

Supporting information for

**New trifluoromethylated derivatives of [60]fullerene, $C_{60}(CF_3)_n$ with
 $n = 12$ and 14**

*N. A. Omelyanyuk, A. A. Goryunkov, N. B. Tamm, S. M. Avdoshenko, I. N. Ioffe, L. N. Sidorov,
E. Kemnitz and S. I. Troyanov*

Chem. Commun.

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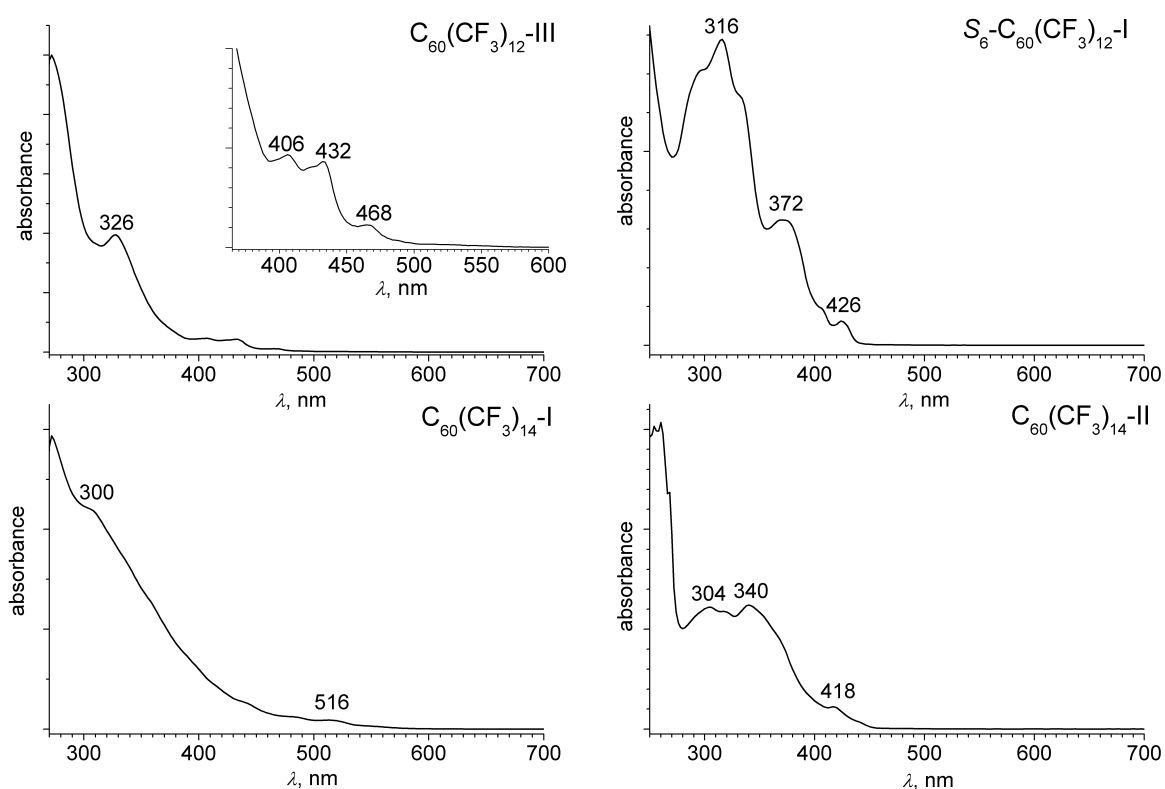
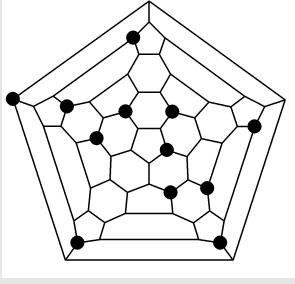
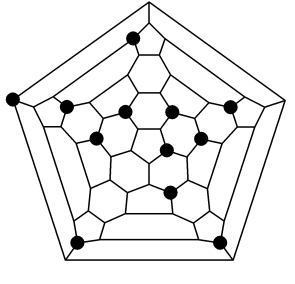
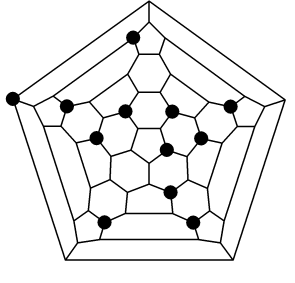
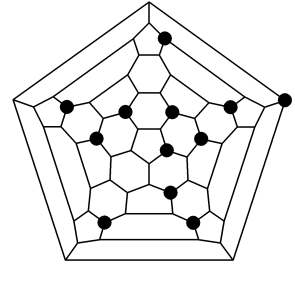
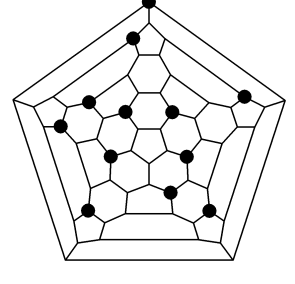
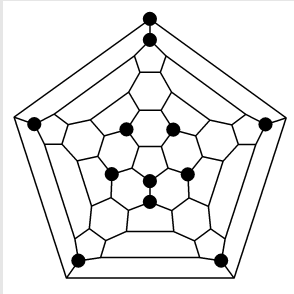
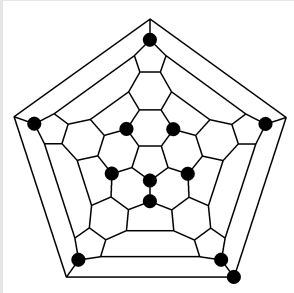
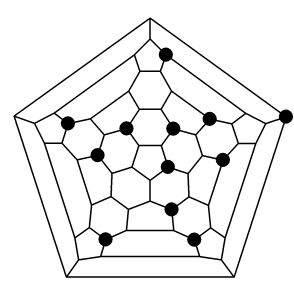
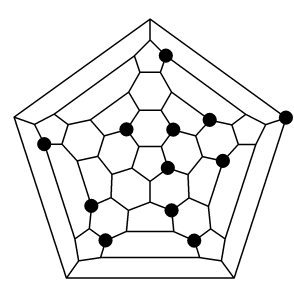
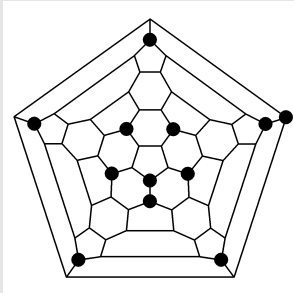
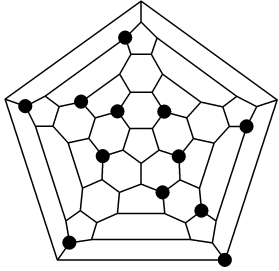
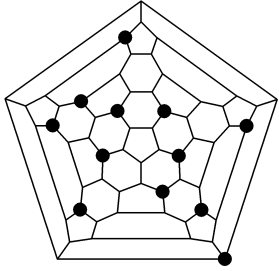
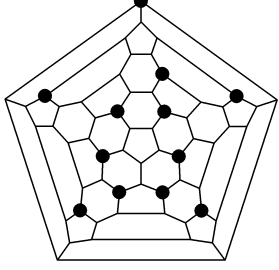
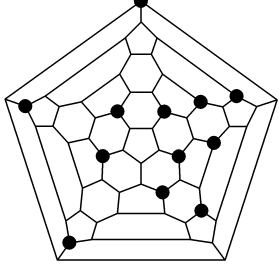
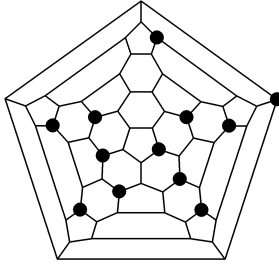


