Electronic Supplementary Material (ESI) for CrystEngComm.

Ab initio investigation on novel Bipyrazolate based MOF affinity towards H_2 and CO_2

Supportig Materials

J. Baima, R. Macchieraldo, and S. Casassa
Dipartimento Chimica IFM and Centre of Excellence NIS (Nanostructured Interfaces and Surfaces), Università degli Studi di Torino, via P. Giuria 5, I-10125 Torino, Italy.

C. Pettinari
School of Pharmacy, Università di Camerino, Italy

The main crystallographic data of the two structures together with the geometrical parameters, as optimized at the B3LYP plus a Grimme posteriori correction level, are summarized in Table I.

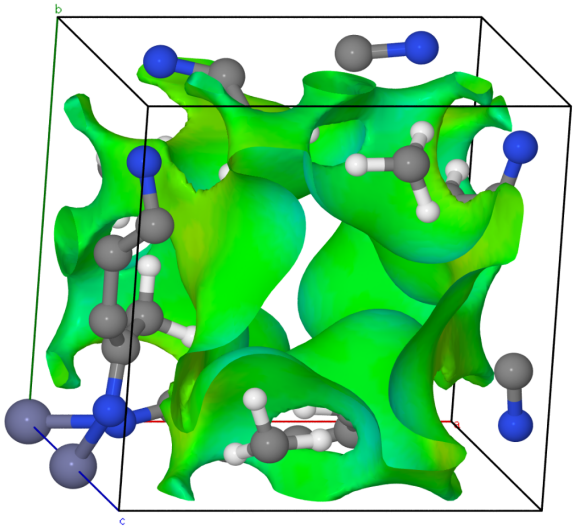

FIG. 1. Tilted view of the electrostatic potential of Zn(Me_4BPZ) projected on a charge density isosurface of 0.003 a.u. Minimum and maximum values of the potential have been set to -0.073 (red) and 0.067 (blue) a.u. respectively.

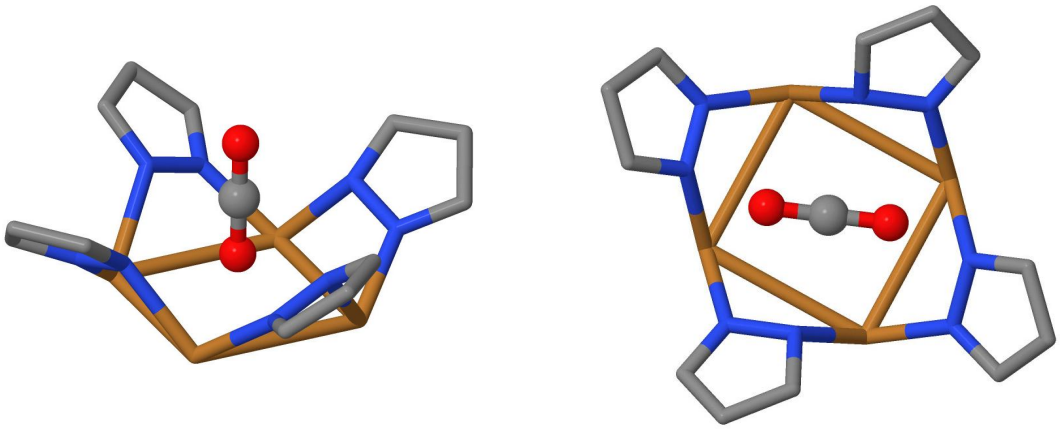

FIG. 2. Adsorption structures a (left) and b (right) of a CO_2 molecule near the metal site and nitrogen atoms of Cu(Me_4BPZ).

[1] A. Tabacaru, C. Pettinari, I. Timokhin, F. Marchetti, F. Carrasco-Marín, F. J. Maldonado-Hodar, S. Galli, and N. Masciocchi, Crystal Growth & Design **13**, 3087 (2013).

	Zn(Me_4BPZ)		Cu(Me_4BPZ)	
Empirical formula	$C_{10}H_{12}N_4Zn$		$C_{10}H_{12}CuN_4$	
Crystal system	Tetragonal		Cubic	
Space Group	P-42c		Im-3m	
Symm Op	8		4	
	Exp[a]	Opt	Exp[a]	Opt
a [Å]	8.8118(5)	8.8027	13.4614(3)	14.4926
c [Å]	7.3668(5)	7.2518	13.4614(3)	11.6336
α [deg]	90	90	90	90
V [Å^3]	572.01(7)	561.93	2439.3(1)	2444
Optimized coordinates of atoms in the asymmetric unit (Å)				
M≡Zn/Cu	0.0000 0.0000 0.0000		-2.3903 0.0000 0.0000	
Cu			-0.0000 2.3900 0.0000	
C	-3.6939 0.0000 1.8241		-3.1440 -1.7879 -2.4453	
C	-2.8361 -0.5622 0.8655		1.7856 3.1416 2.4476	
C	-3.1697 -1.3450 -0.3651		-2.1874 -3.6162 -1.6262	
C			3.6147 2.1872 1.6278	
C			-3.9636 -0.8127 -3.2221	
C			0.8096 3.9594 3.2252	
C			-1.8573 -4.9985 -1.1643	
C			4.9973 1.8585 1.1657	
C			-3.2028 -3.1880 -2.5024	
C			3.1856 3.2014 2.5048	
N	-1.5627 -0.3420 1.2295		-2.1522 -1.4058 -1.6059	
N			1.4044 2.1502 1.6072	
N			-1.5652 -2.5404 -1.1427	
N			2.5395 1.5644 1.1438	
H	-2.7616 -0.8863 -1.2674		-3.4280 0.1269 -3.3426	
H	-2.7442 -2.3514 -0.3103		-0.1299 3.4231 3.3441	
H	-4.2500 -1.4303 -0.4811		-4.1882 -1.2242 -4.2088	
H			1.2204 4.1822 4.2127	
H			-4.9209 -0.6024 -2.7373	
H			0.5992 4.9175 2.7423	
H			-2.7787 -5.5642 -1.0151	
H			5.5620 2.7805 1.0165	
H			-1.2464 -5.5579 -1.8757	
H			5.5574 1.2482 1.8770	
H			-1.3248 -4.9678 -0.2108	
H			4.9670 1.3262 0.2121	

TABLE I. Geometrical information on the two bipyralozated-based MOFs. [a] Experimental data are from Ref. [1]. Atomic position in cartesian coordinates (Å) of the atoms in the asymmetric units are given: the total number of atoms in the unit cell can be derived by multipling the number of atoms in the asymmetric unit for the number of symmetry operators (Symm Op).