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Crystal engineering of 1-halopolyynes by end-group manipulation.

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Streszczenie

Polyynes are compounds with two or more conjugated carbon–carbon triple bonds. Such molecules are usually regarded as models of carbyne—a hypothetical one-dimensional allotropic form of carbon. 1-Halopolyynes are rare representatives of such species, but few interesting crystal-to-crystal reactions have been recently reported for them. Herein, we present 11 new X-ray structures of 1-halopolyynes, nearly doubling the number of such compounds characterized with the use of single-crystal X-ray diffraction. The influence of an end-group on packing motifs in crystal structures of the 1-halopolyynes were thoroughly examined. Especially the strength of halogen bond as a function of polyyne chain length was analyzed with the support of theoretical calculations. Moreover, the compound **CNC_8I** is the longest 1-halopolyyne characterized to date with the use of rentgenostructural analysis. In addition to that, the compounds **NO_2C_6Br** and **$MeC(O)C_6Br$** are the first 1-bromohexatriynes characterized by means of X-ray single-crystal diffraction.

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