

**Electronic supporting information for
Probing the influence of pH dependent citric acid towards the
morphology of rock salt: A computational study**

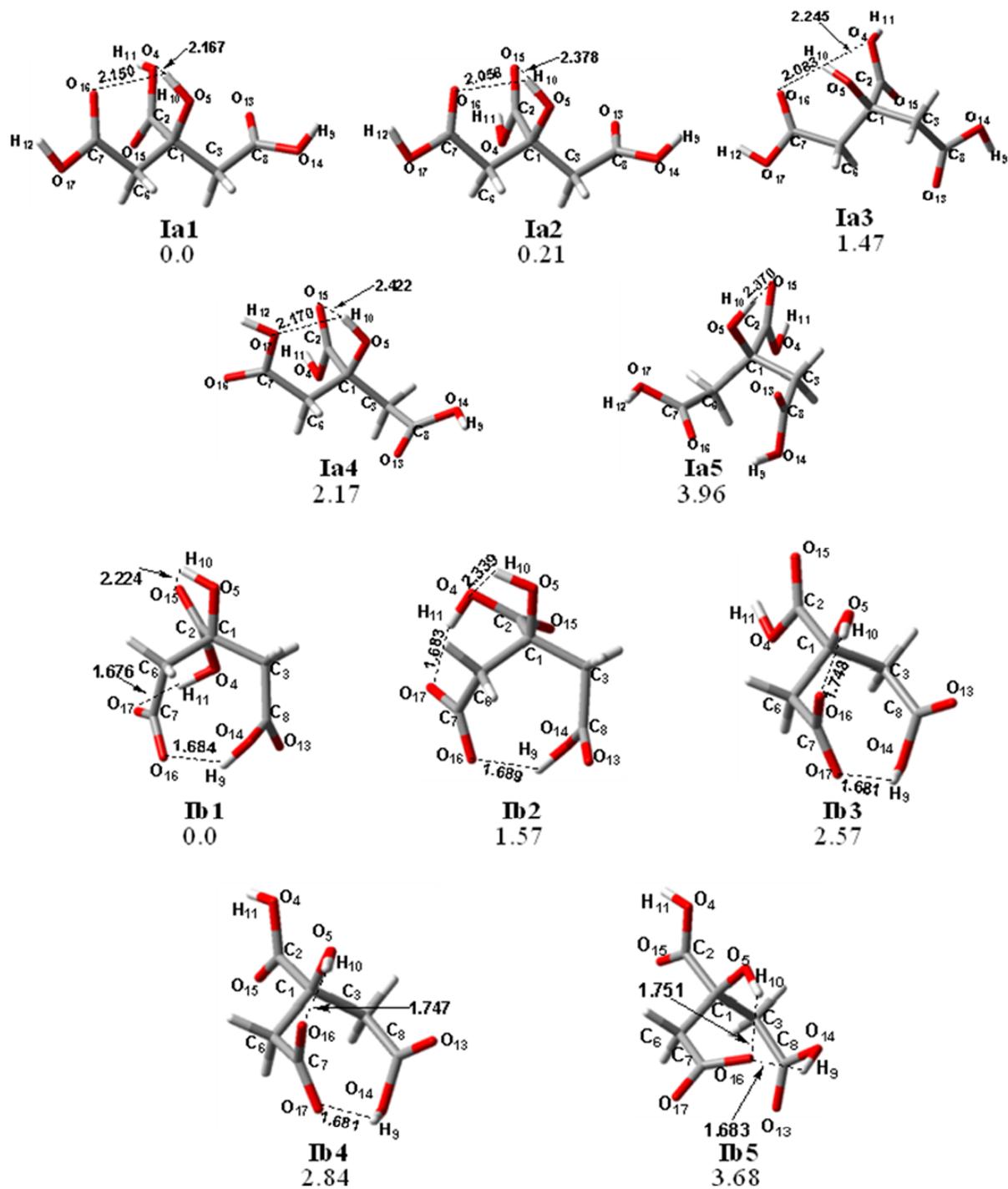
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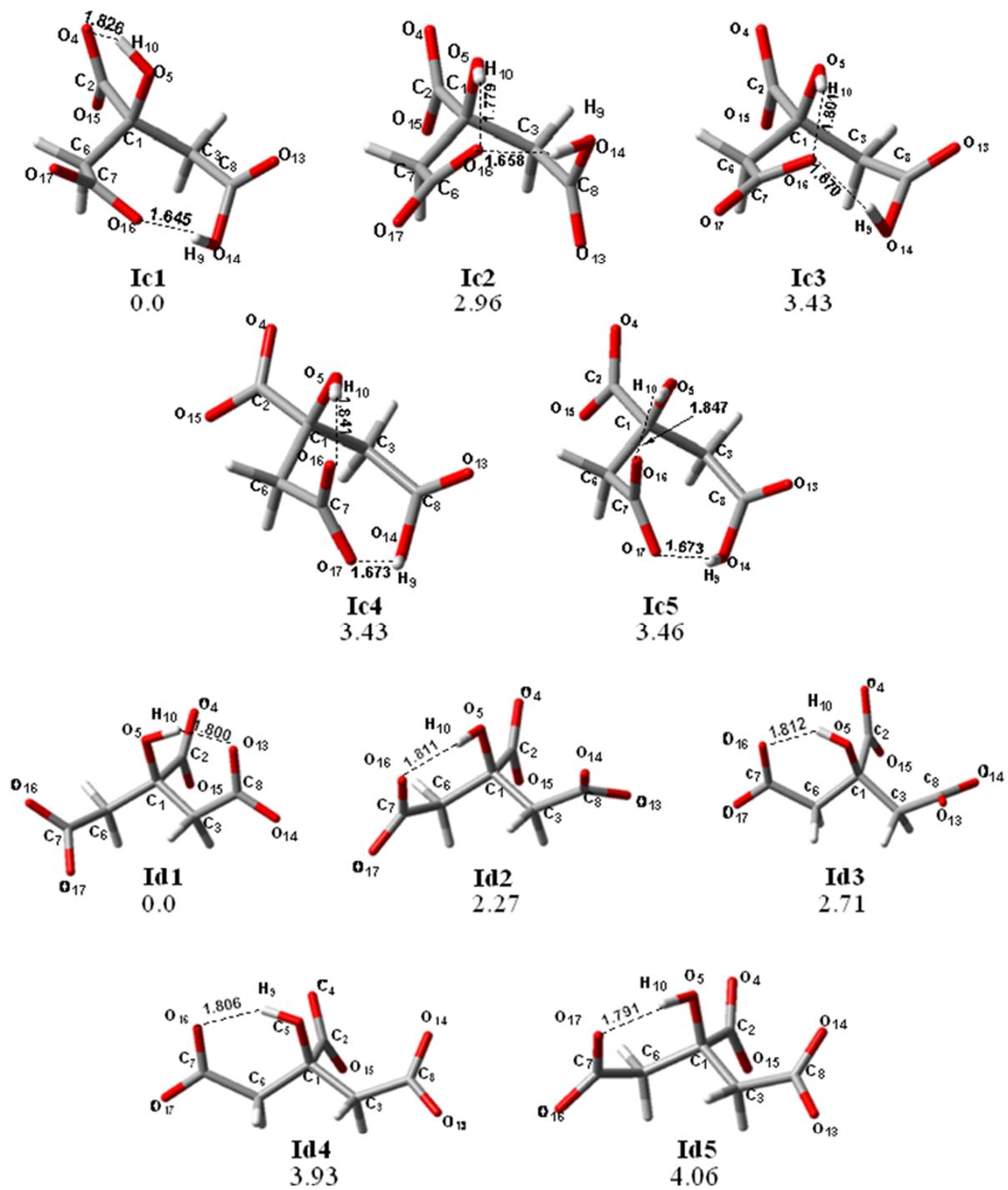
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1. Geometries from **Ia1** to **Ia5** and from **Ib1** to **Ib5** Figure S1 (part A)
2. Geometries from **Ic1** to **Ic5** and from **Id1** to **Id5** Figure S1 (part B)
3. Geometries from **IIa1** to **IIa5** and from **IIb1** to **IIb5** Figure S2 (part A)
4. Geometries from **IIc1** to **IIc5** and from **IId1** to **IId5** Figure S2 (part B)
5. Geometries from **IIIa1** to **IIIa5** and from **IIIb1** to **IIIb5** Figure S3 (part A)
6. Geometries from **IIIc1** to **IIIc5** and from **IIId1** to **IIId5** Figure S3 (part B)

