BOOK OF ABSTRACTS

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The NH···O Interaction of Coordinated Ammonia and Ethylenediamine

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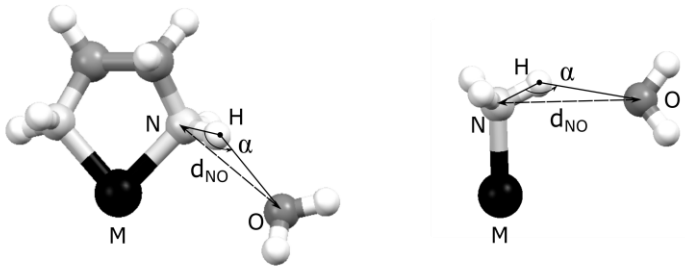
The Cambridge Structural Database (CSD) search was used to find contacts of coordinated ammonia and coordinated ethylenediamine with water molecule.[1,2] The criteria for contacts were the d_{HO} distance less than 4.0 Å and the angle α (N-H···O) larger than 110°. The results from CSD search have shown that the peak of d_{HO} distance for coordinated ammonia is in the 2.0 Å to 2.2 Å range, while the most abundant d_{HO} distance for ethylenediamine is shorter, lying within the 1.8 Å to 2.0 Å range. The distribution of α angle for coordinated ammonia is without clear preference while for ethylenediamine tendency for more linear angle is pronounced. The interaction energy of free ammonia and of free ethylenediamine with water molecule are the same, -2.3 kcal/mol. The interaction energies for coordinated ammonia and coordinated ethylenediamine are significantly stronger. The interaction energies for singly and doubly charged ammonia complexes are -5.0 kcal/mol and -10.7 kcal/mol, respectively. The interaction energies for neutral, singly and doubly charged ethylenediamine are -6.7 kcal/mol, -11.8 kcal/mol and -19.9 kcal/mol, respectively. The interaction for ethylenediamine is stronger than for ammonia molecule due to somewhat stronger electrostatic interactions.



(a) (b)

Figure 1. The geometrical parameters used for search and analysis of CSD data were d_{NO} distance and α angle for hydrogen bond between ethylenediamine complex and water (a), and ammonia complex and water (b).

References

[1] Živković, Jelena M.; Veljković, Dušan Ž.; Zarić Snežana D., *Cryst. Growth Des.*, **2022**, *22*, 148.
[2] Živković, Jelena M.; Milovanović, Milan R.; Zarić Snežana D., *Cryst. Growth Des.*, **2022**, *22*, 5198.

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