

Supporting information

Diamondoid ether clusters in helium nanodroplets

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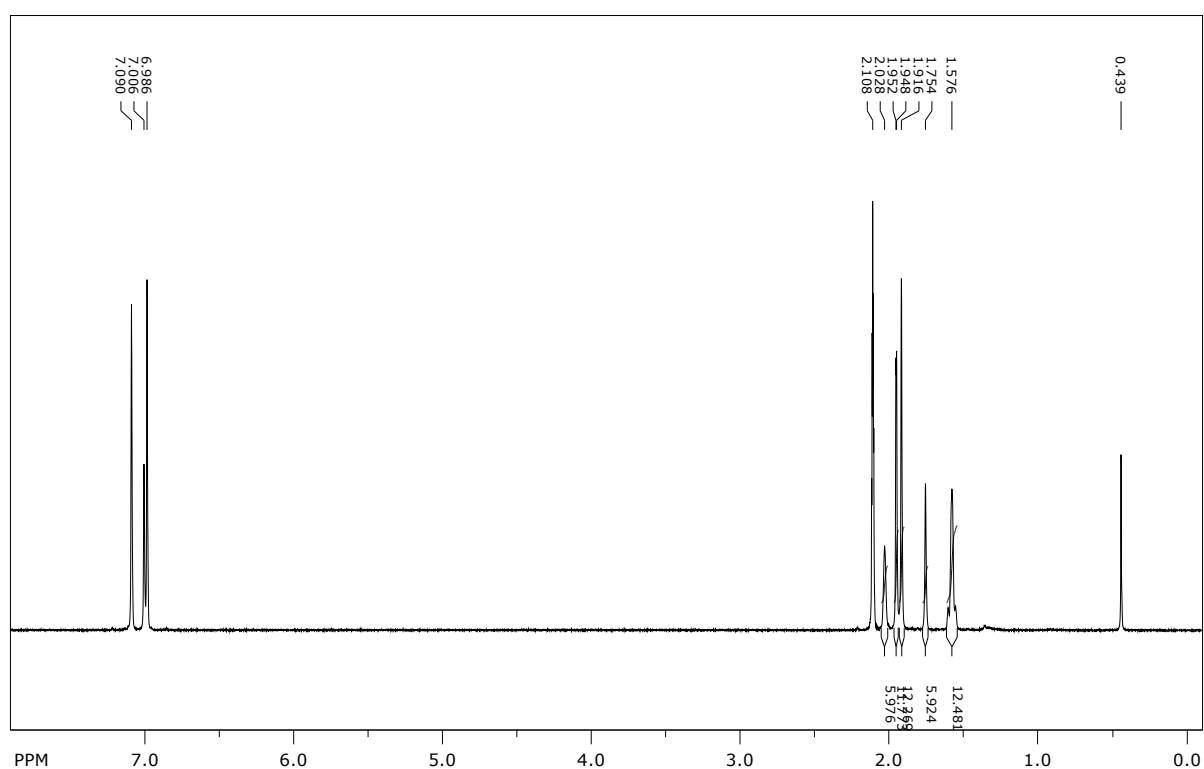
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SpinWorks 4: JA-102

