Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Synthesis, structure and gas adsorption properties of a stable microporous metal-organic framework assembled from T-shaped pyridyl dicarboxylate ligand

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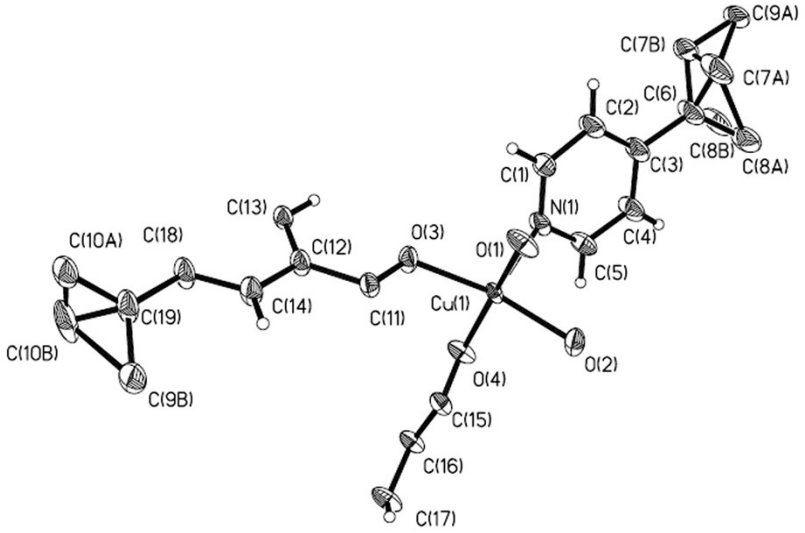

Fig.S1 Representations of the asymmetric units of compounds **1** showing ellipsoid at the 50% probability level.

