

## Supporting Information for

### TADDOLs & Methylcyclohexanones: Selectivity, Resolution and Kinetics of decomposition

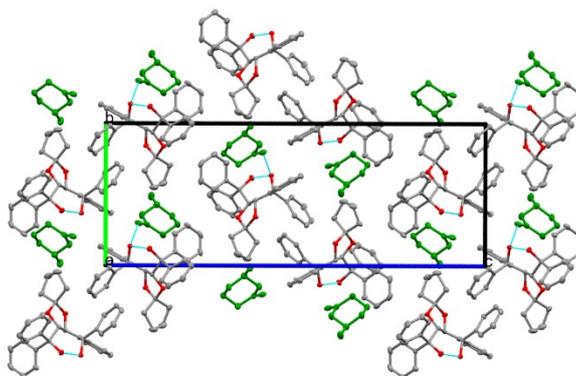
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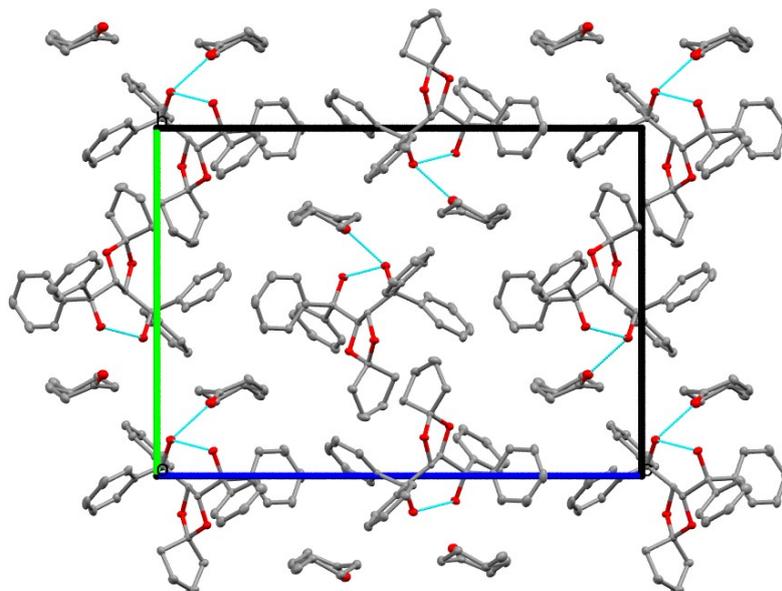
**Table S1.** Structure codes for combinations of hosts and guests.

	<b>H1</b>	<b>H2</b>	<b>H3</b>
2-MeCHN	I	IV	VII
3-MeCHN	II	V	VIII*
4-MeCHN	III	VI	IX

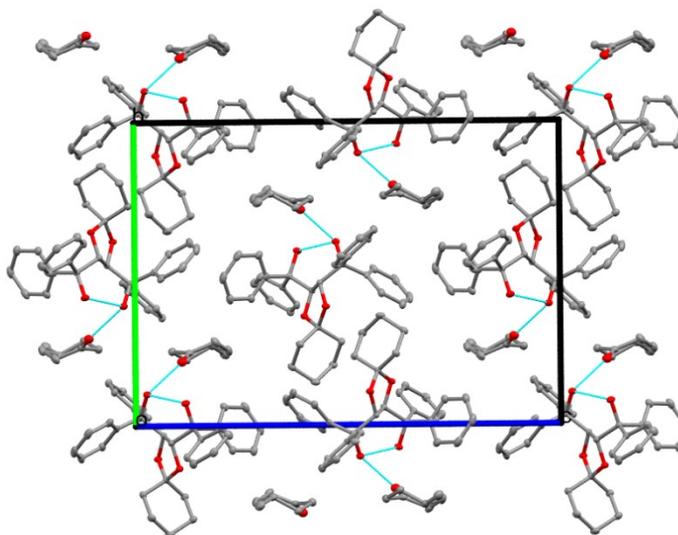
\*No crystals obtained despite several crystallization attempts lasting over 5 months.