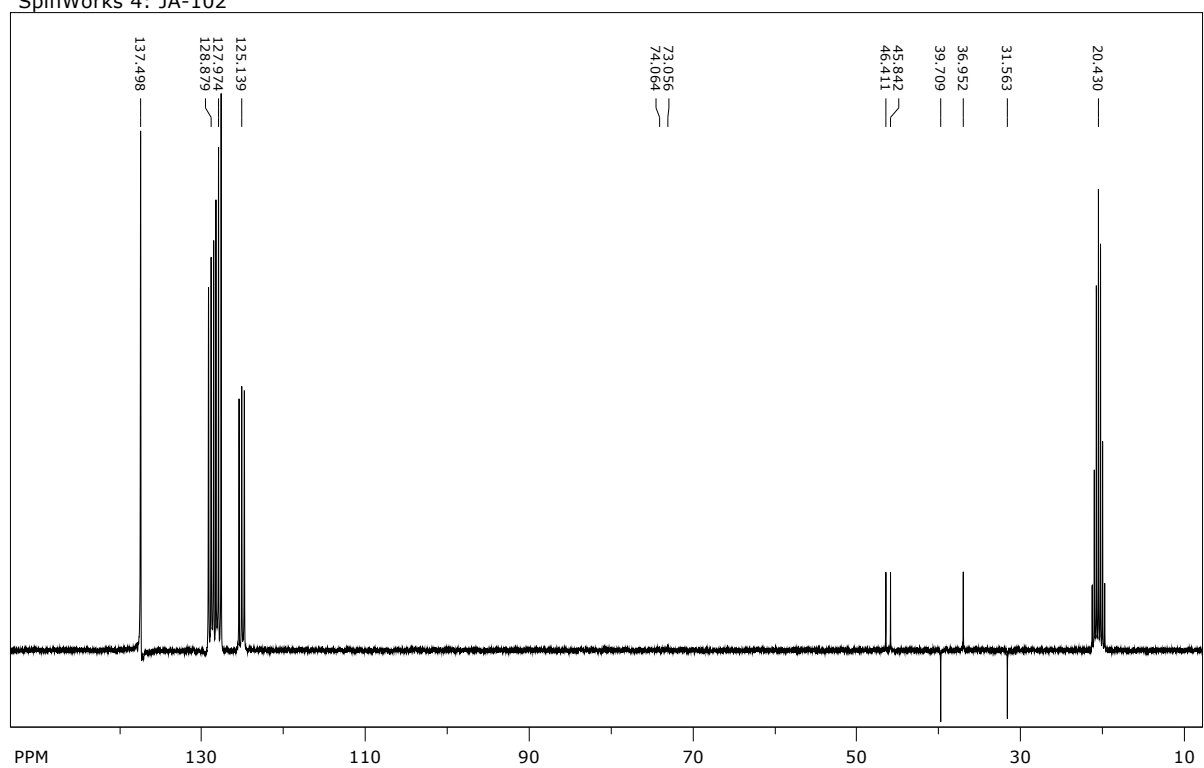
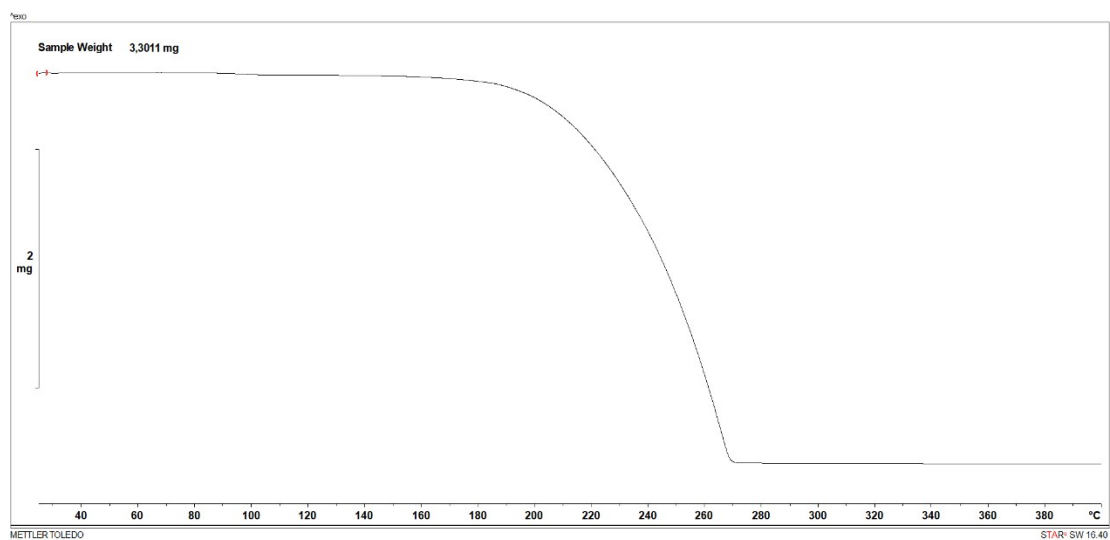
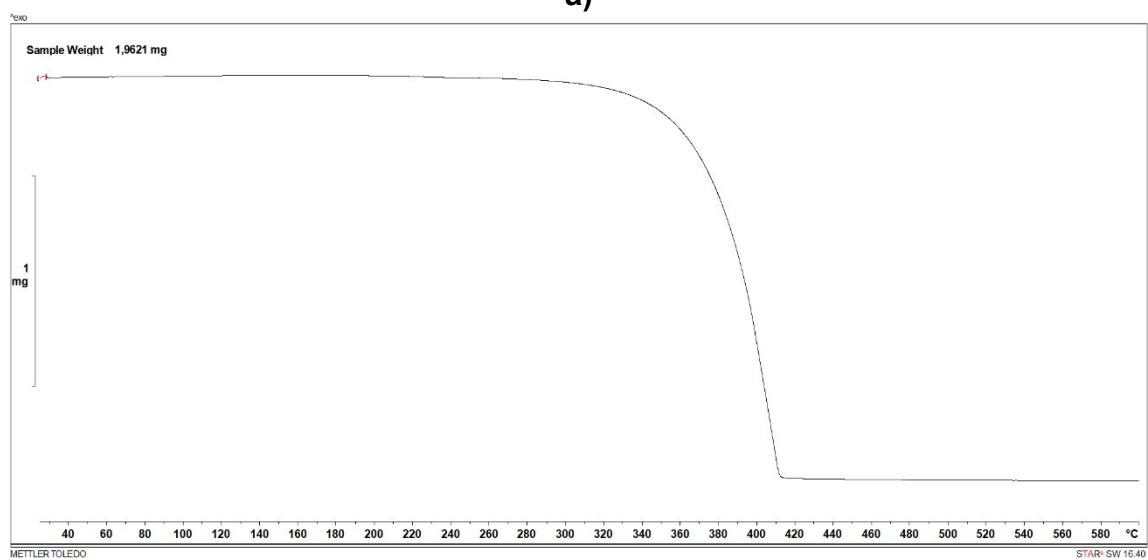