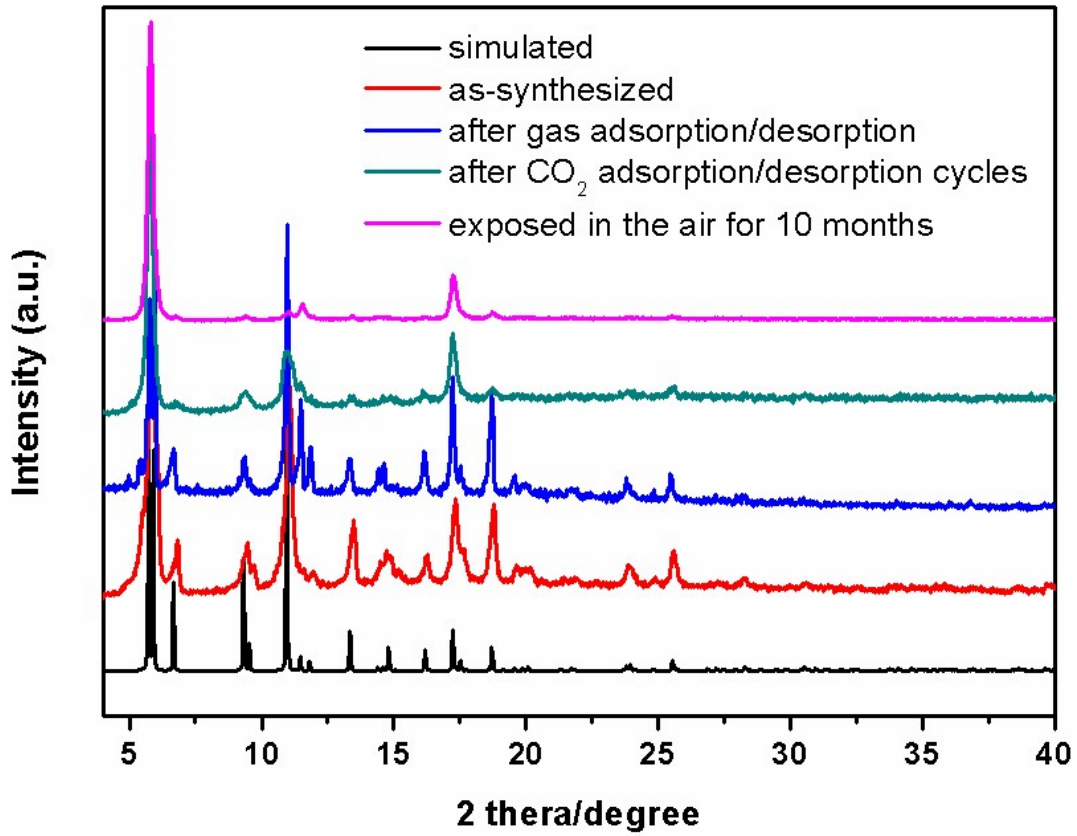

Fig.S2 Powder X-ray diffraction patterns of the simulated, as-synthesized, after gas adsorption/desorption measurements, after CO_2 adsorption/desorption cycles and exposed in the air for 10 months of compound **1**.

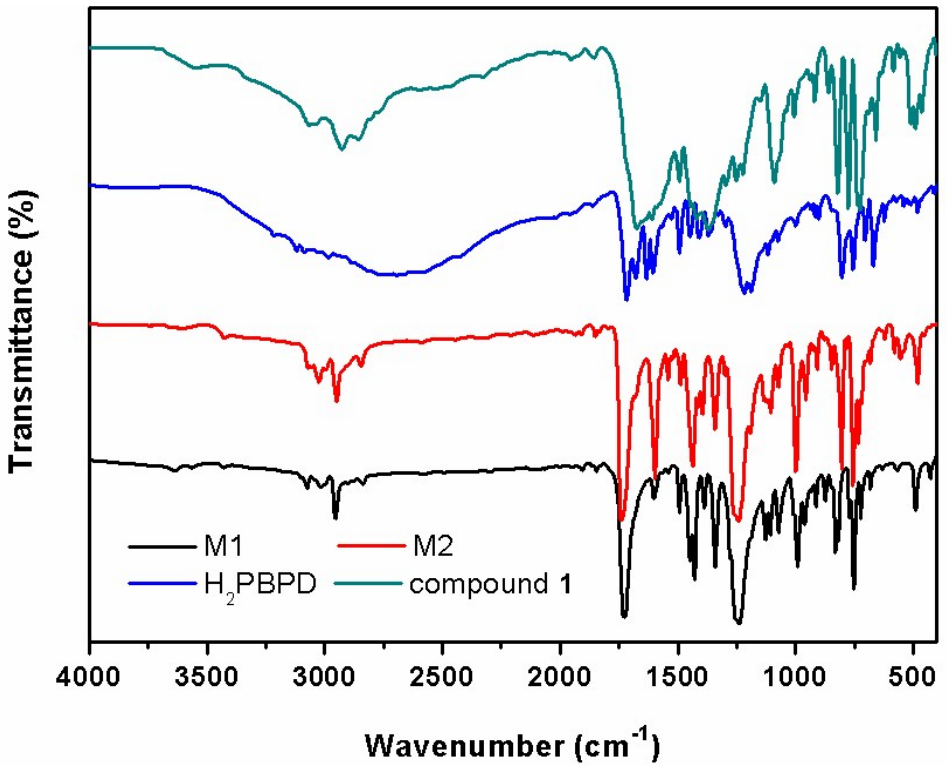

Fig.S3 Infra-red spectra of M1, M2, H_2PBPD and compound **1**.

