Supporting Material

On the Different Roles of Anions and Cations in the Solvation of Enzymes in Ionic Liquids

Marco Klähn,* Geraldine S. Lim, Abirami Seduraman and Ping Wu

Institute of High Performance Computing, 1 Fusionopolis Way, #16-16, Connexis, Singapore 138632, Rep. of Singapore

* To whom correspondence should be addressed. Phone: (65) 6419 1468. Fax: (65) 6463 2536. E-mail: marco@ihpc.a-star.edu.sg.

Complete reference (48):

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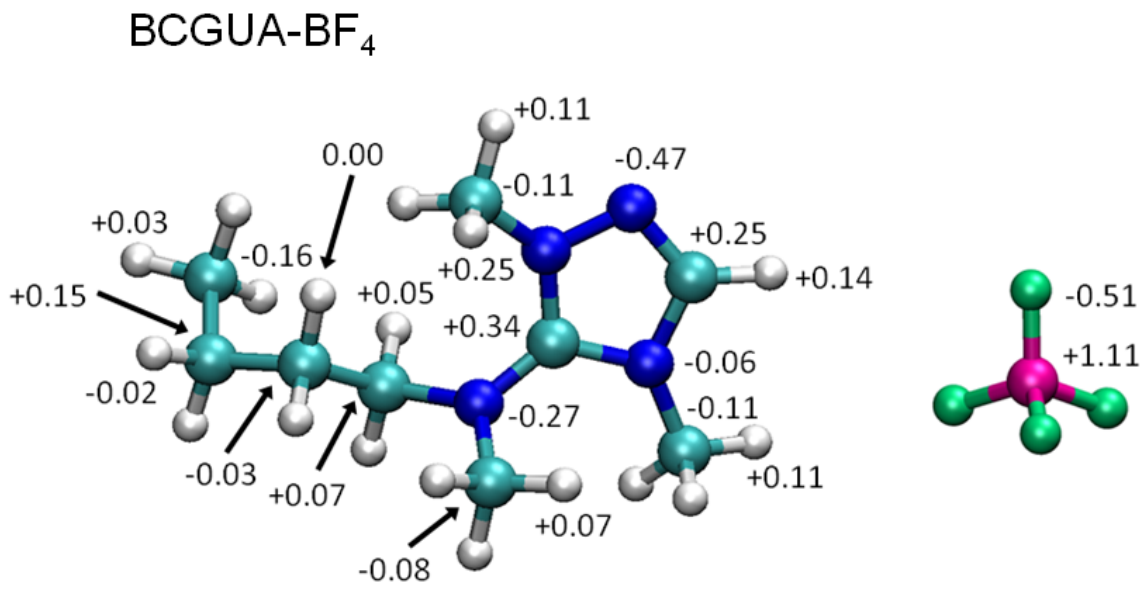

Figure S1. Liquid phase partial charges for BCGUA-BF_4 that were used for the force field. The given partial charges reproduce the electrostatic potential of the ions (ESP charges) in the actual liquid phase and were derived with a QM/MM approach. For chemically equivalent atoms, only the average charge is displayed. Partial charges are given as fractions of the elementary charge.

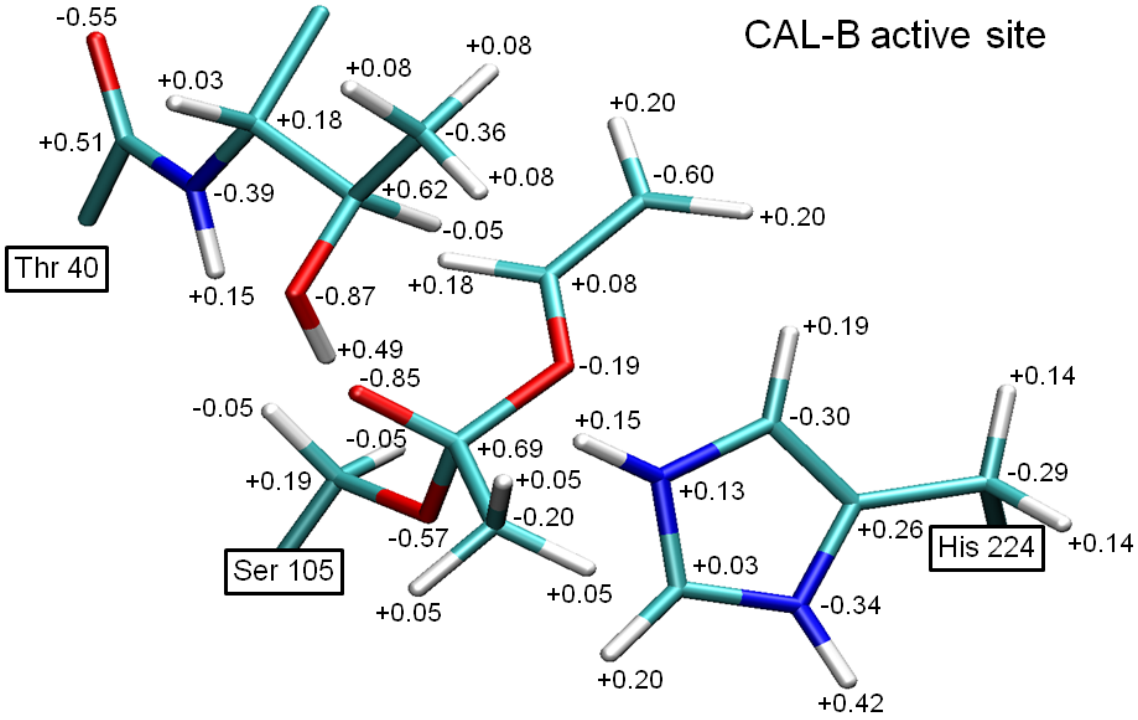

Figure S2. Partial charges in the active site of CAL-B for Ser 105, His 224 and Thr 40 that were used for the force field. The displayed structure represents a reaction intermediate, in which Ser 105 was acetylated with vinyl acetate. The latter two residues form strong hydrogen bonds with the substrate. The given partial charges reproduce the electrostatic potential of the residues (ESP charges) in the active site of CAL-B solvated in water, and were derived with a QM/MM approach. For chemically equivalent atoms, the average charge is displayed. Partial charges are given as fractions of the elementary charge.