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Degeneracy of Topologic Distance Descriptors for Cubic Molecular Graphs: Examples of Small Fullerenes

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ANNEXE 1.

Number of Topological Classes (No TC), Distance Sum (DS), Corresponding Topological Classes for the 18 fullerenes having more than one topological class.

The numbering of the vertices is indicated in ANNEXE 3.

No		No TC	DS	Corresponding TC	Atoms with the same DS value
2	C ₂₄ (D _{6d})	2	66	1	1-6, 19-24
			68	2	7-18
3	C ₂₆ (D _{3h})	4	75	3, 4	5-20, 22, 23
			78	1, 2	1-4, 21, 24-26
4	C ₂₈ (T _d)	3	85	1, 2	1-6, 8, 10, 12-26, 28
			87	3	7, 9, 11, 27
5	C ₃₀ (D _{5h})	3	93	3	11-20
			95	2	6-10, 21-25
			99	1	1-5, 26-30
6	C ₃₂ (D ₃)	6	102	5	11, 13, 15, 18, 20, 22
			104	6	12, 14, 16, 17, 19, 21
			106	3, 4	5-10, 23-26, 28, 29
			107	2	2-4, 27, 30, 32
			112	1	1, 31
7	C ₃₄ (C _{3v})	8	108	1	1
			112	2	2-4
			113	8	29-34
			116	6	17, 20, 21, 24, 25, 28
			117	3	5, 6, 8, 9, 11, 12
			118	4, 7	7, 10, 13, 18, 19, 22, 23, 26, 27
			120	5	14-16
8	C ₃₆ (D _{6h})	3	126	2	5, 6, 10, 18-23, 26-28
			128	1, 3	1-4, 7-9, 11-17, 24, 25, 29-36
9	C ₃₈ (D _{3h})	5	129	5	12-15, 21, 22
			133	4	6, 7, 9, 11, 19, 20, 29-34
			143	3	3, 4, 8, 10, 17, 18, 26-28, 35-37
			152	1, 2	1, 2, 5, 16, 23-25, 38
10	C ₃₈ (C _{3v})	10	133	10	34
			135	9	32, 33, 35
			137	2, 3	2-10
			138	4	11-16
			139	1, 7, 8	1, 26-31, 36-38
			141	5, 6	17-25
11	C ₄₀ (T _d)	3	150	1, 2, 3	1-40
12	C ₄₀ (C _{3v})	10	143	6	18-20
			145	5, 9	16, 17, 30-36
			147	7	21, 23, 29
			149	8	22, 24, 28
			152	2, 4	6-8, 13-15, 25-27, 37-39

			154	1	1-5, 9
			155	6	18-20
			165	10	40
13	$C_{40}(D_{5d})$	3	144	1	1-5, 31, 32, 38-40
			148	2	6, 9, 12, 15, 18, 33-37
			153	3	7, 8, 10, 11, 13, 14, 16, 17, 19-30
14	$C_{42}(D_3)$	7	159	1, 3	1, 3, 5, 7, 9, 11, 13-15, 40-42
			160	2	2, 6, 10, 17, 19, 38
			161	7	22-24, 32, 33, 36
			163	4, 6	4, 8, 12, 16, 18, 21, 25, 29, 30, 34, 37, 39
			165	5	20, 26-28, 31, 35
15	$C_{44}(T)$	5	173	3, 5	3, 9, 15, 21-26, 29-33, 43, 44
			174	2, 4	2, 4-7, 10-13, 16-18, 20, 27, 28, 34-42
			179	1	1, 8, 14, 19
16	$C_{44}(D_{3h})$	6	171	5	17-19, 29, 37, 44
			172	4	11-16, 28, 30, 32, 36, 39, 43
			173	6	20-25
			174	3	5-10, 27, 31, 33, 35, 40, 42
			177	2	2-4, 26, 34, 41
			179	1	1, 38
17	$C_{46}(C_3)$	16	180	16	42
			182	9	23, 28, 31
			184	1, 5, 8, 13, 14	1, 3, 6, 12, 13, 17, 22, 29, 30, 36, 39-41, 43, 44
			186	2, 10	2, 9, 11, 24, 27, 32
			187	4	5, 14, 18
			188	3, 7, 12, 15	4, 8, 10, 16, 19, 21, 34, 35, 37, 38, 45, 46
			189	6	7, 15, 20
			192	11	25, 26, 33
18	$C_{48}(D_3)$	8	193	5	13, 17, 30, 43, 45, 48
			196	6	14, 18, 22, 26, 32, 34
			197	4	9-11, 33, 35, 47
			198	2	2, 4, 5, 39-41
			199	1	1, 3, 6, 36-38
			201	3, 7	7, 8, 12, 15, 19, 21, 23-25, 42, 44, 46
			203	8	16, 20, 27-29, 31
19	$C_{50}(D_{5h})$	4	210	1, 2	1-10, 21-23, 44-50
			211	3	11-20, 24, 25, 28-30, 35, 38, 41-43
			213	4	26, 27, 31-34, 36, 37, 39, 40

ANNEXE 2.