List of Legends:



Part A

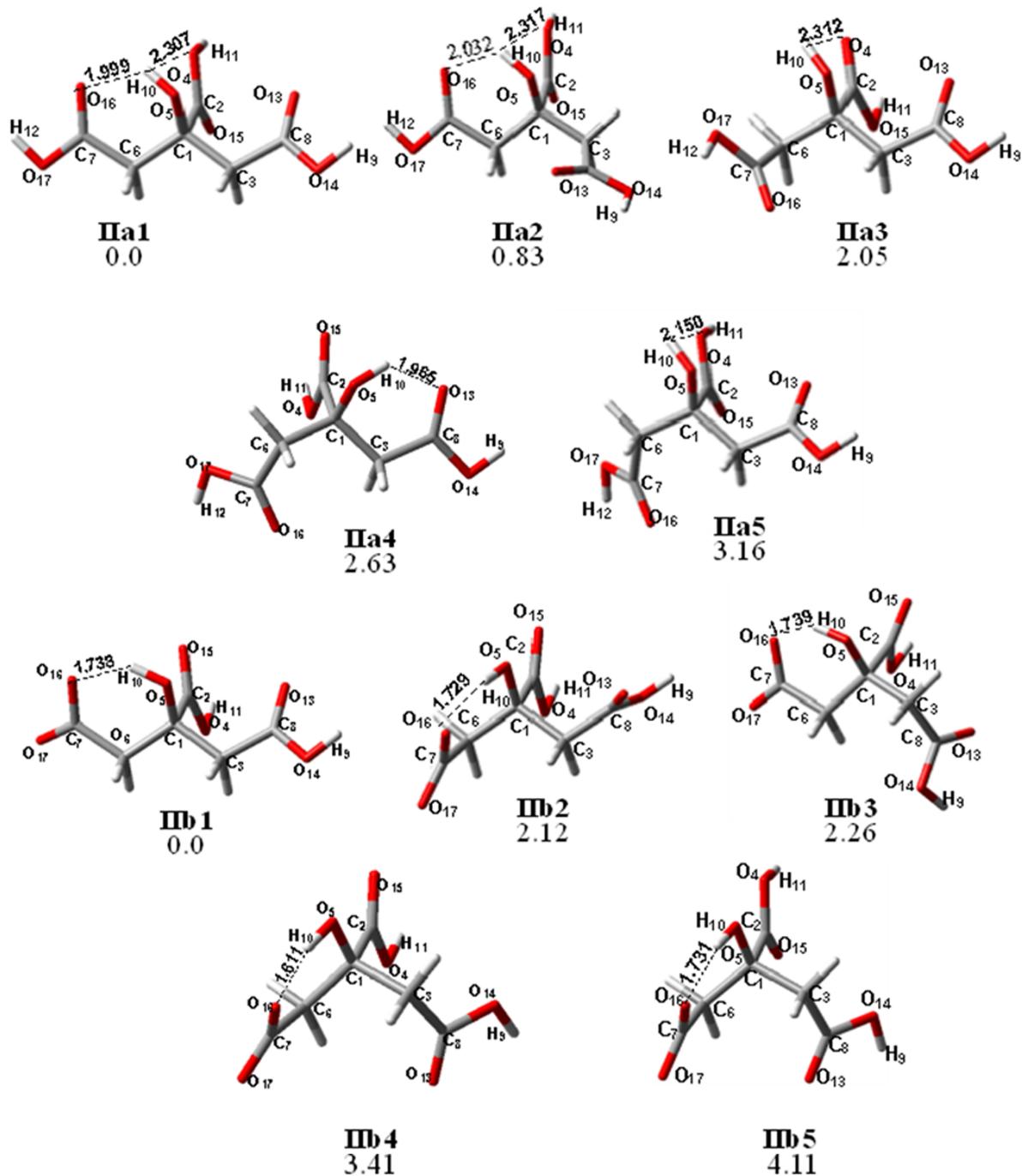


Part B

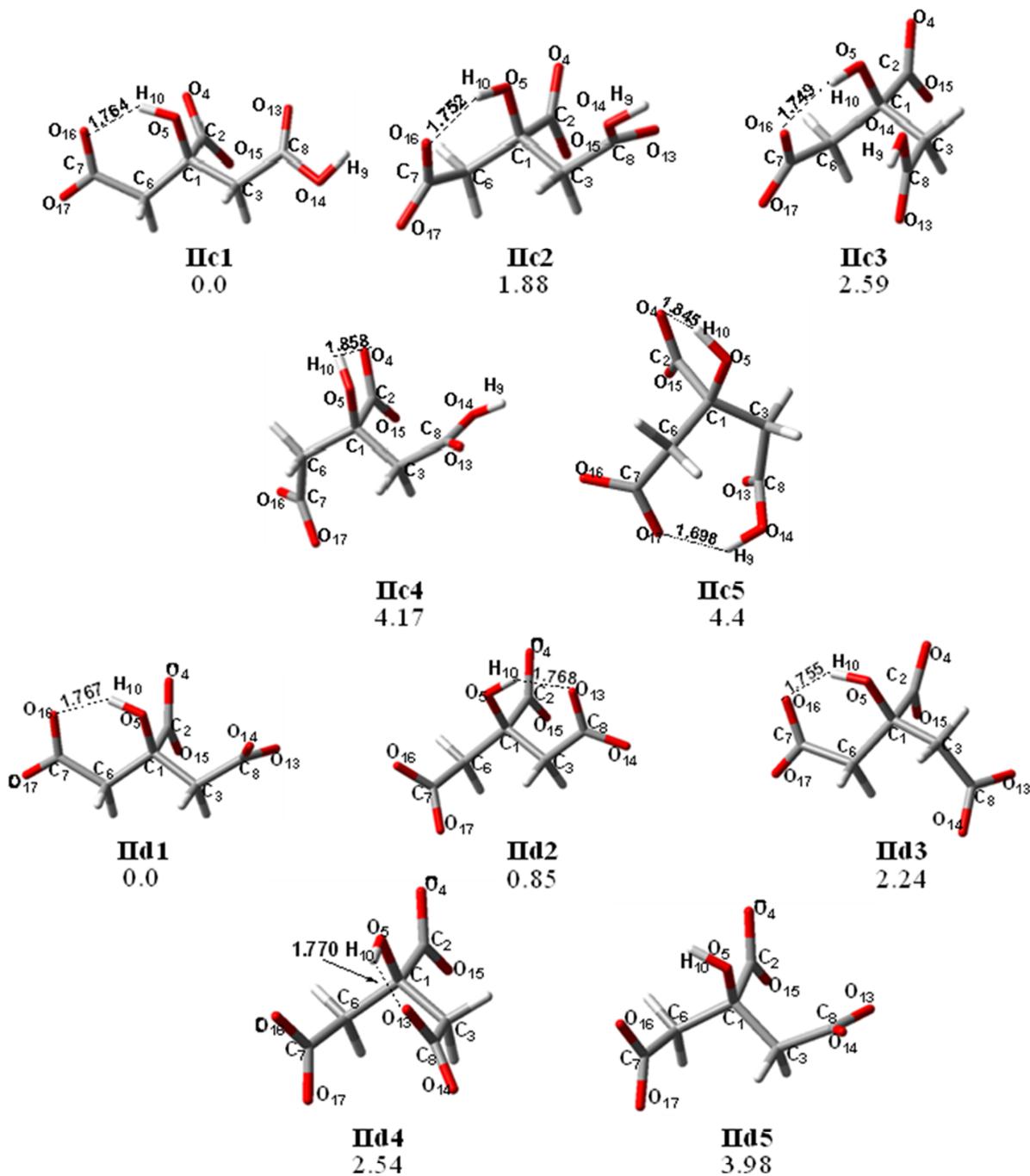
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Fig. S1: Selected conformers after clusterization for citric acid **Ia1** to **Ia5**, dihydrogen citrate from **Ib1** to **Ib5**, hydrogen citrate from **Ic1** to **Ic5** and citrate from **Id1** to **Id5** in the MM2* gas phase calculations. Relative energies are given in kcal/mol.

