Carbon Dioxide Uptake by $[Cu(bpca)]^+$: Synthesis, Crystal Structure, and Magnetic Properties of $\{[Na(H_2O)_2][Cu_2(bpca)_2(CO_3)(HCO_3)]\}_n$ [Hbpca = Bis(2-pyridylcarbonyl)amide]

Rafaela M. R. da Silva,[a] Iara M.L. Rosa,[a] Willian X. C. Oliveira,[b] Odivaldo Cambraia Alves,[c] Evelyn C.S. Santos,[d] Flávio Garcia,[d] Henrique C. Silva Junior,[c] Glaucio B. Ferreira,[c] Guilherme P. Guedes,[c], Walace D. do Pim,[e] Miguel Julve,[f*] and Maria Vanda Marinho.[a*]

[a]*Instituto de Química, Universidade Federal de Alfenas, Campus Santa Clara, Alfenas, MG, 37133-840, Brazil.* maria.marinho@unifal-mg.edu.br
[b]*Departamento de Química - ICEx, Universidade Federal de Minas Gerais, Campus Pampulha, Belo Horizonte, MG, 31270-901, Brazil.*
[c]*Instituto de Química, Universidade Federal Fluminense, Niterói, Rio de Janeiro, RJ 24020-141, Brazil.*
[d]*Centro Brasileiro de Pesquisas Físicas (CBPF), Urca, Rio de Janeiro, RJ 22290-180, Brazil.*

[e]*Departamento de Química, Centro Federal de Educação Tecnológica de Minas Gerais, Belo Horizonte, MG, 30421-169, Brazil.*

[f]*Instituto de Ciencia Molecular (ICMol)/Departament de Química Inorgànica, Universitat de Valencia, C/ Catedrático José Beltrán 2, 46980 Paterna, València, Spain. miguel.julve@uv.es*

Table S1. Polymeric chains containing the $[Cu(bpca)]^+$ unit in the last 45 years.

Compound	Formula	Metal ion Counter ion Geometry	Reagents*	Methodology	Year	Reference
1	$[Cu\{(NC_5H_4CO)_2N\}]ClO_4$	Cu^{2+} ClO_4^- trigonal bipyramidal	$[Cu(H_2O)_6][ClO_4]_2$; tptz	Stirring/heating	1988	[1]
2	Cu(bpca)(CN)	Cu^{2+} CN^- square pyramidal	$Cu(bpca)_2·H_2O$; NaCN	Stirring/heating	2005	[2]
3	$[Cu(bpca)](ClO_4)$	Cu^{2+} ClO_4^- trigonal bipyramidal	$Cu(bpca)(N_3)$; $Fe(ClO_4)_3·H_2O$	Stirring/heating	2055	[2]
4	$[Cu(bpcam)(CN)(H_2O)]$	Cu^{2+} CN^- square pyramidal	$[Cu(bpcam)(H_2O)_3]NO_3·2H_2O$; KCN	Diffusion	2008	[3]
5	$[Cu(bpca)(tcm)]_n$	Cu^{2+} $C_4N_3^-$ square pyramidal	$[Cu(bpcam)(H_2O)_3]NO_3·2H_2O$; Ktcm	Diffusion	2008	[3]
6	$[Cu(bpcam)(tcm)]_n$	Cu^{2+} $C_4N_3^-$ square pyramidal	$[Cu(bpcam)(H_2O)_3]NO_3·2H_2O$; Ktcm	Diffusion	2008	[4]
7	[(BPCA)Cu(MA)]	Cu^{2+} MA^- square pyramidal	HBPCA; $Cu(ClO_4)_2·6H_2O$; HMA	Stirring/heating	2010	[5]
8	$[(BPCA)Cu(MPA)(H_2O)]$	Cu^{2+} MPA^- square pyramidal	HBPCA; $Cu(ClO_4)_2·6H_2O$; HMPA	Stirring/heating	2010	[5]
9	$[(BPCA)Cu(BA)]_n$	Cu^{2+} BA^-	HBPCA; $Cu(ClO_4)_2·6H_2O$; HBA	Stirring/heating	2010	[5]

