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

Supplementary Information for "Accurate Three-body Noncovalent Interactions: the Insights from Energy Decomposition"

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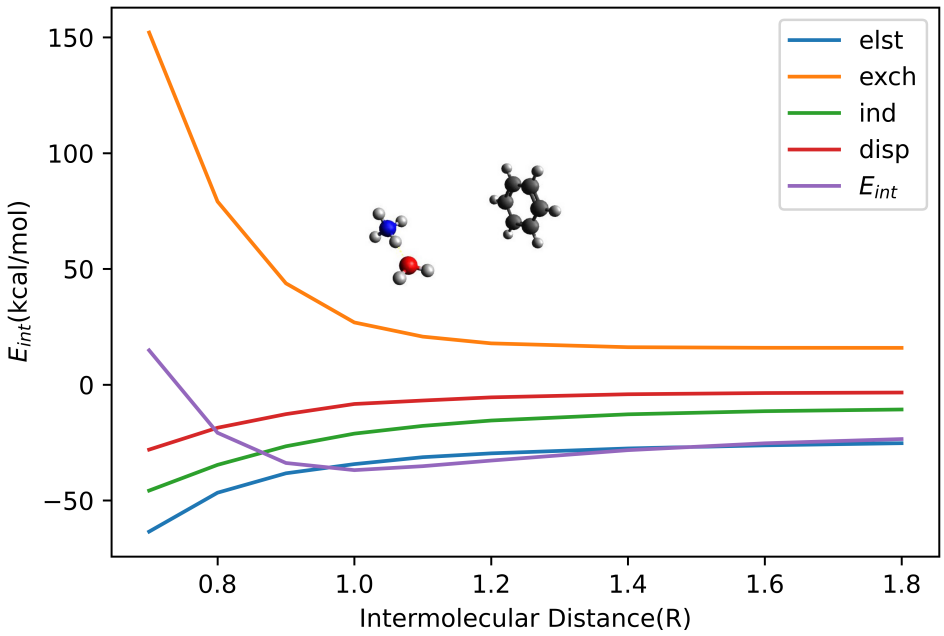

Figure 1: Two-body SAPT(DFT) energy decompositions along the radial benchmark potential energy curves for the ammonium-benzene-water complex 4.1. They are obtained by shifting C_6H_6 relative to the center of mass of the entire complex. The relative geometry of the other two molecules stays unchanged.

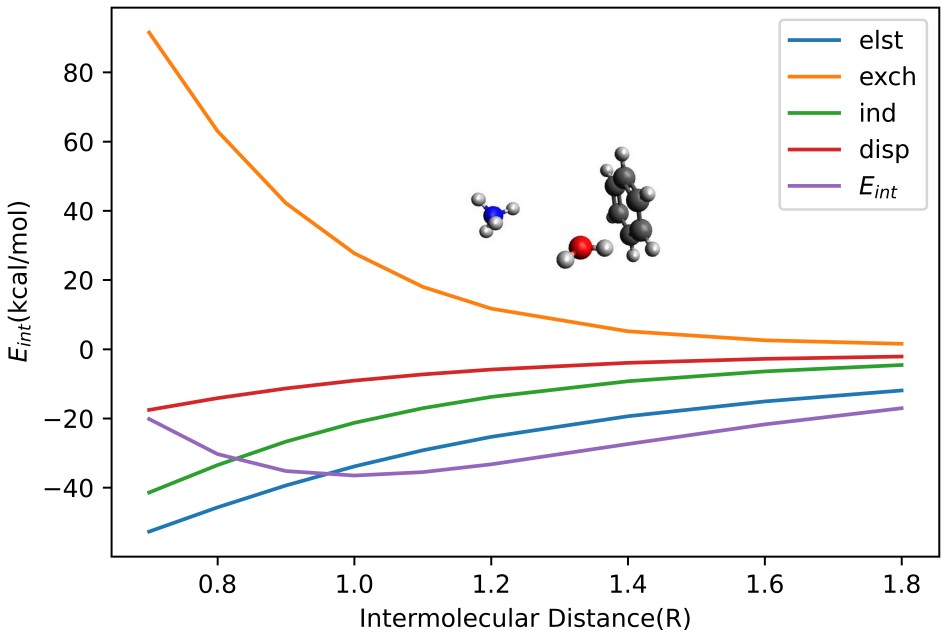

Figure 2: Two-body SAPT(DFT) energy decompositions along the radial benchmark potential energy curves for the ammonium-benzene-water complex 4.1. They are obtained by shifting NH_4^+ relative to the center of mass of the entire complex. The relative geometry of the other two molecules stays unchanged.