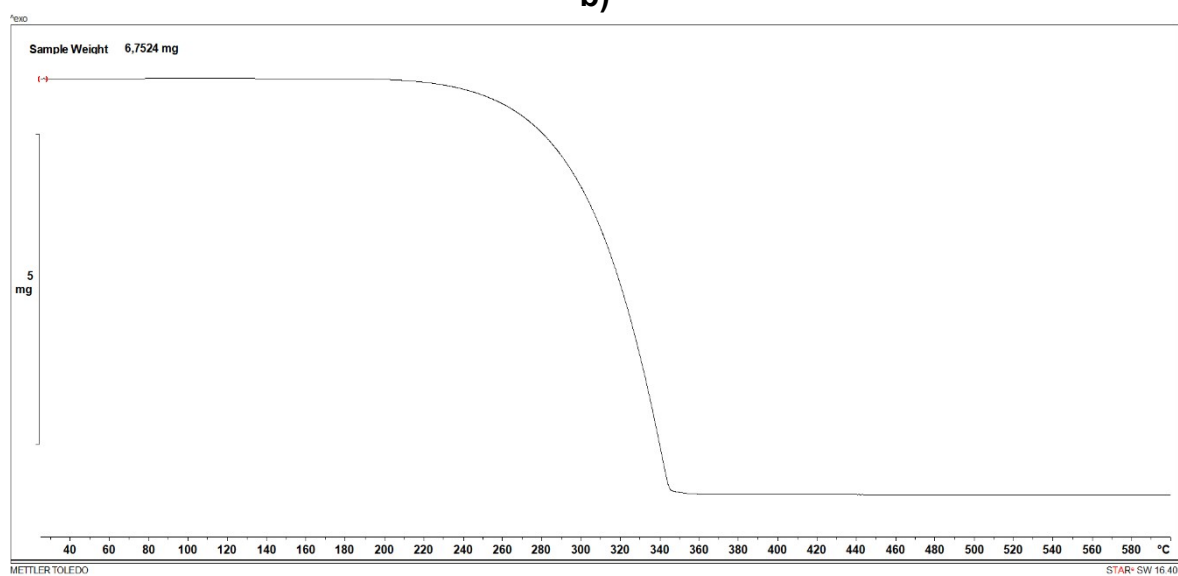
Figure S1. ¹H (600 MHz, toluen-*d*₈, 70 °C) and ¹³C NMR (75 MHz, toluen-*d*₈, 70 °C) spectra of 4,9-bis(1-adamantyloxy)diamantane (**2**).



