## Role of Four-membered Rings in C<sub>32</sub> Fullerene Stability and Mechanisms of Generalized Stone-Wales Transformation: A Density Functional Theory Investigation

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## **Electronic Supplementary Information**

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Table S1 Heat of formation of 364 C <sub>32</sub> fullerenes obtained at AM1 level	. [c	<i>a</i> ]
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	1-1-1[b]	$\begin{array}{c} \text{Ring Index}^{[c]}\\ \text{sym}\\ (n_4, n_5, n_6) \end{array}$	DA [d]	AII		85:C <sub>1</sub>	(3, 6, 9)	5	109.9	0.3193
	label <sup>es</sup> .sym		$PA \stackrel{(n)}{=} 2$	$\Delta m_f$	P	$7:C_{I}$	(1, 10, 7)	11	110	0.0419
_	32:D <sub>4d</sub>	(2, 8, 8)	8	0	0.6458	$55:C_s$	(2, 8, 8)	6	110.1	0.1951
	1: <i>D</i> <sub>3</sub>	(0, 12, 6)	15	19.4	0.3639	93: <i>C</i> <sub>2</sub>	(4, 4, 10)	1	110.3	0.2484
	$5:C_s$	(1, 10, 7)	12	21.8	0.3792	$70:C_{I}$	(3, 6, 9)	4	111.2	0.1665
	33: <i>C</i> <sub>s</sub>	(1, 10, 7)	11	39.5	0.3879	64: <i>C</i> <sub>1</sub>	(3, 6, 9)	4	111.5	0.0954
	$6:C_2$	(0, 12, 6)	16	46.5	0.2527	$22:C_{I}$	(2, 8, 8)	10	111.7	0.1759
	59: <i>C</i> <sub>s</sub>	(3, 6, 9)	4	46.8	0.6165	$11:C_{I}$	(2, 8, 8)	7	112.6	0.0518
	9: <i>C</i> <sub>2</sub>	(2, 8, 8)	9	53.5	0.2524	30:D <sub>2</sub>	(0, 12, 6)	18	113.6	0.0000
	$12:C_{s}$	(2, 8, 8)	8	54.6	0.4374	$66:C_1$	(3, 6, 9)	5	114.1	0.2965
	$2:C_{I}$	(1, 10, 7)	11	60.6	0.2313	52: <i>C</i> <sub>1</sub>	(2, 8, 8)	6	115.1	0.1272
	15: <i>C</i> <sub>1</sub>	(2, 8, 8)	6	62.9	0.4900	71: <i>C</i> <sub>1</sub>	(3, 6, 9)	3	115.4	0.2610
	$18:C_2$	(2, 8, 8)	6	63.9	0.4305	43: <i>C</i> <sub>1</sub>	(2, 8, 8)	6	115.5	0.0169
	41: <i>C</i> <sub>s</sub>	(2, 8, 8)	7	72.3	0.2055	177: <i>C</i> <sub>1</sub>	(2, 8, 8)	8	116.1	0.5059
	17: <i>C</i> <sub>1</sub>	(2, 8, 8)	7	73.3	0.5031	$98:C_1$	(2, 8, 8)	8	116.3	0.0713
	$105:C_{2v}$	(1, 10, 7)	10	73.8	0.1981	67: <i>C</i> <sub>1</sub>	(3, 6, 9)	4	116.4	0.0705
	34: <i>C</i> <sub>1</sub>	(1, 10, 7)	12	74.2	0.2485	35: <i>C</i> <sub>1</sub>	(1, 10, 7)	13	117.5	0.0526
	$27:C_2$	(2, 8, 8)	7	78.0	0.4373	54: <i>C</i> <sub>1</sub>	(2, 8, 8)	7	117.8	0.2228
	58:C1	(3, 6, 9)	5	79.1	0.3916	$88:C_{I}$	(3, 6, 9)	3	118.6	0.3082
	36: <i>C</i> <sub>s</sub>	(1, 10, 7)	12	79.5	0.1811	91: <i>C</i> <sub>2</sub>	(2, 8, 8)	4	120.7	0.1514
	$16:C_{I}$	(2, 8, 8)	7	81.6	0.3656	77: <i>C</i> <sub>1</sub>	(3, 6, 9)	7	120.8	0.1618
	$20:C_{I}$	(2, 8, 8)	8	82.0	0.3390	72: <i>C</i> <sub>1</sub>	(3, 6, 9)	3	120.8	0.2224
	23: <i>C</i> <sub>1</sub>	(2, 8, 8)	9	82.5	0.1824	$68:C_{I}$	(2, 8, 8)	8	121.5	0.0519
	37: <i>C</i> <sub>1</sub>	(1, 10, 7)	12	82.7	0.2937	$8:C_I$	(1, 10, 7)	12	123.2	0.1131
	3: <i>C</i> <sub>1</sub>	(1, 10, 7)	11	83.3	0.1989	76: <i>C</i> <sub>1</sub>	(3, 6, 9)	7	123.4	0.058
	31: <i>C</i> <sub>2v</sub>	(1, 10, 7)	14	84.5	0.0147	95: <i>C</i> <sub>1</sub>	(1, 10, 7)	11	123.8	0.2301
	29: <i>C</i> <sub>1</sub>	(2, 8, 8)	9	85.9	0.0417	130: <i>C</i> <sub>2</sub>	(2, 8, 8)	5	125.2	0.1609
	$4:C_2$	(0, 12, 6)	17	86.8	0.0117	116: <i>D</i> <sub>2</sub>	(2, 8, 8)	9	125.8	0.0443
	$13:C_{s}$	(1, 10, 7)	12	87.2	0.0183	62: <i>C</i> <sub>1</sub>	(3, 6, 9)	5	126.1	0.2354
	25:C <sub>1</sub>	(2, 8, 8)	9	88.2	0.1457	74: <i>C</i> <sub>1</sub>	(3, 6, 9)	2	126.3	0.3222
	96:C <sub>2v</sub>	(2, 8, 8)	11	89.2	0.3579	46: <i>C</i> <sub>1</sub>	(3, 6, 9)	3	126.5	0.1585
	89: <i>C</i> <sub>1</sub>	(3, 6, 9)	6	90.9	0.4566	$10:C_2$	(2, 8, 8)	8	127.3	0.1529
	99: <i>C</i> <sub>1</sub>	(2, 8, 8)	7	94.3	0.3806	87: <i>C</i> 1	(4, 4, 10)	3	128.3	0.2483
	$26:C_{I}$	(1, 10, 7)	12	94.4	0.0445	136: <i>C</i> <sub>1</sub>	(3, 6, 9)	4	128.6	0.3174
	94:D <sub>2h</sub>	(0, 12, 6)	18	96.6	0.0000	61:D <sub>2</sub>	(2, 8, 8)	8	128.7	0.0518
	57: <i>C</i> <sub>1</sub>	(3, 6, 9)	6	98.5	0.1450	19: <i>C</i> <sub>1</sub>	(2, 8, 8)	8	128.7	0.0504
	126: <i>C</i> <sub>2v</sub>	(4, 4, 10)	0	100.1	0.3531	44: <i>C</i> <sub>1</sub>	(2, 8, 8)	5	129.2	0.2759
	179: <i>C</i> <sub>2</sub>	(4, 4, 10)	5	100.2	0.4299	49: <i>C</i> <sub>1</sub>	(1, 10, 7)	12	129.4	0.0334
	$100:C_{1}$	(2, 8, 8)	7	100.2	0.3356	90: <i>C</i> <sub>1</sub>	(2, 8, 8)	9	130.0	0.178
	107:D <sub>3h</sub>	(0, 12, 6)	18	101.1	0.3943	146: <i>C</i> <sub>1</sub>	(3, 6, 9)	3	131.0	0.1392
	14: <i>C</i> <sub>2</sub>	(2, 8, 8)	7	102.1	0.1379	$40:C_{I}$	(2, 8, 8)	6	131.1	0.0923
	65: <i>C</i> <sub>3</sub>	(3, 6, 9)	3	104.3	0.6603	$60:C_{I}$	(3, 6, 9)	4	131.3	0.1936
	78: <i>C</i> <sub>s</sub>	(3, 6, 9)	6	107.9	0.0930	215:C <sub>s</sub>	(3, 6, 9)	2	135.5	0.2419

$\begin{array}{c c c c c c c c c c c c c c c c c c c $										
144.C,         (3, 6, 9)         4         136.S         0.2136         113.C,         (3, 6, 9)         5         154.7         0.3385           21.C,         (3, 6, 9)         4         135.5         0.0847         183.C,         (2, 8, 5)         8         156.9         0.1936           56.C,         (3, 6, 9)         3         137.9         0.1536         158.C,         (4, 4, 10)         1         157.8         0.3061           100.C,         (3, 6, 9)         4         138.7         0.3507         239.C,         (2, 8, 8)         8         157.7         0.2788           232.C,         (4, 4, 10)         1         138.8         0.2229         144.C,         (3, 6, 9)         4         18.8         0.331           84.C,         (2, 8, 8)         0         135.9         0.2316         112.C,         (2, 8, 8)         0.160         0.333           171.D,         (4, 4, 10)         2         140.4         0.2311         120.C,         (2, 8, 8)         5         160.9         0.160           183.C,         (2, 8, 8)         6         140.9         0.2313         161.6         0.1612           192.C,         (2, 8, 8)         7         140         0	$102:C_1$	(2, 8, 8)	7	135.8	0.1442	159: <i>C</i> <sub>1</sub>	(4, 4, 10)	1	154.3	0.2142
