Supporting information for

Selective synthesis and crystal structure of $C_{70}(CF_3)_{10}[C(CO_2Et)_2]$

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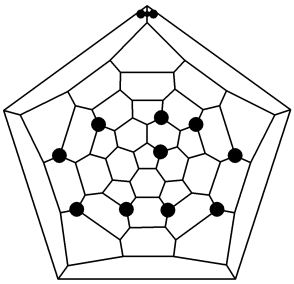
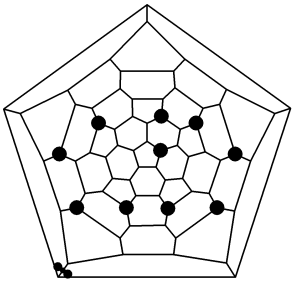
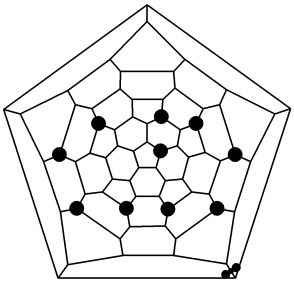
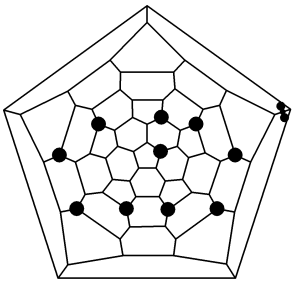
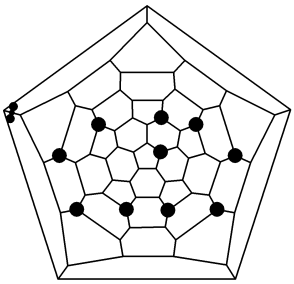
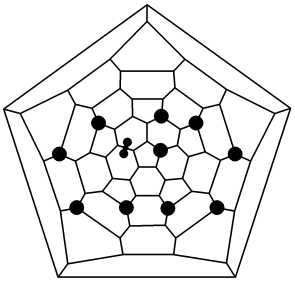
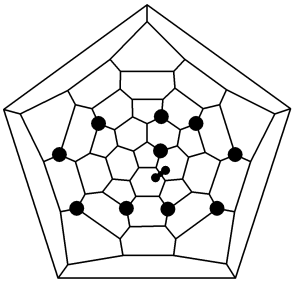
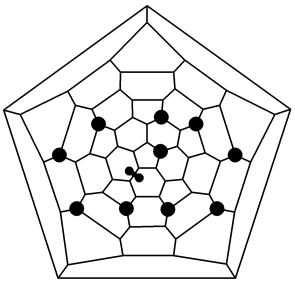
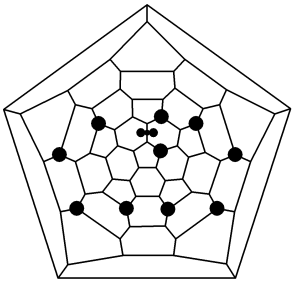
Table 1. Schlegel diagrams, relative energies at the DFT and AM1 (in parentheses) levels of theory of some isomers of $C_{70}(CF_3)_{10}CR_2$ (R= H, CO_2Et). The black circles denote attached CF_3 groups, black dumb-bell denotes attached CR_2 fragment.

№№	*Schlegel Diagrams of $C_{70}(CR_2)$*	*ΔE, kJ·mol^{-1} DFT (AM1)*		*Isomer abbreviation*
		R= H	*R= CO_2Et*	
1		0.0 (0.0)	0.0 (0.0)	*a*-$C_{70}(CF_3)_{10}[CR_2]$
2		8.9 (11.5)	6.5 (12.8)	*c*-$C_{70}(CF_3)_{10}[CR_2]$
3		10.8 (11.7)	12.7 (16.3)	*d*-$C_{70}(CF_3)_{10}[CR_2]$
4		12.6 (14.9)	15.4 (20.9)	*e*-$C_{70}(CF_3)_{10}[CR_2]$

