An Intermolecular Potential for Binding of Protonated Peptides Ions with Perfluorinated Hydrocarbon Surfaces

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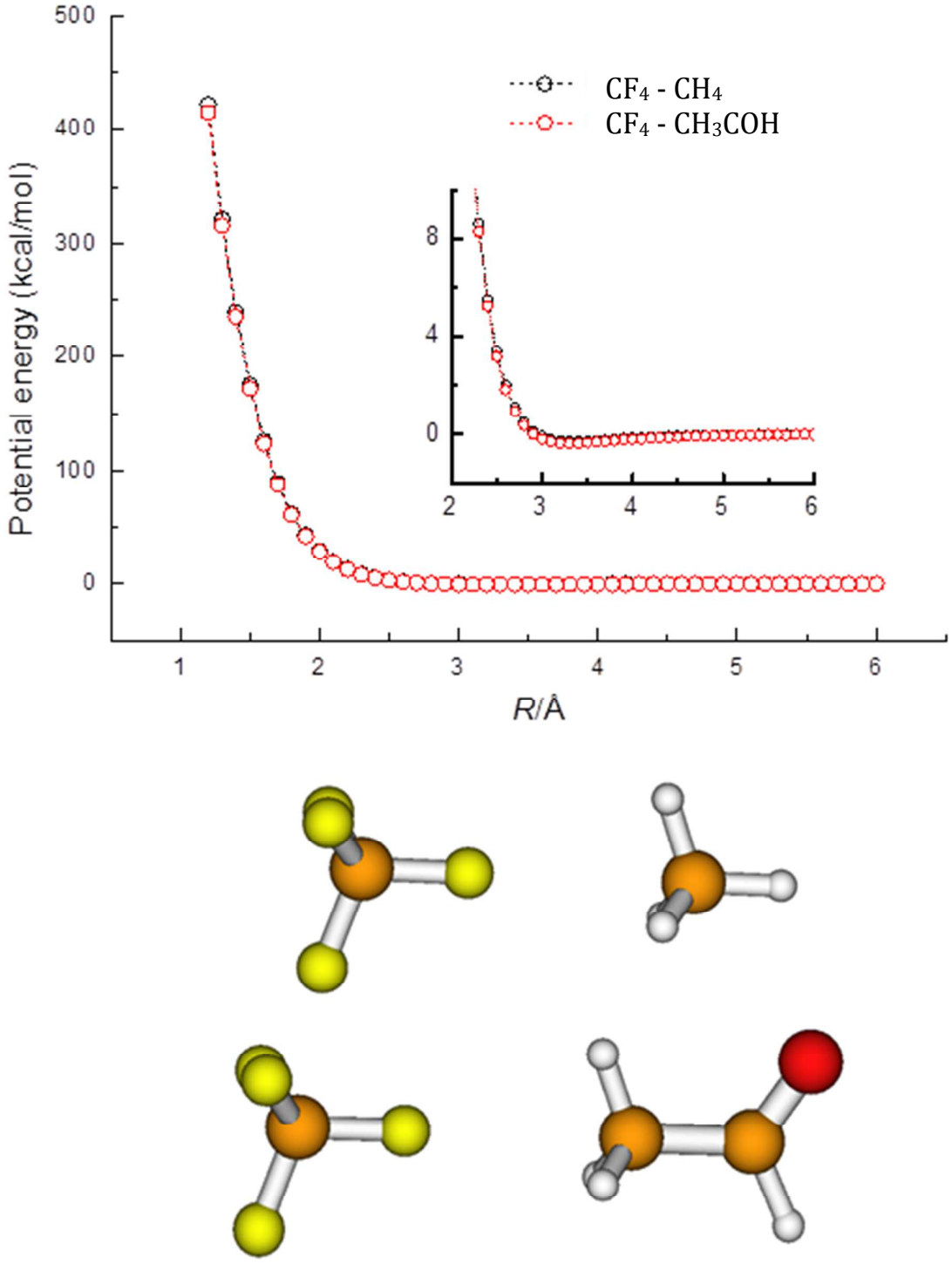

Figure S1: Comparison of MP2/aug-cc-pVTZ potential energy curves for a F-atom of CF_4 interacting with a C-atom of CH_4 and CH_3CHO.

