 5.6581                             | 9.40E-19                                | 1.96                                                                                                                                                                              | 1.84E-18                                                             |                                                              |
| 556.67                             | 13.5243                            | 2.25E-18                                | 2.01                                                                                                                                                                              | 4.52E-18                                                             |                                                              |
| 598.2269                           | 4.2681                             | 7.09E-19                                | 1.36                                                                                                                                                                              | 9.64E-19                                                             |                                                              |
| 703.5139                           | 67.0509                            | 1.11E-17                                | 0.51                                                                                                                                                                              | 5.68E-18                                                             |                                                              |

|           |          |          |        |          |
|-----------|----------|----------|--------|----------|
| 769.5506  | 20.7684  | 3.45E-18 | 3.03   | 1.05E-17 |
| 861.4057  | 49.3219  | 8.19E-18 | 3.17   | 2.60E-17 |
| 890.8248  | 27.6878  | 4.60E-18 | 3.1    | 1.43E-17 |
| 951.2928  | 29.5471  | 4.91E-18 | 2.81   | 1.38E-17 |
| 1096.6125 | 143.963  | 2.39E-17 | 2.1    | 5.02E-17 |
| 1153.7092 | 31.2775  | 5.20E-18 | 1.79   | 9.30E-18 |
| 1170.2955 | 63.9873  | 1.06E-17 | 1.52   | 1.62E-17 |
| 1181.9137 | 76.9045  | 1.28E-17 | 1.52   | 1.94E-17 |
| 1231.2477 | 117.0335 | 1.94E-17 | 1.26   | 2.45E-17 |
| 1242.6526 | 82.9909  | 1.38E-17 | 0.906  | 1.25E-17 |
| 1283.5077 | 179.9606 | 2.99E-17 | 0.411  | 1.23E-17 |
| 1295.1777 | 185.0271 | 3.07E-17 | 0.207  | 6.36E-18 |
| 1338.9988 | 233.7203 | 3.88E-17 | 0.231  | 8.97E-18 |
| 1382.2846 | 5.8471   | 9.71E-19 | 0.181  | 1.76E-19 |
| 1411.1375 | 24.2039  | 4.02E-18 | 0.098  | 3.94E-19 |
| 1429.3203 | 109.774  | 1.82E-17 | 0.0907 | 1.65E-18 |
| 1450.8948 | 16.9089  | 2.81E-18 | 0.0569 | 1.60E-19 |
| 1492.8319 | 2.4752   | 4.11E-19 | 0.0528 | 2.17E-20 |

**Table S7.** Ectotoxicity towards aquatic organisms of CF<sub>3</sub>CF<sub>2</sub>CF<sub>2</sub>CH<sub>2</sub>OH, CF<sub>3</sub>CHF<sub>2</sub>CF<sub>2</sub>CH<sub>2</sub>OH, and their transformation products. (unit: mg/L)

|  | Acute toxicity <sup>a</sup> (mg/L)                      | Chronic toxicity (ChV) <sup>b</sup> (mg/L) | Classification     |
|--|---------------------------------------------------------|--------------------------------------------|--------------------|
|  | <b>LC<sub>50</sub>&gt;100 or EC<sub>50</sub>&gt;100</b> | <b>ChV&gt;10</b>                           | <b>Not harmful</b> |

|                                                                    | 10 < LC <sub>50</sub> (or EC <sub>50</sub> ) < 100 |                                |                                       | 1 < ChV < 10  |         |                | Harmful         |
|--------------------------------------------------------------------|----------------------------------------------------|--------------------------------|---------------------------------------|---------------|---------|----------------|-----------------|
|                                                                    | 1 < LC <sub>50</sub> (or EC <sub>50</sub> ) < 10   |                                |                                       | 0.1 < ChV < 1 |         |                | Toxic           |
|                                                                    | LC <sub>50</sub> < 1 or EC <sub>50</sub> < 1       |                                |                                       | ChV < 0.1     |         |                | Very toxic      |
| Compound                                                           | Fish<br>(LC <sub>50</sub> )                        | Daphnid<br>(LC <sub>50</sub> ) | Green<br>Algae<br>(EC <sub>50</sub> ) | Fish          | Daphnid | Green<br>Algae | ECOSAR<br>Class |
| CF <sub>3</sub> CF <sub>2</sub> CF <sub>2</sub> CH <sub>2</sub> OH | 198.09                                             | 111.54                         | 80.27                                 | 19.17         | 10.63   | 20.64          | Organics        |
| CF <sub>3</sub> CHFCF <sub>2</sub> CH <sub>2</sub> OH              | 342.81                                             | 187.57                         | 119.89                                | 32.08         | 16.50   | 28.91          | Organics        |
| CF <sub>3</sub> CF <sub>2</sub> CF <sub>2</sub> COOH               | 1322.59                                            | 760.59                         | 597.14                                | 131.23        | 76.85   | 160.87         | Organics-acid   |
| CF <sub>3</sub> CHFCF <sub>2</sub> COOH                            | 2303.71                                            | 1287.32                        | 897.61                                | 220.97        | 120.08  | 226.84         | Organics-acid   |
| CF <sub>3</sub> CF <sub>2</sub> CF <sub>2</sub> CHO                | 13.00                                              | 22.22                          | 33.03                                 | 2.06          | 3.17    | 11.64          | Aldehydes       |
| CF <sub>3</sub> CHFCF <sub>2</sub> CHO                             | 17.19                                              | 34.31                          | 47.54                                 | 3.08          | 4.62    | 15.65          | Aldehydes       |

<sup>a</sup>Criteria set by the European Union (described in Annex VI of Directive 67/548/EEC)

<sup>b</sup>Criteria set by the Chinese hazard evaluation guidelines for new chemical substances (HJ/T 154–2004)

### **Coordinates of all the stationary points**

A

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.624037 | -0.236456 | 0.013164  |
| C | -0.320464 | 0.591449  | -0.027010 |
| C | 0.990003  | -0.216086 | 0.019712  |
| C | 2.217555  | 0.666639  | 0.194760  |
| H | 2.168292  | 1.470410  | -0.548888 |
| H | 2.193209  | 1.101997  | 1.193136  |
| F | -2.656769 | 0.572292  | -0.199820 |
| F | -1.775718 | -0.814101 | 1.196312  |
| F | -1.610606 | -1.170292 | -0.929638 |
| F | -0.341056 | 1.432653  | 1.025273  |
| F | -0.330071 | 1.323387  | -1.155045 |
| F | 0.896783  | -1.123656 | 1.012226  |

|                  |           |           |           |
|------------------|-----------|-----------|-----------|
| F                | 1.101835  | -0.902654 | -1.146690 |
| O                | 3.384190  | -0.097139 | 0.089648  |
| H                | 3.427050  | -0.487228 | -0.788755 |
| OH               |           |           |           |
| O                | 0.000000  | 0.000000  | 0.108003  |
| H                | 0.000000  | 0.000000  | -0.864024 |
| H <sub>2</sub> O |           |           |           |
| O                | 0.000000  | 0.000000  | 0.116565  |
| H                | 0.000000  | 0.761616  | -0.466258 |
| H                | 0.000000  | -0.761616 | -0.466258 |
| PA1              |           |           |           |
| C                | 1.583398  | -0.229567 | -0.021154 |
| C                | 0.273513  | 0.591290  | 0.022149  |
| C                | -1.027360 | -0.242025 | 0.018670  |
| C                | -2.256276 | 0.662285  | -0.166434 |
| H                | -2.211056 | 1.423118  | 0.623321  |
| H                | -2.175926 | 1.110545  | -1.162821 |
| F                | 2.610413  | 0.593736  | 0.155376  |
| F                | 1.717112  | -0.830699 | -1.194547 |
| F                | 1.593690  | -1.141757 | 0.941026  |
| F                | 0.271543  | 1.408640  | -1.046940 |
| F                | 0.290648  | 1.344614  | 1.133393  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| F | -0.952037 | -1.146606 | -0.976156 |
| F | -1.101712 | -0.907651 | 1.183767  |
| O | -3.364948 | -0.138507 | -0.042895 |

#### PA2

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.596703 | -0.201174 | -0.007449 |
| C | -0.271995 | 0.596301  | -0.043917 |
| C | 1.009716  | -0.250660 | 0.086589  |
| C | 2.208397  | 0.578877  | 0.338289  |
| H | 2.222186  | 1.309548  | 1.131220  |
| F | -2.594601 | 0.599818  | -0.366300 |
| F | -1.840896 | -0.657520 | 1.212041  |
| F | -1.542810 | -1.223402 | -0.853921 |
| F | -0.303660 | 1.484617  | 0.967624  |
| F | -0.226081 | 1.267455  | -1.203661 |
| F | 0.783920  | -1.183466 | 1.064274  |
| F | 1.187013  | -0.956037 | -1.063073 |
| O | 3.402809  | 0.113410  | -0.053615 |
| H | 3.292879  | -0.540065 | -0.756237 |

#### ERA1

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.86842000  | 0.21528500  | -0.22715400 |
| C | 0.58637800  | -0.06354800 | 0.58905900  |
| C | -0.66880200 | -0.42688000 | -0.22713900 |
| C | -1.81788500 | -0.91341700 | 0.64857000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.52753400 | -1.87302900 | 1.07686600  |
| H | -1.96115800 | -0.18750500 | 1.45669000  |
| F | 2.80705000  | 0.68633000  | 0.58749200  |
| F | 1.63099100  | 1.11908000  | -1.17100200 |
| F | 2.31859600  | -0.89547300 | -0.79211200 |
| F | 0.31545100  | 1.03515100  | 1.31593900  |
| F | 0.85834400  | -1.07655800 | 1.43401400  |
| F | -1.04731400 | 0.68848300  | -0.91089900 |
| F | -0.32943600 | -1.35484100 | -1.14358700 |
| O | -2.96835800 | -1.10260300 | -0.11744100 |
| H | -3.37211400 | -0.23999200 | -0.27060100 |
| O | -3.16146100 | 1.75866700  | 0.09006300  |
| H | -2.89244300 | 2.36382700  | -0.62254400 |

#### TSA1

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.22217900  | -1.48247600 | -0.22141400 |
| C | 0.19134400  | -0.34028600 | -0.07878700 |
| C | -1.28196400 | -0.77709700 | 0.02727000  |
| C | -2.20230200 | 0.37935700  | 0.40470700  |
| H | -1.96956900 | 0.67217200  | 1.43392300  |
| H | -2.01238200 | 1.22821300  | -0.25944600 |
| F | 2.41391500  | -0.95963600 | -0.48672800 |
| F | 0.87925800  | -2.29372800 | -1.21452000 |
| F | 1.30559200  | -2.18064600 | 0.90196800  |
| F | 0.31849300  | 0.46982200  | -1.14284900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| F | 0.50810800  | 0.35879000  | 1.02926100  |
| F | -1.65170700 | -1.29411000 | -1.16924500 |
| F | -1.36859900 | -1.76857300 | 0.93748100  |
| O | -3.52855300 | -0.03298800 | 0.37438900  |
| H | -4.00217300 | 0.19909200  | -0.58960000 |
| O | -4.03935100 | 0.20341600  | -1.80883300 |
| H | -3.74169900 | -0.67341300 | -2.09657300 |

#### TSA2

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 0.279383  | 2.148403  | 0.341692  |
| C | -1.117628 | 1.487882  | 0.309585  |
| C | -1.349918 | 0.475806  | -0.829018 |
| C | -2.807380 | 0.063138  | -0.973493 |
| H | -3.156054 | -0.353061 | 0.076228  |
| H | -3.433253 | 0.918462  | -1.225368 |
| F | 0.401098  | 2.848648  | 1.463721  |
| F | 0.432518  | 2.966749  | -0.688273 |
| F | 1.227196  | 1.220301  | 0.309593  |
| F | -2.033575 | 2.466899  | 0.211540  |
| F | -1.297635 | 0.855912  | 1.488223  |
| F | -0.896991 | 1.026482  | -1.975188 |
| F | -0.597768 | -0.621820 | -0.579582 |
| O | -2.967131 | -0.926789 | -1.913605 |
| H | -2.523881 | -1.726992 | -1.607092 |
| O | -3.262193 | -1.331930 | 1.070905  |

|   |           |           |          |
|---|-----------|-----------|----------|
| H | -2.602589 | -1.006102 | 1.705821 |
|---|-----------|-----------|----------|

EPA1

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.90982800  | 0.21614100  | -0.22843000 |
| C | 0.60054200  | 0.05693900  | 0.57615200  |
| C | -0.61552300 | -0.46603700 | -0.20987300 |
| C | -1.79662400 | -0.80084700 | 0.69874100  |
| H | -1.52601800 | -1.63565800 | 1.36067900  |
| H | -2.04001700 | 0.06512600  | 1.32944700  |
| F | 2.81034300  | 0.83329700  | 0.52911700  |
| F | 1.70033100  | 0.94054700  | -1.32034300 |
| F | 2.39103400  | -0.96878000 | -0.57767300 |
| F | 0.28347400  | 1.25324500  | 1.09734200  |
| F | 0.85014200  | -0.79704400 | 1.58993000  |
| F | -0.97266100 | 0.47961100  | -1.10829500 |
| F | -0.23543400 | -1.56074600 | -0.90479700 |
| O | -2.90417700 | -1.13814800 | -0.02209300 |
| H | -4.38087700 | 1.25307000  | -0.18131600 |
| O | -3.47418700 | 1.52797400  | -0.02574200 |
| H | -3.06057900 | 1.54049900  | -0.89319400 |

EPA2

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.60577000 | 0.37664900  | -0.09858100 |
| C | -0.39087200 | -0.30433600 | 0.57018000  |
| C | 0.67337800  | -0.88637100 | -0.40351100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.98519200  | -1.18932500 | 0.20082100  |
| H | 1.60295700  | 2.78820500  | 0.45710500  |
| H | 2.17918100  | -2.18506600 | 0.56892000  |
| F | -2.54790000 | 0.60677000  | 0.80884600  |
| F | -2.10955000 | -0.38705500 | -1.05717300 |
| F | -1.24376400 | 1.54873900  | -0.62479000 |
| F | -0.84068500 | -1.29613800 | 1.35005900  |
| F | 0.18947900  | 0.62651700  | 1.35690700  |
| F | 0.14533900  | -2.00476400 | -0.93813500 |
| F | 0.79992900  | 0.04305500  | -1.41132500 |
| O | 2.82331400  | -0.22525600 | 0.56906900  |
| H | 2.55471000  | 0.66122600  | 0.24144700  |
| O | 2.02176800  | 2.26154900  | -0.22923000 |
| H | 1.39527900  | 2.23147900  | -0.95913300 |
| B |             |             |             |
| C | 1.62525200  | -0.11724800 | 0.00374700  |
| C | 0.35596800  | 0.54507200  | -0.53254800 |
| C | -0.93843500 | -0.16181900 | -0.12254400 |
| C | -2.17288900 | 0.72066800  | -0.22381900 |
| H | -2.02150700 | 1.59411600  | 0.41740800  |
| H | -2.28331800 | 1.05513500  | -1.25696300 |
| F | 1.62220200  | -1.42081800 | -0.26850000 |
| F | 1.75440600  | 0.04803500  | 1.31432800  |
| F | 0.34291500  | 1.83454800  | -0.06891000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -3.32355400 | -0.00188800 | 0.11054600  |
| H | -3.25036900 | -0.29985800 | 1.02240700  |
| F | 2.69469000  | 0.42906800  | -0.58433400 |
| H | 0.41332600  | 0.55734800  | -1.62378800 |
| F | -0.84231300 | -0.61357600 | 1.16117200  |
| F | -1.07068700 | -1.25633200 | -0.90847200 |

#### PB1

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.58458400  | -0.11188600 | -0.01492900 |
| C | 0.29552700  | 0.53798200  | -0.52082800 |
| C | -0.97798300 | -0.18538600 | -0.06287900 |
| C | -2.20433300 | 0.73887900  | -0.14598600 |
| H | -2.05684200 | 1.53412500  | 0.59203500  |
| H | -2.22855400 | 1.14479000  | -1.16693500 |
| F | 2.63035900  | 0.43374300  | -0.64237800 |
| F | 1.57699500  | -1.41779700 | -0.27553100 |
| F | 1.75103200  | 0.06767000  | 1.28843000  |
| F | 0.27965400  | 1.82901100  | -0.06806300 |
| F | -1.14444600 | -1.26195700 | -0.86241500 |
| F | -0.83941200 | -0.63796900 | 1.20139400  |
| O | -3.31344600 | -0.02626500 | 0.11037000  |
| H | 0.31854600  | 0.53937800  | -1.61326300 |

#### PB2

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 1.60572700 | -0.08207700 | -0.03846900 |
| C | 0.29016000 | 0.54382500  | -0.50824600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.96630900 | -0.20873000 | -0.06657200 |
| C | -2.19358700 | 0.33538700  | -0.68754900 |
| H | -2.24949700 | 0.50083200  | -1.75304600 |
| F | 2.60617200  | 0.76502700  | -0.28859400 |
| F | 1.84875000  | -1.21067500 | -0.70497300 |
| F | 1.60640700  | -0.34951000 | 1.26308500  |
| F | 0.22568800  | 1.81161800  | -0.00674900 |
| F | -0.77857800 | -1.54027900 | -0.35148400 |
| F | -1.09901400 | -0.14211600 | 1.28895600  |
| O | -3.36875900 | 0.17100200  | -0.06486300 |
| H | -3.22108000 | 0.00911700  | 0.87589000  |
| H | 0.31988100  | 0.58501900  | -1.60108500 |

### PB3

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.67028800  | -0.10562700 | -0.00479300 |
| C | 0.34462400  | 0.54384200  | -0.26412400 |
| C | -0.96667700 | -0.16025500 | -0.09714200 |
| C | -2.16794000 | 0.77336900  | -0.11043100 |
| H | -2.02285000 | 1.53024500  | 0.66789600  |
| H | -2.21643900 | 1.27002300  | -1.08054900 |
| F | 1.60514700  | -1.40451500 | -0.27322700 |
| F | 2.04341300  | 0.04312900  | 1.27303000  |
| F | 0.34500000  | 1.85367800  | -0.06751500 |
| O | -3.35070400 | 0.04807900  | 0.05603600  |
| H | -3.32052900 | -0.41108600 | 0.90109600  |

|      |             |             |             |
|------|-------------|-------------|-------------|
| F    | 2.62111500  | 0.44649200  | -0.76087700 |
| F    | -0.96677100 | -0.84076300 | 1.09846500  |
| F    | -1.08305000 | -1.10710800 | -1.05629700 |
| ERB1 |             |             |             |
| C    | -1.87442200 | 0.15617300  | -0.12299600 |
| C    | -0.73760800 | -0.51579200 | 0.64641500  |
| C    | 0.59610100  | -0.54730700 | -0.10392100 |
| C    | 1.79368800  | -0.78124700 | 0.80697700  |
| H    | 1.84635100  | 0.04950700  | 1.51721600  |
| H    | 1.62053500  | -1.70794100 | 1.35986700  |
| F    | -1.96770700 | -0.34612700 | -1.35313500 |
| F    | -1.70670000 | 1.47114700  | -0.20899600 |
| O    | 2.96333700  | -0.93132800 | 0.06083000  |
| H    | 3.27843700  | -0.05274000 | -0.18270900 |
| F    | -3.03248500 | -0.06630200 | 0.50709100  |
| F    | 0.77059900  | 0.62789100  | -0.78442600 |
| F    | 0.51398400  | -1.52059300 | -1.03943200 |
| O    | 2.93145200  | 1.93743600  | -0.12529500 |
| H    | 2.53543600  | 2.34473100  | -0.91524800 |
| H    | -1.03585900 | -1.54460200 | 0.86330000  |
| F    | -0.58544300 | 0.16634200  | 1.82494700  |
| ERB2 |             |             |             |
| C    | -1.54994500 | -0.35302600 | 0.15311100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.29284700 | -0.21317500 | -0.70692700 |
| C | 0.99113500  | -0.02848100 | 0.10195200  |
| C | 2.25806900  | -0.25164700 | -0.70705000 |
| H | 2.22129400  | -1.26203200 | -1.12531500 |
| H | 2.28258400  | 0.47117100  | -1.52459300 |
| F | -1.59945200 | 0.60556200  | 1.08583500  |
| F | -1.60177900 | -1.53089500 | 0.76256300  |
| F | -0.18989200 | -1.35441400 | -1.46011700 |
| O | 3.39308200  | -0.03447700 | 0.08250400  |
| H | 3.40142500  | -0.67526400 | 0.79987600  |
| F | -2.63653300 | -0.23763200 | -0.61233600 |
| H | -0.42381400 | 0.64975700  | -1.36311900 |
| F | 1.00373500  | -0.88130000 | 1.16627300  |
| F | 0.97840000  | 1.22839200  | 0.61965500  |
| O | -0.71825100 | 2.85687500  | -0.61162500 |
| H | -0.90892400 | 2.84774300  | 0.34275200  |

#### TSB1

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.50794700  | 0.77912700  | -0.26745500 |
| C | 0.14550900  | 1.47156000  | -0.30315600 |
| C | -1.03761300 | 0.52121900  | -0.50236900 |
| C | -2.37182800 | 1.13667100  | -0.09724800 |
| H | -2.34111100 | 1.41342800  | 0.95938600  |
| H | -2.52679300 | 2.04364600  | -0.69488500 |
| F | 1.65499300  | -0.01198100 | -1.32862000 |

|      |             |             |             |
|------|-------------|-------------|-------------|
| F    | 1.67036600  | 0.05636500  | 0.83338600  |
| O    | -3.41554200 | 0.26523500  | -0.38710700 |
| H    | -3.68582800 | -0.34410400 | 0.48789700  |
| F    | 2.47424100  | 1.70175600  | -0.29744100 |
| F    | -0.84198300 | -0.62619400 | 0.20523700  |
| F    | -1.06831000 | 0.17023300  | -1.80907300 |
| O    | -3.42895000 | -1.05931100 | 1.43967000  |
| H    | -2.71036900 | -1.64572700 | 1.15631400  |
| H    | 0.15420400  | 2.19224200  | -1.12505200 |
| F    | -0.00561700 | 2.14213400  | 0.88163100  |
| TSB2 |             |             |             |
| C    | 1.30297000  | 1.10721800  | 0.46430800  |
| C    | -0.10927000 | 0.52091200  | 0.40231800  |
| C    | -0.32951100 | -0.49751300 | -0.71948200 |
| C    | -1.77637900 | -0.94481800 | -0.85090000 |
| H    | -2.10458700 | -1.37597500 | 0.19695800  |
| H    | -2.42391100 | -0.09788500 | -1.08446400 |
| F    | 1.42308400  | 1.83771100  | 1.57428400  |
| F    | 1.51654700  | 1.90524000  | -0.58036900 |
| F    | 2.24130900  | 0.16841100  | 0.48379600  |
| F    | -0.35387400 | -0.10276700 | 1.59999500  |
| F    | 0.09125500  | 0.05848400  | -1.88039400 |
| F    | 0.44088400  | -1.59154400 | -0.49419400 |
| O    | -1.94039900 | -1.92135000 | -1.80500200 |
| H    | -1.46251400 | -2.71258700 | -1.52902400 |

|   |             |             |            |
|---|-------------|-------------|------------|
| O | -2.19890800 | -2.32824900 | 1.22069600 |
| H | -1.48673100 | -2.00986000 | 1.80046400 |
| H | -0.80718000 | 1.35453400  | 0.28539700 |

#### TSB3

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.84062200  | 0.25970200  | 0.09695100  |
| C | 0.52000900  | 0.86325300  | -0.37022300 |
| C | -0.75093100 | 0.43711700  | 0.35831400  |
| C | -1.99986200 | 1.10053100  | -0.19961100 |
| H | -1.84257000 | 2.18426000  | -0.19601900 |
| H | -2.13509700 | 0.76405700  | -1.22917900 |
| F | 1.80351700  | -1.06564200 | 0.06444700  |
| F | 2.15731600  | 0.65372800  | 1.32552600  |
| F | 0.63545500  | 2.21234700  | -0.34963200 |
| O | -3.13047100 | 0.71659500  | 0.52886600  |
| H | -3.03231300 | 1.01398300  | 1.43843600  |
| F | 2.81267700  | 0.67087100  | -0.72985100 |
| H | 0.37873400  | 0.51634900  | -1.51522300 |
| F | -0.63214400 | 0.76315600  | 1.67879600  |
| F | -0.84977400 | -0.90621500 | 0.29220800  |
| O | 0.37857200  | 0.36719300  | -2.81635800 |
| H | 1.26545000  | 0.70341200  | -3.03125400 |

