



STRUCTURAL
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Supporting information for article:

Cocrystals of 1,4-diethynylbenzene with 1,3-diacetylbenzene and benzene-1,4-dicarbaldehyde exhibiting strong nonconventional alkyne–carbonyl C—H···O hydrogen bonds between the components

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Two cocrystals with strong nonconventional alkyne...carbonyl C-H...O hydrogen bonds between the components

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The following two scatter plots were prepared using the results from a search of the Cambridge Structural Database (Version 5.37) using Excel. The search criteria were: crystal structures that contain alkyne *sp*-C-H...O=C carbonyl contacts with O...H distances equal to, or less than, the sum of the van der Waals radii of 2.72 Å.

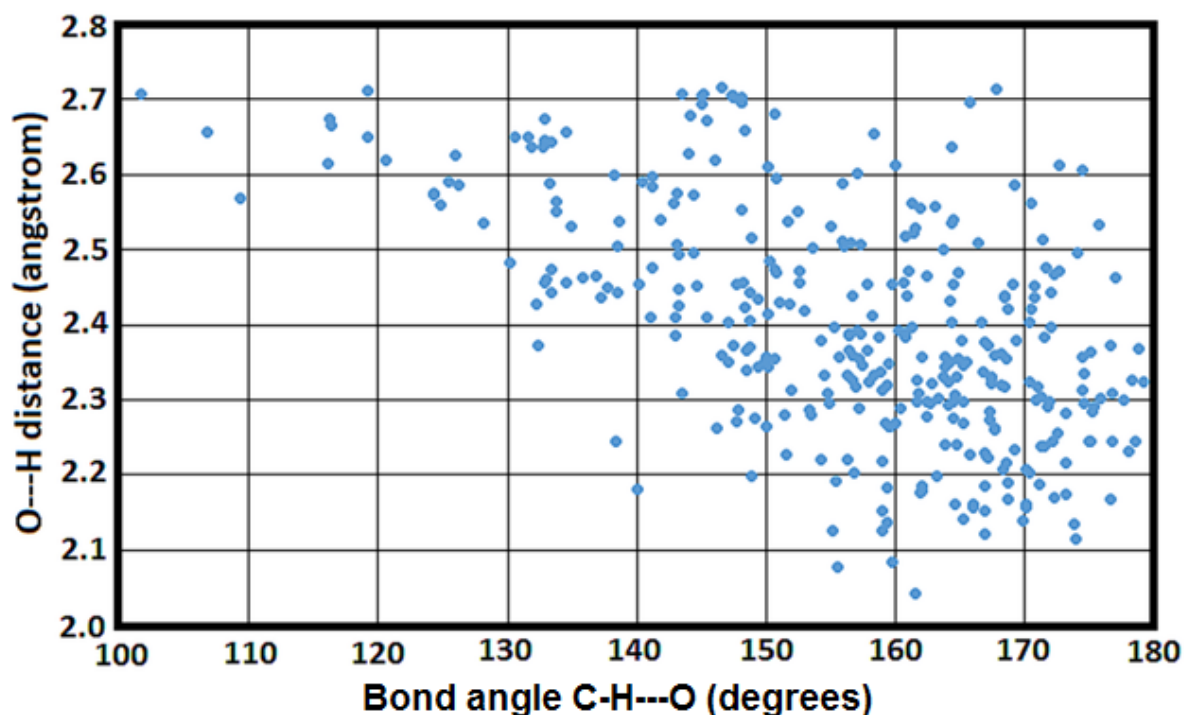


Figure S1 Scatter plot of the C-H...O bond angle vs. the distance (O...H) for X-ray structures with short alkyne *sp*-C-H...O=C interactions.

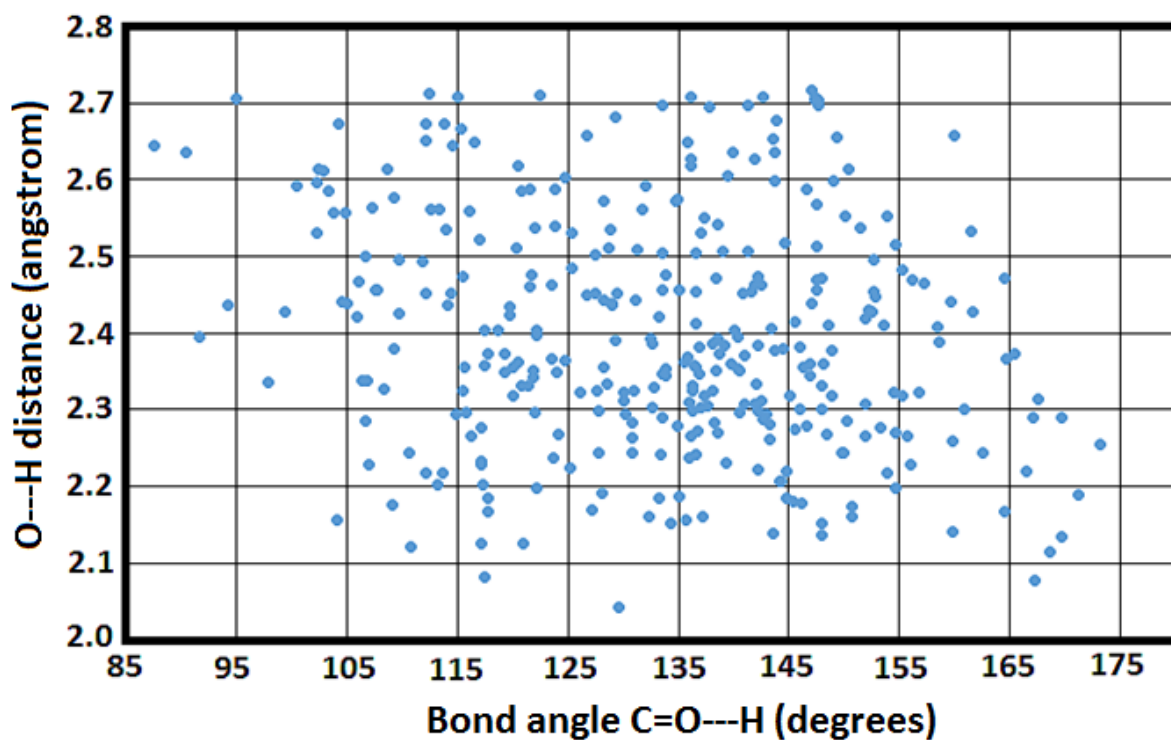


Figure S2 Scatter plot of the C=O...H bond angle vs. the distance (O...H) for X-ray structures with short alkyne sp -C-H...O=C interactions.