



**A Combined Study on the Crystal Structure and Hydrogen Bonds of  
[NH<sub>2</sub>(C<sub>2</sub>H<sub>5</sub>)<sub>2</sub>][4-CH<sub>3</sub>-C<sub>6</sub>H<sub>4</sub>-S(O)<sub>2</sub>NHP(O)(O)(N(C<sub>2</sub>H<sub>5</sub>)<sub>2</sub>)]·H<sub>2</sub>O**

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In the present work, we report on the synthesis and structure determination of the title hydrated salt, [NH<sub>2</sub>(C<sub>2</sub>H<sub>5</sub>)<sub>2</sub>][4-CH<sub>3</sub>-C<sub>6</sub>H<sub>4</sub>-S(O)<sub>2</sub>NHP(O)(O)(N(C<sub>2</sub>H<sub>5</sub>)<sub>2</sub>)]·H<sub>2</sub>O. In the anion of this salt, each of the phosphorus and sulfur atoms has a distorted tetrahedral configuration with the bond angles in range of 102.99(6)° to 117.28(7)° at the P atom and 106.47(7)° to 119.42(7)° for S atom. The P1—N1 and P1—N2 bond lengths are 1.7085(14) Å and 1.6495(14) Å, respectively; whereas, P1—O3 and P1—O2 have almost equal bond lengths (1.4960(12) Å and 1.4957(9) Å). The S=O bond lengths of 1.4355(12) Å and 1.4351(12) Å are standard for sulfonamide compounds [1–3]. The asymmetric unit of the title hydrated salt contains three components including one [NH<sub>2</sub>(C<sub>2</sub>H<sub>5</sub>)<sub>2</sub>]<sup>+</sup> cation, one [4-CH<sub>3</sub>-C<sub>6</sub>H<sub>4</sub>-S(O)<sub>2</sub>NHP(O)(O)(N(C<sub>2</sub>H<sub>5</sub>)<sub>2</sub>)]<sup>−</sup> anion and one H<sub>2</sub>O molecule which are involving in hydrogen bonding interaction forming linear arrangement along to the *a* axis. In this aggregation, both oxygen atom of P(O)(O) group acts as double-hydrogen bond acceptor; so that the O2 atom is cooperating in the O...(H—N)(H—O) grouping (where the N—H unit is related to the anion). The O3 atom is formed an O...(H—N)(H—N) grouping (the N—H units are related to two neighboring cations). Moreover, the oxygen atoms of S(O)(O) group cooperates in the O4...H—N<sub>cation</sub> and O1...H—O hydrogen bonds. Computational studies using the NBO method showed a positive character for H atom and a negative character for N and O atoms. The N atom in S(O)<sub>2</sub>NHP(O) moiety has large negative charge caused by the  $\pi$  electrons of P=O and S=O with a resonance property. The nature of hydrogen bond formation was confirmed by the AIM method through the Laplacian ( $\nabla^2$ ) and electron density ( $\rho$ ) analysis. Computed values of  $\rho$  at the B3LYP/6-311++G(d,p) level of the theory are 0.088 and 0.027 for the bond critical points of O3...H—N<sub>cation</sub> and O1...H—O hydrogen bonds, respectively. Accordingly, greater strength for the hydrogen bond of O3...H—N<sub>cation</sub> is achieved.

**References:**

- [1] S. Ibrahim, M. N. Tahir, N. Iqbal, D. Shahwar, M. A. Raza, *Acta. Cryst.* E67 (2011) o298.
- [2] M. Pourayoubi, S. Sadeghi Seragi, G. Bruno, H. Amiri Rudbari, *Acta. Cryst.* E67 (2011) o1285.
- [3] M. Pourayoubi, H. Fadaei, A. Tarahhomi, M. Parvez, *Acta. Cryst.* E67 (2011) o2795.