#### EPB1

|   |             |            |             |
|---|-------------|------------|-------------|
| C | -1.91406600 | 0.16865300 | -0.13915600 |
|---|-------------|------------|-------------|

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.74735300 | -0.21887100 | 0.76886600  |
| C | 0.53373600  | -0.59954100 | 0.02311900  |
| C | 1.77327100  | -0.55476500 | 0.91148000  |
| H | 1.94284500  | 0.47469100  | 1.25752600  |
| H | 1.62390700  | -1.18265100 | 1.80272400  |
| F | -2.12334800 | -0.77617400 | -1.05457400 |
| F | -1.70236400 | 1.32476700  | -0.75505800 |
| O | 2.89229600  | -0.95229400 | 0.24081500  |
| H | 4.08423400  | 1.24690200  | -0.65706600 |
| F | -3.02446000 | 0.29242700  | 0.59412700  |
| F | 0.71719400  | 0.21804800  | -1.04607100 |
| F | 0.36975000  | -1.85431100 | -0.46589100 |
| O | 3.24898100  | 1.67408200  | -0.45164600 |
| H | 2.68250700  | 1.49196500  | -1.20675800 |
| H | -1.06166900 | -1.06991400 | 1.37861800  |
| F | -0.48961400 | 0.84989300  | 1.58588400  |

#### EPB2

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.63508700  | 0.10772400  | -0.04543600 |
| C | 0.37217500  | -0.31446500 | -0.79348800 |
| C | -0.71308800 | -0.96761700 | 0.09034400  |
| C | -2.08745900 | -0.92129200 | -0.44954100 |
| H | -0.77368000 | 2.58123600  | 0.09780000  |
| H | -2.49996000 | -1.79162400 | -0.93562700 |
| F | 2.59260200  | 0.43840100  | -0.91588900 |

|      |             |             |             |
|------|-------------|-------------|-------------|
| F    | 2.08986100  | -0.87730700 | 0.72096100  |
| F    | 1.41122800  | 1.18068200  | 0.72257900  |
| F    | -0.12365800 | 0.81909000  | -1.38835200 |
| F    | -0.34120800 | -2.26246400 | 0.24965400  |
| F    | -0.66031500 | -0.37710300 | 1.33652800  |
| O    | -2.79753100 | 0.20196300  | -0.48852300 |
| H    | -2.34499100 | 0.95299100  | -0.04323400 |
| O    | -1.45387300 | 2.25317900  | 0.69415800  |
| H    | -0.97747100 | 1.92877800  | 1.46516500  |
| H    | 0.65045200  | -1.03030400 | -1.56979100 |
| EPB3 |             |             |             |
| C    | -1.69924100 | -0.30007500 | 0.03159600  |
| C    | -0.36142800 | -0.08707800 | -0.59534700 |
| C    | 0.94644300  | -0.40682400 | 0.04883300  |
| C    | 2.14109000  | 0.21388500  | -0.65789500 |
| H    | 2.09734600  | -0.08007100 | -1.71305400 |
| H    | 2.06174000  | 1.29748600  | -0.58292400 |
| F    | -1.62741100 | -1.26983000 | 0.93973000  |
| F    | -2.60082600 | -0.64112100 | -0.89394600 |
| F    | -0.35988200 | 0.68256000  | -1.66761500 |
| O    | 3.33237200  | -0.18534900 | -0.04049400 |
| H    | 3.39274800  | -1.14510900 | -0.06966100 |
| F    | -2.17173700 | 0.79885100  | 0.64198200  |
| H    | 0.34633700  | 2.26871300  | 1.42161800  |

|   |             |             |            |
|---|-------------|-------------|------------|
| F | 1.11630500  | -1.77099700 | 0.06478200 |
| F | 0.91568700  | -0.04692100 | 1.36389000 |
| O | 0.28087900  | 2.46583100  | 0.48290900 |
| H | -0.41458900 | 3.12280900  | 0.40217100 |

#### A-(PCM)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.62201800 | -0.23788500 | 0.00968600  |
| C | -0.32024900 | 0.59453900  | -0.02223900 |
| C | 0.99382400  | -0.20874200 | 0.01441300  |
| C | 2.22616900  | 0.67239500  | 0.15887700  |
| H | 2.19477900  | 1.44386900  | -0.61616500 |
| H | 2.19604800  | 1.14799400  | 1.13872500  |
| F | -2.65967600 | 0.57528100  | -0.16176500 |
| F | -1.75809000 | -0.85516700 | 1.17603700  |
| F | -1.62491300 | -1.14217400 | -0.96234600 |
| F | -0.34913000 | 1.42371900  | 1.03793800  |
| F | -0.33842700 | 1.33452100  | -1.14456000 |
| F | 0.91525400  | -1.09787100 | 1.03188600  |
| F | 1.07588000  | -0.92708700 | -1.13337800 |
| O | 3.38345000  | -0.11537700 | 0.09221200  |
| H | 3.52713800  | -0.39168500 | -0.81898400 |

#### OH-(PCM)

|   |            |            |             |
|---|------------|------------|-------------|
| O | 0.00000000 | 0.00000000 | 0.10816800  |
| H | 0.00000000 | 0.00000000 | -0.86534100 |

H<sub>2</sub>O-(PCM)

|   |            |             |             |
|---|------------|-------------|-------------|
| O | 0.00000000 | 0.00000000  | 0.11762800  |
| H | 0.00000000 | 0.76018100  | -0.47051000 |
| H | 0.00000000 | -0.76018100 | -0.47051000 |

PA1-(PCM)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.57952200  | -0.23316400 | -0.02146400 |
| C | 0.27516300  | 0.59844800  | 0.01993000  |
| C | -1.02975800 | -0.22892000 | 0.01819500  |
| C | -2.26158200 | 0.66885200  | -0.15990200 |
| H | -2.23106300 | 1.42227700  | 0.63579800  |
| H | -2.18997100 | 1.12491400  | -1.15232000 |
| F | 2.61379300  | 0.58299600  | 0.14540500  |
| F | 1.70657400  | -0.84585400 | -1.19052000 |
| F | 1.58845300  | -1.13939800 | 0.94788600  |
| F | 0.28157000  | 1.41139100  | -1.04951100 |
| F | 0.30054000  | 1.34912800  | 1.13193000  |
| F | -0.95676100 | -1.13876400 | -0.97555200 |
| F | -1.09826800 | -0.90271200 | 1.18351700  |
| O | -3.36026900 | -0.15369700 | -0.04530300 |

PA2-(PCM)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.59248000 | -0.20035100 | -0.00135600 |
| C | -0.26939300 | 0.60137600  | -0.04639700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.01232800  | -0.24878900 | 0.07460000  |
| C | 2.20873300  | 0.57121700  | 0.34759500  |
| H | 2.20609100  | 1.31398300  | 1.12966500  |
| F | -2.59316600 | 0.58599400  | -0.38509000 |
| F | -1.84348800 | -0.62964000 | 1.22775600  |
| F | -1.53096100 | -1.24379900 | -0.82188300 |
| F | -0.30180700 | 1.49250900  | 0.96057400  |
| F | -0.23373000 | 1.26987700  | -1.20954700 |
| F | 0.76921300  | -1.19969200 | 1.04065200  |
| F | 1.18240200  | -0.94307100 | -1.08067000 |
| O | 3.40951900  | 0.11298400  | -0.02901600 |
| H | 3.32646000  | -0.54816700 | -0.73031900 |

ERA1-(PCM)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.87625100  | 0.26282200  | -0.22609700 |
| C | 0.61968500  | -0.11670500 | 0.58990200  |
| C | -0.65374900 | -0.40143300 | -0.22904400 |
| C | -1.79066000 | -0.96590800 | 0.61181400  |
| H | -1.48782000 | -1.94695500 | 0.97763900  |
| H | -1.95127800 | -0.29874300 | 1.46447100  |
| F | 2.84241900  | 0.62841500  | 0.61114500  |
| F | 1.61592400  | 1.27612700  | -1.04384800 |
| F | 2.30584500  | -0.76983200 | -0.93938000 |
| F | 0.36428600  | 0.89486700  | 1.43801600  |
| F | 0.92611700  | -1.21233300 | 1.30974800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| F | -1.03745500 | 0.76366000  | -0.81126300 |
| F | -0.32755200 | -1.25177900 | -1.23109900 |
| O | -2.93684300 | -1.11373100 | -0.17742100 |
| H | -3.35405800 | -0.24396900 | -0.25284500 |
| O | -3.35021100 | 1.68197100  | 0.16592500  |
| H | -3.42582900 | 2.30895800  | -0.57662800 |

TSA1-(PCM)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.23356600  | -1.49007400 | -0.19403600 |
| C | 0.21594700  | -0.33288900 | -0.06600600 |
| C | -1.26392200 | -0.75845700 | 0.00040000  |
| C | -2.18978300 | 0.38582700  | 0.39288700  |
| H | -1.96262900 | 0.67182100  | 1.42502900  |
| H | -2.01002900 | 1.24563700  | -0.25854600 |
| F | 2.43524000  | -0.98747600 | -0.45488400 |
| F | 0.88784200  | -2.30641100 | -1.18297200 |
| F | 1.30043200  | -2.18196200 | 0.93568600  |
| F | 0.37857100  | 0.47915300  | -1.12334700 |
| F | 0.52065500  | 0.35231800  | 1.05171500  |
| F | -1.61100200 | -1.24634400 | -1.21340900 |
| F | -1.37063800 | -1.77863700 | 0.88353700  |
| O | -3.51308700 | -0.04513500 | 0.35735400  |
| H | -3.99479600 | 0.20824200  | -0.59340200 |
| O | -4.08320400 | 0.20362500  | -1.81533900 |
| H | -3.93257600 | -0.71132900 | -2.10366400 |

## TSA2-(PCM)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.30448900  | 2.12896600  | 0.31617300  |
| C | -1.08769100 | 1.45518400  | 0.31231000  |
| C | -1.33725400 | 0.46349900  | -0.84093700 |
| C | -2.78820200 | 0.02483900  | -0.96041000 |
| H | -3.10510100 | -0.42755300 | 0.07211900  |
| H | -3.43880400 | 0.87512300  | -1.15959100 |
| F | 0.45543100  | 2.80675300  | 1.44827900  |
| F | 0.41881100  | 2.97203500  | -0.70071500 |
| F | 1.26248200  | 1.21358400  | 0.23299400  |
| F | -2.01101900 | 2.42931600  | 0.25536900  |
| F | -1.22761800 | 0.79936900  | 1.47946500  |
| F | -0.92484000 | 1.04698700  | -1.98996200 |
| F | -0.55378300 | -0.62331300 | -0.64242600 |
| O | -2.95140200 | -0.92385800 | -1.94738400 |
| H | -2.38693400 | -1.68718300 | -1.76995800 |
| O | -3.37417900 | -1.28119100 | 1.18515100  |
| H | -2.96018900 | -0.76056900 | 1.89521300  |

## EPA1-(PCM)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.83699500 | -0.18931200 | -0.21864800 |
| C | -0.49309200 | -0.16165400 | 0.54921600  |
| C | 0.64186100  | 0.60996100  | -0.15943500 |
| C | 1.84278600  | 0.82229200  | 0.76776100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.50714600  | 1.47072500  | 1.58365700  |
| H | 2.15907700  | -0.16815700 | 1.11282800  |
| F | -2.65809600 | -1.04316100 | 0.38194000  |
| F | -1.65087100 | -0.58293600 | -1.47289900 |
| F | -2.40058500 | 1.01101100  | -0.21971700 |
| F | -0.09659600 | -1.42866300 | 0.73451100  |
| F | -0.72630200 | 0.39856500  | 1.74825900  |
| F | 1.00206800  | -0.09666100 | -1.25271800 |
| F | 0.14791800  | 1.79117500  | -0.58852600 |
| O | 2.81645400  | 1.42969300  | 0.00326600  |
| H | 3.84762400  | -2.32102100 | -0.13671000 |
| O | 2.95723000  | -1.95861600 | -0.14304400 |
| H | 2.81149100  | -1.68183700 | -1.05256300 |

EPA2-(PCM)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.63630100 | 0.44254100  | -0.10000200 |
| C | -0.42059200 | -0.24607000 | 0.56012200  |
| C | 0.60529000  | -0.89787800 | -0.40676700 |
| C | 1.88192700  | -1.30679800 | 0.21453600  |
| H | 2.04544200  | 2.70880100  | 0.42871500  |
| H | 1.97440900  | -2.30381300 | 0.61864500  |
| F | -2.53075800 | 0.75413400  | 0.83431600  |
| F | -2.21107000 | -0.36602000 | -0.98390100 |
| F | -1.26673900 | 1.56058100  | -0.71329200 |
| F | -0.88427900 | -1.19969900 | 1.38458800  |

|   |            |             |             |
|---|------------|-------------|-------------|
| F | 0.20971300 | 0.68792700  | 1.29821500  |
| F | 0.00054800 | -1.97822700 | -0.95110300 |
| F | 0.81368800 | 0.01634100  | -1.40623700 |
| O | 2.78628700 | -0.40530100 | 0.59184500  |
| H | 2.60583400 | 0.50369600  | 0.24419800  |
| O | 2.42246500 | 2.10493900  | -0.21980400 |
| H | 1.94242900 | 2.26810100  | -1.03850300 |

#### B-(PCM)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.62446000  | -0.11837000 | -0.01593100 |
| C | 0.34948100  | 0.54462500  | -0.53577900 |
| C | -0.94011300 | -0.15331200 | -0.10047800 |
| C | -2.18994100 | 0.68176800  | -0.32523700 |
| H | -2.08436400 | 1.62276300  | 0.21964500  |
| H | -2.27370200 | 0.89515500  | -1.39172400 |
| F | 1.63915800  | -1.41969500 | -0.30337400 |
| F | 1.75730000  | 0.02290100  | 1.30182700  |
| F | 0.34806800  | 1.82878500  | -0.05231200 |
| O | -3.33068500 | -0.03849100 | 0.06271600  |
| H | -3.36412900 | -0.07856500 | 1.02417400  |
| F | 2.69273500  | 0.44583900  | -0.58803400 |
| H | 0.39138400  | 0.56748100  | -1.62653900 |
| F | -0.86324600 | -0.49056100 | 1.21995000  |
| F | -1.02813000 | -1.32362100 | -0.78502700 |

## PB1-(PCM)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.57895800  | -0.11596600 | -0.02618400 |
| C | 0.29636100  | 0.54789200  | -0.53060600 |
| C | -0.97823700 | -0.16712800 | -0.06815800 |
| C | -2.22152900 | 0.71771000  | -0.23897500 |
| H | -2.09446500 | 1.58745400  | 0.41247600  |
| H | -2.26549300 | 1.00761400  | -1.29552200 |
| F | 2.63634300  | 0.42337000  | -0.63659200 |
| F | 1.56925700  | -1.42349800 | -0.28480700 |
| F | 1.74099100  | 0.05400500  | 1.28410600  |
| F | 0.29389600  | 1.83004700  | -0.05066700 |
| F | -1.10731200 | -1.30208700 | -0.79432800 |
| F | -0.86241500 | -0.54390100 | 1.22953900  |
| O | -3.30582800 | -0.04964700 | 0.12039900  |
| H | 0.31642200  | 0.56563700  | -1.62186100 |

## PB2-(PCM)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.59807200  | -0.09160500 | -0.05687500 |
| C | 0.28983900  | 0.55693500  | -0.51359600 |
| C | -0.96808500 | -0.18403800 | -0.05448400 |
| C | -2.19117700 | 0.32942500  | -0.69864100 |
| H | -2.21615300 | 0.53597800  | -1.75794300 |
| F | 2.61237000  | 0.74855200  | -0.27373600 |
| F | 1.83872700  | -1.20986000 | -0.74051500 |
| F | 1.59128600  | -0.39067400 | 1.24312500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| F | 0.25106200  | 1.81901000  | 0.01604500  |
| F | -0.76825700 | -1.53178100 | -0.28370000 |
| F | -1.09858300 | -0.07880700 | 1.30127000  |
| O | -3.37926600 | 0.12835100  | -0.11138800 |
| H | -3.26938400 | -0.05360200 | 0.83217300  |
| H | 0.30832700  | 0.61855300  | -1.60395000 |

PB3-(PCM)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.66619900  | -0.10182500 | 0.00072800  |
| C | 0.34421300  | 0.55318800  | -0.25023800 |
| C | -0.96614500 | -0.15389100 | -0.09593600 |
| C | -2.16733700 | 0.77831900  | -0.06360600 |
| H | -2.03019200 | 1.49700900  | 0.74873500  |
| H | -2.21154000 | 1.31740500  | -1.01047200 |
| F | 1.60015700  | -1.39757000 | -0.29687000 |
| F | 2.04089200  | 0.00980000  | 1.28399700  |
| F | 0.34952200  | 1.86233100  | -0.07286200 |
| O | -3.34811100 | 0.03464000  | 0.06836800  |
| H | -3.40632200 | -0.30809800 | 0.96640700  |
| F | 2.62543100  | 0.46091500  | -0.73706300 |
| F | -0.94502400 | -0.89989700 | 1.05775800  |
| F | -1.09638300 | -1.06204300 | -1.10132600 |

ERB1-(PCM)

|   |             |            |             |
|---|-------------|------------|-------------|
| C | -1.89022400 | 0.13312700 | -0.13190200 |
|---|-------------|------------|-------------|

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.73706200 | -0.38852400 | 0.72440100  |
| C | 0.58349400  | -0.55249700 | -0.03020600 |
| C | 1.78340200  | -0.74913900 | 0.88374900  |
| H | 1.86401600  | 0.12376900  | 1.53701900  |
| H | 1.60244500  | -1.63468700 | 1.49590500  |
| F | -2.04281300 | -0.60296400 | -1.23226800 |
| F | -1.70666000 | 1.40137500  | -0.49657100 |
| O | 2.94367800  | -0.95880100 | 0.12632900  |
| H | 3.25394100  | -0.09474300 | -0.17784800 |
| F | -3.02954100 | 0.07937300  | 0.56502100  |
| F | 0.79628100  | 0.53616400  | -0.82919300 |
| F | 0.45184800  | -1.61315700 | -0.86869000 |
| O | 3.02864400  | 1.86058600  | -0.29954000 |
| H | 2.91438400  | 2.22234600  | -1.19745000 |
| H | -1.02907600 | -1.35303500 | 1.14535200  |
| F | -0.56044200 | 0.51745900  | 1.74019600  |

ERB2-(PCM)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.53838100  | -0.36141200 | -0.15386400 |
| C | 0.28657800  | -0.22482500 | 0.71458300  |
| C | -0.99518000 | -0.02091800 | -0.09344600 |
| C | -2.26791200 | -0.26034700 | 0.70101900  |
| H | -2.25252500 | -1.28487400 | 1.07988400  |
| H | -2.28483900 | 0.43079200  | 1.54478300  |
| F | 1.58097800  | 0.58106500  | -1.09766700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| F | 1.58997600  | -1.55053100 | -0.75275000 |
| F | 0.18107900  | -1.38342800 | 1.44294100  |
| O | -3.39382100 | 0.00132600  | -0.09560800 |
| H | -3.50484200 | -0.71605700 | -0.72806700 |
| F | 2.63454200  | -0.24226700 | 0.59976600  |
| H | 0.42223200  | 0.62161200  | 1.38957700  |
| F | -0.99272300 | -0.84154800 | -1.18489300 |
| F | -0.97632800 | 1.25103900  | -0.57966400 |
| O | 0.78075800  | 2.85006600  | 0.61727000  |
| H | 0.99555700  | 3.01343200  | -0.31882100 |

TSB1-(PCM)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.51965900  | 0.79737400  | -0.30090500 |
| C | 0.15276500  | 1.48089500  | -0.28685600 |
| C | -1.02409000 | 0.52251500  | -0.47562900 |
| C | -2.36785000 | 1.14144500  | -0.11653100 |
| H | -2.36263400 | 1.45548800  | 0.92953900  |
| H | -2.52216000 | 2.02470200  | -0.74723400 |
| F | 1.65797000  | 0.02909300  | -1.38081600 |
| F | 1.70863700  | 0.04265400  | 0.77987200  |
| O | -3.39835100 | 0.24503400  | -0.39660000 |
| H | -3.68312600 | -0.32545400 | 0.48861600  |
| F | 2.48552700  | 1.71986800  | -0.31935600 |
| F | -0.83358900 | -0.60217000 | 0.27161800  |
| F | -1.03232900 | 0.11934400  | -1.77126400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -3.47451800 | -1.06041100 | 1.45410300  |
| H | -2.81510800 | -1.71513600 | 1.17207300  |
| H | 0.13263700  | 2.23098100  | -1.08033200 |
| F | 0.02987600  | 2.10007700  | 0.93081700  |

TSB2-(PCM)

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.30143500  | 1.10463600  | 0.44655100  |
| C | -0.10383300 | 0.50055600  | 0.41261600  |
| C | -0.32956900 | -0.49569200 | -0.72725600 |
| C | -1.76439800 | -0.97938600 | -0.84691600 |
| H | -2.06765300 | -1.44139200 | 0.18247600  |
| H | -2.44086800 | -0.14569100 | -1.03620000 |
| F | 1.45191800  | 1.81403700  | 1.56626300  |
| F | 1.49004700  | 1.92048600  | -0.58904200 |
| F | 2.25398900  | 0.17302500  | 0.42567400  |
| F | -0.28521000 | -0.16834000 | 1.59854300  |
| F | 0.05881000  | 0.08915400  | -1.88874400 |
| F | 0.47561000  | -1.57823200 | -0.54811100 |
| O | -1.91253100 | -1.92453600 | -1.84211300 |
| H | -1.31655400 | -2.66647000 | -1.67932100 |
| O | -2.29721900 | -2.28386100 | 1.32528200  |
| H | -1.66791900 | -1.86823700 | 1.93999600  |
| H | -0.82326900 | 1.31990500  | 0.34468900  |

TSB3-(PCM)

|                     |             |             |             |
|---------------------|-------------|-------------|-------------|
| C                   | 1.88846900  | 0.25697300  | 0.16951200  |
| C                   | 0.58349400  | 0.85046800  | -0.35511100 |
| C                   | -0.70619700 | 0.43287500  | 0.34619000  |
| C                   | -1.94382900 | 1.09624600  | -0.23637900 |
| H                   | -1.80632400 | 2.18019800  | -0.20427500 |
| H                   | -2.03948000 | 0.77908700  | -1.27595300 |
| F                   | 1.86124300  | -1.07151500 | 0.12684200  |
| F                   | 2.13089900  | 0.63603200  | 1.42434900  |
| F                   | 0.69546700  | 2.19873400  | -0.35173400 |
| O                   | -3.08910100 | 0.67703600  | 0.45591500  |
| H                   | -3.11370100 | 1.11060700  | 1.31513500  |
| F                   | 2.90213800  | 0.68270100  | -0.58585000 |
| H                   | 0.47279800  | 0.46005900  | -1.49420800 |
| F                   | -0.61212000 | 0.73695600  | 1.67227200  |
| F                   | -0.80844900 | -0.91658300 | 0.26603600  |
| O                   | 0.30177200  | 0.17879200  | -2.75805800 |
| H                   | 0.70211200  | 0.96603000  | -3.16848700 |
| OH-H <sub>2</sub> O |             |             |             |
| O                   | -1.61261700 | 0.00038000  | 0.00551600  |
| H                   | -0.63435100 | -0.00773100 | -0.01544200 |
| O                   | 1.24109200  | -0.00062000 | -0.02514200 |
| H                   | 1.79596500  | 0.77437100  | 0.08551600  |
| H                   | 1.81058200  | -0.76472000 | 0.08693600  |