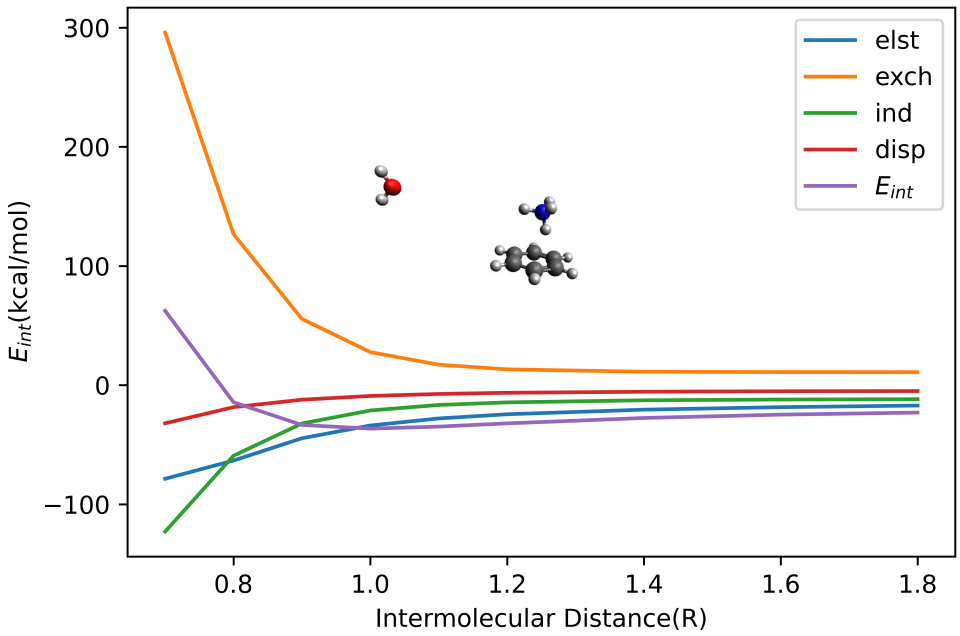

Figure 3: Two-body SAPT(DFT) energy decompositions along the radial benchmark potential energy curves for the ammonium-benzene-water complex 4.1. They are obtained by shifting H_2O relative to the center of mass of the entire complex. The relative geometry of the other two molecules stays unchanged.

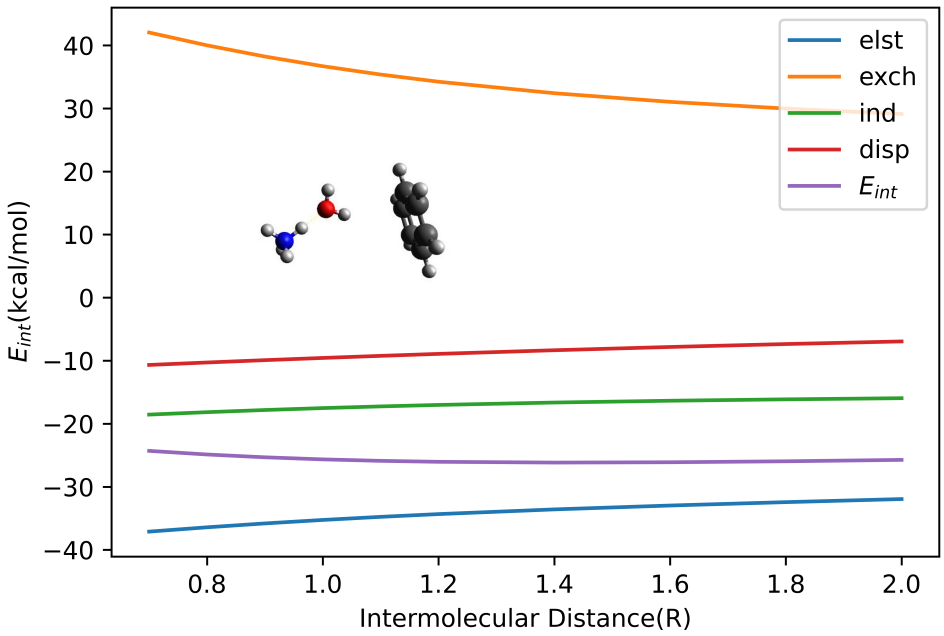

Figure 4: Two-body SAPT(DFT) energy decompositions along the radial benchmark potential energy curves for the ammonium-benzene-water complex 4.2. They are obtained by shifting C_6H_6 relative to the center of mass of the entire complex. The relative geometry of the other two molecules stays unchanged.