**Fig. S1.** Packing of **V** viewed down [0 1 0] showing the 3-methylcyclohexanone guest located in cavities.



**Fig. S2.** Packing of VI viewed down [1 0 0], showing the guest 4-MeCHN located in channels.



**Fig. S3.** Packing of IX viewed down [1 0 0], showing the guest 4-MeCHN located in channels.

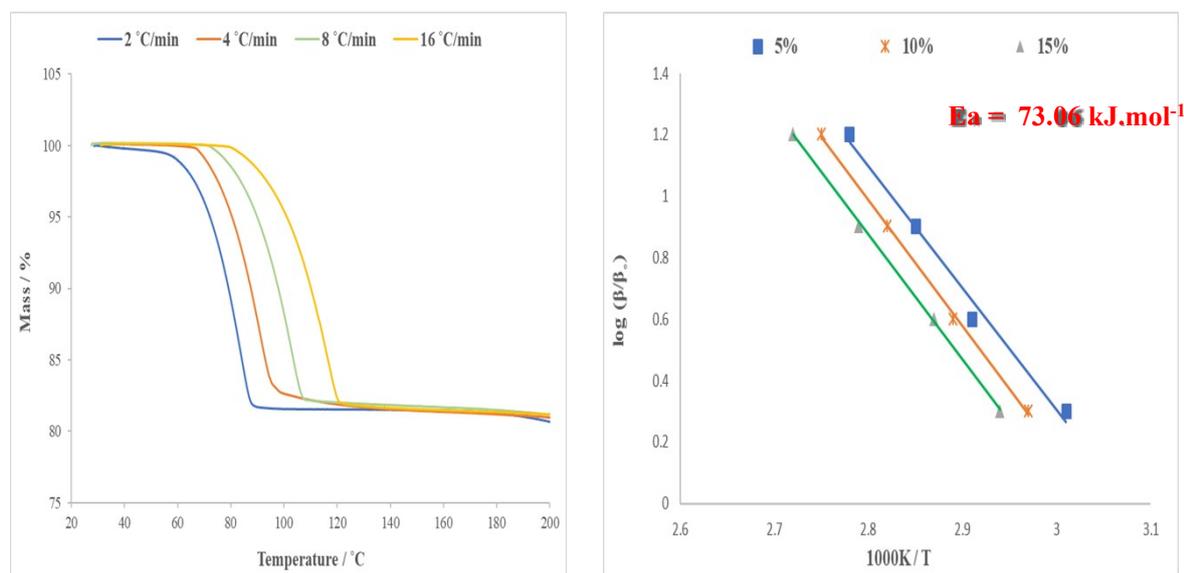
**Table S2. Lists of the H-bond details for intramolecular bond O-H...O(Host)for Structures I - IX.**

<b>Structure</b>	<b>Donor</b>	<b>Acceptor</b>	<b>O...O (Å)</b>	<b>O...H (Å)</b>
I [H1.2-MeCHN]	O13A	O19A	2.72(8)	0.97(3)
	O13B	O19B	2.63(1)	0.84(5)
II [H1.3-MeCHN]	O13A	O19A	2.75(3)	0.82(6)
III [H1.4-MeCHN]	O19A	O13A	2.69(3)	0.85(3)
IV [H2.2-MeCHN]	O21A	O13A	2.67(2)	0.97(3)
V [H2.3-MeCHN]	O21A	O13A	2.69(2)	0.84(3)
VI [H2.4-MeCHN]	O13A	O21A	2.71(2)	0.90(3)
VII [H3.2-MeCHN]	O22A	O13A	2.66(7)	0.71(7)
	O22A	O13B	2.65(5)	0.88(6)
IX [H3.4-MeCHN]	O22A	O13A	2.72(2)	0.97(3)

