

## Supplementary Information

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

Bruno Landeros-Rivera,<sup>a</sup> Ilich A. Ibarra,<sup>b</sup> Mariana L. Díaz-Ramírez,<sup>b</sup> Rubicelia Vargas,<sup>a\*</sup> Hugo A. Lara-García,<sup>c\*</sup> Jorge Garza<sup>1</sup> and Ana Martínez<sup>d\*</sup>

Figure SI1. (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