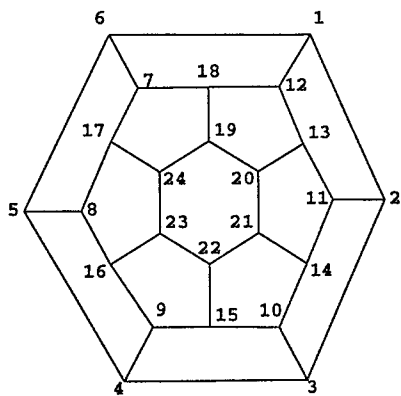
Number of Topological Classes (No TC), Distance Degree Sum (DDS), Corresponding Topological Classes for the 18 fullerenes having more than one topological class. The numbering of the vertices is indicated in Figure in ANNEXE 3.

No		No TC	DDS	Corresponding TC	Atoms with the same DDS value
2	C ₂₄ (D _{6d})	2	1 3 6 6 5 3	2	7-18
			1 3 6 7 5 2	1	1-6, 19-24
3	C ₂₆ (D _{3h})	4	1 3 6 6 5 5	2	2-4, 21, 24, 26
			1 3 6 6 6 3 1	1	1, 25
			1 3 6 7 6 3	3, 4	5-20, 22, 23
4	C ₂₈ (T _d)	3	1 3 6 6 6 6	3	7, 9, 11, 27
			1 3 6 7 6 5	2	2, 4, 6, 8, 10, 12, 19-22, 24, 25
			1 3 6 7 7 3 1	1	1, 3, 5, 13-18, 23, 26, 28
5	C ₃₀ (D _{5h})	3	1 3 6 6 6 6 2	1	1-5, 26-30
			1 3 6 7 7 5 1	2	6-10, 21-25
			1 3 6 8 7 4 1	3	11-20
6	C ₃₂ (D ₃)	6	1 3 6 6 6 6 3 1	1	1, 31
			1 3 6 7 7 5 3	2	2-4, 27, 30, 32
			1 3 6 7 7 6 2	3, 4	5-10, 23-26, 28, 29
			1 3 6 7 8 6 1	6	12, 14, 16, 17, 19, 21
			1 3 6 8 8 5 1	5	11, 13, 15, 18, 20, 22
7	C ₃₄ (C _{3v})	8	1 3 6 6 7 7 4	5	14-16
			1 3 6 7 7 6 4	4, 7	7, 10, 13, 18, 19, 22, 23, 26, 27
			1 3 6 7 7 7 3	3	5, 6, 8, 9, 11, 12
			1 3 6 8 8 6 2	8	29-34
			1 3 6 7 8 6 3	6	17, 20, 21, 24, 25, 28
			1 3 6 8 9 5 2	2	2-4
8	C ₃₆ (D _{6h})	3	1 3 6 7 8 7 3 1	1, 3	1-4, 7-9, 11-17, 24, 25, 29-36
			1 3 6 8 8 6 3 1	2	5, 6, 10, 18-23, 26-28
9	C ₃₈ (D _{3h})	5	1 3 6 6 6 6 5 5	2	2, 5, 16, 23-25
			1 3 6 6 6 6 6 3 1	1	1, 38
			1 3 6 7 7 7 5 2	3	3, 4, 8, 10, 17, 18, 26-28, 35-37
			1 3 6 8 9 8 3	4	6, 7, 9, 11, 19, 20, 29-34
			1 3 6 9 10 7 2	5	12-15, 21, 22
10	C ₃₈ (C _{3v})	10	1 3 6 6 9 9 3 1	1	1
			1 3 6 7 8 7 4 2	5, 6	17-25
			1 3 6 7 8 7 6	8	27, 30, 37
			1 3 6 7 8 8 4 1	7	26, 28, 29, 31, 36, 38
			1 3 6 7 9 8 3 1	2	2-4
			1 3 6 8 8 6 5 1	4	11-16
			1 3 6 8 8 7 4 1	3	5-10
			1 3 6 8 9 7 3 1	9	32, 33, 35
1 3 6 9 9 6 3 1	10	34			
11	C ₄₀ (T _d)	3	1 3 6 6 9 9 6	2	7, 10, 13, 40
			1 3 6 7 9 8 4 2	3	8, 9, 11, 12, 14-21
			1 3 6 8 8 7 5 2	1	1-6, 22-39

