

## RRKM-ME for Unimolecular Reactions Involving Intermediates with Multiple Configurations: Ozonolysis of Cyclopentene

Hanhao Chen,<sup>a</sup> Lingyu Wang,<sup>\* b</sup> and Liming Wang <sup>\* a,c</sup>

<sup>a</sup> School of Chemistry & Chemical Engineering, South China University of Technology, Guangzhou 510640, China

<sup>b</sup> School of Chemistry & Chemical Engineering, Zhoukou Normal University, Zhoukou, 466001, China

<sup>c</sup> Guangdong Provincial Key Laboratory of Atmospheric Environment and Pollution Control, South China University of Technology, Guangzhou 510006, China

**\* Corresponding author:** Liming Wang (E-mail: [wanglm@scut.edu.cn](mailto:wanglm@scut.edu.cn)), Lingyu Wang (E-mail: [wangly1029@163.com](mailto:wangly1029@163.com))

**\* Corresponding author**

Liming Wang (E-mail: [wanglm@scut.edu.cn](mailto:wanglm@scut.edu.cn)),

Lingyu Wang (E-mail: [wangly1029@163.com](mailto:wangly1029@163.com))

Figure S1-3. Time profiles of species in assessment model #3 at different barriers.

Figure S4. Time profiles of product formation in ozonolysis of cyclopentene (include MC- and SC-RRKM-ME).

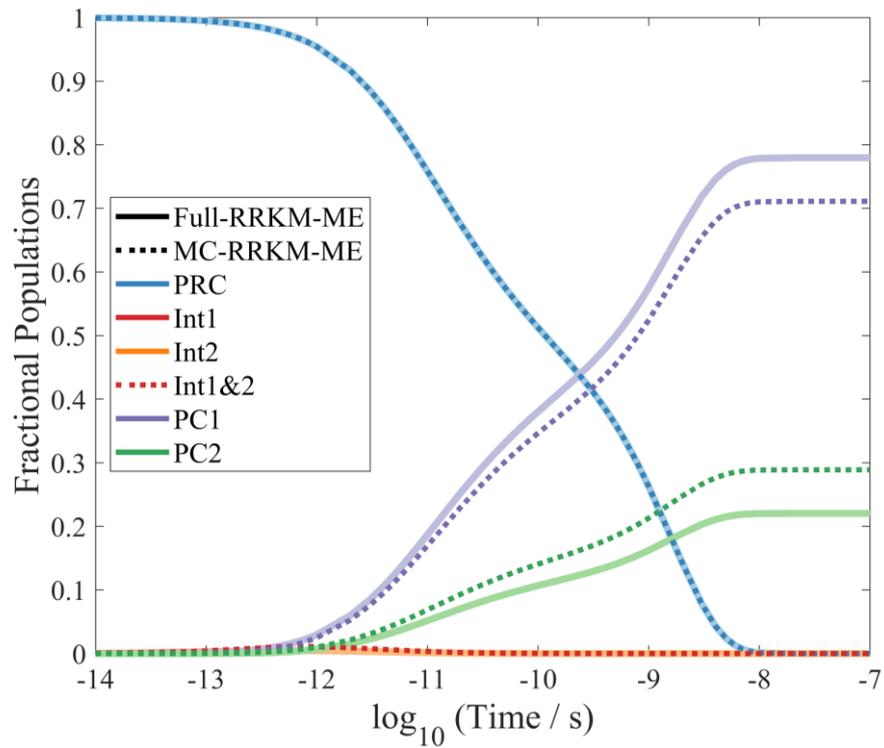


Figure S1. Time profiles of species for assessment at  $E^\ddagger(\text{TS}_{\text{Int}}) = 1RT$  and  $E^\ddagger(\text{TS}_1) = 5RT$

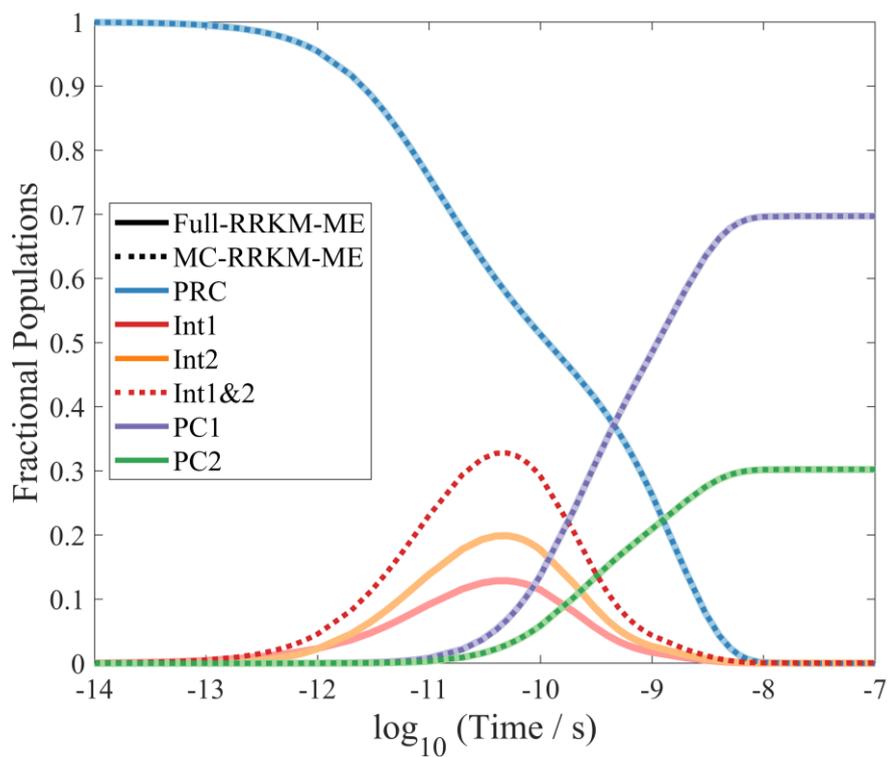


Figure S2. Time profiles of species for assessment at  $E^\ddagger(\text{TS}_{\text{Int}}) = 4RT$  and  $E^\ddagger(\text{TS}_1) = 33RT$

