

Supplementary Material (ESI) for PCCP
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Valence electronic structure and conformational flexibility of Epichlorohydrin

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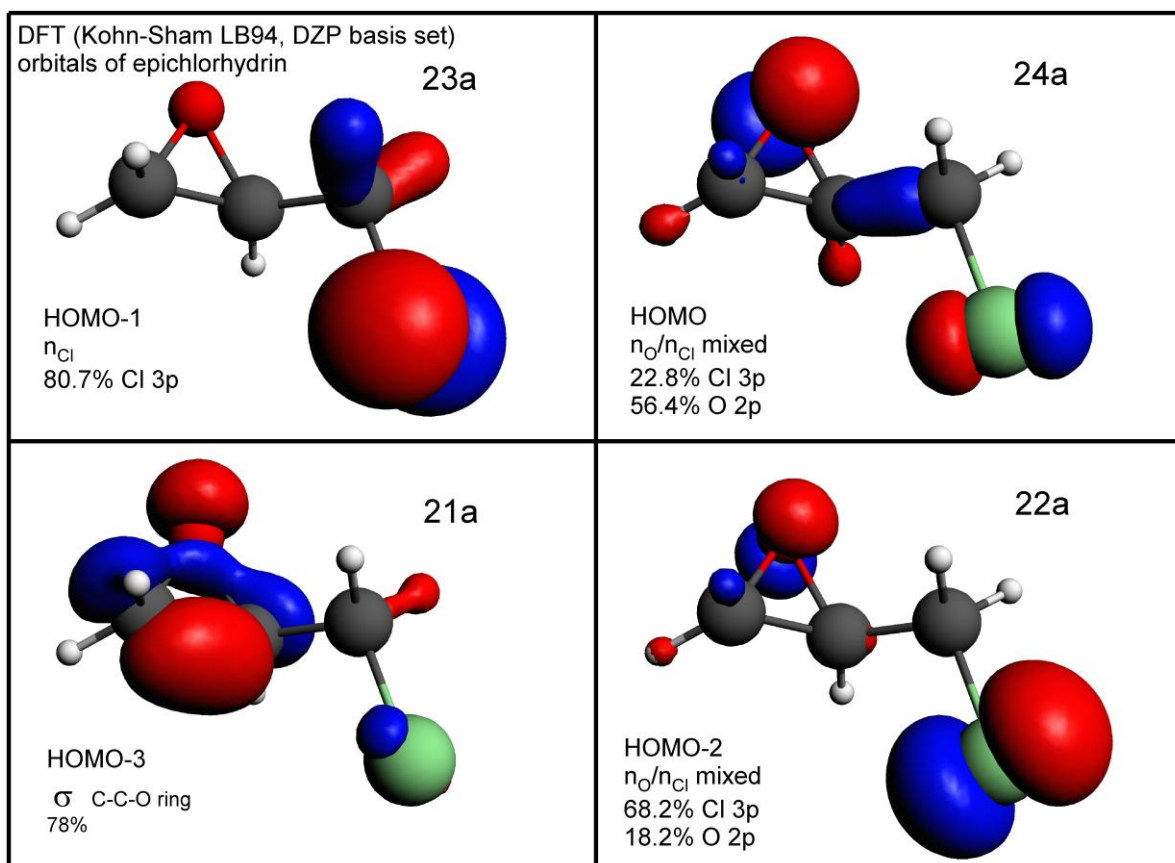
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Contents:



Caption: Pictures of the four outermost Kohn-Shan DFT MOs with their main character, in terms of AO contributions, for the *gauche-II* conformer of epichlorohydrin.