

Effect of organic solvent and brönsted acid on 5-hydroxymethylfurfural preparation from glucose over CrCl_3

Yan Yang^a, Wentao Liu^a, Ningning Wang^a, Haijun Wang^{a,*}, Zhanxin Song^a,
Wei Li^a

^a *The Key Laboratory of Food Colloids and Biotechnology, Ministry of Education, School
of Chemical and Material Engineering, Jiangnan University, Wuxi 214122, Jiangsu,
China.*

Corresponding Author E-mail: wanghj329@outlook.com

Electronic Supplementary Information

Contents

- S1. IL characterization
- S2. Configurations of chromium(III) complexes
- S3. The optimized geometries of the intermediates and transition states

S1. IL characterization

Figure S1. [NMP]HSO₄ ¹H NMR

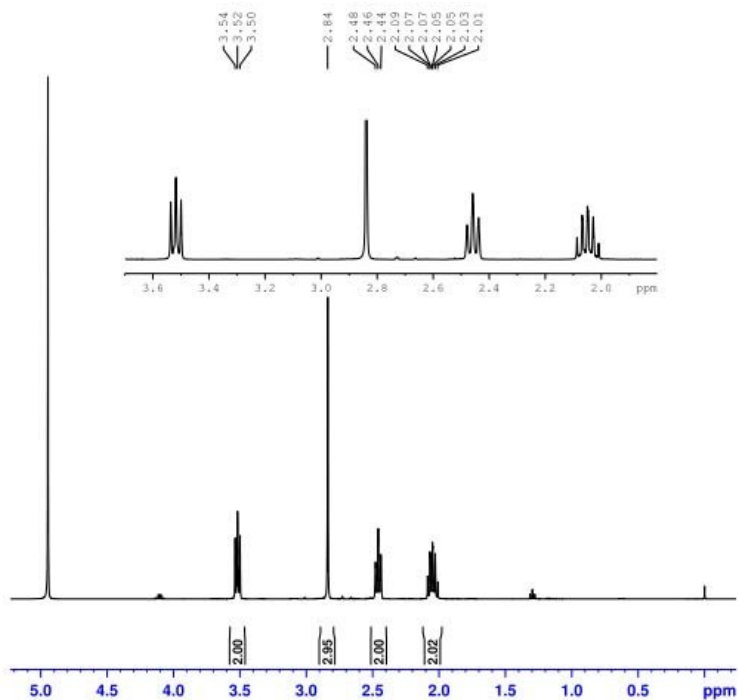


Figure S2. [NMP]HSO₄ IR

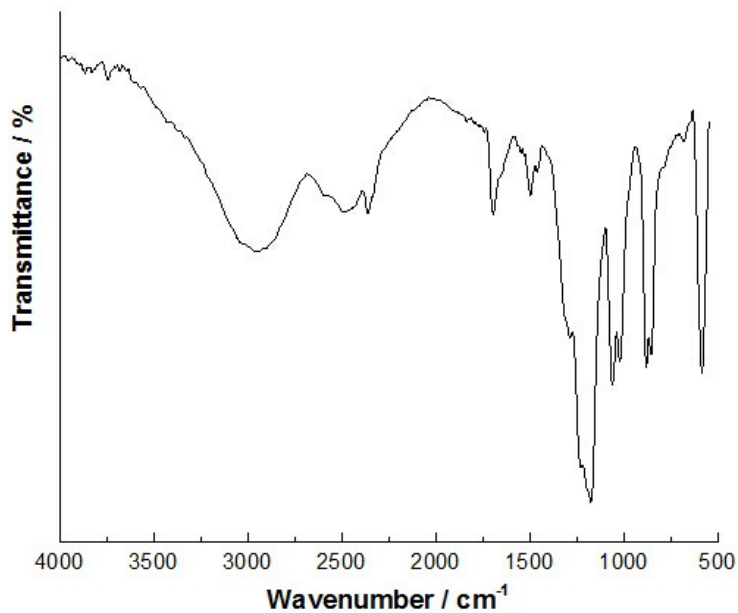
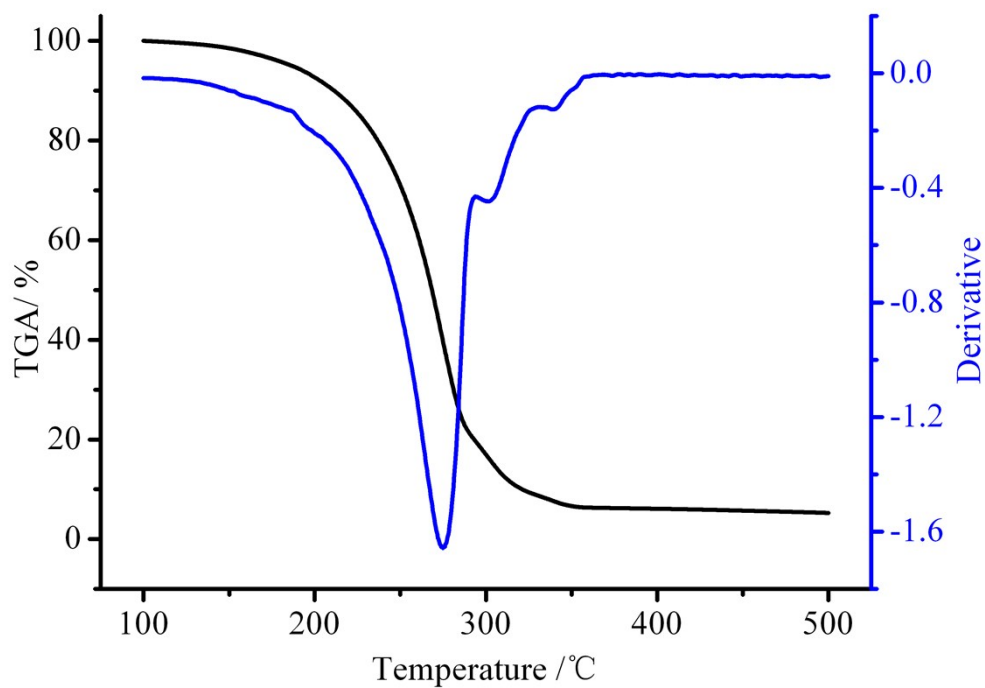
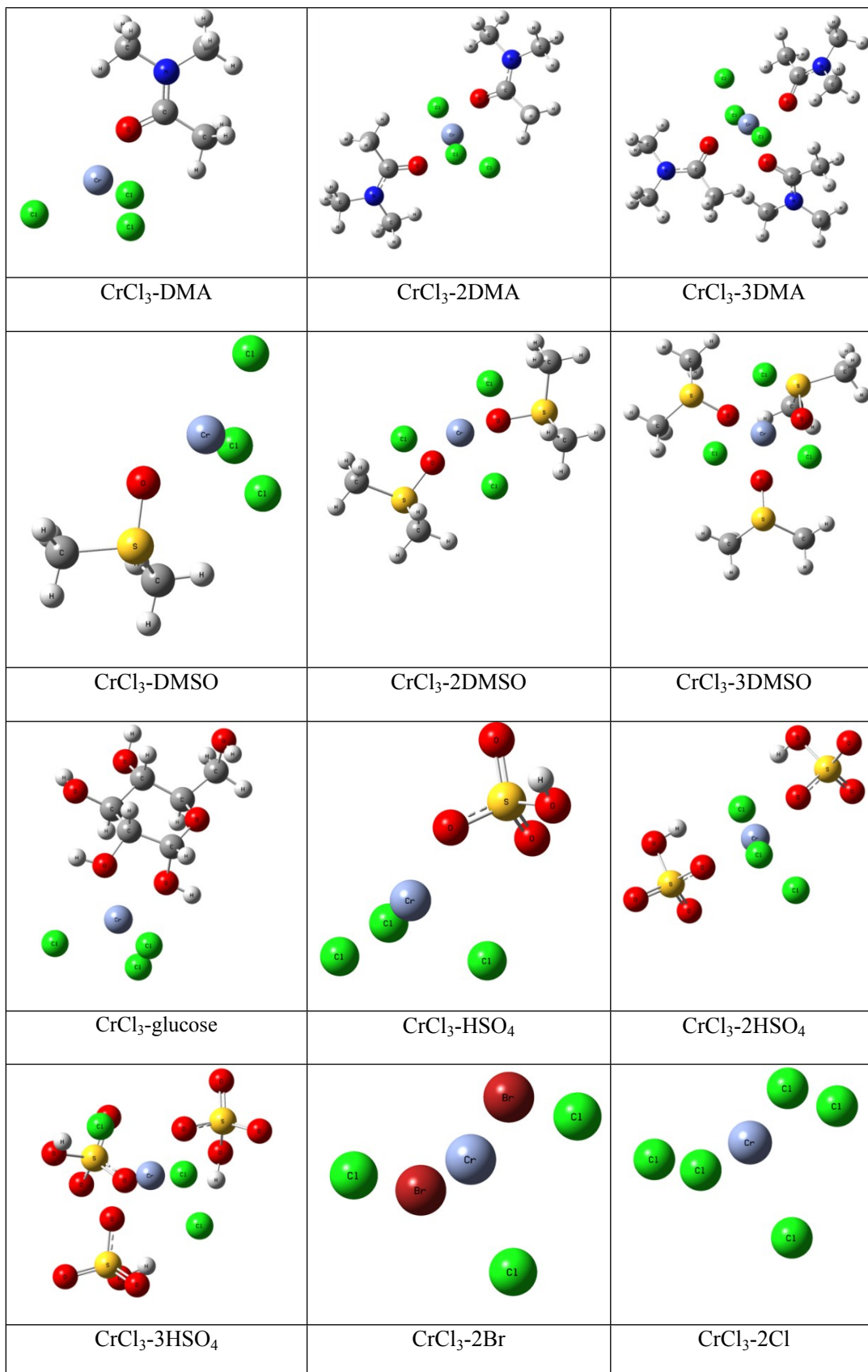


