Crystallographic Analysis of Analogous Silicon- and Carbon-Containing Di(Cyanate Ester)s and Tri(Cyanate Ester)s

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Cyanate esters are versatile, thermosetting monomers that are commercially important due to their outstanding physical properties such as fire and heat resistivity. This class of molecules also possesses relatively low melting points, allowing for improved processability and manufacturing. While studies of this class of polymers are prominent, the monomers tend to shy away from focus. In an effort to understand organic crystal engineering of these compounds, four structures of silicon- and carbon-containing di(cyanate ester)s and tri(cyanate ester)s are presented and analyzed using single-crystal X-ray diffraction. This data, in concert with extensive thermodynamic and computational studies, assist in understanding how a subtle change, such as exchanging quaternary central carbon for a silicon, affects the molecular degrees of freedom. From a crystallographic standpoint, this affects the packing efficiency and intermolecular interactions.