		square pyramidal				
10	$[Cu(bpca)(CF_3SO_3)(H_2O)]\cdot H_2O$	Cu^{2+} $CFSO_3^-$ square pyramidal	$Cu(CF_3SO_3)_2$; tptz	Stirring/heating	2013	[6]
11	$[Cu(bpca)(EtH_2opba)]_n$	Cu^{2+} $CFSO_3^-$ Octahedral	$[Cu(bpca)(CF_3SO_3)(H_2O)]\cdot H_2O$; EtH_2opba	Stirring/heating	2013	[6]
12	$[Cu(bpca)Cl]_n$	Cu^{2+} Cl^- square pyramidal	$[Cu(tptz)Cl_2]\cdot 2H_2O$	Stirring/heating	2014	[7]
13	$[\{Cu(bpca)]_2[Pd(opba)]\}\cdot 1.75dmso\cdot 0,25H_2O$	Cu^{2+} $opba^-$ Square planar	$[Cu(bpca)(H_2O)_2]NO_3\cdot 2H_2O$; $K_2[Pd(opba)]\cdot 2H_2O$	Stirring/heating	2015	[8]
14	$\{[Cu(bpca)]_2[Pd(opba)]\}_n$	Cu^{2+} $opba^-$ Square planar	$[Cu(bpca)(H_2O)_2]NO_3\cdot 2H_2O$; $K_2[Pd(opba)]\cdot 2H_2O$	Stirring/heating	2015	[8]
15	$[\{Cu(bpca)\}_2(H_2ppba)]\cdot 1.33dmf\cdot 0.66dmso\}_n$	Cu^{2+} $ppba^-$ Octahedral	$[\{K_2(H_2O)_2\}\{Pd_2(ppba)_2\}]$	Diffusion	2016	[9]

*Abbreviations: NC_5H_4CO = bpca= bis(2-pyridylcarbonyl)amidate; bpcam = bis(2-pyrimidylcarbonyl)amidate; tptz = 2,4,6-Tris(2-pyridyl)-l,3,5-triazine; tcm = tricyanomethanide; MA = racemic mandelate; MPA = racemic a-methoxy phenylacetate; BA = benzilate anion; H_4opba = N,N'-1,2-phenylenebis(oxamic acid); EtH_3opba = monoethyl ester derivative of the H_4opba; H_4mpba =1,3-phenylenebis(oxamic acid); H_4opba = 1,2- phenylenebis(oxamic acid); Hbpca = bis(2-pyridylcarbonyl)amide; dmso = dimethyl sulfoxide; = dimethylformamide; H_4ppba = N,N'-1,4-phenylenebis(oxamic acid.

Table S2. Values of the spin moment calculated for the singlet and nonet states of **1**.

		Singlet state **Spin Density**			
Cu_2	**N_5**	**N_4**	**N_6**	**O_8**	**O_9**
0.622	0.076	0.069	0.067	0.115	0.004
Cu_1	**N_2**	**N_1**	**N_3**	**O_5**	**O_6**
0.660	0.085	0.074	0.078	0.063	0.000
$Cu_{2'}$	**$N_{5'}$**	**$N_{4'}$**	**$N_{6'}$**	**$O_{8'}$**	**$O_{9'}$**
0.622	0.076	0.069	0.067	0.115	0.004
$Cu_{1'}$	**$N_{2'}$**	**$N_{1'}$**	**$N_{3'}$**	**$O_{5'}$**	**$O_{6'}$**
0.660	0.085	0.074	0.078	0.063	0.000
		Nonet state **Spin Density**			
Cu_2	**N_5**	**N_4**	**N_6**	**O_8**	**O_9**
-0.622	-0.076	-0.069	-0.067	-0.115	-0.004
Cu_1	**N_2**	**N_1**	**N_3**	**O_5**	**O_6**
-0.660	-0.085	-0.074	-0.078	-0.063	-0.000
$Cu_{2'}$	**$N_{5'}$**	**$N_{4'}$**	**$N_{6'}$**	**$O_{8'}$**	**$O_{9'}$**
0.622	0.076	0.069	0.067	0.115	0.004
$Cu_{1'}$	**$N_{2'}$**	**$N_{1'}$**	**$N_{3'}$**	**$O_{5'}$**	**$O_{6'}$**
0.660	0.085	0.074	0.078	0.063	0.000

Table S3. Values of the spin moment calculated for nonet state of **1** with a totally antiferromagnetic organization.

