The van der Waals - London Discussions

University of Strasbourg October 26-27th 2023

General Information and Abstracts

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Group picture of a meeting on Magnetism showing **Fritz London** and his fellows all standing on the steps of the **Aula of the University of Strasbourg**. ©AIP Emilio Segrè Visual Archives.

«Conference on Magnetism in Strasbourg, 21 May 1939.

Appearing in the photo: Hitkel, Mlle Hildebrand, Mme Forrer, Ristorcelli, Persoz, Maxim, Spilmann, Guillaud, Trombe, Schultz, Establier, Forrer, Mott, Fallot, Preisach, Simon, Hilpert, Forestier, Melle Theron, Hocart, Malleman, Manebach, Lapp, Mlle Amiot, Gerlach, Von Handel, London, Becker, Ollivier, Suksmith, Bates, Opechowski, Mme Lapp, Aime Cotton, Mlle Serres, Krishnan, P. Weiss, Barrett, Cabrera, Bauer, Abraham, Bizetti. »

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We finally thank all the participants and the speakers for taking part to this inaugural meeting, which opens the way to future editions.

Dr Jean-Pierre Djukic, chairman

Dr Yann Cornaton, secretary

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Poster Abstract

Antiparallel Noncovalent Interactions

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In spite of being quite different substances, benzene and water can form similar noncovalent interactions. Analysis of the data in the crystal structures in the Cambridge Structural Database (CSD) revealed similarities in benzene/benzene and water/water interactions, since both benzene/benzene and water/water can form antiparallel interactions.

The quantum chemical calculations of potential surface of water/water interactions showed that the minimum is hydrogen bond. Analysis of the data in the crystal structures in the Cambridge Structural Database (CSD) revealed antiparallel water/water interactions, in addition to classical hydrogen bonds (1). The geometries of all water/water contacts in the CSD were analyzed and for all contacts interaction energies were calculated at accurate CCSD(T)/CBS level. The results showed that the most frequent water/water contacts are hydrogen bonds; hydrogen bonds are 70% of all attractive water/water interactions. In addition, water/water contacts with antiparallel interactions are 20% of all attractive water/water contacts. In these contacts O-H bonds of water molecules are in antiparallel orientation (Figure).

The quantum chemical calculations of potential surface of benzene/benzene interactions showed two minima stacking (parallel displaced) geometry and T-shaped geometry. Analysis of all benzene/benzene contacts in the crystal structures in the CSD revealed the most frequent benzene/benzene geometries (2). Majority of the benzene/benzene interactions in the CSD are stacking interactions with large horizontal displacements, and not geometries that are minima on benzene/benzene potential surface. In benzene/benzene interactions at large horizontal displacements two C-H bonds are in the antiparallel orientation (Figure).

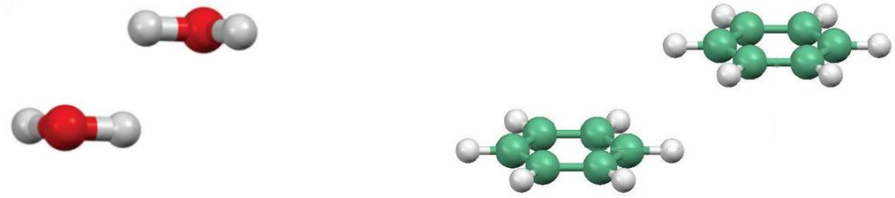

Figure. W**ater–water antiparallel O-H interaction and benzene/benzene antiparallel C-H interaction**

In these O-H and C-H antiparallel interactions two dipoles are in antiparallel orientation enabling close contact of positive and negative regions of the dipoles. Symmetry Adapted Perturbation Theory (SAPT) analysis showed that electrostatic is the largest attractive force in the antiparallel interactions. Antiparallel interactions are also possible between O-H and C-H bonds; in the crystal structures from the CSD these interactions are observed as one of the types of water benzene interactions (3).

References:

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