## ERA1-w

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.87976300 | 0.22364500  | -0.13817200 |
| C | -0.65527500 | -0.37606800 | 0.58703400  |
| C | 0.50025200  | -0.85596800 | -0.30875100 |
| C | 1.67075000  | -1.42781700 | 0.49017000  |
| H | 1.84698400  | -0.79134300 | 1.36428800  |
| H | 1.37659700  | -2.42316500 | 0.82741100  |
| F | -2.79024800 | 0.57527700  | 0.76122300  |
| F | -2.41918300 | -0.63918200 | -0.98072600 |
| F | -1.51911000 | 1.32102000  | -0.81470800 |
| F | -1.08257100 | -1.40817500 | 1.33299900  |
| F | -0.18758500 | 0.58705900  | 1.40766800  |
| F | 0.01476500  | -1.76582800 | -1.17755300 |
| F | 0.90548500  | 0.21661800  | -1.04029800 |
| O | 2.79816900  | -1.53961300 | -0.31853900 |
| H | 3.20629300  | -0.66404000 | -0.35321600 |
| O | 3.03472800  | 1.16959100  | 0.62238300  |
| H | 2.46045200  | 1.88326600  | 0.25762500  |
| O | 1.14800800  | 2.94446000  | -0.37315000 |
| H | 0.48966600  | 2.44724600  | -0.86866800 |
| H | 0.66301200  | 3.58868400  | 0.14788100  |

## TSA2-w

|   |             |            |            |
|---|-------------|------------|------------|
| C | -0.41330600 | 2.44884700 | 0.84271400 |
| C | -1.64425800 | 1.73016700 | 0.24643200 |

|        |             |             |             |
|--------|-------------|-------------|-------------|
| C      | -1.33091600 | 0.56916000  | -0.71755800 |
| C      | -2.55818200 | -0.26169800 | -1.05250200 |
| H      | -2.89934700 | -0.81592700 | -0.03793000 |
| H      | -3.37832200 | 0.37560000  | -1.38830100 |
| F      | -0.80987100 | 3.54070700  | 1.48226500  |
| F      | 0.44680600  | 2.78752700  | -0.10348500 |
| F      | 0.20361500  | 1.65339700  | 1.72131100  |
| F      | -2.37785300 | 2.64105600  | -0.41144700 |
| F      | -2.37061300 | 1.26399300  | 1.28113100  |
| F      | -0.78963200 | 1.09465400  | -1.83339200 |
| F      | -0.37692800 | -0.21328300 | -0.14254700 |
| O      | -2.28351000 | -1.23714900 | -1.98261900 |
| H      | -1.91538400 | -2.00015300 | -1.51997000 |
| O      | -2.83077800 | -1.86065300 | 0.78631600  |
| H      | -2.19362300 | -1.53993100 | 1.46112300  |
| O      | -0.87769700 | -0.97581800 | 2.63334400  |
| H      | -0.08190000 | -0.66902200 | 2.18926800  |
| H      | -1.07783000 | -0.30718300 | 3.29344600  |
| EPA2-w |             |             |             |
| C      | -1.76565800 | 0.42785300  | 0.07963500  |
| C      | -0.55507900 | -0.42765900 | 0.51358500  |
| C      | 0.32720600  | -1.01862600 | -0.61882200 |
| C      | 1.36768800  | -1.96654500 | -0.16780700 |
| H      | 3.83412100  | 1.36478900  | 0.83429500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.10722800  | -3.01368600 | -0.11030300 |
| F | -2.34529900 | 0.95048400  | 1.15606900  |
| F | -2.65784300 | -0.29393700 | -0.57664100 |
| F | -1.37063500 | 1.43909900  | -0.70455200 |
| F | -1.03936800 | -1.43501000 | 1.25749900  |
| F | 0.22402100  | 0.35163500  | 1.28832400  |
| F | -0.50176400 | -1.62837800 | -1.49378200 |
| F | 0.88733700  | 0.06583800  | -1.24722100 |
| O | 2.39553800  | -1.56175400 | 0.56666100  |
| H | 2.60764600  | -0.59826000 | 0.46850600  |
| O | 3.08033500  | 0.97702300  | 0.38733000  |
| H | 2.47102700  | 1.69648400  | 0.14042500  |
| O | 1.23087400  | 2.82971700  | -0.48236900 |
| H | 0.78150700  | 2.32288100  | -1.16678100 |
| H | 0.53150600  | 3.13018900  | 0.10407000  |

#### ERB1-w

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.96938000 | 0.08324400  | -0.19399100 |
| C | -0.91932000 | -0.52264600 | 0.73433700  |
| C | 0.39449800  | -0.88510100 | 0.03198200  |
| C | 1.58482100  | -0.95891100 | 0.97796600  |
| H | 1.72141300  | 0.03800900  | 1.41052200  |
| H | 1.33629800  | -1.65965700 | 1.77997100  |
| F | -3.13944700 | 0.17906100  | 0.43844200  |
| F | -2.13731600 | -0.65747500 | -1.28105700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| F | -1.62305600 | 1.32411500  | -0.57348800 |
| F | -0.68653900 | 0.40109700  | 1.72076200  |
| F | 0.19532200  | -2.06706400 | -0.59467200 |
| F | 0.65677600  | 0.03160600  | -0.95086200 |
| O | 2.71512900  | -1.42748400 | 0.31506800  |
| H | 3.10572700  | -0.68409700 | -0.16840300 |
| O | 3.32454500  | 1.11453500  | -0.81812700 |
| H | 2.58747800  | 1.68220900  | -0.49534000 |
| O | 1.12907600  | 2.47201800  | 0.22527700  |
| H | 0.29187000  | 2.21115000  | -0.17274100 |
| H | 1.00942000  | 3.36603000  | 0.55357000  |
| H | -1.33758200 | -1.42777600 | 1.18079100  |

TSB2-w

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.40469000 | 2.40800300  | 0.85216600  |
| C | -1.64221800 | 1.74143600  | 0.25237800  |
| C | -1.33635100 | 0.58442700  | -0.70060300 |
| C | -2.55337500 | -0.27038700 | -1.00951500 |
| H | -2.86654600 | -0.83973700 | 0.00488900  |
| H | -3.39703300 | 0.35072100  | -1.31894100 |
| F | -0.76202200 | 3.52390900  | 1.49024800  |
| F | 0.47657700  | 2.72348700  | -0.08769800 |
| F | 0.19331900  | 1.61267200  | 1.74682100  |
| F | -2.39942600 | 1.28545900  | 1.30046400  |
| F | -0.84509000 | 1.12728000  | -1.84128100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| F | -0.34698200 | -0.19924800 | -0.18595100 |
| O | -2.28995400 | -1.23383200 | -1.95543100 |
| H | -1.90855200 | -1.99858400 | -1.50664100 |
| O | -2.79844600 | -1.91082400 | 0.79496300  |
| H | -2.18110000 | -1.59032200 | 1.48901800  |
| O | -0.90503800 | -0.93351400 | 2.63749800  |
| H | -0.09380600 | -0.74270000 | 2.15698200  |
| H | -1.14534100 | -0.10162400 | 3.05474800  |
| H | -2.20481300 | 2.50310300  | -0.29321400 |

EPB2-w

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.83828200 | 0.20068600  | 0.21279100  |
| C | -0.57772200 | -0.50577500 | 0.71110700  |
| C | 0.30361300  | -1.15994200 | -0.37079300 |
| C | 1.46256800  | -1.93169500 | 0.14054800  |
| H | 3.70124400  | 1.66269400  | 0.53179000  |
| H | 1.30323400  | -2.97899300 | 0.35989700  |
| F | -2.46910900 | 0.76267200  | 1.24783400  |
| F | -2.67471800 | -0.64953900 | -0.36991800 |
| F | -1.56028400 | 1.18044400  | -0.65904100 |
| F | 0.17769100  | 0.43923900  | 1.35294600  |
| F | -0.49088500 | -1.98887600 | -1.09174800 |
| F | 0.72426500  | -0.15061400 | -1.20429700 |
| O | 2.47173400  | -1.34128600 | 0.77071900  |
| H | 2.60696000  | -0.39296100 | 0.51333800  |

|                                  |             |             |             |
|----------------------------------|-------------|-------------|-------------|
| O                                | 2.97795400  | 1.16463100  | 0.14818100  |
| H                                | 2.28754600  | 1.79784700  | -0.12404200 |
| O                                | 0.90322200  | 2.70568200  | -0.77547900 |
| H                                | 0.49500600  | 2.04543000  | -1.34598900 |
| H                                | 0.21214500  | 2.94470700  | -0.15178100 |
| H                                | -0.89313000 | -1.27052900 | 1.42551400  |
| O <sub>2</sub> ( <sup>3</sup> P) |             |             |             |
| O                                | 0.00000000  | 0.00000000  | 0.59437700  |
| O                                | 0.00000000  | 0.00000000  | -0.59437700 |
| NO                               |             |             |             |
| N                                | 0.00000000  | 0.00000000  | -0.60707500 |
| O                                | 0.00000000  | 0.00000000  | 0.53119100  |
| NO <sub>2</sub>                  |             |             |             |
| O                                | 1.09082300  | -0.13825200 | 0.00000000  |
| N                                | 0.00000000  | 0.31525900  | 0.00000000  |
| O                                | -1.09082300 | -0.13760000 | 0.00000000  |
| HO <sub>2</sub>                  |             |             |             |
| H                                | -0.87903600 | -0.87314600 | 0.00000000  |
| O                                | 0.05494000  | 0.70807100  | 0.00000000  |
| O                                | 0.05494000  | -0.59892800 | 0.00000000  |

HNO<sub>2</sub>

|   |             |             |            |
|---|-------------|-------------|------------|
| O | 1.08389300  | -0.21812900 | 0.00000000 |
| O | -1.08374000 | -0.21937500 | 0.00000000 |
| N | 0.00000000  | 0.30715300  | 0.00000000 |
| H | -0.00122700 | 1.34996300  | 0.00000000 |

c-HONO

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | -0.15964600 | -0.51618100 | 0.00000600  |
| O | 1.06882000  | 0.06853300  | -0.00000600 |
| H | 0.92720300  | 1.03445200  | 0.00003200  |
| O | -1.04503000 | 0.25381900  | -0.00000300 |

t-HONO

|   |             |             |             |
|---|-------------|-------------|-------------|
| N | 0.16099100  | 0.48056000  | 0.00000700  |
| O | -1.01681200 | -0.25470600 | -0.00000500 |
| H | -1.71042900 | 0.41717200  | 0.00000400  |
| O | 1.08974900  | -0.21793100 | -0.00000200 |

HNO<sub>3</sub>

|   |             |             |            |
|---|-------------|-------------|------------|
| O | -0.96006600 | 0.84163500  | 0.00000000 |
| O | 1.16525200  | 0.44150800  | 0.00000000 |
| N | 0.00000000  | 0.14585200  | 0.00000000 |
| O | -0.27938500 | -1.20711300 | 0.00000000 |
| H | 0.59359900  | -1.62919400 | 0.00000000 |

## HCOOH

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.13549700 | 0.39888500  | -0.00032300 |
| O | 1.11106900  | -0.08896600 | 0.00000400  |
| H | 1.05208100  | -1.05523500 | 0.00041800  |
| O | -1.12710000 | -0.26517000 | 0.00007100  |
| H | -0.11085000 | 1.49501500  | 0.00091400  |

CF<sub>3</sub>CF<sub>2</sub>CF<sub>2</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.01516800  | -0.38603300 | 0.00058900  |
| C | -0.10856000 | 0.67723600  | -0.00087600 |
| C | -1.51914300 | 0.12635100  | -0.00042100 |
| F | 2.20164700  | 0.20396600  | 0.00032700  |
| F | 0.91280800  | -1.15295200 | -1.07932900 |
| F | 0.91211700  | -1.15073100 | 1.08196800  |
| F | 0.05067200  | 1.43500600  | 1.09437200  |
| F | -1.86028100 | -0.52120700 | 1.09021300  |
| F | -1.85965600 | -0.52470900 | -1.08914200 |
| F | 0.05104900  | 1.43225900  | -1.09793700 |

CF<sub>3</sub>CHFCF<sub>2</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.99060600  | -0.27377400 | 0.03998200  |
| C | -0.10638900 | 0.54676100  | -0.64626900 |
| C | -1.49331200 | 0.21390500  | -0.17813400 |
| F | 2.17260200  | -0.03044100 | -0.52606400 |
| F | 0.72015300  | -1.57529100 | -0.09553000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| F | 1.08412900  | 0.00670900  | 1.33379800  |
| F | 0.14959300  | 1.86481200  | -0.39370700 |
| F | -1.69504800 | 0.23569100  | 1.12337600  |
| F | -2.02020200 | -0.86536700 | -0.72781000 |
| H | -0.04648000 | 0.35362200  | -1.72005100 |

PA2-O<sub>2</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.00394500  | 0.02126000  | -0.08292900 |
| C | 0.56234700  | -0.46537000 | 0.20098000  |
| C | -0.52805900 | 0.59752400  | -0.06494400 |
| C | -1.86098000 | 0.32929800  | 0.66327200  |
| H | -1.72312300 | 0.44232500  | 1.73708400  |
| F | 2.39397500  | 0.89417900  | 0.83477700  |
| F | 2.06239500  | 0.59022900  | -1.28166000 |
| F | 0.33119500  | -1.54030400 | -0.55852200 |
| O | -2.83808300 | 1.16372000  | 0.22829400  |
| H | -2.97638600 | 1.01517000  | -0.71782100 |
| F | 2.82697300  | -1.01871200 | -0.05754100 |
| F | -0.74760800 | 0.67378100  | -1.39091100 |
| F | -0.06772000 | 1.79456100  | 0.35145200  |
| O | -2.20050600 | -1.07285000 | 0.48045800  |
| O | -2.71621400 | -1.27933000 | -0.69436900 |
| F | 0.49794800  | -0.82107600 | 1.49878300  |

PA2-O<sub>2</sub>-NO<sub>2</sub>

|     |             |             |             |
|-----|-------------|-------------|-------------|
| C   | 0.50418800  | 0.98778000  | 0.07227300  |
| C   | -1.00603100 | 1.10186500  | 0.35837600  |
| O   | -1.61037600 | 0.41965300  | -0.73360900 |
| O   | -2.97545600 | 0.34121500  | -0.51666400 |
| O   | -2.38511600 | -1.61644800 | 0.44276000  |
| N   | -3.29691900 | -0.94722200 | 0.09800200  |
| O   | -4.46804100 | -1.08874900 | 0.15535800  |
| F   | 1.15652000  | 1.54150900  | 1.11173700  |
| F   | 0.78992300  | 1.70985800  | -1.03113800 |
| C   | 1.03144300  | -0.45196900 | -0.11393700 |
| C   | 2.56870200  | -0.58257700 | 0.02817400  |
| F   | 0.69479900  | -0.90373700 | -1.32548900 |
| F   | 0.46739300  | -1.22992800 | 0.82596500  |
| F   | 2.93965300  | -1.78825400 | -0.38285700 |
| F   | 2.94116000  | -0.43142200 | 1.29099200  |
| F   | 3.17629800  | 0.33301400  | -0.71884900 |
| O   | -1.38903600 | 2.41140000  | 0.44831300  |
| H   | -1.13527100 | 2.87705600  | -0.35917700 |
| H   | -1.24361400 | 0.60696300  | 1.30133100  |
| AP1 |             |             |             |
| C   | 1.76267000  | -0.09880500 | -0.05850200 |
| C   | 0.33737100  | 0.47641900  | -0.23517500 |
| C   | -0.77467200 | -0.35284100 | 0.45042300  |
| C   | -2.16518200 | 0.08750700  | -0.06111900 |

|     |             |             |             |
|-----|-------------|-------------|-------------|
| F   | 2.64818500  | 0.80512700  | -0.45790500 |
| F   | 1.91819200  | -1.19643100 | -0.78404700 |
| F   | 1.98447600  | -0.38509100 | 1.21906800  |
| O   | -2.60093000 | -0.71481900 | -1.02328900 |
| H   | -3.45502600 | -0.38172500 | -1.33456100 |
| O   | -2.71751300 | 1.04711800  | 0.37429300  |
| F   | 0.07390600  | 0.53482300  | -1.55330500 |
| F   | 0.31767600  | 1.71643100  | 0.26390000  |
| F   | -0.55580200 | -1.65472900 | 0.20240100  |
| F   | -0.71536100 | -0.14794600 | 1.77130600  |
| AP2 |             |             |             |
| C   | -1.56345900 | -0.08402800 | -0.10801700 |
| C   | -0.16164000 | 0.51635600  | 0.13783300  |
| C   | 1.02019100  | -0.46986300 | 0.07272800  |
| C   | 2.35508800  | 0.23658100  | 0.40422400  |
| H   | 2.52641000  | 0.40665700  | 1.48074900  |
| F   | -2.46480900 | 0.88843000  | -0.04237500 |
| F   | -1.84838800 | -0.99415400 | 0.81330900  |
| F   | -1.62175600 | -0.64466100 | -1.30785300 |
| O   | 3.11896800  | 0.54020300  | -0.45370800 |
| F   | -0.16001300 | 1.07575600  | 1.36365200  |
| F   | 0.04438800  | 1.47777700  | -0.77363700 |
| F   | 0.82454100  | -1.44211100 | 0.99100900  |
| F   | 1.07278800  | -1.01909800 | -1.14318200 |

## IM1A

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.56258800 | -0.17885800 | 0.08248700  |
| C | -1.05467600 | -0.50828000 | -0.04052700 |
| C | -0.13655800 | 0.73595200  | -0.01195100 |
| C | 1.25519100  | 0.51891700  | -0.63247100 |
| H | 1.15924100  | 0.34756400  | -1.70543000 |
| F | -3.01510500 | 0.39498700  | -1.02304700 |
| F | -2.76581200 | 0.63534800  | 1.11272900  |
| F | -0.73425700 | -1.32843100 | 0.96366100  |
| O | 2.05460100  | 1.61979800  | -0.45021400 |
| H | 2.11607700  | 1.81446600  | 0.49431900  |
| F | -3.23811400 | -1.30330700 | 0.28294500  |
| F | 0.00770100  | 1.14295000  | 1.26606800  |
| F | -0.74065900 | 1.72637400  | -0.69670000 |
| O | 1.74500800  | -0.64081700 | 0.00865800  |
| O | 2.88777900  | -1.06013000 | -0.68975900 |
| O | 3.96499800  | -0.12157300 | 0.96315400  |
| N | 4.10250400  | -0.71883500 | -0.01123000 |
| F | -0.87155000 | -1.14734100 | -1.21123600 |

## IM2A

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 2.62187100 | -0.24275300 | -0.00215100 |
| C | 1.09801900 | -0.51833300 | 0.02015200  |
| C | 0.23053200 | 0.76046700  | -0.03635500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.20669800 | 0.58365800  | 0.48324000  |
| H | -1.19144300 | 0.38753000  | 1.55611000  |
| F | 3.02597400  | 0.27545900  | 1.14858700  |
| F | 2.91765500  | 0.59800600  | -0.98785800 |
| F | 0.81007500  | -1.30554900 | -1.01934700 |
| O | -1.95231700 | 1.71709000  | 0.27100200  |
| H | -1.93982700 | 1.93565600  | -0.67010000 |
| F | 3.26735400  | -1.38461400 | -0.20283300 |
| F | 0.18928300  | 1.20378000  | -1.31012500 |
| F | 0.82480100  | 1.70933000  | 0.71301200  |
| O | -1.69905800 | -0.54110800 | -0.21416800 |
| O | -2.90617400 | -0.91117300 | 0.38194600  |
| O | -4.97829700 | -0.62279800 | 0.02751900  |
| N | -3.96275500 | -0.32572600 | -0.42207700 |
| F | 0.81985500  | -1.17168300 | 1.16398800  |

#### IM3A

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.43636600  | -0.36627600 | 0.09577100  |
| C | 0.89654300  | -0.47884800 | -0.01696700 |
| C | 0.17314500  | 0.88542500  | -0.11374100 |
| C | -1.30328400 | 0.84756300  | 0.31441000  |
| H | -1.37356700 | 0.63682800  | 1.38015400  |
| F | 2.79100600  | 0.10533600  | 1.28203700  |
| F | 2.89871900  | 0.44032000  | -0.85370200 |
| F | 0.61937300  | -1.21576300 | -1.09482500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.92631500 | 2.04005800  | 0.06611800  |
| H | -1.79253900 | 2.28863800  | -0.85763700 |
| F | 2.97206400  | -1.56934000 | -0.06112000 |
| F | 0.25623400  | 1.33726800  | -1.38177100 |
| F | 0.80976100  | 1.76638800  | 0.68103500  |
| O | -1.84746400 | -0.21993800 | -0.45285200 |
| N | -3.05667000 | -0.75399700 | 0.05891100  |
| O | -3.56870100 | -1.50241900 | -0.70106300 |
| O | -3.38586100 | -0.40478400 | 1.15023000  |
| F | 0.44983500  | -1.11732100 | 1.08265700  |

#### IM4A

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -2.26087000 | 1.43073800  | 0.17994000  |
| C | -2.12719900 | 0.23414300  | -0.42384200 |
| H | -2.01747200 | 0.40853300  | -1.50649900 |
| C | -0.78807000 | -0.40117100 | 0.06115400  |
| C | 0.42635000  | 0.54561100  | -0.05620400 |
| C | 1.79639700  | -0.17309200 | -0.00509000 |
| O | -3.16046200 | -0.66699800 | -0.24671100 |
| H | -3.33166000 | -0.77189700 | 0.69647600  |
| F | -0.93158500 | -0.77141100 | 1.34939400  |
| F | -0.54656600 | -1.50582500 | -0.66357000 |
| F | 0.39479100  | 1.43610100  | 0.93935500  |
| F | 0.35187400  | 1.19277800  | -1.23436500 |
| F | 1.84384600  | -0.98970200 | 1.04154200  |

|   |            |             |             |
|---|------------|-------------|-------------|
| F | 2.00453000 | -0.87108300 | -1.11241500 |
| F | 2.75810200 | 0.73364300  | 0.11206900  |

TS-PA2-O<sub>2</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.46846900  | 0.62821600  | -0.11810600 |
| C | 1.81121800  | 0.49389300  | 0.63267500  |
| H | 1.73152500  | 0.32746900  | 1.71338800  |
| O | 2.79503600  | 1.07762100  | 0.12680400  |
| H | 3.38036600  | 0.02524600  | -0.41339300 |
| O | 3.29140400  | -1.09073200 | -0.49220700 |
| O | 2.22511900  | -1.27062600 | 0.16659000  |
| C | -0.69049500 | -0.13994700 | 0.54645400  |
| C | -2.00443700 | -0.18936700 | -0.26515100 |
| F | -2.95779000 | -0.72346300 | 0.48893000  |
| F | -2.37481300 | 1.03241200  | -0.62567800 |
| F | -1.84946400 | -0.93614300 | -1.34900400 |
| F | 0.61077800  | 0.22079300  | -1.39084500 |
| F | 0.14634800  | 1.93545800  | -0.12933000 |
| F | -0.30804100 | -1.40612700 | 0.78013900  |
| F | -0.94623000 | 0.45045000  | 1.72748700  |

