Supporting Information:

Ground state potential energy surfaces around selected atoms from resonant inelastic x-ray scattering

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S1 Calculated C=O potential energy curves of acetone and the acetone-chloroform complex

In Figure S1 we present calculated potential energy curves along the C=O bond distance of acetone and the acetone-chloroform complex. A small but clear effect of the hydrogen bond in the acetone-chloroform complex can be observed. This effect is in line with the trend observed in the potentials extracted from the experimental data in the main paper.

The curves in Figure S1 were calculated using the ORCA software package [1]. For this, in a first step, the acetone molecule and acetone-chloroform complex were geometry optimized using the BP86 functional and def2-TZVP basis sets for all atoms. For the optimized structures, the potential energy surface was scanned along the C=O bond distance coordinate using the standard ORCA routine with the same functional and basis sets as for the geometry optimization.

References

[1] F. Neese. The ORCA program system. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, 2(1):73–78, Jan. 2012.

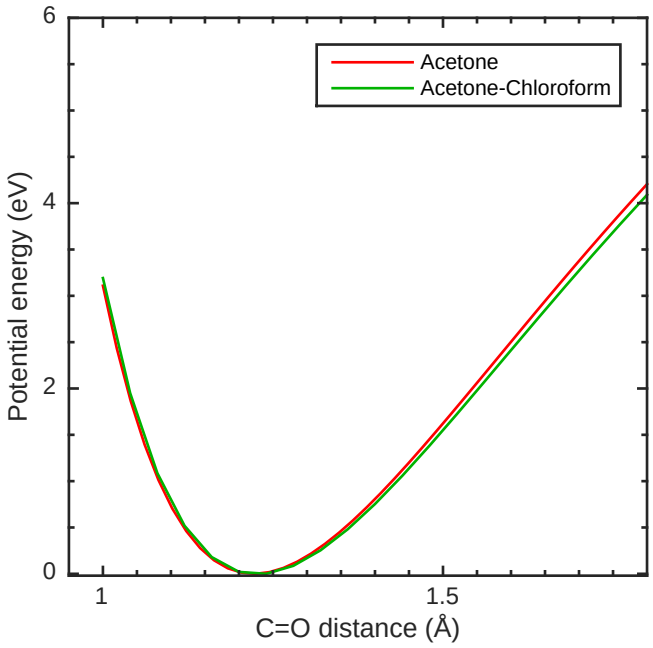

Figure S1: Calculated C=O potential energy curves for acetone and the hydrogen bonded acetone-chloroform comlex.