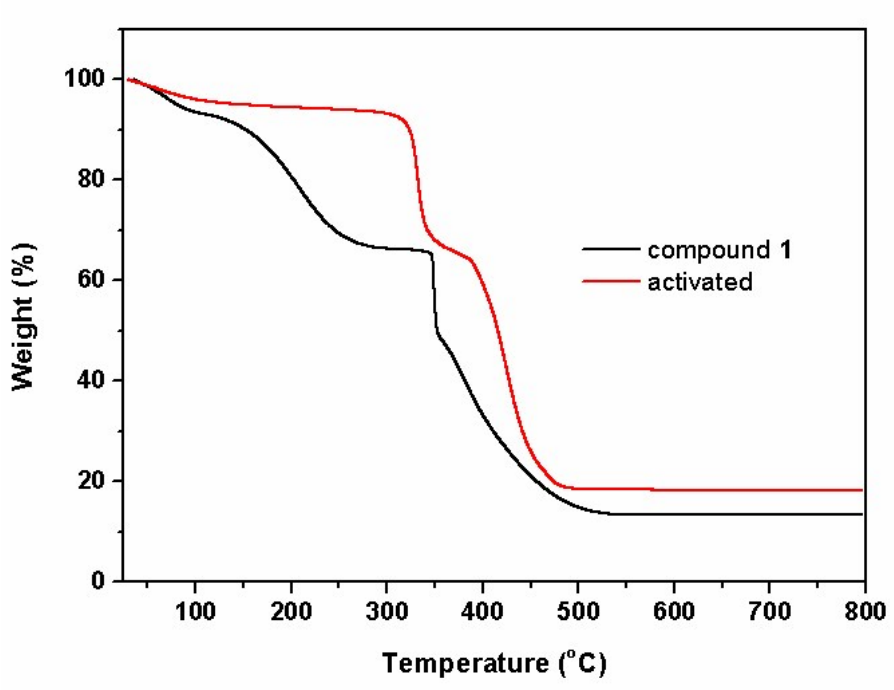

Fig. S4 TGA curves of compound **1** and activated.

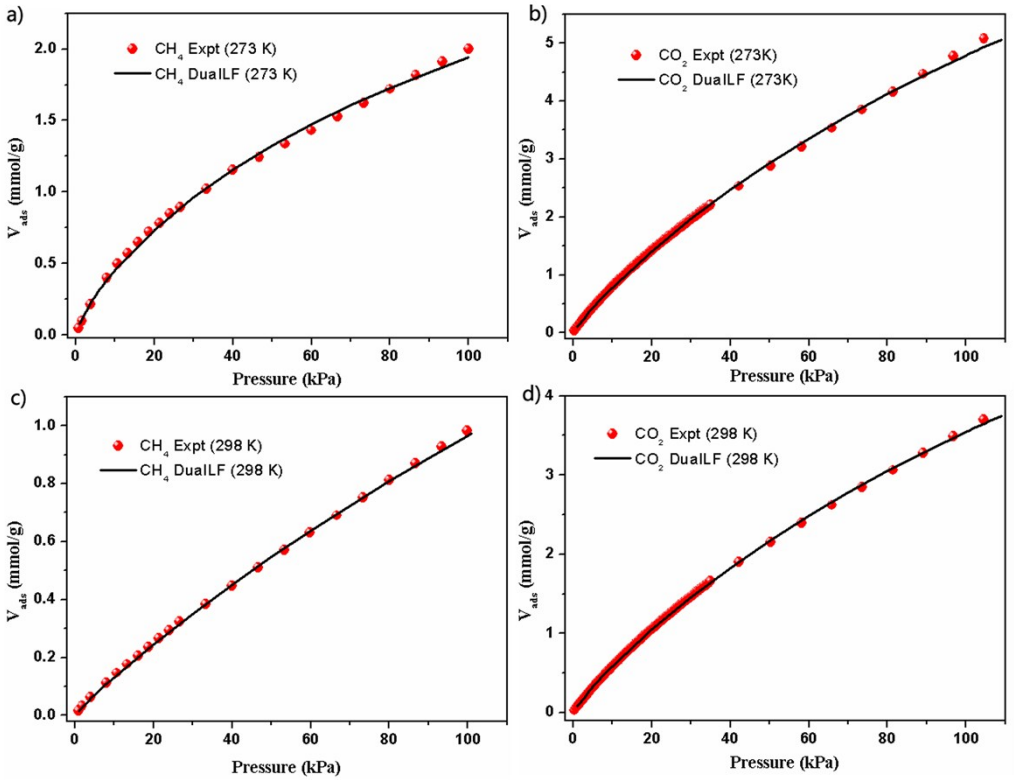

Fig. S5 Measured CH_4 and CO_2 isotherms at 273 K and 298 K along with the DSLF fits for compound **1**.