S1:C,       (3, 6, 9)       4       1365       0241       241.C,       (3, 6, 9)       5       137.0       01847         21:C,       (2, 8, 8)       10       137.6       0078       97.C,       (2, 8, 8)       8       156.9       0195         47.C,       (3, 6, 9)       3       137.9       01536       138.C,       (4, 4, 10)       1       157.0       0278         223.C,       (4, 4, 10)       1       138.8       0249       184.C,       (3, 6, 9)       4       158.4       02331         84.C,       (4, 4, 10)       2       138.8       02326       112.C,       (2, 8, 8)       6       158.9       0616         169.C,       (2, 8, 8)       9       139.9       00319       174.C,       (3, 6, 9)       3       1606.0       1608.0       1608.0       1608.0       1608.0       1608.0       1608.0       1608.0       1608.0       1608.0       161.4       00921       133.4       160.9       3       160.9       160.0       160.1       161.4       00921       133.5.7       141.0       01835       151.0       161.0       161.4       01071       141.0       183.6       142.2       12.8.8       161.1       01017	144: <i>C</i> 1	(3, 6, 9)	4	136.5	0.2136	113: <i>C</i> <sub>1</sub>	(3, 6, 9)	5	154.5	0.2458
21.C,       (2, 8, 8)       10       137.6       0.0847       183.C,       (2, 8, 8)       8       156.9       0.1995         56.C,       (1, 6, 9)       5       137.6       0.0778       97.C,       (2, 8, 8)       9       157.4       0.0878         47.C,       (3, 6, 9)       4       138.7       0.3507       239.C,       (2, 8, 8)       8       158.7       0.2788         232.C,       (4, 4, 10)       1       138.8       0.3256       112.C,       (2, 8, 8)       8       158.7       0.659         81.C,       (2, 8, 8)       9       139       0.0319       174.C,       (3, 6, 9)       3       1666       0.169         1690,C       (2, 8, 8)       6       140.9       0.2811       120.C,       (2, 8, 8)       6       161.0       0.169         1632,C,       (2, 8, 8)       6       140.7       0.0373       161.C,       (3, 6, 9)       3       161.7       0.161.0       0.161         92.C,       (2, 8, 8)       5       141.5       0.1563       150.C,       (3, 6, 9)       3       161.7       0.131         92.C,       (2, 8, 8)       5       141.5       0.1563       150.C,       (3, 6, 9) </td <td>51:<i>C</i><sub>1</sub></td> <td>(3, 6, 9)</td> <td>4</td> <td>136.5</td> <td>0.2481</td> <td>241:<i>C</i><sub>1</sub></td> <td>(3, 6, 9)</td> <td>5</td> <td>154.7</td> <td>0.3385</td>	51: <i>C</i> <sub>1</sub>	(3, 6, 9)	4	136.5	0.2481	241: <i>C</i> <sub>1</sub>	(3, 6, 9)	5	154.7	0.3385
56.C,       (3, 6, 9)       5       137.6       0.0778       97.C,       (2, 8, 8)       9       157.4       0.0878         47.C,       (3, 6, 9)       3       137.9       0.1536       158.C,       (4, 4, 10)       1       157.5       0.0068         160.C,       (3, 6, 9)       4       138.8       0.2326       1184.C,       (3, 6, 9)       4       158.4       0.8331         232.C,       (4, 4, 10)       1       138.8       0.2326       112.C,       (2, 8, 8)       8       159.7       0.1699         169.C,       (2, 8, 8)       9       139       0.0519       174.C,       (3, 6, 9)       3       160.9       0.2353         171.D,       (4, 4, 10)       2       140.4       0.2811       120.C,       (2, 8, 8)       5       160.9       0.196         83.C,       (3, 6, 9)       5       140.5       0.178       154.C,       (3, 6, 9)       3       161.4       0.0962         155.C,       (3, 8, 9)       141.5       0.1856       150.C,       (3, 6, 9)       3       161.6       0.117         92.C,       (3, 6, 9)       5       141.7       0.0715       364.C,       (5, 2, 11)       0       16	21: <i>C</i> <sub>1</sub>	(2, 8, 8)	10	137.6	0.0847	183: <i>C</i> <sub>1</sub>	(2, 8, 8)	8	156.9	0.1995
47.C,       (3, 6, 9)       3       1379       0.1536       158C,       (4, 4, 10)       1       157.5       0.3006         160C,       (1, 6, 9)       4       138.7       0.3507       239.C,       (2, 8, 8)       8       157.7       0.2788         23.5C,       (4, 4, 10)       1       138.8       0.2429       184.C,       (2, 8, 8)       6       158.9       0.031         84.C,       (2, 8, 8)       9       139       0.0319       174.C,       (3, 6, 9)       3       160.6       0.2533         171.D,       (4, 4, 10)       2       140.4       0.2811       120.C,       (2, 8, 8)       5       160.8       0.1096         23.C,       (2, 8, 8)       6       140.7       0.0373       101.C,       (3, 6, 9)       3       161.4       0.1017         24.C,       (3, 8, 9)       5       140.5       0.1563       130.C,       (3, 6, 9)       3       163.4       0.2266         79.C,       (3, 6, 9)       5       141.7       0.0715       364.C,       (5, 2, 11)       0       163.5       0.152         148.C,       (2, 8, 8)       7       143.5       0.169       3       165.0       0.165	56: <i>C</i> <sub>1</sub>	(3, 6, 9)	5	137.6	0.0778	97: <i>C</i> <sub>1</sub>	(2, 8, 8)	9	157.4	0.0878
169:C. $(3, 6, 9)$ $4$ $138.7$ $0.3507$ $229.C.$ $(2, 8, 8)$ $8$ $157.7$ $0.2788$ $223.C_1$ $(4, 4, 10)$ $1$ $138.8$ $0.2429$ $184.C_1$ $(3, 6, 9)$ $4$ $158.4$ $0.2331$ $84.C_1$ $(4, 4, 10)$ $2$ $138.8$ $0.2326$ $112.C_1$ $(2, 8, 8)$ $6$ $158.9$ $0.053$ $81.C_2$ $(2, 8, 8)$ $0$ $139$ $0.0619$ $174.C_1$ $(3, 6, 9)$ $3$ $160.6$ $0.2331$ $171.D_2$ $(4, 4, 10)$ $2$ $1404$ $0.0371$ $174.C_1$ $(3, 6, 9)$ $3$ $160.9$ $0.1802$ $28.C_2$ $(2, 8, 8)$ $6$ $140.7$ $0.0373$ $101.C_1$ $(3, 6, 9)$ $3$ $160.9$ $0.1802$ $28.C_2$ $(2, 8, 8)$ $7$ $141.0$ $0.1836$ $142C_2$ $(2, 8, 8)$ $6$ $161.6$ $0.017$ $92.C_1$ $(2, 8, 8)$ $7$ $141.0$ $0.1836$ $142C_1$ $(3, 6, 9)$ $3$ $163.4$ $0.2264$ $179.C_1$ $(3, 6, 9)$ $5$ $141.7$ $0.0715$ $364.C_1$ $(5, 2, 11)$ $0$ $165.5$ $0.5152$ $148.C_1$ $(2, 8, 8)$ $7$ $144.0$ $0.0795$ $364.C_1$ $(5, 2, 11)$ $0$ $165.5$ $0.5152$ $19.C_1$ $(4, 4, 10)$ $1$ $143.6$ $0.2814$ $357.C_1$ $(5, 2, 11)$ $0$ $165.5$ $0.1127$ $148.C_1$ $(2, 8, 8)$ $7$ $144.2$ $0.1092$ $135.C_1$ $(6, 0, 12.2)$	47: <i>C</i> <sub>1</sub>	(3, 6, 9)	3	137.9	0.1536	$158:C_{I}$	(4, 4, 10)	1	157.5	0.3006