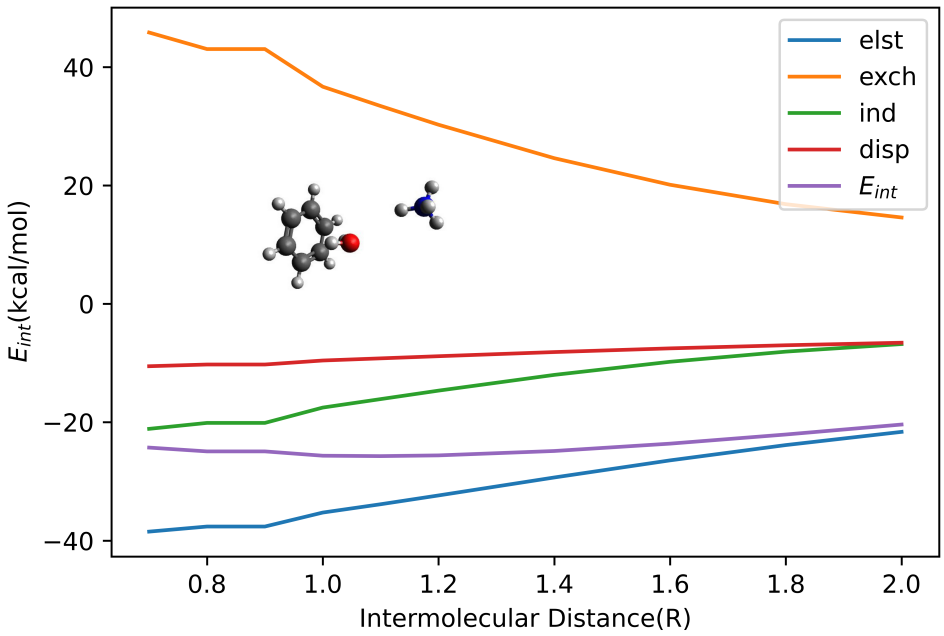

Figure 5: Two-body SAPT(DFT) energy decompositions along the radial benchmark potential energy curves for the ammonium-benzene-water complex 4.2. They are obtained by shifting NH_4^+ relative to the center of mass of the entire complex. The relative geometry of the other two molecules stays unchanged.

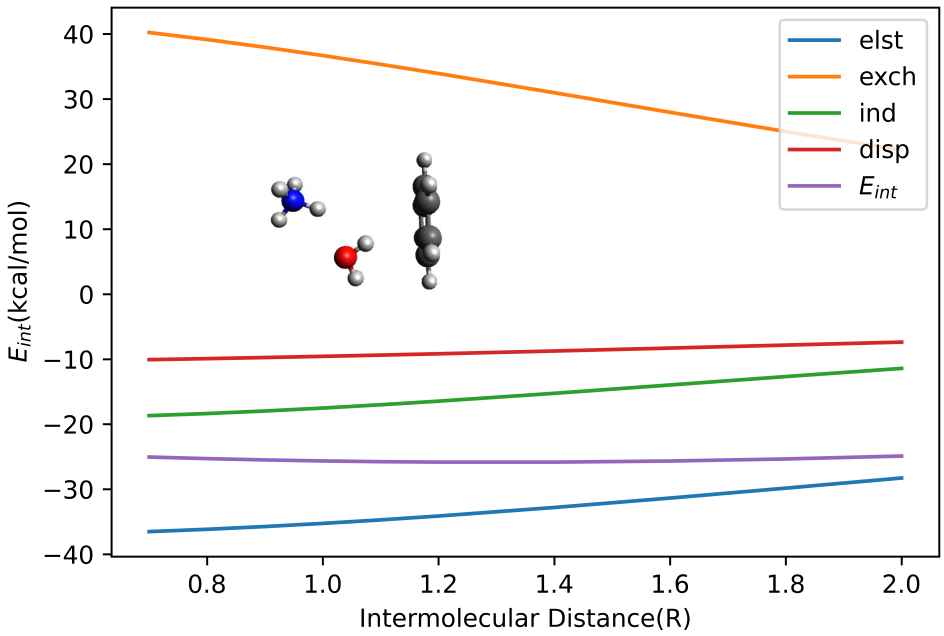

Figure 6: Two-body SAPT(DFT) energy decompositions along the radial benchmark potential energy curves for the ammonium-benzene-water complex 4.2. They are obtained by shifting H_2O relative to the center of mass of the entire complex. The relative geometry of the other two molecules stays unchanged.

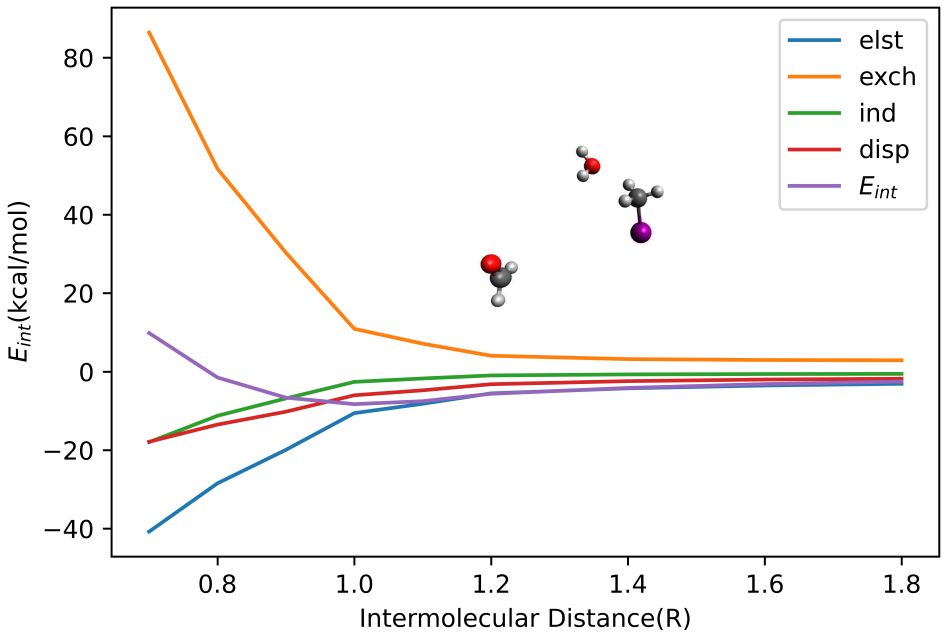

Figure 7: Two-body SAPT(DFT) energy decompositions along the radial benchmark potential energy curves for the iodomethane-formaldehyde-water complex 1.1. They are obtained by shifting HCHO relative to the center of mass of the entire complex. The relative geometry of the other two molecules stays unchanged.