Figure S3. [NMP]HSO₄ TGA



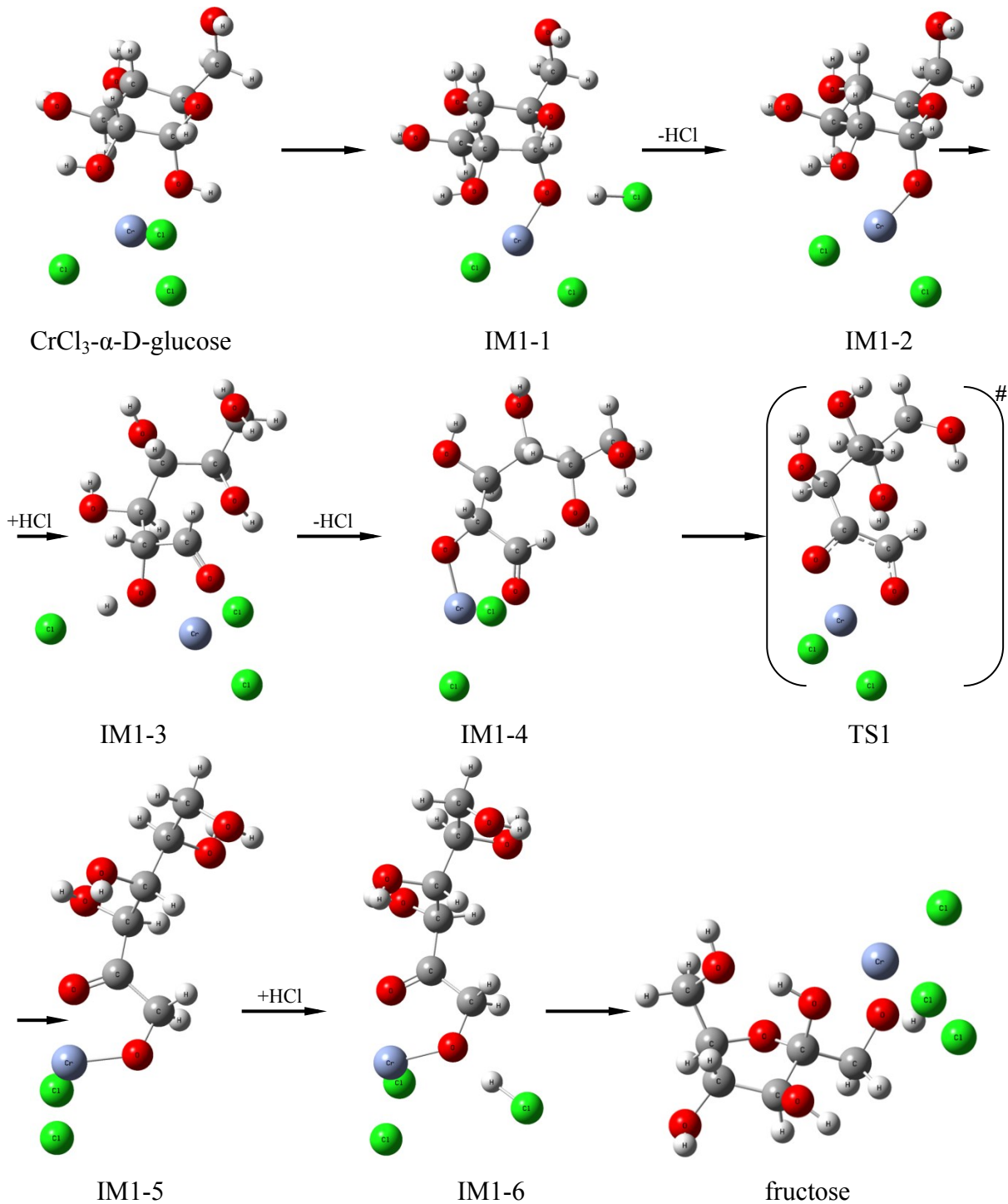
S2. Configurations of chromium(III) complexes