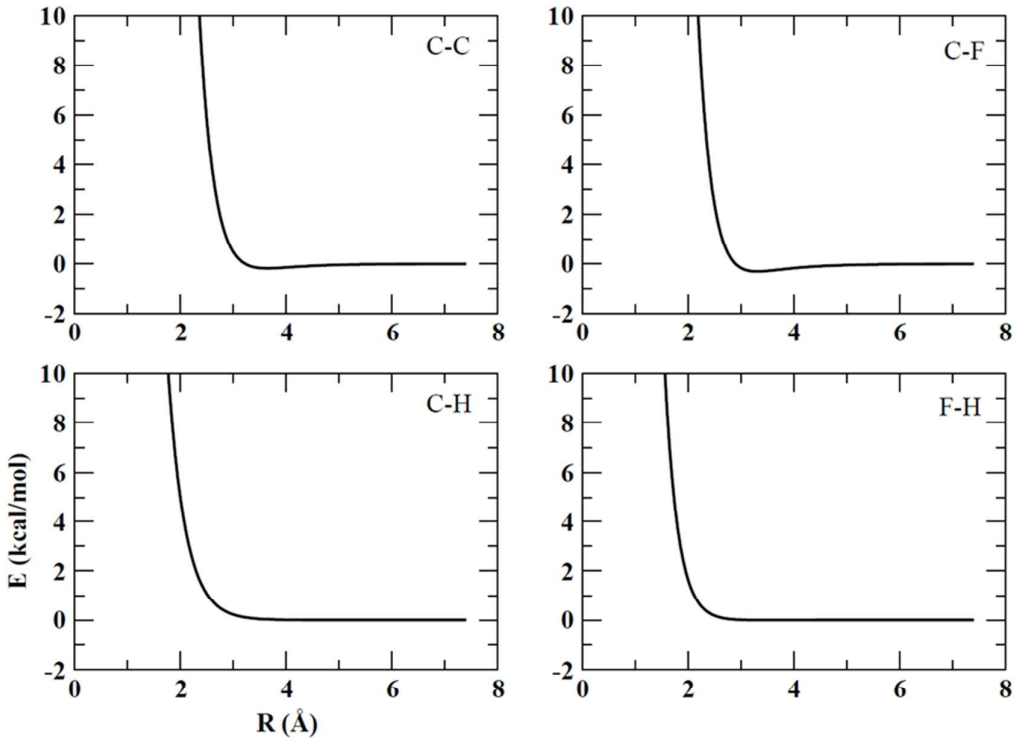

Figure S2. Two-body potentials obtained from the CH_4/CF_4 fitting.

