approximant [4] and the Hume-Rothery mechanism for the formation of the quasicrystal [5]. For Al-Co-Ni, Ni and Co are located in the most inner and second inner parts, respectively, of the columnar model cluster, indicating the tendency of the close distribution of Ni atoms and the separated distribution of Co atoms. This is consistent with a recent study on the formation of the quasiperiodic Al-Co-Ni surfaces by the scanning tunneling microscopy [6]. The chemical bond and formation of the quasicrystals has been discussed in terms of local clusters around the transition metals.

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Keywords: decagonal quasicrystals, *ab-initio* cluster calculation, transition-metal clusters

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Ni(II) thiosemicarbazone complexes : Structural and theoretical investigation

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MM: Molecular Modelling DFT: Density Functional Theory Heterocyclic thiosemicarbazone and their metal complexes are among the most widely studied compounds for their potential antitumoral, antibacterial and antifungal activities (1). Some of these activities are closely related to the stability of molecular geometry (2) and especially when these activities are enhanced by the presence of some metallic ions (3). Therefore we were interested in single X-ray Crystallographic studies of some Ni(II) thiosemicarbazone complexes. These studies were supplemented by theoretical calculations (MM and DFT) in order to investigate more about the transmission of electronic effects between the redox unit and a metal center.

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Keywords: complexes, single-X ray diffraction, DFT

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Prediction and experimental determination of the crystal structure of $SiBr_4$

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The crystal structure of $SiBr_4$ is unknown hitherto, although the structures of all other EX_4 compounds (with E = C, Si, Ge, Sn, Pb and X = F, Cl, Br, I) are published. Possible crystal structures of $SiBr_4$ were predicted with force-field methods using the program CRYSCA[1]. Low-energy structures were post-optimised using the program package Cerius[2]. All calculations were performed with a Dreiding/X6 [2] force-field which was modified for Si-Br bond lengths. Calculations were performed in those space groups statistically most frequent for molecular compounds and for EX_4 compounds resp. $P1$ (Z = 1), $P\bar{1}$ (Z = 2), $P2_1$ (Z = 2), Cc (Z = 4), $P2_1/c$ (Z = 4), $P2_12_12_1$ (Z = 4), $Pna2_1$ (Z = 4), $Pca2_1$ (Z = 4) and $Pbca$ (Z = 8). In many cases higher symmetries (supergroups) were reached during the optimisation. Several possible polymorphs were found within an energy range of 5 kJ/mol above the global minimum. X-ray powder diagrams of $SiBr_4$ revealed the existence of two polymorphs; their structures were determined from X-ray powder data: the cubic high temperature phase crystallises in $Pa\bar{3}$ (Z = 8), the low temperature phase in $P2_1/c$ (Z = 4). Both phases had been predicted in the calculations.

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Keywords: lattice energy calculations, crystal structure prediction, crystal structure solution

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Computation of diffuse magnetic neutron diffraction single crystal patterns

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Magnetic diffuse scattering is observed in the paramagnetic state or in frustrated magnetic systems where long-range order is impeded by geometric constraints. This diffuse scattering can easily be probed using neutron diffraction and single crystal diffraction in particular allows to obtain very detailed maps in reciprocal space. The amount of information available from reciprocal space surveys of magnetic diffuse scattering can potentially give detailed insight into the interaction between the magnetic ions. Yet, very few such studies have been carried out likely due to the lack of software tools, methodology or computational resources. Here, we present Monte-Carlo simulations on model systems supported by experimental data. This allows phase diagrams to be explored and the effect of varying exchange constants to be simulated and compared to the data. Due to the finite size of the model crystal obtained, direct Fourier summation leads to noisy reciprocal space reconstructions. We have therefore extended the method of averaging over Fourier transforms of many small parts of the model crystal ('lots') to include magnetic diffuse scattering leading to high quality, smooth simulated patterns [1].

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