**Table S3. Lists of the H-bond details for intermolecular bond O-H...O=C(Guest) for Structures I - IX.**

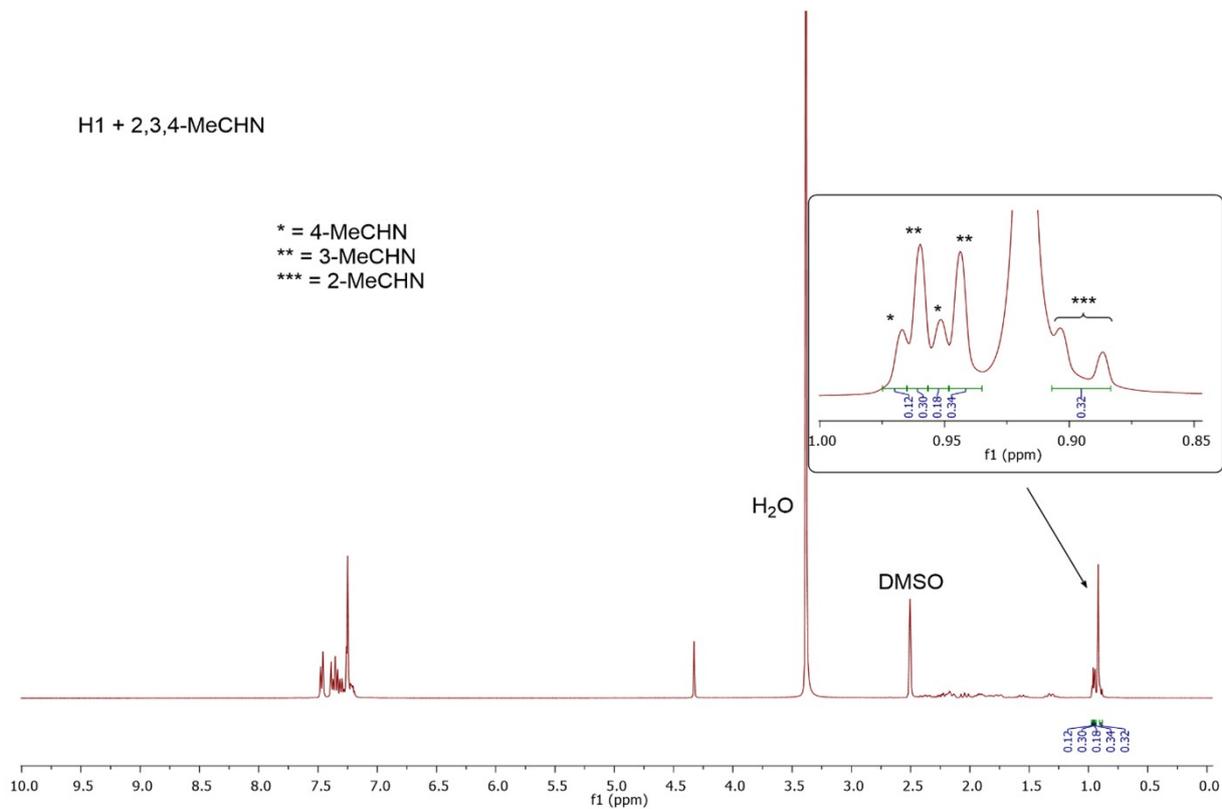
Structure	Donor	Acceptor	O...O (Å)	O-H (Å)
I [H1.2-MeCHN]	O19A	O1X	2.86(3)	0.97(3)
	O19A	O1Y	2.88(6)	0.97(3)
	O19B	O1W	2.75(4)	0.97(3)
	O19B	O1Z	2.56(5)	0.97(3)
II [H1.3-MeCHN]	O19A	O1X	2.73(4)	0.75(6)
III [H1.4-MeCHN]	O13A	O1X	2.62(2)	0.86(3)
IV [H2.2-MeCHN]	O13A	O1X	2.76(1)	0.97(3)
	O13A	O1Y	2.80(1)	0.97(3)
V [H2.3-MeCHN]	O13A	O1X	2.77(2)	0.78(3)
VI [H2.4-MeCHN]	O21A	O1X	2.76(2)	0.90(4)
VII [H3.2-MeCHN]	O13A	O1X	2.79(2)	0.80(8)
	O13A	O1Y	2.62(1)	0.80(8)
	O13B	O1Z	2.76(1)	0.84(9)
	O13B	O1W	2.69(3)	0.84(9)
IX [H3.4-MeCHN]	O13A	O1X	2.72(2)	0.97(3)