a)



b)



c)

Figure S2. TG curves for ethers: (a) 1, (b) 2, (c) 3.

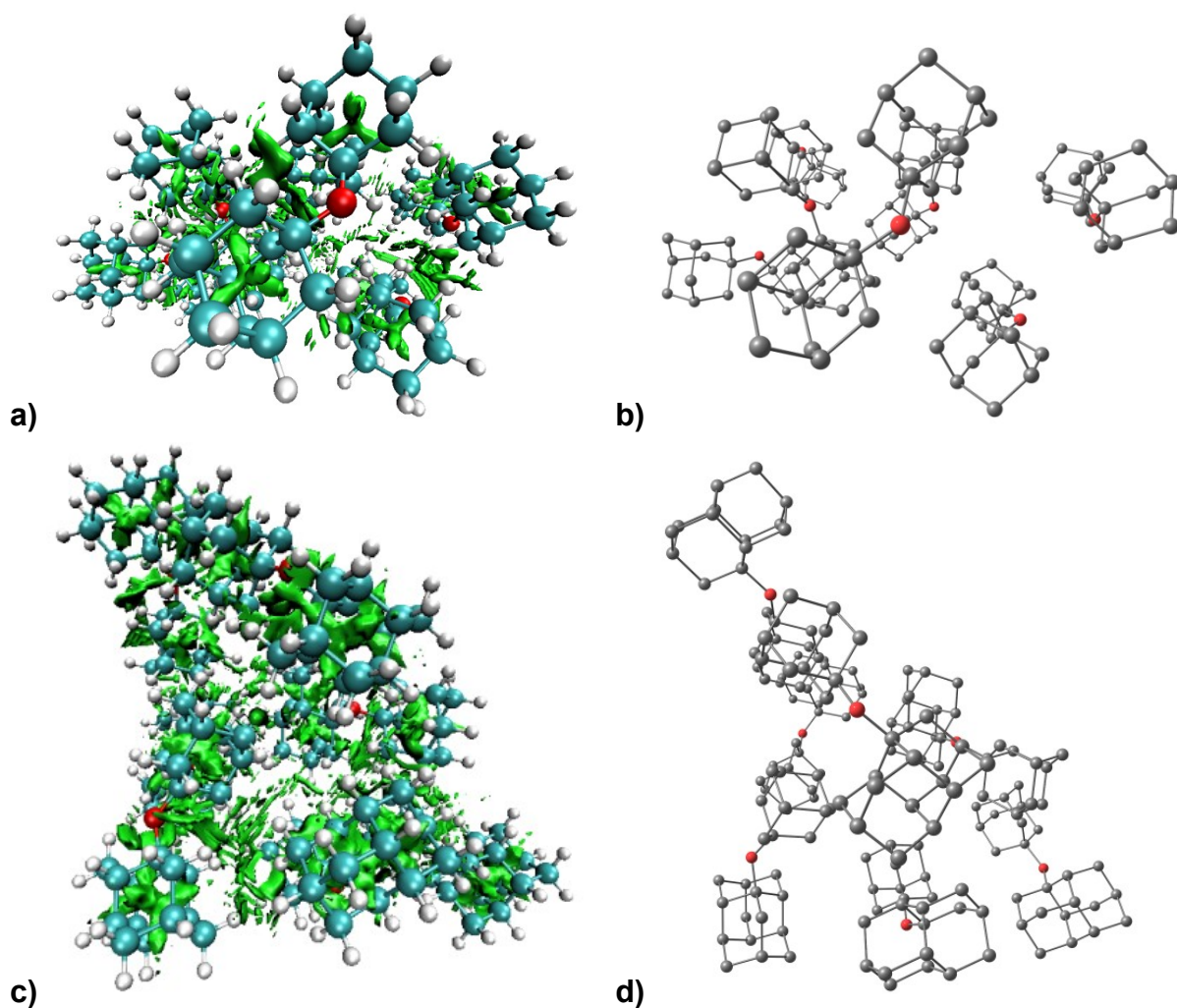


Figure S3. NCI plots of the computed structure of **CL1** (a) and **CL3** (c) with non-covalent interactions depicted in green, and the corresponding molecules building **CL1** (b) and **CL3** (d) depicted without hydrogen atoms for clarity.

Table S1. Electronic energies, zero-point vibrational energies, enthalpies and Gibbs energies of ethers **1–3** and clusters **CL1–CL3** in Hartree computed using the GFN2-xTB method at 0.4 K.

compound	E	$ZPVE$	H	G
1	-62.330173	0.462195	-61.867972	-61.867986
2	-105.676053	0.755918	-104.920130	-104.920144
3	-72.982695	0.533355	-72.449334	-72.449349
CL1	-436.399649	3.250816	-433.148827	-433.148800
CL2	-317.071649	2.277312	-314.794332	-314.794326
CL3	-510.975191	3.751655	-507.223531	-507.223503

Table S2. Electronic energies of ethers **1–3** and clusters **CL1–CL3** in Hartree and interaction energies, $\Delta H(0\text{ K})$,^a for clusters **CL1–CL3** in kcal mol⁻¹ computed at the B3LYP-gCP-D3(BJ)-ABC/def2-TZVPP level of theory.

compound	<i>E</i>	compound	<i>E</i>	ΔH
1	-855.263900	CL1	-5986.934860	-45.2
3	-1474.722022	CL2	-4424.206671	-19.5
3	-1010.080285	CL3	-7070.655192	-47.1

^a Interaction energies are defined as a difference between the energy of the cluster and the energy of the corresponding number of ether molecules. *ZPVE* taken from GFN2-xTB computations.

Table S3. Geometries of ethers **1–3** and clusters **CL1–CL3** in Cartesian coordinates in Å computed using the GFN2-xTB method at 0.4 K.

