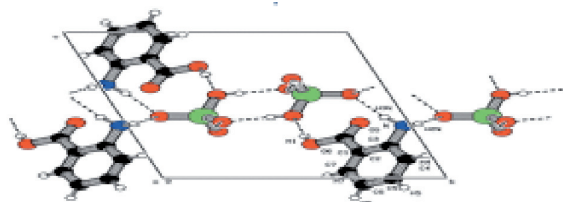


electrical, magnetic and optical properties and the hydrogen bonding richness of these structures. This kind of hydrogen bonding appears in the active sites of several biological systems and is observed in similar previously studied hybrid compounds [1, 2, 3].

The combination of the matrix cation and the anion mineral anions allowed us to obtain original structures (hybrid compounds) [4, 5]. Presenting strong hydrogen bond, average and low. Several crystals were already isolated in this system. This study consists in studying the influences of hydrogen bond in the geometry of the crystal structures.

Our current domain of research involve the study of the hydrogen connections in a series of hybrids compound, to do it; we are going to use the potentialities which offer the ADF software (Amsterdam Density Functional) to study this type chap of compounds, under solid.



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Keywords: X-ray of diffraction, hybrid compounds, hydrogen bond.

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A charge density investigation into an Rh...C-C sigma interaction

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Developing an understanding of structure and bonding in transition metal complexes containing metal centres coordinated to saturated bonds (e.g. C-H, H-H, C-C) is of significant interest due to their potential catalysis applications. We have been investigating transition metal catalysed approaches for C-C bond activation: this process is both thermodynamically and kinetically unfavourable due to the strength of the C-C bond. One approach to overcome this is to use strained systems such as cyclopropanes, for which the reduction in strain is thought to provide the driving force to break the C-C bond [1]. The intermediates in this process are believed to involve M...C-C sigma interactions.

Experimental insight into the electron distribution within a system can be obtained through accurate, high resolution, charge density investigations [2]. The nature of the bonding and interactions can then be studied using powerful tools such as Bader's quantum theory of atoms in molecules (AIM) which classifies interactions on the basis of the topological properties of the electron density and its Laplacian at bond critical points (bcp) [3]. A large number of organic species have been successfully studied in this manner however the analysis of the

topological properties around heavy atoms is more challenging with bcp's often appearing in regions of charge depletion or missing where chemical intuition would expect them to be present.

We have previously reported experimental charge density studies for Rh(C₇H₈)(PR₃)Cl (R = PPh₃, P^tBu₃ and PCy₃) [4] these have served as precursors for our current study into [Rh(Binor-S)(PCy₃)]([HCB₁₁Me₁₁]) which contains a Rh...C-C sigma interaction. Particular attention will be paid to the nature of the interactions around the rhodium metal centre.

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Charge density measurements of the anomeric effect in disaccharides

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The anomeric effect was first identified as the preference for pyranose rings to adopt the more hindered axial α -anomeric conformation in solution over the less hindered equatorial β -anomeric conformation. It is now recognized as a specific example of a 'generalized anomeric effect' in which systems with a R-Y-C-X linkage, where Y is an element with lone pairs and X is an electronegative element, show a preference for a *gauche* rather than a *trans* conformation. Several electronic models for the origin of the anomeric effect have been proposed, and it continues to be a topic of experimental and theoretical study and debate. In disaccharides, an additional complication exists because, in addition to the normal anomeric effect, the oxygen of the glycosidic linkage can give rise to an exo-anomeric effect which, depending on the torsion angles, may act with or against the normal effect.

Recently, an accurate experimental and theoretical determination of the charge density distribution of sucrose has been reported¹, and we have conducted similar charge density measurements of α,α -trehalose² and methyl- β -cellobioside. In addition to the determining the deformation density, the charge distribution has been analyzed using the *Atoms in Molecules*³ formalism. These studies allow the predictions of various electronic models for the anomeric effect to be compared with the actual charge density distribution.

The α -pyranose ring of sucrose shows variations in the total electron density at the bond critical points as well as variations in the bond lengths which are consistent with a model for the anomeric effect which involves a $n \rightarrow \sigma^*$ overlap between a lone pair orbital on the Y atom with the σ^* antibonding orbital of the C-X bond. In trehalose, the exo-anomeric effect is in competition with normal anomeric effect, resulting in less variation in the density at the bond critical points.

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Keywords: charge_density, anomeric_effect, topology