

Synthesis and molecular structure of seven isomers of $C_{70}(C_2F_5)_{10}$

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Selected crystallographic data

Crystallographic data and some details of data collection and structure refinement for seven isomers of $C_{70}(C_2F_5)_{10}$ are given in Table 1S. Structure I contains two crystallographically independent $C_{70}(C_2F_5)_{10}$ molecules along with a toluene molecule disordered around an inversion centre. Structure II contains a half of hexane molecule near an inversion centre so that the whole C_6H_{14} molecule is centrosymmetric. The isomer V was obtained as Vt or Vb dependent on the solvent used for growing crystals (toluene or benzene, respectively). The data for the modification Vt are given in Table 1. Unit cells and packing diagrams are very similar for the both crystalline solvates. The only small difference is the presence of either two independent toluene or two independent benzene molecules in the crystal lattice. One of the toluene molecules in structure Vt is disordered. CIF files are provided for the both solvates. Crystal structures of other four isomers are solvent free. Two C_2F_5 groups in the structure of isomer IV are positionally disordered.

Table 1S. Crystallographic data and some details of data collection and refinement for six isomers of C₇₀(C₂F₅)₁₀.

Isomer /	C ₇₀ (C ₂ F ₅) ₁₀ (I)	C ₇₀ (C ₂ F ₅) ₁₀ (II)	C ₇₀ (C ₂ F ₅) ₁₀ (III)	C ₇₀ (C ₂ F ₅) ₁₀ (IV)	C ₇₀ (C ₂ F ₅) ₁₀ (Vt)	C ₇₀ (C ₂ F ₅) ₁₀ (VI)	C ₇₀ (C ₂ F ₅) ₁₀ (VII)
Solvent in the lattice	0.25 C ₆ H ₅ (CH ₃)	0.5 C ₆ H ₁₄	-	-	C ₆ H ₅ (CH ₃)	-	-
M	2053.93	2073.99	2030.90	2030.90	2123.03	2030.90	2030.90
Crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic	Triclinic	Triclinic	Monoclinic
Space group	<i>P2₁/c</i>	<i>P-1</i>	<i>P2₁/n</i>	<i>Cc</i>	<i>P-1</i>	<i>P-1</i>	<i>P2₁/n</i>
<i>a</i> / Å	14.4559(1)	14.6171(1)	13.9259(2)	26.1672(4)	15.3403(1)	13.0480(1)	19.465(1)
<i>b</i> / Å	24.2760(1)	15.2530(1)	20.1946(4)	12.5034(2)	22.1951(1)	13.1964(1)	16.290(1)
<i>c</i> / Å	39.0100(2)	17.4577(2)	24.0235(5)	40.3019(6)	22.8553(1)	21.2378(2)	20.626(3)
<i>α</i> / °	90	82.2610(4)	90	90	79.9992(2)	83.0458(5)	90
<i>β</i> / °	90.7544(2)	84.5166(5)	105.538(8)	95.1204(6)	78.8229(2)	73.4163(5)	98.860(4)
<i>γ</i> / °	90	62.3042(5)	90	90	70.0532(2)	70.4461(4)	90
Volume / Å ³	13688.7(1)	3412.53(5)	6509.2(2)	13133.3(4)	7127.23(6)	3301.30(5)	6462(1)
Z	8	2	4	8	4	2	4
<i>D_c</i> / g cm ⁻³ ; μ / mm ⁻¹	1.993 ; 0.212	2.018 ; 0.214	2.072 ; 0.222	2.054 ; 0.220	1.979 ; 0.207	2.043 ; 0.219	2.087 ; 0.223
Crystal size / mm	0.2x0.03x0.03	0.09x0.05x0.05	0.1x0.03x0.01	0.06x0.04x0.03	0.1x0.07x0.05	0.06x0.04x0.03	0.04x0.03x0.02
Temperature / K	100(2)	100(2)	100(2)	100(2)	100(2)	100(2)	100(2)
Area detector, λ / Å	MAR225, 0.910	MAR225, 0.905	MAR225, 0.910	MAR225, 0.905	MAR225, 0.905	MAR225, 0.910	MAR225, 0.910
Refls collected / independent	113452 / 25962	28865 / 11484	30346 / 8143	58085 / 19937	84499 / 24088	32982 / 10483	10173 / 5702
Data / parameters	25959 / 2541	11481 / 1290	8140 / 1261	19929 / 2578	24085 / 2713	10489 / 1289	5701 / 912
R ₁ [I ≥ 2σ(I)] / wR ₂ (all)	0.087 / 0.219	0.059 / 0.156	0.053 / 0.154	0.094 / 0.249	0.067 / 0.178	0.066 / 0.168	0.153 / 0.355
Δρ (max / min) / e Å ⁻³	1.062 / -0.555	0.749 / -0.784	0.905 / -0.437	1.086 / -0.415	1.118 / -0.633	0.699 / -0.511	0.616 / -0.556