№№	*Schlegel Diagrams of* $C_{70}(CR_2)$	ΔE, kJ·mol^{-1} DFT (AM1)		*Isomer abbreviation*
		R= H	*R= CO_2Et*	
5		11.1 (20.4)	17.1 (22.1)	*b*-$C_{70}(CF_3)_{10}[CR_2]$
6		19.3 (15.1)	18.2 (28.0)	*b′*-$C_{70}(CF_3)_{10}[CR_2]$
7		0.5 (13.7)	23.1 (49.3)	*d′*-$C_{70}(CF_3)_{10}[CR_2]$
8		23.9 (21.3)	24.9 (29.6)	*c′*-$C_{70}(CF_3)_{10}[CR_2]$
9		-23.1 (18.8)	49.6 (80.7)	*a′*-$C_{70}(CF_3)_{10}[CR_2]$

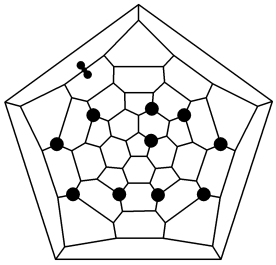
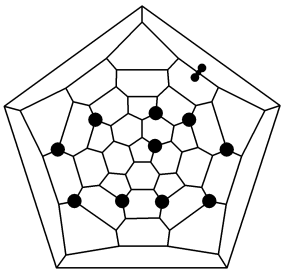
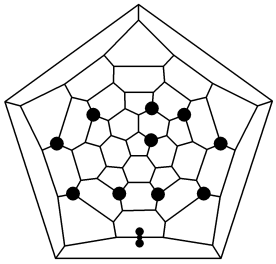
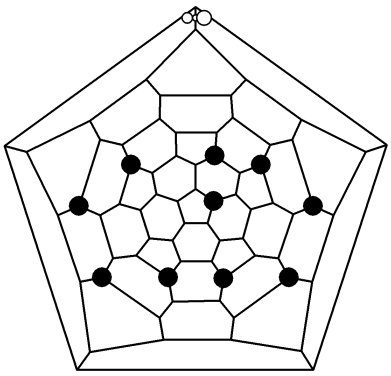
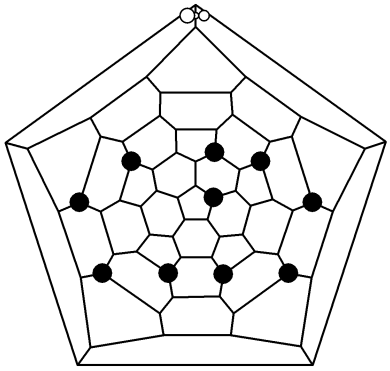
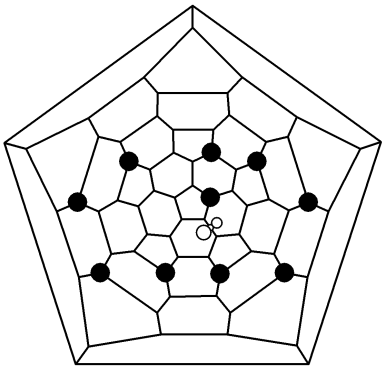
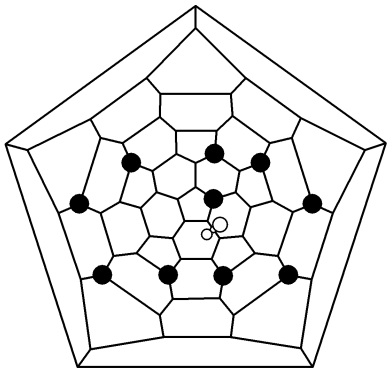
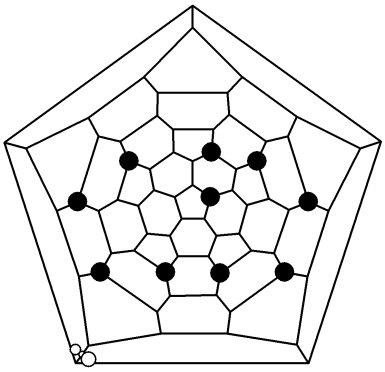
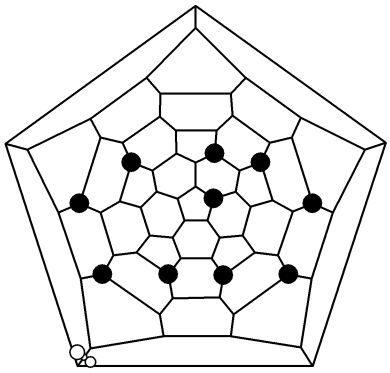