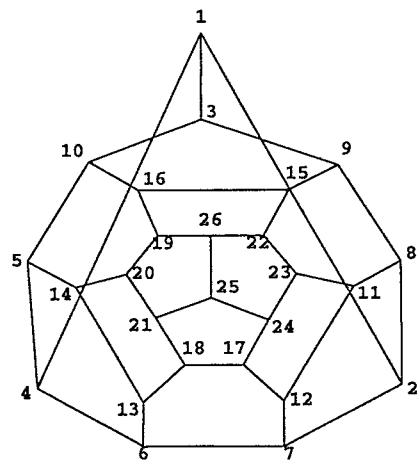
12	$C_{40} (C_{3v})$	10	1 3 6 6 6 6 6 6	10	40
			1 3 6 7 7 7 7 2	3	10-12
			1 3 6 7 8 7 5 3	1	1-5, 9
			1 3 6 7 8 8 5 2	2, 4	6-8, 13-15, 25-27, 37-39
			1 3 6 8 8 7 6 1	8	22, 24, 28
			1 3 6 8 9 7 5 1	7	21, 23, 29
			1 3 6 8 9 9 3 1	9	30-32
			1 3 6 8 10 7 4 1	5	16, 17, 33-36
			1 3 6 9 9 8 3 1	6	18-20
13	$C_{40} (D_{5d})$	3	1 3 6 7 8 7 6 2	3	7, 8, 10, 11, 13, 14, 16, 17, 19-30
			1 3 6 8 8 8 5 1	2	6, 9, 12, 15, 18, 33-37
			1 3 6 8 10 8 3 1	1	1-5, 31, 32, 38-40
14	$C_{42} (D_3)$	7	1 3 6 7 8 8 6 3	5	20, 26-28, 31, 35
			1 3 6 7 9 8 5 3	4, 6	4, 8, 12, 16, 18, 21, 25, 29, 30, 34, 37, 39
			1 3 6 8 8 8 6 2	7	22-24, 32, 33, 36
			1 3 6 8 9 7 6 2	2	2, 6, 10, 17, 19, 38
			1 3 6 8 9 8 5 2	1, 3	1, 3, 5, 7, 9, 11, 13-15, 40-42
15	$C_{44} (T)$	5	1 3 6 6 9 9 6 3 1	1	1, 8, 14, 19
			1 3 6 7 9 9 6 3	2	2, 4, 7, 10, 13, 18, 20, 27, 28, 35, 40, 42
			1 3 6 8 8 8 7 3	4	5, 6, 11, 12, 16, 17, 34, 36-39, 41
			1 3 6 8 9 8 5 4	3	3, 9, 15, 21, 23, 24, 26, 29, 31-33, 43
			1 3 6 9 9 6 6 3 1	5	22, 25, 30, 44
16	$C_{44} (D_{3h})$	6	1 3 6 6 9 9 6 3 1	1	1, 38
			1 3 6 7 9 8 5 5	2	2-4 26, 34, 41
			1 3 6 7 10 9 6 2	5	17-19, 29, 37, 44
			1 3 6 8 8 8 7 3	3	5-10, 27, 31, 33, 35, 40, 42
			1 3 6 8 9 8 5 4	6	20-25
			1 3 6 8 9 8 6 3	4	11-16, 28, 30, 32, 36, 39, 43
17	$C_{46} (C_3)$	16	1 3 6 7 8 8 7 6	11	25, 26, 33
			1 3 6 7 8 9 8 4	6	7, 15, 20
			1 3 6 7 9 9 6 5	3, 12	4, 10, 19, 34, 37, 46
			1 3 6 7 9 9 7 3 1	7	8, 16, 21
			1 3 6 7 9 9 7 4	4	5, 14, 18
			1 3 6 8 8 8 8 3 1	15	35, 38, 45
			1 3 6 8 9 8 7 3 1	2, 10	2, 9, 11, 24, 27, 32
			1 3 6 8 9 9 6 4	1, 13	1, 3, 12, 36, 39, 44
			1 3 6 8 10 8 5 5	8	22, 29, 30
			1 3 6 8 10 8 6 3 1	5, 14	8, 16, 21, 40, 41, 43
			1 3 6 9 9 8 6 4	9	23, 28, 31
1 3 6 9 9 9 6 3	16	42			
18	$C_{48} (D_3)$	8	1 3 6 7 8 9 8 6	8	16, 20, 27-29, 31
			1 3 6 7 9 9 7 6	3	7, 8, 12, 23, 42, 44
			1 3 6 7 9 9 8 4 1	7	15, 19, 21, 24, 25, 46
			1 3 6 8 9 8 8 4 1	1	1, 3, 6, 36-38
			1 3 6 8 9 9 7 4 1	2	2, 4, 5, 39-41
			1 3 6 8 9 9 8 3 1	4	9-11, 33, 35, 47
			1 3 6 8 10 9 6 4 1	6	14, 18, 22, 26, 32, 34
			1 3 6 9 10 8 6 5	5	13, 17, 30, 43, 45, 48
19	$C_{50} (D_{5h})$	4	1 3 6 8 9 9 8 5 1	3	11-20, 24, 25, 28-30, 35, 38, 41-43
			1 3 6 8 9 9 8 6	2	6-10, 21-23, 44, 45
			1 3 6 8 10 9 7 4 2	1	1-5, 46-50
			1 3 6 7 10 9 7 6 1	4	26, 27, 31-34, 36, 37, 39, 40