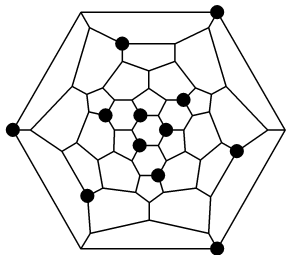
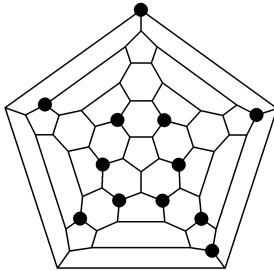
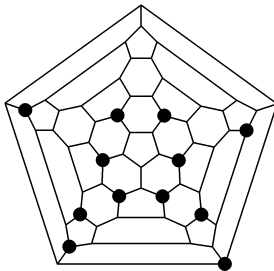
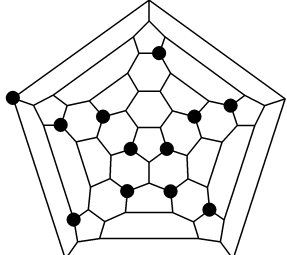
Figure 1. UV/Vis spectra of isolated S₆-C₆₀(CF₃)₁₂-I, C₆₀(CF₃)₁₂-III and C₆₀(CF₃)₁₄-I, II (hexane solution, 270-700 nm range, 2 nm resolution)

