Interactions and Reactivity in Crystalline Intermediates of Mechanochemical Cyclorhodation Reactions

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Supplementary information

Contents

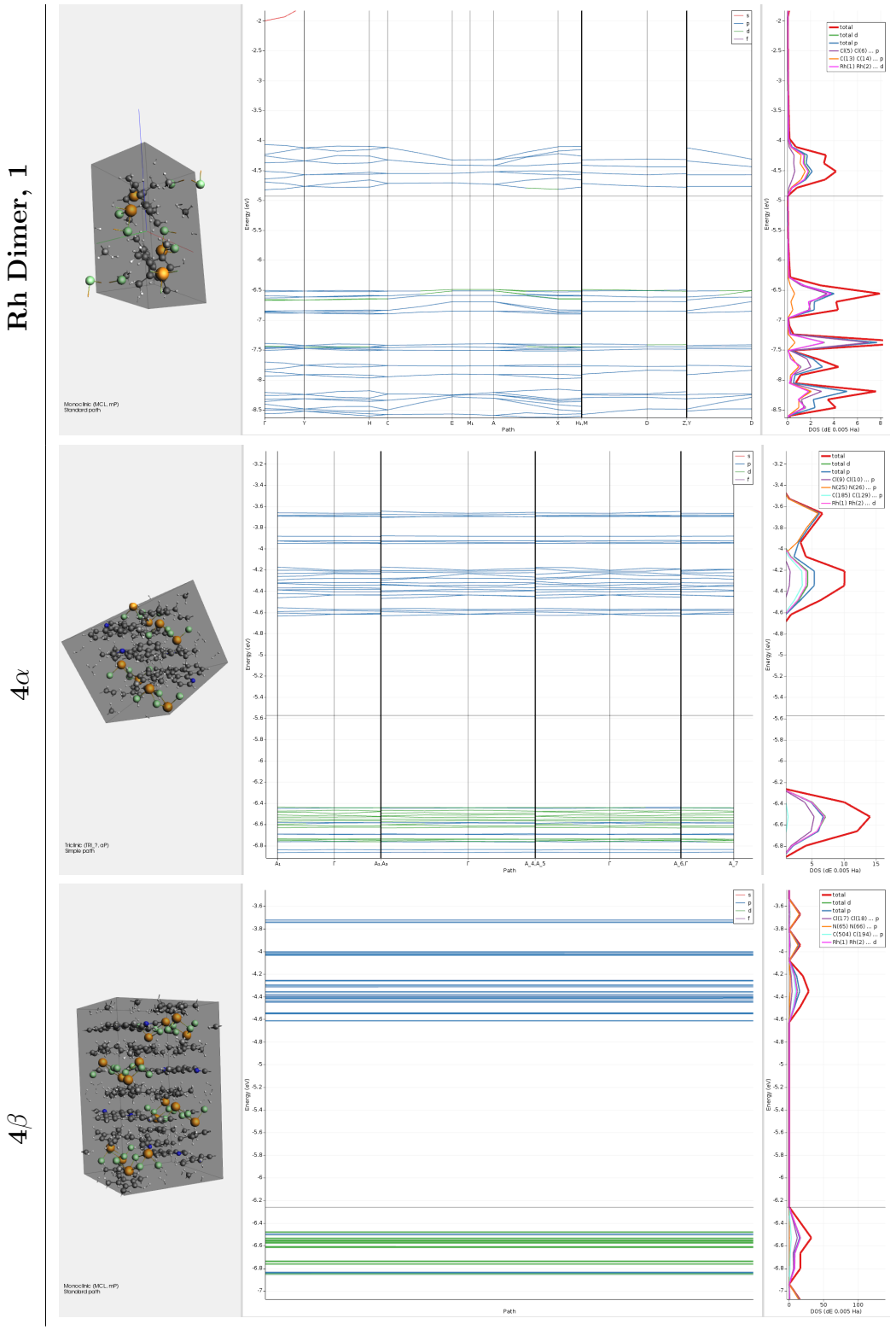

Figure S1: Band structure and Density of states (DOS) of the rhodium dimer, **1** (top), **4**α (middle) and **4**β (bottom) with their corresponding dominant character. The Fermi level is plotted as a horizontal gray line in all the cases. All calculations using the AMS–BAND program[1]

