

Electronic Supplementary Information.

Figure Captions.

Figure A: Computed (MP2/6-31+G*) structures of doubly-hydrated complexes of conformer 2 of 1-(R)-phenylethylamine. Relative energies (in kJ mol^{-1}) computed through MP2/6-311++G** single-point calculations, include a zero-point correction (B3LYP/6-31+G*).

Figure B: Convergence plots of R_{01} (CIS using the velocity representation of the transition dipole moments) versus number of basis functions for the two conformers of 1-phenylethylamine.

Figure C: Convergence plots of R_{01} (CIS using the velocity representation of the transition dipole moments) versus number of basis functions for the singly hydrated complexes of 1-phenylethylamine.

Figure D: Convergence plots of R_{01} (CIS using the velocity representation of the transition dipole moments) versus number of basis functions for doubly hydrated complexes of conformer 1 of 1-phenylethylamine.

Figure E: Convergence plots of R_{01} (CIS using the velocity representation of the transition dipole moments) versus number of basis functions for doubly hydrated complexes of conformer 2 of 1-phenylethylamine.

Figure F: Convergence plots of R_{01} (CIS using the velocity representation of the transition dipole moments) versus number of basis functions for bare and singly hydrated complexes of protonated 1-phenylethylamine.

Figure G: Convergence plots of R_{01} (CIS using the velocity representation of the transition dipole moments) versus number of basis functions for doubly and triply hydrated complexes of protonated 1-phenylethylamine.

Figure H: Convergence plots of R_{01} (CIS using the velocity representation of the transition dipole moments) versus number of basis functions for bare 1-phenylethanol and its singly and doubly hydrated complexes.

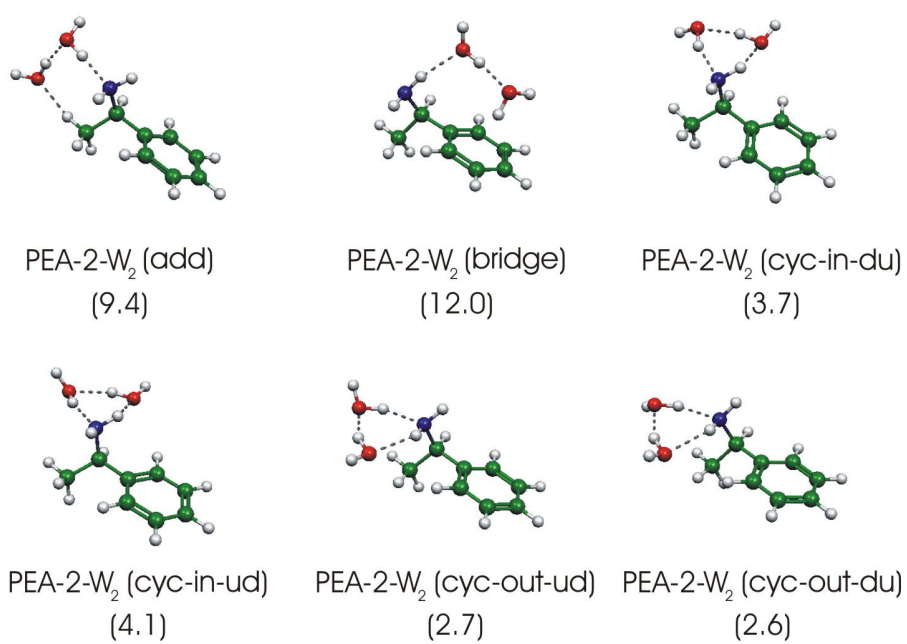


Figure A.

