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A Search for Isostructural "Bridge-Flipped" Isomers. W.H. Ojala, J.M. Spude, T.M. Arola, M.K. Kuspa, Y. Moua, H.M. Sexe, B.L. Sanders, N. Herrera, and J.M. Smieja, Dept. of Chemistry, Univ. of St. Thomas, St. Paul, MN 55105 USA; C.R. Ojala, Dept. of Chemistry, Normandale Community College, Bloomington, MN 55431 USA.

We designate as "bridge-flipped" isomers those pairs of molecules related by reversal of a bridge of atoms connecting two major parts of the individual molecules. This kind of isomerism is found among the benzylideneanilines (Ar-CH=N-Ar' vs. Ar-N=CH-Ar') and the phenylhydrazones (Ar-CH=N-NH-Ar' vs. Ar-NH-N=CH-Ar') (Ar = aryl). We are examining compounds of both types to identify isostructural pairs of bridge-flipped isomers for co-crystallization experiments. Published structures of isomeric pairs are numerous, but isostructural examples are rare. We describe here the influence of structural features that might encourage isostructuralism if they were to operate similarly on both isomers, including disorder, similarity in conformation (in particular, planarity) and similarity in such intermolecular influences on packing as hydrogen bonding and Lewis acid-base interactions. In practice we have found some of these to be occasionally structure-differentiating, and we have obtained isostructural pairs in their absence.

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