TS-PA2-O<sub>2</sub>-NO<sub>2</sub>

|   |             |            |            |
|---|-------------|------------|------------|
| C | -0.39705100 | 1.09114200 | 0.10974700 |
| C | 1.15264900  | 1.21681600 | 0.03508700 |
| H | 1.52785600  | 0.45757700 | 0.91124100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.57841800  | 2.47213200  | 0.38101500  |
| H | 1.90765300  | 2.92622400  | -0.40411300 |
| O | 1.61142700  | 0.67383700  | -1.05223300 |
| O | 3.06586700  | -0.27811500 | -0.72557100 |
| O | 2.44196700  | -0.57992900 | 1.30854500  |
| N | 2.73755900  | -1.12333700 | 0.21525300  |
| O | 2.70676700  | -2.29210100 | 0.00483500  |
| C | -0.90772400 | -0.29071500 | -0.36479300 |
| C | -2.33651800 | -0.62970400 | 0.12737600  |
| F | -2.77698000 | -1.69668800 | -0.52389800 |
| F | -2.33305900 | -0.89186300 | 1.42559200  |
| F | -0.07985000 | -1.24530600 | 0.10075900  |
| F | -0.90851300 | -0.32372200 | -1.69946800 |
| F | -0.79035500 | 1.29850700  | 1.37590700  |
| F | -0.94806400 | 2.04445000  | -0.65518800 |
| F | -3.15230400 | 0.39103800  | -0.11160700 |

TS1A

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.56102600 | -0.30475100 | 0.06082600  |
| C | -1.03341700 | -0.50079700 | -0.10075400 |
| C | -0.21278000 | 0.79575400  | 0.08829400  |
| C | 1.18903800  | 0.76305000  | -0.54451000 |
| H | 1.10609300  | 0.73035100  | -1.63117400 |
| F | -3.06444000 | 0.36688600  | -0.96491000 |
| F | -2.81914900 | 0.35571300  | 1.18512000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| F | -0.64547100 | -1.41658200 | 0.79056500  |
| O | 1.90259400  | 1.88966000  | -0.20842700 |
| H | 1.89460400  | 1.99954000  | 0.75062000  |
| F | -3.14839200 | -1.49356700 | 0.11661200  |
| F | -0.09528900 | 1.04695300  | 1.41113100  |
| F | -0.89724900 | 1.81680700  | -0.46329800 |
| O | 1.76361200  | -0.43061500 | -0.06879900 |
| O | 2.89417100  | -0.70517800 | -0.85886500 |
| O | 4.36852700  | -1.10728800 | 0.74970900  |
| N | 4.09028100  | -0.25817900 | 0.05227100  |
| F | -0.81387500 | -0.96674400 | -1.34382300 |

#### TS2A

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 2.11293600  | 0.65694300  | -0.27215700 |
| O | 2.44834700  | -1.36034700 | -1.01369000 |
| N | 2.62605800  | -1.65935200 | 0.04257900  |
| O | 2.75297400  | -1.71767400 | 1.16318100  |
| C | 1.16673700  | 1.55987600  | -0.53879500 |
| H | 0.93293200  | 1.68728600  | -1.60952000 |
| C | -0.15860800 | 1.13998000  | 0.15011800  |
| C | -0.60131000 | -0.29381500 | -0.22198800 |
| C | -2.09094400 | -0.61606400 | 0.04145800  |
| O | 1.47349200  | 2.85765600  | -0.07320000 |
| H | 1.97668500  | 2.72511000  | 0.73766300  |
| F | -0.02937600 | 1.17985400  | 1.49583500  |

|      |             |             |             |
|------|-------------|-------------|-------------|
| F    | -1.18127100 | 1.96184200  | -0.18796300 |
| F    | 0.11587600  | -1.21011800 | 0.48349300  |
| F    | -0.37142200 | -0.52410100 | -1.52945500 |
| F    | -2.43183900 | -0.26637900 | 1.27492300  |
| F    | -2.87343600 | 0.00776200  | -0.82541100 |
| F    | -2.28289500 | -1.92990500 | -0.09409100 |
| TS3A |             |             |             |
| C    | 2.27728300  | -0.56632400 | 0.15334200  |
| C    | 0.84284000  | -0.30980500 | -0.36884300 |
| C    | 0.20211000  | 0.99222600  | 0.16831600  |
| C    | -1.34309200 | 0.97309800  | 0.07649800  |
| H    | -1.67396200 | 0.16412900  | 0.82714900  |
| F    | 2.25961900  | -0.90540100 | 1.43393600  |
| F    | 3.01668300  | 0.52629900  | -0.00078400 |
| F    | 0.89114300  | -0.26970700 | -1.70207400 |
| O    | -1.89999900 | 2.15935800  | 0.51670500  |
| H    | -1.87341000 | 2.80336500  | -0.20021400 |
| F    | 2.82126900  | -1.55715800 | -0.54142400 |
| F    | 0.67781400  | 2.03652800  | -0.53324000 |
| F    | 0.56710600  | 1.15817100  | 1.45201100  |
| O    | -1.72443800 | 0.52882200  | -1.10202600 |
| N    | -2.88343500 | -1.01269100 | 0.34140100  |
| O    | -2.96085800 | -0.72872700 | -0.83971200 |
| O    | -3.53330400 | -1.85121800 | 0.88679900  |

|      |             |             |             |
|------|-------------|-------------|-------------|
| F    | 0.07807300  | -1.35314300 | 0.01527000  |
| TS4A |             |             |             |
| C    | -2.05200100 | -0.90595200 | -0.09315800 |
| C    | -0.60605200 | -0.39152000 | 0.10255100  |
| C    | -0.46460000 | 1.14908900  | 0.05627500  |
| C    | 0.97949500  | 1.60185900  | -0.31261400 |
| H    | 1.09682200  | 1.35638000  | -1.38717100 |
| F    | -2.44823000 | -0.74443800 | -1.34800900 |
| F    | -2.88046600 | -0.25614300 | 0.71597700  |
| F    | -0.16565800 | -0.86081600 | 1.27449000  |
| O    | 1.05338000  | 2.99153000  | -0.22537700 |
| H    | 1.15547300  | 3.21924400  | 0.70556500  |
| F    | -2.09932400 | -2.20265600 | 0.19783600  |
| F    | -0.80554400 | 1.64310100  | 1.26122400  |
| F    | -1.34337200 | 1.62588900  | -0.84967000 |
| O    | 1.84690700  | 0.91347000  | 0.43049900  |
| O    | 3.09554400  | -0.28502000 | -0.62419700 |
| O    | 3.44561000  | -2.29360500 | 0.20596100  |
| N    | 3.06498000  | -1.19214200 | 0.08242900  |
| F    | 0.14484500  | -0.93410300 | -0.88616000 |
| TS5A |             |             |             |
| C    | 2.06507000  | -0.78988300 | 0.11489100  |
| C    | 0.66481100  | -0.29814700 | -0.32493500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.33452400  | 1.14965200  | 0.11003100  |
| C | -1.21142200 | 1.43662300  | 0.08250200  |
| H | -1.57796500 | 0.79078600  | 0.97269100  |
| F | 2.10964600  | -0.98537500 | 1.42563800  |
| F | 2.98928300  | 0.09913200  | -0.22708600 |
| F | 0.59388900  | -0.40716600 | -1.65165900 |
| O | -1.40449800 | 2.76081300  | 0.47069800  |
| H | -1.76568800 | 3.22165300  | -0.29476200 |
| F | 2.33217600  | -1.94225500 | -0.49145100 |
| F | 0.96840700  | 1.99529700  | -0.71314200 |
| F | 0.81329900  | 1.33805600  | 1.35521300  |
| O | -1.77211100 | 1.02448400  | -0.99971200 |
| N | -3.03393700 | -1.47111700 | -0.07349200 |
| O | -2.95625700 | -2.57295300 | 0.30769100  |
| O | -2.94749700 | -0.37480600 | 0.29357600  |
| F | -0.23934300 | -1.14262100 | 0.23177100  |

#### TS6A

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.20222700 | 0.85755200  | -0.15776900 |
| C | 1.16676100  | 0.97130600  | 0.53541800  |
| H | 1.15675500  | 0.72274800  | 1.60178600  |
| O | 1.95568300  | 1.82391300  | 0.06542300  |
| H | 3.03752700  | 1.23589300  | 0.21407300  |
| O | 1.83929500  | -0.67633800 | 0.06444600  |
| O | 3.78588600  | 0.34935200  | 0.23798700  |

|      |             |             |             |
|------|-------------|-------------|-------------|
| N    | 3.11316800  | -0.72583700 | -0.01262300 |
| O    | 3.67054800  | -1.72691300 | -0.28841700 |
| C    | -0.97754700 | -0.45748000 | 0.11069000  |
| C    | -2.51593800 | -0.30214100 | 0.01173500  |
| F    | -0.93282700 | 1.88057100  | 0.34792700  |
| F    | -0.07297900 | 1.03184500  | -1.47162900 |
| F    | -0.60845000 | -1.39175600 | -0.76653800 |
| F    | -2.83471400 | 0.31979300  | -1.11773000 |
| F    | -2.99138000 | 0.38416200  | 1.04100700  |
| F    | -3.07306700 | -1.50613500 | 0.01304300  |
| F    | -0.68925500 | -0.87995800 | 1.35798100  |
| TS7A |             |             |             |
| C    | 2.27841900  | -0.52280200 | 0.14645800  |
| C    | 0.80830600  | -0.36207100 | -0.31218300 |
| C    | 0.18780000  | 1.01351000  | 0.02313500  |
| C    | -1.34524700 | 1.00288300  | -0.07510700 |
| H    | -1.72347900 | 0.22874700  | 0.94805600  |
| F    | 2.35484300  | -0.61314900 | 1.46632800  |
| F    | 3.00119500  | 0.51228100  | -0.26408800 |
| F    | 0.76536100  | -0.56146300 | -1.63206100 |
| O    | -1.87776200 | 2.23982700  | 0.23138300  |
| H    | -2.37211300 | 2.55553000  | -0.53395600 |
| F    | 2.77735100  | -1.63321100 | -0.38353500 |
| F    | 0.68704300  | 1.92715200  | -0.82840800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| F | 0.56926800  | 1.36400300  | 1.26802600  |
| O | -1.86109000 | 0.29026800  | -0.98713300 |
| N | -2.88475900 | -0.97430500 | 0.07310100  |
| O | -3.63129500 | -1.78148900 | -0.33550200 |
| O | -2.56469900 | -0.72386400 | 1.21727600  |
| F | 0.08849600  | -1.32352300 | 0.30398100  |

# TS8A

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.12969500 | -0.32876500 | -0.15858400 |
| C | -0.68102200 | -0.29314700 | 0.38721800  |
| C | 0.15217400  | 0.90644400  | -0.11834500 |
| C | 1.67337900  | 0.71384200  | 0.14508000  |
| H | 1.91290600  | -0.24546900 | -0.65501200 |
| F | -2.81961000 | -1.24825200 | 0.50520900  |
| F | -2.14088000 | -0.63986200 | -1.44729400 |
| F | -2.71312000 | 0.85180900  | 0.01031300  |
| O | 2.34439900  | 1.79442900  | -0.38263300 |
| H | 3.10785100  | 1.96381000  | 0.18283900  |
| O | 2.02508400  | 0.18302800  | 1.22764300  |
| O | 3.05171200  | -1.85019400 | 0.11746800  |
| O | 2.62468500  | -1.47743900 | -0.93533400 |
| F | -0.74618100 | -0.26082200 | 1.71988500  |
| F | -0.07884000 | -1.43510400 | -0.00231600 |
| F | -0.06903200 | 1.06097400  | -1.43755700 |
| F | -0.26309500 | 2.01490500  | 0.50985000  |

TS9A

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.85119400  | -0.13637200 | -0.01302300 |
| C | 0.44902900  | 0.52225900  | -0.04411900 |
| C | -0.70082900 | -0.48095300 | 0.09603500  |
| F | 2.78283800  | 0.80393400  | 0.03680900  |
| F | 2.04361000  | -0.87502200 | -1.09742900 |
| F | 1.95682200  | -0.91064500 | 1.06273400  |
| C | -2.34138900 | 0.35250500  | -0.46173600 |
| O | -2.30112300 | 1.38827100  | 0.22100700  |
| O | -3.23474800 | -0.64215500 | -0.21372100 |
| H | -2.05616000 | 0.34355200  | -1.52480600 |
| H | -3.62788300 | -0.47591100 | 0.65374400  |
| F | 0.38980600  | 1.40173200  | 0.95431700  |
| F | -0.89529100 | -0.87067900 | 1.33737700  |
| F | -0.55599500 | -1.52580900 | -0.70026600 |
| F | 0.32520700  | 1.15635600  | -1.22133900 |

TS10A

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.79931700  | -0.14917300 | -0.03803600 |
| F | 1.91406300  | -0.99930800 | 0.97515200  |
| C | 0.41449000  | 0.54450100  | -0.00842000 |
| C | -0.77447400 | -0.43849000 | 0.09859800  |
| C | -2.14809300 | 0.24876500  | -0.13321300 |
| O | -2.33628900 | 1.41838700  | 0.11945200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| F | 2.74427000  | 0.77666600  | 0.06775200  |
| F | 1.97383700  | -0.80492200 | -1.17733900 |
| O | -3.10321500 | -0.69467100 | -0.20025700 |
| H | -3.96181600 | -0.25558900 | -0.12703300 |
| H | -1.84426700 | 0.41002200  | -1.77012600 |
| F | 0.39446500  | 1.37086200  | 1.04112200  |
| F | 0.30510100  | 1.25847300  | -1.14184100 |
| F | -0.58927500 | -1.44744600 | -0.76916000 |
| F | -0.78971800 | -0.95185500 | 1.34098300  |

#### TS11A

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.77318100 | -0.30964700 | 0.01043400  |
| C | 0.50065400  | 0.55659800  | 0.10087500  |
| C | 1.83268700  | -0.21331700 | -0.05563900 |
| F | 1.80363700  | -0.96243400 | -1.15143900 |
| F | 2.05102200  | -0.98935200 | 0.99643900  |
| F | 2.82850500  | 0.65835100  | -0.15583300 |
| C | -2.00778300 | 0.48846800  | 0.47831400  |
| O | -2.51580500 | 1.31278800  | -0.26954700 |
| H | -2.17003500 | 0.47804800  | 1.56477900  |
| O | -3.31535200 | -0.83265200 | 0.12821900  |
| H | -3.39672900 | -0.79224700 | -0.84339600 |
| F | 0.51047200  | 1.15100800  | 1.31149400  |
| F | 0.44911500  | 1.50225500  | -0.84286500 |
| F | -0.60791600 | -1.39135100 | 0.79325200  |

|                                     |             |             |             |
|-------------------------------------|-------------|-------------|-------------|
| F                                   | -0.93464000 | -0.70842000 | -1.26156500 |
| PB2-O <sub>2</sub>                  |             |             |             |
| C                                   | -1.99469800 | -0.06896200 | 0.10669100  |
| C                                   | -0.74259100 | -0.09073900 | -0.77038800 |
| C                                   | 0.46492500  | 0.60207100  | -0.12487200 |
| C                                   | 1.83459300  | 0.13240000  | -0.66606500 |
| H                                   | 1.81007300  | 0.05745600  | -1.75321100 |
| F                                   | -2.24587900 | 1.17481300  | 0.51472600  |
| F                                   | -1.86996100 | -0.85465200 | 1.16717100  |
| F                                   | -0.45497900 | -1.39353800 | -1.05607100 |
| O                                   | 2.83614100  | 0.96614100  | -0.28687200 |
| H                                   | 2.94787100  | 0.89567600  | 0.67217800  |
| F                                   | -3.04098100 | -0.49607400 | -0.60358200 |
| H                                   | -0.97262300 | 0.43707900  | -1.69973300 |
| F                                   | 0.46364900  | 0.45966200  | 1.21923800  |
| F                                   | 0.34887000  | 1.92407700  | -0.38654100 |
| O                                   | 2.05105600  | -1.23344300 | -0.20163400 |
| O                                   | 2.61715900  | -1.25362600 | 0.96526700  |
| PB2-O <sub>2</sub> -NO <sub>2</sub> |             |             |             |
| C                                   | 0.53344600  | 0.95550800  | 0.10328400  |
| C                                   | -0.97900800 | 1.14044600  | 0.31850700  |
| O                                   | -1.57733600 | 0.40110700  | -0.74399400 |
| O                                   | -2.92040700 | 0.21806000  | -0.46654600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -2.12047400 | -1.64215400 | 0.53584700  |
| N | -3.10205800 | -1.06722300 | 0.19470600  |
| O | -4.24925500 | -1.32104300 | 0.29936300  |
| F | 1.14372500  | 1.38964900  | 1.22704000  |
| F | 0.92416100  | 1.75903700  | -0.91129600 |
| C | 0.96432700  | -0.49098000 | -0.18742900 |
| C | 2.44052800  | -0.74466500 | 0.13311900  |
| F | 0.77481500  | -0.74443100 | -1.51082800 |
| F | 2.80764400  | -1.91694400 | -0.37995800 |
| F | 2.62595500  | -0.79462800 | 1.45307200  |
| F | 3.23246200  | 0.19800700  | -0.37151200 |
| O | -1.34738800 | 2.45464000  | 0.33128200  |
| H | -1.00783100 | 2.89152500  | -0.46041000 |
| H | -1.25641900 | 0.70025800  | 1.27884800  |
| H | 0.36293000  | -1.18415700 | 0.40745900  |

BP1

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.73446300  | -0.50480700 | -0.04691300 |
| C | 2.13405300  | 0.13972500  | 0.04639700  |
| O | 2.35732500  | 0.86615100  | -1.05176600 |
| H | 3.23993300  | 1.25836200  | -0.99180900 |
| O | 2.87956700  | -0.00985900 | 0.95767500  |
| C | -0.34014200 | 0.55499200  | -0.30435900 |
| C | -1.76543100 | 0.06677200  | -0.04880700 |
| F | -2.63166100 | 0.98917900  | -0.47590700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| F | -1.99202400 | -1.06162500 | -0.72090500 |
| F | -0.10354600 | 1.61145300  | 0.53147100  |
| F | 0.73560700  | -1.38347600 | -1.07693900 |
| F | 0.49384200  | -1.17991600 | 1.08166300  |
| F | -1.99658600 | -0.14609500 | 1.23940300  |
| H | -0.26340900 | 0.88551900  | -1.34244300 |

## BP2

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.98094100 | 0.41126100  | -0.10932900 |
| C | -2.31545500 | -0.28969500 | -0.43386200 |
| H | -2.52157300 | -0.38824300 | -1.51600000 |
| O | -3.05632600 | -0.66403000 | 0.41577800  |
| C | 0.21179100  | -0.41281900 | -0.60293100 |
| H | 0.29722700  | -0.29519900 | -1.68652400 |
| C | 1.54492200  | -0.00902700 | 0.02701300  |
| F | 2.54332200  | -0.61979800 | -0.61615200 |
| F | 1.72150700  | 1.30734100  | -0.08223700 |
| F | 1.61213100  | -0.34893400 | 1.30577700  |
| F | -0.89588300 | 0.65718700  | 1.20245000  |
| F | -0.97639700 | 1.59916700  | -0.77122400 |
| F | -0.01434200 | -1.72859000 | -0.30628500 |

## IM1B

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.26442800 | -0.50738500 | -0.13567300 |
| C | -0.75857100 | -0.48354400 | 0.14377000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.13797400 | 0.90883200  | -0.05981700 |
| C | 1.37565500  | 0.89774000  | -0.33563300 |
| H | 1.54956300  | 0.49951300  | -1.33822700 |
| F | -2.49396000 | -0.42193600 | -1.44728700 |
| F | -2.90355800 | 0.48776200  | 0.47294600  |
| F | -0.56794000 | -0.86639200 | 1.43474900  |
| O | 1.91825000  | 2.15225600  | -0.28756500 |
| H | 1.69914800  | 2.56122600  | 0.55928500  |
| F | -2.77680400 | -1.65794800 | 0.29718100  |
| H | -0.28104600 | -1.20555200 | -0.52456600 |
| F | -0.37325300 | 1.67313600  | 1.02924800  |
| F | -0.72708500 | 1.51021400  | -1.11720800 |
| O | 1.90469200  | 0.01793100  | 0.64453000  |
| O | 3.20432800  | -0.35055600 | 0.26876100  |
| O | 2.18829100  | -2.07141900 | -0.58872100 |
| N | 3.22902300  | -1.60832400 | -0.38501000 |

## IM2B

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.37962800 | -0.65370200 | 0.02893400  |
| C | -1.01763200 | -0.39165100 | -0.61582200 |
| C | -0.37715700 | 0.92582600  | -0.15595400 |
| C | 1.15546500  | 1.00014000  | -0.32205600 |
| H | 1.44319500  | 0.62449000  | -1.30769800 |
| F | -3.16417400 | 0.41628200  | -0.09717000 |
| F | -2.26872500 | -0.95818500 | 1.31497300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| F | -0.21614400 | -1.45883900 | -0.34121000 |
| O | 1.61010200  | 2.29194100  | -0.22417300 |
| H | 1.38129700  | 2.64235800  | 0.64580500  |
| F | -2.97049500 | -1.68043600 | -0.58770600 |
| H | -1.16604600 | -0.32517900 | -1.69705700 |
| F | -0.68203500 | 1.20790500  | 1.13279700  |
| F | -0.92190000 | 1.90591000  | -0.91265600 |
| O | 1.65938500  | 0.16572200  | 0.69763200  |
| O | 3.02144600  | -0.04867200 | 0.45991000  |
| O | 4.23548100  | -1.61411900 | -0.28635200 |
| N | 3.12217200  | -1.35400900 | -0.14415100 |

#### IM3B

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.29711200 | -0.55723700 | 0.03992000  |
| C | -1.04424000 | -0.16223900 | -0.73893000 |
| C | -0.26385800 | 0.99578600  | -0.08919600 |
| C | 1.25818000  | 0.91808900  | -0.29602300 |
| H | 1.48825400  | 0.70112400  | -1.33792100 |
| F | -3.05364100 | 0.52086500  | 0.24841300  |
| F | -2.00409400 | -1.11506000 | 1.20608100  |
| F | -0.26259700 | -1.27460200 | -0.87385100 |
| O | 1.88592800  | 2.08806800  | 0.04352400  |
| H | 1.66266400  | 2.32097400  | 0.95383900  |
| F | -3.00535500 | -1.43504400 | -0.67259700 |
| H | -1.35696300 | 0.16803900  | -1.73251700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| F | -0.51042800 | 1.09784300  | 1.23861700  |
| F | -0.70959900 | 2.14136500  | -0.65342800 |
| O | 1.66499300  | -0.15327400 | 0.54686800  |
| N | 2.76601700  | -0.90442000 | 0.08072300  |
| O | 3.14458800  | -1.68508800 | 0.88583700  |
| O | 3.15918200  | -0.68019100 | -1.02400600 |

#### IM4B

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.79617900  | -0.06933100 | 0.02714000  |
| C | 0.49438600  | 0.35773600  | -0.65391400 |
| C | -0.73963400 | -0.36736800 | -0.09907700 |
| C | -2.08997300 | 0.39204300  | -0.30466800 |
| H | -2.09738400 | 0.78454900  | -1.33497400 |
| F | 1.89744000  | -1.39820300 | 0.04176000  |
| F | 1.87391300  | 0.38223600  | 1.27179900  |
| F | 0.38396200  | 1.70852900  | -0.52052100 |
| O | -3.15830100 | -0.48218200 | -0.19272800 |
| H | -3.25714400 | -0.74139400 | 0.73062200  |
| F | 2.83375200  | 0.42097800  | -0.65506700 |
| H | 0.57244500  | 0.10795000  | -1.71559500 |
| F | -0.61263600 | -0.63231700 | 1.22379500  |
| F | -0.81319200 | -1.55551600 | -0.73225200 |
| O | -2.09830000 | 1.43706300  | 0.54740800  |

#### TS-PB2-O<sub>2</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.39282200 | 0.70527200  | -0.12255700 |
| C | -1.77087700 | 0.38110300  | -0.73444500 |
| H | -1.75469400 | 0.06161300  | -1.78374400 |
| O | -2.76456600 | 0.96031300  | -0.24341600 |
| H | -3.22139900 | -0.04545100 | 0.48833300  |
| O | -3.03381300 | -1.12536500 | 0.71482900  |
| O | -2.00299000 | -1.32160900 | 0.00505000  |
| C | 0.76770800  | -0.05755700 | -0.77049000 |
| H | 1.04540700  | 0.46085000  | -1.69202800 |
| C | 2.01065700  | -0.14861400 | 0.11380000  |
| F | 3.02932000  | -0.63640000 | -0.59861700 |
| F | 2.34973400  | 1.06338000  | 0.55156500  |
| F | 1.82055400  | -0.94665900 | 1.15562800  |
| F | -0.44209600 | 0.50530500  | 1.20853300  |
| F | -0.17114200 | 2.02741700  | -0.32496500 |
| F | 0.37514600  | -1.33137100 | -1.07460100 |

