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Supporting information for article:

D-Mannosamine hydrochloride (2-amino-2-deoxy-D-mannose hydrochloride): ionic hydrogen bonding in saccharides involving chloride and ammonium ions

Jieye Lin, Allen G. Oliver and Anthony S. Serianni

Table S1 The rigid-body vibration analysis of (I).

Atom-Atom		**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**
1	O1	0	4	4	4	4	8	-5	5	4	0	4	2
2	O3	5	0	6	2	3	3	1	1	-3	0	0	0
3	O4	5	3	0	2	7	1	7	2	1	-1	1	5
4	O5	2	4	4	0	1	2	0	0	3	1	0	6
5	O6	5	6	4	3	0	2	1	1	1	5	2	-4
6	N2	3	3	4	3	6	0	5	0	1	3	3	3
7	C1	-1	4	4	-1	4	2	0	0	2	1	1	4
8	C2	2	2	4	2	5	-1	-2	0	-1	0	0	4
9	C3	4	-1	2	3	5	2	3	-2	0	-2	3	3
10	C4	4	2	-1	2	4	3	3	3	-2	0	-2	0
11	C5	4	4	2	-1	2	4	2	3	3	-2	0	-1
12	C6	5	5	3	2	-1	5	4	4	4	3	-1	0

The entries highlighted in grey represent Del(A,B)×1000 values, which should be near zero. The remaining entries represent distances (A–B) in angstroms. Negative entries indicate bonded atoms. (Hirshfeld, 1976; Rosenfield, 1978). Atoms of the minor α-anomer (disordered region) are omitted for clarity.