223.C; $(4, 4, 10)$ 1138.80.2429184.C; $(3, 6, 9)$ 4158.40.233184.C; $(4, 4, 10)$ 2138.80.2326112.C; $(2, 8, 8)$ 6158.90.05381.C; $(2, 8, 8)$ 91390.0319174.C; $(3, 6, 9)$ 3160.60.2333171.D; $(4, 4, 10)$ 2140.40.2811120.C; $(2, 8, 8)$ 5160.90.1609180.C; $(3, 6, 9)$ 5140.50.0718154.C; $(3, 6, 9)$ 3160.70.962128.C; $(2, 8, 8)$ 6140.70.0373101.C; $(3, 6, 9)$ 3161.70.030192.C; $(2, 8, 8)$ 7141.00.1836142.C; $(2, 8, 8)$ 6161.60.101792.C; $(2, 8, 8)$ 5143.50.178240.C; $(3, 6, 9)$ 3161.70.30163.C; $(3, 6, 9)$ 5141.70.715364.C; $(2, 8, 8)$ 6163.60.135180.C; $(3, 6, 9)$ 5141.70.715364.C; $(2, 8, 8)$ 6163.50.1512180.C; $(3, 6, 9)$ 2143.80.2619183.C; $(2, 8, 8)$ 6163.50.1627190.C; $(2, 8, 8)$ 7144.0.179886.C; $(3, 6, 9)$ 3167.10.464191.C; $(2, 8, 8)$ 7144.0.1798356.C; $(6, 0, 12)$ 0165.10.000018	$160:C_1$	(3, 6, 9)	4	138.7	0.3507	239: <i>C</i> <sub>1</sub>	(2, 8, 8)	8	157.7	0.2788
84.C; $(4, 4, 10)$ 2138.80.2326 $112.C;$ $(2, 8, 8)$ 6 $158.9$ 0.05381.C; $(2, 8, 8)$ 10138.90.0816 $109.C;$ $(2, 8, 8)$ 8 $159.7$ 0.1609169.C; $(2, 8, 8)$ 91390.0319 $174.C;$ $(3, 6, 9)$ 3160.60.2353171.D; $(4, 4, 10)$ 2140.50.0718 $154.C;$ $(2, 8, 8)$ 5160.80.102028.C; $(2, 8, 8)$ 6140.70.0373101.C; $(3, 6, 9)$ 3161.40.0902153.C; $(2, 8, 8)$ 7141.00.1836142.C; $(2, 8, 8)$ 6161.60.101792.C; $(2, 8, 8)$ 5141.70.715364.C; $(5, 2, 11)$ 0163.50.3152148.C; $(2, 8, 8)$ 5143.50.478118.C; $(2, 8, 8)$ 6163.60.1394119.C; $(3, 6, 9)$ 3141.50.1788240.C; $(3, 6, 9)$ 3161.40.0961119.C; $(3, 6, 9)$ 5143.50.478118.C; $(2, 8, 8)$ 6163.60.1394119.C; $(3, 6, 9)$ 1143.60.2814357.C; $(5, 2, 11)$ 0163.50.1227145.C; $(2, 8, 8)$ 814420.1082123.C; $(4, 4, 10)$ 1164.50.1671119.C; $(2, 8, 8)$ 814420.1082123.C; $(4, 4, 10)$ 1167.00.031	223:C <sub>1</sub>	(4, 4, 10)	1	138.8	0.2429	$184:C_{I}$	(3, 6, 9)	4	158.4	0.2331
$81:C_1$ $(2, 8, 8)$ $10$ $138.9$ $0.0816$ $109:C_1$ $(2, 8, 8)$ $8$ $1597$ $0.1609$ $169:C_1$ $(2, 8, 8)$ $9$ $139$ $0.0319$ $174:C_1$ $(3, 6, 9)$ $3$ $160.6$ $0.2333$ $171:D_2$ $(4, 4, 10)$ $2$ $140.4$ $0.2811$ $120:C_1$ $(2, 8, 8)$ $5$ $160.8$ $0.1096$ $83:C_1$ $(3, 6, 9)$ $5$ $140.5$ $0.0718$ $164.C_1$ $(3, 6, 9)$ $3$ $160.9$ $0.1802$ $28:C_2$ $(2, 8, 8)$ $6$ $161.4$ $0.0961$ $101:C_1$ $(3, 6, 9)$ $3$ $161.6$ $0.017$ $92:C_2$ $(2, 8, 8)$ $6$ $114.5$ $0.1583$ $150:C_1$ $(3, 6, 9)$ $3$ $163.6$ $0.2266$ $79:C_1$ $(3, 6, 9)$ $3$ $141.5$ $0.1583$ $118:C_1$ $(2, 8, 8)$ $6$ $163.6$ $0.1651$ $180:C_2$ $(2, 8, 8)$ $5$ $143.5$ $0.0478$ $118:C_1$ $(2, 8, 8)$ $6$ $163.6$ $0.1671$ $119:C_2$ $(3, 6, 9)$ $2$ $143.8$ $0.2199$ $163:C_1$ $(4, 4.10)$ $1$ $164.5$ $0.1667$ $111:C_1$ $(2, 8, 8)$ $7$ $144$ $0.1798$ $86:C_1$ $(3, 6, 9)$ $4$ $165.1$ $0.0201$ $119:C_2$ $(2, 8, 8)$ $7$ $144.9$ $0.0795$ $14:C_2$ $(1, 10, 7)$ $13$ $167.1$ $0.0312$ $114:C_1$ $(1, 6, 7)$ $13$ $169.9$ $0.0351$ $167.1$ $0.0312$	84: <i>C</i> 1	(4, 4, 10)	2	138.8	0.2326	112: <i>C</i> <sub>1</sub>	(2, 8, 8)	6	158.9	0.053
$169\cdotC$ , $(2, 8, 8)$ 919 $0.0319$ $174\cdotC$ , $(3, 6, 9)$ 3 $160.6$ $0.2333$ $171\cdotD_2$ $(4, 4, 10)$ 2 $140.4$ $0.2811$ $120\cdotC_7$ , $(2, 8, 8)$ 5 $160.8$ $0.1096$ $83\cdotC_7$ $(3, 6, 9)$ 5 $140.5$ $0.0718$ $154\cdotC_7$ , $(3, 6, 9)$ 3 $160.9$ $0.1802$ $28\cdotC_7$ $(2, 8, 8)$ 6 $140.7$ $0.0373$ $101\cdotC_7$ , $(3, 6, 9)$ 3 $161.4$ $0.0962$ $153\cdotC_7$ $(2, 8, 8)$ 7 $141.0$ $0.1836$ $142\cdotC_7$ , $(2, 6, 9)$ 3 $161.7$ $0.0301$ $62\cdotC_7$ $(3, 6, 9)$ 3 $141.5$ $0.1788$ $240\cdotC_7$ , $(3, 6, 9)$ 3 $163.4$ $0.2266$ $79\cdotC_7$ $(3, 6, 9)$ 5 $141.7$ $0.0715$ $364\cdotC_7$ , $(5, 2, 11)$ 0 $163.5$ $0.3152$ $148\cdotC_7$ $(2, 8, 8)$ 5 $143.5$ $0.0478$ $118\cdotC_7$ , $(2, 8, 8)$ 6 $163.6$ $0.1667$ $111\cdotC_7$ $(2, 8, 8)$ 7 $144$ $0.1798$ $86\cdotC_7$ , $(3, 6, 9)$ 4 $165$ $0.1677$ $111\cdotC_7$ $(2, 8, 8)$ 7 $144.2$ $0.1795$ $36\cdotC_7$ , $(1, 4, 10)$ 1 $164.5$ $0.1671$ $111\cdotC_7$ $(2, 8, 8)$ 7 $144.2$ $0.1795$ $36\cdotC_7$ , $(3, 6, 9)$ 3 $1671$ $0.3012$ $120\cdotC_7$ $(2, 8, 8)$ 7 $144.2$ $0.1795$ $36\cdotC_7$ , $(1, 0, 17)$ $13$ $160.0$ $0.31$	81: <i>C</i> <sub>1</sub>	(2, 8, 8)	10	138.9	0.0816	109: <i>C</i> <sub>1</sub>	(2, 8, 8)	8	159.7	0.1609
$171:D_2$ $(4, 4, 10)$ $2$ $140.4$ $0.2811$ $120.c$ $(2, 8, 8)$ $5$ $160.8$ $0.1096$ $83:C_1$ $(3, 6, 9)$ $5$ $140.5$ $0.0718$ $154:C_1$ $(3, 6, 9)$ $3$ $160.9$ $0.1802$ $28:C_2$ $(2, 8, 8)$ $6$ $140.7$ $0.0373$ $101:C_2$ $(3, 6, 9)$ $6$ $161.4$ $0.0962$ $153:C_2$ $(2, 8, 8)$ $7$ $141.0$ $0.1836$ $142:C_2$ $(2, 8, 8)$ $6$ $161.6$ $0.1017$ $92:C_2$ $(2, 8, 8)$ $9$ $141.5$ $0.1563$ $150:C_1$ $(3, 6, 9)$ $3$ $161.7$ $0.301$ $63:C_1$ $(3, 6, 9)$ $3$ $141.5$ $0.1788$ $240:C_1$ $(3, 6, 9)$ $3$ $163.4$ $0.2266$ $79:C_1$ $(3, 6, 9)$ $5$ $143.5$ $0.0478$ $118:C_2$ $(2, 8, 8)$ $6$ $163.6$ $0.1465$ $110:C_2$ $(4, 4, 10)$ $1$ $143.5$ $0.2619$ $163:C_1$ $(4, 4.10)$ $1$ $164.5$ $0.1667$ $111:C_1$ $(2, 8, 8)$ $7$ $144.3$ $0.0795$ $35:C_2$ $(6, 0, 12)$ $0$ $165.1$ $0.0000$ $168:C_1$ $(2, 8, 8)$ $7$ $144.3$ $0.0795$ $35:C_2$ $(1, 10.7)$ $13$ $167.0$ $0.312$ $73:C_1$ $(2, 8, 8)$ $7$ $144.3$ $0.0795$ $35:C_2$ $(1, 10.7)$ $13$ $167.0$ $0.312$ $73:C_1$ $(3, 6, 9)$ $2$ $146.8$ $0.1232$ $189:C_1$ $(3, 6, 9)$ </td <td>169:<i>C</i><sub>s</sub></td> <td>(2, 8, 8)</td> <td>9</td> <td>139</td> <td>0.0319</td> <td><math>174:C_{I}</math></td> <td>(3, 6, 9)</td> <td>3</td> <td>160.6</td> <td>0.2353</td>	169: <i>C</i> <sub>s</sub>	(2, 8, 8)	9	139	0.0319	$174:C_{I}$	(3, 6, 9)	3	160.6	0.2353