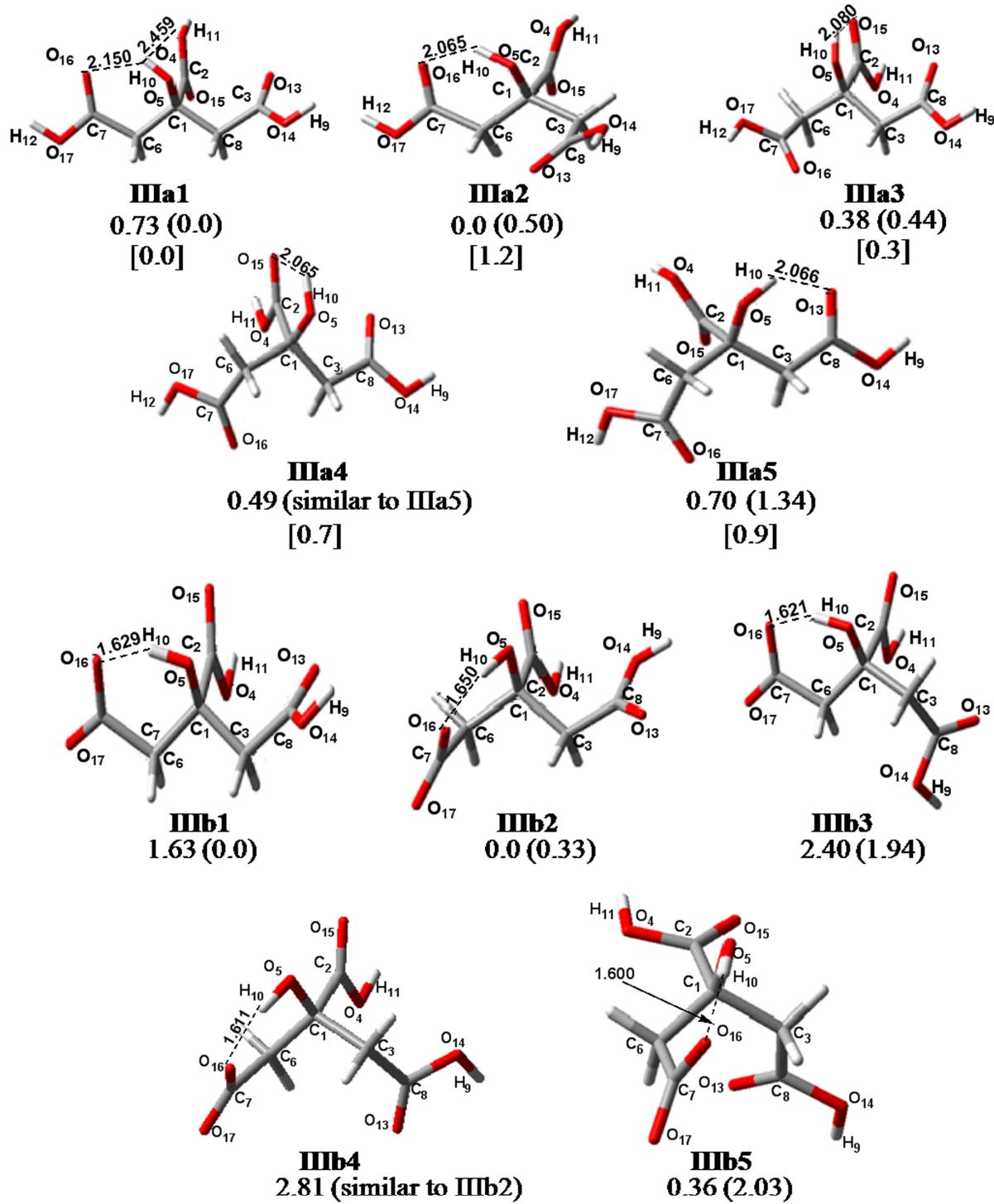


Part A

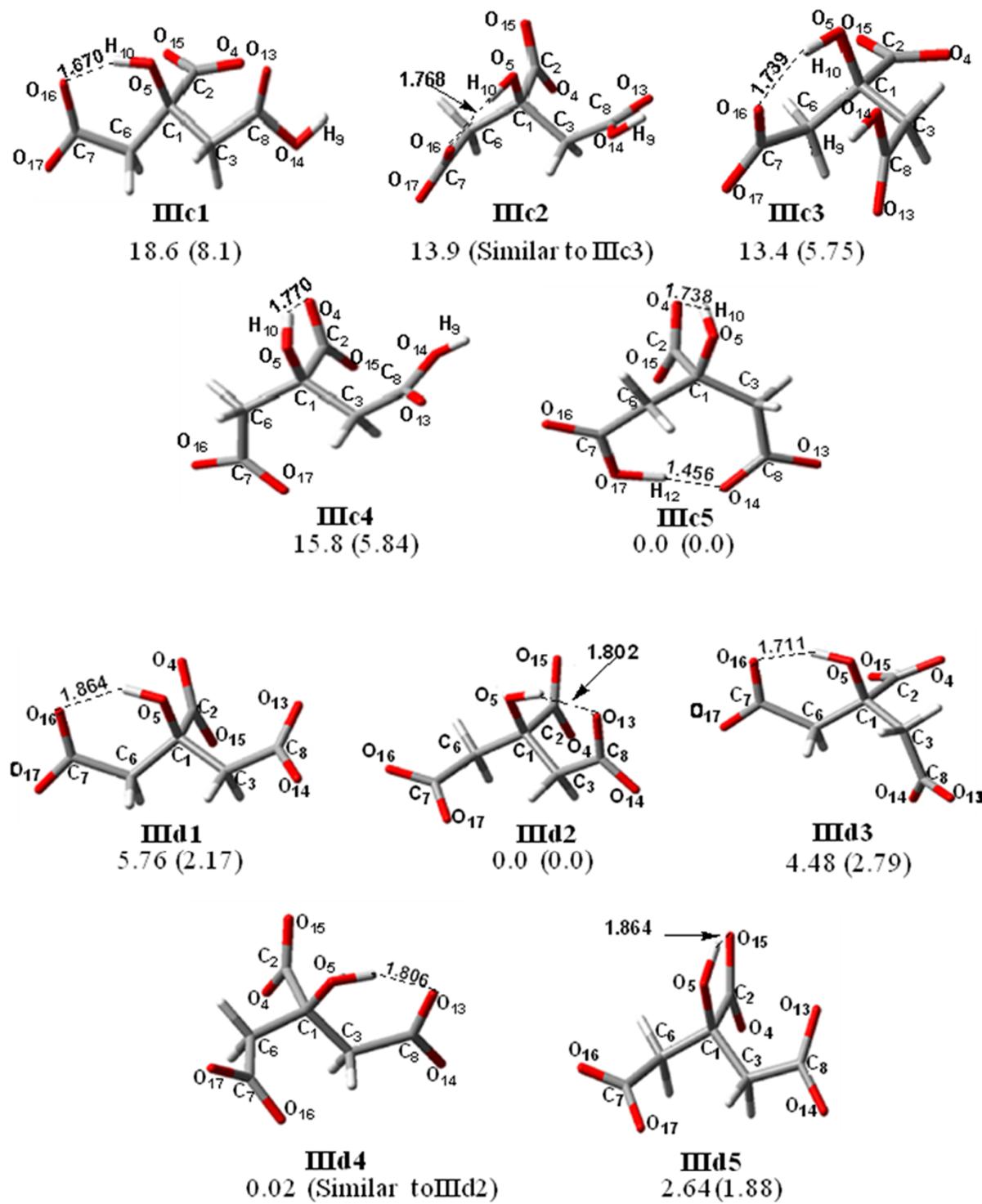


Part B

Fig. S2: Selected conformers after clusterization for citric acid **IIa1** to **IIa5**, dihydrogen citrate from **IIb1** to **IIb5**, hydrogen citrate from **IIc1** to **IIc5** and citrate from **IIId1** to **IIId5** in MM2* aqueous phase calculation. Relative energies are given in kcal/mol.



Part A



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Relative energies of gas phase and aqueous phase () are given in kcal/mol. Relative MP2 energies in aqueous phase are given in [].