Table 1. The Schlegel diagrams, relative energies (at the DFT and AM1 levels of theory), and IUPAC lowest-locant abbreviation for the most stable isomers of $C_{60}(CF_3)_{12}$ within the gap of $50 \text{ kJ}\cdot\text{mol}^{-1}$. The fields with experimentally observed isomers are shadowed. The energies from the ref. [S1] are given in the parentheses.

N_0N_0	Schlegel Diagrams of $C_{60}(CF_3)_{12}$	$\Delta\Delta_f H_0^\circ \text{ kJ}\cdot\text{mol}^{-1}$		IUPAC lowest-locant abbreviation for dodeca(trifluoromethyl)(C_{60} - I_h)[5,6]fullerene
		DFT	AM1	
1		0.0 (0.0)	0.0 (0.0)	1, 6, 11, 16, 18, 26, 36, 44, 46, 49, 54, 60
2		22.7 (21.1)	23.2 (22.8)	1, 6, 8, 11, 16, 18, 23, 36, 46, 49, 54, 60
3		25.7 (20.0)	23.7 (23.0)	1, 6, 8, 11, 16, 18, 23, 28, 31, 36, 54, 60
4		29.0 (18.8)	24.2 (22.5)	1, 6, 8, 11, 16, 18, 23, 28, 31, 36, 41, 57
5		31.4 (32.1)	42.9 (45.7)	1, 3, 7, 10, 13, 17, 23, 28, 35, 40, 50, 60

$N_2.N_2$	<i>Schlegel Diagrams of</i> $C_{60}(CF_3)_{12}$	$\Delta \Delta_f H_0^\circ \text{ kJ}\cdot\text{mol}^{-1}$		<i>IUPAC lowest-locant abbreviation for</i> <i>dodeca(trifluoromethyl)(C₆₀-I_n)[5,6]fullerene</i>
		<i>DFT</i>	<i>AMI</i>	
6		32.5 (32.6)	49.5 (43.8)	1, 6, 9, 12, 15, 18, 43, 46, 49, 52, 55, 60
7		32.7	49.9	1, 6, 9, 12, 15, 18, 43, 46, 49, 52, 55, 57
8		32.8	45.8	1, 3, 7, 10, 13, 17, 23, 28, 35, 40, 48, 58
9		34.0	46.9	1, 3, 7, 10, 13, 17, 28, 35, 43, 48, 55, 58
10		34.1	50.9	1, 6, 9, 12, 15, 18, 43, 46, 49, 52, 55, 56

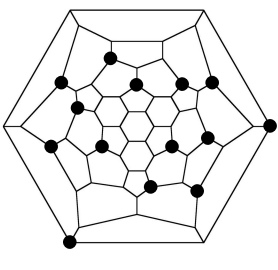
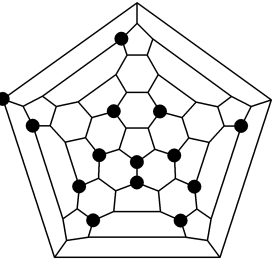
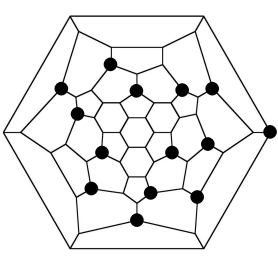
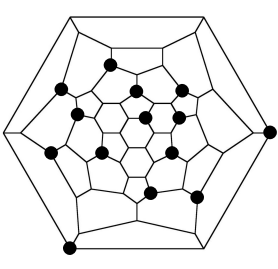
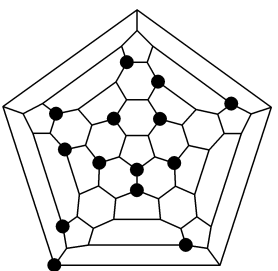
$N_2.N_2$	<i>Schlegel Diagrams of</i> $C_{60}(CF_3)_{12}$	$\Delta \Delta_f H_0^\circ \text{ kJ}\cdot\text{mol}^{-1}$		<i>IUPAC lowest-locant abbreviation for</i> <i>dodeca(trifluoromethyl)(C₆₀-I_h)[5,6]fullerene</i>
		<i>DFT</i>	<i>AMI</i>	
11		35.5 (35.5)	30.7 (33.2)	1, 3, 7, 11, 17, 24, 34, 45, 50, 52, 55, 57
12		36.1	44.3	1, 3, 7, 10, 13, 17, 28, 35, 43, 50, 55, 60
13		38.7	44.6	1, 3, 7, 10, 14, 17, 28, 31, 43, 46, 52, 55
14		39.7 (39.8)	54.8 (53.3)	1, 3, 6, 11, 13, 18, 24, 27, 33, 51, 54, 60
15		41.9 (42.0)	45.5 (39.8)	1, 6, 12, 15, 18, 23, 25, 32, 35, 41, 45, 57