$83:C_i$ $(3, 6, 9)$ $5$ $140.5$ $0.0718$ $154:C_i$ $(3, 6, 9)$ $3$ $160.9$ $0.1802$ $28:C_i$ $(2, 8, 8)$ $6$ $140.7$ $0.0373$ $101:C_i$ $(3, 6, 9)$ $6$ $161.4$ $0.0962$ $153:C_i$ $(2, 8, 8)$ $7$ $141.0$ $0.1836$ $142:C_i$ $(2, 8, 8)$ $6$ $161.6$ $0.1017$ $92:C_i$ $(2, 8, 8)$ $9$ $141.5$ $0.1663$ $150:C_i$ $(3, 6, 9)$ $3$ $161.7$ $0.0301$ $63:C_i$ $(3, 6, 9)$ $3$ $141.5$ $0.1788$ $240:C_i$ $(3, 6, 9)$ $3$ $163.4$ $0.2266$ $79:C_i$ $(3, 6, 9)$ $5$ $141.7$ $0.0715$ $364:C_i$ $(5, 2, 11)$ $0$ $163.5$ $0.3152$ $18:C_i$ $(4, 4, 10)$ $1$ $143.6$ $0.2814$ $35:C_i$ $(4, 4, 10)$ $1$ $164.5$ $0.1667$ $111:C_i$ $(2, 8, 8)$ $7$ $144$ $0.1798$ $86:C_i$ $(3, 6, 9)$ $4$ $165$ $0.1727$ $145:C_i$ $(2, 8, 8)$ $7$ $144.3$ $0.0795$ $35:C_i$ $(6, 0.12)$ $0$ $165.1$ $0.0000$ $168:C_i$ $(3, 6, 9)$ $4$ $145.8$ $0.2159$ $42:C_i$ $(1, 10, 7)$ $13$ $167.0$ $0.312$ $73:C_i$ $(3, 6, 9)$ $2$ $146.8$ $0.1233$ $189:C_i$ $(3, 6, 9)$ $3$ $167.1$ $0.0965$ $114:C_i$ $(1, 10, 7)$ $13$ $146.9$ $0.2952$ $151:C_i$ $(3, 6, 9)$ <	171:D <sub>2</sub>	(4, 4, 10)	2	140.4	0.2811	$120:C_{I}$	(2, 8, 8)	5	160.8	0.1096
$28.C_{7}$ $(2, 8, 8)$ $6$ $140.7$ $0.0373$ $101:C_{7}$ $(3, 6, 9)$ $6$ $161.4$ $0.0962$ $153.C_{7}$ $(2, 8, 8)$ $7$ $141.0$ $0.1836$ $142.C_{7}$ $(2, 8, 8)$ $6$ $161.6$ $0.1017$ $92.C_{7}$ $(2, 8, 8)$ $9$ $141.5$ $0.1563$ $150.C_{7}$ $(3, 6, 9)$ $3$ $161.7$ $0.0301$ $63.C_{7}$ $(3, 6, 9)$ $3$ $141.5$ $0.1788$ $240.C_{7}$ $(3, 6, 9)$ $3$ $163.4$ $0.2266$ $79.C_{7}$ $(3, 6, 9)$ $5$ $141.7$ $0.0715$ $364.C_{7}$ $(5, 2, 11)$ $0$ $163.5$ $0.3152$ $148.C_{7}$ $(2, 8, 8)$ $5$ $143.5$ $0.0478$ $118.C_{7}$ $(2, 8, 8)$ $6$ $163.6$ $0.1667$ $111.C_{7}$ $(3, 6, 9)$ $2$ $143.8$ $0.2619$ $163.C_{7}$ $(4, 4, 10)$ $1$ $164.5$ $0.1677$ $111.C_{7}$ $(2, 8, 8)$ $8$ $144.2$ $0.1082$ $123.C_{7}$ $(3, 6, 9)$ $4$ $165.1$ $0.0224$ $210.C_{7}$ $(2, 8, 8)$ $8$ $144.2$ $0.1082$ $123.C_{7}$ $(4, 4, 10)$ $1$ $167.1$ $0.0405$ $141.C_{7}$ $(1, 10, 7)$ $13$ $146.9$ $0.0936$ $363.C_{7}$ $(5, 2, 11)$ $0$ $167.1$ $0.0405$ $24.C_{7}$ $(2, 8, 8)$ $8$ $147.1$ $0.1299$ $138.C_{7}$ $(4, 4, 10)$ $1$ $167.7$ $0.834$ $173.C_{7}$ $(4, 4, 10)$ $3$ $148.0$	83: <i>C</i> 1	(3, 6, 9)	5	140.5	0.0718	154: <i>C</i> <sub>1</sub>	(3, 6, 9)	3	160.9	0.1802
153.C; $(2, 8, 8)$ 7141.00.1836142.C; $(2, 8, 8)$ 6161.60.101792.C; $(2, 8, 8)$ 9141.50.1563150.C; $(3, 6, 9)$ 3161.70.030163.C; $(3, 6, 9)$ 3141.50.1788240.C; $(3, 6, 9)$ 3163.40.226679.C; $(3, 6, 9)$ 5141.70.0715364.C; $(5, 2, 11)$ 0163.50.3152148.C; $(2, 8, 8)$ 5143.50.0478118.C; $(2, 8, 8)$ 6163.60.1667111.C; $(2, 8, 8)$ 71440.179886.C; $(3, 6, 9)$ 41650.1727145.C; $(2, 8, 8)$ 8144.20.1082123.C; $(2, 8, 8)$ 8165.10.2624210.C; $(2, 8, 8)$ 7144.30.0795356.C; $(6, 0, 12)$ 0163.10.0001168.C; $(3, 6, 9)$ 2146.80.1233189.C; $(3, 6, 9)$ 3167.10.2956141.C; $(1, 10, 7)$ 13146.90.0936363.C; $(5, 2, 11)$ 0167.10.001524.C; $(2, 8, 8)$ 8147.10.1299138.C; $(4, 4, 10)$ 1167.70.0834173.C; $(4, 4, 10)$ 3148.00.2652151.C; $(3, 6, 9)$ 3167.10.0565178.C; $(2, 8, 8)$ 7148.70.0497110.C; $(2, 8, 8)$ 6168.60.165 <td><math>28:C_2</math></td> <td>(2, 8, 8)</td> <td>6</td> <td>140.7</td> <td>0.0373</td> <td><math>101:C_{I}</math></td> <td>(3, 6, 9)</td> <td>6</td> <td>161.4</td> <td>0.0962</td>	$28:C_2$	(2, 8, 8)	6	140.7	0.0373	$101:C_{I}$	(3, 6, 9)	6	161.4	0.0962
92: $C_7$ (2, 8, 8)9141.50.1563150: $C_7$ (3, 6, 9)3161.70.030163: $C_7$ (3, 6, 9)5141.70.0715364: $C_7$ (3, 6, 9)3163.40.226679: $C_7$ (3, 6, 9)5141.70.0715364: $C_7$ (5, 2, 11)0163.50.3152148: $C_7$ (2, 8, 8)5143.50.0478118: $C_7$ (2, 8, 8)6163.60.1465180: $C_7$ (4, 4, 10)1143.60.2814357: $C_7$ (5, 2, 11)0163.90.3945119: $C_7$ (2, 8, 8)71440.179886: $C_7$ (3, 6, 9)41650.1727145: $C_7$ (2, 8, 8)8144.20.1082123: $C_7$ (2, 8, 8)8165.10.2624210: $C_7$ (2, 8, 8)7144.30.0795356: $C_7$ (6, 0, 12)0165.10.0000168: $C_7$ (3, 6, 9)2146.80.1233189: $C_7$ (3, 6, 9)3167.10.2956141: $C_7$ (1, 10, 7)13146.90.0936363: $C_7$ (5, 2, 11)0167.10.040524: $C_7$ (2, 8, 8)8147.10.1299138: $C_7$ (3, 6, 9)3167.90.0756141: $C_7$ (1, 10, 7)13146.90.0936363: $C_7$ (5, 2, 11)0167.10.040524: $C_7$ (2, 8, 8)7144.80.2652151: $C_7$ (3, 6, 9)3	153: <i>C</i> <sub>1</sub>	(2, 8, 8)	7	141.0	0.1836	142: <i>C</i> <sub>2</sub>	(2, 8, 8)	6	161.6	0.1017
$63:C_i$ $(3, 6, 9)$ $3$ $141.5$ $0.1788$ $240:C_i$ $(3, 6, 9)$ $3$ $163.4$ $0.2266$ $79:C_i$ $(3, 6, 9)$ $5$ $141.7$ $0.0715$ $364:C_i$ $(5, 2, 11)$ $0$ $163.5$ $0.3152$ $148:C_i$ $(2, 8, 8)$ $5$ $143.5$ $0.0478$ $118:C_i$ $(2, 8, 8)$ $6$ $163.6$ $0.1465$ $180:C_i$ $(4, 4, 10)$ $1$ $143.6$ $0.2814$ $357:C_i$ $(5, 2, 11)$ $0$ $163.9$ $0.3945$ $119:C_i$ $(2, 8, 8)$ $7$ $144$ $0.1798$ $8e:C_i$ $(3, 6, 9)$ $4$ $165$ $0.1677$ $111:C_i$ $(2, 8, 8)$ $7$ $144$ $0.1798$ $8e:C_i$ $(3, 6, 9)$ $4$ $165$ $0.1727$ $145:C_i$ $(2, 8, 8)$ $7$ $144.3$ $0.0795$ $356:C_i$ $(6, 0, 12)$ $0$ $165.1$ $0.0000$ $168:C_i$ $(3, 6, 9)$ $4$ $1458$ $0.2159$ $42:C_i$ $(1, 10, 7)$ $13$ $167.0$ $0.0312$ $73:C_i$ $(3, 6, 9)$ $2$ $1468$ $0.1233$ $189:C_i$ $(3, 6, 9)$ $3$ $167.1$ $0.0006$ $24:C_i$ $(1, 10, 7)$ $13$ $1469$ $0.0936$ $363:C_i$ $(5, 2, 11)$ $0$ $167.1$ $0.0405$ $24:C_i$ $(2, 8, 8)$ $8$ $147.1$ $0.1299$ $138:C_i$ $(4, 4, 10)$ $1$ $167.7$ $0.8344$ $173:C_i$ $(4, 4, 10)$ $3$ $1480$ $0.2652$ $151:C_i$ $(3, 6, 9)$ <	92: <i>C</i> <sub>2</sub>	(2, 8, 8)	9	141.5	0.1563	$150:C_s$	(3, 6, 9)	3	161.7	0.0301
