Supplementary information for:

Computational and experimental studies on the adsorption of CO, N_2 and CO_2 on Mg-MOF-74

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	Mg	**C**	**O**	**H**	**CO**	**ΔE_{nocpc}**	**BSSE**	**ΔE_{cpc}**	**Mg---C**	**C-O**
1	85-11G(d)	6-31G(d,p)	84-11G(d,p)	6-31G(d,p)	6-31G(d,p)	-33.22	15.71	17.51	2.456	1.133
2	“	“	“	“	6-311G(d,p)	-24.73	10.57	14.16	2.526	1.124
3	“	“	“	“	TZVP	-24.79	10.89	13.90	2.533	1.123
4	“	“	“	“	QZVP	-26.61	12.08	14.53	2.529	1.123
5	“	“	“	“	QZVPP	-27.15	12.37	14.77	2.515	1.121
6	TZV	“	“	“	TZVP	-23.39	8.16	15.23	2.553	1.123
7	“	“	“	“	QZVP	-24.88	9.40	15.38	2.540	1.123
8	QZVP	“	“	“	TZVP	-22.75	7.82	14.93	2.558	1.123
9	“	“	“	“	QZVP	-24.03	8.90	15.13	2.552	1.123
10	“	TZVP	“	“	TZVP	-21.02	4.75	16.27	2.555	1.123
11	TZVP	“	“	“	“	-21.43	4.87	16.56	2.554	1.123
12	QZVP	“	TZVP	“	“	-21.27	3.92	17.35	2.545	1.123
13	***TZVP***	***“***	***“***	***TZVP***	***“***	***-21.63***	***4.08***	***17.55***	***2.540***	***1.123***
14	“	“	“	“	TZVPP	-21.52	3.93	17.59	2.539	1.121
15	“	“	“	“	QZVP	-21.86	3.86	18.00	2.529	1.122

Table S1. Adsorption of CO molecules in MOF-74; the basis sets for the atoms in the bulk and in the molecule are indicated. ΔE_{nocpc} is the variation energy before BSSE (basis set superposition error) and ΔE_{cpc} is the binding energy (both in kJ/mol per CO molecule). Mg---C and C-O are distances expressed in Å. For this preliminary study, calculations were performed at B3LYP level of theory.

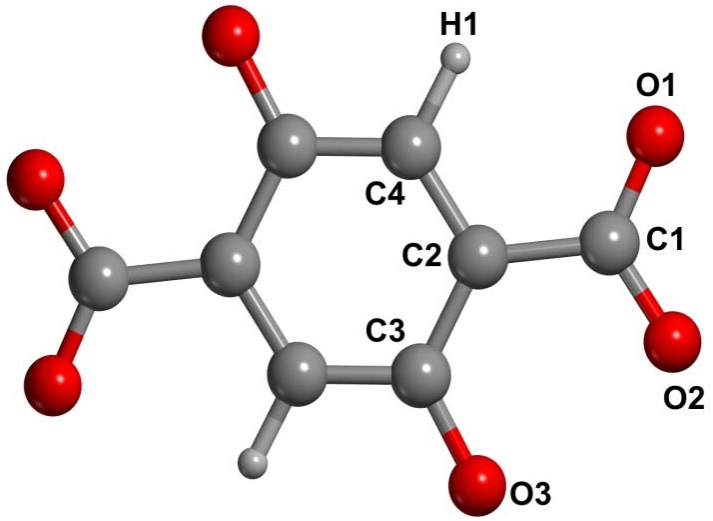

Figure S1. Organic linker of Mg-MOF-74. Only irreducible atoms are indicated. Atomic labels refer to distances reported in Table S2 below.

	Mg-MOF-74	**Mg-MOF-74/CO**	**Mg-MOF-74/N_2**	**Mg-MOF-74/CO_2**
a	26.212	26.259	26.269	26.236
c	6.932	6.984	6.968	6.992
V	4125.0	4170.4	4164.5	4168.3
C1-O1	1.257	1.257	1.257	1.260
C1-O2	1.282	1.280	1.281	1.278
C1-C2	1.491	1.500	1.498	1.497
C2-C3	1.427	1.430	1.429	1.429
C2-C4	1.400	1.402	1.402	1.402
C3-O3	1.348	1.343	1.345	1.342
C4-H1	1.081	1.081	1.081	1.081

Table S2. Cell parameters (Å) and unit cell volumes ($Å^3$) for Mg-MOF-74 bulk (reported for reference) and with the presence of the adsorbed molecule. Inter-atomic distances (Å) of the organic linker are also reported. When the three molecular species are adsorbed, distances do not change, showing that no interaction occurs of the adduct with the organic part of Mg-MOF-74. Atomic labels refer to Figure S1.