Direct and Indirect Effects of Dispersion Interactions on the Electric Properties of Weakly Bound Complexes

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Table S1. Interaction energies (in kJ·mol^{-1}) of the canonical form of p-aminobenzoic acid (pABA-c) with benzene (Be) obtained with various atomic basis sets by selected WF-based and DFT methods using the equilibrium geometry. CP stands for the counterpoise-corrected values.

Basis sets	HF	B3LYP-D	B97-D	ωB97XD	B2PLYP-D	M06-2X	LC-BOP-LRD	MP2	SCS-MP2
Sadlej POL	10.5	-32.7	-33.7	-33.5	-82.8	-28.1	-28.5	-83.2	-73.7
Sadlej POL (CP)	18.7	-17.6	-20.3	-21.8	-26.8	-16.6	-21.4	-26.9	-16.9
apc1/aug-cc-pVDZ	11.8	-28.6	-32.0	-36.4	-71.3	-36.1	-37.7	-46.9	-37.2
apc1/aug-cc-pVDZ (CP)	18.9	-15.2	-17.8	-21.4	-24.4	-19.0	-22.3	-26.7	-16.6
pc2/cc-pVTZ	16.4	-17.2	-19.2	-21.1	-33.6	-17.2	-23.2	-31.9	-22.3
pc2/cc-pVTZ (CP)	19.3	-16.1	-18.2	-20.2	-23.0	-16.0	-21.4	-23.8	-14.3
apc2/aug-cc-pVTZ	17.6	-18.5	-19.7	-21.9	-24.1	-17.9	-22.7	-37.2	-27.4
apc2/aug-cc-pVTZ (CP)	18.9	-17.7	-18.7	-20.9	-18.1	-16.8	-21.3	-28.7	-18.3

Table S2. Interaction energies (in kJ·mol^{-1}) of the zwitter-ionic form of p-aminobenzoic acid (pABA-z) with benzene (Be) obtained with various atomic basis sets by selected WF-based and DFT methods f the equilibrium geometry. CP stands for the counterpoise-corrected values.

Basis sets	HF	B3LYP-D	B97-D	ωB97XD	B2PLYP-D	M06-2X	LC-BOP-LRD	MP2	SCS-MP2
Sadlej POL	-32.3	-95.9	-90.4	-92.9	-150.4	-88.2	-43.9	-150.8	-136.4
Sadlej POL (CP)	-21.3	-75.2	-72.1	-76.8	-80.9	-72.3	-76.5	-81.0	-66.0
apc1/aug-cc-pVDZ	-31.2	-82.6	-88.4	-96.5	-134.7	-97.3	-98.3	-109.8	-95.1
apc1/aug-cc-pVDZ (CP)	-21.5	-81.9	-70.3	-77.5	-77.3	-76.0	-77.2	-81.0	-66.0
pc2/cc-pVTZ	-27.0	-76.0	-72.3	-77.2	-92.5	-74.5	-79.6	-95.1	-80.2
pc2/cc-pVTZ (CP)	-21.4	-74.2	-70.5	-75.5	-78.4	-72.6	-75.1	-80.7	-66.0
apc2/aug-cc-pVTZ	-22.9	NA	-72.2	-77.6	NA	-75.5	-79.1	-98.3	-83.6
apc2/aug-cc-pVTZ (CP)	-21.3	NA	-70.9	-76.4	NA	-73.7	-75.7	-86.4	-70.8

Table S3. Basis set dependence of the induced longitudinal dipole moment values (in a.u.) of the canonical form of p-aminobenzoic acid (pABA-c) with benzene (Be) calculated using the Sadlej's POL, aug-cc-pVXZ and Jensen's (aug)-pc-n series of atomic basis sets for WF-based and DFT methods, respectively. The optimized geometry of the complex is used. CP stands for the counterpoise-corrected values.

Basis set	RHF	B3LYP	CAM-B3LYP	LC-BOP	LC-BOP-LRD	MP2	SCS-MP2
Sadlej's POL	-0.106	-0.058	-0.112	-0.108	-0.112	-0.106	-0.105
Sadlej's POL (CP)	-0.108	-0.060	-0.117	-0.108	-0.111		
aug-pc-1/aug-cc-pVDZ	-0.107	-0.050	-0.106	-0.100	-0.103	-0.105	-0.103
aug-pc-1/aug-cc-pVDZ (CP)	-0.107	-0.055	-0.110	-0.105	-0.109		
pc-2/cc-pVTZ	-0.107	-0.053	-0.108	-0.101	-0.104	-0.108	-0.106
pc-2/cc-pVTZ (CP)	-0.104	-0.055	-0.109	-0.104	-0.107		
aug-pc-2/aug-cc-pVTZ	-0.108	-0.059	-0.112	-0.107	-0.110	-0.106	-0.104

Table S4. Basis set dependence of the induced longitudinal polarizability values (in a.u.) of the canonical form of p-aminobenzoic acid (pABA-c) with benzene (Be) calculated using the Sadlej's POL, aug-cc-pVXZ and Jensen's (aug)-pc-n series of atmoic basis sets for WF-based and DFT methods, respectively. The optimized geometry of the complex is used. CP stands for the counterpoise-corrected values.

