Synthesis and Crystal Structure
Determination of a Guanidine Adduct of Sodium Guanidinate,
$\text{NaCN}_3\text{H}_4(\text{CN}_3\text{H}_5)_2$

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Well-grown single crystals of $\text{NaCN}_3\text{H}_4(\text{CN}_3\text{H}_5)_2$ were synthesized from guanidine and sodium hydride. The new compound crystallizes in the monoclinic space group $P2_1/n$ (no. 14) with $Z = 4$ and $a = 6.2007(4)$, $b = 9.6261(8)$, $c = 15.7630(11)$ Å and $\beta = 93.783(3)^\circ$ at 293 K. The asymmetric unit comprises two sodium cations on special positions, one guanidinate anion and two symmetry-independent guanidine molecules. The structure is built up from columns of face-sharing $\text{NaN}_6$ octahedra oriented along the crystallographic $a$ axis. The coordinating organic ligand anions and molecules are connected by hydrogen bonds from amino H atoms to imino N atoms to generate a tube-like motif. These tubes are then linked by two more hydrogen bonds to form a three-dimensional network.

Key words: Guanidinate, Guanidine Adduct, Sodium, Crystal Structure, Hydrogen Bonds