		Nonet state **Spin Density**			
Cu_2	**N_5**	**N_4**	**N_6**	**O_8**	**O_9**
0.623	0.076	0.070	0.067	0.115	0.005
Cu_1	**N_2**	**N_1**	**N_3**	**O_5**	**O_6**
-0.659	-0.085	-0.074	-0.078	-0.063	-0.000
$Cu_{2'}$	**$N_{5'}$**	**$N_{4'}$**	**$N_{6'}$**	**$O_{8'}$**	**$O_{9'}$**
-0.623	-0.076	-0.070	-0.067	-0.115	-0.005
$Cu_{1'}$	**$N_{2'}$**	**$N_{1'}$**	**$N_{3'}$**	**$O_{5'}$**	**$O_{6'}$**
0.659	0.085	0.074	0.078	0.063	0.000

Table S4. Values of the spin moment calculated for nonet state of **1** in antiferromagnetic chains but with a ferromagnetic organization between them.

		Nonet state Spin Density			
Cu_2	**N_5**	**N_4**	**N_6**	**O_8**	**O_9**
-0.623	-0.076	-0.070	-0.067	-0.115	-0.004
Cu_1	**N_2**	**N_1**	**N_3**	**O_5**	**O_6**
0.659	0.085	0.074	0.078	0.063	0.000
$Cu_{2'}$	**$N_{5'}$**	**$N_{4'}$**	**$N_{6'}$**	**$O_{8'}$**	**$O_{9'}$**
-0.623	-0.076	-0.070	-0.067	-0.115	-0.004
$Cu_{1'}$	**$N_{2'}$**	**$N_{1'}$**	**$N_{3'}$**	**$O_{5'}$**	**$O_{6'}$**
0.659	0.085	0.074	0.078	0.063	0.000

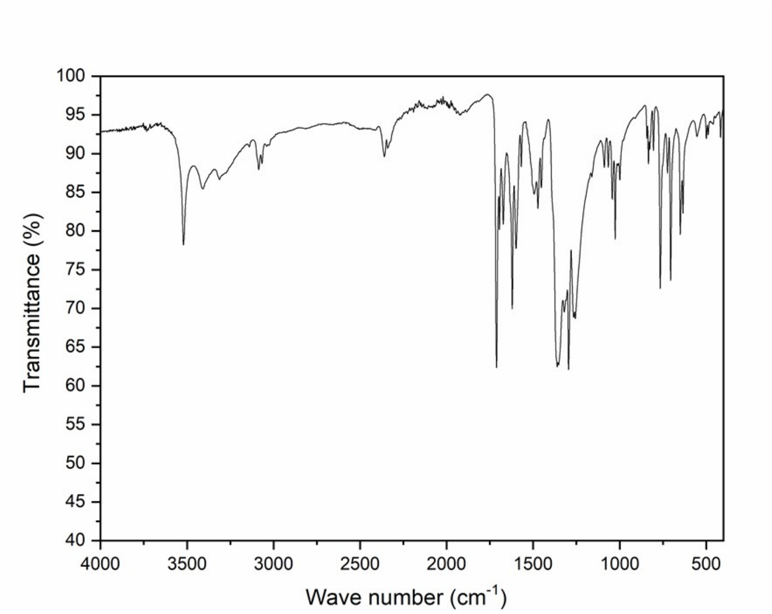


Figure S1. IR spectrum of **1**.

