04.2-01 INFLUENCE OF CRYSTALLOGRAPHIC TRANS-FORMATIONS ON THE CHEMICAL REACTIVITY OF IRON OXIDES DURING GASEOUS REDUCTION. By J. <u>Heizmann</u>, P. Becker, J. Bessières et A. Bessières, Laboratoire de Métallurgie Structurale, Université de Metz, 57045 Metz Cedex, France.

The reaction diagram for the reduction of iron oxide shows that there are several possible ways of obtaining iron. These are: either a chain of single reactions

$$\operatorname{Fe}_2^{0_3} \xrightarrow{1} \operatorname{Fe}_3^{0_4} \xrightarrow{2} \operatorname{Fe}_{1-x^0} \xrightarrow{3} \operatorname{Fe}_{1-x^0}$$

or a combination of single and double reactions

$$Fe_2O_3 \xrightarrow{1} Fe_3O_4 \xrightarrow{2} Fe$$
; $Fe_2O_3 \xrightarrow{1} Fe_{1-x}O \xrightarrow{2} Fe$
or a triple reaction $Fe_2O_3 \xrightarrow{1} Fe$

The structure relationships between the different oxides are studied by $X - \tau ay$ texture goniometry and the reduction kinetics are deduced from thermogravimetric analysis.

The authors determine the structure relationships between each pair of oxides within a single reduction and the kinetics of each single reaction. They show that the latter depends on the distribution of the orientations around the ideal orientations defined by the structure relationships. The authors show that the structure relationships which were found for single reduction are preserved when the reduction is progressing within a double or a triple reaction. In these cases the chemical kinetics of the second or third reaction which are progressing within the overall reaction depends strongly on the degradation of the crystal structures.

04.2-02 TRANSFORMATIONS AFFECTING MgC12.6H20 ON MgO SUBSTRATES. <u>Pronob Bardhan</u>, Corning Glass Works, Sullivan Park, DV-19, Corning, New York, 14831.

Magnesium oxychloride cements are well known for their acoustic and elastic properties. However, they are not durable. While works by Walter-Levy (Acta Cryst. (1953) 6, 40), Cole (Aust. J. Chem. (1955) 8, 215, 234) and Sorrell and Armstrong (J. Am. Cer. Soc., (1976), 59, 51) have helped identify the structure and temperature range of stability of some of the phases, little is known of the morphological aspects of the transformation. The latter is reported in this paper.

A saturated solution of MgCl₂.6 H₂O was allowed to react with a polycrystalline MgO substrate in the presence of water. The sequence of hydration products suggests the formation of an initial layer of Mg(OH)₂ at the solution/ crystal interface. The subsequent reaction products, lying in layers, are readily explained as a slice through the MgO-MgCl₂-H₂O phase diagram. Some useful and practical consequences of the resulting composite formation will be discussed. 04.2-03 INTERMEDIATES IN THE SYNTHESIS OF BIOLOGICAL-LY ACTIVE TERPENOIDS. CRYSTAL STRUCTURE OF DIELS-ALDER ADDUCTS OF o- AND p-BENZOQUINONES. By <u>A. Mugnoli</u>, Istituto di Chimica Fisica, Università di Genova, Italy, and A. Moretto, F. Orsini and F. Pelizzoni, Centro C.N.R. and Istituto di Chimica Organica, Università di Milano, Italy.

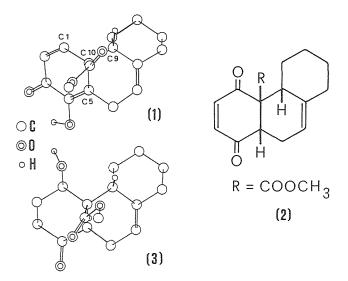
Although 9,10-syn pimarane diterpenoids are rather uncommon in nature, several related compounds have been recently isolated, and for some of them a specific biological activity has been reported (P. On'okoko and M.Vanhaelen, Phytochemistry (1980) 19,303 and references quoted therein; N.F. Roque, G.B. Zoghbi and H.E. Gottlieb, Phytochemistry, in the press). Compounds (1) and (2), which 'appear as useful intermediates in a simple, convergent synthesis of such diterpenoids, have been obtained via Diels-Alder reaction of vinylcyclohexene with o- and pcarbomethoxy benzoquinone. The correct regio- and stereoselectivity (endo) of the reaction have been established by X-ray analysis of compounds (1) and (3), a highly crystalline derivative of (2). To our knowledge, (1) is the first normal Diels-Alder adduct obtained from an o-benzoquinone.

Compound (1), $C_{16}H_{18}O_4$, mp 122-124°C, crystallizes in

space group C2/c with a = 14.284, b = 8.624, c = 22.639Å,

$$\beta = 93.07^{\circ}$$
, $Z = 8$. Compound (3), $C_{16}H_{22}O_4$, mp 155°C,
crystallizes in space group P2₁/n with a = 9.021, b =

20.909, c = 7.544 Å, β = 93.15°, Z = 4. Intensities were collected by four-circle diffractometry using MoKK radiation. Both structures were solved by direct methods (G.M. Sheldrick, SHELX 76, University of Cambridge, 1976) and refined by full-matrix least-squares calculations. The current value of the R index for both compounds is 0.06 over about 1400 and 1500 observed reflections, respectively. The refinement is in progress. The orientation of the carbomethoxy group in (1) and in (3) is quite different and can be referred back to the different hydrogen bonding pattern in the two crystals.



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