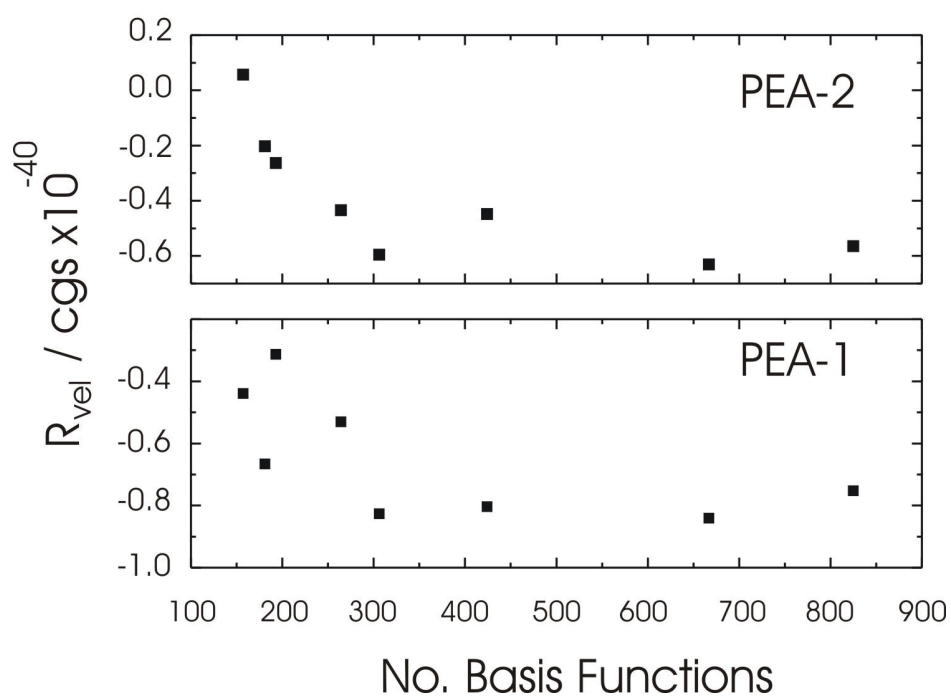


Figure B.

