



0°0° 0°-30° 0°60° 30°30° 30°-30° 30°60° 60°60°

The coefficients of $V(\theta_1, \theta_2)$ have been obtained by solving the system of seven equations corresponding to the values of θ_1 and θ_2 for non-equivalent conformations. The energy values for these conformations have been obtained by the SCF INDO open shell calculations (JPople; J.Chem. Phys., 47 (1967) 2026). This method is analogous to the CNDO/2 (J. Pople, J.Chem.Phys., 44(1966)3289) and gives reasonable results in the case of rotation of groups involved in localized bonds (C.Sieiro, J.Mol.Struct. 24 (1975)345). Solving the Schrödinger equation with $V = V(\theta_1, \theta_2)$, we obtain the rotational levels and the corresponding population analysis.

0° 0°	-4.668
0° -30°	-4.294
0° 60°	-3.919
30° 30°	-4.099
30° -30°	-2.988
30° 60°	-2.302
60° 60°	0.000

The INDO results are shown in Table 1.

The free rotation can be explained by the population analysis and by the tunnel effect.

21.3-02 MÖSSBAUER AND ELECTRON DIFFRACTION STUDIES OF CATION DISTRIBUTION IN CELADONITE. By L.G. Dainyak, A.S. Bookin, V.A. Drits and S.I. Tsipursky, Geological Institute of the USSR Academy of Sciences, Moscow, USSR.

A study of a celadonite of composition $\{Ca_{0.10}K_{0.89}\}\{Si_{0.96}Al_{0.04}\}\{Al_{0.05}Fe_{0.95}Fe_{0.26}Mg_{0.73}\}O_{10}(OH)_2$ is reported. Its structure as derived from electron diffraction data is characterized by its strict dioctahedral nature with vacant positions in space group C2. Moreover, the preference of cations of a given valency to one of the *cis* positions is about 60%.

Interpretation of the Mössbauer spectrum of celadonite was made according to the procedure developed earlier (Bookin, Dainyak, Drits, Phys. Chem. Minerals (1978) 3, 58). The electric field gradients (EFG) were calculated for each possible configuration of the nearest cation surrounding Fe and taking into account the presence of non-equivalent *cis* position and the corresponding geometry of Fe^{3+} octahedra. The ratio between them was used for computer simulation of spectra, corresponding to different variants of cation distribution over octahedral sheets of celadonite. Comparison of the simulated and experimental spectra allowed us to select the most probable model of cation distribution which was used as a first approximation during computer fitting of experimental spectrum of celadonite. The final fitting process allowed us to conclude that the distribution of isomorphous cations over *cis* positions within each 2:1 layer in the structure has an almost ideal degree of order (~90%) when each R^{3+} cation is surrounded by the R^{2+} cation and vice versa. The disturbances in the ideal order result from the pairs of R^{3+} cations occupying adjacent *cis* octahedra along the *b* axis, Table 1.

Table 1.

Fe	Δ	δ^*	r	S%	S_A/S_B	S_B/S_F
1. Results of EFG calculation						
Fe^{3+}	A [#]	0.36	-	0.27		
	B	0.52	-	0.27	2.0	3.0
	F	0.17	-	0.27		
2. Results of fitting of spectra (T=77 K)						
Fe^{3+}	A	0.37	0.30	0.27	44.1	
	B	0.59	0.30	0.27	20.5	2.15
	F	0.18	0.30	0.27	6.8	
	X [†]	1.15	0.31	0.27	9.6	
Fe^{2+}	2.57	1.07	0.38	19.0	$\chi^2 = 1.11$	

* Isomer shift δ (mm/sec) is relative to α -Fe.

Symbols A, B and F correspond to configurations of ($3R^{2+}$), ($2R^{2+}1R^{3+}$) and ($3R^{3+}$).

† Corresponds to presence of Fe^{3+} octahedra with deficiency of hydroxyls.

Discrepancies between the electronographic and Mössbauer data are presumably related to the effect of averaging in the diffraction methods.