Electronic supplementary information (ESI)

Crystal structure and physical properties of 1-methyl-3-(carboxymethyl) benzimidazolium betaine·$CuBr_2$ in crystal and water solution

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Table S1 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3).

	x	*y*	*z*	*U(eq)*
Cu(1)	0	10000	10000	26(1)
Br(1)	2693(1)	8207(1)	9244(1)	42(1)
N(1)	1178(3)	16529(2)	5392(2)	30(1)
C(2)	1170(3)	16203(3)	6924(3)	29(1)
N(3)	2351(3)	14616(3)	7710(2)	28(1)
C(4)	3191(3)	13853(3)	6624(3)	29(1)
C(5)	2434(3)	15077(3)	5142(3)	30(1)
C(6)	2962(4)	14728(4)	3776(3)	43(1)
C(7)	4263(4)	13108(4)	3973(4)	52(1)
C(8)	5027(4)	11903(4)	5458(4)	50(1)
C(9)	4505(3)	12232(3)	6816(3)	40(1)
C(10)	55(4)	18157(3)	4165(3)	44(1)
C(11)	2585(3)	13763(3)	9430(3)	33(1)
C(12)	1694(3)	12299(3)	10134(2)	26(1)
O(1)	1875(2)	11474(2)	11573(2)	39(1)
O(2)	837(2)	12067(2)	9162(2)	34(1)
H(2)	439	16976	7389	35
H(6)	2466	15541	2784	52
H(7)	4641	12812	3091	62
H(8)	5921	10840	5532	60
H(9)	5003	11415	7806	48
H(101)	-697	18952	4648	66
H(102)	-664	17822	3610	66
H(103)	791	18761	3436	66
H(111)	2098	14682	9884	39
H(112)	3843	13235	9718	39

U(eq) is defined as one third of the trace of the orthogonalized *Uij* tensor.

Table S2 Bond lengths (Å) and angles (°)

Cu(1)-O(2)	1.9293(15)
Cu(1)-O(1)	2.9492(19)
Cu(1)-Br(1)	2.4125(3)
N(1)-C(2)	1.321(3)
N(1)-C(5)	1.390(3)
N(1)-C(10)	1.469(3)
C(2)-N(3)	1.330(3)
N(3)-C(4)	1.391(3)
N(3)-C(11)	1.461(3)
C(4)-C(9)	1.386(3)
C(4)-C(5)	1.395(3)
C(5)-C(6)	1.389(3)
C(6)-C(7)	1.380(4)
C(7)-C(8)	1.395(4)
C(8)-C(9)	1.374(4)
C(11)-C(12)	1.527(3)
C(12)-O(1)	1.230(3)
C(12)-O(2)	1.268(3)
Br(1)-O(2)	3.0803(16)
Br(1)`-O(2)	3.0978(16)
O(2)#1-Cu(1)-O(2)	180.00(9)
O(2)#1-Cu(1)-Br(1)	90.33(5)
O(2)-Cu(1)-Br(1)	89.67(5)
O(2)#1-Cu(1)-Br(1)#1	89.67(5)
O(2)-Cu(1)-Br(1)#1	90.33(5)
Br(1)-Cu(1)-Br(1)#1	180.0
C(2)-N(1)-C(5)	108.41(19)
C(2)-N(1)-C(10)	125.6(2)
C(5)-N(1)-C(10)	126.0(2)
N(1)-C(2)-N(3)	110.5(2)
C(2)-N(3)-C(4)	108.31(19)
C(2)-N(3)-C(11)	125.0(2)
C(4)-N(3)-C(11)	126.41(19)
C(9)-C(4)-N(3)	131.7(2)
C(9)-C(4)-C(5)	122.1(2)
N(3)-C(4)-C(5)	106.2(2)
C(6)-C(5)-N(1)	132.0(2)
C(6)-C(5)-C(4)	121.5(2)
N(1)-C(5)-C(4)	106.5(2)
C(7)-C(6)-C(5)	116.3(3)
C(6)-C(7)-C(8)	121.9(3)
C(9)-C(8)-C(7)	122.2(3)
C(8)-C(9)-C(4)	116.0(3)
N(3)-C(11)-C(12)	113.13(19)
O(1)-C(12)-O(2)	126.8(2)
O(1)-C(12)-C(11)	117.3(2)
O(2)-C(12)-C(11)	115.95(18)
C(12)-O(2)-Cu(1)	115.85(13)