$79:C_i$ $(3, 6, 9)$ $5$ $141.7$ $0.0715$ $364.C_i$ $(5, 2, 11)$ $0$ $163.5$ $0.3152$ $148.C_2$ $(2, 8, 8)$ $5$ $143.5$ $0.0478$ $118.C_i$ $(2, 8, 8)$ $6$ $163.6$ $0.1465$ $180:C_i$ $(4, 4, 10)$ $1$ $143.6$ $0.2814$ $357:C_i$ $(5, 2, 11)$ $0$ $163.9$ $0.3945$ $119:C_2$ $(3, 6, 9)$ $2$ $143.8$ $0.2619$ $163.C_i$ $(4, 4, 10)$ $1$ $164.5$ $0.1667$ $111:C_i$ $(2, 8, 8)$ $7$ $144$ $0.1798$ $86:C_i$ $(3, 6, 9)$ $4$ $165$ $0.1727$ $145:C_i$ $(2, 8, 8)$ $7$ $144.3$ $0.0795$ $356:C_3$ $(6, 0, 12)$ $0$ $165.1$ $0.0000$ $168:C_i$ $(3, 6, 9)$ $4$ $145.8$ $0.2159$ $42:C_i$ $(1, 10, 7)$ $13$ $167.0$ $0.0312$ $73:C_i$ $(3, 6, 9)$ $2$ $146.8$ $0.1233$ $189:C_i$ $(3, 6, 9)$ $3$ $167.1$ $0.00512$ $24:C_2$ $(2, 8, 8)$ $8$ $147.1$ $0.1299$ $138:C_i$ $(4, 4, 10)$ $1$ $167.7$ $0.0354$ $173:C_i$ $(3, 6, 9)$ $2$ $148.8$ $0.2652$ $151:C_i$ $(3, 6, 9)$ $3$ $167.9$ $0.0756$ $178:C_i$ $(3, 6, 9)$ $4$ $148.8$ $0.2402$ $134:C_i$ $(4, 4, 10)$ $1$ $169.3$ $0.1312$ $82:C_i$ $(4, 4, 10)$ $2$ $149.3$ $0.0893$ $172:C_i$ $($	63: <i>C</i> <sub>1</sub>	(3, 6, 9)	3	141.5	0.1788	240:C <sub>s</sub>	(3, 6, 9)	3	163.4	0.2266
148. $C_2$ (2, 8, 8)5143.50.0478118. $C_1$ (2, 8, 8)6163.60.1465180. $C_1$ (4, 4, 10)1143.60.2814357. $C_1$ (5, 2, 11)0163.90.3945119. $C_2$ (3, 6, 9)2143.80.2619163. $C_1$ (4, 4, 10)1164.50.1667111: $C_1$ (2, 8, 8)71440.179886. $C_1$ (3, 6, 9)41650.1727145. $C_1$ (2, 8, 8)7144.30.0795356. $C_2$ (6, 0, 12)0165.10.0000168. $C_1$ (3, 6, 9)4145.80.215942. $C_1$ (1, 10, 7)13167.00.031273. $C_1$ (3, 6, 9)2146.80.1233189. $C_1$ (3, 6, 9)3167.10.040524. $C_2$ (2, 8, 8)8147.10.1299138. $C_1$ (4, 4, 10)1167.70.0834173. $C_1$ (4, 4, 10)3148.00.2652151. $C_1$ (3, 6, 9)3167.90.0756178. $C_1$ (3, 6, 9)2148.10.1672108. $C_1$ (2, 8, 8)6168.60.165114. $C_1$ (3, 6, 9)4148.80.2402134. $C_1$ (3, 6, 9)3169.20.247953. $C_2$ (2, 8, 8)7148.70.0497110. $C_1$ (2, 8, 8)6168.60.165114. $C_1$ (3, 6, 9)4148.80.2402134. $C_1$ (3, 6, 9)3169	79: <i>C</i> <sub>1</sub>	(3, 6, 9)	5	141.7	0.0715	364: <i>C</i> <sub>s</sub>	(5, 2, 11)	0	163.5	0.3152
180. $C_i$ (4, 4, 10)1143.60.2814357; $C_i$ (5, 2, 11)0163.90.3945119; $C_2$ (3, 6, 9)2143.80.2619163; $C_i$ (4, 4, 10)1164.50.1667111; $C_i$ (2, 8, 8)8144.20.1082123; $C_i$ (2, 8, 8)8165.10.2624210; $C_i$ (2, 8, 8)7144.30.0795356; $C_i$ (6, 0, 12)0165.10.0000168; $C_i$ (3, 6, 9)4145.80.215942; $C_i$ (1, 10, 7)13167.00.031273; $C_i$ (3, 6, 9)2146.80.1233189; $C_i$ (3, 6, 9)3167.10.2956141; $C_i$ (1, 10, 7)13146.90.0936363; $C_i$ (5, 2, 11)0167.10.003224; $C_2$ (2, 8, 8)8147.10.1299138; $C_i$ (4, 4, 10)1167.70.0834173; $C_i$ (4, 4, 10)3148.00.2652151; $C_i$ (3, 6, 9)3167.90.0756178; $C_i$ (3, 6, 9)2148.10.1672108; $C_i$ (2, 8, 8)6168.60.163114; $C_i$ (3, 6, 9)4148.80.2402134; $C_i$ (3, 6, 9)3169.20.247953; $C_i$ (2, 8, 8)7144.30.0993172; $C_i$ (4, 4, 10)1169.30.134282; $C_i$ (4, 4, 10)2149.30.0893172; $C_i$ (3, 6, 9)3 </td <td>148:<i>C</i><sub>2</sub></td> <td>(2, 8, 8)</td> <td>5</td> <td>143.5</td> <td>0.0478</td> <td>118:<i>C</i><sub>1</sub></td> <td>(2, 8, 8)</td> <td>6</td> <td>163.6</td> <td>0.1465</td>	148: <i>C</i> <sub>2</sub>	(2, 8, 8)	5	143.5	0.0478	118: <i>C</i> <sub>1</sub>	(2, 8, 8)	6	163.6	0.1465
119: $C_2$ (3, 6, 9)2143.80.2619163: $C_1$ (4, 4, 10)1164.50.1667111: $C_1$ (2, 8, 8)71440.179886: $C_1$ (3, 6, 9)41650.1727145: $C_1$ (2, 8, 8)8144.20.1082123: $C_2$ (2, 8, 8)8165.10.2624210: $C_1$ (2, 8, 8)7144.30.0795356: $C_2$ (6, 0, 12)0165.10.0000168: $C_1$ (3, 6, 9)4145.80.215942: $C_2$ (1, 10, 7)13167.00.031273: $C_1$ (3, 6, 9)2146.80.1233189: $C_1$ (3, 6, 9)3167.10.2956141: $C_1$ (1, 10, 7)13146.90.0936363: $C_2$ (5, 2, 11)0167.10.003224: $C_2$ (2, 8, 8)8147.10.1299138: $C_1$ (4, 4, 10)1167.70.0834173: $C_1$ (4, 4, 10)3148.00.2652151: $C_2$ (3, 6, 9)3167.90.0756178: $C_1$ (3, 6, 9)2148.70.0497110: $C_7$ (2, 8, 8)6168.60.163114: $C_7$ (3, 6, 9)4148.80.2402134: $C_7$ (3, 6, 9)3169.20.247953: $C_4$ (2, 8, 8)7149.30.0893172: $C_7$ (4, 4, 10)1169.30.131282: $C_1$ (4, 4, 10)2149.30.0593191: $C_7$ (3, 6, 9)3	$180:C_{I}$	(4, 4, 10)	1	143.6	0.2814	357:C <sub>s</sub>	(5, 2, 11)	0	163.9	0.3945
111: $C_1$ (2, 8, 8)71440.1798 $86C_1$ (3, 6, 9)41650.1727145: $C_1$ (2, 8, 8)8144.20.1082123: $C_1$ (2, 8, 8)8165.10.2624210: $C_1$ (2, 8, 8)7144.30.0795 $356:C_3$ (6, 0, 12)0165.10.0000168: $C_1$ (3, 6, 9)2146.80.2159 $42:C_4$ (1, 10, 7)13167.00.031273: $C_n$ (3, 6, 9)2146.80.1233189: $C_1$ (3, 6, 9)3167.10.2956141: $C_1$ (1, 10, 7)13146.90.0936363: $C_7$ (5, 2, 11)0167.10.040524: $C_2$ (2, 8, 8)8147.10.1299138: $C_1$ (4, 4, 10)1167.90.0756178: $C_7$ (3, 6, 9)2148.10.1672108: $C_7$ (2, 8, 8)11168.50.097645: $C_1$ (2, 8, 8)7148.70.0497110: $C_1$ (2, 8, 8)6168.60.165114: $C_7$ (3, 6, 9)3169.20.2479134: $C_7$ (3, 6, 9)3169.20.247953: $C_4$ (4, 4, 10)2149.30.0893172: $C_1$ (4, 4, 10)1169.30.134220: $C_7$ (4, 4, 10)2149.30.0893172: $C_7$ (4, 4, 10)2169.30.1318104: $C_7$ (2, 8, 8)7149.90.1747106: $C_7$ (2, 8, 8)81	119: <i>C</i> <sub>2</sub>	(3, 6, 9)	2	143.8	0.2619	163: <i>C</i> <sub>1</sub>	(4, 4, 10)	1	164.5	0.1667
145: $C_r$ (2, 8, 8)8144.20.1082123: $C_s$ (2, 8, 8)8165.10.2624210: $C_r$ (2, 8, 8)7144.30.0795356: $C_s$ (6, 0, 12)0165.10.0000168: $C_r$ (3, 6, 9)4145.80.215942: $C_s$ (1, 10, 7)13167.00.031273: $C_s$ (3, 6, 9)2146.80.1233189: $C_r$ (3, 6, 9)3167.10.2956141: $C_s$ (1, 10, 7)13146.90.0936363: $C_r$ (5, 2, 11)0167.10.040524: $C_s$ (2, 8, 8)8147.10.1299138: $C_r$ (4, 4, 10)1167.70.0834173: $C_r$ (4, 4, 10)3148.00.2652151: $C_r$ (3, 6, 9)3167.90.0756178: $C_r$ (3, 6, 9)2148.10.1672108: $C_r$ (2, 8, 8)11168.50.097645: $C_r$ (2, 8, 8)7148.70.0497110: $C_r$ (2, 8, 8)6168.60.165114: $C_r$ (3, 6, 9)4148.80.2402134: $C_r$ (3, 6, 9)3169.20.247953: $C_r$ (2, 8, 8)7149.30.0893172: $C_r$ (4, 4, 10)1169.30.134282: $C_r$ (4, 4, 10)2149.30.0893191: $C_s$ (3, 6, 9)5169.90.576147: $C_r$ (2, 8, 8)7149.90.1747106: $C_r$ (2, 8, 8)8<	$111:C_1$	(2, 8, 8)	7	144	0.1798	86: <i>C</i> 1	(3, 6, 9)	4	165	0.1727