TS-PB2-O<sub>2</sub>-NO<sub>2</sub>

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.45487800 | 1.05444000  | 0.08873000  |
| C | 1.09439000  | 1.24310600  | -0.00311700 |
| H | 1.47778000  | 0.52025800  | 0.89096100  |
| O | 1.48273000  | 2.52990200  | 0.27371100  |
| H | 1.88817300  | 2.91068300  | -0.51443400 |
| O | 1.57656000  | 0.66671000  | -1.06061000 |
| O | 3.03099700  | -0.26956500 | -0.66804600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 2.24985900  | -0.64368400 | 1.30254000  |
| N | 2.64008700  | -1.14532300 | 0.21619300  |
| O | 2.64694000  | -2.30676900 | -0.02675600 |
| C | -0.87362400 | -0.39903400 | 0.35544200  |
| C | -2.34126900 | -0.67080300 | 0.01470200  |
| F | -2.68653900 | -1.86937700 | 0.48581100  |
| F | -3.12513500 | 0.24545700  | 0.58166000  |
| F | -0.11529500 | -1.26965700 | -0.37159600 |
| F | -0.89636600 | 1.79636200  | 1.11863900  |
| F | -1.02235500 | 1.54141600  | -1.03212700 |
| F | -2.55053300 | -0.66563900 | -1.29474500 |
| H | -0.72494400 | -0.59972400 | 1.42009000  |

#### TS1B

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.22092300 | -0.64860500 | 0.03614700  |
| C | -0.93151200 | -0.23787100 | -0.67472800 |
| C | -0.29907500 | 1.04013500  | -0.10217400 |
| C | 1.21792100  | 1.16450200  | -0.34762900 |
| H | 1.45465400  | 0.89821800  | -1.38019600 |
| F | -3.05834500 | 0.38553600  | 0.10667000  |
| F | -1.98869000 | -1.10064800 | 1.26104200  |
| F | -0.07090400 | -1.29850500 | -0.60813400 |
| O | 1.65817700  | 2.45085900  | -0.14313800 |
| H | 1.51488800  | 2.68813300  | 0.78134700  |
| F | -2.81714600 | -1.62273700 | -0.65651700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.17091400 | -0.04523100 | -1.72355100 |
| F | -0.53587400 | 1.16363600  | 1.22568500  |
| F | -0.91696100 | 2.08047700  | -0.70810000 |
| O | 1.79618900  | 0.24559400  | 0.54778400  |
| O | 3.08652300  | -0.07596500 | 0.08901000  |
| O | 2.95285400  | -2.28064400 | 0.34474000  |
| N | 2.87774800  | -1.51980800 | -0.49146700 |

# TS2B

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 2.11717100  | 0.64157200  | -0.42899200 |
| O | 2.48684100  | -1.37992300 | -1.08282700 |
| N | 2.58701700  | -1.68973500 | -0.01599600 |
| O | 2.59001300  | -1.70585800 | 1.11429100  |
| C | 1.13386100  | 1.53447300  | -0.59719900 |
| H | 0.84937800  | 1.71911100  | -1.65093800 |
| C | -0.15403500 | 1.05463400  | 0.11160600  |
| C | -0.66540800 | -0.28728000 | -0.43851500 |
| C | -2.12684800 | -0.59784000 | -0.11178400 |
| O | 1.46184100  | 2.80574500  | -0.07806600 |
| H | 2.04601900  | 2.63168200  | 0.66803800  |
| F | 0.06182400  | 0.92056800  | 1.44224000  |
| F | -1.15708300 | 1.95486900  | -0.05216800 |
| F | 0.07502000  | -1.32719600 | 0.09406800  |
| F | -2.40410100 | -0.43792400 | 1.17787700  |
| F | -2.94628600 | 0.17010400  | -0.82635900 |

|      |             |             |             |
|------|-------------|-------------|-------------|
| F    | -2.38714900 | -1.87302300 | -0.43107500 |
| H    | -0.55687800 | -0.30543900 | -1.52627300 |
| TS3B |             |             |             |
| C    | -2.27938300 | -0.59054000 | -0.03461100 |
| C    | -0.81603800 | -0.39489600 | -0.43356600 |
| C    | -0.25676300 | 0.98106200  | -0.03602800 |
| C    | 1.28096800  | 1.00684400  | 0.09686800  |
| H    | 1.68840400  | 0.24775300  | -0.91609200 |
| F    | -3.01207400 | 0.44009500  | -0.45458700 |
| F    | -2.42418900 | -0.71912700 | 1.27675800  |
| F    | -0.09443200 | -1.40788100 | 0.13189100  |
| O    | 1.79876900  | 2.26189600  | -0.16457800 |
| H    | 2.39022000  | 2.49151200  | 0.56132600  |
| F    | -2.74969600 | -1.69967700 | -0.61155600 |
| H    | -0.74994300 | -0.47907900 | -1.52188400 |
| F    | -0.79911000 | 1.41035000  | 1.12523500  |
| F    | -0.63495800 | 1.84844000  | -0.99820700 |
| O    | 1.78930600  | 0.29427700  | 1.01160300  |
| N    | 2.81135100  | -0.99270900 | -0.03493500 |
| O    | 3.52998900  | -1.82234300 | 0.37873900  |
| O    | 2.48809800  | -0.75581200 | -1.18333600 |
| TS4B |             |             |             |
| C    | -2.15685900 | -0.71970800 | -0.08098500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.74981800 | -0.31495400 | -0.52859000 |
| C | -0.26723100 | 1.00443300  | 0.09669000  |
| C | 0.89738800  | 1.65621800  | -0.69092000 |
| H | 0.46158400  | 1.98271200  | -1.65537000 |
| F | -3.07089900 | 0.06096300  | -0.65696200 |
| F | -2.30429500 | -0.64807300 | 1.23863800  |
| F | 0.09645600  | -1.32761000 | -0.16454100 |
| O | 1.31409500  | 2.81696900  | -0.04310500 |
| H | 1.76466600  | 2.56519500  | 0.77035300  |
| F | -2.39606300 | -1.97703700 | -0.45725500 |
| H | -0.75558500 | -0.23014000 | -1.61833000 |
| F | 0.14270700  | 0.77091800  | 1.36770400  |
| F | -1.30983200 | 1.86064200  | 0.15483400  |
| O | 1.85305600  | 0.74810000  | -0.94652600 |
| O | 2.51144600  | -0.39299300 | 0.55134900  |
| O | 3.31499600  | -2.37077700 | 0.05922300  |
| N | 2.83100800  | -1.30604300 | -0.08330000 |

#### TS5B

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.04703700 | -0.86101500 | 0.00912100  |
| C | -0.67296000 | -0.37862900 | -0.45272500 |
| C | -0.40988000 | 1.10539400  | -0.14450100 |
| C | 1.12467200  | 1.44560400  | -0.01768700 |
| H | 1.56926900  | 0.87494500  | -0.93211200 |
| F | -2.99750300 | -0.04279000 | -0.43972100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| F | -2.12943000 | -0.93693600 | 1.33017200  |
| F | 0.26014000  | -1.19500400 | 0.13117200  |
| O | 1.29225800  | 2.80391900  | -0.28323000 |
| H | 1.73278700  | 3.17475800  | 0.48943900  |
| F | -2.27919800 | -2.08117700 | -0.48664200 |
| H | -0.61771100 | -0.50560800 | -1.53675700 |
| F | -1.03156100 | 1.49547200  | 0.98319500  |
| F | -0.94919800 | 1.80574900  | -1.16492000 |
| O | 1.65988100  | 0.97053300  | 1.04921000  |
| N | 3.00126700  | -1.43953600 | 0.11027800  |
| O | 2.95550600  | -2.53012200 | -0.31176500 |
| O | 2.90220000  | -0.33724000 | -0.24634900 |

TS6B

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.31680700  | 0.89328200  | 0.06936500  |
| C | -1.12747700 | 1.04799800  | -0.43360200 |
| H | -1.21563500 | 0.97628900  | -1.52435500 |
| O | -1.91670800 | 1.74552400  | 0.24183400  |
| H | -2.96201700 | 1.19614800  | 0.01448500  |
| O | -1.75531700 | -0.71382700 | -0.25084000 |
| O | -3.71632200 | 0.28622800  | -0.17243500 |
| N | -3.02678300 | -0.80205700 | -0.15190500 |
| O | -3.56000900 | -1.85128300 | -0.06024900 |
| C | 0.92630500  | -0.51179300 | -0.08878100 |
| C | 2.45696900  | -0.48064400 | -0.17010800 |

|   |            |             |             |
|---|------------|-------------|-------------|
| F | 1.02753300 | 1.76872100  | -0.69286900 |
| F | 0.39737400 | 1.27944600  | 1.34173300  |
| F | 0.57820700 | -1.25402000 | 0.99434000  |
| F | 2.99636800 | 0.28215000  | 0.77505000  |
| F | 2.84652700 | -0.02392600 | -1.36193200 |
| F | 2.92744300 | -1.71812200 | -0.02924400 |
| H | 0.55528700 | -0.99245300 | -0.99821500 |

#### TS7B

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.28935100  | -0.61282800 | 0.01245300  |
| C | 0.83714500  | -0.44541100 | 0.45728700  |
| C | 0.27829500  | 0.96302400  | 0.19253200  |
| C | -1.26313000 | 0.97661000  | -0.00731600 |
| H | -1.67625300 | 0.24205000  | 0.78429900  |
| F | 3.03499600  | 0.36770800  | 0.52219900  |
| F | 2.40967700  | -0.60659100 | -1.30782600 |
| F | 0.09128600  | -1.40084000 | -0.17304500 |
| O | -1.82969100 | 2.20796800  | 0.27666300  |
| H | -1.80527800 | 2.75032700  | -0.51981300 |
| F | 2.76120500  | -1.77655500 | 0.46479100  |
| H | 0.79325800  | -0.61918500 | 1.53573900  |
| F | 0.86148100  | 1.54391800  | -0.88024400 |
| F | 0.58682000  | 1.72025200  | 1.26417400  |
| O | -1.57427900 | 0.43791100  | -1.16343500 |
| N | -2.82850700 | -0.98684500 | 0.31999500  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -2.84215700 | -0.78894200 | -0.87885700 |
| O | -3.51278900 | -1.78002200 | 0.89308500  |

TS8B

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.07796600  | 0.47448000  | -0.11309600 |
| C | 0.69745500  | 0.27831400  | 0.52004800  |
| C | -0.13931000 | -0.78475600 | -0.20586700 |
| C | -1.65439000 | -0.63338600 | 0.12990100  |
| H | -1.89883300 | 0.36411300  | -0.60983900 |
| F | 2.84582900  | 1.18727000  | 0.70915300  |
| F | 1.96486900  | 1.14742600  | -1.26044300 |
| F | 2.68985100  | -0.68018400 | -0.35830900 |
| O | -2.35611900 | -1.67765400 | -0.41895800 |
| H | -3.10424900 | -1.86467800 | 0.16120000  |
| O | -1.96717600 | -0.14377300 | 1.24711800  |
| O | -3.01080700 | 1.96547000  | 0.26482100  |
| O | -2.55982500 | 1.66845900  | -0.80363500 |
| F | 0.87183600  | -0.11710600 | 1.80860200  |
| F | 0.03728300  | -0.66806900 | -1.54133800 |
| F | 0.26622800  | -2.00818700 | 0.15852900  |
| H | 0.18112200  | 1.24228400  | 0.50221800  |

TS9B

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 1.84678700 | -0.03952100 | -0.13012500 |
| C | 0.44992900 | 0.57332900  | -0.28797900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.65342600 | -0.39278100 | 0.12128300  |
| F | 2.77222500  | 0.89902500  | -0.30600700 |
| F | 2.03722600  | -0.99207400 | -1.04456200 |
| F | 2.01333700  | -0.57402600 | 1.07734400  |
| C | -2.30774500 | 0.18831200  | -0.65757700 |
| O | -2.20952300 | 1.41788900  | -0.51018400 |
| O | -3.22111600 | -0.55463700 | 0.02122100  |
| H | -2.08424700 | -0.29988300 | -1.62054700 |
| H | -3.55304300 | -0.01910100 | 0.75424500  |
| F | 0.38050400  | 1.66502900  | 0.51249100  |
| F | -0.86936900 | -0.42426600 | 1.41916200  |
| F | -0.47275600 | -1.62131300 | -0.34311800 |
| H | 0.31861800  | 0.86555100  | -1.33339500 |

#### TS10B

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.78845100  | -0.06351200 | -0.16152900 |
| F | 1.96093200  | -0.70690300 | 0.98954500  |
| C | 0.42007600  | 0.61639200  | -0.24861800 |
| C | -0.73002300 | -0.31229100 | 0.16486100  |
| C | -2.09581700 | 0.22083300  | -0.34581100 |
| O | -2.25627000 | 1.39011000  | -0.64353800 |
| F | 2.74688500  | 0.85412700  | -0.27442300 |
| F | 1.93131300  | -0.93643000 | -1.16108300 |
| O | -3.07799900 | -0.62747500 | -0.01186800 |
| H | -3.92446200 | -0.18295400 | -0.15732200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -1.75189400 | -0.29761200 | -1.87678800 |
| F | 0.42284800  | 1.69027200  | 0.58592400  |
| F | -0.50907900 | -1.55890300 | -0.30032300 |
| F | -0.79966600 | -0.38035700 | 1.50504500  |
| H | 0.27529800  | 0.95470200  | -1.27821900 |

#### TS11B

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.71216400  | -0.28598500 | -0.16332800 |
| C | -0.56032200 | 0.45253000  | -0.59823500 |
| C | -1.83728400 | -0.09826800 | 0.03983000  |
| F | -1.90480800 | 0.18236600  | 1.33373100  |
| F | -1.90486700 | -1.41942200 | -0.11959500 |
| F | -2.90008500 | 0.44878100  | -0.55679300 |
| C | 1.97502400  | 0.53208100  | -0.49260100 |
| O | 2.36902500  | 1.40421700  | 0.26865700  |
| H | 2.28089300  | 0.47844400  | -1.54862900 |
| O | 3.26615500  | -0.72336300 | 0.10023300  |
| H | 3.19279700  | -0.63826500 | 1.06955800  |
| F | -0.46350000 | 1.77046100  | -0.25949100 |
| F | 0.75355200  | -1.45918400 | -0.83302000 |
| F | 0.68263500  | -0.55093000 | 1.15711100  |
| H | -0.65896000 | 0.36219900  | -1.68353300 |

#### H<sub>4</sub>SiO<sub>4</sub>

|    |            |            |             |
|----|------------|------------|-------------|
| Si | 0.00004700 | 0.00003900 | -0.00001400 |
|----|------------|------------|-------------|

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 0.61495600  | -1.24191700 | 0.87071100  |
| H | 0.01534200  | -1.90775400 | 1.21014300  |
| O | -1.24162700 | -0.61549400 | -0.87070800 |
| H | -1.90797800 | -0.01622400 | -1.20976900 |
| O | -0.61575200 | 1.24219600  | 0.86975800  |
| H | -0.01655100 | 1.90783700  | 1.21026600  |
| O | 1.24250700  | 0.61521400  | -0.86979200 |
| H | 1.90785800  | 0.01561100  | -1.21019100 |

H<sub>6</sub>Si<sub>2</sub>O<sub>7</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | -1.45963300 | 0.00140200  | 0.10372500  |
| O  | 0.00003600  | -0.00008200 | 0.84351000  |
| O  | -1.68819200 | -1.42848600 | -0.65755400 |
| H  | -0.88849200 | -1.83247000 | -1.01520100 |
| O  | -1.33009200 | 1.27984000  | -0.93102000 |
| H  | -2.08877800 | 1.54502000  | -1.45353400 |
| Si | 1.45966000  | -0.00133400 | 0.10369200  |
| O  | 1.68877500  | 1.42909800  | -0.65638000 |
| H  | 0.88930700  | 1.83376100  | -1.01372700 |
| O  | 1.32986800  | -1.27875100 | -0.93233900 |
| H  | 2.08846600  | -1.54304700 | -1.45545000 |
| O  | 2.71803200  | -0.25890800 | 1.10143300  |
| H  | 3.11446000  | 0.49441600  | 1.54195900  |
| O  | -2.71807100 | 0.25719300  | 1.10185600  |
| H  | -3.11819500 | -0.49785000 | 1.53608000  |

H<sub>12</sub>Si<sub>6</sub>O<sub>18</sub>

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | -3.04190000 | 0.25896200  | -0.16989300 |
| Si | -1.74800900 | -2.50810100 | -0.14768800 |
| Si | 1.29599000  | -2.76451500 | -0.15581600 |
| Si | 3.04172700  | -0.25910600 | -0.16995400 |
| Si | 1.74817900  | 2.50803100  | -0.14822000 |
| Si | -1.29608300 | 2.76485800  | -0.15635800 |
| O  | -2.45461100 | -1.15448900 | -0.72198800 |
| O  | -0.23648100 | -2.72359000 | -0.71039900 |
| O  | 2.21418800  | -1.54925900 | -0.72809000 |
| O  | 2.45614800  | 1.15502300  | -0.72224400 |
| O  | 0.23624900  | 2.72043200  | -0.71156000 |
| O  | -2.21819500 | 1.55191200  | -0.72726300 |
| O  | -2.85310700 | 0.29990800  | 1.46978500  |
| H  | -2.58651100 | -0.53488900 | 1.88381000  |
| O  | -4.59391200 | 0.35516700  | -0.64529400 |
| H  | -4.96951900 | 1.20980400  | -0.86077200 |
| O  | -1.67032600 | -2.29419100 | 1.48676900  |
| H  | -0.80984200 | -2.47798000 | 1.89287600  |
| O  | -2.62258600 | -3.80653600 | -0.58654700 |
| H  | -3.53861000 | -3.69419400 | -0.84383700 |
| O  | 1.16197000  | -2.59542300 | 1.48078500  |
| H  | 1.76729900  | -1.95734300 | 1.88783800  |
| O  | 2.00764300  | -4.15406400 | -0.61162900 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.47048900  | -4.93153800 | -0.76985900 |
| O | 2.85424000  | -0.29945700 | 1.46973600  |
| H | 2.58681900  | 0.53536100  | 1.88315900  |
| O | 4.59355700  | -0.35986900 | -0.64493200 |
| H | 4.96275300  | -1.21512600 | -0.86853200 |
| O | 1.67017100  | 2.29518700  | 1.48627900  |
| H | 0.80896800  | 2.47766400  | 1.89171800  |
| O | 2.62148500  | 3.80736700  | -0.58719300 |
| H | 3.53662200  | 3.69500200  | -0.84772600 |
| O | -1.16168000 | 2.59583600  | 1.48027100  |
| H | -1.76825400 | 1.95886200  | 1.88725900  |
| O | -2.00412000 | 4.15632900  | -0.61239800 |
| H | -1.46392200 | 4.93030100  | -0.77763700 |

I-1

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | -3.14697100 | -0.44612200 | -0.04003400 |
| O  | -4.72120000 | -0.88292300 | 0.04271400  |
| H  | -5.38479700 | -0.24883500 | -0.23323000 |
| O  | -2.99264000 | 0.59654400  | -1.27849900 |
| H  | -2.25635600 | 1.22177800  | -1.25465400 |
| O  | -2.58412900 | 0.34907800  | 1.30310700  |
| H  | -2.28754200 | -0.20069200 | 2.03280300  |
| O  | -2.27838900 | -1.82909400 | -0.09438800 |
| H  | -2.62317900 | -2.57656300 | -0.58456900 |
| C  | 2.72910000  | -0.96944500 | 0.01835000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.21100400  | 0.47717300  | -0.14272000 |
| C | 0.70135400  | 0.68058900  | 0.07996600  |
| C | 0.30524200  | 2.15159600  | 0.13677600  |
| H | 0.70758000  | 2.57550500  | 1.06152900  |
| H | 0.75262200  | 2.66680600  | -0.71483200 |
| F | 4.00487900  | -1.01587500 | -0.35164400 |
| F | 2.64221100  | -1.35792500 | 1.28361100  |
| F | 2.03235200  | -1.80171900 | -0.74294100 |
| F | 2.51544900  | 0.89004400  | -1.38471700 |
| F | 2.88068800  | 1.24801900  | 0.73772800  |
| F | 0.36232200  | 0.06341500  | 1.24224000  |
| F | 0.03610400  | 0.05936400  | -0.91377500 |
| O | -1.08307200 | 2.28844500  | 0.03854600  |
| H | -1.52153000 | 1.82391400  | 0.77282800  |

I-2

|    |            |             |             |
|----|------------|-------------|-------------|
| Si | 2.93692100 | -0.48572700 | 0.00777600  |
| O  | 2.38253500 | -1.72743300 | -0.91375800 |
| H  | 1.62849200 | -1.56615300 | -1.48325100 |
| O  | 2.95615800 | 0.90191300  | -0.83592700 |
| H  | 2.35651600 | 1.62326100  | -0.60532900 |
| O  | 2.01368700 | -0.21281800 | 1.34996800  |
| H  | 2.10136200 | -0.83406900 | 2.07553500  |
| O  | 4.41193200 | -0.96808700 | 0.52480100  |
| H  | 4.91201800 | -1.56197200 | -0.03658800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -2.48606300 | -1.02942800 | -0.21701300 |
| C | -1.83360100 | 0.13029900  | 0.56829300  |
| C | -0.82120400 | 0.98166300  | -0.21928100 |
| C | -0.06694400 | 1.96806400  | 0.65630200  |
| H | -0.79576300 | 2.62019000  | 1.14705400  |
| H | 0.50943600  | 1.41344700  | 1.39497000  |
| F | -3.43050300 | -1.58391500 | 0.53344400  |
| F | -3.03718700 | -0.57814900 | -1.33697300 |
| F | -1.58522200 | -1.95525700 | -0.51884000 |
| F | -1.21437000 | -0.39976100 | 1.63670600  |
| F | -2.81621200 | 0.94073800  | 1.00172000  |
| F | -1.49275400 | 1.66187200  | -1.18341300 |
| F | 0.03412800  | 0.14652100  | -0.85628600 |
| O | 0.85030600  | 2.69233600  | -0.13003700 |
| H | 0.38004300  | 3.22616500  | -0.77866400 |