**Details of the thermogravimetric analysis (TGA) and the decomposition reaction of H1.(3-MeCHN).**

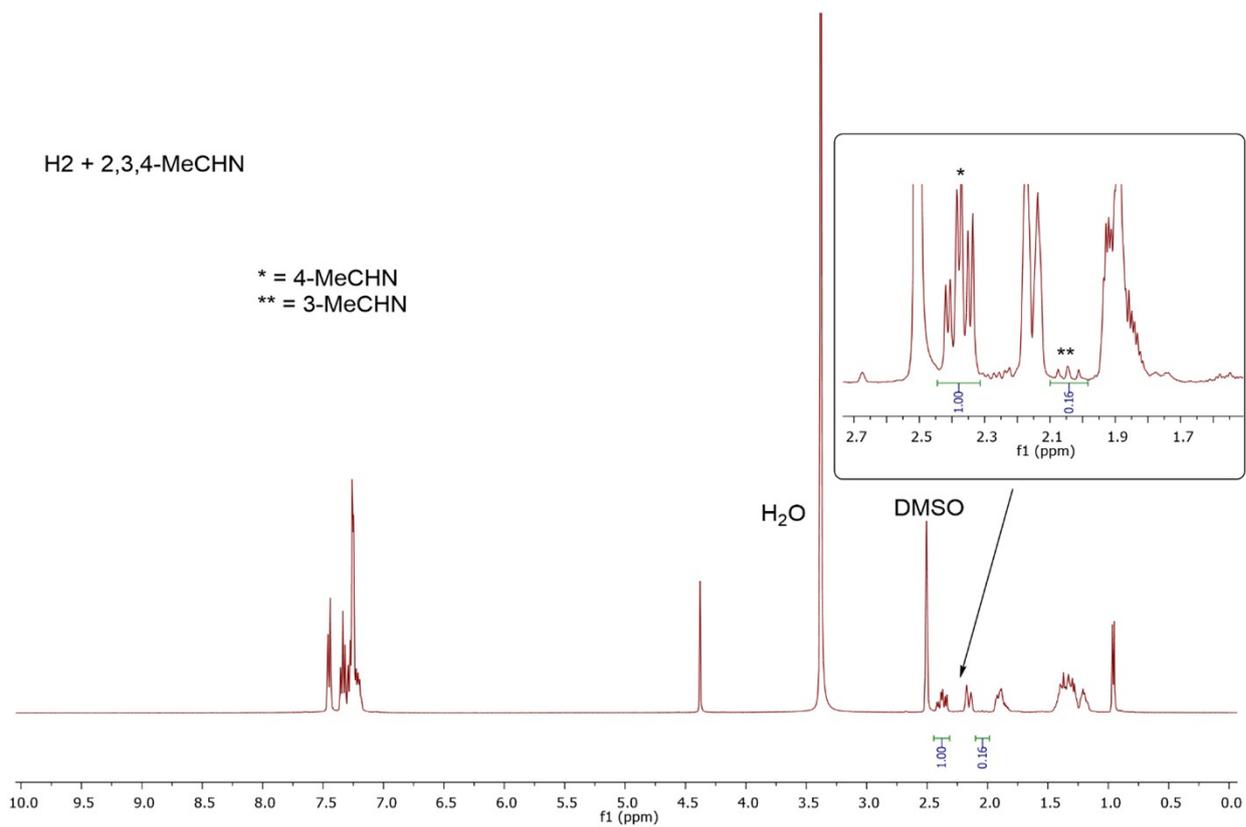


**Fig. S4. TGA traces collected at various heating rates of 2, 4, 8, and 16 °C/min and (b) plots of log( $\beta/\beta_0$ ) versus 1000 K / T at 5%, 10%, and 15% extent of the guest desorption reaction of structure H1.(3-MeCHN).**