$210:C_1$ $(2, 8, 8)$ 7 $144.3$ $0.0795$ $356:C_3$ $(6, 0, 12)$ 0 $165.1$ $0.0000$ $168:C_t$ $(3, 6, 9)$ 4 $145.8$ $0.2159$ $42:C_s$ $(1, 10, 7)$ $13$ $167.0$ $0.0312$ $73:C_s$ $(3, 6, 9)$ 2 $146.8$ $0.1233$ $189:C_t$ $(3, 6, 9)$ 3 $167.1$ $0.2956$ $141:C_s$ $(1, 10, 7)$ $13$ $146.9$ $0.0936$ $363:C_t$ $(5, 2, 11)$ 0 $167.1$ $0.0405$ $24:C_2$ $(2, 8, 8)$ 8 $147.1$ $0.1299$ $138:C_t$ $(4, 4, 10)$ 1 $167.7$ $0.0834$ $173:C_t$ $(4, 4, 10)$ 3 $148.0$ $0.2652$ $151:C_t$ $(3, 6, 9)$ 3 $167.9$ $0.0756$ $178:C_t$ $(3, 6, 9)$ 2 $148.1$ $0.1672$ $108:C_t$ $(2, 8, 8)$ 11 $168.5$ $0.0976$ $45:C_t$ $(2, 8, 8)$ 7 $148.7$ $0.0497$ $110:C_t$ $(2, 8, 8)$ 6 $168.6$ $0.165$ $114:C_t$ $(3, 6, 9)$ 4 $148.8$ $0.2402$ $134:C_t$ $(4, 4, 10)$ 1 $169.3$ $0.1342$ $82:C_t$ $(4, 4, 10)$ 2 $149.3$ $0.0893$ $172:C_t$ $(4, 4, 10)$ 2 $169.3$ $0.1318$ $104:C_t$ $(2, 8, 8)$ 7 $149.9$ $0.1747$ $106:C_t$ $(2, 8, 8)$ 8 $170.0$ $0.0861$ $200:C_t$ $(4, 4, 10)$ 3 $149.9$ $0.3559$ $133:C_t$ $(3, 6, 9)$ 3 $170.4$ <	145: <i>C</i> <sub>1</sub>	(2, 8, 8)	8	144.2	0.1082	123: <i>C</i> <sub>s</sub>	(2, 8, 8)	8	165.1	0.2624
$168.C_t$ $(3, 6, 9)$ $4$ $145.8$ $0.2159$ $42:C_s$ $(1, 10, 7)$ $13$ $167.0$ $0.0312$ $73:C_s$ $(3, 6, 9)$ $2$ $146.8$ $0.1233$ $189:C_t$ $(3, 6, 9)$ $3$ $167.1$ $0.2956$ $141:C_s$ $(1, 10, 7)$ $13$ $146.9$ $0.0936$ $363:C_t$ $(5, 2, 11)$ $0$ $167.1$ $0.0405$ $24:C_2$ $(2, 8, 8)$ $8$ $147.1$ $0.1299$ $138:C_t$ $(4, 4, 10)$ $1$ $167.7$ $0.0834$ $173:C_t$ $(4, 4, 10)$ $3$ $148.0$ $0.2652$ $151:C_t$ $(3, 6, 9)$ $3$ $167.9$ $0.0756$ $178:C_t$ $(3, 6, 9)$ $2$ $148.1$ $0.1672$ $108:C_t$ $(2, 8, 8)$ $11$ $168.5$ $0.0976$ $45:C_t$ $(2, 8, 8)$ $7$ $148.7$ $0.0497$ $110:C_t$ $(2, 8, 8)$ $6$ $168.6$ $0.165$ $114:C_t$ $(3, 6, 9)$ $4$ $148.8$ $0.2402$ $134:C_t$ $(3, 6, 9)$ $3$ $169.2$ $0.2479$ $53:C_s$ $(2, 8, 8)$ $8$ $149.2$ $0.0987$ $164:C_t$ $(4, 4, 10)$ $1$ $169.3$ $0.1342$ $82:C_t$ $(4, 4, 10)$ $2$ $149.3$ $0.0893$ $172:C_t$ $(4, 4, 10)$ $2$ $169.3$ $0.1342$ $82:C_t$ $(4, 4, 10)$ $3$ $149.9$ $0.5593$ $191:C_s$ $(3, 6, 9)$ $5$ $169.9$ $0.0576$ $147:C_t$ $(2, 8, 8)$ $7$ $149.9$ $0.559$ $133:C_t$	210: <i>C</i> <sub>1</sub>	(2, 8, 8)	7	144.3	0.0795	356: <i>C</i> <sub>3</sub>	(6, 0, 12)	0	165.1	0.0000
$73:C_s$ $(3, 6, 9)$ $2$ $146.8$ $0.1233$ $189:C_t$ $(3, 6, 9)$ $3$ $167.1$ $0.2956$ $141:C_s$ $(1, 10, 7)$ $13$ $146.9$ $0.0936$ $363:C_t$ $(5, 2, 11)$ $0$ $167.1$ $0.0405$ $24:C_t$ $(2, 8, 8)$ $8$ $147.1$ $0.1299$ $138:C_t$ $(4, 4, 10)$ $1$ $167.7$ $0.0834$ $173:C_t$ $(4, 4, 10)$ $3$ $148.0$ $0.2652$ $151:C_t$ $(3, 6, 9)$ $3$ $167.9$ $0.0756$ $178:C_t$ $(3, 6, 9)$ $2$ $148.1$ $0.1672$ $108:C_t$ $(2, 8, 8)$ $11$ $168.5$ $0.0976$ $45:C_t$ $(2, 8, 8)$ $7$ $148.7$ $0.0497$ $110:C_t$ $(2, 8, 8)$ $6$ $168.6$ $0.165$ $114:C_t$ $(3, 6, 9)$ $4$ $148.8$ $0.2402$ $134:C_t$ $(3, 6, 9)$ $3$ $169.2$ $0.2479$ $53:C_s$ $(2, 8, 8)$ $8$ $149.2$ $0.0987$ $164:C_t$ $(4, 4, 10)$ $1$ $169.3$ $0.1342$ $82:C_t$ $(4, 4, 10)$ $2$ $149.3$ $0.0893$ $172:C_t$ $(4, 4, 10)$ $2$ $169.3$ $0.1318$ $104:C_t$ $(2, 8, 8)$ $7$ $149.9$ $0.1747$ $106:C_t$ $(2, 8, 8)$ $8$ $170.0$ $0.0861$ $200:C_t$ $(4, 4, 10)$ $3$ $149.9$ $0.3559$ $133:C_t$ $(3, 6, 9)$ $3$ $170.4$ $0.1034$ $38:C_t$ $(1, 10, 7)$ $13$ $150.3$ $0.0982$ $208:C_2$ <t< td=""><td><math>168:C_{I}</math></td><td>(3, 6, 9)</td><td>4</td><td>145.8</td><td>0.2159</td><td><math>42:C_s</math></td><td>(1, 10, 7)</td><td>13</td><td>167.0</td><td>0.0312</td></t<>	$168:C_{I}$	(3, 6, 9)	4	145.8	0.2159	$42:C_s$	(1, 10, 7)	13	167.0	0.0312
141: $C_s$ (1, 10, 7)13146.90.0936 $363:C_1$ (5, 2, 11)0167.10.0405 $24:C_2$ (2, 8, 8)8147.10.1299 $138:C_1$ (4, 4, 10)1167.70.0834 $173:C_1$ (4, 4, 10)3148.00.2652 $151:C_1$ (3, 6, 9)3167.90.0756 $178:C_1$ (3, 6, 9)2148.10.1672 $108:C_1$ (2, 8, 8)11168.50.0976 $45:C_1$ (2, 8, 8)7148.70.0497 $110:C_1$ (2, 8, 8)6168.60.165 $114:C_1$ (3, 6, 9)4148.80.2402 $134:C_1$ (3, 6, 9)3169.20.2479 $53:C_s$ (2, 8, 8)8149.20.0987164:C_1(4, 4, 10)1169.30.1342 $82:C_1$ (4, 4, 10)2149.30.0893172:C_1(4, 4, 10)2169.30.1318 $104:C_1$ (2, 8, 8)9149.80.0593191:C_s(3, 6, 9)5169.90.0576 $147:C_1$ (2, 8, 8)7149.90.1747106:C_1(2, 8, 8)8170.00.0861 $200:C_1$ (4, 4, 10)3149.90.3559133:C_1(3, 6, 9)3170.40.1034 $38:C_1$ (1, 10, 7)13150.30.0982 $208:C_2$ (2, 8, 8)7171.10.005 $39:C_1$ (2, 8, 8)7150.80.0961 $251:D_2$ (4, 4, 10)0171.9	73: <i>C</i> <sub>s</sub>	(3, 6, 9)	2	146.8	0.1233	189: <i>C</i> <sub>1</sub>	(3, 6, 9)	3	167.1	0.2956
$24:C_2$ $(2, 8, 8)$ 8 $147.1$ $0.1299$ $138:C_1$ $(4, 4, 10)$ $1$ $167.7$ $0.0834$ $173:C_1$ $(4, 4, 10)$ $3$ $148.0$ $0.2652$ $151:C_1$ $(3, 6, 9)$ $3$ $167.9$ $0.0756$ $178:C_1$ $(3, 6, 9)$ $2$ $148.1$ $0.1672$ $108:C_1$ $(2, 8, 8)$ $11$ $168.5$ $0.0976$ $45:C_1$ $(2, 8, 8)$ $7$ $148.7$ $0.0497$ $110:C_1$ $(2, 8, 8)$ $6$ $168.6$ $0.165$ $114:C_1$ $(3, 6, 9)$ $4$ $148.8$ $0.2402$ $134:C_1$ $(3, 6, 9)$ $3$ $169.2$ $0.2479$ $53:C_s$ $(2, 8, 8)$ $8$ $149.2$ $0.0987$ $164:C_1$ $(4, 4, 10)$ $1$ $169.3$ $0.1342$ $82:C_1$ $(4, 4, 10)$ $2$ $149.3$ $0.0893$ $172:C_1$ $(4, 4, 10)$ $2$ $169.3$ $0.1318$ $104:C_1$ $(2, 8, 8)$ $9$ $149.3$ $0.0593$ $191:C_s$ $(3, 6, 9)$ $5$ $169.9$ $0.0576$ $147:C_1$ $(2, 8, 8)$ $7$ $149.9$ $0.1747$ $106:C_1$ $(2, 8, 8)$ $8$ $170.0$ $0.0861$ $200:C_1$ $(4, 4, 10)$ $3$ $149.9$ $0.3559$ $133:C_1$ $(3, 6, 9)$ $3$ $170.4$ $0.1034$ $38:C_1$ $(1, 10, 7)$ $13$ $150.3$ $0.0982$ $208:C_2$ $(2, 8, 8)$ $7$ $171.1$ $0.005$ $39:C_1$ $(2, 8, 8)$ $7$ $150.8$ $0.0961$ $251:D_2$ $(4,$	$141:C_s$	(1, 10, 7)	13	146.9	0.0936	363: <i>C</i> <sub>1</sub>	(5, 2, 11)	0	167.1	0.0405
$173:C_I$ $(4, 4, 10)$ $3$ $148.0$ $0.2652$ $151:C_I$ $(3, 6, 9)$ $3$ $167.9$ $0.0756$ $178:C_I$ $(3, 6, 9)$ $2$ $148.1$ $0.1672$ $108:C_I$ $(2, 8, 8)$ $11$ $168.5$ $0.0976$ $45:C_I$ $(2, 8, 8)$ $7$ $148.7$ $0.0497$ $110:C_I$ $(2, 8, 8)$ $6$ $168.6$ $0.165$ $114:C_I$ $(3, 6, 9)$ $4$ $148.8$ $0.2402$ $134:C_I$ $(3, 6, 9)$ $3$ $169.2$ $0.2479$ $53:C_s$ $(2, 8, 8)$ $8$ $149.2$ $0.0987$ $164:C_I$ $(4, 4, 10)$ $1$ $169.3$ $0.1342$ $82:C_I$ $(4, 4, 10)$ $2$ $149.3$ $0.0893$ $172:C_I$ $(4, 4, 10)$ $2$ $169.3$ $0.1342$ $82:C_I$ $(4, 4, 10)$ $2$ $149.3$ $0.0893$ $191:C_s$ $(3, 6, 9)$ $5$ $169.9$ $0.576$ $147:C_I$ $(2, 8, 8)$ $7$ $149.9$ $0.1747$ $106:C_I$ $(2, 8, 8)$ $8$ $170.0$ $0.0861$ $200:C_I$ $(4, 4, 10)$ $3$ $149.9$ $0.3559$ $133:C_I$ $(3, 6, 9)$ $3$ $172.0$ $0.3393$ $32:C_I$ $(1, 10, 7)$ $13$ $150.3$ $0.0982$ $208:C_2$ $(2, 8, 8)$ $7$ $171.4$ $0.1034$ $38:C_I$ $(1, 10, 7)$ $13$ $150.5$ $0.2082$ $75:C_I$ $(4, 4, 10)$ $3$ $172.0$ $0.3393$ $124:C_I$ $(2, 8, 8)$ $5$ $152.6$ $0.121$ $132:C_I$	$24:C_2$	(2, 8, 8)	8	147.1	0.1299	$138:C_{I}$	(4, 4, 10)	1	167.7	0.0834