ANNEXE 3.

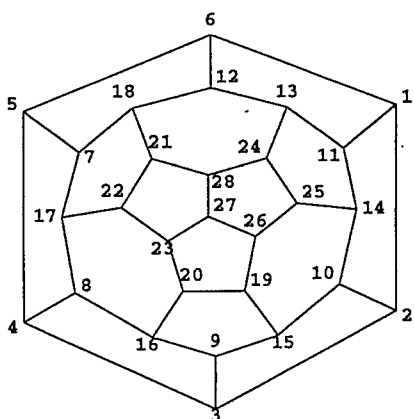
Atom numbering of C_{24} to C_{50} fullerenes having more than one topological classes



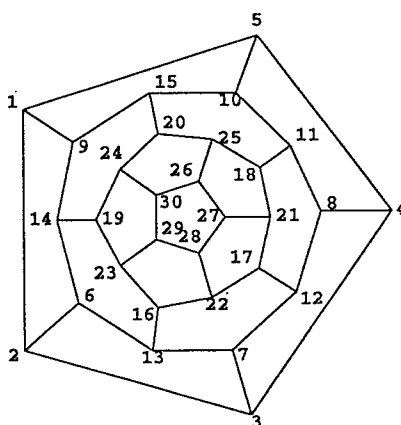
2 C_{24} (D_{6d})



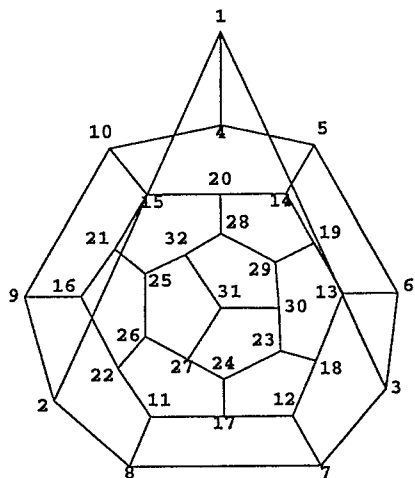
3 C_{26} (D_{3h})



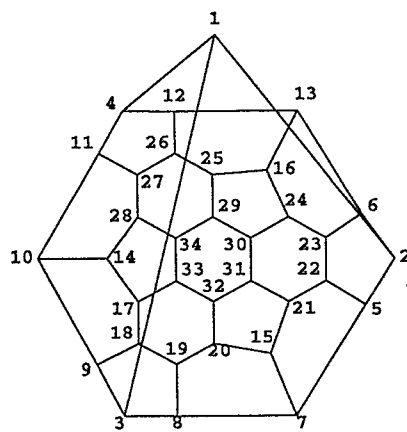
4 C_{28} (T_d)