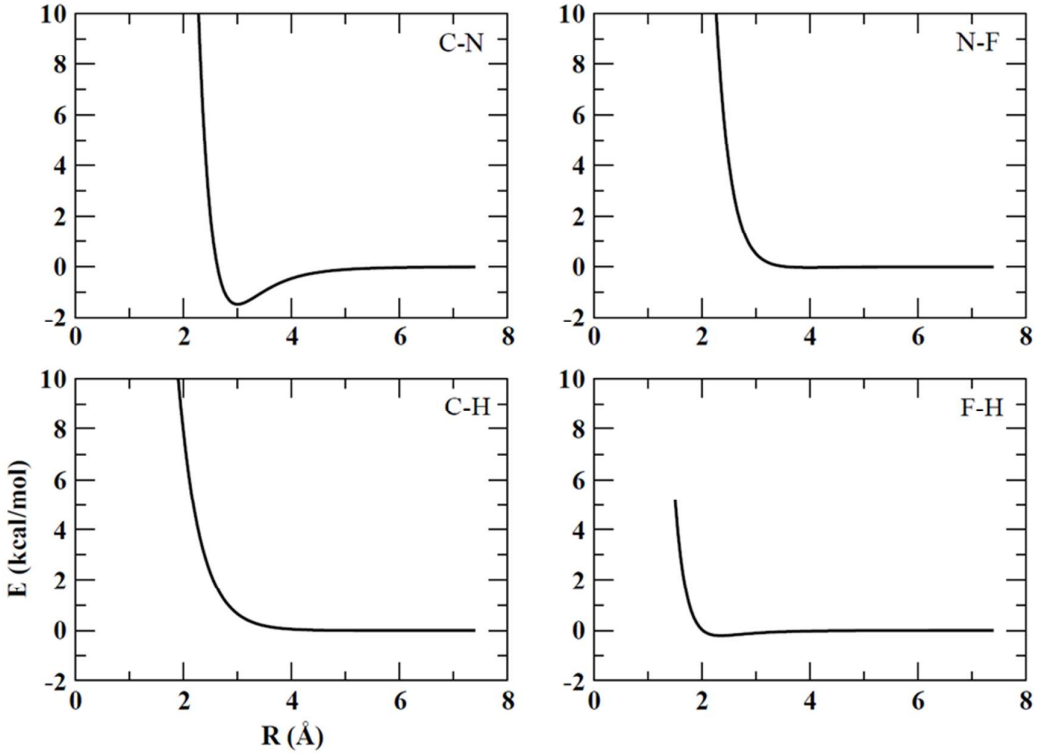

Figure S3. Two-body potentials obtained from the NH_3/CF_4 fitting.

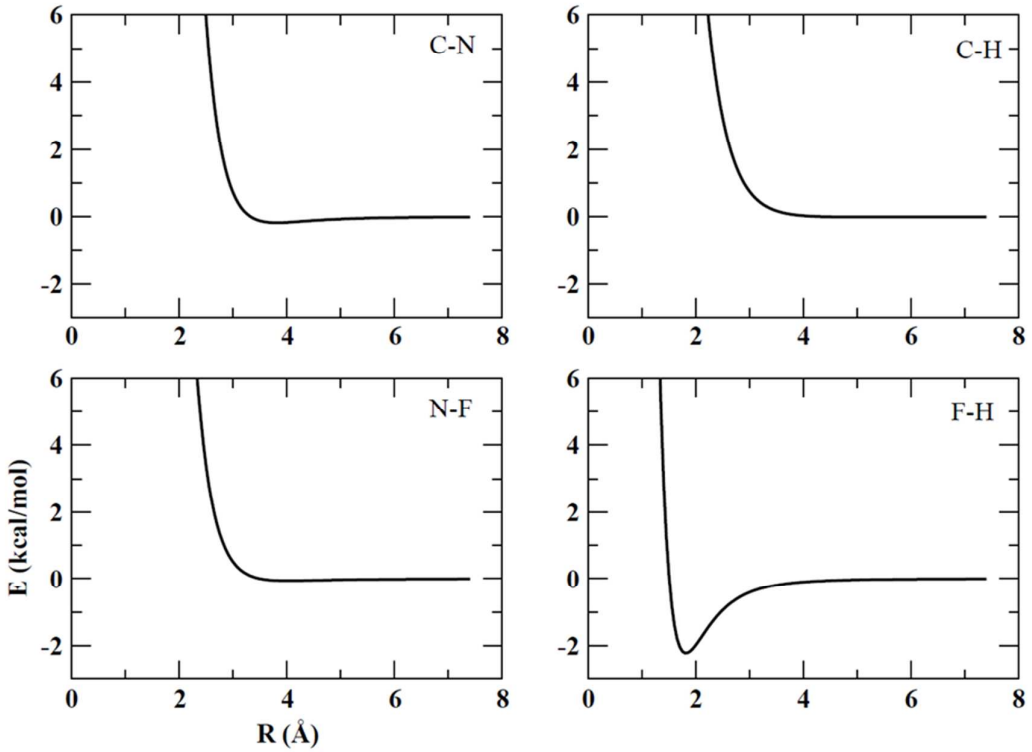

Figure S4. Two-body potentials obtained from the NH_4^+/CF_4 fitting.