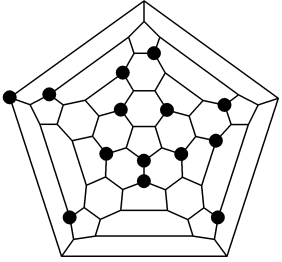
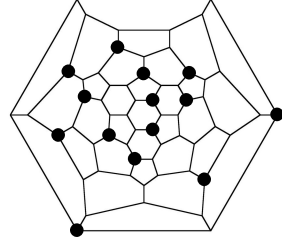
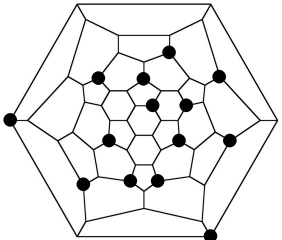
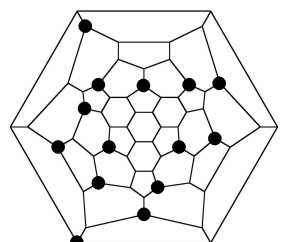
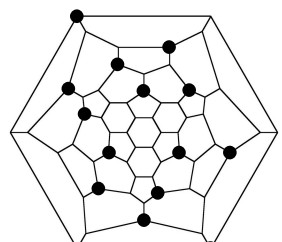
N_2, N_2	<i>Schlegel Diagrams of</i> $C_{60}(CF_3)_{12}$	$\Delta \Delta_f H_0^\circ \text{ kJ}\cdot\text{mol}^{-1}$		<i>IUPAC lowest-locant abbreviation for</i> <i>dodeca(trifluoromethyl)(C₆₀-I_h)[5,6]fullerene</i>
		<i>DFT</i>	<i>AMI</i>	
16		44.2	45.5	1, 6, 8, 11, 18, 23, 33, 46, 49, 51, 54, 60
17		45.8	50.0	1, 3, 7, 10, 14, 17, 21, 28, 31, 42, 52, 55
18		45.9	46.2	1, 3, 7, 10, 14, 17, 21, 28, 31, 36, 39, 42
19		46.7	49.8	1, 3, 7, 11, 13, 17, 23, 27, 35, 40, 50, 60