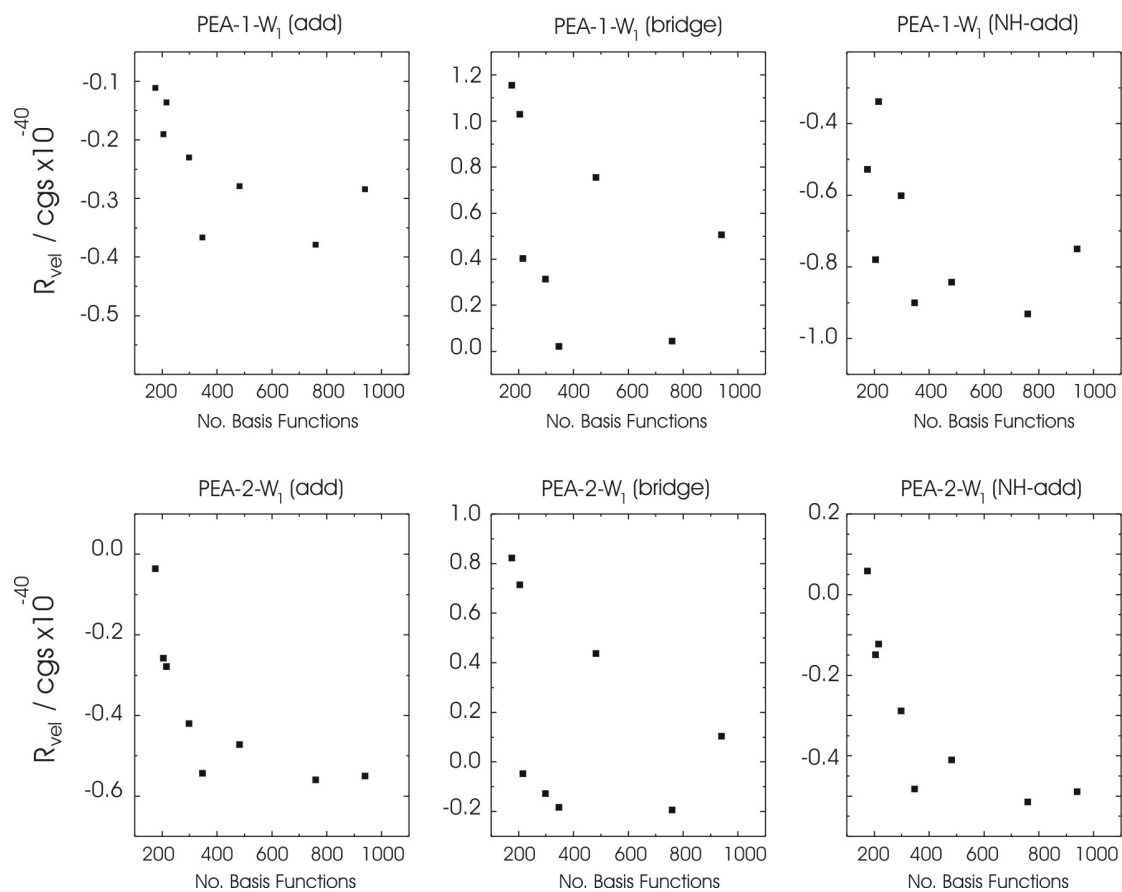


Figure C.

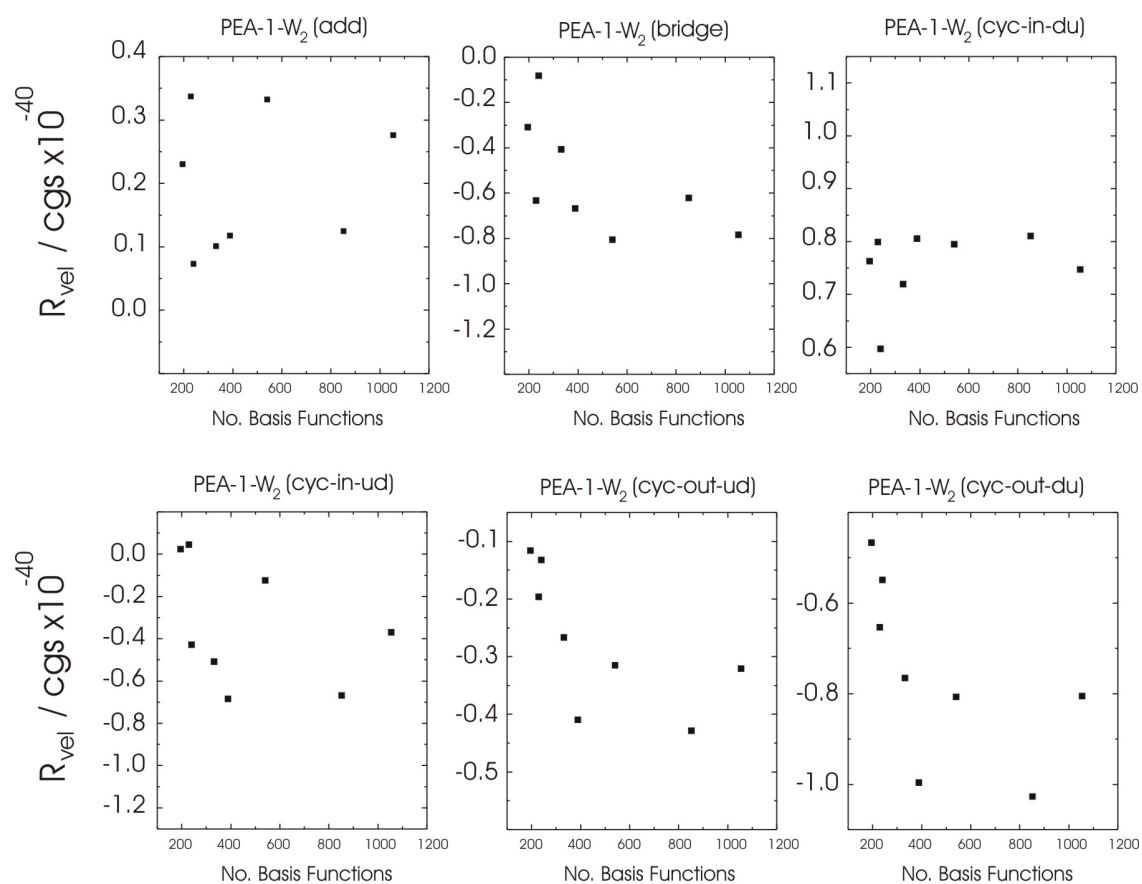


Figure D.