I-3

|    |            |             |             |
|----|------------|-------------|-------------|
| Si | 3.58283000 | -0.38436700 | -0.02935000 |
| O  | 3.81307900 | -1.99900300 | -0.00537700 |
| H  | 4.21365800 | -2.41554900 | 0.75893500  |
| O  | 3.09736200 | 0.08363600  | 1.45978600  |
| H  | 3.07069200 | 1.02686300  | 1.64319600  |
| O  | 4.88344200 | 0.52255500  | -0.41351700 |
| H  | 5.15738900 | 0.60133100  | -1.32835900 |
| O  | 2.44007100 | -0.10450200 | -1.18647800 |

|     |             |             |             |
|-----|-------------|-------------|-------------|
| H   | 1.84453300  | -0.81206200 | -1.44619200 |
| C   | -3.27135600 | -0.51770900 | -0.25181600 |
| C   | -1.99667300 | -0.17829600 | 0.55184100  |
| C   | -0.99603800 | 0.76656900  | -0.13991900 |
| C   | 0.12857500  | 1.21015800  | 0.78342500  |
| H   | -0.30382200 | 1.82040300  | 1.57690900  |
| H   | 0.58262100  | 0.31450500  | 1.22546200  |
| F   | -3.96130500 | -1.44643300 | 0.40324000  |
| F   | -4.03754600 | 0.55394000  | -0.39511400 |
| F   | -2.95304600 | -0.98969400 | -1.45141200 |
| F   | -1.36814200 | -1.33549000 | 0.82925800  |
| F   | -2.38699100 | 0.38297500  | 1.71197500  |
| F   | -1.67674000 | 1.82229400  | -0.62859900 |
| F   | -0.47204000 | 0.10026900  | -1.20545700 |
| O   | 1.05685200  | 1.98949400  | 0.08797100  |
| H   | 1.46410100  | 1.43312800  | -0.59433100 |
| I-4 |             |             |             |
| Si  | 3.08020000  | -0.46670600 | -0.04086900 |
| O   | 3.16543100  | 0.01514900  | 1.52401600  |
| H   | 3.74081100  | -0.46313800 | 2.12219500  |
| O   | 4.58111200  | -0.91743600 | -0.51333400 |
| H   | 4.66110400  | -1.55346700 | -1.22535400 |
| O   | 2.13973200  | -1.78513600 | -0.30482700 |
| H   | 1.19274900  | -1.70677300 | -0.17656100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 2.47590800  | 0.80958100  | -0.86576400 |
| H | 2.33202600  | 1.62801400  | -0.37599100 |
| C | -2.49106000 | -1.09631400 | 0.21756200  |
| C | -2.00388700 | 0.17680400  | -0.51099800 |
| C | -0.89234400 | 0.96349900  | 0.20824900  |
| C | -0.26346700 | 2.03179000  | -0.67081200 |
| H | 0.24481400  | 1.54793800  | -1.50365400 |
| H | -1.06252500 | 2.68096100  | -1.04418000 |
| F | -3.55793800 | -1.57573000 | -0.40837900 |
| F | -1.54184900 | -2.02721100 | 0.20835900  |
| F | -2.81512400 | -0.81914900 | 1.47307500  |
| F | -3.05868300 | 0.98861900  | -0.68739500 |
| F | -1.54623100 | -0.20172900 | -1.71949200 |
| F | 0.03361600  | 0.07487900  | 0.64129300  |
| F | -1.42573400 | 1.54457400  | 1.31097400  |
| O | 0.70902100  | 2.74291000  | 0.05092400  |
| H | 0.31061900  | 3.16685700  | 0.81765700  |

I-5

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | -3.00580700 | -0.27132500 | -0.02761600 |
| O  | -2.64474700 | 0.73691700  | -1.26892200 |
| H  | -2.97304200 | 1.63746100  | -1.24458500 |
| O  | -2.15210800 | 0.27579900  | 1.26409400  |
| H  | -2.35365400 | -0.08749500 | 2.12853400  |
| O  | -4.58372000 | -0.26226000 | 0.40403800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -5.19254900 | -0.83915100 | -0.05978700 |
| O | -2.64569400 | -1.79499100 | -0.48683500 |
| H | -1.79533800 | -1.98493900 | -0.88630500 |
| C | 2.23881300  | -1.33436200 | -0.08429800 |
| C | 1.09573700  | -0.33833200 | 0.21642900  |
| C | 1.43208400  | 1.14524800  | -0.03284600 |
| C | 0.19996600  | 2.03180300  | -0.07909100 |
| H | -0.37099200 | 1.77835300  | -0.97189300 |
| H | -0.41782900 | 1.81035400  | 0.79756600  |
| F | 1.89819700  | -2.53700100 | 0.37309000  |
| F | 2.45159200  | -1.42807000 | -1.38919800 |
| F | 3.35754300  | -0.95008800 | 0.51609600  |
| F | 0.73216200  | -0.50001200 | 1.49505100  |
| F | 0.05177600  | -0.68354700 | -0.57610600 |
| F | 2.14215500  | 1.22675500  | -1.17897800 |
| F | 2.24805800  | 1.55555500  | 0.97277000  |
| O | 0.57830500  | 3.37900600  | -0.16884300 |
| H | 1.03546600  | 3.62971900  | 0.63917800  |

I-6

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | -3.02484600 | -0.01274600 | 0.00837700  |
| O  | -2.20766000 | 1.35879000  | -0.39257800 |
| H  | -2.44480200 | 2.16112900  | 0.07727900  |
| O  | -2.82094700 | -0.21738600 | 1.61792400  |
| H  | -3.44118800 | -0.77405900 | 2.09103000  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -4.64176700 | 0.06489100  | -0.24468700 |
| H | -4.97735100 | -0.14369500 | -1.11780700 |
| O | -2.45233100 | -1.20363600 | -0.94824200 |
| H | -1.53130900 | -1.21621200 | -1.21351200 |
| C | 1.80524800  | -1.61582000 | 0.06922000  |
| C | 0.97401900  | -0.32533000 | -0.10624400 |
| C | 1.74592800  | 0.99924500  | 0.03027800  |
| C | 0.83024800  | 2.21089600  | 0.09633000  |
| H | 0.12025600  | 2.14991200  | -0.73484700 |
| H | 0.27312000  | 2.17028100  | 1.03212200  |
| F | 1.05274600  | -2.65694400 | -0.28098000 |
| F | 2.88136300  | -1.58698100 | -0.70582400 |
| F | 2.17692300  | -1.76686700 | 1.33052800  |
| F | -0.01775800 | -0.35655700 | 0.80037900  |
| F | 0.41393300  | -0.36969100 | -1.33741300 |
| F | 2.56400900  | 1.11570600  | -1.04756600 |
| F | 2.53309600  | 0.91328300  | 1.12241600  |
| O | 1.58788500  | 3.38862000  | 0.09499000  |
| H | 2.05619800  | 3.45936800  | -0.74215200 |

## II-1

|    |             |            |             |
|----|-------------|------------|-------------|
| Si | -2.20342800 | 1.57729800 | -0.27554400 |
| O  | -1.82028600 | 0.00921500 | -0.49523600 |
| O  | -3.79167700 | 1.85496100 | -0.48304600 |
| H  | -4.35325800 | 1.07466400 | -0.39149900 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| O  | -1.39453300 | 2.56732300  | -1.27895300 |
| H  | -0.43674500 | 2.52144700  | -1.29176200 |
| Si | -2.53343300 | -1.44976500 | -0.30709200 |
| O  | -2.41941900 | -2.41215100 | -1.61918900 |
| H  | -1.67052100 | -3.00757000 | -1.67796100 |
| O  | -4.12703400 | -1.04216200 | -0.14013600 |
| H  | -4.78883400 | -1.73556600 | -0.14966800 |
| O  | -1.89989000 | -2.22667500 | 0.97181300  |
| H  | -1.37140700 | -1.69611500 | 1.58897400  |
| O  | -1.76551900 | 1.86312100  | 1.31175300  |
| H  | -2.14524100 | 2.63003500  | 1.74608100  |
| C  | 0.96929100  | -0.13214000 | 2.18159000  |
| C  | 1.33712700  | -0.08978900 | 0.70368000  |
| H  | 1.45142800  | -1.00149100 | 2.63051000  |
| H  | 1.35882800  | 0.77548700  | 2.65333200  |
| C  | 2.85883200  | -0.04621600 | 0.47000300  |
| C  | 3.32133400  | -0.04251700 | -1.00392800 |
| O  | -0.41245200 | -0.26710200 | 2.34196000  |
| H  | -0.86644200 | 0.55807400  | 2.07903800  |
| F  | 4.64480200  | 0.06527700  | -1.03988800 |
| F  | 2.79296300  | 0.98598900  | -1.65714800 |
| F  | 2.96948800  | -1.16842100 | -1.60816300 |
| F  | 3.34644200  | 1.06432000  | 1.05371500  |
| F  | 3.41170400  | -1.11991500 | 1.06374100  |
| F  | 0.80178300  | 1.02281800  | 0.12884800  |

|   |            |             |            |
|---|------------|-------------|------------|
| F | 0.84006400 | -1.16258900 | 0.05779000 |
|---|------------|-------------|------------|

II-2

|    |             |            |             |
|----|-------------|------------|-------------|
| Si | -2.10033700 | 1.20631900 | -0.68302300 |
|----|-------------|------------|-------------|

|   |             |             |            |
|---|-------------|-------------|------------|
| O | -1.43268800 | -0.10954200 | 0.03846300 |
|---|-------------|-------------|------------|

|   |             |            |             |
|---|-------------|------------|-------------|
| O | -3.72165000 | 1.07276600 | -0.68747200 |
|---|-------------|------------|-------------|

|   |             |            |             |
|---|-------------|------------|-------------|
| H | -4.08210500 | 0.20716100 | -0.45662600 |
|---|-------------|------------|-------------|

|   |             |            |             |
|---|-------------|------------|-------------|
| O | -1.54826500 | 1.36115600 | -2.20499700 |
|---|-------------|------------|-------------|

|   |             |            |             |
|---|-------------|------------|-------------|
| H | -0.64351700 | 1.64537800 | -2.34688600 |
|---|-------------|------------|-------------|

|    |             |             |            |
|----|-------------|-------------|------------|
| Si | -1.85782600 | -1.60189400 | 0.53244900 |
|----|-------------|-------------|------------|

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -1.04211400 | -2.74788100 | -0.29723900 |
|---|-------------|-------------|-------------|

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.72376000 | -2.55427300 | -1.18086800 |
|---|-------------|-------------|-------------|

|   |             |             |            |
|---|-------------|-------------|------------|
| O | -3.48885700 | -1.62602100 | 0.27892700 |
|---|-------------|-------------|------------|

|   |             |             |            |
|---|-------------|-------------|------------|
| H | -4.00665000 | -2.35764400 | 0.61955400 |
|---|-------------|-------------|------------|

|   |             |             |            |
|---|-------------|-------------|------------|
| O | -1.59617900 | -1.87410500 | 2.11827000 |
|---|-------------|-------------|------------|

|   |             |             |            |
|---|-------------|-------------|------------|
| H | -0.76089600 | -2.27021100 | 2.37389300 |
|---|-------------|-------------|------------|

|   |             |            |            |
|---|-------------|------------|------------|
| O | -1.69043000 | 2.53558100 | 0.21697000 |
|---|-------------|------------|------------|

|   |             |            |            |
|---|-------------|------------|------------|
| H | -2.43285800 | 3.01197300 | 0.59792300 |
|---|-------------|------------|------------|

|   |            |            |            |
|---|------------|------------|------------|
| C | 1.01337500 | 1.66591800 | 1.64609600 |
|---|------------|------------|------------|

|   |            |            |            |
|---|------------|------------|------------|
| C | 1.70310700 | 1.14587700 | 0.39340500 |
|---|------------|------------|------------|

|   |            |            |            |
|---|------------|------------|------------|
| H | 0.10656100 | 1.07308900 | 1.80176200 |
|---|------------|------------|------------|

|   |            |            |            |
|---|------------|------------|------------|
| H | 1.69483200 | 1.51721200 | 2.48753100 |
|---|------------|------------|------------|

|   |            |             |            |
|---|------------|-------------|------------|
| C | 2.04953900 | -0.36034600 | 0.45622800 |
|---|------------|-------------|------------|

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 2.25493500 | -1.04526800 | -0.91251700 |
|---|------------|-------------|-------------|

|   |            |            |            |
|---|------------|------------|------------|
| O | 0.74873000 | 3.02601700 | 1.50789000 |
|---|------------|------------|------------|

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -0.06162300 | 3.10152100  | 0.98196800  |
| F | 2.71546100  | -2.27575400 | -0.72520300 |
| F | 3.12346600  | -0.36470300 | -1.64644900 |
| F | 1.10105800  | -1.12801700 | -1.57571800 |
| F | 3.17606300  | -0.51084200 | 1.16858900  |
| F | 1.06813700  | -1.03565000 | 1.09508100  |
| F | 2.84639000  | 1.81201500  | 0.15069100  |
| F | 0.89944500  | 1.34995200  | -0.69321000 |

### II-3

|    |            |             |             |
|----|------------|-------------|-------------|
| Si | 1.56508200 | -0.20131600 | 0.28847000  |
| O  | 3.08056200 | -0.51254000 | 0.83312300  |
| O  | 1.19469700 | -1.29148600 | -0.87258000 |
| H  | 1.94226200 | -1.59390000 | -1.40112700 |
| O  | 1.66363900 | 1.35321900  | -0.22033700 |
| H  | 0.88334300 | 1.88629200  | -0.42875200 |
| Si | 4.46831900 | -0.25638500 | 0.00656800  |
| O  | 4.66615900 | 1.34880100  | -0.24344400 |
| H  | 3.84126800 | 1.83881800  | -0.35339200 |
| O  | 4.21937300 | -1.10929200 | -1.38308800 |
| H  | 4.91060200 | -1.14248600 | -2.04607200 |
| O  | 5.80110800 | -0.83109900 | 0.74334600  |
| H  | 6.24976700 | -0.27111800 | 1.37851000  |
| O  | 0.42639300 | -0.29004400 | 1.46136000  |
| H  | 0.07355500 | -1.15450500 | 1.68241900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -1.56597000 | 2.06243800  | 0.57855800  |
| C | -2.20733200 | 0.98634100  | -0.28013700 |
| H | -2.35541300 | 2.64897600  | 1.05824200  |
| H | -0.94108700 | 1.58510800  | 1.33320500  |
| C | -3.14508900 | 0.05315900  | 0.50952900  |
| C | -3.52929900 | -1.25442500 | -0.21927600 |
| O | -0.72767800 | 2.85631900  | -0.23074500 |
| H | -1.24975300 | 3.29049400  | -0.91356400 |
| F | -4.51664800 | -1.84758600 | 0.44346700  |
| F | -2.49349800 | -2.07956500 | -0.26492800 |
| F | -3.93765700 | -0.99248000 | -1.45454000 |
| F | -2.55217300 | -0.28860200 | 1.66901700  |
| F | -4.27231700 | 0.72654800  | 0.79499600  |
| F | -1.26253600 | 0.24010800  | -0.88854100 |
| F | -2.93517600 | 1.57980000  | -1.26315000 |

#### II-4

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | -3.26736200 | -0.67107200 | -0.23602500 |
| O  | -3.11703500 | 0.96496200  | -0.30259000 |
| O  | -3.33128800 | -1.14147000 | 1.33394600  |
| H  | -2.82854800 | -0.58852500 | 1.94222800  |
| O  | -1.90563500 | -1.18210400 | -0.99585500 |
| H  | -1.52262200 | -2.04587800 | -0.79589900 |
| Si | -1.75019600 | 1.77502200  | 0.08274800  |
| O  | -0.59056500 | 1.50811600  | -1.03631900 |

|      |             |             |             |
|------|-------------|-------------|-------------|
| H    | -0.59387400 | 0.63058100  | -1.43907400 |
| O    | -1.36109100 | 1.13778400  | 1.56356100  |
| H    | -0.67712700 | 1.57323200  | 2.07695800  |
| O    | -1.94117500 | 3.38080600  | 0.25799300  |
| H    | -1.82964200 | 3.94425500  | -0.50919300 |
| O    | -4.58637000 | -1.22537700 | -1.00573400 |
| H    | -5.43176600 | -1.19879100 | -0.55573500 |
| C    | 0.50312900  | -1.75175100 | 0.89696600  |
| C    | 1.59790900  | -1.25279800 | -0.03126100 |
| H    | 0.95462600  | -1.99682900 | 1.86397900  |
| H    | -0.23809200 | -0.96349000 | 1.03353600  |
| C    | 2.39908400  | -0.07833000 | 0.56637700  |
| C    | 3.30202300  | 0.68367000  | -0.42852200 |
| O    | -0.14398000 | -2.85829000 | 0.31770200  |
| H    | 0.47741800  | -3.58639000 | 0.21669300  |
| F    | 4.06543800  | 1.53667600  | 0.24741400  |
| F    | 2.57555400  | 1.36013600  | -1.30055700 |
| F    | 4.08590200  | -0.17161600 | -1.07655100 |
| F    | 1.53905100  | 0.80968100  | 1.10356300  |
| F    | 3.17457500  | -0.55832400 | 1.55433500  |
| F    | 1.08856000  | -0.87469500 | -1.22318200 |
| F    | 2.46421600  | -2.26892800 | -0.27953600 |
| II-5 |             |             |             |
| Si   | -1.98805700 | 0.73069000  | 0.38769800  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| O  | -2.97233100 | -0.53835600 | 0.04490900  |
| O  | -2.88574000 | 2.03315700  | 0.75368500  |
| H  | -3.79461800 | 2.03856000  | 0.42954500  |
| O  | -1.03625600 | 1.05984900  | -0.90954900 |
| H  | -0.44824200 | 0.36844600  | -1.23044200 |
| Si | -4.54998200 | -0.85212000 | -0.20309300 |
| O  | -4.75968300 | -1.70025400 | -1.58331600 |
| H  | -4.24097400 | -1.49728300 | -2.36303200 |
| O  | -5.23322600 | 0.64821300  | -0.21637600 |
| H  | -6.18856100 | 0.73174100  | -0.20504800 |
| O  | -5.25555400 | -1.71603100 | 0.98385400  |
| H  | -5.29472700 | -2.67054800 | 0.90535100  |
| O  | -0.95494900 | 0.36163300  | 1.59839200  |
| H  | -1.29228800 | 0.13621100  | 2.46665300  |
| C  | 1.78468600  | 1.94060500  | 0.29726200  |
| C  | 2.49303900  | 0.80149700  | -0.42534500 |
| H  | 1.07132800  | 1.50124900  | 1.00405600  |
| H  | 2.54343900  | 2.49562100  | 0.85118300  |
| C  | 3.09259700  | -0.23959600 | 0.54015200  |
| C  | 4.04909000  | -1.27333900 | -0.09524700 |
| O  | 1.18502900  | 2.80190700  | -0.62177800 |
| H  | 0.31878900  | 2.44031500  | -0.85567200 |
| F  | 4.33702300  | -2.20970400 | 0.80428500  |
| F  | 5.17968600  | -0.69857100 | -0.47973500 |
| F  | 3.47729400  | -1.85383900 | -1.14479300 |

|   |            |             |             |
|---|------------|-------------|-------------|
| F | 3.78380400 | 0.40742800  | 1.49930400  |
| F | 2.08651300 | -0.91404000 | 1.12111500  |
| F | 3.48052300 | 1.26250800  | -1.21851300 |
| F | 1.61555900 | 0.13730400  | -1.23572800 |

## II-6

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | -1.47322100 | 0.11113800  | -0.19448000 |
| O  | -2.96411400 | 0.44022000  | -0.78194000 |
| O  | -1.22098600 | -1.50396300 | -0.16902400 |
| H  | -2.01178400 | -2.03113800 | -0.00215200 |
| O  | -1.52335100 | 0.77095700  | 1.31832900  |
| H  | -0.81218200 | 0.56660200  | 1.92846800  |
| Si | -4.38825000 | 0.08914500  | -0.05581600 |
| O  | -4.58353200 | 1.04544500  | 1.25726300  |
| H  | -3.77004900 | 1.26963000  | 1.72377500  |
| O  | -4.20940600 | -1.50846600 | 0.31528900  |
| H  | -4.94652400 | -1.99337300 | 0.68983500  |
| O  | -5.69123100 | 0.26339700  | -1.01291300 |
| H  | -6.11911300 | 1.11990400  | -1.05674900 |
| O  | -0.27789400 | 0.83215200  | -1.03446400 |
| H  | 0.06393000  | 0.41997400  | -1.83095100 |
| C  | 2.33184700  | 2.20112500  | 0.40090100  |
| C  | 2.90209500  | 0.91715100  | -0.18022700 |
| H  | 1.26017300  | 2.21177300  | 0.20269900  |
| H  | 2.50987900  | 2.19250000  | 1.48375500  |

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 2.49946300 | -0.34494900 | 0.62302400  |
| C | 2.52945400 | -1.66181200 | -0.18235300 |
| O | 2.90150400 | 3.31337500  | -0.22773200 |
| H | 3.85139300 | 3.31023000  | -0.07533000 |
| F | 2.33907200 | -2.68584900 | 0.63957600  |
| F | 3.71417600 | -1.79635000 | -0.77063300 |
| F | 1.58004800 | -1.67290800 | -1.10573600 |
| F | 3.32767600 | -0.47353700 | 1.67058800  |
| F | 1.24812800 | -0.19289700 | 1.11492800  |
| F | 4.25882300 | 0.98070900  | -0.17238600 |
| F | 2.53316600 | 0.75593600  | -1.47030700 |

### III-1

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | 4.83116300  | -1.46513200 | 0.59505600  |
| Si | 4.79592600  | 1.58991200  | 0.53652400  |
| Si | 2.29514900  | 3.12483200  | -0.32211400 |
| Si | -0.07609900 | 1.41298500  | -1.16881700 |
| Si | -0.06756600 | -1.60902900 | -1.18980900 |
| Si | 2.39937800  | -3.12081200 | -0.22921900 |
| O  | 5.02760000  | 0.05362500  | 0.04266700  |
| O  | 3.76050700  | 2.41535100  | -0.41035600 |
| O  | 1.19481600  | 2.42066500  | -1.29788800 |
| O  | 0.26428000  | -0.08342900 | -1.69325700 |
| O  | 1.28069200  | -2.52061100 | -1.24748500 |
| O  | 3.83690300  | -2.36239300 | -0.33244400 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 4.09182700  | -1.39120600 | 2.06927700  |
| H | 4.06901600  | -0.51658200 | 2.48522000  |
| O | 6.30640000  | -2.14910700 | 0.64218600  |
| H | 6.39793000  | -3.08817600 | 0.47608600  |
| O | 4.13760800  | 1.46197600  | 2.04537400  |
| H | 3.35748600  | 2.01003100  | 2.21434000  |
| O | 6.20779200  | 2.39636700  | 0.51275000  |
| H | 7.03084600  | 1.91367600  | 0.59892700  |
| O | 1.80460800  | 2.92379500  | 1.24058300  |
| H | 0.92011400  | 2.55184100  | 1.36798000  |
| O | 2.41333500  | 4.68228300  | -0.76727200 |
| H | 3.26931300  | 5.11225500  | -0.75620600 |
| O | -0.47559800 | 1.34534000  | 0.42980800  |
| H | -0.60703500 | 0.43889100  | 0.75710400  |
| O | -1.31886100 | 2.05006100  | -2.03863600 |
| H | -1.17039900 | 2.86171600  | -2.52761500 |
| O | -0.52075400 | -1.44575000 | 0.40324600  |
| H | 0.01283100  | -1.96869000 | 1.02308000  |
| O | -1.17854800 | -2.34712000 | -2.10846800 |
| H | -2.02421400 | -1.88733200 | -2.15898400 |
| O | 1.78339400  | -2.85916000 | 1.28220800  |
| H | 2.40416500  | -2.49364500 | 1.93059000  |
| O | 2.66533900  | -4.68946100 | -0.56316400 |
| H | 1.97122900  | -5.20950600 | -0.97024400 |
| C | -7.20850600 | -0.04856100 | 0.88878700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -5.68972100 | 0.21068800  | 1.00017300  |
| C | -4.86758000 | -0.05119200 | -0.27555200 |
| C | -3.36953300 | 0.00767200  | -0.02433600 |
| H | -3.12481400 | 0.95588300  | 0.46559800  |
| H | -3.07888900 | -0.82025200 | 0.62308300  |
| F | -7.80144600 | 0.37583000  | 1.99993400  |
| F | -7.71777100 | 0.60810800  | -0.14568800 |
| F | -7.45356600 | -1.34345400 | 0.74648500  |
| F | -5.51404400 | 1.49330200  | 1.36217900  |
| F | -5.21585300 | -0.57805300 | 1.98448600  |
| F | -5.20959500 | 0.88015900  | -1.19658100 |
| F | -5.22017300 | -1.25782000 | -0.76985900 |
| O | -2.68495700 | -0.14213600 | -1.24187100 |
| H | -2.68588000 | 0.69428100  | -1.73273700 |