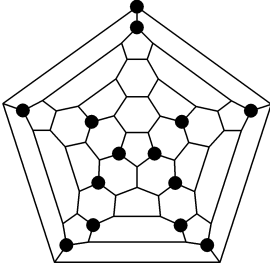
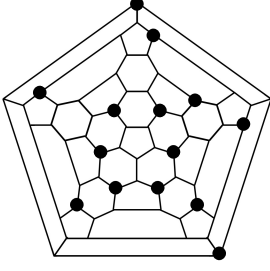
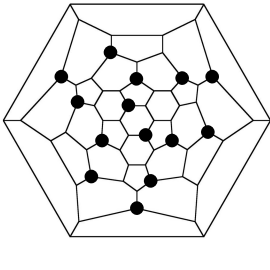
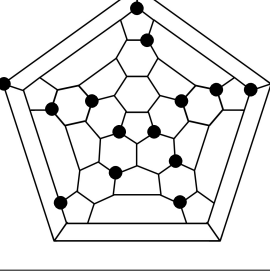
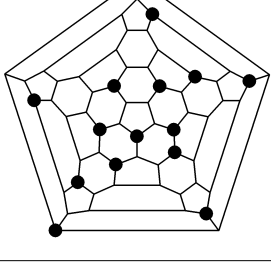
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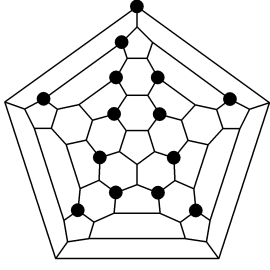
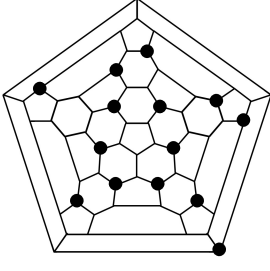
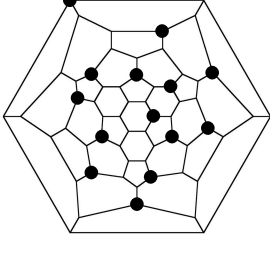
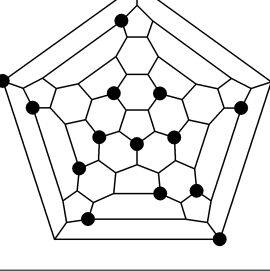
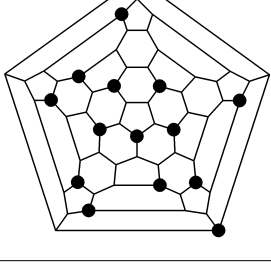
[S1] Kareev, I. E., Shustova, N. B., Peryshkov, D. V., Lebedkin, S. F., Miller, S. M., Anderson, O. P., Popov, A. A., Boltalina, O. V., Strauss, S. H., *Chem. Commun.*, 2007, 1650.

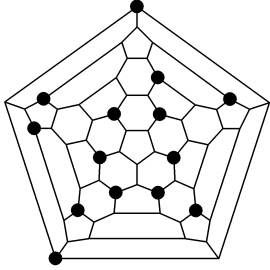
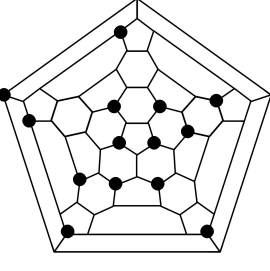
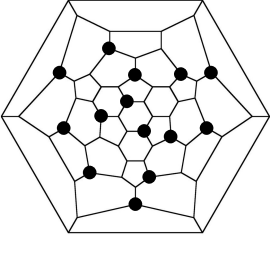
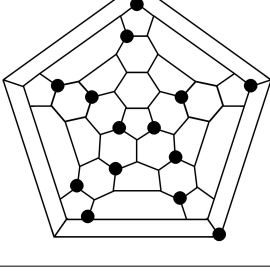
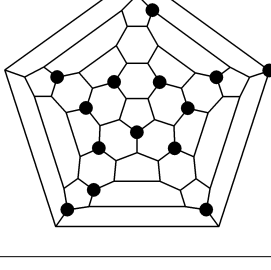
Table 2. The Schlegel diagrams, relative energies (at the DFT and AM1 levels of theory), and IUPAC lowest-locant abbreviation for the most stable isomers of $C_{60}(CF_3)_{14}$ within the gap of $25 \text{ kJ}\cdot\text{mol}^{-1}$. The fields with experimentally observed isomers are shadowed.

N_0N_0	Schlegel Diagrams of $C_{60}(CF_3)_{14}$	$\Delta \Delta_f H_0^\circ \text{ kJ}\cdot\text{mol}^{-1}$		IUPAC lowest-locant abbreviation for tetradeca(trifluoromethyl)(C_{60} - I_h)[5,6]fullerene
		DFT	AM1	
1		0.0	0.5	1, 3, 6, 11, 13, 18, 26, 33, 41, 44, 46, 49, 51, 57
2		0.4	16.6	1, 3, 7, 10, 11, 14, 17, 24, 27, 31, 36, 39, 47, 59
3		2.2	0.0	1, 3, 6, 8, 11, 13, 18, 23, 33, 41, 46, 49, 51, 57
4		4.4	3.0	1, 3, 8, 11, 13, 21, 23, 33, 38, 41, 46, 49, 51, 57
5		7.1	19.0	1, 3, 7, 8, 11, 14, 17, 24, 27, 31, 36, 39, 47, 59