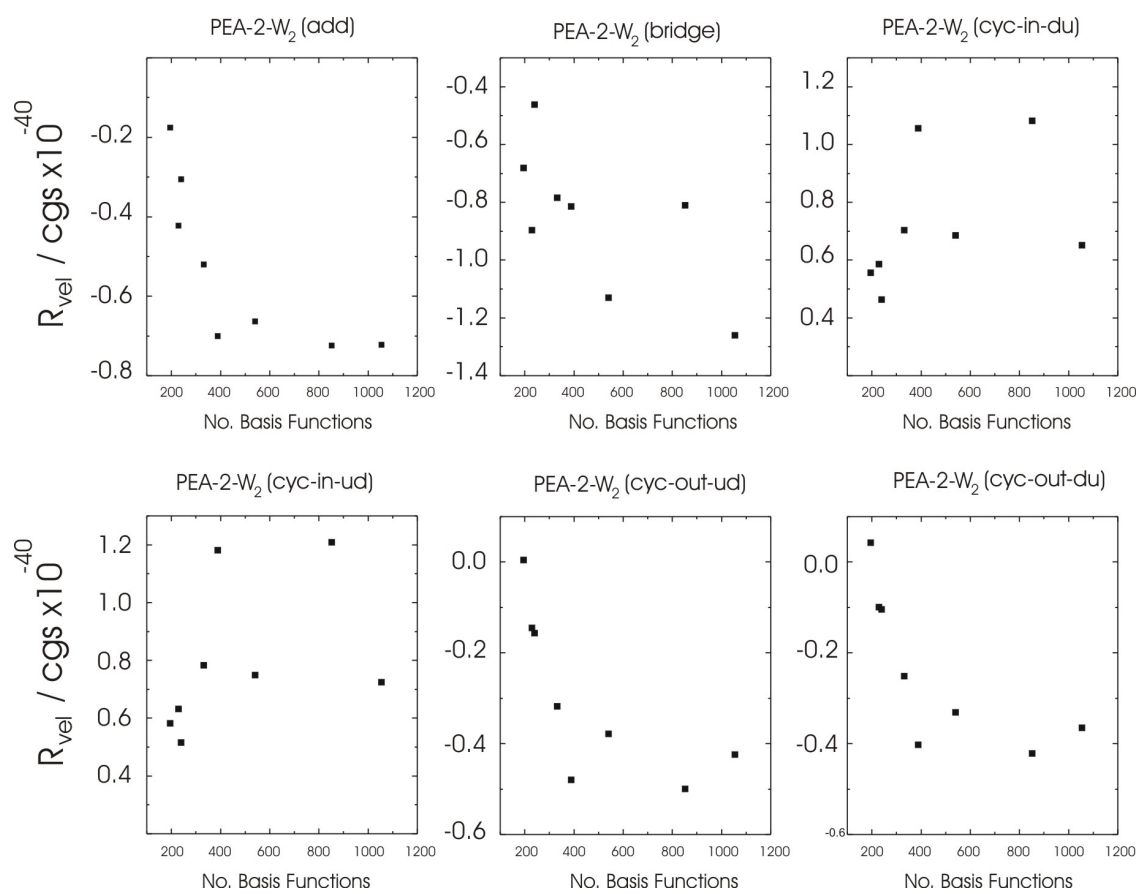


Figure E.