### III-2

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | 2.94789600  | 1.60685600  | -0.93556300 |
| Si | 0.68481100  | 3.06774800  | 0.36986800  |
| Si | -1.23542900 | 1.43390800  | 2.04387800  |
| Si | -0.42611400 | -1.46570100 | 1.58023500  |
| Si | 1.69643100  | -2.93403300 | 0.18519000  |
| Si | 3.83996500  | -1.31068500 | -1.02847700 |
| O  | 1.38837100  | 1.93170200  | -0.58426800 |
| O  | -0.76697600 | 2.47510300  | 0.86726600  |
| O  | -1.26306100 | -0.08477100 | 1.42909700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 0.64531200  | -1.67792800 | 0.38012200  |
| O | 2.75969400  | -2.53595300 | -0.98497400 |
| O | 3.17409800  | 0.10080700  | -1.49937000 |
| O | 3.83400300  | 1.66174400  | 0.45965600  |
| H | 3.56719500  | 2.32936000  | 1.10517300  |
| O | 3.39503200  | 2.71793100  | -2.03872900 |
| H | 4.23617600  | 2.64262600  | -2.49147400 |
| O | 1.65956800  | 3.31332300  | 1.66539500  |
| H | 1.33164400  | 2.96059600  | 2.50428700  |
| O | 0.48262800  | 4.45783600  | -0.43828600 |
| H | 0.21685200  | 4.38914600  | -1.36044500 |
| O | -0.07907800 | 1.53461300  | 3.20387200  |
| H | 0.20475700  | 0.69598900  | 3.59400500  |
| O | -2.68589500 | 1.84036100  | 2.64189500  |
| H | -3.46066100 | 1.77419900  | 2.07977800  |
| O | 0.35022600  | -1.31609700 | 3.03161900  |
| H | 1.08031300  | -1.93062400 | 3.17770600  |
| O | -1.37524900 | -2.80045200 | 1.50788400  |
| H | -2.14262100 | -2.89108500 | 2.07565500  |
| O | 2.47990700  | -3.10751500 | 1.62484100  |
| H | 3.30219900  | -2.60139000 | 1.68442500  |
| O | 0.88652200  | -4.28238300 | -0.20409700 |
| H | -0.02946300 | -4.34390600 | 0.08342200  |
| O | 4.34077500  | -1.14644400 | 0.53566800  |
| H | 4.46984400  | -0.23719300 | 0.84234100  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 5.02414300  | -1.65519800 | -2.08595400 |
| H | 5.29809900  | -2.56418600 | -2.21406600 |
| C | -4.12334900 | -1.40343000 | -0.62322900 |
| C | -3.00674500 | -0.77881000 | -1.48967700 |
| C | -2.94489300 | 0.76674200  | -1.45818100 |
| C | -1.59148300 | 1.33218500  | -1.85567800 |
| H | -0.82391900 | 0.89882200  | -1.20773500 |
| H | -1.38993300 | 1.04833100  | -2.88995300 |
| F | -4.20847000 | -2.70227100 | -0.88393200 |
| F | -3.85809700 | -1.25330700 | 0.67230700  |
| F | -5.29117700 | -0.83252200 | -0.89176200 |
| F | -1.83636100 | -1.29706200 | -1.07676300 |
| F | -3.20515600 | -1.16369300 | -2.76058500 |
| F | -3.25183600 | 1.18203700  | -0.18680300 |
| F | -3.92545900 | 1.23468100  | -2.25022100 |
| O | -1.62388000 | 2.73288600  | -1.78343300 |
| H | -1.78757000 | 2.96859200  | -0.86019300 |

### III-3

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | 4.36886800  | -1.89721000 | 0.10375900  |
| Si | 4.76384000  | 1.12632600  | 0.29541800  |
| Si | 2.39087800  | 2.99843900  | -0.15410000 |
| Si | -0.36598600 | 1.81100800  | -0.67791800 |
| Si | -0.78602200 | -1.19979800 | -0.81147800 |
| Si | 1.60353400  | -3.06289200 | -0.45806300 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 4.75115800  | -0.37712600 | -0.33520500 |
| O | 3.74096200  | 2.14114500  | -0.46321800 |
| O | 1.09401400  | 2.46500000  | -0.98432500 |
| O | -0.52029800 | 0.33240300  | -1.32317000 |
| O | 0.44652400  | -2.18939100 | -1.20189700 |
| O | 3.10617700  | -2.50019200 | -0.73440200 |
| O | 3.87880000  | -1.87684100 | 1.67958600  |
| H | 4.00975300  | -1.03995200 | 2.15001600  |
| O | 5.68373700  | -2.81989000 | -0.14845300 |
| H | 5.57469000  | -3.72549700 | -0.44121200 |
| O | 4.25653600  | 0.94640200  | 1.85546600  |
| H | 3.57432500  | 1.56832500  | 2.14985600  |
| O | 6.25497300  | 1.76121600  | 0.16951900  |
| H | 7.01091000  | 1.18118700  | 0.07134500  |
| O | 2.10793700  | 2.77822700  | 1.45681100  |
| H | 1.19256600  | 2.59565300  | 1.71404000  |
| O | 2.61071900  | 4.55102900  | -0.58269400 |
| H | 3.48895500  | 4.93251100  | -0.55130600 |
| O | -0.53095200 | 1.74308600  | 0.95240900  |
| H | -0.85057300 | 0.89763900  | 1.30441700  |
| O | -1.49609900 | 2.82144100  | -1.32487200 |
| H | -1.17789100 | 3.50941600  | -1.91506000 |
| O | -0.87586900 | -1.08736600 | 0.83236600  |
| H | -0.34565900 | -1.73393500 | 1.32203200  |
| O | -2.11031300 | -1.81199100 | -1.52298800 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.89849800 | -1.27121000 | -1.60427200 |
| O | 1.28102900  | -2.91912900 | 1.15521400  |
| H | 2.04450500  | -2.71697400 | 1.71702300  |
| O | 1.57224300  | -4.59703000 | -0.99708400 |
| H | 0.74180400  | -4.98276400 | -1.27893200 |
| C | -5.18015300 | -1.43219600 | 0.78921000  |
| C | -5.26559100 | -0.18285400 | -0.11559600 |
| C | -4.37861600 | 1.00449900  | 0.31198400  |
| C | -4.75077100 | 2.31744800  | -0.36226500 |
| H | -4.74842600 | 2.14772600  | -1.44660800 |
| H | -5.76155500 | 2.58169500  | -0.04899800 |
| F | -5.81058800 | -2.44217400 | 0.19914400  |
| F | -3.91077700 | -1.76723200 | 0.97775600  |
| F | -5.75537600 | -1.19976600 | 1.95967500  |
| F | -4.89565700 | -0.55602100 | -1.36384500 |
| F | -6.54826300 | 0.20985200  | -0.16006900 |
| F | -3.09370300 | 0.67211600  | -0.02141900 |
| F | -4.42540300 | 1.10903700  | 1.65186300  |
| O | -3.88555900 | 3.32939200  | 0.03605900  |
| H | -3.02357400 | 3.19718200  | -0.38993500 |

#### III-4

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | 2.65698700  | 2.73597200  | -0.24265300 |
| Si | -0.07891800 | 2.29717100  | 1.03002000  |
| Si | -1.00318200 | -0.50708600 | 1.69212100  |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | 0.72584900  | -2.82765300 | 0.71389200  |
| Si | 3.35635900  | -2.38421000 | -0.76629800 |
| Si | 4.44556900  | 0.43573300  | -1.16441700 |
| O  | 1.05535400  | 2.46151900  | -0.12841700 |
| O  | -0.93307000 | 0.92316300  | 0.88500200  |
| O  | -0.47636700 | -1.72885700 | 0.74949400  |
| O  | 1.75864900  | -2.60908600 | -0.52507700 |
| O  | 3.68922800  | -0.97050100 | -1.50215700 |
| O  | 3.41442400  | 1.69875800  | -1.23869300 |
| O  | 3.34541800  | 2.46901500  | 1.23459800  |
| H  | 2.76078000  | 2.56700500  | 1.99906500  |
| O  | 2.81314100  | 4.26523600  | -0.77626000 |
| H  | 3.62913100  | 4.54885800  | -1.19059100 |
| O  | 0.72447300  | 2.33238200  | 2.46389900  |
| H  | 0.59068500  | 1.55826100  | 3.03379200  |
| O  | -1.16462700 | 3.51762100  | 0.86513300  |
| H  | -0.82728800 | 4.39392400  | 0.66041200  |
| O  | 0.03921300  | -0.35004700 | 2.95986500  |
| H  | 0.67206800  | -1.07645100 | 3.07062700  |
| O  | -2.50471600 | -0.79135500 | 2.22365600  |
| H  | -3.25046400 | -0.31037000 | 1.85750500  |
| O  | 1.54977300  | -2.59432600 | 2.12720300  |
| H  | 2.51529800  | -2.64223200 | 2.05833500  |
| O  | 0.11390900  | -4.32532900 | 0.54957500  |
| H  | -0.73783300 | -4.53949900 | 0.93224800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 4.02170200  | -2.35614400 | 0.74500100  |
| H | 4.61691000  | -1.61543400 | 0.93271100  |
| O | 3.94369400  | -3.56796900 | -1.71252400 |
| H | 3.51837400  | -4.42636700 | -1.71680200 |
| O | 5.00178800  | 0.31180100  | 0.38061400  |
| H | 4.72170700  | 1.01122900  | 0.98941400  |
| O | 5.66070000  | 0.66466300  | -2.21717900 |
| H | 5.76538700  | 0.06163500  | -2.95413800 |
| C | -5.00640300 | -1.37806000 | -0.69274600 |
| C | -3.96719800 | -0.36468300 | -1.22002600 |
| C | -4.15688900 | 1.09196000  | -0.75834400 |
| C | -3.21072600 | 2.06268400  | -1.45126800 |
| H | -2.19400800 | 1.66487100  | -1.35363700 |
| H | -3.48301000 | 2.09658300  | -2.50747300 |
| F | -4.62923800 | -2.60672700 | -1.02640000 |
| F | -5.08375000 | -1.30320000 | 0.63534900  |
| F | -6.20253700 | -1.14506200 | -1.20935100 |
| F | -2.75389300 | -0.78342900 | -0.81007300 |
| F | -4.00197000 | -0.40418000 | -2.56359900 |
| F | -3.93944000 | 1.12406700  | 0.58901000  |
| F | -5.44433400 | 1.43576200  | -0.95572800 |
| O | -3.35404100 | 3.33513700  | -0.90381100 |
| H | -2.78043200 | 3.39707600  | -0.12675000 |

III-5

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | 0.73442200  | 3.00318700  | 0.68356900  |
| Si | -0.90942300 | 0.66893700  | 1.76557600  |
| Si | -0.17621600 | -2.24992700 | 1.31045300  |
| Si | 2.40880200  | -2.84839600 | -0.19293200 |
| Si | 4.13098200  | -0.56053500 | -1.23997800 |
| Si | 3.30026100  | 2.34753000  | -0.83539600 |
| O  | -0.43927100 | 1.88658700  | 0.79299000  |
| O  | -0.79869500 | -0.76669300 | 0.98357500  |
| O  | 0.81024000  | -2.66829300 | 0.06951200  |
| O  | 3.01193900  | -1.74936800 | -1.22937900 |
| O  | 3.49710600  | 0.90083500  | -1.56584000 |
| O  | 1.74169400  | 2.72289600  | -0.57546600 |
| O  | 1.68910900  | 2.89928800  | 2.02694700  |
| H  | 1.36185400  | 2.31209400  | 2.72483300  |
| O  | 0.04050000  | 4.45904500  | 0.49361200  |
| H  | 0.47011500  | 5.11639900  | -0.05470300 |
| O  | 0.16593300  | 0.71139200  | 3.01386400  |
| H  | 0.39920800  | -0.13953100 | 3.40825400  |
| O  | -2.42497800 | 0.90098500  | 2.29984400  |
| H  | -3.14704300 | 0.40073300  | 1.91495500  |
| O  | 0.68984100  | -2.11943700 | 2.69849200  |
| H  | 1.62424900  | -2.36459400 | 2.62228100  |
| O  | -1.35960800 | -3.33925700 | 1.48882300  |
| H  | -1.95271900 | -3.47904100 | 0.73768200  |
| O  | 3.11001900  | -2.63370100 | 1.28719700  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 3.87996500  | -2.04474700 | 1.30219300  |
| O | 2.71121600  | -4.30671900 | -0.85077800 |
| H | 2.25084100  | -5.08034400 | -0.52350600 |
| O | 4.75084300  | -0.53872200 | 0.28989400  |
| H | 4.80913000  | 0.33748200  | 0.70180700  |
| O | 5.24491800  | -0.86856300 | -2.38456200 |
| H | 5.40615100  | -1.77262900 | -2.65701700 |
| O | 4.05915700  | 2.19020200  | 0.62340900  |
| H | 3.56259400  | 2.52756700  | 1.38489100  |
| O | 3.92467500  | 3.52219700  | -1.77186700 |
| H | 4.66763500  | 3.32814400  | -2.34460900 |
| C | -4.96040000 | 1.23083000  | -0.74548900 |
| C | -3.77396200 | 0.38201300  | -1.25401000 |
| C | -3.78139900 | -1.09982700 | -0.84127200 |
| C | -2.64586800 | -1.89692000 | -1.46266300 |
| H | -2.72690000 | -1.83394100 | -2.55065300 |
| H | -1.69592600 | -1.46900000 | -1.14078400 |
| F | -4.78146900 | 2.49071000  | -1.11144300 |
| F | -6.10317800 | 0.79292800  | -1.25611900 |
| F | -5.02829900 | 1.17204600  | 0.58219200  |
| F | -3.76460700 | 0.45219900  | -2.59728800 |
| F | -2.64424700 | 0.93377700  | -0.78139300 |
| F | -4.96587600 | -1.65065700 | -1.20702800 |
| F | -3.71899000 | -1.16142300 | 0.51067000  |
| O | -2.70309700 | -3.22723700 | -1.00246500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -3.49531600 | -3.65604000 | -1.34187600 |
|---|-------------|-------------|-------------|

### III-6

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | 4.51640300  | -1.42325300 | 0.37903800  |
| Si | 4.39752200  | 1.63038400  | 0.40237800  |
| Si | 1.82921900  | 3.09533700  | -0.37956200 |
| Si | -0.66591200 | 1.49361500  | -1.09212000 |
| Si | -0.53967700 | -1.55005400 | -1.06183700 |
| Si | 2.03665000  | -3.03169300 | -0.38259600 |
| O  | 4.68711500  | 0.11513700  | -0.12516100 |
| O  | 3.30923900  | 2.42543400  | -0.50912300 |
| O  | 0.71180600  | 2.34329400  | -1.29258500 |
| O  | -0.49203600 | -0.02671800 | -1.64637800 |
| O  | 0.86234700  | -2.34567600 | -1.28305700 |
| O  | 3.47381300  | -2.28240500 | -0.53485000 |
| O  | 3.85520100  | -1.40406100 | 1.89125100  |
| H  | 3.80786900  | -0.53563600 | 2.31868400  |
| O  | 5.98661600  | -2.11573600 | 0.32781900  |
| H  | 6.06721500  | -3.03949500 | 0.08747300  |
| O  | 3.77322200  | 1.44598200  | 1.91970500  |
| H  | 2.98431600  | 1.97244600  | 2.11661000  |
| O  | 5.77413100  | 2.49514300  | 0.36937400  |
| H  | 6.61833100  | 2.04400200  | 0.40736300  |
| O  | 1.41735000  | 2.90873600  | 1.20960500  |
| H  | 0.51776600  | 2.59734900  | 1.38350300  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.88192200  | 4.64507100  | -0.86588500 |
| H | 2.69742600  | 5.14065700  | -0.78085000 |
| O | -0.99113300 | 1.45640700  | 0.52368400  |
| H | -1.07079100 | 0.56352800  | 0.89868900  |
| O | -1.88389800 | 2.25774300  | -1.86243600 |
| H | -1.67393900 | 2.85299400  | -2.58435000 |
| O | -0.78952400 | -1.36461000 | 0.56218100  |
| H | -0.24466000 | -1.92698400 | 1.13381500  |
| O | -1.68861400 | -2.42299300 | -1.81071900 |
| H | -2.52863300 | -2.01773400 | -2.03300800 |
| O | 1.52996500  | -2.87629000 | 1.18157400  |
| H | 2.18897800  | -2.52703500 | 1.80074300  |
| O | 2.25399700  | -4.57537500 | -0.84445900 |
| H | 1.51971900  | -5.06518100 | -1.21697800 |
| C | -4.54772900 | -1.72657700 | 0.49425500  |
| C | -3.97549600 | -0.28979700 | 0.53828600  |
| C | -5.00832200 | 0.84997600  | 0.48670100  |
| C | -4.36926000 | 2.21237700  | 0.26746500  |
| H | -3.55471700 | 2.32936600  | 0.99167300  |
| H | -3.94020300 | 2.24800300  | -0.73346900 |
| F | -3.60886300 | -2.58994900 | 0.85286100  |
| F | -5.58168000 | -1.84586000 | 1.31517400  |
| F | -4.93727800 | -2.01973800 | -0.74418700 |
| F | -3.24054000 | -0.15684400 | 1.65085600  |
| F | -3.15935600 | -0.16300600 | -0.53942500 |

|   |             |            |             |
|---|-------------|------------|-------------|
| F | -5.67891700 | 0.85027900 | 1.66829600  |
| F | -5.90223500 | 0.55711100 | -0.48151900 |
| O | -5.34057800 | 3.21705700 | 0.36634700  |
| H | -5.69040800 | 3.23009700 | 1.26206400  |

#### ER-I-1

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | -3.14968500 | -0.26577900 | -0.26720100 |
| O  | -4.74417600 | -0.57878200 | -0.42008900 |
| H  | -5.31814200 | 0.11591900  | -0.74692100 |
| O  | -2.76172700 | 0.83462300  | -1.40081000 |
| H  | -2.00478700 | 1.41547100  | -1.25603500 |
| O  | -2.68798100 | 0.33429200  | 1.19832500  |
| H  | -2.25146500 | -0.28519300 | 1.80267400  |
| O  | -2.39532800 | -1.73215300 | -0.37361800 |
| H  | -2.74815800 | -2.37698100 | -0.99071100 |
| C  | 2.86808500  | -0.73208700 | -0.51342300 |
| C  | 2.15890100  | 0.25823600  | 0.43648400  |
| C  | 0.83680400  | 0.85423000  | -0.07737600 |
| C  | 0.29995700  | 1.96491800  | 0.81640400  |
| H  | 0.30514900  | 1.60638700  | 1.85098700  |
| H  | 0.97216400  | 2.82000600  | 0.73305600  |
| F  | 3.90032800  | -1.27635100 | 0.12131000  |
| F  | 2.03526100  | -1.69769900 | -0.88354700 |
| F  | 3.31688200  | -0.10752100 | -1.59330100 |
| F  | 3.01557700  | 1.26823500  | 0.68466400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| F | 1.90762700  | -0.38390800 | 1.58906900  |
| F | -0.06992600 | -0.15532900 | -0.15154800 |
| F | 1.02256900  | 1.30497100  | -1.33695400 |
| O | -0.97804300 | 2.33776200  | 0.38469000  |
| H | -1.63303400 | 1.80617900  | 0.86870800  |
| O | -0.83559400 | -1.69738100 | 1.93452500  |
| H | -1.14068400 | -2.01113800 | 1.05509700  |

#### TS-I-1

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | -3.14137300 | -0.43126700 | -0.01313300 |
| O  | -4.71854700 | -0.82992100 | 0.14633600  |
| H  | -5.38326700 | -0.20625900 | -0.15030600 |
| O  | -2.99909500 | 0.48795400  | -1.34857000 |
| H  | -2.25488300 | 1.09682600  | -1.41815100 |
| O  | -2.53382200 | 0.48568100  | 1.22775100  |
| H  | -2.25863900 | 0.02976900  | 2.02720500  |
| O  | -2.29561800 | -1.82716700 | 0.03754600  |
| H  | -2.66576900 | -2.61108800 | -0.37066800 |
| C  | 2.76513900  | -0.93487900 | -0.05784300 |
| C  | 2.23530900  | 0.50567400  | -0.23722700 |
| C  | 0.72365400  | 0.70041200  | -0.02119500 |
| C  | 0.31478900  | 2.16890200  | -0.02227300 |
| H  | 0.70511700  | 2.63215100  | 0.98200200  |
| H  | 0.80472100  | 2.70358800  | -0.83746800 |
| F  | 4.04460700  | -0.97069400 | -0.41365500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| F | 2.66814500  | -1.31009100 | 1.21082200  |
| F | 2.08427500  | -1.77996500 | -0.81799500 |
| F | 2.54664200  | 0.91336900  | -1.47672600 |
| F | 2.89525900  | 1.28878400  | 0.64603400  |
| F | 0.39094800  | 0.11497400  | 1.15499500  |
| F | 0.06642900  | 0.04184500  | -0.99908400 |
| O | -1.04836200 | 2.32480200  | -0.12318100 |
| H | -1.50544900 | 1.86160900  | 0.60620600  |
| O | 1.02876000  | 2.97456500  | 2.31233600  |
| H | 1.81463500  | 2.41752000  | 2.43995700  |

#### EP-I-1

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | 3.88541200  | -0.75326500 | -0.03282500 |
| O  | 4.48704900  | 0.50573000  | -0.85878100 |
| H  | 4.21269600  | 1.41557700  | -0.62594700 |
| O  | 4.30450900  | -0.60755300 | 1.54808000  |
| H  | 3.90023100  | -1.19298300 | 2.19310800  |
| O  | 2.20475200  | -0.82458400 | -0.06229600 |
| H  | 1.80779600  | -1.43243300 | -0.69503400 |
| O  | 4.35441800  | -2.15766800 | -0.74840200 |
| H  | 5.21371700  | -2.19799100 | -1.17461800 |
| C  | -3.74980300 | -0.67197100 | -0.05249600 |
| C  | -2.75260800 | 0.52329800  | -0.18835500 |
| C  | -1.28133800 | 0.25608500  | 0.24028900  |
| C  | -0.48018200 | 1.48973900  | 0.29768400  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 2.37681400  | 2.67612900  | 0.02957900  |
| H | -0.92936900 | 2.44114100  | 0.53330600  |
| F | -4.91283300 | -0.33069800 | -0.62459300 |
| F | -3.27805000 | -1.76143200 | -0.66857500 |
| F | -3.98294900 | -0.96335700 | 1.22892400  |
| F | -3.24705900 | 1.54362600  | 0.56120400  |
| F | -2.75886100 | 0.91320000  | -1.48494200 |
| F | -0.72647200 | -0.64346000 | -0.64589900 |
| F | -1.31153700 | -0.42596500 | 1.45302600  |
| O | 0.85833800  | 1.43102700  | 0.35932700  |
| H | 1.23828400  | 0.52434900  | 0.20036500  |
| O | 3.29825500  | 2.91111100  | -0.16432300 |
| H | 3.26892800  | 3.67727600  | -0.74507100 |

P-I-1

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | -3.36269800 | -0.39266900 | -0.04923000 |
| O  | -4.87860200 | -0.70146200 | 0.47348800  |
| H  | -5.50540700 | 0.02168500  | 0.52740700  |
| O  | -3.45484000 | 0.84157900  | -1.10959600 |
| H  | -2.70337200 | 1.42842200  | -1.23707600 |
| O  | -2.31669600 | 0.12214100  | 1.13114000  |
| H  | -1.83768500 | -0.54053500 | 1.63685000  |
| O  | -2.74661500 | -1.80054700 | -0.59017300 |
| H  | -3.32447100 | -2.43449800 | -1.01703100 |
| C  | 2.89612300  | -0.89935000 | -0.01333100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.30227900  | 0.52519800  | -0.11733900 |
| C | 0.78240500  | 0.61768100  | 0.11802200  |
| C | 0.23011500  | 1.92339900  | -0.28149700 |
| H | 0.69596300  | 2.53211700  | -1.03943500 |
| F | 4.22248500  | -0.81462200 | -0.01273800 |
| F | 2.50543400  | -1.48620400 | 1.11225200  |
| F | 2.52208000  | -1.64240500 | -1.04444000 |
| F | 2.58721500  | 0.98828400  | -1.34981600 |
| F | 2.92612600  | 1.30026600  | 0.78226600  |
| F | 0.54064400  | 0.37888800  | 1.44236900  |
| F | 0.18731000  | -0.43185900 | -0.53681900 |
| O | -1.04379600 | 2.20091000  | 0.01789000  |
| H | -1.41004700 | 1.55648800  | 0.66373000  |