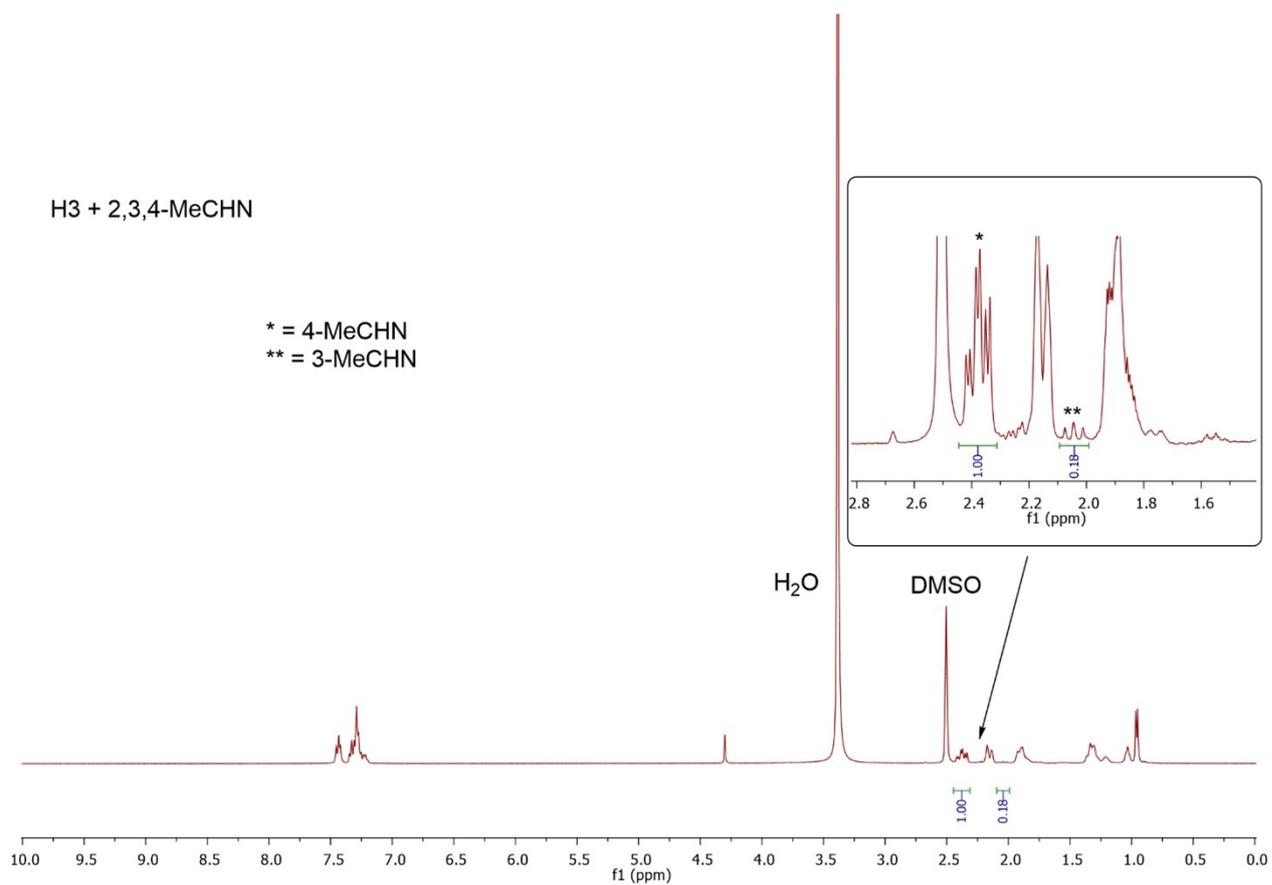
NMR results with appropriate peaks identifying the guests molecules for H1.2,3,4-MeCHN, H2.2,3,4-MeCHN, and H3.2,3,4-MeCHN are shown in **Figs S5, Fig S6 and Fig S7** respectively.



**Fig. S5. . <sup>1</sup>H NMR of H1.2,3,4-MeCHN in d<sub>6</sub>.DMSO.**



**Fig. S6.** <sup>1</sup>H NMR of H<sub>2</sub>.2,3,4-MeCHN in d<sub>6</sub>.DMSO.



**Fig. S7. <sup>1</sup>H NMR of H3.2,3,4-MeCHN in d<sub>6</sub>.DMSO.**