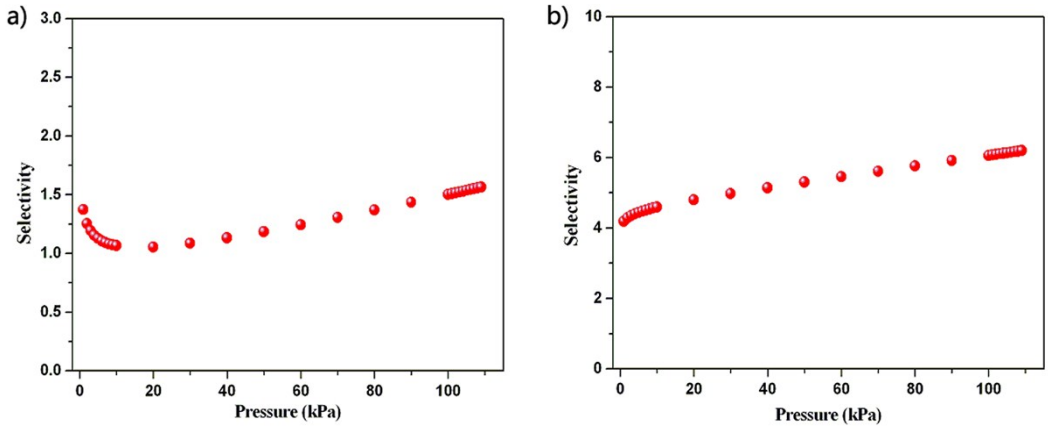

Fig. S6 IAST predicted equimolar gas mixture adsorption selectivities at 273 K (a) and 298 K (b) for compound **1**.

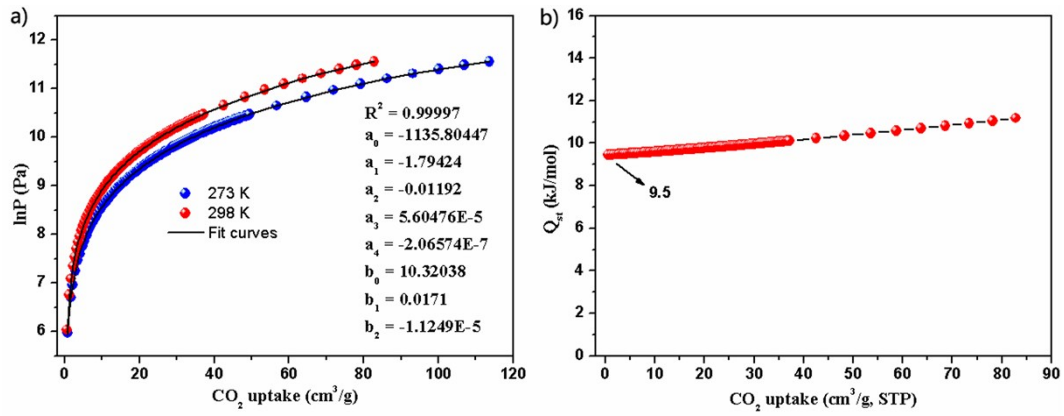

Fig.S7 (a) Nonlinear curves fitting of CO_2 for compound **1** at 273 K and 298 K; (b) Isosteric heat of CO_2 for for compound **1**.