#### ER-II-1

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | -2.15464000 | 1.47927400  | -0.29224200 |
| O  | -1.88484600 | -0.11602000 | -0.46810000 |
| O  | -3.73794200 | 1.78093900  | -0.51398600 |
| H  | -4.32432200 | 1.02254700  | -0.38981700 |
| O  | -1.27215700 | 2.39769500  | -1.33757400 |
| H  | -1.60804400 | 2.52835100  | -2.22677500 |
| Si | -2.65022500 | -1.54399500 | -0.24900400 |
| O  | -2.56315200 | -2.53305900 | -1.54361700 |
| H  | -1.84579100 | -3.16847500 | -1.57235500 |
| O  | -4.22700500 | -1.06953200 | -0.10122800 |

|         |             |             |             |
|---------|-------------|-------------|-------------|
| H       | -4.91822000 | -1.73292900 | -0.07097000 |
| O       | -2.05215000 | -2.30809000 | 1.05252100  |
| H       | -1.45697900 | -1.79996700 | 1.62713700  |
| O       | -1.59476000 | 1.89283100  | 1.20238600  |
| H       | -0.96793500 | 2.63054300  | 1.24383100  |
| C       | 0.91601900  | -0.16177800 | 2.13641800  |
| C       | 1.29498900  | -0.30874900 | 0.66717700  |
| H       | 1.44707200  | -0.92953100 | 2.70244000  |
| H       | 1.24802200  | 0.82454700  | 2.47415400  |
| C       | 2.82018800  | -0.34097800 | 0.45247200  |
| C       | 3.29262500  | -0.26538500 | -1.01689900 |
| O       | -0.45826400 | -0.35173800 | 2.31848000  |
| H       | -0.92773200 | 0.45730600  | 2.03776500  |
| F       | 4.60343100  | -0.47883000 | -1.06347400 |
| F       | 3.04090800  | 0.93124600  | -1.52972900 |
| F       | 2.68277200  | -1.18886700 | -1.75039800 |
| F       | 3.36826700  | 0.70011500  | 1.10744800  |
| F       | 3.29976200  | -1.47918800 | 0.98338900  |
| F       | 0.80444600  | 0.73016700  | -0.06037200 |
| F       | 0.77055500  | -1.44198800 | 0.15831500  |
| O       | 0.69575000  | 3.35936000  | 0.41307500  |
| H       | 0.30404400  | 3.16204500  | -0.46522600 |
| TS-II-1 |             |             |             |
| Si      | -2.42319600 | 1.03709800  | -0.00877600 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| O  | -1.81975700 | -0.45653300 | -0.29767100 |
| O  | -4.04947500 | 0.95033100  | 0.00469300  |
| H  | -4.42057300 | 0.08412100  | 0.21671600  |
| O  | -1.92936200 | 2.16633200  | -1.07316700 |
| H  | -2.43105900 | 2.29953000  | -1.87846000 |
| Si | -2.19813700 | -2.01835600 | -0.01568600 |
| O  | -2.13338600 | -2.96623400 | -1.34170300 |
| H  | -1.30981500 | -3.41830100 | -1.53204100 |
| O  | -3.78228700 | -1.92212900 | 0.44287500  |
| H  | -4.28286700 | -2.72850900 | 0.57698600  |
| O  | -1.20940500 | -2.64586100 | 1.11416800  |
| H  | -0.69429600 | -2.03448500 | 1.65876100  |
| O  | -1.78593300 | 1.46972000  | 1.45294800  |
| H  | -1.26510500 | 2.27979000  | 1.54562000  |
| C  | 1.12572400  | 0.30359400  | 2.02878900  |
| C  | 1.43913800  | 0.17605300  | 0.53800900  |
| H  | 1.95019600  | -0.08443000 | 2.63049500  |
| H  | 1.05244400  | 1.45985700  | 2.24256100  |
| C  | 2.90118300  | 0.54075900  | 0.22179700  |
| C  | 3.26874000  | 0.61538500  | -1.27712800 |
| O  | -0.05389200 | -0.30706000 | 2.37878200  |
| H  | -0.80131200 | 0.27721000  | 2.10207400  |
| F  | 4.58274500  | 0.77412500  | -1.39178400 |
| F  | 2.66564700  | 1.64570300  | -1.85341000 |
| F  | 2.91588000  | -0.50235800 | -1.89721200 |

|   |            |             |             |
|---|------------|-------------|-------------|
| F | 3.15667900 | 1.75502400  | 0.76101500  |
| F | 3.70681500 | -0.35940800 | 0.80493000  |
| F | 0.64953100 | 0.99686200  | -0.19380300 |
| F | 1.21910100 | -1.08827600 | 0.12872100  |
| O | 0.62104800 | 2.82099800  | 2.15983600  |
| H | 1.20725400 | 3.12065000  | 1.44375700  |

#### EP-II-1

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | -2.85790600 | 1.50130400  | -0.11279100 |
| O  | -3.39298400 | 0.05225800  | -0.66435400 |
| O  | -3.68192700 | 1.90094900  | 1.25103300  |
| H  | -4.05816400 | 1.15636700  | 1.74007800  |
| O  | -3.01565300 | 2.72312600  | -1.19553300 |
| H  | -3.84652000 | 3.20478000  | -1.20306900 |
| Si | -3.97114400 | -1.37350800 | -0.10270400 |
| O  | -5.28368900 | -1.92255300 | -0.91728000 |
| H  | -5.13609700 | -2.50190700 | -1.66873700 |
| O  | -4.45673700 | -0.98390100 | 1.43666700  |
| H  | -4.88732600 | -1.65300900 | 1.97433600  |
| O  | -2.81689900 | -2.53336400 | -0.17845600 |
| H  | -1.89584700 | -2.25319000 | -0.06482200 |
| O  | -1.23156400 | 1.28093700  | 0.10687400  |
| H  | -0.64304300 | 2.06356700  | 0.21101700  |
| C  | 1.02774100  | -1.43682600 | 0.14476500  |
| C  | 2.03486800  | -0.38278800 | -0.00835000 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 1.29618700  | -2.48098300 | 0.13647500  |
| H | 1.42563100  | 2.83268000  | 0.43814600  |
| C | 3.48395600  | -0.90393500 | 0.20281000  |
| C | 4.63804400  | 0.08281700  | -0.16929400 |
| O | -0.27843900 | -1.15609500 | 0.14146900  |
| H | -0.51724200 | -0.18097200 | 0.12980400  |
| F | 5.80081800  | -0.43300500 | 0.24620200  |
| F | 4.46577500  | 1.27143900  | 0.42665800  |
| F | 4.70763100  | 0.26990900  | -1.48899600 |
| F | 3.63753100  | -1.23676900 | 1.50604000  |
| F | 3.66512400  | -2.02439200 | -0.54245800 |
| F | 1.82243900  | 0.65829200  | 0.89157600  |
| F | 1.97984100  | 0.24950500  | -1.24861900 |
| O | 0.57885600  | 3.28524800  | 0.34234200  |
| H | 0.68131900  | 3.90025700  | -0.39159700 |

#### P-II-1

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | -2.66940800 | 1.64094900  | -0.01967400 |
| O  | -3.12197300 | 0.21425500  | -0.66333700 |
| O  | -3.62404200 | 2.00129900  | 1.25100900  |
| H  | -4.03961300 | 1.24449200  | 1.68534400  |
| O  | -2.66382200 | 2.89004000  | -1.06032800 |
| H  | -3.46420100 | 3.40488600  | -1.17313100 |
| Si | -3.83126800 | -1.17873600 | -0.18533800 |
| O  | -5.12315300 | -1.60102000 | -1.08245100 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -4.98856100 | -2.17690400 | -1.83665000 |
| O | -4.37138900 | -0.78965800 | 1.32761000  |
| H | -4.88299700 | -1.43111700 | 1.82364100  |
| O | -2.76314600 | -2.40391900 | -0.22969500 |
| H | -1.83637900 | -2.19156700 | -0.05176900 |
| O | -1.08536800 | 1.37587000  | 0.39030200  |
| H | -0.49696200 | 2.11252900  | 0.57318400  |
| C | 1.04709000  | -1.38750700 | 0.23647000  |
| C | 1.97876200  | -0.26813600 | 0.01416300  |
| H | 1.34259700  | -2.41117000 | 0.07162500  |
| C | 3.44426000  | -0.66304200 | 0.28503900  |
| C | 4.49903100  | 0.34468600  | -0.22984800 |
| O | -0.26347200 | -1.13338300 | 0.29545000  |
| H | -0.47153700 | -0.16593800 | 0.36128500  |
| F | 5.68976300  | 0.00899900  | 0.25636200  |
| F | 4.20452300  | 1.57478800  | 0.17547200  |
| F | 4.56432600  | 0.32572000  | -1.55303800 |
| F | 3.61706500  | -0.80301200 | 1.60739700  |
| F | 3.69915800  | -1.84629500 | -0.30690600 |
| F | 1.66383800  | 0.78165700  | 0.82872400  |
| F | 1.91279300  | 0.24257800  | -1.25765300 |

#### ER-III-1

|    |             |             |            |
|----|-------------|-------------|------------|
| Si | -4.58029500 | 2.16348200  | 0.26261000 |
| Si | -5.22539300 | -0.82185600 | 0.39840500 |

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | -3.08934700 | -2.94715000 | -0.11860600 |
| Si | -0.30357900 | -1.92413800 | -0.84593000 |
| Si | 0.35762700  | 1.02013800  | -1.02130800 |
| Si | -1.76109000 | 3.12999200  | -0.40866600 |
| O  | -5.06549700 | 0.68192600  | -0.20747800 |
| O  | -4.33054500 | -1.92784700 | -0.39371700 |
| O  | -1.77382900 | -2.59692000 | -1.01353600 |
| O  | -0.25139600 | -0.43340300 | -1.47139600 |
| O  | -0.74584600 | 2.19204000  | -1.26848700 |
| O  | -3.32819100 | 2.73372900  | -0.61078800 |
| O  | -4.01545100 | 2.05525200  | 1.81055700  |
| H  | -4.22021400 | 1.22951600  | 2.27403800  |
| O  | -5.85766800 | 3.15745000  | 0.10709800  |
| H  | -5.71951700 | 4.07061400  | -0.14740800 |
| O  | -4.67349000 | -0.71846300 | 1.95134900  |
| H  | -4.05729000 | -1.41151900 | 2.22918700  |
| O  | -6.77456700 | -1.30284500 | 0.29175000  |
| H  | -7.47548200 | -0.64993300 | 0.27904600  |
| O  | -2.69885500 | -2.73483100 | 1.47202300  |
| H  | -1.76364200 | -2.60078900 | 1.67522000  |
| O  | -3.53226800 | -4.46744700 | -0.47550400 |
| H  | -4.46178000 | -4.68859900 | -0.54518700 |
| O  | 0.00412200  | -1.84996200 | 0.78688100  |
| H  | 0.30227400  | -0.96707700 | 1.07256100  |
| O  | 0.81619800  | -2.91031100 | -1.51779700 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 0.53631200  | -3.69241500 | -1.99721600 |
| O | 0.60263400  | 0.88758000  | 0.62031200  |
| H | 0.13645500  | 1.55881600  | 1.14519800  |
| O | 1.67978400  | 1.43687800  | -1.85492400 |
| H | 2.38358800  | 0.78050700  | -1.90154000 |
| O | -1.36114000 | 2.85549000  | 1.17175800  |
| H | -2.10773700 | 2.70645700  | 1.77150400  |
| O | -1.59433600 | 4.68222200  | -0.86182400 |
| H | -0.77706900 | 4.96634600  | -1.27335100 |
| C | 7.19833800  | 0.63456900  | 0.38636000  |
| C | 5.81651900  | 0.18200100  | 0.90775900  |
| C | 4.80409900  | -0.27047600 | -0.15970200 |
| C | 3.42585700  | -0.55273600 | 0.41633600  |
| H | 3.51375300  | -1.32742300 | 1.18329900  |
| H | 3.02320200  | 0.36295600  | 0.85161300  |
| F | 7.99155000  | 0.87820600  | 1.42468200  |
| F | 7.75049100  | -0.31343900 | -0.35941800 |
| F | 7.08619700  | 1.74337300  | -0.33151000 |
| F | 6.01066600  | -0.83879400 | 1.76172100  |
| F | 5.28622600  | 1.21434000  | 1.59128600  |
| F | 5.28741600  | -1.37924900 | -0.76226800 |
| F | 4.71821400  | 0.69661700  | -1.10458200 |
| O | 2.57356800  | -0.94404400 | -0.62933300 |
| H | 2.66779300  | -1.89481500 | -0.79268700 |
| O | 2.36038600  | -3.54348800 | 0.62114500  |

|          |             |             |             |
|----------|-------------|-------------|-------------|
| H        | 1.53381900  | -3.12284900 | 0.93624400  |
| TS-III-1 |             |             |             |
| Si       | 3.64853400  | -0.60624900 | -0.94489700 |
| Si       | 4.16085300  | 2.39999500  | -0.74734400 |
| Si       | 1.92120500  | 4.41352300  | -1.27764400 |
| Si       | -0.78113800 | 3.22946600  | -2.06974200 |
| Si       | -1.30869500 | 0.26265200  | -2.32485900 |
| Si       | 0.90760100  | -1.73210800 | -1.69346200 |
| O        | 4.07539700  | 0.90182900  | -1.38323600 |
| O        | 3.22926400  | 3.47841800  | -1.53627500 |
| O        | 0.64728300  | 3.99214000  | -2.20249000 |
| O        | -0.75407400 | 1.75130400  | -2.73208200 |
| O        | -0.15575700 | -0.85934700 | -2.56683100 |
| O        | 2.44431100  | -1.22006300 | -1.85578800 |
| O        | 3.03831100  | -0.55152200 | 0.58861200  |
| H        | 3.20490700  | 0.26764700  | 1.07804500  |
| O        | 4.97684000  | -1.53350500 | -1.08455400 |
| H        | 4.88809900  | -2.46096200 | -1.30766700 |
| O        | 3.59094700  | 2.24668100  | 0.79429100  |
| H        | 2.93274200  | 2.90126100  | 1.06943300  |
| O        | 5.68948700  | 2.94669100  | -0.81993700 |
| H        | 6.41629000  | 2.32436900  | -0.86763400 |
| O        | 1.52313300  | 4.15949500  | 0.30491500  |
| H        | 0.59541100  | 3.97573200  | 0.50205800  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 2.26117000  | 5.96216600  | -1.62459100 |
| H | 3.16359500  | 6.27890900  | -1.56805200 |
| O | -1.09316300 | 3.07740500  | -0.44695100 |
| H | -1.32396200 | 2.16388900  | -0.19278000 |
| O | -1.93824800 | 4.15991100  | -2.76630400 |
| H | -1.68625000 | 4.99397300  | -3.16729000 |
| O | -1.60937600 | 0.35760900  | -0.69016000 |
| H | -1.14070800 | -0.30782700 | -0.16029100 |
| O | -2.59644300 | -0.18133600 | -3.20003800 |
| H | -3.32882400 | 0.44334600  | -3.20940000 |
| O | 0.44996800  | -1.50561700 | -0.12144200 |
| H | 1.16958100  | -1.31638300 | 0.49973900  |
| O | 0.86795500  | -3.28526900 | -2.16876700 |
| H | 0.07570300  | -3.63713200 | -2.57660900 |
| C | -8.23454400 | 2.07212700  | -0.11647900 |
| C | -6.71710900 | 2.23388300  | 0.13029400  |
| C | -5.83971900 | 2.20872300  | -1.13538400 |
| C | -4.35819300 | 2.08081900  | -0.82638800 |
| H | -4.10083300 | 2.97590400  | -0.07041400 |
| H | -4.12510700 | 1.14048300  | -0.32761700 |
| F | -8.88584300 | 2.31123200  | 1.01596900  |
| F | -8.64545100 | 2.93439900  | -1.03881100 |
| F | -8.51914300 | 0.84026400  | -0.51593700 |
| F | -6.51998100 | 3.39371600  | 0.76693000  |
| F | -6.32608000 | 1.22525000  | 0.93517400  |

|   |             |            |             |
|---|-------------|------------|-------------|
| F | -6.05506700 | 3.34162000 | -1.83807300 |
| F | -6.24024300 | 1.17214100 | -1.91127500 |
| O | -3.60156700 | 2.18443000 | -1.98384400 |
| H | -3.62313400 | 3.08696600 | -2.34241900 |
| O | -3.61626800 | 4.08392800 | 0.50029000  |
| H | -2.68234100 | 3.96272500 | 0.23952600  |

#### EP-III-1

|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | -4.81005700 | 1.40445100  | 0.80222500  |
| Si | -4.63892500 | -1.64475700 | 0.82118100  |
| Si | -2.17852200 | -3.05981000 | -0.31394300 |
| Si | 0.03790300  | -1.38076700 | -1.59916000 |
| Si | -0.10471400 | 1.64498600  | -1.48471800 |
| Si | -2.49904800 | 3.08491800  | -0.27162600 |
| O  | -5.01402400 | -0.13706300 | 0.32197600  |
| O  | -3.68570900 | -2.44118800 | -0.23002900 |
| O  | -1.26644700 | -2.34004700 | -1.44914500 |
| O  | -0.40271400 | 0.12762300  | -2.00465100 |
| O  | -1.46865300 | 2.52906900  | -1.40422000 |
| O  | -3.91768500 | 2.28767700  | -0.23934600 |
| O  | -3.94876800 | 1.39933300  | 2.21167400  |
| H  | -3.83987300 | 0.53284800  | 2.63225400  |
| O  | -6.28899000 | 2.06367500  | 0.94860300  |
| H  | -6.41205800 | 2.99393400  | 0.75534100  |
| O  | -3.80346200 | -1.44485700 | 2.23095900  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| H | -2.95411800 | -1.90805400 | 2.28529500  |
| O | -6.00347100 | -2.50929700 | 1.00526100  |
| H | -6.84329600 | -2.05405800 | 1.07710700  |
| O | -1.49899100 | -2.74597000 | 1.16018000  |
| H | -0.59773800 | -2.39670700 | 1.14101100  |
| O | -2.26332200 | -4.64938700 | -0.63830800 |
| H | -3.11414400 | -5.08871000 | -0.61482600 |
| O | 0.73762000  | -1.35113700 | -0.07701300 |
| H | 0.86687600  | -0.44637000 | 0.26064700  |
| O | 1.07014900  | -1.94648900 | -2.71369300 |
| H | 1.76445800  | -2.55719300 | -2.44125200 |
| O | 0.48215000  | 1.46436800  | 0.06066500  |
| H | -0.02940800 | 1.93204100  | 0.74129800  |
| O | 0.92615800  | 2.42883200  | -2.46221000 |
| H | 1.69173200  | 1.92859600  | -2.76056500 |
| O | -1.72630900 | 2.81787800  | 1.16578700  |
| H | -2.28614000 | 2.47671800  | 1.88006000  |
| O | -2.83969600 | 4.64899300  | -0.55447600 |
| H | -2.20275200 | 5.19734500  | -1.01420900 |
| C | 6.62917000  | 0.03935500  | 1.52081300  |
| C | 5.13430200  | 0.06827900  | 1.13099600  |
| C | 4.81598700  | 0.52374600  | -0.31145400 |
| C | 3.36106700  | 0.77839800  | -0.50249100 |
| H | 3.97573900  | -2.68890900 | -0.59537000 |
| H | 2.90140300  | 1.62881500  | -0.02079600 |

|   |            |             |             |
|---|------------|-------------|-------------|
| F | 6.75343100 | -0.54037400 | 2.71080500  |
| F | 7.32256800 | -0.66231300 | 0.63059400  |
| F | 7.12481700 | 1.26447900  | 1.59343500  |
| F | 4.65223100 | -1.18234900 | 1.29333200  |
| F | 4.50350600 | 0.88311900  | 1.99195700  |
| F | 5.25021500 | -0.43483900 | -1.16080000 |
| F | 5.56588300 | 1.63877500  | -0.54805500 |
| O | 2.75099000 | 0.33757700  | -1.61675800 |
| H | 3.05691300 | -0.56430900 | -1.83488300 |
| O | 3.15988900 | -2.37126100 | -0.99106200 |
| H | 2.54272500 | -2.17606600 | -0.26869300 |

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|    |             |             |             |
|----|-------------|-------------|-------------|
| Si | -4.60137300 | -0.75953000 | -0.94435000 |
| Si | -4.02082900 | 2.18570400  | -0.38559200 |
| Si | -1.36723300 | 3.04438800  | 0.85671900  |
| Si | 0.48964600  | 0.74035800  | 1.57882600  |
| Si | -0.09987400 | -2.21768300 | 1.24027400  |
| Si | -2.67649800 | -3.00581000 | -0.17797200 |
| O  | -4.55876900 | 0.66331100  | -0.15671200 |
| O  | -2.94746900 | 2.65536500  | 0.74488800  |
| O  | -0.53895700 | 1.97810400  | 1.77675300  |
| O  | -0.13945600 | -0.71579300 | 1.89917900  |
| O  | -1.60594300 | -2.79826800 | 1.03325600  |
| O  | -3.94120500 | -1.98386300 | -0.09696200 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | -3.66862700 | -0.63944400 | -2.30200700 |
| H | -3.46204600 | 0.26039400  | -2.59463800 |
| O | -6.16763800 | -1.07336700 | -1.25202600 |
| H | -6.45756000 | -1.97845600 | -1.37256200 |
| O | -3.25987900 | 2.15518800  | -1.85019300 |
| H | -2.38358800 | 2.56585700  | -1.88088200 |
| O | -5.26678400 | 3.22781700  | -0.32090200 |
| H | -6.14811500 | 2.92534900  | -0.54370000 |
| O | -0.76926000 | 2.97782600  | -0.67703400 |
| H | -0.00578600 | 2.39797800  | -0.81520600 |
| O | -1.21445600 | 4.51435000  | 1.52786200  |
| H | -1.99249800 | 5.05984900  | 1.64881000  |
| O | 0.96144200  | 0.81669700  | 0.00303100  |
| H | 1.15942500  | -0.03014900 | -0.42542900 |
| O | 1.76431000  | 0.91756100  | 2.60996200  |
| H | 2.07370900  | 1.80097100  | 2.82275900  |
| O | 0.61006700  | -2.01906800 | -0.24328000 |
| H | 0.06230500  | -2.29862400 | -0.99364200 |
| O | 0.69103400  | -3.26158600 | 2.19645700  |
| H | 1.56331800  | -2.97913100 | 2.48890400  |
| O | -1.83091100 | -2.67561700 | -1.55797500 |
| H | -2.26781000 | -2.07664900 | -2.18228600 |
| O | -3.27612700 | -4.51579200 | -0.12813700 |
| H | -2.76065400 | -5.21633400 | 0.27338400  |
| C | 5.88579300  | 0.72035900  | -1.56159500 |

|   |            |             |             |
|---|------------|-------------|-------------|
| C | 4.65565600 | -0.11773200 | -1.14301900 |
| C | 4.52589300 | -0.39441500 | 0.36905000  |
| C | 3.48244300 | -1.40589400 | 0.64813700  |
| H | 3.44672400 | -2.33021800 | 0.09363100  |
| F | 5.75182500 | 1.08118800  | -2.83387000 |
| F | 5.97808300 | 1.81433400  | -0.81458100 |
| F | 7.00019900 | 0.01442500  | -1.43884600 |
| F | 3.55464500 | 0.52836500  | -1.55707800 |
| F | 4.72893500 | -1.29613800 | -1.79116600 |
| F | 4.22663600 | 0.76752600  | 1.00259400  |
| F | 5.76476200 | -0.76174700 | 0.82378100  |
| O | 2.89047500 | -1.41673600 | 1.85413700  |
| H | 2.83959800 | -0.52380200 | 2.25486900  |