Basis set	RHF	B3LYP	CAM-B3LYP	LC-BOP	LC-BOP-LRD	MP2	SCS-MP2
Sadlej's POL	-18.9	-14.3	-20.6	-19.2	-18.6	-19.8	-19.8
Sadlej's POL (CP)	-19.2	-14.3	-20.6	-19.5	-19.0		
aug-pc-1/aug-cc-pVDZ	-18.6	-13.3	-19.7	-18.5	-17.9	-19.3	-19.4
aug-pc-1/aug-cc-pVDZ (CP)	-19.2	-14.0	-20.3	-19.2	-18.6		
pc-2/cc-pVTZ	-16.2	-11.7	-17.8	-16.8	-16.3	-17.9	-17.9
pc-2/cc-pVTZ (CP)	-18.7	-14.0	-20.0	-18.9	-18.5		
aug-pc-2/aug-cc-pVTZ	-19.1	-14.1	-20.4	-19.3	-18.7	-19.9	-19.9

Table S5. Basis set dependence of the induced longitudinal first hyperpolarizability values (in a.u.) of the canonical form of p-aminobenzoic acid (pABA-c) with benzene (Be) calculated using the Sadlej's POL, aug-cc-pVXZ and Jensen's (aug)-pc-n series of atomic basis sets for WF-based and DFT methods, respectively. The optimized geometry of the complex is used.. CP stands for the counterpoise-corrected values.

Basis set	**RHF**	**B3LYP**	**CAM-B3LYP**	**LC-BOP**	**LC-BOP-LRD**	**MP2**	**SCS-MP2**
Sadlej's POL	-133	-112	-178	-162	-138±15	NA	-164
Sadlej's POL (CP)	-130	-106	-171	-165	-153±10		
aug-pc-1/aug-cc-pVDZ	-138	-111	-180	-168	-171	-201	-203
aug-pc-1/aug-cc-pVDZ (CP)	-131	-102	-171	-160	-167		
pc-2/cc-pVTZ	-131	-131	-196	-178	-182	-179	-184
pc-2/cc-pVTZ (CP)	-121	-111	-176	-163	-166		
aug-pc-2/aug-cc-pVTZ	-131	-105	-170	-158	-165	-183	-188

Table S6. Basis set dependence of the induced longitudinal dipole moment values (in a.u.) of the zwitter-ionic form of p-aminobenzoic acid (pABA-z) with benzene (Be) calculated using the Sadlej's POL, aug-cc-pVXZ and Jensen's (aug)-pc-n series of atomic basis sets for WF-based and DFT methods, respectively. The optimized geometry of the complex is used.. CP stands for the counterpoise-corrected values.

Basis set	RHF	B3LYP	CAM-B3LYP	LC-BOP	LC-BOP-LRD	MP2	SCS-MP2
Sadlej's POL	-0.761	-0.667	-0.722	-0.751	-0.753	-0.752	-0.751
Sadlej's POL (CP)	-0.760	-0.666	-0.720	-0.748	-0.746		
aug-pc-1/aug-cc-pVDZ	-0.762	-0.669	-0.726	-0.752	-0.754	-0.755	-0.754
aug-pc-1/aug-cc-pVDZ (CP)	-0.761	-0.665	-0.721	-0.747	-0.745		
pc-2/cc-pVTZ	-0.771	-0.673	-0.729	-0.753	-0.756	-0.766	-0.765
pc-2/cc-pVTZ (CP)	-0.748	-0.661	-0.715	-0.739	-0.737		
aug-pc-2/aug-cc-pVTZ	-0.760	-0.668	-0.721	-0.746	-0.748	-0.750	-0.749

Table S7. Basis set dependence of the induced longitudinal polarizability values (in a.u.) of the zwitter-ionic form of p-aminobenzoic acid (pABA-z) with benzene (Be) calculated using the Sadlej's POL, aug-cc-pVXZ and Jensen's (aug)-pc-n series of atomic basis sets for WF-based and DFT methods, respectively. The optimized geometry of the complex is used.. CP stands for the counterpoise-corrected values.

Basis set	RHF	B3LYP	CAM-B3LYP	LC-BOP	LC-BOP-LRD	MP2	SCS-MP2
Sadlej's POL	-17.6	-32.1	-22.9	-18.6	-18.1	-19.8	-19.5
Sadlej's POL (CP)	-17.8	-31.9	-22.8	-19.0	-18.6		
aug-pc-1/aug-cc-pVDZ	-12.5	-31.5	-22.1	-18.1	-17.5	-18.9	-18.6
aug-pc-1/aug-cc-pVDZ (CP)	-17.8	-32.0	-22.7	-18.8	-18.3		
pc-2/cc-pVTZ	-14.5	-28.7	-20.1	-16.4	-15.8	-17.0	-16.8
pc-2/cc-pVTZ (CP)	-17.4	-31.3	-22.5	-18.6	-18.3		
aug-pc-2/aug-cc-pVTZ	-17.7	-31.4	-22.6	-18.8	-18.2	-19.5	-19.2

Table S8. Basis set dependence of the induced longitudinal first hyperpolarizability values (in a.u.) of the zwitter-ionic form of p-aminobenzoic acid (pABA-z) with benzene (Be) calculated using the Sadlej's POL, aug-cc-pVXZ and Jensen's (aug)-pc-n series of atomic basis sets for WF-based and DFT methods, respectively. The optimized geometry of the complex is used.. CP stands for the counterpoise-corrected values.

Basis set	**RHF**	**B3LYP**	**CAM-B3LYP**	**LC-BOP**	**LC-BOP-LRD**	**MP2**	**SCS-MP2**
Sadlej's POL	-109	-3005	-707	-314	-333	-352	-315
Sadlej's POL (CP)	-105	-2974	-693	-288	-268		
aug-pc-1/aug-cc-pVDZ	-102	-3078	-731	-309	-368	-349	-317
aug-pc-1/aug-cc-pVDZ (CP)	-105	-3034	-710	-294	-329		
pc-2/cc-pVTZ	-103	-2583	-667	-281	-276	-330	-301
pc-2/cc-pVTZ (CP)	-113	-2724	-672	-280	-274		
aug-pc-2/aug-cc-pVTZ	-105	-2947	-688	-281	-283	-343	-311