A Structural Investigation of a Vermiculite-Piperidine Complex*

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* This research was partially supported by Petroleum Research Fund 2413-C administered by the American Chemical Society.

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Abstract: A vermiculite-piperidine complex was investigated by a single crystal three dimensional X-ray diffraction procedure. The complex was prepared by ion exchange of a Na-vermiculite at pH 8. A total of 453 reflections was observed and used in the least squares refinement of the structure. The complex is monoclinic, *C*2/*m*, *a* = 5 · 346(2) Å, *b* = 9 · 256(3) Å, *c* = 17 · 57(1) Å, β = 96 · 29(9) ° . The final *R* value was 0 · 17 using anisotropic temperature factors for the silicate atoms and isotropic temperature factors for the carbon atoms. The occupancy factors of the *C* atoms were considered as variable parameters. The diffraction data were of poor quality because of stacking faults. The results show that the molecules are randomly distributed over the crystallographic sites in the interlayer space and the peaks appearing in the electron density maps can be interpreted as being due to 2 piperidine molecules and two H_2O molecules. The orientation of the organic molecules is ambiguous. The electron density peaks fit a model in which the molecules are vertical and their planes form a small dihedral angle, and also fit a model in which the plane of the molecules is parallel to (001). It is quite possible that both types of orientations are present.

Clays and Clay Minerals; February 1974 v. 22; no. 1; p. 91-95; DOI: 10.1346/CCMN.1974.0220113

Clay Minerals Society (www.clays.org)