$C_{12}F_{12}$	*hP*48	(176) $P6_3/m - i^2h^4$

$C_{12}F_{12}$ [2]
Structural features: $C_{12}F_{12}$ molecules (a central C_6 hexagon sharing edges with three coplanar C_4 squares, two F bonded to each outer C). See Fig. IV.70.

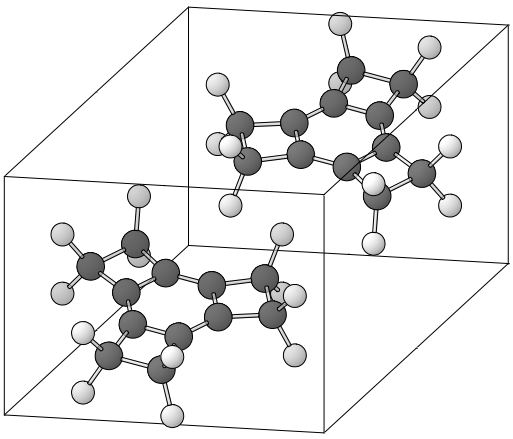

Fig. IV.70. **$C_{12}F_{12}$**

Arrangement of $C_{12}F_{12}$ molecules (C atoms dark, F atoms light). For clarity, atoms located in the cell but belonging to molecules with the central hexagon in a neighboring cell are omitted.

Thummel R.P. et al. (1977) [1]
$C_{12}F_{12}$
$a = 0.8966$, $c = 0.8671$ nm, $c/a = 0.967$, $V = 0.6037$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
F1	12*i*	1	0.017	0.256	0.1252		single atom C
F2	12*i*	1	0.1209	0.595	0.126		single atom C
C3	6*h*	*m*..	0.0302	0.5086	$^1/_4$		tetrahedron F_2C_2
C4	6*h*	*m*..	0.3398	0.0298	$^1/_4$		tetrahedron F_2C_2
C5	6*h*	*m*..	0.4921	0.2123	$^1/_4$		coplanar triangle C_3
C6	6*h*	*m*..	0.6126	0.1585	$^1/_4$		coplanar triangle C_3

Experimental: single crystal, diffractometer, X-rays, R = 0.035, T = 238 K

Remarks: Perfluoro-triethanobenzene, perfluorobenzo[1,2:3,4:5,6]tricyclobutene.

References: [1] Thummel R.P., Korp J.D., Bernal I., Harlow R.L., Soulen R.L. (1977), J. Am. Chem. Soc. 99, 6916-6918. [2] Cobbledick R.E., Einstein F.W.B. (1976), Acta Crystallogr. B 32, 1908-1909.