N_1, N_2	<i>Schlegel Diagrams of</i> $C_{60}(CF_3)_{14}$	$\Delta \Delta_f H_0^\circ \text{ kJ}\cdot\text{mol}^{-1}$		<i>IUPAC lowest-locant abbreviation for</i> <i>tetradeca(trifluoromethyl)(C₆₀-I_b)[5,6]fullerene</i>
		<i>DFT</i>	<i>AMI</i>	
6		8.3	18.7	1, 3, 7, 8, 11, 14, 17, 24, 27, 31, 47, 52, 55, 59
7		9.0	3.9	1, 3, 8, 11, 13, 16, 21, 23, 36, 38, 41, 46, 49, 57
8		9.4	18.0	1, 3, 7, 10, 13, 28, 33, 38, 43, 48, 51, 53, 55, 58
9		10.4	18.7	1, 3, 6, 11, 13, 18, 22, 25, 33, 41, 46, 49, 51, 57
10		12.2	19.6	1, 3, 6, 11, 13, 18, 24, 27, 33, 41, 46, 49, 51, 57

N_1, N_2	<i>Schlegel Diagrams of</i> $C_{60}(CF_3)_{14}$	$\Delta \Delta_f H_0^\circ \text{ kJ}\cdot\text{mol}^{-1}$		<i>IUPAC lowest-locant abbreviation for</i> <i>tetradeca(trifluoromethyl)(C₆₀-I_n)[5,6]fullerene</i>
		<i>DFT</i>	<i>AMI</i>	
11		13.0	23.0	1, 3, 7, 10, 14, 17, 28, 31, 43, 46, 49, 52, 55, 56
12		13.7	17.8	1, 3, 7, 10, 13, 28, 33, 38, 43, 46, 49, 51, 53, 55
13		14.0	9.1	1, 3, 7, 10, 17, 23, 28, 30, 33, 38, 40, 50, 53, 60
14		16.0	22.9	1, 3, 7, 10, 13, 17, 23, 28, 35, 40, 43, 50, 55, 60
15		16.0	22.6	1, 2, 7, 10, 20, 24, 27, 29, 34, 37, 39, 48, 51, 59

N_1, N_2	<i>Schlegel Diagrams of</i> $C_{60}(CF_3)_{14}$	$\Delta \Delta_f H_0^\circ \text{ kJ}\cdot\text{mol}^{-1}$		<i>IUPAC lowest-locant abbreviation for</i> <i>tetradeca(trifluoromethyl)(C₆₀-I_b)[5,6]fullerene</i>
		<i>DFT</i>	<i>AMI</i>	
16		16.1	20.4	1, 3, 7, 8, 11, 13, 17, 24, 27, 32, 36, 39, 51, 59
17		16.4	18.7	1, 3, 7, 10, 13, 17, 28, 32, 36, 39, 43, 46, 51, 59
18		16.5	18.9	1, 3, 7, 10, 13, 23, 28, 33, 38, 40, 48, 51, 53, 58
19		16.6	18.6	1, 3, 7, 10, 13, 17, 28, 32, 34, 43, 46, 52, 55, 59
20		19.5	20.2	1, 3, 7, 10, 13, 17, 28, 33, 35, 43, 46, 49, 55, 60

$N_u.N_b$	Schlegel Diagrams of $C_{60}(CF_3)_{14}$	$\Delta \Delta_f H_o^\circ \text{ kJ}\cdot\text{mol}^{-1}$		IUPAC lowest-locant abbreviation for tetradeca(trifluoromethyl)(C_{60} - I_b)[5,6]fullerene
		DFT	AMI	
21		19.9	24.4	1, 3, 7, 10, 14, 17, 23, 28, 31, 40, 43, 49, 52, 55
22		22.0	23.5	1, 3, 6, 8, 11, 13, 18, 23, 33, 46, 49, 51, 54, 60
23		22.8	14.0	1, 3, 7, 10, 14, 17, 21, 28, 31, 36, 39, 42, 45, 57
24		23.4	23.4	1, 3, 7, 10, 13, 17, 28, 32, 36, 39, 43, 48, 55, 58
25		24.0	24.5	1, 3, 7, 10, 13, 17, 28, 32, 38, 43, 48, 53, 55, 58