Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Estimating successive pK_a values of polyprotic acids from *ab initio* molecular dynamics using metadynamics: the dissociation of phthalic acid and its isomers

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SUPPLEMENTARY INFORMATION

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CONTENTS:

Table S1: The number of water molecules and dimension of the simulation cell for the acid molecules investigated.

Movie S1: Movie file of the configurations along the trajectory of the dissociation of benzoic acid.

Figure S1: Structure of the contact-ion pair formed during the dissociation of benzoic acid.

Movie S2: Movie file of the configurations along the trajectory of the first dissociation of phthalic acid.

Movie S2: Movie file of the configurations along the trajectory of the second dissociation of phthalic acid.

Figure S2: The O-H distances of the contact-ion pair formed during the first and second dissociation reaction of phthalic acid.

Figure S3: The free energy profiles for the first and second acid dissociation of (a) isophthalic acid (b) terephthalic acid.

Table S1: The number of water molecules and dimension of the simulation cell for the acid molecules investigated.

Acid	**Cell size (Å)**	**No. of water molecules**
Benzoic	11.97	52
Phthalic	11.94	51
Isophthalic	11.94	51
Terephthalic	11.94	51

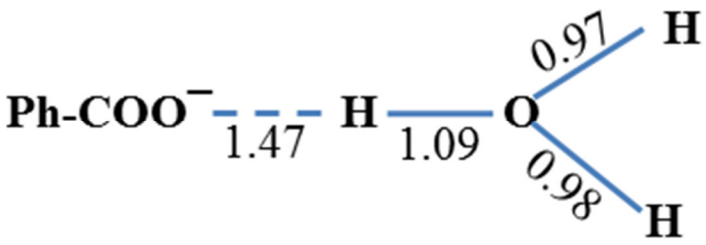

Figure S1: Structure of the contact-ion pair formed during the dissociation of benzoic acid. Distances are given in angstroms.

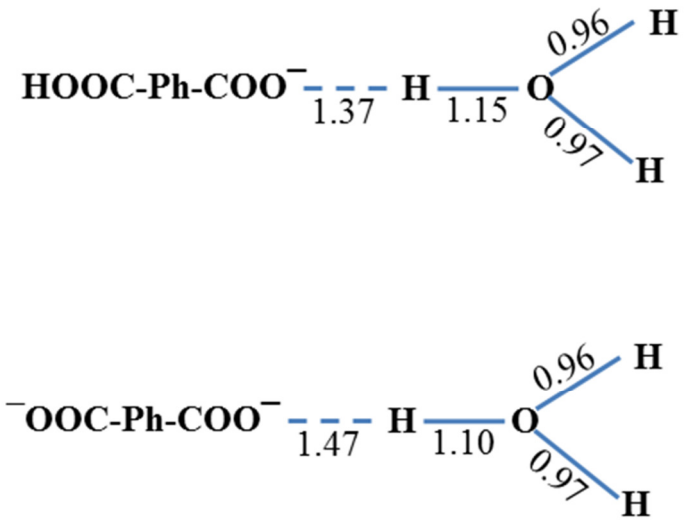

Figure S2: The O-H distances (in angstroms) of the contact-ion pair formed during the first and second dissociation reaction of phthalic acid.

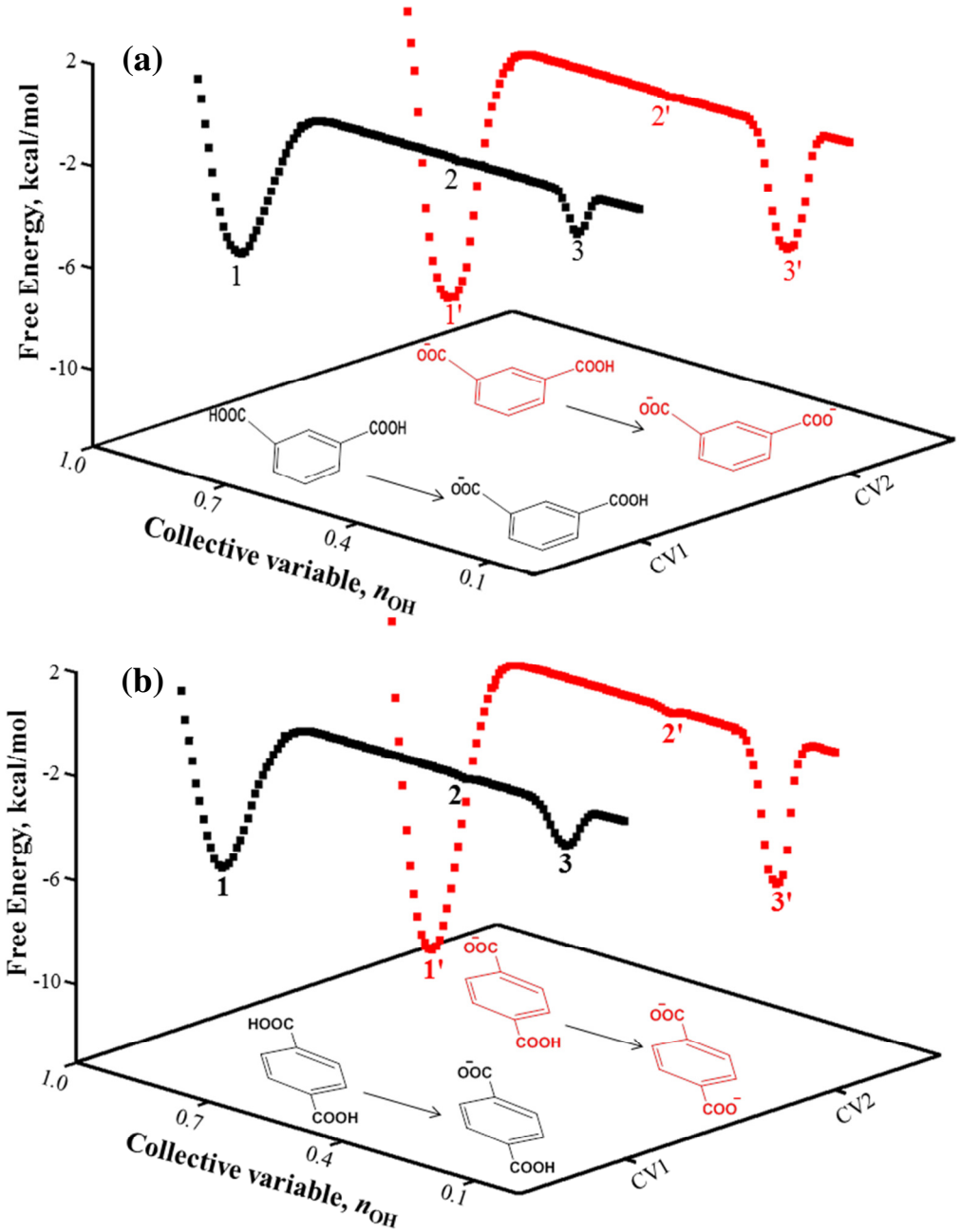

Figure S3: The free energy profiles for the first and second acid dissociation of (a) isophthalic acid (b) terephthalic acid.