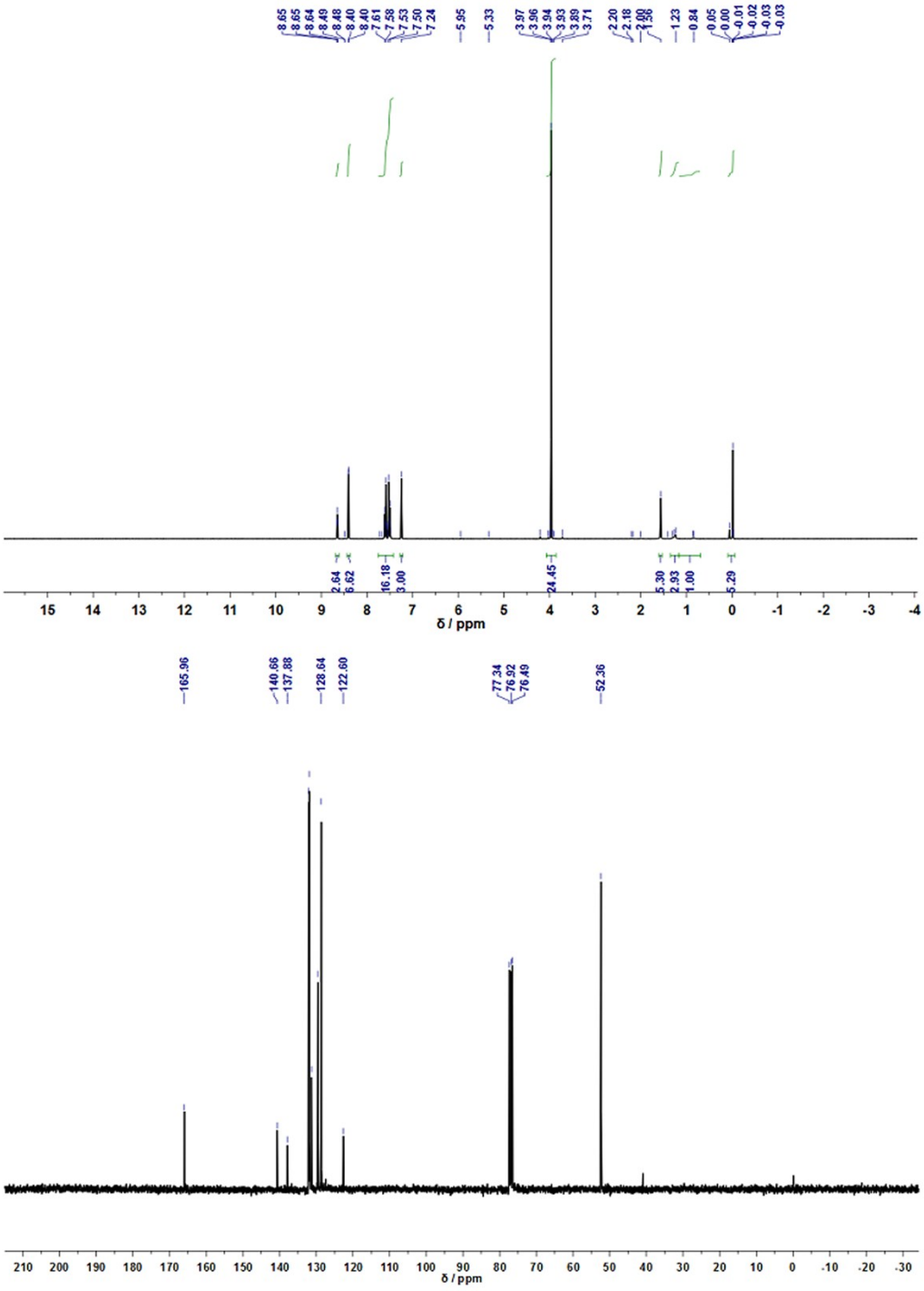

Fig.S8 The ^{1}H and ^{13}C NMR spectra of M1.