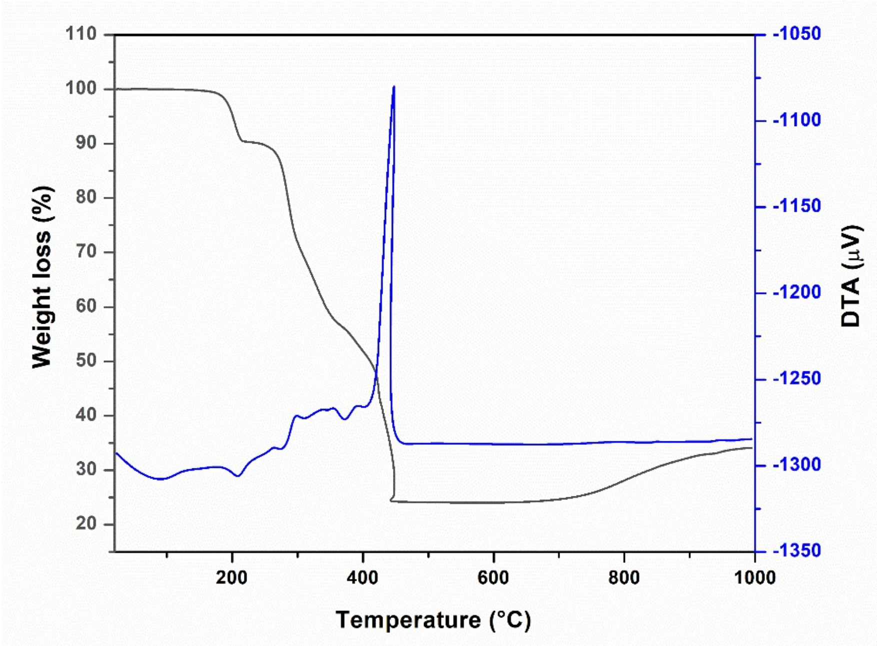


Figure S2. TG and DTA curves for **1**.

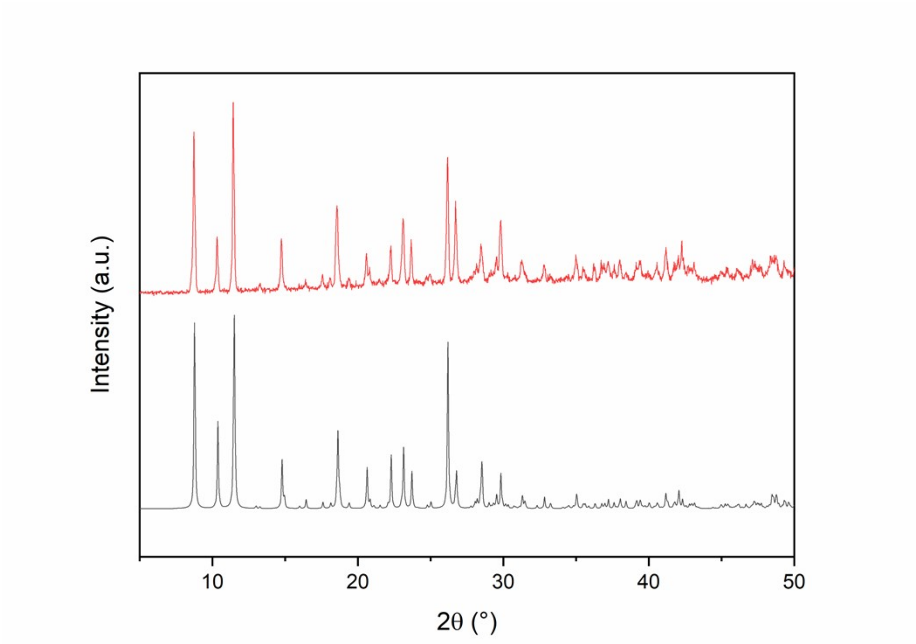
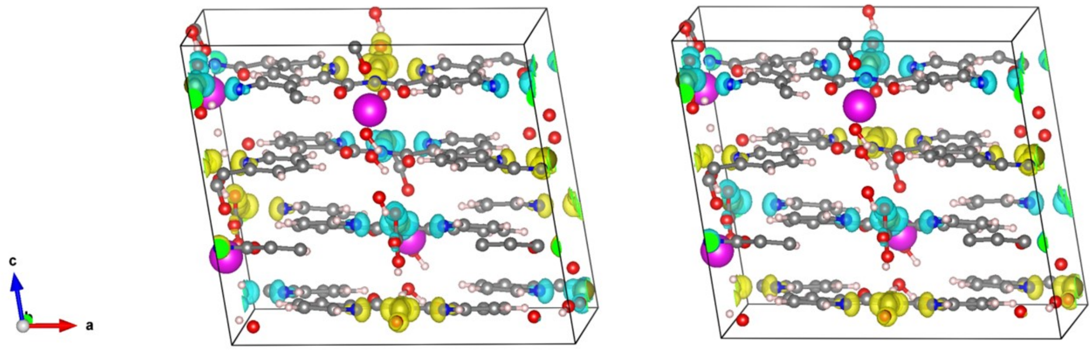


Figure S3. PXRD calculated (black) and experimental (red) patterns of **1**.



(a) (b)

Figure S4. Spin moment in the unit cell of **1** for the singlet state (E_{BS}) (a) totally antiferromagnetic and (b) with antiferromagnetic chains but with a ferromagnetic organization between them. Atoms are represented by CPK color scheme: carbon (grey) oxygen (red), nitrogen (blue), copper (olive), pink (Na), hydrogen (white), positive spin density (yellow), and negative spin density (blue).

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