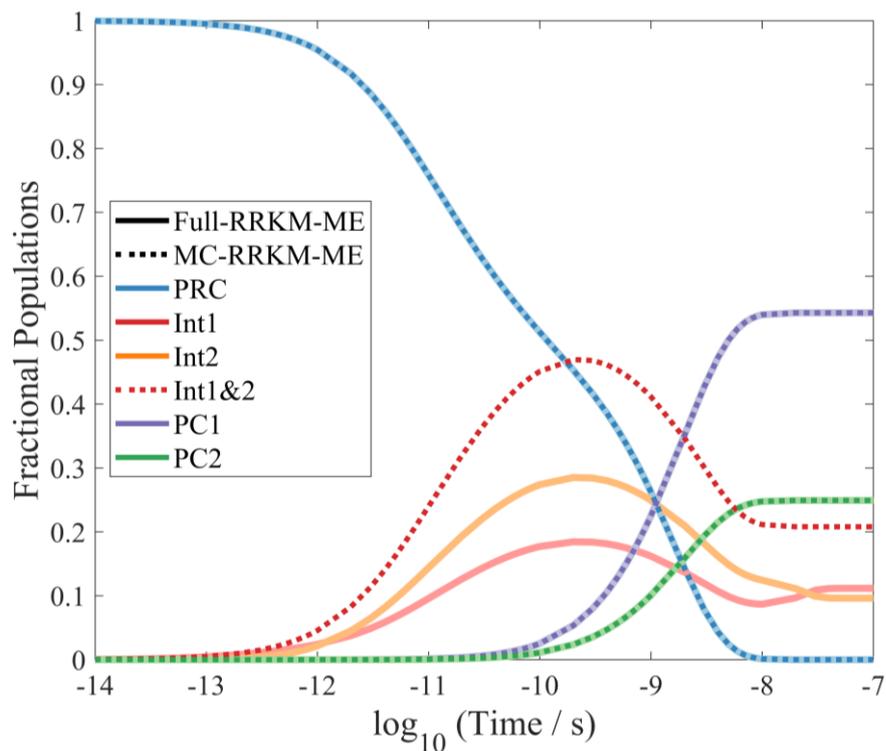


Figure S3. Time profiles of species for assessment at  $E^\ddagger(\text{TS}_{\text{Int}}) = 5RT$  and  $E^\ddagger(\text{TS}_1) = 43RT$

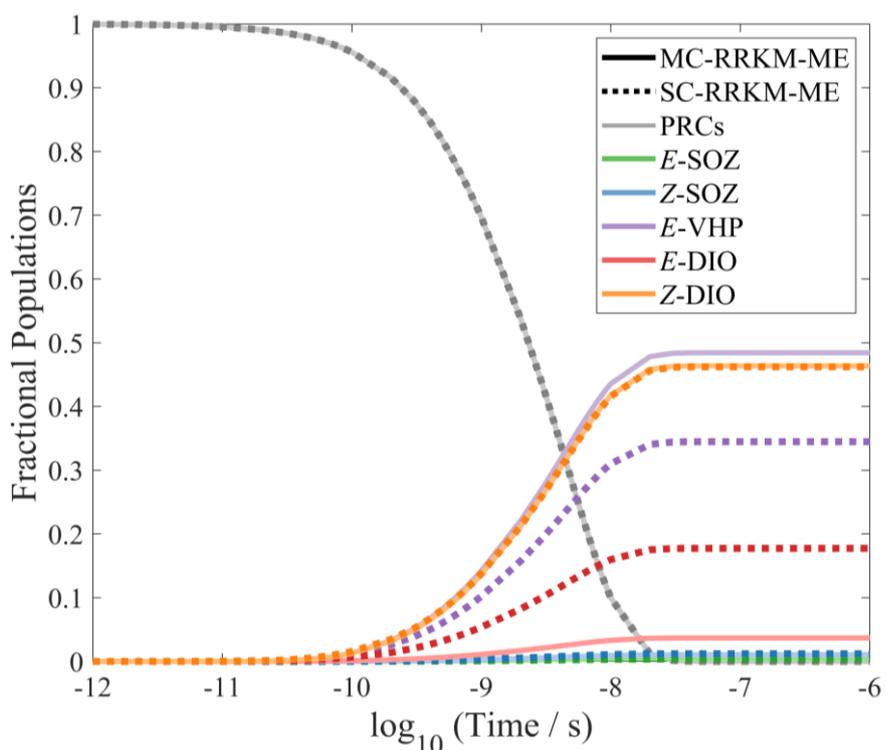


Figure S4. Time profiles of product formation in ozonolysis of cyclopentene (include MC- and SC-RRKM-ME).