$178:C_I$ $(3, 6, 9)$ $2$ $148.1$ $0.1672$ $108:C_I$ $(2, 8, 8)$ $11$ $168.5$ $0.0976$ $45:C_I$ $(2, 8, 8)$ $7$ $148.7$ $0.0497$ $110:C_I$ $(2, 8, 8)$ $6$ $168.6$ $0.165$ $114:C_I$ $(3, 6, 9)$ $4$ $148.8$ $0.2402$ $134:C_I$ $(3, 6, 9)$ $3$ $169.2$ $0.2479$ $53:C_s$ $(2, 8, 8)$ $8$ $149.2$ $0.0987$ $164:C_I$ $(4, 4, 10)$ $1$ $169.3$ $0.1342$ $82:C_I$ $(4, 4, 10)$ $2$ $149.3$ $0.0893$ $172:C_I$ $(4, 4, 10)$ $2$ $169.3$ $0.1318$ $104:C_I$ $(2, 8, 8)$ $9$ $149.8$ $0.0593$ $191:C_s$ $(3, 6, 9)$ $5$ $169.9$ $0.0576$ $147:C_I$ $(2, 8, 8)$ $7$ $149.9$ $0.1747$ $106:C_I$ $(2, 8, 8)$ $8$ $170.0$ $0.0861$ $200:C_I$ $(4, 4, 10)$ $3$ $149.9$ $0.3559$ $133:C_I$ $(3, 6, 9)$ $3$ $170.4$ $0.1034$ $38:C_I$ $(1, 10, 7)$ $13$ $150.3$ $0.0982$ $208:C_2$ $(2, 8, 8)$ $7$ $171.1$ $0.005$ $39:C_I$ $(2, 8, 8)$ $7$ $150.8$ $0.0961$ $251:D_2$ $(4, 4, 10)$ $3$ $172.0$ $0.3393$ $124:C_I$ $(2, 8, 8)$ $5$ $152.6$ $0.121$ $132:C_I$ $(2, 8, 8)$ $7$ $173.4$ $0.1201$ $157:C_I$ $(4, 4, 10)$ $1$ $152.7$ $0.3232$ $69:C_2$ $(4$	173:C <sub>1</sub>	(4, 4, 10)	3	148.0	0.2652	151: <i>C</i> <sub>1</sub>	(3, 6, 9)	3	167.9	0.0756
$45:C_I$ $(2, 8, 8)$ 7 $148.7$ $0.0497$ $110:C_I$ $(2, 8, 8)$ 6 $168.6$ $0.165$ $114:C_I$ $(3, 6, 9)$ 4 $148.8$ $0.2402$ $134:C_I$ $(3, 6, 9)$ 3 $169.2$ $0.2479$ $53:C_s$ $(2, 8, 8)$ 8 $149.2$ $0.0987$ $164:C_I$ $(4, 4, 10)$ 1 $169.3$ $0.1342$ $82:C_I$ $(4, 4, 10)$ 2 $149.3$ $0.0893$ $172:C_I$ $(4, 4, 10)$ 2 $169.3$ $0.1318$ $104:C_I$ $(2, 8, 8)$ 9 $149.8$ $0.0593$ $191:C_s$ $(3, 6, 9)$ 5 $169.9$ $0.0576$ $147:C_I$ $(2, 8, 8)$ 7 $149.9$ $0.1747$ $106:C_I$ $(2, 8, 8)$ 8 $170.0$ $0.0861$ $200:C_I$ $(4, 4, 10)$ 3 $149.9$ $0.3559$ $133:C_I$ $(3, 6, 9)$ 3 $170.4$ $0.1034$ $38:C_I$ $(1, 10, 7)$ $13$ $150.3$ $0.0982$ $208:C_2$ $(2, 8, 8)$ 7 $171.1$ $0.005$ $39:C_I$ $(2, 8, 8)$ 7 $150.8$ $0.0961$ $251:D_2$ $(4, 4, 10)$ 3 $172.0$ $0.3393$ $124:C_I$ $(2, 8, 8)$ 5 $152.6$ $0.121$ $132:C_I$ $(2, 8, 8)$ 7 $173.4$ $0.1201$ $157:C_I$ $(4, 4, 10)$ 1 $152.7$ $0.3456$ $155:C_I$ $(3, 6, 9)$ 2 $173.8$ $0.1924$ $217:C_I$ $(3, 6, 9)$ 2 $152.7$ $0.3276$ $245:C_I$ $(4, 4, 10)$ 0 $173.8$	$178:C_{I}$	(3, 6, 9)	2	148.1	0.1672	$108:C_1$	(2, 8, 8)	11	168.5	0.0976
$114:C_I$ $(3, 6, 9)$ 4 $148.8$ $0.2402$ $134:C_I$ $(3, 6, 9)$ 3 $169.2$ $0.2479$ $53:C_s$ $(2, 8, 8)$ 8 $149.2$ $0.0987$ $164:C_I$ $(4, 4, 10)$ 1 $169.3$ $0.1342$ $82:C_I$ $(4, 4, 10)$ 2 $149.3$ $0.0893$ $172:C_I$ $(4, 4, 10)$ 2 $169.3$ $0.1318$ $104:C_I$ $(2, 8, 8)$ 9 $149.8$ $0.0593$ $191:C_s$ $(3, 6, 9)$ 5 $169.9$ $0.0576$ $147:C_I$ $(2, 8, 8)$ 7 $149.9$ $0.1747$ $106:C_I$ $(2, 8, 8)$ 8 $170.0$ $0.0861$ $200:C_I$ $(4, 4, 10)$ 3 $149.9$ $0.3559$ $133:C_I$ $(3, 6, 9)$ 3 $170.4$ $0.1034$ $38:C_I$ $(1, 10, 7)$ $13$ $150.3$ $0.0982$ $208:C_2$ $(2, 8, 8)$ 7 $171.1$ $0.005$ $39:C_I$ $(2, 8, 8)$ 7 $150.8$ $0.0961$ $251:D_2$ $(4, 4, 10)$ 3 $172.0$ $0.3393$ $124:C_I$ $(2, 8, 8)$ 5 $152.6$ $0.121$ $132:C_I$ $(2, 8, 8)$ 7 $173.4$ $0.1201$ $157:C_I$ $(4, 4, 10)$ 1 $152.7$ $0.3232$ $69:C_2$ $(4, 4, 10)$ 2 $173.8$ $0.4168$ $125:C_I$ $(3, 6, 9)$ 2 $152.7$ $0.3236$ $155:C_I$ $(3, 6, 9)$ 2 $173.8$ $0.1224$ $217:C_I$ $(3, 6, 9)$ 2 $152.9$ $0.3276$ $245:C_I$ $(4, 4, 10)$ 0 $173.8$ <t< td=""><td>45:<i>C</i><sub>1</sub></td><td>(2, 8, 8)</td><td>7</td><td>148.7</td><td>0.0497</td><td><math>110:C_{I}</math></td><td>(2, 8, 8)</td><td>6</td><td>168.6</td><td>0.165</td></t<>	45: <i>C</i> <sub>1</sub>	(2, 8, 8)	7	148.7	0.0497	$110:C_{I}$	(2, 8, 8)	6	168.6	0.165
$53:C_s$ $(2, 8, 8)$ $8$ $149.2$ $0.0987$ $164:C_I$ $(4, 4, 10)$ $1$ $169.3$ $0.1342$ $82:C_I$ $(4, 4, 10)$ $2$ $149.3$ $0.0893$ $172:C_I$ $(4, 4, 10)$ $2$ $169.3$ $0.1318$ $104:C_I$ $(2, 8, 8)$ $9$ $149.8$ $0.0593$ $191:C_s$ $(3, 6, 9)$ $5$ $169.9$ $0.0576$ $147:C_I$ $(2, 8, 8)$ $7$ $149.9$ $0.1747$ $106:C_I$ $(2, 8, 8)$ $8$ $170.0$ $0.0861$ $200:C_I$ $(4, 4, 10)$ $3$ $149.9$ $0.3559$ $133:C_I$ $(3, 6, 9)$ $3$ $170.4$ $0.1034$ $38:C_I$ $(1, 10, 7)$ $13$ $150.3$ $0.0982$ $208:C_2$ $(2, 8, 8)$ $7$ $171.1$ $0.005$ $39:C_I$ $(2, 8, 8)$ $7$ $150.8$ $0.0961$ $251:D_2$ $(4, 4, 10)$ $0$ $171.9$ $0.1376$ $167:C_I$ $(3, 6, 9)$ $3$ $151.5$ $0.2082$ $75:C_I$ $(4, 4, 10)$ $3$ $172.0$ $0.3393$ $124:C_I$ $(2, 8, 8)$ $5$ $152.6$ $0.121$ $132:C_I$ $(2, 8, 8)$ $7$ $173.4$ $0.1201$ $157:C_I$ $(4, 4, 10)$ $1$ $152.7$ $0.3232$ $69:C_2$ $(4, 4, 10)$ $2$ $173.8$ $0.4168$ $125:C_I$ $(3, 6, 9)$ $2$ $152.9$ $0.3276$ $245:C_I$ $(4, 4, 10)$ $0$ $173.8$ $0.2348$ $217:C_I$ $(3, 6, 9)$ $2$ $152.9$ $0.3276$ $245:C_I$	$114:C_{I}$	(3, 6, 9)	4	148.8	0.2402	134: <i>C</i> <sub>1</sub>	(3, 6, 9)	3	169.2	0.2479
$82:C_I$ $(4, 4, 10)$ $2$ $149.3$ $0.0893$ $172:C_I$ $(4, 4, 10)$ $2$ $169.3$ $0.1318$ $104:C_I$ $(2, 8, 8)$ $9$ $149.8$ $0.0593$ $191:C_s$ $(3, 6, 9)$ $5$ $169.9$ $0.0576$ $147:C_I$ $(2, 8, 8)$ $7$ $149.9$ $0.1747$ $106:C_I$ $(2, 8, 8)$ $8$ $170.0$ $0.0861$ $200:C_I$ $(4, 4, 10)$ $3$ $149.9$ $0.3559$ $133:C_I$ $(3, 6, 9)$ $3$ $170.4$ $0.1034$ $38:C_I$ $(1, 10, 7)$ $13$ $150.3$ $0.0982$ $208:C_2$ $(2, 8, 8)$ $7$ $171.1$ $0.005$ $39:C_I$ $(2, 8, 8)$ $7$ $150.8$ $0.0961$ $251:D_2$ $(4, 4, 10)$ $0$ $171.9$ $0.1376$ $167:C_I$ $(3, 6, 9)$ $3$ $151.5$ $0.2082$ $75:C_I$ $(4, 4, 10)$ $3$ $172.0$ $0.3393$ $124:C_I$ $(2, 8, 8)$ $5$ $152.6$ $0.121$ $132:C_I$ $(2, 8, 8)$ $7$ $173.4$ $0.1201$ $157:C_I$ $(4, 4, 10)$ $1$ $152.7$ $0.3232$ $69:C_2$ $(4, 4, 10)$ $2$ $173.8$ $0.4168$ $125:C_I$ $(3, 6, 9)$ $2$ $152.9$ $0.3276$ $245:C_I$ $(4, 4, 10)$ $0$ $173.8$ $0.2348$ $217:C_I$ $(3, 6, 9)$ $2$ $152.9$ $0.3276$ $245:C_I$ $(4, 4, 10)$ $0$ $173.8$ $0.2348$	53: <i>C</i> <sub>s</sub>	(2, 8, 8)	8	149.2	0.0987	164: <i>C</i> <sub>1</sub>	(4, 4, 10)	1	169.3	0.1342