Figure S9. Configurations of chromium(III) complexes

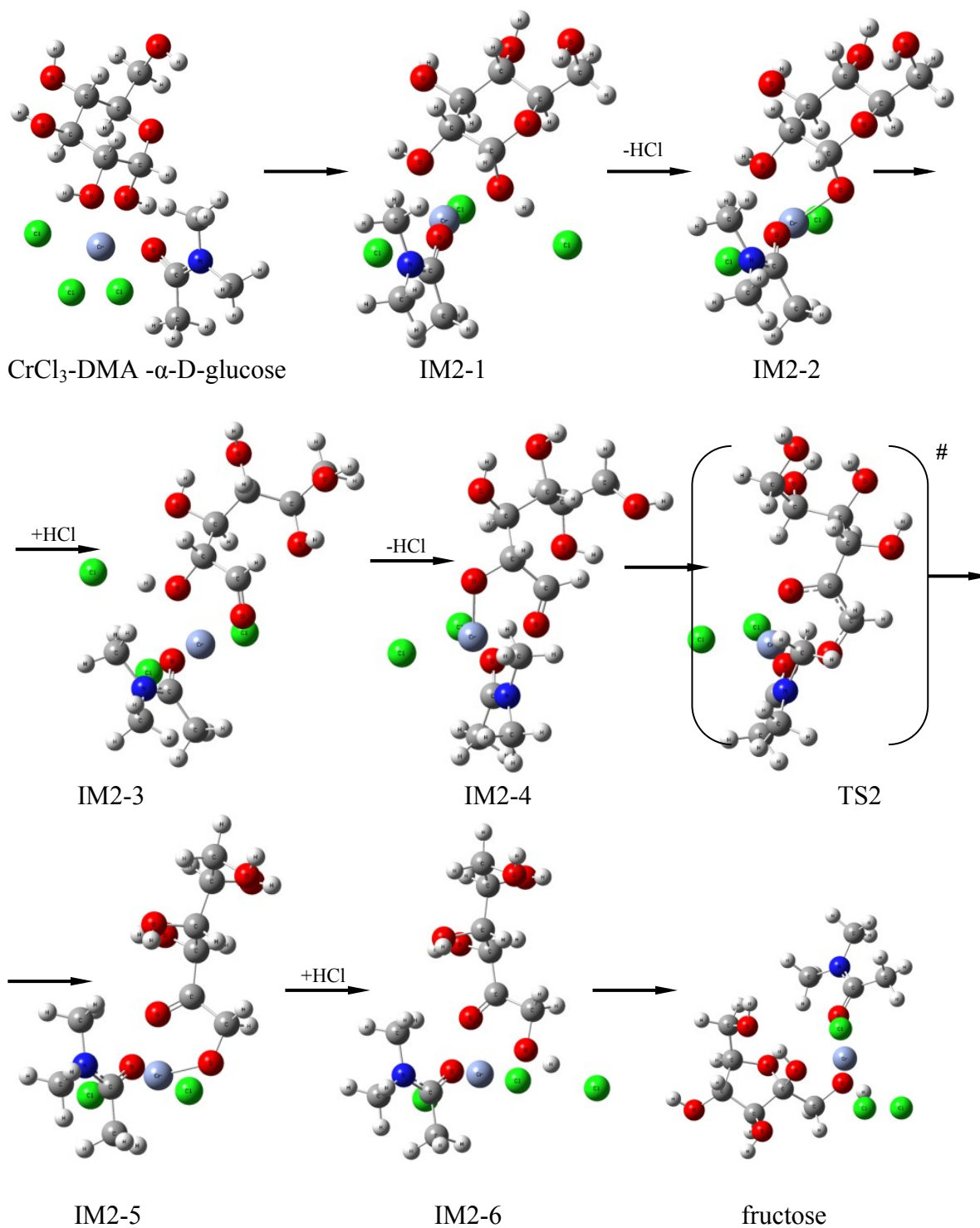


S3. The optimized geometries of the intermediates and transition states

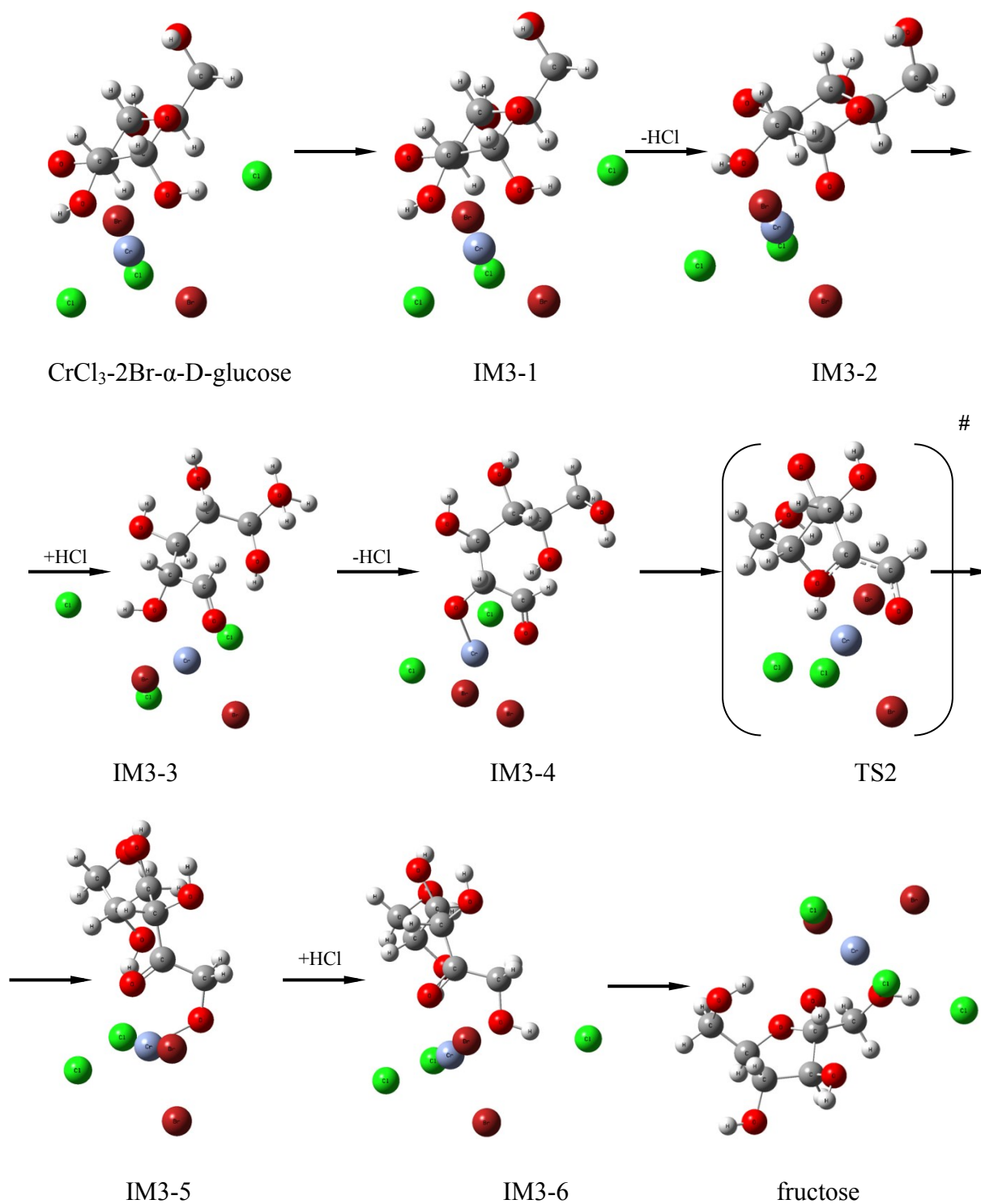
S3.1 Optimized geometries of the intermediates and transition states during glucose isomerization by CrCl_3 .



S3.2 Optimized geometries of the intermediates and transition states during glucose isomerization by CrCl_3 -DMA



S3.3 Optimized geometries of the intermediates and transition states during glucose isomerization by $\text{CrCl}_3\cdot 2\text{Br}$ in DMA



S3.4 Optimized geometries of the intermediates and transition states during glucose isomerization by $\text{CrCl}_3\cdot 2\text{Cl}$ in DMA.

