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Selectivity of Butanol Isomers by Enclathration.

Hong Su[a], Peter W. Linder[a], Luigi R. Nassimbeni[a]. [a]Department of Chemistry, University of Cape Town, Private Bag, Rondebosch 7701, South Africa. E-mail: hong.su@uct.ac.za

Quantifying the process of molecular recognition in solid state inclusion chemistry is a difficult task. We employed the idea of the selectivity coefficient, first termed by Ward[1], which defines the selectivity coefficient of a given host for two guests A and B as

$$K_{A:B} = \left(K_{B:A}\right)^{-1} = Z_A/Z_B * X_B/X_A$$

where X_A, X_B are the mole fractions in the liquid mixture and Z_A, Z_B are the mole fractions of the guests in the crystal grown from the liquid mixture. The selectivities, determined by competition experiments as previously described[2,3], may yield a quantitative measure of the relative affinity of the host for a particular guest from a mixture of guests. Selectivity experiments have since been performed on a number of host-guest systems[4,5]. We now present the results of the selectivity of butanol isomers by the host 1,1-bis(4-hydroxyphenyl)cyclohexane. The host forms inclusion compounds with 1-butanol, 2-butanol and iso-butanol which all have host:guest stoichiometries of 1:1 and similar packings. The structures are stabilised by host···host and host···guest hydrogen bonds. Competition experiments show preferred selectivity in the sequence 2-butanol > iso-butanol > 1-butanol. This correlates with thermal stabilities measured by DSC but not with the calculated lattice energies.

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About Crystal Structure of Mountainite.

R.G. Askerov[a], M.I. Chiragov[a], K.G. Ragimov[a], A.F.Shirinova[a]. [a]Department of Geology. Baku State University. Baku,Azerbaijan. E-mail: mchiragov@yandex.ru

Alkali calcium silicates - rhodezite and mountainite for the first time are established in Kimberley Southern Africa and described in works. In literature parameters of elementary cells, results chemical, electromicroscopic, radiographic and thermal analyses are resulted. The method of comparative crystallchemistry [1], using similarity of parameters of an elementary cell of minerals of family of rhodezite-macdonaldite simulates structure of mountainite. It is visible, that parameters *a* and *b* of rhodezite, delhayelite and hidrodelhayelite almost identical, and the parameter *c* of the specified minerals (in monteragianite *b*) is approximately equal ~ 23.9Å. Parameters of a cell *a* and *b* macdonaldite are the double parameters of the previous minerals and parameters $b_{mout}=b_{macd}=2b$ (rhodezite, delhayelite, hidrodelhayelite) = 13.10Å. Comparison of parameters mountainite and macdonaldite, it is possible to establish, that $a_{mount} \approx a_{macd} \cdot sin$ β = 13.6Å. Experimentally established parameter mountainite a_{mount}=13.51Å. The interrelation between *c* and β parameters of mountainite with parameters *a* and *c* of macdonaldite is traced. Having allocated parameter C_{mount} of mountainite along a diagonal formed $1/4$ $1/4$ a_{macd} and $1/2c_{macd}$ we shall receive parameter C_{mount} of mountainite, equal 12.25Å, thus the corner β between $1/2c_{macd}$ and c_{mount} will be 17 ° or, accordingly, 107°. If instead of $1/4a_{macd}$ to present $1/4a_{mounl}$ and value of a diagonal 12.25Å to increase till 13.51Å then the corner between parameters C_{macd} and c_{mount} will make 14°, i.e. β =104 °. The established law in cell parameters and feature of structural minals allow to assume, that structural elements of minerals of family rhodezite-macdonaldite are kept and in structure of mountainite. In family of rhodezite-macdonaldite a siliconoxygen radical - a tetrahedral double layer with composition $|Si_8O_{19}|$ or $|Si_{16}O_{38}|$. By results of chemical analyses it is established, that composition a siliconoxygen radical of mountainite $|Si_{16}O_{40}|$. The radical with such structure corresponds to a onestoreyed tetrahedral sheets which turns out decomposition Si-0 of a radical of rhodezite-macdonaldite type. In structure of mountainite atoms of calcium and sodium create octahedric walls. Continuous octahedric walls from both sides are connected with a tetrahedral layer composition $|Si_{16}O_{40}|$, which repeating in parameter c=13.5lÅ, formed structural types of mountainite. On crystallochemistry to reasons it is probable, that in untied with a octahedral layer free vertices of tetrahedrons settle down (OH) - groups. On the basis of the described structure of mountainite the crystallochemistry formula of a mineral can be presented in the following kind: $K_2Na_2Ca_2|Si_8O_{18}$ (OH)$_2$ |(OH)$_2$ ·3H$_2$0 (z=4).From predicted model of structure of mountainite coordinates of basic atoms and distances between them which are in limits are determined: Si - O(OH) = l.562 - 1.665Å; (Si - O, OH)$_{av}$ =1.608Å; Ca - O(OH) = 2.310 - 2.402Å; (Ca - O, OH)$_{av}$ = 2.352Å; Na - O(OH) = 2.261 - 2.40Å; (Na - O, OH)$_{av}$ = 2.342Å;K - O(OH) = 3.06 - 3.62Å; (K - O, OH, H$_2$0)$_{av}$ = 3.22Å. The specified interatoms distances will be coordinated to corresponding distances in known structures of alkaline calcium and rareearth silicates.

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