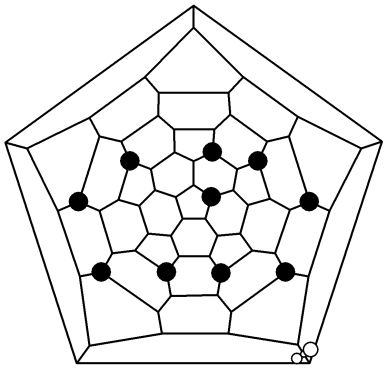
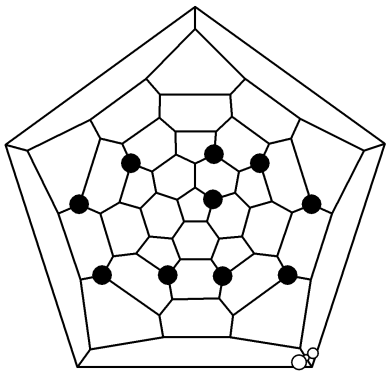
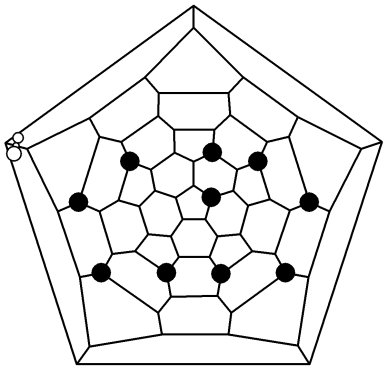
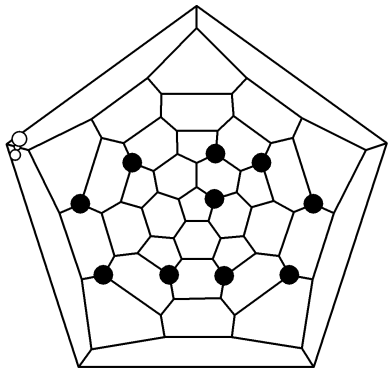
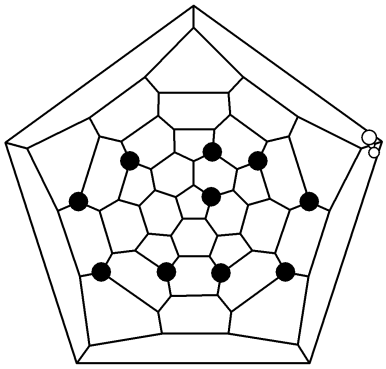
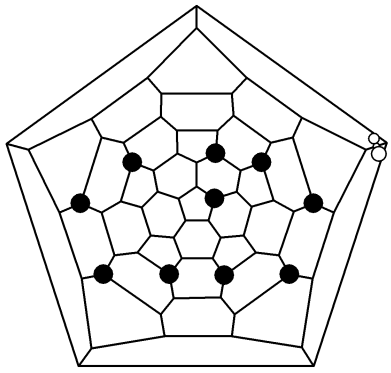
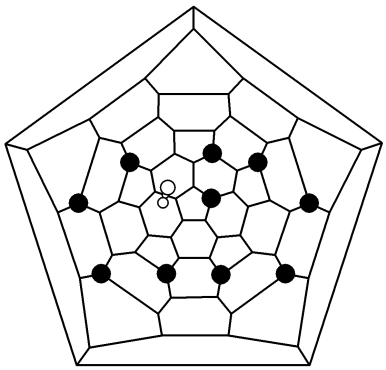
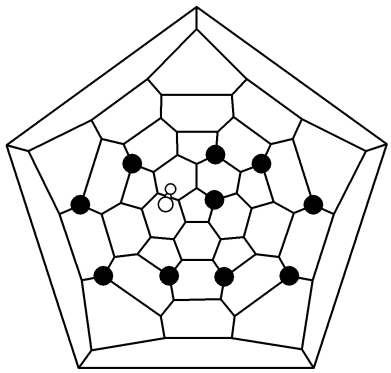
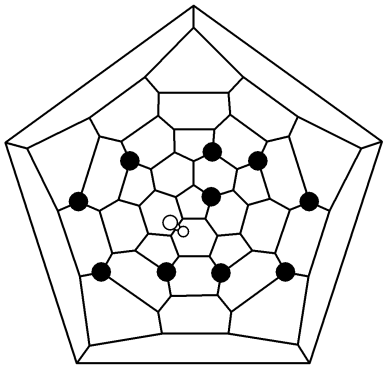
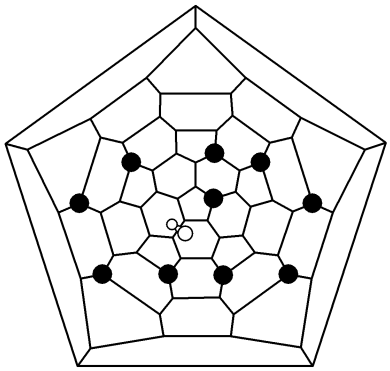
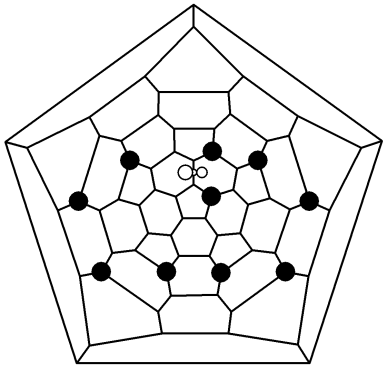
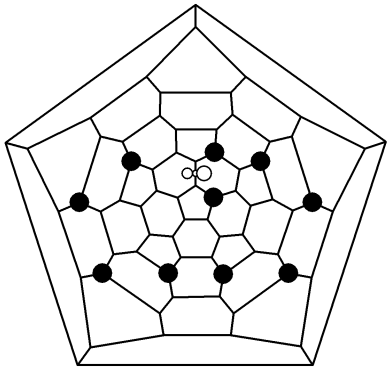
№№	*Schlegel Diagrams of $C_{70}(CR_2)$*	*ΔE, kJ·mol^{-1} DFT (AM1)*		*Isomer abbreviation*
		R= H	*R= CO_2Et*	
10		20.6 (60.1)	> 20	*g*-$C_{70}(CF_3)_{10}[CR_2]$
11		21.6 (61.9)	> 20	*i*-$C_{70}(CF_3)_{10}[CR_2]$
12		40.3 (85.6)	> 20	*h*-$C_{70}(CF_3)_{10}[CR_2]$