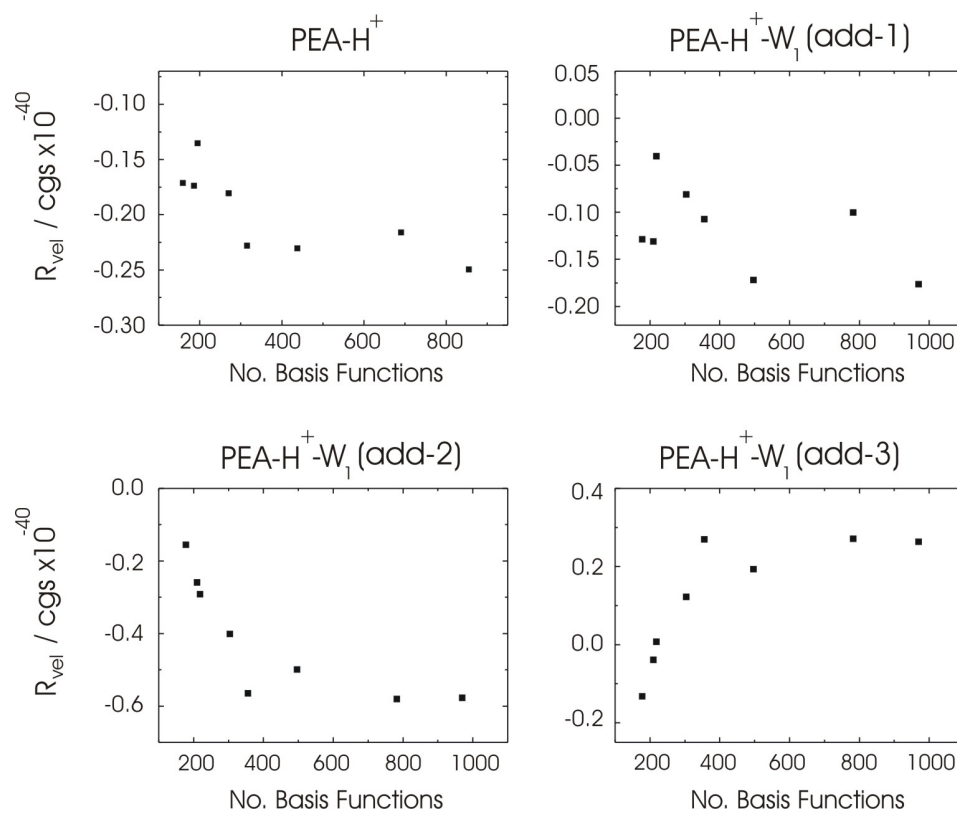


Figure F.