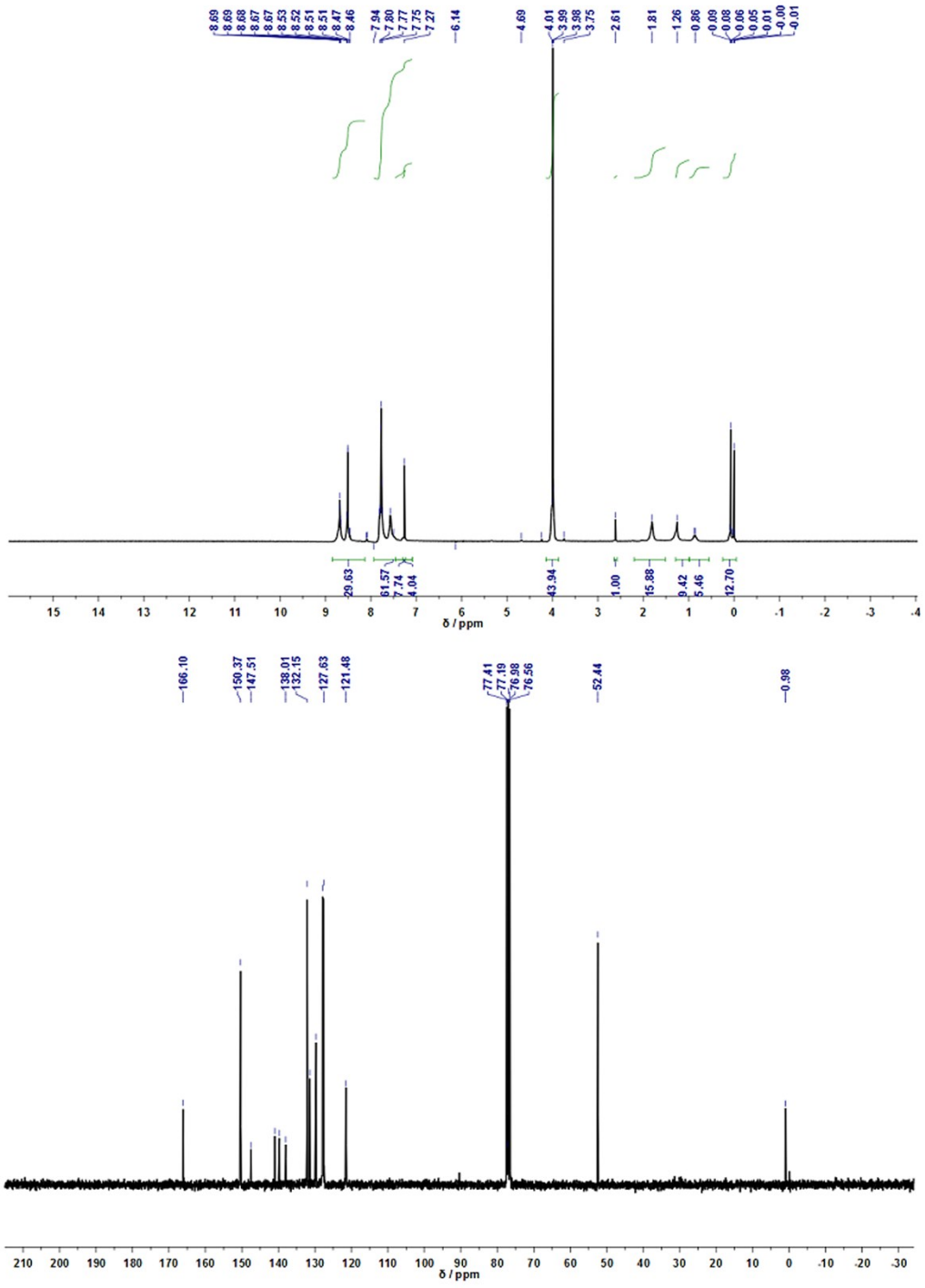

Fig.S9 The ^{1}H and ^{13}C NMR spectra of M2.