Table 2. Schlegel diagrams, relative energies at the DFT and AM1 (in parentheses) levels of theory for some isomers of $C_{70}(CF_3)_{10}CHCO_2Et$. The black circles denote attached CF_3 groups; empty dumb-bell denotes attached $CH(CO_2Et)$ fragment, where small and large circles correspond H and CO_2Et groups.

№№ (isomer)	*Schlegel Diagrams of $C_{70}(CF_3)_{10}CHCO_2Et$ #1*	$\Delta\Delta_f H^o_0$ **kJ·mol^{-1}**	*Schlegel Diagrams of $C_{70}(CF_3)_{10}CHCO_2Et$ #2*	$\Delta\Delta_f H^o_0$ **kJ·mol^{-1}**
1 (*a*)		0.1 (0.0)		0.0 (0.3)
2 (*d′*)		2.8 (16.2)		19.4 (35.1)
3 (*c*)		10.5 (12.7)		10.8 (11.7)

№№ (isomer)	*Schlegel Diagrams of $C_{70}(CF_3)_{10}CHCO_2Et$ #1*	$\Delta\Delta_f H_0^o$ kJ·mol^{-1}	*Schlegel Diagrams of $C_{70}(CF_3)_{10}CHCO_2Et$ #2*	$\Delta\Delta_f H_0^o$ kJ·mol^{-1}
4 (*d*)		11.2 (14.3)		10.9 (12.8)
5 (*b*)		14.9 (18.2)		15.5 (16.2)
6 (*e*)		15.3 (16.2)		15.4 (16.5)
7 (*b′*)		21.6 (23.4)		19.1 (21.9)

№№ (isomer)	*Schlegel Diagrams of $C_{70}(CF_3)_{10}CHCO_2Et$ #1*	$\Delta\Delta_f H_0^o$ kJ·mol^{-1}	*Schlegel Diagrams of $C_{70}(CF_3)_{10}CHCO_2Et$ #2*	$\Delta\Delta_f H_0^o$ kJ·mol^{-1}
8 (*c′*)		25.0 (25.1)		25.5 (22.9)
9 (*a′*)		-14.7 (24.7)		34.3 (61.5)