Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

In situ cryocrystallization and solid-state structures of furfural and some derivatives

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Comparison of X–C–O and X–C=C angles for 2-substituted furans with X = N and X = O from the Cambridge Structure Database (CSD)

Parameter values for 2N-furans in the CSD version 5.4 (November 2018)

Refcode	*O-C-N*	*C=C-N*
BAYFIT	117,961	132,185
DAGTIP	118,631	128,887
WUBPAM	114,173	133,957
WUBPAM	115,944	130,834
WUBPAM	114,635	132,821
WUBPAM	117,103	131,638
WUBPIU	115,347	132,641
WUBPIU	116,209	132,319
WUBPIU	116,74	131,615
WUBPIU	116,467	132,364
WUCFAD	114,473	132,724
AVERAGE	116,15	132,00
STDEV	1,43	1,30

Parameter values for 2O-furans in the CSD version 5.4 (November 2018)

Refcode	*O-C-O*	*C=C-O*
CIDKAD	115,130	133,395
CIDKEH	115,387	131,418
AVERAGE	115,26	132,41
STDEV	0,18	1,40