M13.0F Strong Closed Shell Interactions in Crystals

Chair: A.Vegas
Co-Chair: P. Pyykko

Attendance: 31

The 13OF microsymposium, dedicated to Strong Closed-Shell Interactions, was celebrated with a significant attendance of delegates. It was chaired by Dr. Angel Vegas, being the co-chairman Prof. P. Pyykkö. The act started with a litle delay, as the photographer (Dr. Bill Duax) ran out of film and went outside to get some more. In spite of being celebrated the last day, a total of 70 scientists followed with great interest the sessions. Well known scientists of both theory and experimental crystallography and crystal chemistry were among the attendants. The discussions after each conference were vibrant.

Lyudmila G. Kuz'mina (Russian Academy of Sciences, Moscow) opened the microsymposium with a review of her long experience in the synthesis of Au(I) compounds. The tendency of the Au atoms to form clusters (d^{10}-d^{10} interactions) was shown and interesting reactions were shown, in which the "strength" of these "weak" interactions was made evident.

Nino Runeberg (University of Helsinki, Finland) analyzed the contributions to the interaction energy between closed-shell centers, particularly d^{10} metal centers. He concluded that the aurophilic interaction is mainly a consequence of the dynamic electron correlation contribution strengthened by relativistic effects.

Vladimir G. Tsirelson (Mendeleev University, Moscow, Russia), and Victor Luaña (University of Oviedo, Spain) adopted a fully different perspective by discussing on chemical bonding, instead of binding, using the concepts of the Atoms in Molecules (AIM) theory. They showed both experimental and calculated electron density maps of rare gases and of fully ionic compounds where closed-shell bonding occurs. They showed the apearance of anion-anion and cation-cation bonding features.

Angel Vegas, from the CSIC (Research Council) in Madrid (Spain), presented a comparison between the cation arrays of ionic solids and the structure of the corresponding metals. In an over-whelming number of ionic compounds, cations reproduce, both topology and distances, of the parent metal structure. This empirical evidence is still waiting for an explanation.

We have been able to obtain an empirical trend of many atoms: their capacity to form aggregates and in spite of being charged with charges of the same sign. However, we have not yet a satisfactory explanation for the formation of these anion-anion and cation-cation bonds.