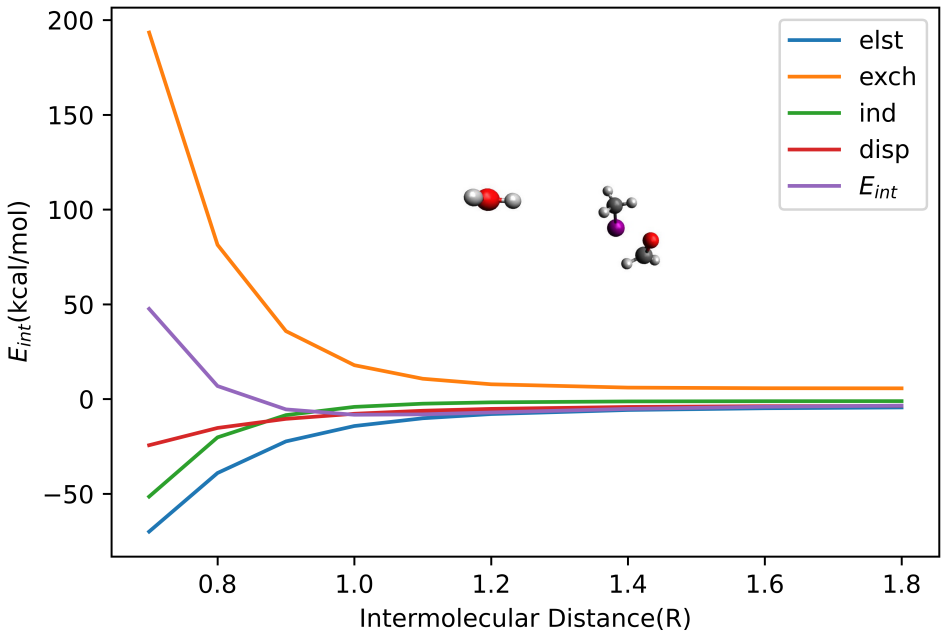

Figure 8: Two-body SAPT(DFT) energy decompositions along the radial benchmark potential energy curves for the iodomethane-formaldehyde-water complex 1.1. They are obtained by shifting H_2O relative to the center of mass of the entire complex. The relative geometry of the other two molecules stays unchanged.

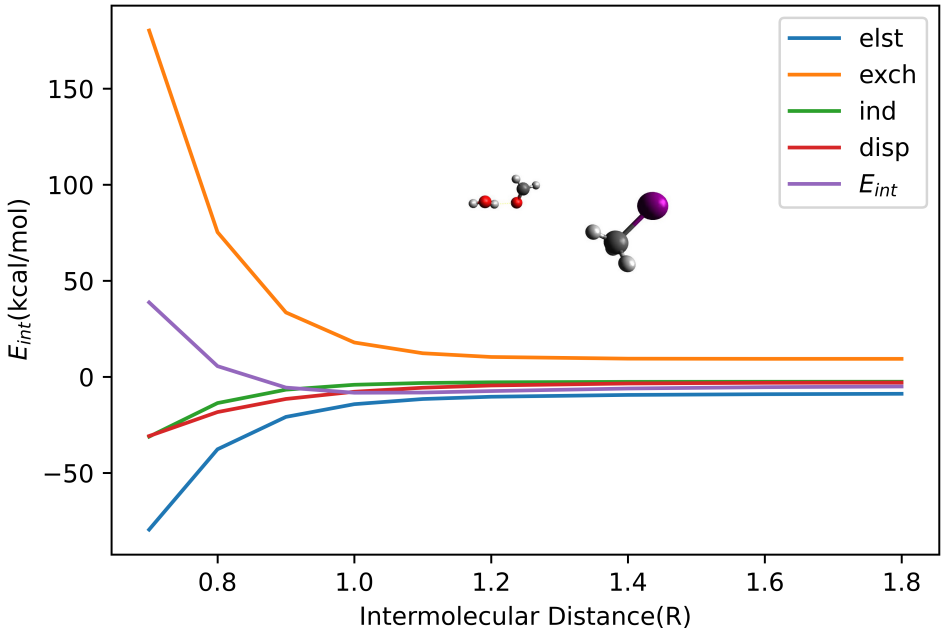

Figure 9: Two-body SAPT(DFT) energy decompositions along the radial benchmark potential energy curves for the iodomethane-formaldehyde-water complex 1.1. They are obtained by shifting CH_3I relative to the center of mass of the entire complex. The relative geometry of the other two molecules stays unchanged.