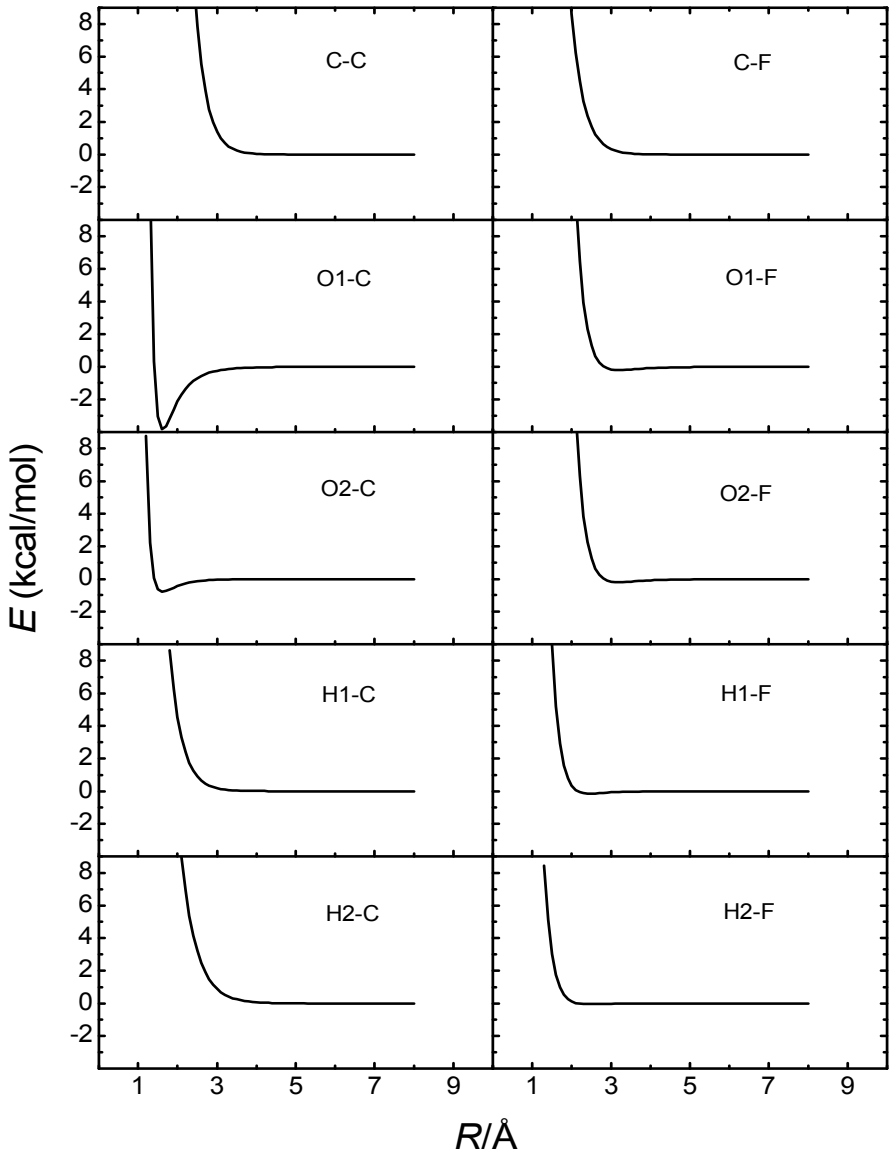

Figure S5. Two-body potentials obtained from the HCOOH/CF_4 fitting. O1 and O2 are carbonyl and hydroxyl oxygens, respectively. H1 and H2 are the carbonyl and hydroxyl hydrogens, respectively.