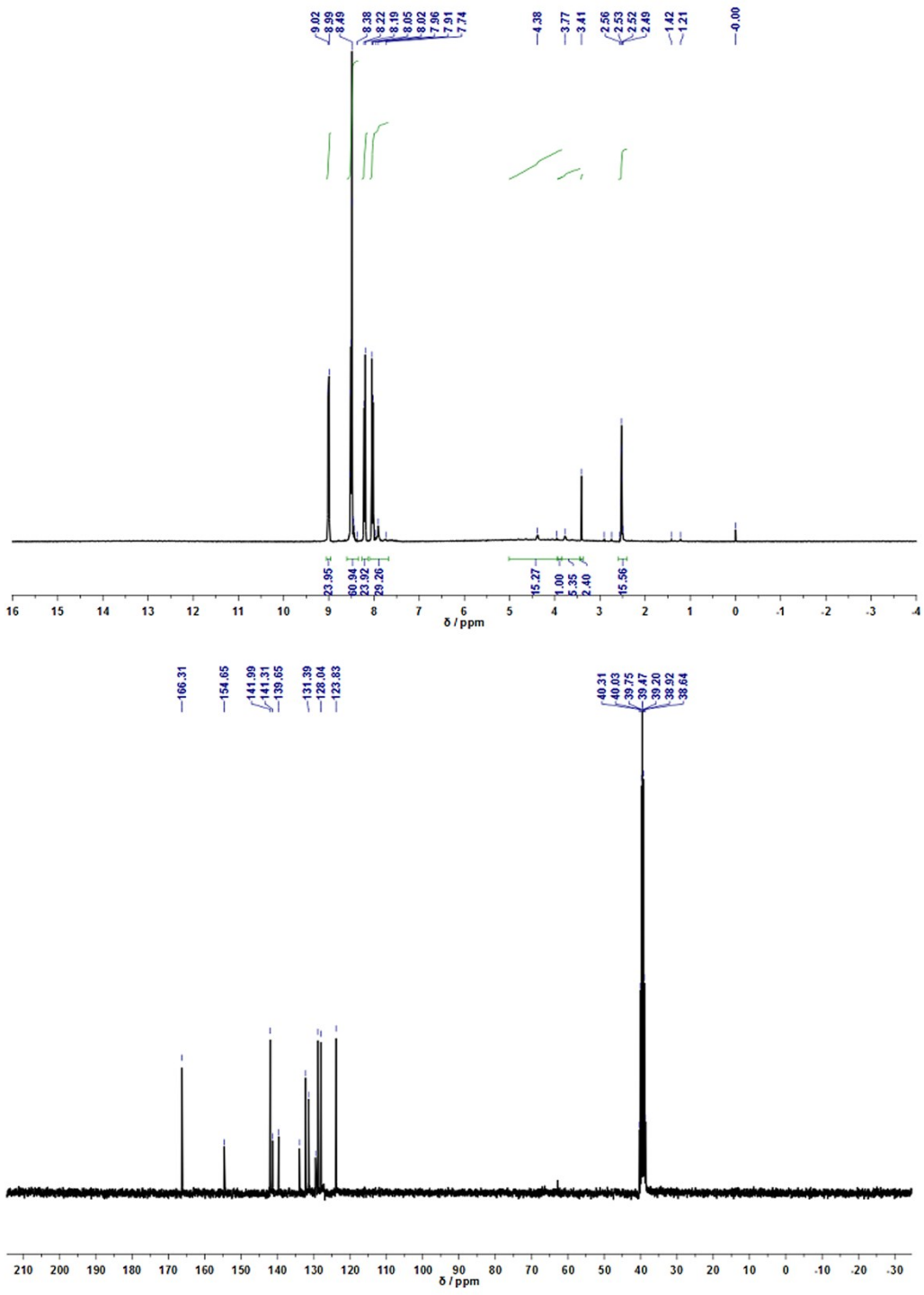

Fig.S10 The ^{1}H and ^{13}C NMR spectra of H_2PBPD.