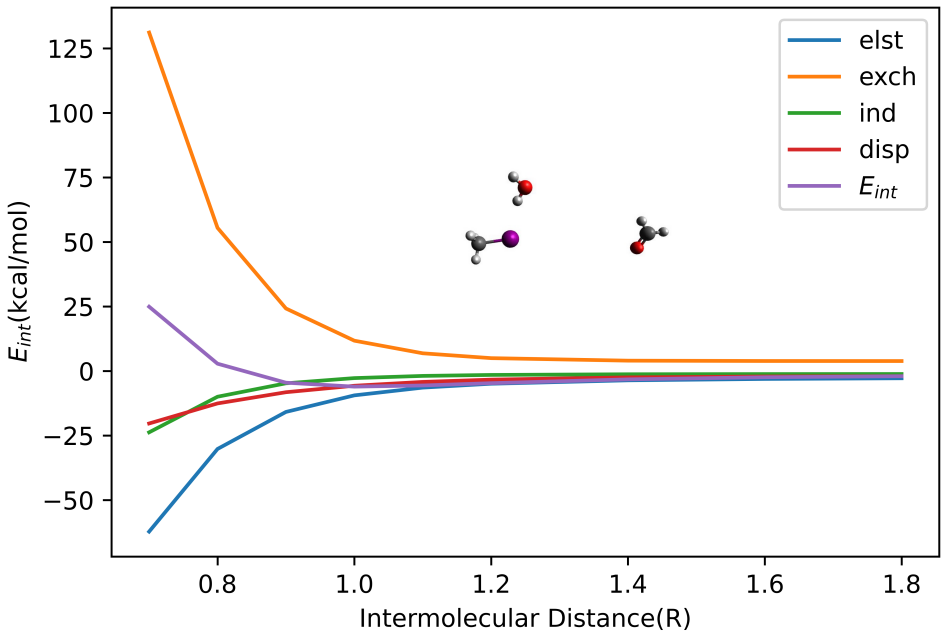

Figure 10: Two-body SAPT(DFT) energy decompositions along the radial benchmark potential energy curves for the iodomethane-formaldehyde-water complex complex 1.2. They are obtained by shifting HCHO relative to the center of mass of the entire complex. The relative geometry of the other two molecules stays unchanged.

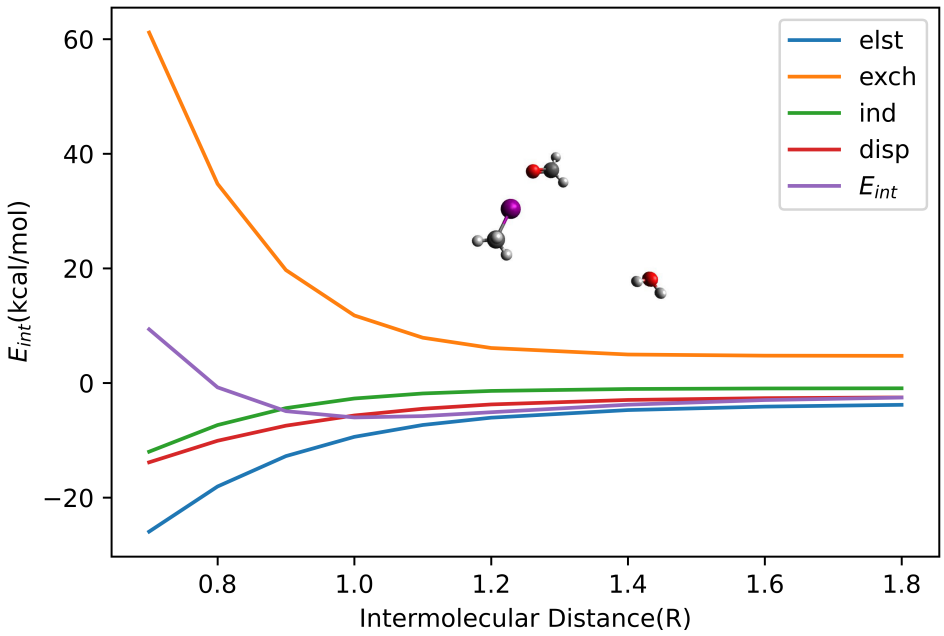

Figure 11: Two-body SAPT(DFT) energy decompositions along the radial benchmark potential energy curves for the iodomethane-formaldehyde-water complex complex 1.2. They are obtained by shifting H_2O relative to the center of mass of the entire complex. The relative geometry of the other two molecules stays unchanged.

