VIBRATIONAL SPECTROSCOPY OF PARTIALLY BONDED COMPLEXES: A MATRIX ISOLATION INFRARED STUDY OF CH3CN - BF3

NATHAN P. WELLS AND JAMES A. PHILLIPS, *Department of Chemistry, University of Wisconsin-Eau Claire, 105 Garfield Avenue, Eau Claire, WI 54702-4004*.

The complex formed from acetonitrile and boron trifluoride has been called a "partially bonded molecule" since its B-N bond distance and N-B-F bond angle are intermediate between those characteristic of a weak, non-bonded interaction and a *bona fide* donor-acceptor bond.[a] Furthermore, complexes among this class have been shown to be quite sensitive to chemical medium, and in particular, undergo dramatic structural rearrangement upon crystallization, which includes a substantial contraction of the donor - acceptor bond. In fact, the C-N stretching frequency of $CH_3CN - BF_3$ was recently observed in solid argon[b] at a value very near that of the crystalline complex.[c] This seemed to indicate that the inert matrix environment caused a nearly full contraction of the B-N dative bond. We have undertaken a re-examination of the complex, with an eye toward vibrational modes involving motion of the BF_3 moiety, which should be rather sensitive to the effects of complexation. We have observed and identified several new absorption features in argon matrices seeded with 0.1 to 1.0 percent CH_3CN and BF_3 that we assign to the 1:1 complex. The basis for these assignments is: dependence on both component species, consistent relative intensities across a wide range of conditions, and isotope shifts consistent with recent calculations[d] on the gas-phase complex. Our observations of the BF_3 antisymmetric stretching mode (ν_{13}) indicate that, contrary to the previous study, matrix-isolated $CH_3CN - BF_3$ more closely resembles the gas-phase complex than the crystalline species. Recently obtained spectra of two additional isotopic forms of the complex provide further support for our assignments, and will also be discussed.

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[b] Beattie, I. R.; Jones, P. J. *Agnew. Chem. Int. Ed. Engl.* **1996**, *35*, 1527.
[c] Swanson, D. F.; Schriver, D. F. *Inorg. Chem.* **1970**, *9*, 1406.
[d] Cheong, B.; Cho, H. *J. Mol. Struct. (Theochem)* **2000**, *486*, 185.