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$(CH_3)_3N$-$CB_{10}H_{12}$ – A Commensurately Modulated Carbaborane Compound. Charles F. Campana, Bruker AXS Inc., 5465 East Cheryl Parkway, Madison, WI 53711, USA, Ludger Häming, Bruker AXS Gmbh, Oestliche Rheinbrueckenstr. 50, D-76187 Karlsruhe, Germany, John C. Huffman, Indiana Univ., Molecular Structure Center, Chemistry, A421, 800 E. Kirkwood Ave., Bloomington, IN 47405.

Previous attempts to determine the structure of $(CH_3)_3N$-$CB_{10}H_{12}$ with conventional point detector diffractometers indicated an apparent orthorhombic unit cell of approximate dimensions: a = 6.9212(6) Å, b = 10.4905(10) Å, c = 16.1290(16) Å volume = 1171.08(19) $Å^3$. This structure could not be successfully refined due to an ambiguous space group and severe disorder problems.

A later dataset collected on an early Siemens SMART system indicated a possible super-cell with dimensions of a = 48.4485(48) Å, b = 10.4905(10) Å, c = 16.1290(16) Å, volume = 8197.6(2) $Å^3$. However, careful exploration of reciprocal space with the RLATT program revealed that the original unit cell was correct with additional weak satellite reflections present at 3/7 and 4/7 intervals in the a* direction. The structure was refined in both the sub-cell and super-cell using SHELXTL.

We have recently recollected data using a Bruker Kappa APEX II system and used the APEX2 software to carry out integration and absorption correction calculations on the main reflections as well as the satellite reflections. The data were output in a format suitable for refinement with JANA2000. Results of the JANA2000 refinement will be presented.