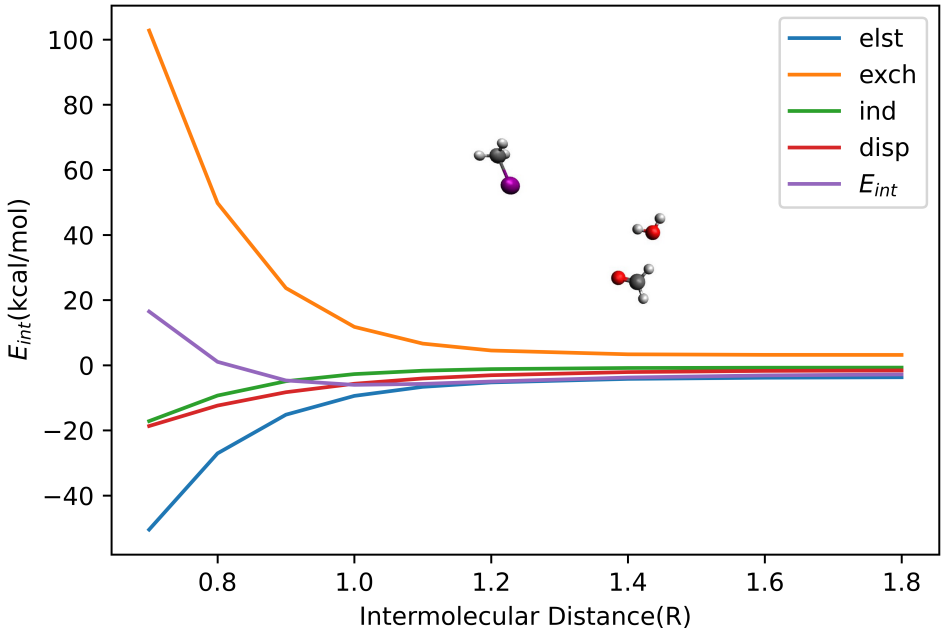

Figure 12: Two-body SAPT(DFT) energy decompositions along the radial benchmark potential energy curves for the iodomethane-formaldehyde-water complex 1.2. They are obtained by shifting CH_3I relative to the center of mass of the entire complex. The relative geometry of the other two molecules stays unchanged.

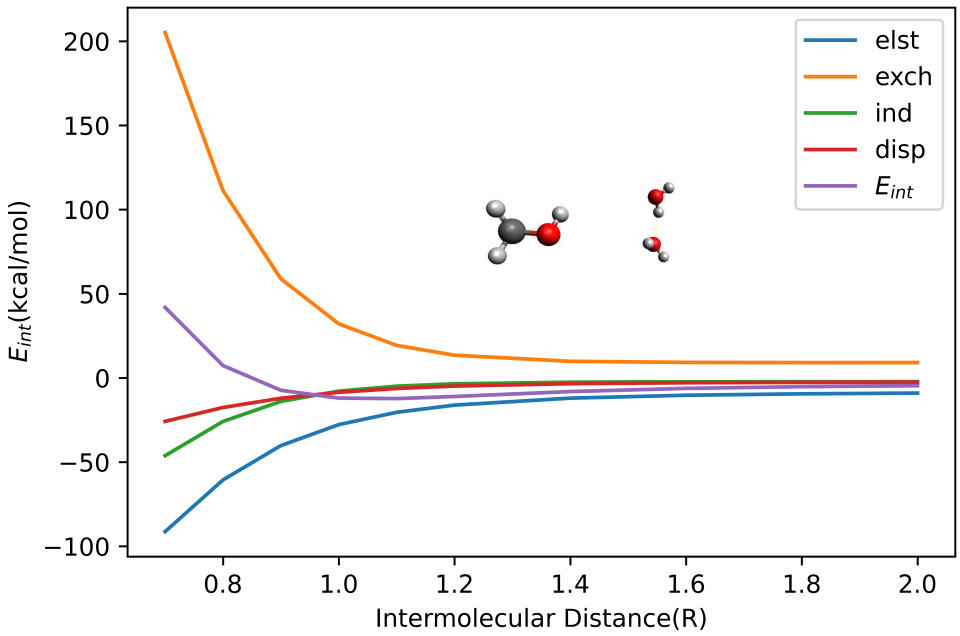

Figure 13: Two-body SAPT(DFT) energy decompositions along the radial benchmark potential energy curves for the water-water-methanol 3.1. They are obtained by shifting CH_3OH relative to the center of mass of the entire complex. The relative geometry of the other two molecules stays unchanged.