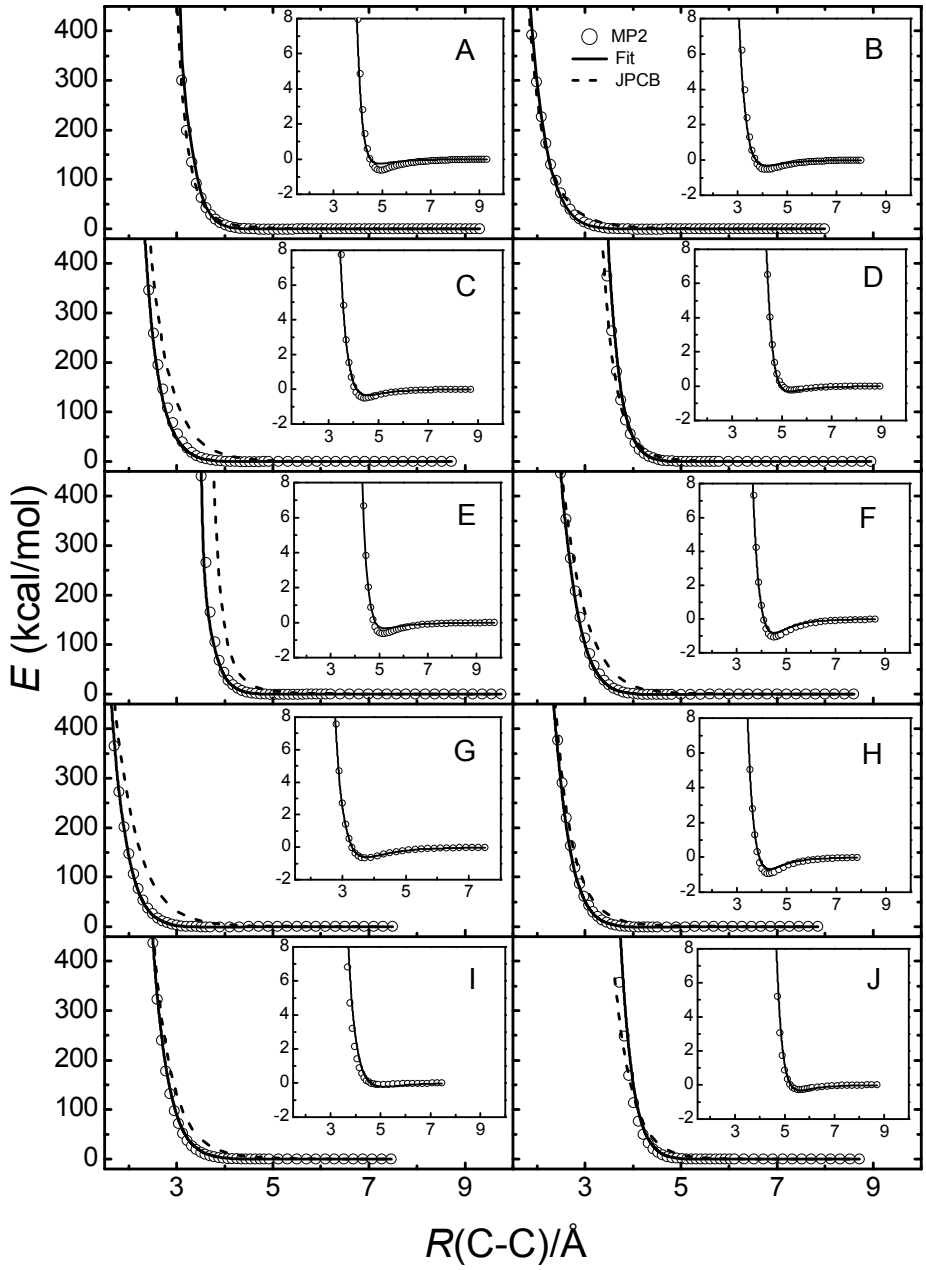

Figure S6. For the $HCOOH/CF_4$ system: a comparison between our present potential (solid lines) and that reported in JPC B 2005, 109, 8320 (dashed lines). The insets do not show the JPC-B data.