Symmetry transformations used to generate equivalent atoms:
#1 -*x*, 2-*y*, 2-*z*

Table S3 Torsion angles (deg)

C(5)-N(1)-C(2)-N(3)	0.1(3)
C(10)-N(1)-C(2)-N(3)	-179.6(2)
N(1)-C(2)-N(3)-C(4)	0.1(3)
N(1)-C(2)-N(3)-C(11)	-174.4(2)
C(2)-N(3)-C(4)-C(9)	-179.7(3)
C(11)-N(3)-C(4)-C(9)	-5.3(4)
C(2)-N(3)-C(4)-C(5)	-0.3(2)
C(11)-N(3)-C(4)-C(5)	174.2(2)
C(2)-N(1)-C(5)-C(6)	179.5(3)
C(10)-N(1)-C(5)-C(6)	-0.8(4)
C(2)-N(1)-C(5)-C(4)	-0.2(3)
C(10)-N(1)-C(5)-C(4)	179.4(2)
C(9)-C(4)-C(5)-C(6)	0.1(4)
N(3)-C(4)-C(5)-C(6)	-179.5(2)
C(9)-C(4)-C(5)-N(1)	179.9(2)
N(3)-C(4)-C(5)-N(1)	0.3(2)
N(1)-C(5)-C(6)-C(7)	-179.4(2)
C(4)-C(5)-C(6)-C(7)	0.3(4)
C(5)-C(6)-C(7)-C(8)	-1.1(4)
C(6)-C(7)-C(8)-C(9)	1.6(4)
C(7)-C(8)-C(9)-C(4)	-1.2(4)
N(3)-C(4)-C(9)-C(8)	179.8(3)
C(5)-C(4)-C(9)-C(8)	0.4(3)
C(2)-N(3)-C(11)-C(12)	100.1(3)
C(4)-N(3)-C(11)-C(12)	-73.5(3)
N(3)-C(11)-C(12)-O(1)	177.79(19)
N(3)-C(11)-C(12)-O(2)	-2.4(3)
O(1)-C(12)-O(2)-Cu(1)	-8.7(3)
C(11)-C(12)-O(2)-Cu(1)	171.51(15)
O(2)#1-Cu(1)-O(2)-C(12)	-118(100)
Br(1)-Cu(1)-O(2)-C(12)	-91.70(15)
Br(1)#1-Cu(1)-O(2)-C(12)	88.30(15)

Symmetry transformations used to generate equivalent atoms:
#1 *-x*, 2-*y*, 2-*z*

Table S4 FT-IR absorption maxima (cm^{-1}) of MBImAcOH Br **(2),** benzimidazolium betaine MBImAcO ligand **(3)** and $Cu(MBImAcO)_2Br_2$ complex **(4).**

Compound			Assignments
(2)	**(3)**	**(4)**	
	3466 3396		$\nu(OH)_2$
	3137 3059 3006 2985	3148 3030 2967 2962	ν(CH)
			$\nu_{as}(CH_2)$
2810			$\nu_s(CH_2)$
			Bz. inplane ring bending
			Ring stretching
1737	1616	1626	(COOH)
1572	1569	1575	ν_{as}(COO)
1487	1488	1487	Bz. CH outplane bending
1465 1451 1430 1410	1466 1414	1468 1437 1423	Ring stretching
1396	1377	1375	υ_s(COO)
1364 1357 1313	1350 1306	1361 1352 1346	Ring stretching
1275	1285	1278	$\delta(CH_2)$
			Bz. inplane ring stretching
			Ring stretching
1203 1190 1113 1036	1204 1170 1094 1028	1204 1166 1131 1092	Bz. inplane CH bending
986	986	981	Im. CH inplane bending
894	902	923	Bz. inplane ring bending
884	872	886	Im. inplane ring bending
864 830	811		Im. CH outplane bending
772	780 760	798 772 757 750	Im. plane ring bending
722	727	736	Bz CH outplane bending
629 601 576	659 591	668 614 572	NH outplane bending + Im. plane ring bending + Im. ring torsion
526	525	530	Ring torsion

Bz – benzimidazole; Im - imidazole