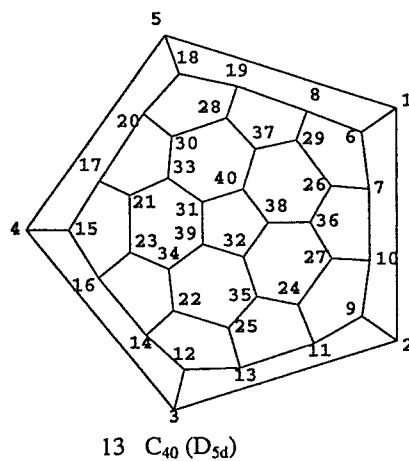
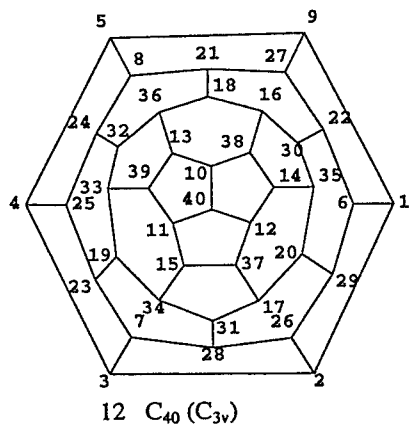
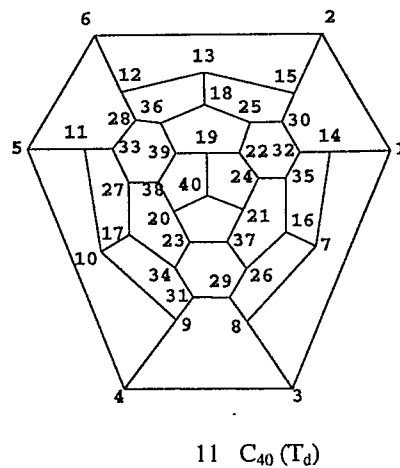
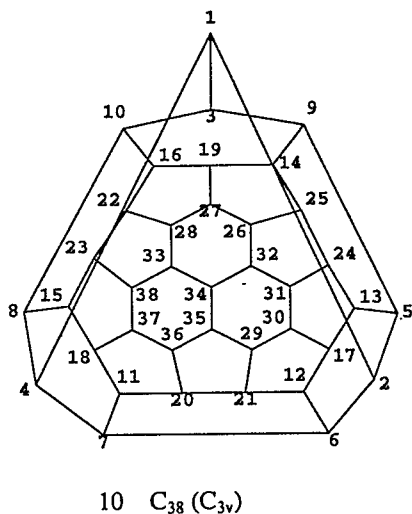
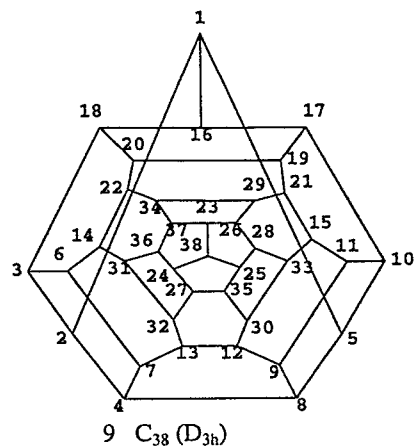
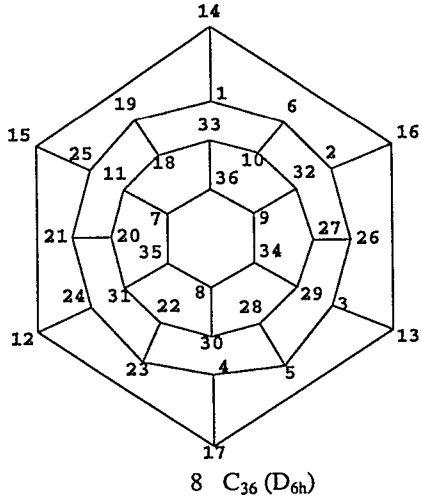
5 C_{30} (D_{5h})

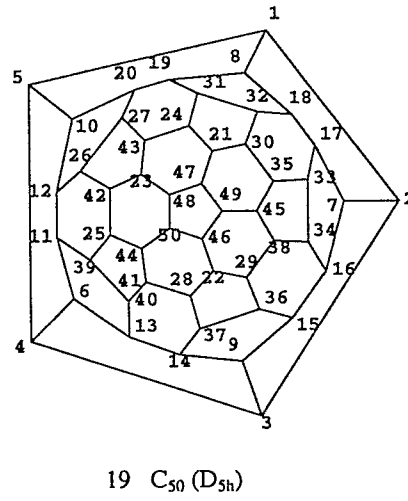
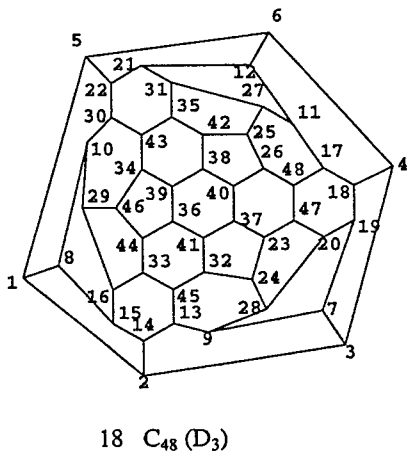
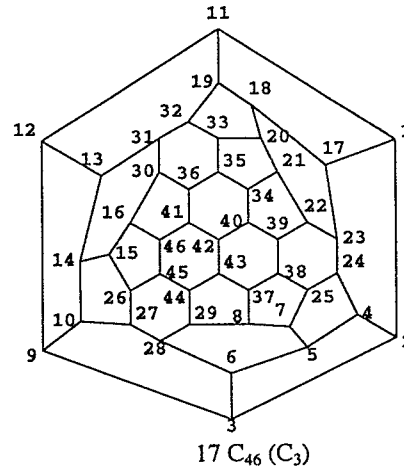
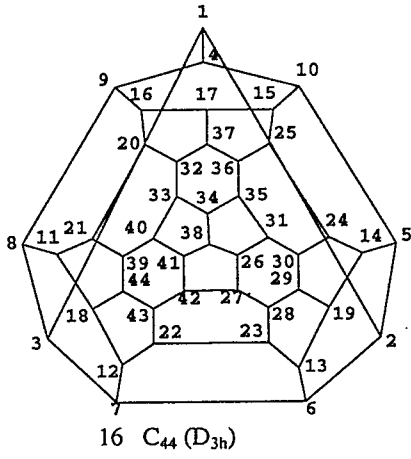
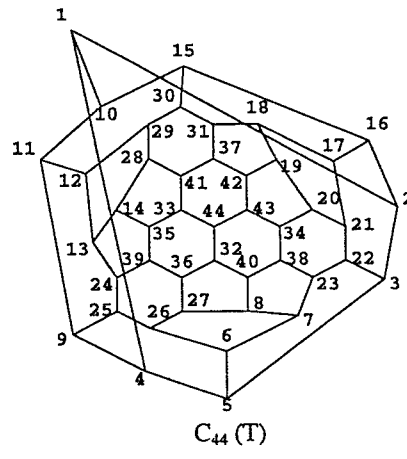
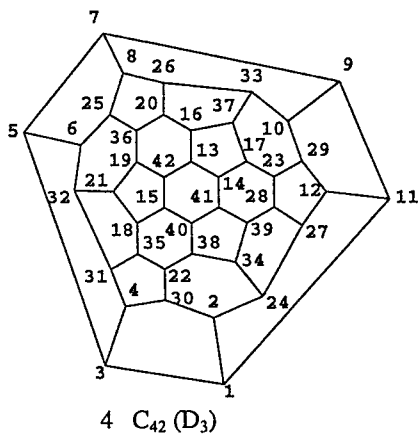


6 C_{32} (D_3)

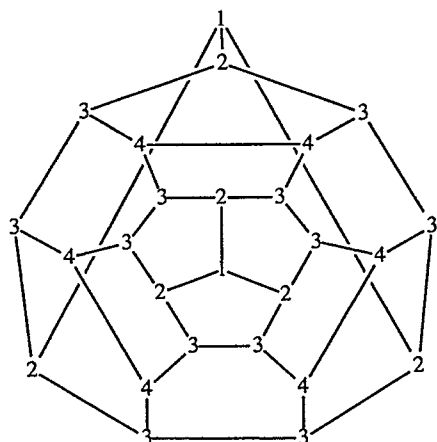


7 C_{34} (C_{3v})

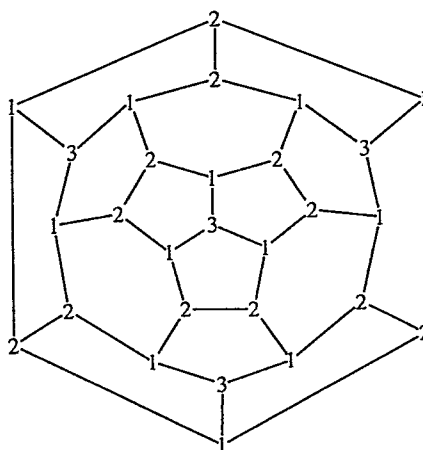




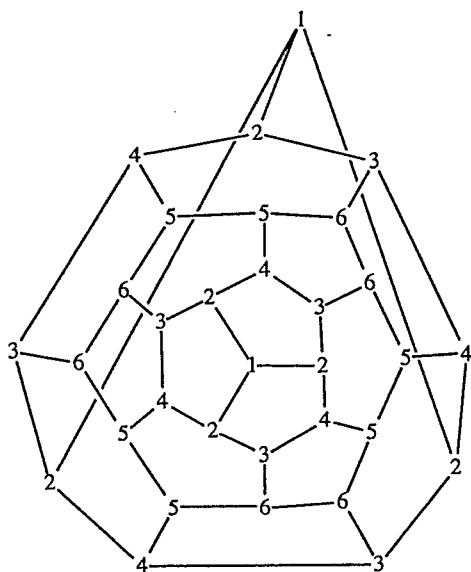
ANNEXE 4. The topological classes of equivalence of atoms in the fullerenes which present DS and/or DDS degenerated values. The degenerated DS and/or DDS values are presented in Tables 1 and 2 of the paper.