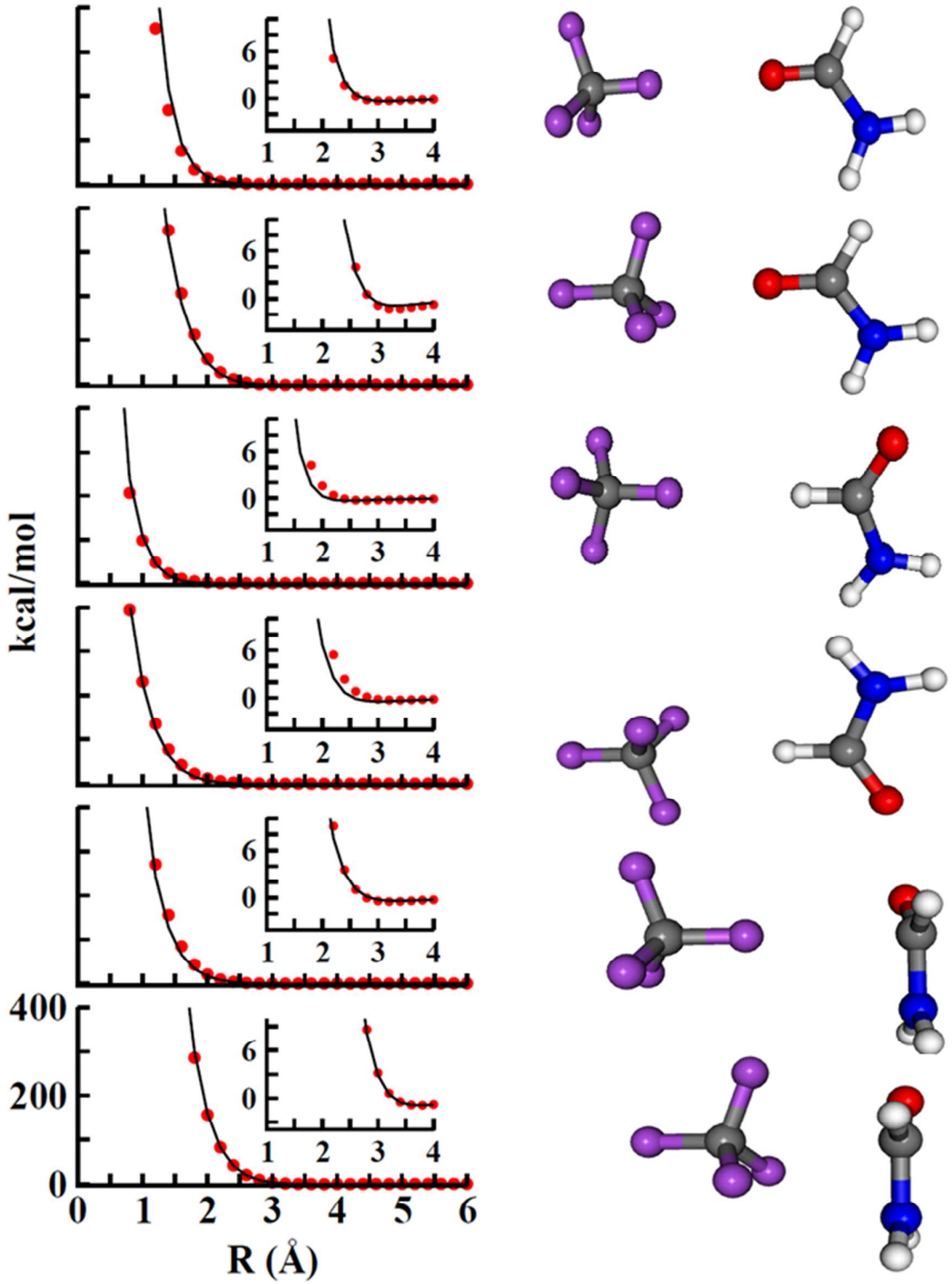

Figure S7: Comparison between IPECs calculated at the MP2/aug-cc-pVTZ level (solid circles) for CF_4 interacting with $HCONH_2$ and those predicted with the analytic potentials (solid lines) using parameters listed in Table 2.

