Computation Studies of Atmospheric Chemistry and Environment

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Introduction

Scope of Studies

- Quantum chemical calculations of the reaction intermediate species and products of oxidation reactions of volatile organic compounds (VOCs) to elucidate the kinetics and mechanism relevant to air pollution in the ambient environment
- Theoretical studies of pre-nucleation species relevant to new particle formation in the atmosphere
- Numerical simulations of regional ozone and particulate matter formation using chemical transport models (CTMs)
Fig. 1. Simulated surface O3 (A and B) and NOx (C and D) distributions at 11 p.m. (A and C) and 3 p.m. (B and D) CDT during the time period of September 7–8, 1993.

The Houston City limit is marked by thin white lines, and the other white lines in C label the county limits near Houston.

Also shown in C are the locations of surface air quality monitoring stations marked by the brown dots. The brown frame encompassing all of the stations is defined as the Houston domain in the text.
Fig. 2. Temporal evolution of simulated (solid lines) and observed (filled circles) surface O3 (A) and NOx (B) concentrations averaged over the Houston domain during September 7–11, 1993.
Fig. 3. Calculated VOC reactivity averaged over the entire episode within the bottom model layer in the Houston domain. AVOC, anthropogenic VOC; BVOC, biogenic VOC.

**Fig. 1.** Structures of hydroxy peroxy nitrites (ROONO) at the B3LYP/6-31G(d,p) level of theory.
Fig. 2. Structures of hydroxy nitrates (RONO$_2$) at the B3LYP/6-31G(d,p) level of theory.

**Fig. 1** Aromatic and Sulfuric Acid Complexes
Table 1. Bonding energies, $D_0$ (in kcal mol$^{-1}$), of the aromatic acid–sulfuric acid complexes. BASA denotes benzoic acid–sulfuric acid complex; PTA-SA, $p$-toluic acid–sulfuric acid complex; and MTA-SA, $m$-toluic acid–sulfuric acid complex. All energies are corrected with the zero-point energies (ZPE). The quantum chemical methods used in the present study are similar to those used by Suh et al.

<table>
<thead>
<tr>
<th>Complex</th>
<th>$D_0$</th>
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<tbody>
<tr>
<td>BA-SA</td>
<td>19.85*</td>
</tr>
<tr>
<td></td>
<td>17.62†</td>
</tr>
<tr>
<td></td>
<td>18.63‡</td>
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<tr>
<td></td>
<td>17.84§</td>
</tr>
<tr>
<td>PTA-SA</td>
<td>19.99*</td>
</tr>
<tr>
<td>MTA-SA</td>
<td>23.72*</td>
</tr>
</tbody>
</table>

* Determined with B3LYP/6-31G(d,p)//B3LYP/6-31G(d,p). † Determined with CCSD(T)/6-31G(d) CF//B3LYP/6-31G(d,p). ‡ Determined with QCISD(T)/6-31G(d)//MP2(full)/6-31G(d). § Determined with G2(MP2, SVP).
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