Table.3. Conformation of N^6-benzoyladeninum molecule in the salt of N6-benzoyladeninum nitrate (NA)(I)

Crystals	Dihedral angle (°)				Torsion angle(°)
	Primidine ring /imdazole ring of adenine (N1-N3-C2-C4-C5-C6/N7-N9-C4-C5-C8)	Purine ring /benzene ring (N1-C2-N3-C4-C5-C6-N7-C8-N9/C11-C12-C13-C14-C15-C16)	Purine ring /amide (N1-C2-N3-C4-C5-C6-N7-C8-N9/N6-H6-C10-O1)	Benzene ring /amide (C11-C12-C13-C14-C15-C16/N6-H6-C10-O1)	(C6-N6-C10-C11)
N^6-benzoyladenine–3-hydroxypyridinium-2-carboxylate(1:1) (Ref. a)	3.00(9)	0.94(8)	21.20(17)	21.45(18)	-176.24(16)
N^6-benzoyladenine–DL-tartaric acid(1:1)(Ref. a)	2.26(10)	9.77(8)	2.93(18)	11.35(9)	-179.08(17)
N^6-benzoyladeninium Nitrate (present)	1.34(14)	52.25(12)	23.7(2)	29.2(2)	-168.8(2)

Ref: a) Karthikeyan *et al.*, 2015.

Table.4. Comparison of dihedral angles (°) between the adenine plane and phenyl ring plane in some related structures

Name of the Compound	**Molecule A (°)**	**Molecule B (°)**	**Reference**
N6-benzyladenine	78.5(3)		a
N6-benzyladeninium oxalate	49.03(8)		b
N6-benzyladeninium p-toluenesulfonate	82.76(11)		c
N6-benzyladeninium sulphosalicylate monohydrate	77.04(10)		d
N6-benzyladeninium 3-hydroxypicolinate	67.91(12)	68.27(13)	e
N6-benzyladeninium nitrate	76.64(16)		f
N6-benzyoladenine	7.4		g
N6-benzyoladenine 3-hydroxypyridinium-2-carboxylate	1.54(7)		h
N6-benzyoladenine (DL)-tartaric acid	9.74(7)		i
N6-benzoyladeninium nitrate	51.57(10)		Present

Ref: a) Raghunathan *et al.*, 1983; b) McHugh & Erxleben,2011; c) Tamilselvi & Muthiah, 2011; d) Xia *et al.*, 2010; e &f) Nirmalram *et al.*, 2011; i) Raghunathan & Pattabhi, 1981; h &i) Karthikeyan *et al.*, 2015.