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Non-traditional Bonding Interactions via Experimental Charge Density. Lee M. Daniels¹, T. Stanley Cameron², Joseph D. Ferrara¹, ¹Rigaku Americas Corp., 9009 New Trails Dr., The Woodlands, TX 77381 USA, ²Dept. of Chemistry, Dalhousie Univ., Halifax, Nova Scotia, Canada B3H 4J3.

Years ago, crystallography revolutionized a lot of thought about Important Science, and provided perhaps the most powerful tool for the study of chemical bonding. Precise positional information giving exact bond distances became routine; more recently advances in charge density studies have provided extensive views of bonding once available only in theory. Direct observation of covalent bonding is now possible, and extension of the analysis provides detailed information about *intermolecular* interactions. Using the criteria proposed by Koch and Popelier, a “bond path” can be constructed between any two atoms or groups in a structure, allowing one to distinguish “bonding” interactions from van der Waals contacts. In this work interactions such as H-H bonding, F-F bonding, I-S bonding, P-N ring bonding, etc. are considered.