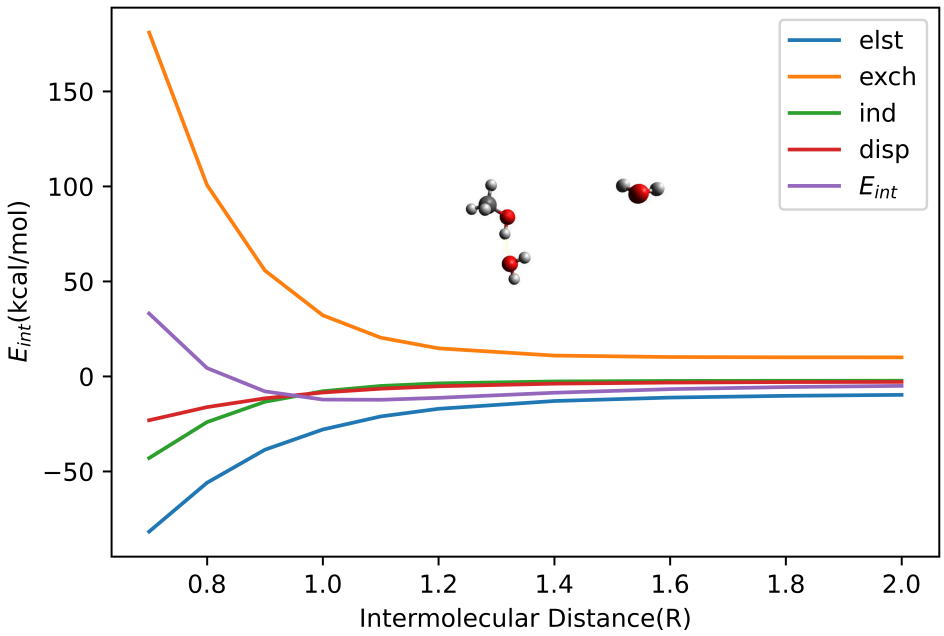

Figure 14: Two-body SAPT(DFT) energy decompositions along the radial benchmark potential energy curves for the water-water-methanol 3.1. They are obtained by shifting H_2O(a) relative to the center of mass of the entire complex. The relative geometry of the other two molecules stays unchanged.

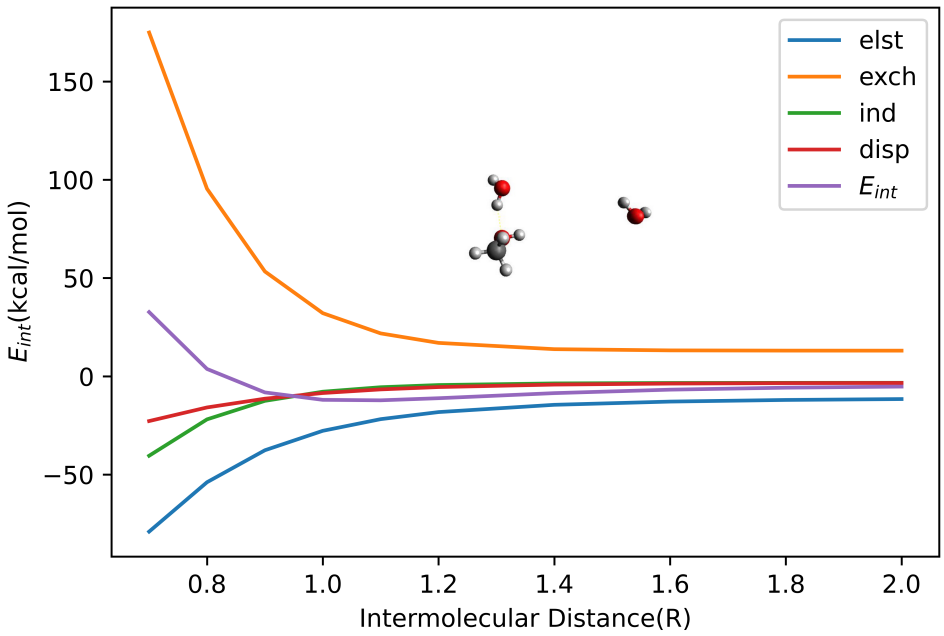

Figure 15: Two-body SAPT(DFT) energy decompositions along the radial benchmark potential energy curves for the water-water-methanol 3.1. They are obtained by shifting H_2O(b) relative to the center of mass of the entire complex. The relative geometry of the other two molecules stays unchanged.

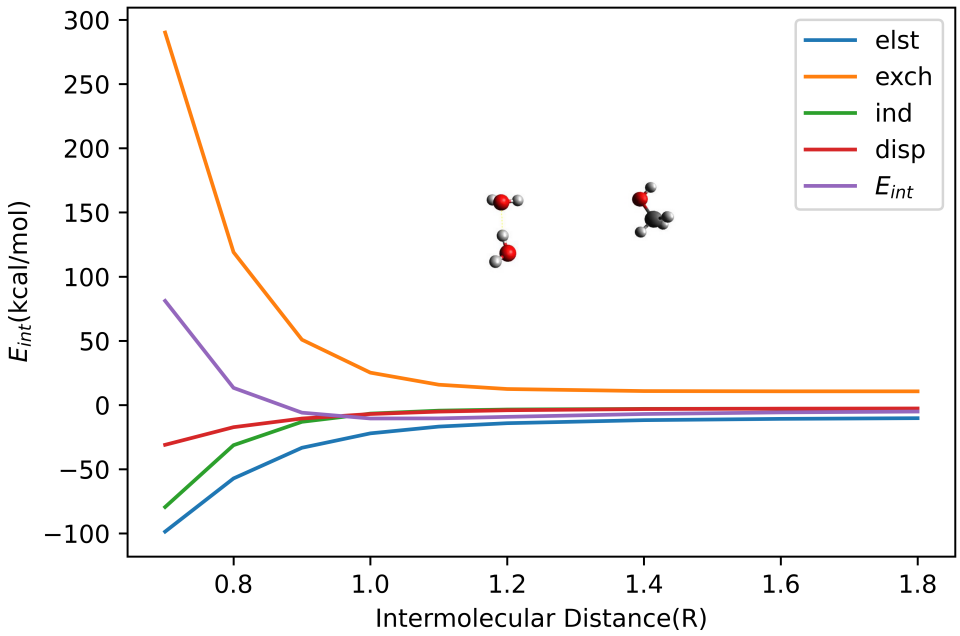

Figure 16: Two-body SAPT(DFT) energy decompositions along the radial benchmark potential energy curves for the water-water-methanol 3.2. They are obtained by shifting CH_3OH relative to the center of mass of the entire complex. The relative geometry of the other two molecules stays unchanged.