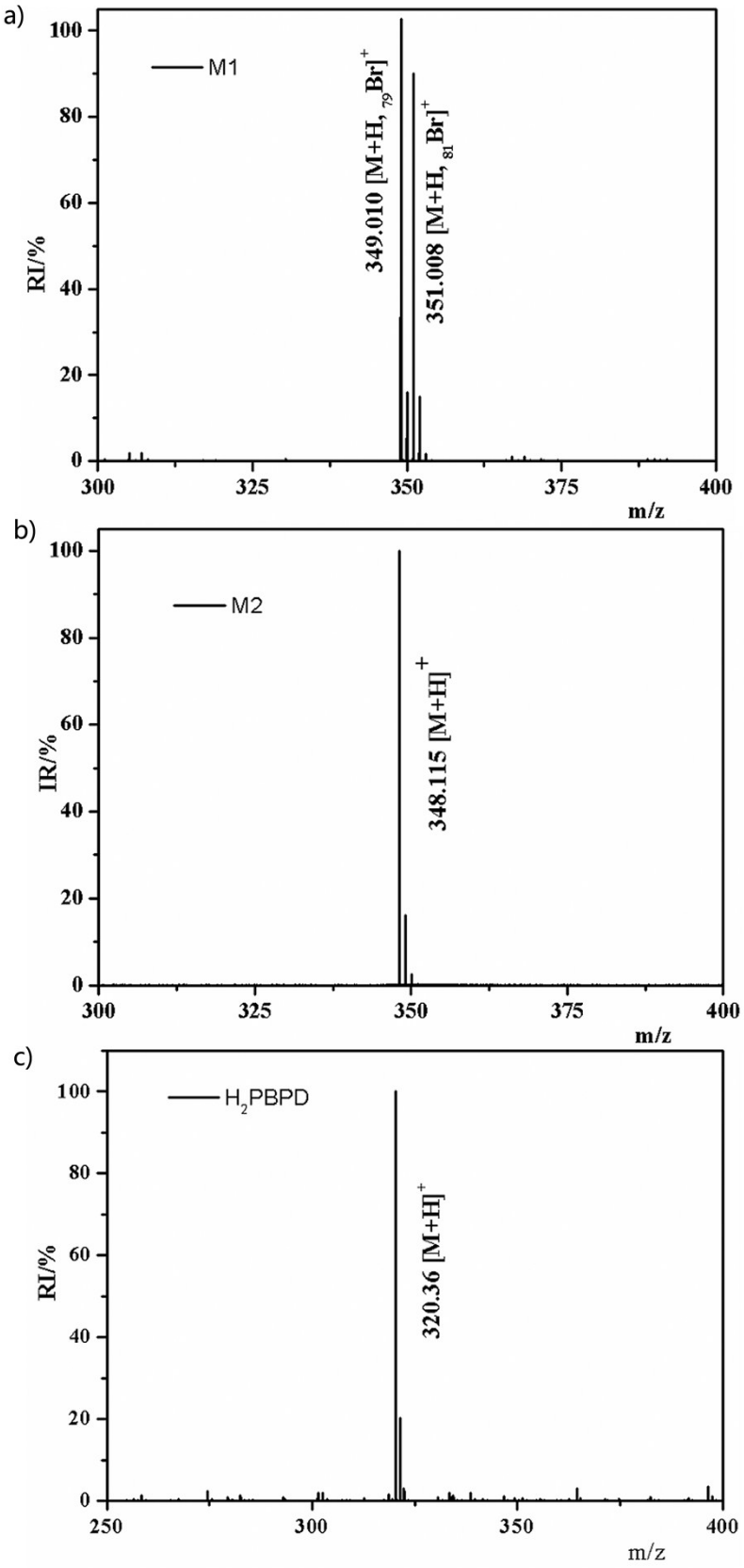

Fig.S11 MS of M1, M2 and H_2PBPD.

Table S1 Crystal Data and Structure Refinement for compound **1.**[a]

Formula	$C_{25}H_{31}N_3O_9Cu$	
Formula weight	580.14	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Hexagonal, *R*-3	
Unit cell dimensions	*a* = 18.9711(9) Å	α = 90°
	b = 18.9711(9) Å	β = 90°
	c = 44.954(2) Å	γ = 120°
Volume	14011.3(11) Å^3	
Z	18	
Calculated density	0.812 mg/cm^3	
Absorption coefficient	0.714 mm^{-1}	
F (000)	3474	
Theta range for data collection	1.32 to 25.33°	
Limiting indices	-20≤h≤22, -22≤k≤22, -49≤l≤53	
Reflections collected / unique	30455 / 5645	
R_{int}	0.0452	
Completeness to theta =25.33	99.1%	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5645/0/262	
Goodness-of-fit on F^2	1.184	
Final *R* indices [$I>2\sigma(I)$][b]	R_1 = 0.0597, wR_2 = 0.2127	
R indices (all data)	R_1 = 0.0735, wR_2 = 0.2315	

[a]Date based on *PLATON/SQUEEZE* mode.

[b]$R_1=\sum||F_o|-|F_c||/\sum|F_o|$. $wR_2=[\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]]^{1/2}$.

Table S2. Selected bond lengths [Å] and angles [deg] for compound **1.**

Bond lengths	
Cu(1)-O(3)	1.953(3)
Cu(1)-O(4)	1.953(3)
Cu(1)-O(2)	1.971(3)
Cu(1)-O(1)	1.971(3)
Cu(1)-N(1)	2.188(3)
N(1)-C(1)	1.333(6)
N(1)-C(5)	1.336(6)
Bond angels	
O(3)-Cu(1)-O(4)	88.39(15)
O(3)-Cu(1)-O(2)	166.66(12)
O(4)-Cu(1)-O(2)	89.53(16)
O(3)-Cu(1)-O(1)	89.47(16)
O(4)-Cu(1)-O(1)	166.75(12)
O(2)-Cu(1)-O(1)	89.54(17)
O(3)-Cu(1)-N(1)	104.03(13)
O(4)-Cu(1)-N(1)	104.09(13)
O(2)-Cu(1)-N(1)	89.25(13)
O(1)-Cu(1)-N(1)	89.11(13)