An Examination of All the Inter-ion Interactions in $(CH_3)_2N(H)CH_2CH_2N(H)(CH_3)_2$ $(SCN)_2$

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N,N,N'N'-tetramethylethylenediammonium $(CH_3)_2N(H)CH_2CH_2N(H)(CH_3)_2]^+$ forms a di-thiocyanate hydrogen bonded salt in space group P-1 with Z = 1. X-ray data were collected on a Saturn 70 with Mo-K_α radiation to $2\theta(max) = 105^o$. The multipole refinement was performed via XD [1] and all the topological interactions were then investigated. Of the 8 unique C-H hydrogen atoms, all but one forms significant interactions to the thiocyanate anion. These interactions constitute 4 (C-H…S), 2(C-H…C), 2(C-H…π(C≡N)), and 2(C-H…N) with two bifurcated C-H interactions. All 10 interactions satisfy all the eight of Koch & Popelier's criteria [2] for a weak interaction, though one interaction of a bifurcated pair is only marginally satisfactory. The N-H…N classical hydrogen bond is found to have weakened in the crystal when compared with the theoretically calculated values for an isolated ion pair.

[1] Koritsanszky T. S., Howard S., Macchi P., Gatti, C., Farrugia L. J., Mallinson P. R., Volkov A., Su Z., Richter T., Hansen N. K., *XD (version 4.10, July): A computer program package for multipole refinement and analysis of electron densities from diffraction data,* 2003. [2] a) Koch U., Popelier P. L. A., *J. Phys. Chem.* 1995, **99**, 9747; b) Popelier P., *Atoms in Molecules*, Prentice Hall, UK, 2000, 151.

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