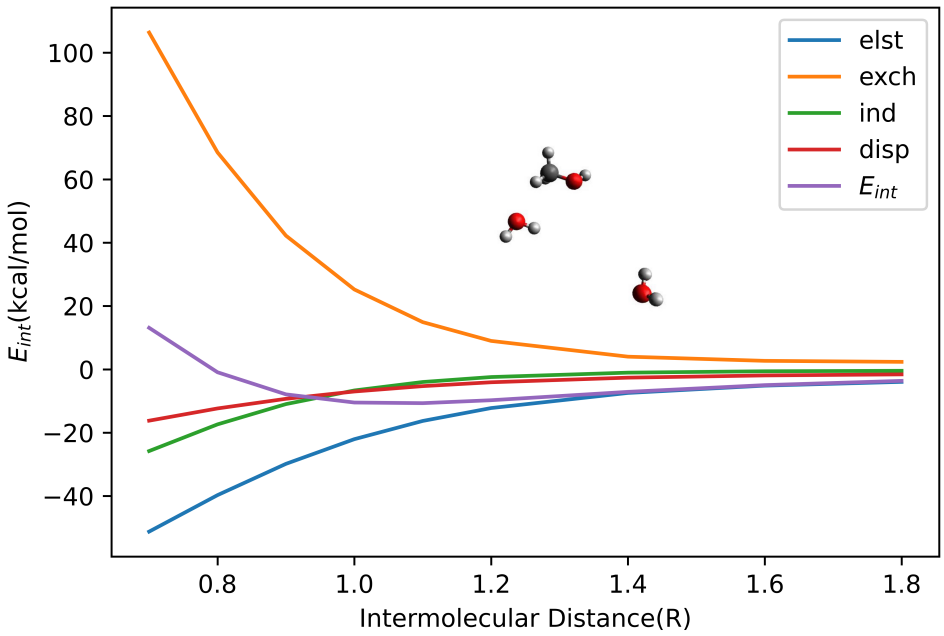

Figure 17: Two-body SAPT(DFT) energy decompositions along the radial benchmark potential energy curves for the water-water-methanol 3.2. They are obtained by shifting H_2O(a) relative to the center of mass of the entire complex. The relative geometry of the other two molecules stays unchanged.

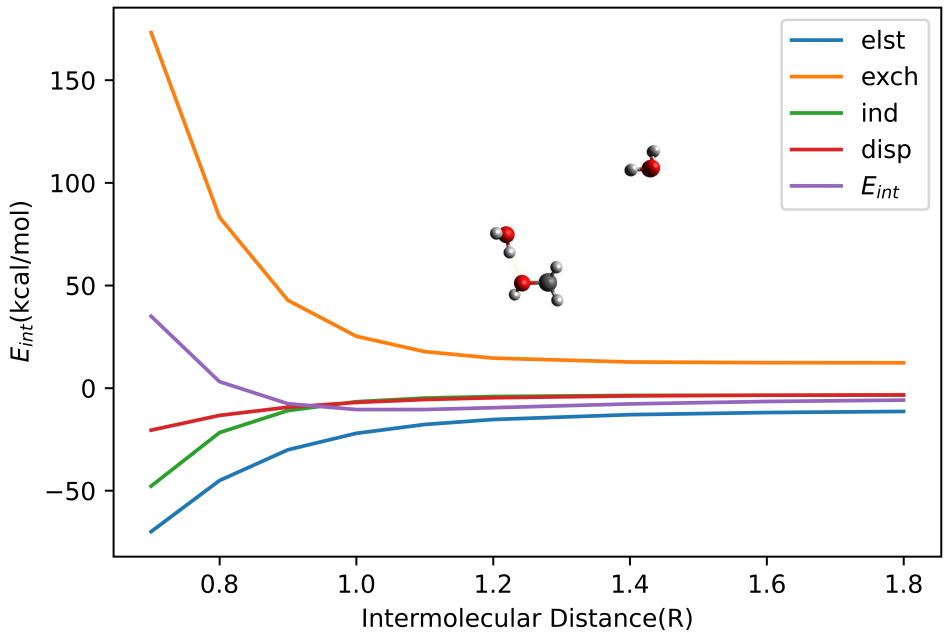

Figure 18: Two-body SAPT(DFT) energy decompositions along the radial benchmark potential energy curves for the water-water-methanol 3.2. They are obtained by shifting H_2O(b) relative to the center of mass of the entire complex. The relative geometry of the other two molecules stays unchanged.