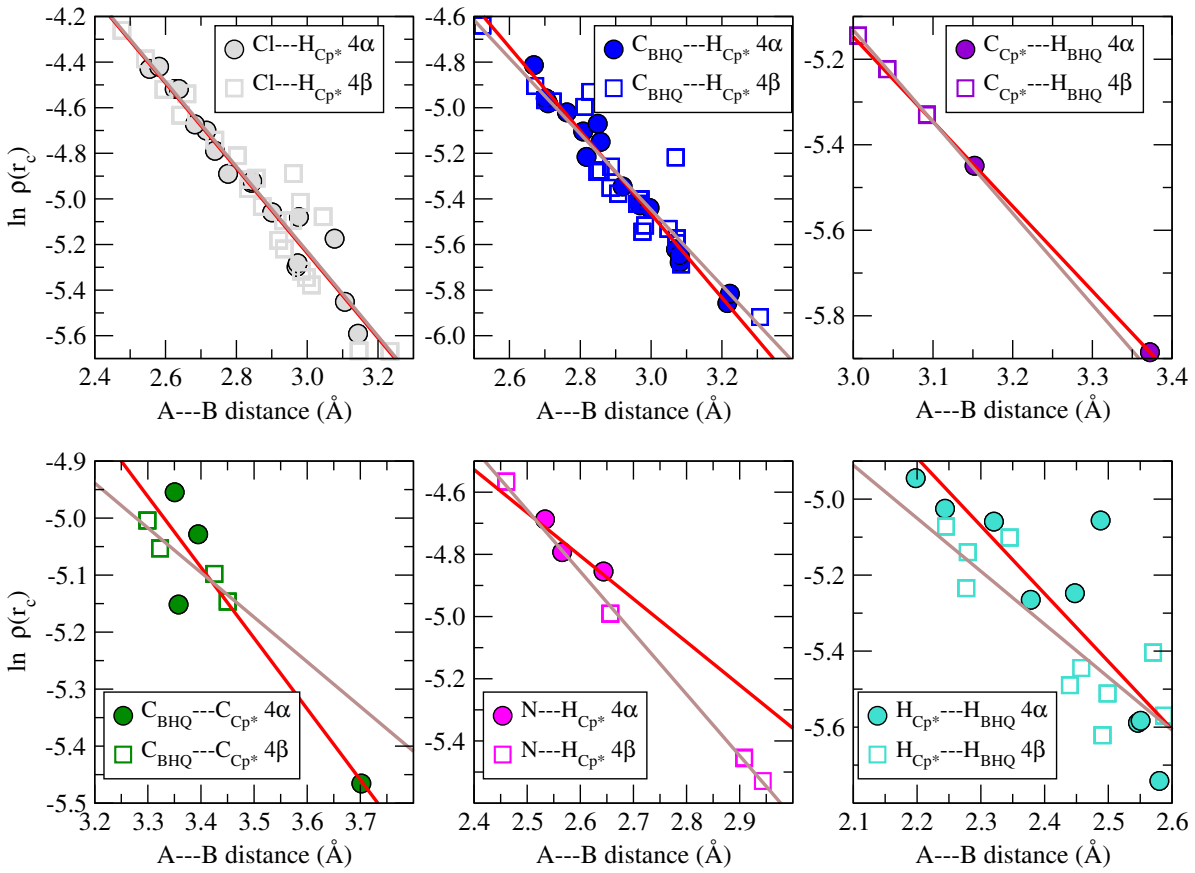

Figure S2: Logarithmic relationships for $[\mathbf{r}, \rho(\mathbf{r_c})]$, $\mathbf{r}$ being the length of the contacts in the subsets of the Cl$\cdots$H, C$\cdots$H, C$\cdots$C, N$\cdots$H and H$\cdots$H interactions found with the topological QTAIM analysis (see Table 4 in the main text). Linear regression for **4**α in red, for **4**β in brown.

References

[1] P. Philipsen, G. te Velde, E. Baerends, J. Berger, P. de Boeij, M. Franchini, J. Groeneveld, E. Kadantsev, R. Klooster, F. Kootstra, M. Pols, P. Romaniello, M. Raupach, D. Skachkov, J. Snijders, C. Verzijl, J. Celis Gil, J. M. Thijssen, G. Wiesenekker, C. A. Peeples, G. Schreckenbach, and T. Ziegler, "Band *(version 2022.102)*, software for chemistry & materials, scm," 2022. Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands.