Supplementary Information

A detailed description of the CO molecule adsorbed in InOF-1

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Figure S11. (a) Negative of the Laplacian of the electron density over the plane defined by the O-H...C centers is presented. Lowest values are in black and highest values are in white. (b) Electron density in the interval [0,0.005] over a plane defined by the O-H...C atoms. This picture is used as the reference for the positions of these atoms. (c) Difference of the electron density in the interval [-0.005, 0.005] between the whole system and each atom. (d) Positive regions of (c) in the interval [0,0.005]. (e) Negative regions of (c) in the region [-0.005,0]. For all cases the highest value is in black and the lowest is in white. The electron density is in atomic units.

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