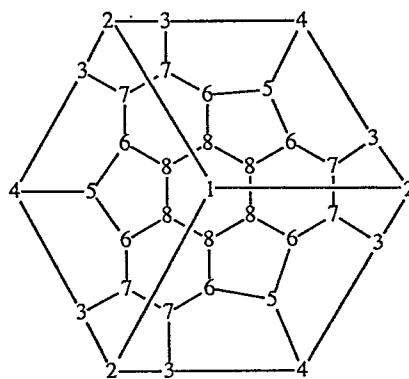
3 $C_{26} (D_{3h})$



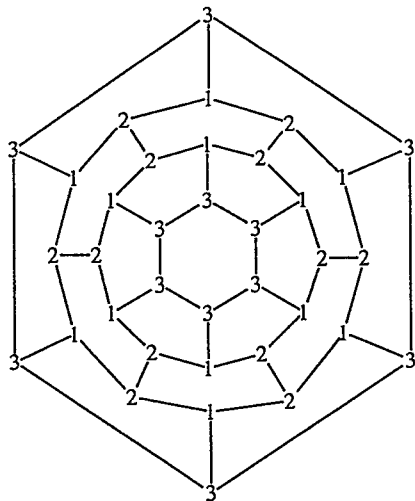
4 $C_{28} (T_d)$



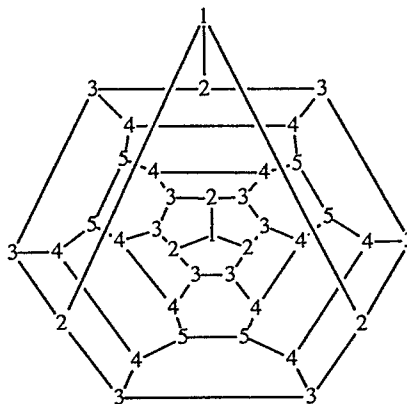
6 $C_{32} (D_3)$



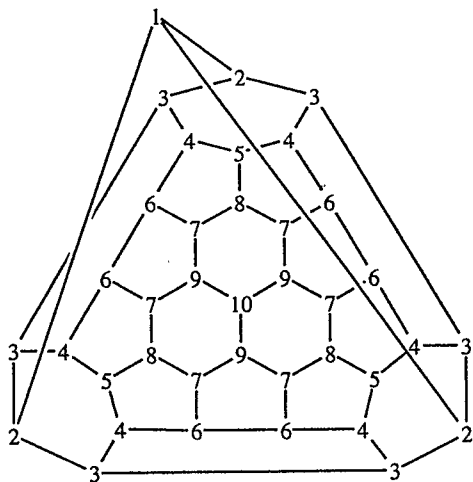
7 $C_{34} (C_{3v})$



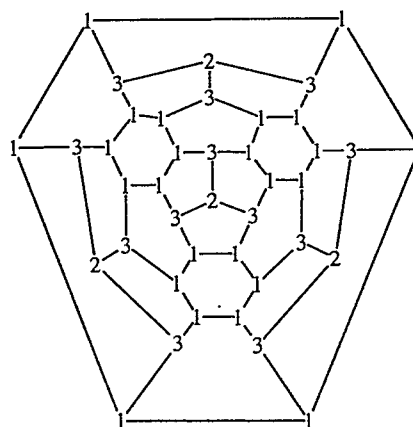
8 $C_{36} (D_{6h})$



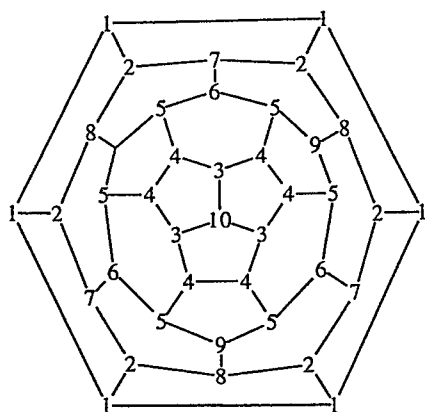
9 $C_{38} (D_{3h})$



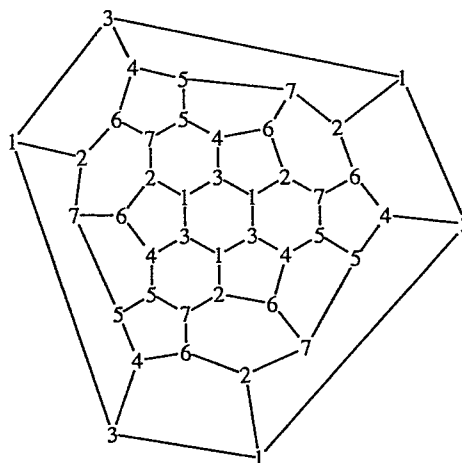
10 $C_{38} (C_{3v})$



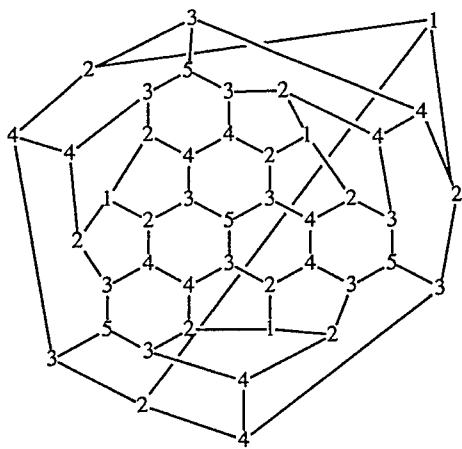
11 $C_{40} (T_d)$



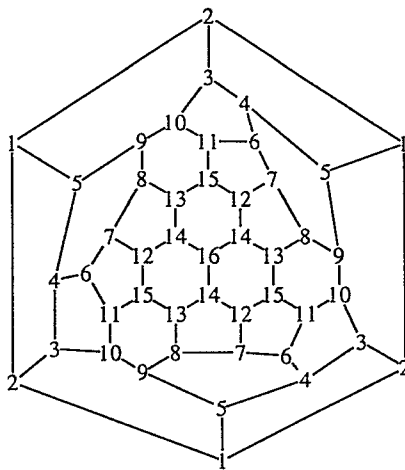
12 $C_{40} (C_{3v})$



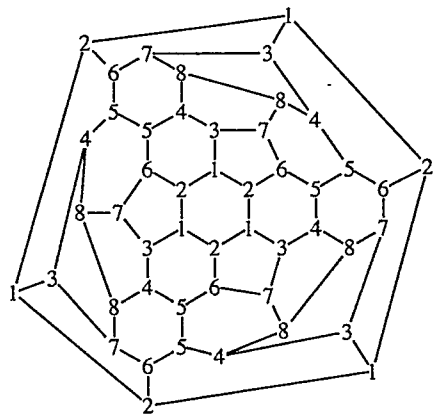
14 $C_{42} (D_3)$



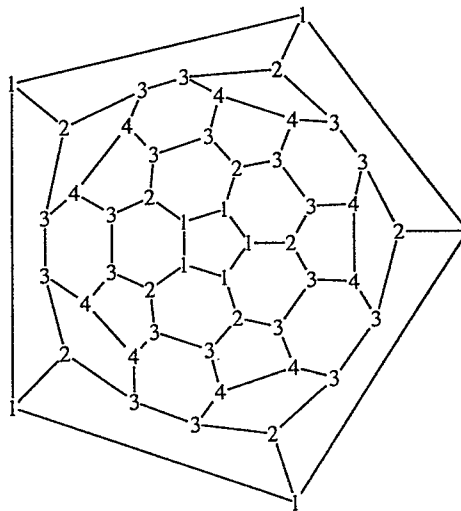
15 $C_{44}(T)$



17 $C_{46}(C_3)$



18 $C_{48}(D_3)$



19 $C_{50}(D_{5h})$