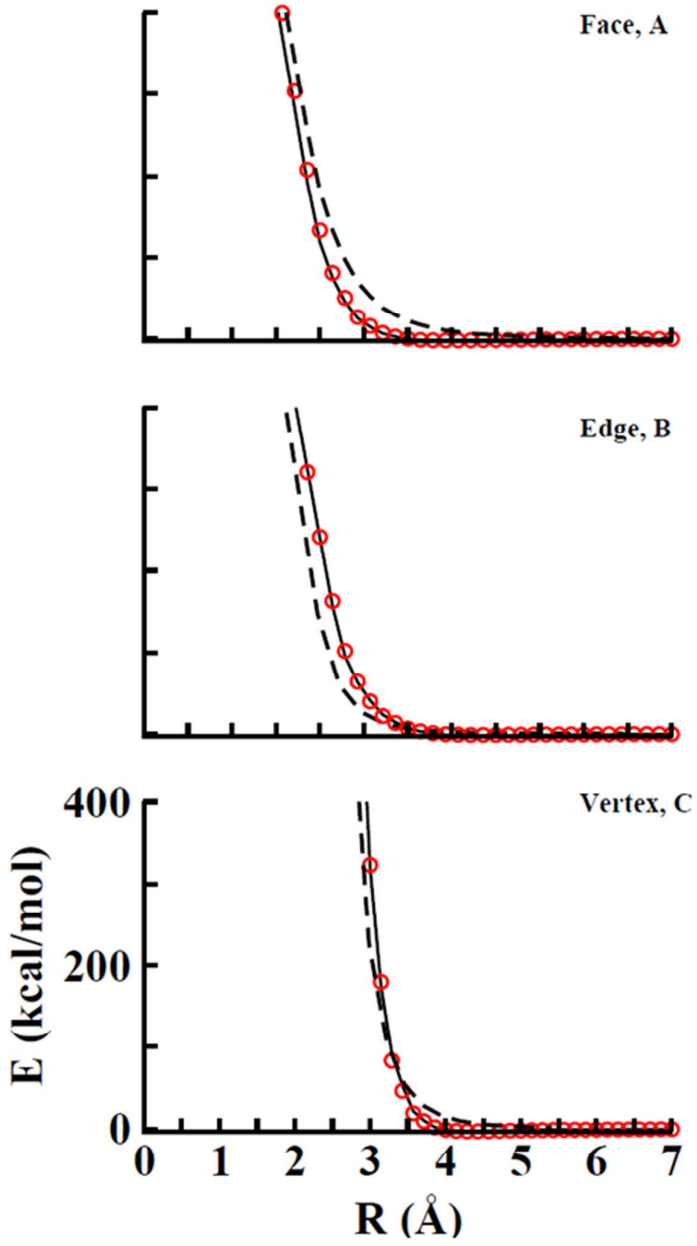

Figure S8: For the NH_4^+/CF_4 system: a comparison between our present potential (solid lines) and that reported in ref. 97 (dashed lines), for the orientations considered in the latter. The points are the MP2 calculations. Both the current and previous identifications are given.

