HIRSCHFELD SURFACE OF A COMPLEX OF CARBAMIDE WITH STRONTIUM NITRATE

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As a result of the interaction of urea with strontium nitrate in a 1:2 ratio, a complex compound of the composition $[Sr((NH_2)_2CO)_2(NO_3)_2]$was synthesized. The molecular (Fig. 1, a) and polymer (Fig. 1, b) structure of the new complex was determined by X-ray diffraction analysis. To characterize the nature of intermolecular interactions (Fig. 2), an analysis of the Hirschfeld surface was performed using the Crystal Explorer17.5[1] program.

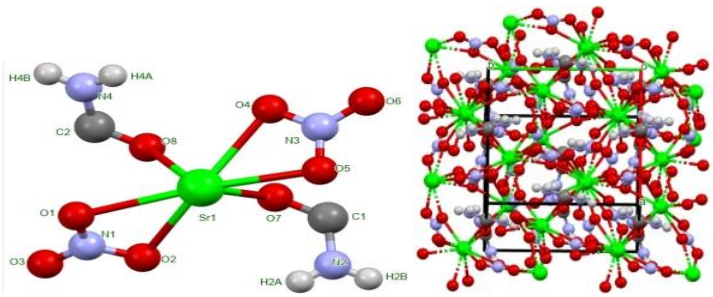


Figure 1. Molecular structure (a) and appearance in the polymer structure (b) of the complex of urea with strontium nitrate.

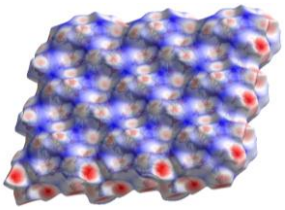


Figure 2. Hirschfeld surfaces of the complex $[Sr((NH_2)_2CO)_2(NO_3)_2]n$

On the Hirschfeld surface of the complex of urea with strontium nitrate, the red color represents the nearest interactions, and the blue color represents the farthest interactions (Fig. 2). Thus, the analysis of the Hirschfeld surface revealed the following interactions: H...O/O...H (54.3%), H...H (17.5%), N...O/O...N (8.6%), O..O (7.3%), O...Sr/Sr...O (5.5%), N...C/C...N (2.6%), H...N/N...H (2.0%), O...C/C...O (1.3%), H...C/C...H (0.5%), N...N (0.4%) which make the main contribution to the formation of crystalline packaging. Hirshfeld's surface analysis shows that the main part of the interactions is O...H/H...O (54.3%) and H...H (17.5%) [2].

REFERENCES

[1]. Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Spackman, P. R., Jayatilaka, D. & Spackman, M. A. 2017, Turner CrystalExplorer17. University of Western Australia. http://Hirshfeldsurface.net.

[2]. A.Bektursinova,Z. Djumanazarova, Z.Uzakbergenova, J.Ashurov,b A. Khan, Sh.Kadirova, B.Torambetov. Synthesis, crystal structure and Hirshfeld surface analysis of $[Sr((NH_2)_2CO)_2(NO_3)_2]$.Acta E Cryst. 2025 E81.https://doi.org/10.1107/S2056989024012386.