10.1071/CH11236_AC

Australian Journal of Chemistry 2011, 64(12), 1624-1627

Accessory Publication

Efficient synthesis of ellagic acid salts using distillable ionic liquids

Shahana A. Chowdhury,[A] *Pamela M. Dean,*[A] *R. Vijayaraghavan,*[A] *and D. R. MacFarlane*[A,B]

[A]School of Chemistry, Monash University, Clayton Campus, Victoria 3800, Australia.

[B]*Corresponding author. Email: douglas.macfarlane@monash.edu*

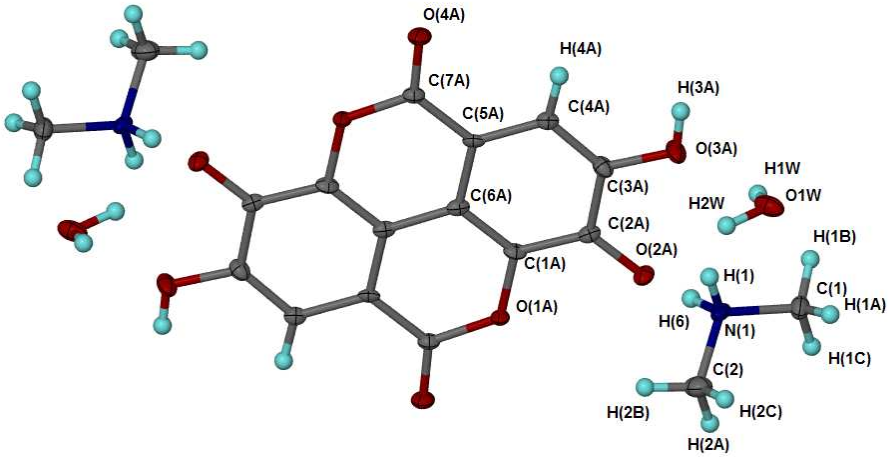

Fig A-1 The unique component and some symmetry-related atoms [symmetry code: -x,1-y,1-z] of (I) comprising the molecular moiety. The schematic displays the numbering scheme and thermal ellipsoids at the 50 % probability level. The hydrogen atoms are shown as spheres of arbitrary size.

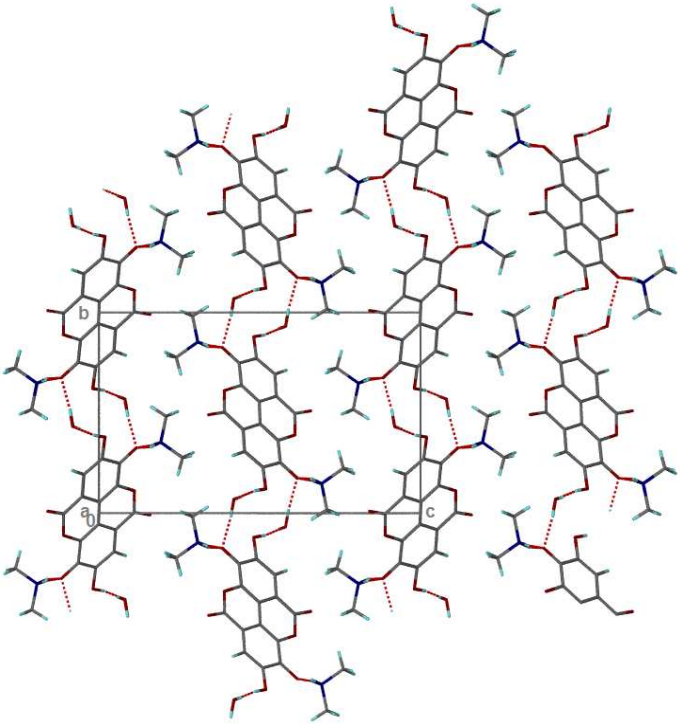

Fig A-2 The extended packing of (I) as viewed down the *a*-axis. Hydrogen bonds are indicated in a dashed red line.

Table 1

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N(1)—H(1)···O(2A)^{ii}	0.93 (4)	1.85 (4)	2.740 (4)	159 (3)
O(1W)—H(1W)···O(3A)^{i}	0.82 (5)	2.55 (4)	3.370 (4)	175 (4)
O(1W)—H(2W)···O(2A)^{iii}	0.94 (6)	1.85 (5)	2.787 (4)	172 (4)
O(3A)—H(3A)···O(1W)^{iv}	0.84	1.86	2.696 (4)	170
N(1)—H(6)···O(2A)	0.95 (4)	1.82 (4)	2.760 (4)	173 (4)

Table 2

Geometrical parameters (Å, °) of selected inter-ring π—π interactions. α is the dihedral angle between planes I and J, CgI is the centroid of plane I and CgJ the centroid of plane J.

CgI	CgJ	Cg···Cg	α	Symmetry position of CgJ
Cg1	Cg1	4.0186 (19)	0.00	-1-X,1-Y,1-Z
Cg1	Cg2	3.541 (2)	1.24	-1+X,Y,Z
Cg1	Cg3	4.0186 (19)	0.00	-1+X,Y,Z
Cg1	Cg3	4.732 (2)	0.00	-1-X,1-Y,1-Z
Cg1	Cg3	4.732 (2)	0.00	1-X,1-Y,1-Z
Cg2	Cg1	3.541 (2)	1.24	1+X,Y,Z
Cg2	Cg2	4.559 (2)	0.00	1-X,1-Y,1-Z
Cg2	Cg3	3.541 (2)	1.24	1-X,1-Y,1-Z
Cg3	Cg1	4.0186 (19)	0.00	1+X,Y,Z
Cg3	Cg1	4.732 (2)	0.00	-1-X,1-Y,1-Z
Cg3	Cg1	4.732 (2)	0.00	1-X,1-Y,1-Z
Cg3	Cg2	3.541 (2)	1.24	1-X,1-Y,1-Z
Cg3	Cg3	4.0186 (19)	0.00	1-X,1-Y,1-Z

Notes: Cg1 is the centroid of ring O1A/C1A/C6A/C6Aa/C5Aa/C7Aa. Cg2 is the centroid of ring C1A/C2A/C3A/C4A/C5A/C6A. Cg3 is the centroid of ring C5A/C6A/C6Aa/C1Aa/O1Aa/C7A.

Structure of Ellagic acid

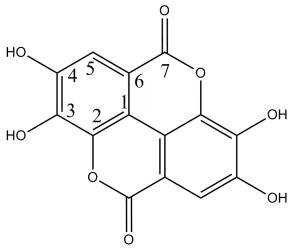

Table 3 : ^{13}C Chemical shifts of the Ellagic acid salt

Carbon	Ellagic acid diammonium salt (ppm)
1	**105.7**
2	**135.6**
3	**--**
4	**149.7**
5	**--**
6	**114.3**
7	**160.8**