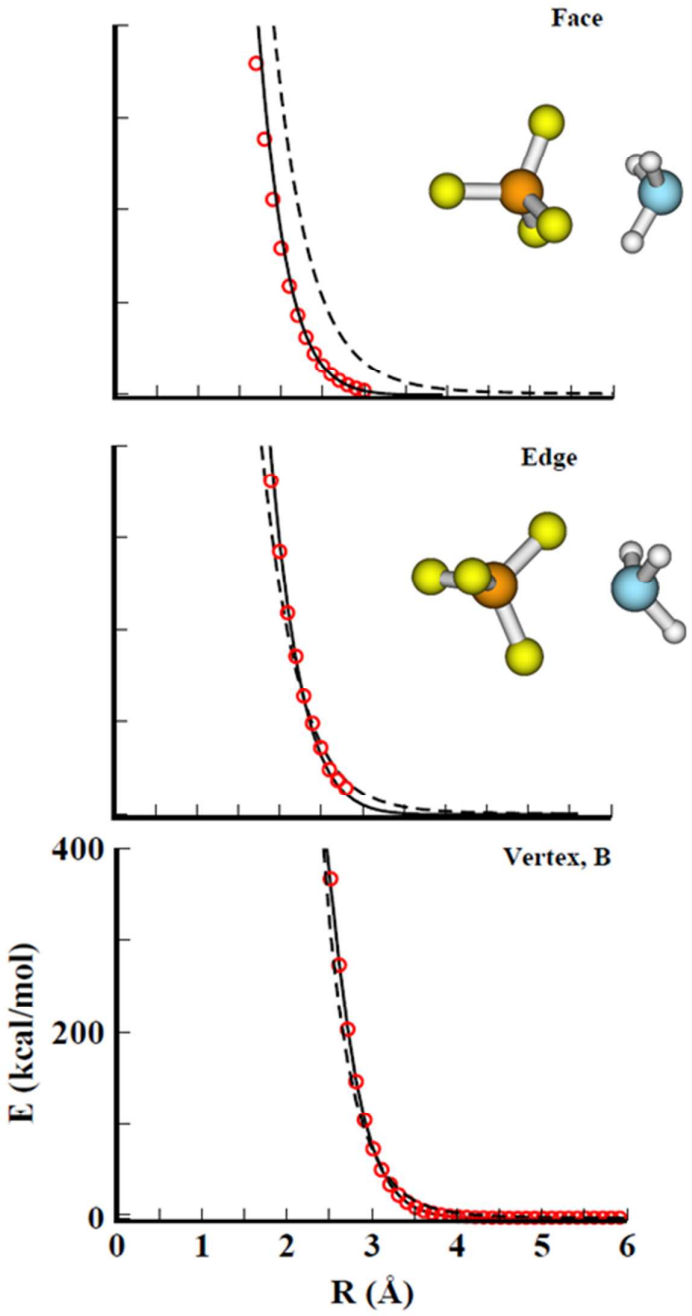

Figure S9: For the NH_3/CF_4 system: a comparison between our present potential (solid line) and that reported in ref. 97 (dashed lines), for the orientations considered in the latter. The points are from MP2 calculations. Both the current and previous identifications of the orientations are given.

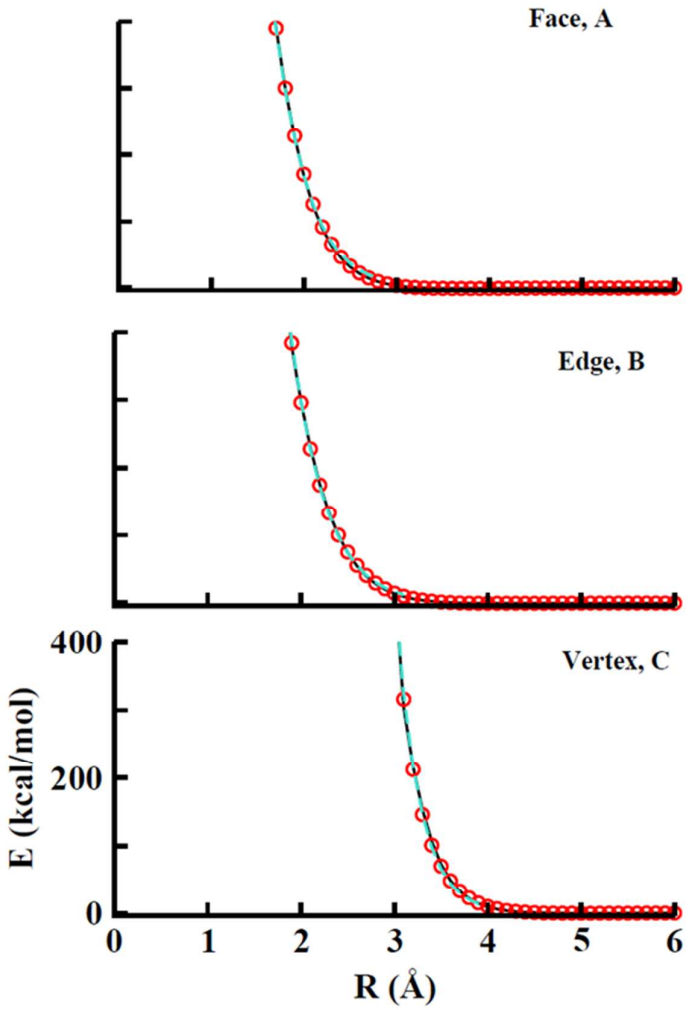

Figure S10: For the CH_4/CF_4 system: a comparison between our present potential (solid lines) and that reported in ref. 97 (dashed lines), for the orientations considered in the latter. The points are from MP2 calculations. Both the current and previous identifications of the orientations are given.