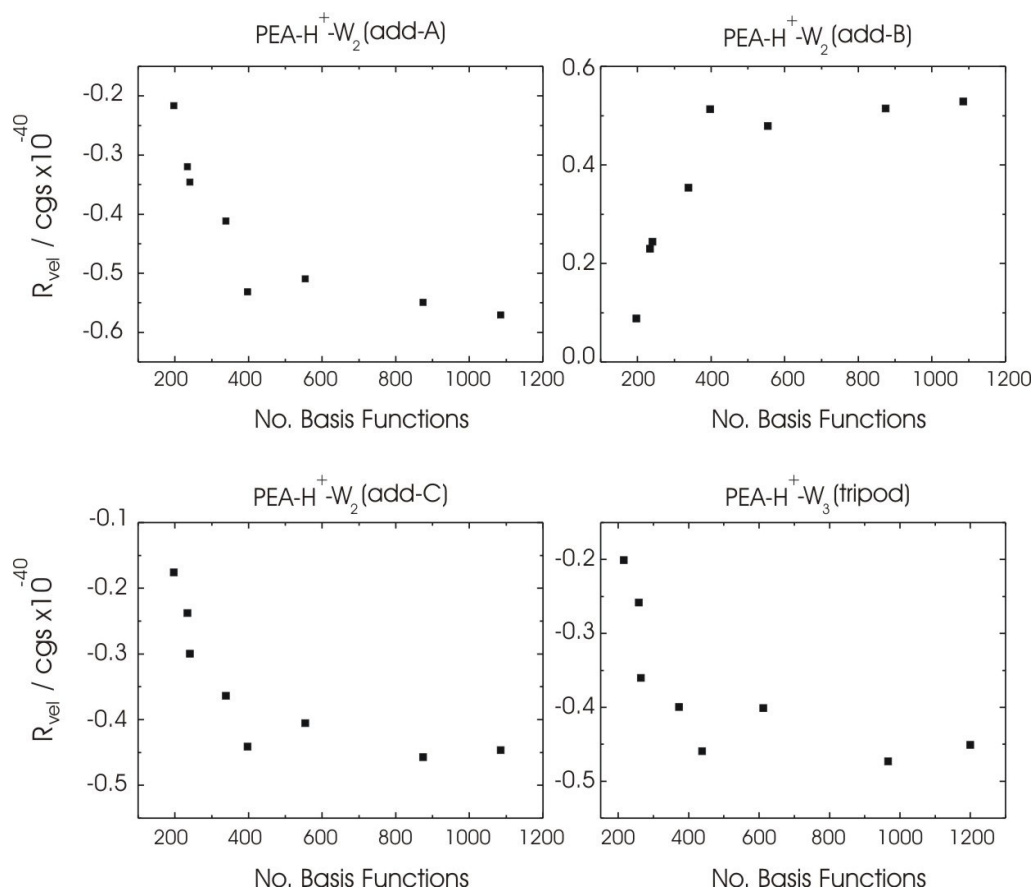


Figure G.

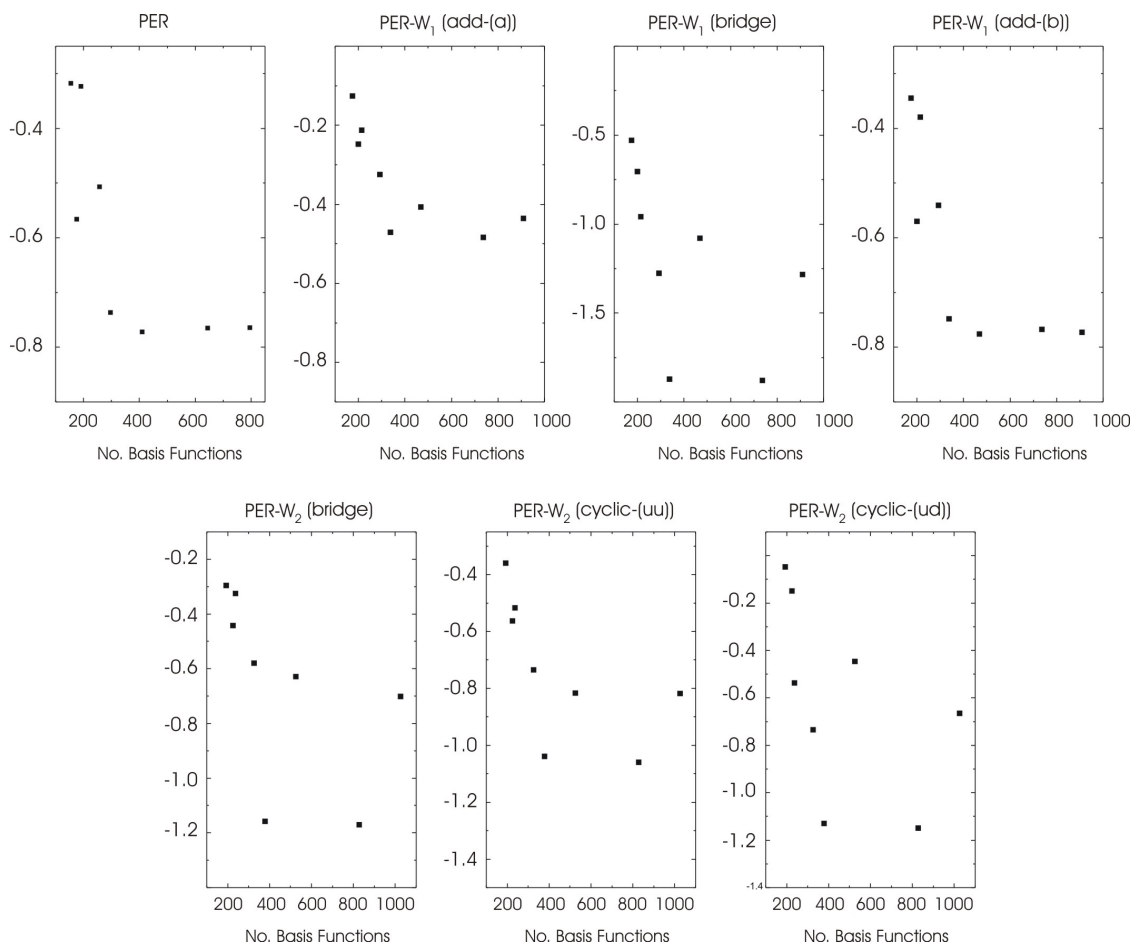


Figure H.