at 293 K. The asymmetric unit contains two unique iron sites (Fe and Fe'); each is located at the crystallographic inversion centers. The main difference in these two molecules is the planarity of the abpt ligand; the dihedral angle between the triazole ring and the uncoordinated pyridine ring is 6.2 and 20.1° for Fe and Fe' complex respectively. The result of temperature-dependent FTIR spectra indicates that Fe undergoes a gradual spin crossover transition in the temperature range of 200 ~ 100 K (T_c = 145 K), while the Fe' remains at high spin state in the temperature range studied. This shows a definite correlation between the spin crossover character and the planarity of the ligand in this complex; this applies to the known crystal structures of polymorph A[1] and B[2]. The closer to the planar of the ligand abpt is, the easier a spin crossover complex will be. The single crystal diffraction data at 90 K were also studied. Comparing to the structure at 293 K, the $Fe\text{-}N_{avg}$ distances change from 2.155(3) to 1.976(3) Å at site Fe and 2.163(2) to 2.181(2) Å at site Fe', it is consistent with the FTIR measurement. Below 50 K, the Fe site can be excited from low spin to high spin state using a green light laser (532 nm), the light induce exited spin state strapping (LIESST) process was monitored by the CN stretching frequency in the range of 1900-2200 cm^{-1}.

[1] Moliner N., Muñoz M. C., Létard S., Létard J., Solans X., Burriel R., Castro M., Kahn O., Real J. A., *Inorganica Chimica Acta*, 1999, **291**, 278-288.
[2] Gaspar A. B., Munoz M. C., Moliner N., Ksenofontov V., Levchenko G., Gütlich P., Real J. A., *Monatshefte Fur Chemie*, 2003, **134**, 285-294.

Keywords: spin crossover, LIESST, FTIR

P.11.16.12
Acta Cryst. (2005). A**61**, C407

The Crystal Structures of the Iron Carbides

Esna du Plessis[a], Gert Kruger[a], Johan de Villiers[b], [a]*Department of Chemistry, University of Johannesburg, Johannesburg, South Africa.* [b]*University of Pretoria, Pretoria, South Africa.* E-mail: gjk@rau.ac.za

Various low temperature iron carbides are formed in the reactor during the Sasol Synthol process to produce hydrocarbons. The small particle sizes of the iron carbides prevented complete structure determination in the past. Modern equipment is available to study the crystal structures of the iron carbides. The improved crystal structures can then be used to characterize the commercial catalyst samples.

Hägg carbide ($\chi\text{-}Fe_5C_2$) and pseudo hexagonal ($\varepsilon'\text{-}Fe_{2.2}C$) iron carbide samples have been prepared from spray-dried hematite. The preparations were done in an Anton Paar reaction chamber mounted on an X'Pert Pro diffractometer.

The samples were characterized using SEM, powder X-ray diffraction and room temperature Mössbauer spectroscopy. Structure determination with powder diffraction (SDPD) was used to determine the structures of the iron carbides. Rietveld refinements with X'Pert Plus and GSAS software were done on the powder X-ray diffractograms.

Keywords: iron carbide, powder diffraction, SDPD

P.11.16.13
Acta Cryst. (2005). A**61**, C407

Classification of White Marble Varieties by Monocrystal X-ray Diffraction

Sonia Mañas-Carpio[a], Manuel Serrano-Ruiz[b], Antonio Romerosa[c], Lourdes Sánchez[b], Valentín Tijeras[b], [a]*Servicio de difracción de rayos X, Servicios Técnicos U. de Almería.* [b]*Centro Tecnológico Andaluz de la Piedra (CTAP), Macael-Almería.* [c]*Área de Química Inorgánica, Universidad de Almería.* E-mail: smcarpio@ual.es

A classification of white marble which was not influenced by human evaluation is of paramount importance for the Spanish marble industry and in particular for the industry of the Spanish area of Macael (Almeria). The Macael-marble is characterized by a nice white color linked to interesting mechanical properties for building that have provided to this class of marble to be a very appreciate material used for centuries in a large variety of Spanish and American palaces for example the Alhambra of Granada. Instead of the economical and cultural importance of this material, no instrumental procedures were developed to differentiate and classify the Macael-marbles from others white marbles characterized by less convenient building properties. As a result of the research collaboration between the "University of Almeria-Servicio de rayos X" and the "Centro Tecnológico Andaluz de la Piedra" (CTAP) a new procedure for marble analysis has been obtained. The method basically consists in determining the cell dimensions of the marbles by monocrystal X-ray diffraction. The analysis and comparison of evaluated marble cell parameters leaded to a reproducible procedure which provides an easy, fast and economical method to a selective identification and classification of the Macael-marbles and of the white marbles in general.

Keywords: white marble, monocrystal X-ray diffraction, marble classification

P11