Glycine-sodium nitrate, GSN: a low temperature redetermination

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As part of research into materials for use in the field of non-linear optics, crystals of glycine-sodium nitrate (I) were prepared. Inorganic salts of amino acids have shown to be useful in nonlinear optics studies [1-3]. The room-temperature crystal structure of (I), refined in space group *Cc*, was reported by Krishnakumar et al. [4] although no mention of the non-linear optical properties of the compound is discussed.

This low-temperature redetermination is presented in the conventional space group *Ia*. The asymmetric unit of (I) consists of one glycine molecule, one sodium cation and one nitrate anion. The structure is polymeric and the complete coordination environment of the sodium centre is shown in Fig. 1. The octa-coordinated sodium centre has essentially distorted hexagonal bipyramidal geometry, with apical glycine ligands. The bonding geometry is unexceptional. The glycine molecule exists as a zwitterion and N—H· · ·O hydrogen bonding secures the location of the N—H H atoms (Table 1). Compound (I) was prepared by dissolving 32.83 g of glycine and 37.16 g of sodium nitrate in100 mL of double-distilled water. Crystals were grown by slow solvent evaporation from a saturated solution over several weeks at a constant temperature of 30°C.

All H atoms were first located from a difference electron density map. N—H H atoms were freely refined. The C—H H atoms were refined as riding, with a C—H distance constrained to be 0.99 $\overset{o}{A}$ and $U_{iso}(H) = 1.2U_{eq}(C)$. Since the largest element in this structure is sodium, the value of the Flack parameter is meaningless due to lack of significant anomalous dispersion. Friedel pairs were thus merged during the final refinement.

Data collection: SMART [5]. Cell refinement: SAINT [5]. Data reduction: SAINT. Program(s) used to solve structure: SHELXTL [6]. Program(s) used to refine structure: SHELXTL. Molecular graphics: ORTEP3 for Windows.

References

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Table 1. *Hydrogen-bonding geometry (Å, °)*

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1N$\cdots$O4^{i}	0.87 (3)	2.32 (3)	2.894 (4)	124 (2)
N1—H2N$\cdots$O1^{ii}	0.85 (4)	1.95 (4)	2.792 (3)	171 (4)
N1—H3N$\cdots$O2^{iii}	0.87 (5)	1.93 (5)	2.793 (4)	169 (4)

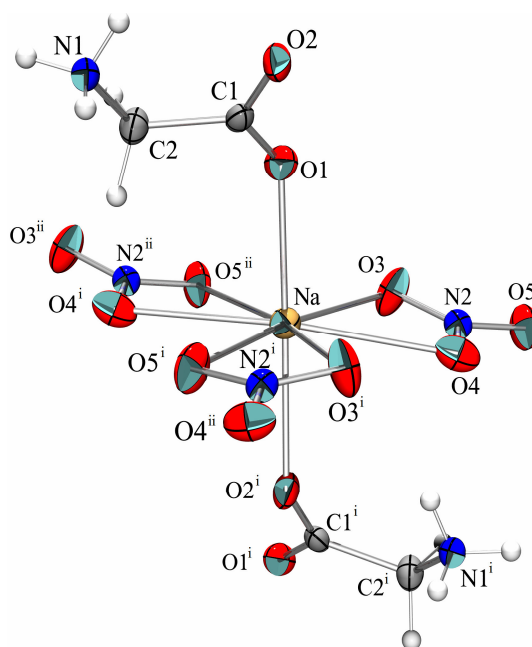Symmetry codes: (i) $x, \frac{1}{2} - y, \frac{1}{2} + z$; (ii) $x - \frac{1}{2}, 1 - y, z$; (iii) $x, 1 + y, z$.

FIG. 1. GSN redefined structure