1			
6	-1.864116000	3.764963000	0.629218000
6	-2.697168000	2.563435000	1.101225000
6	-1.756718000	1.448260000	1.578255000
6	-0.940470000	3.323230000	-0.515147000
1	-1.270526000	4.159761000	1.459397000
1	-2.523024000	4.571493000	0.292337000
6	-0.004294000	2.203955000	-0.028074000
6	-0.824317000	0.987380000	0.444531000
1	-2.326243000	0.584744000	1.931443000
1	-1.140206000	1.790857000	2.413089000
1	0.614454000	2.548590000	0.804839000
1	0.668403000	1.920605000	-0.836858000
6	-3.550255000	2.043335000	-0.065681000
1	-3.347280000	2.865256000	1.927379000
6	-1.695091000	0.475833000	-0.715999000
6	-2.627183000	1.599043000	-1.209259000
1	-4.230822000	2.826670000	-0.413691000
1	-4.169755000	1.203619000	0.264415000
1	-2.286701000	-0.377595000	-0.376398000
1	-1.072480000	0.135912000	-1.545417000
6	-1.787251000	2.794949000	-1.684294000
1	-0.338685000	4.172512000	-0.851509000
1	-1.136642000	2.492162000	-2.511021000
1	-2.440911000	3.585872000	-2.064971000
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6	2.697168000	-2.563433000	1.101227000
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1	2.326240000	-0.584743000	1.931445000
6	1.695089000	-0.475834000	-0.715999000
6	2.627183000	-1.599042000	-1.209257000
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6	3.550254000	-2.043332000	-0.065679000

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1	2.440914000	-3.585872000	-2.064968000

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CL1

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