$104:C_I$ $(2, 8, 8)$ 9 $149.8$ $0.0593$ $191:C_s$ $(3, 6, 9)$ 5 $169.9$ $0.0576$ $147:C_I$ $(2, 8, 8)$ 7 $149.9$ $0.1747$ $106:C_I$ $(2, 8, 8)$ 8 $170.0$ $0.0861$ $200:C_I$ $(4, 4, 10)$ 3 $149.9$ $0.3559$ $133:C_I$ $(3, 6, 9)$ 3 $170.4$ $0.1034$ $38:C_I$ $(1, 10, 7)$ $13$ $150.3$ $0.0982$ $208:C_2$ $(2, 8, 8)$ 7 $171.1$ $0.005$ $39:C_I$ $(2, 8, 8)$ 7 $150.8$ $0.0961$ $251:D_2$ $(4, 4, 10)$ 0 $171.9$ $0.1376$ $167:C_I$ $(3, 6, 9)$ 3 $151.5$ $0.2082$ $75:C_I$ $(4, 4, 10)$ 3 $172.0$ $0.3393$ $124:C_I$ $(2, 8, 8)$ 5 $152.6$ $0.121$ $132:C_I$ $(2, 8, 8)$ 7 $173.4$ $0.1201$ $157:C_I$ $(4, 4, 10)$ 1 $152.7$ $0.3232$ $69:C_2$ $(4, 4, 10)$ 2 $173.8$ $0.4168$ $125:C_I$ $(3, 6, 9)$ 2 $152.9$ $0.3276$ $245:C_I$ $(4, 4, 10)$ 0 $173.8$ $0.2348$	82: <i>C</i> <sub>1</sub>	(4, 4, 10)	2	149.3	0.0893	172: <i>C</i> <sub>1</sub>	(4, 4, 10)	2	169.3	0.1318
$147:C_I$ $(2, 8, 8)$ 7 $149.9$ $0.1747$ $106:C_I$ $(2, 8, 8)$ 8 $170.0$ $0.0861$ $200:C_I$ $(4, 4, 10)$ 3 $149.9$ $0.3559$ $133:C_I$ $(3, 6, 9)$ 3 $170.4$ $0.1034$ $38:C_I$ $(1, 10, 7)$ $13$ $150.3$ $0.0982$ $208:C_2$ $(2, 8, 8)$ 7 $171.1$ $0.005$ $39:C_I$ $(2, 8, 8)$ 7 $150.8$ $0.0961$ $251:D_2$ $(4, 4, 10)$ 0 $171.9$ $0.1376$ $167:C_I$ $(3, 6, 9)$ 3 $151.5$ $0.2082$ $75:C_I$ $(4, 4, 10)$ 3 $172.0$ $0.3393$ $124:C_I$ $(2, 8, 8)$ 5 $152.6$ $0.121$ $132:C_I$ $(2, 8, 8)$ 7 $173.4$ $0.1201$ $157:C_I$ $(4, 4, 10)$ 1 $152.7$ $0.3232$ $69:C_2$ $(4, 4, 10)$ 2 $173.8$ $0.4168$ $125:C_I$ $(3, 6, 9)$ 2 $152.7$ $0.3456$ $155:C_I$ $(3, 6, 9)$ 2 $173.8$ $0.1924$ $217:C_I$ $(3, 6, 9)$ 2 $152.9$ $0.3276$ $245:C_I$ $(4, 4, 10)$ 0 $173.8$ $0.2348$	104: <i>C</i> <sub>1</sub>	(2, 8, 8)	9	149.8	0.0593	191: <i>C</i> <sub>s</sub>	(3, 6, 9)	5	169.9	0.0576
$200:C_I$ $(4, 4, 10)$ $3$ $149.9$ $0.3559$ $133:C_I$ $(3, 6, 9)$ $3$ $170.4$ $0.1034$ $38:C_I$ $(1, 10, 7)$ $13$ $150.3$ $0.0982$ $208:C_2$ $(2, 8, 8)$ $7$ $171.1$ $0.005$ $39:C_I$ $(2, 8, 8)$ $7$ $150.8$ $0.0961$ $251:D_2$ $(4, 4, 10)$ $0$ $171.9$ $0.1376$ $167:C_I$ $(3, 6, 9)$ $3$ $151.5$ $0.2082$ $75:C_I$ $(4, 4, 10)$ $3$ $172.0$ $0.3393$ $124:C_I$ $(2, 8, 8)$ $5$ $152.6$ $0.121$ $132:C_I$ $(2, 8, 8)$ $7$ $173.4$ $0.1201$ $157:C_I$ $(4, 4, 10)$ $1$ $152.7$ $0.3232$ $69:C_2$ $(4, 4, 10)$ $2$ $173.8$ $0.4168$ $125:C_I$ $(3, 6, 9)$ $2$ $152.7$ $0.3456$ $155:C_I$ $(3, 6, 9)$ $2$ $173.8$ $0.1924$ $217:C_I$ $(3, 6, 9)$ $2$ $152.9$ $0.3276$ $245:C_I$ $(4, 4, 10)$ $0$ $173.8$ $0.2348$	147: <i>C</i> <sub>1</sub>	(2, 8, 8)	7	149.9	0.1747	$106:C_{I}$	(2, 8, 8)	8	170.0	0.0861
$38:C_I$ $(1, 10, 7)$ $13$ $150.3$ $0.0982$ $208:C_2$ $(2, 8, 8)$ $7$ $171.1$ $0.005$ $39:C_I$ $(2, 8, 8)$ $7$ $150.8$ $0.0961$ $251:D_2$ $(4, 4, 10)$ $0$ $171.9$ $0.1376$ $167:C_I$ $(3, 6, 9)$ $3$ $151.5$ $0.2082$ $75:C_I$ $(4, 4, 10)$ $3$ $172.0$ $0.3393$ $124:C_I$ $(2, 8, 8)$ $5$ $152.6$ $0.121$ $132:C_I$ $(2, 8, 8)$ $7$ $173.4$ $0.1201$ $157:C_I$ $(4, 4, 10)$ $1$ $152.7$ $0.3232$ $69:C_2$ $(4, 4, 10)$ $2$ $173.8$ $0.4168$ $125:C_I$ $(3, 6, 9)$ $2$ $152.7$ $0.3456$ $155:C_I$ $(3, 6, 9)$ $2$ $173.8$ $0.1924$ $217:C_I$ $(3, 6, 9)$ $2$ $152.9$ $0.3276$ $245:C_I$ $(4, 4, 10)$ $0$ $173.8$ $0.2348$	$200:C_{I}$	(4, 4, 10)	3	149.9	0.3559	133: <i>C</i> <sub>1</sub>	(3, 6, 9)	3	170.4	0.1034
$39:C_I$ $(2, 8, 8)$ 7 $150.8$ $0.0961$ $251:D_2$ $(4, 4, 10)$ 0 $171.9$ $0.1376$ $167:C_I$ $(3, 6, 9)$ 3 $151.5$ $0.2082$ $75:C_I$ $(4, 4, 10)$ 3 $172.0$ $0.3393$ $124:C_I$ $(2, 8, 8)$ 5 $152.6$ $0.121$ $132:C_I$ $(2, 8, 8)$ 7 $173.4$ $0.1201$ $157:C_I$ $(4, 4, 10)$ 1 $152.7$ $0.3232$ $69:C_2$ $(4, 4, 10)$ 2 $173.8$ $0.4168$ $125:C_I$ $(3, 6, 9)$ 2 $152.7$ $0.3456$ $155:C_I$ $(3, 6, 9)$ 2 $173.8$ $0.1924$ $217:C_I$ $(3, 6, 9)$ 2 $152.9$ $0.3276$ $245:C_I$ $(4, 4, 10)$ 0 $173.8$ $0.2348$	38: <i>C</i> <sub>1</sub>	(1, 10, 7)	13	150.3	0.0982	$208:C_2$	(2, 8, 8)	7	171.1	0.005
$167:C_I$ $(3, 6, 9)$ $3$ $151.5$ $0.2082$ $75:C_I$ $(4, 4, 10)$ $3$ $172.0$ $0.3393$ $124:C_I$ $(2, 8, 8)$ $5$ $152.6$ $0.121$ $132:C_I$ $(2, 8, 8)$ $7$ $173.4$ $0.1201$ $157:C_I$ $(4, 4, 10)$ $1$ $152.7$ $0.3232$ $69:C_2$ $(4, 4, 10)$ $2$ $173.8$ $0.4168$ $125:C_I$ $(3, 6, 9)$ $2$ $152.7$ $0.3456$ $155:C_I$ $(3, 6, 9)$ $2$ $173.8$ $0.1924$ $217:C_I$ $(3, 6, 9)$ $2$ $152.9$ $0.3276$ $245:C_I$ $(4, 4, 10)$ $0$ $173.8$ $0.2348$	39: <i>C</i> <sub>1</sub>	(2, 8, 8)	7	150.8	0.0961	251:D <sub>2</sub>	(4, 4, 10)	0	171.9	0.1376
$124:C_I$ $(2, 8, 8)$ $5$ $152.6$ $0.121$ $132:C_I$ $(2, 8, 8)$ $7$ $173.4$ $0.1201$ $157:C_I$ $(4, 4, 10)$ $1$ $152.7$ $0.3232$ $69:C_2$ $(4, 4, 10)$ $2$ $173.8$ $0.4168$ $125:C_I$ $(3, 6, 9)$ $2$ $152.7$ $0.3456$ $155:C_I$ $(3, 6, 9)$ $2$ $173.8$ $0.1924$ $217:C_I$ $(3, 6, 9)$ $2$ $152.9$ $0.3276$ $245:C_I$ $(4, 4, 10)$ $0$ $173.8$ $0.2348$	$167:C_{I}$	(3, 6, 9)	3	151.5	0.2082	75: <i>C</i> <sub>1</sub>	(4, 4, 10)	3	172.0	0.3393
$157:C_I$ $(4, 4, 10)$ 1 $152.7$ $0.3232$ $69:C_2$ $(4, 4, 10)$ 2 $173.8$ $0.4168$ $125:C_I$ $(3, 6, 9)$ 2 $152.7$ $0.3456$ $155:C_I$ $(3, 6, 9)$ 2 $173.8$ $0.1924$ $217:C_I$ $(3, 6, 9)$ 2 $152.9$ $0.3276$ $245:C_I$ $(4, 4, 10)$ 0 $173.8$ $0.2348$	$124:C_{I}$	(2, 8, 8)	5	152.6	0.121	132: <i>C</i> <sub>1</sub>	(2, 8, 8)	7	173.4	0.1201
$125:C_I$ $(3, 6, 9)$ $2$ $152.7$ $0.3456$ $155:C_I$ $(3, 6, 9)$ $2$ $173.8$ $0.1924$ $217:C_I$ $(3, 6, 9)$ $2$ $152.9$ $0.3276$ $245:C_I$ $(4, 4, 10)$ $0$ $173.8$ $0.2348$	157: <i>C</i> <sub>1</sub>	(4, 4, 10)	1	152.7	0.3232	69: <i>C</i> <sub>2</sub>	(4, 4, 10)	2	173.8	0.4168
$217:C_I \qquad (3, 6, 9) \qquad 2 \qquad 152.9 \qquad 0.3276 \qquad 245:C_I \qquad (4, 4, 10) \qquad 0 \qquad 173.8 \qquad 0.2348$	$125:C_{I}$	(3, 6, 9)	2	152.7	0.3456	155: <i>C</i> <sub>1</sub>	(3, 6, 9)	2	173.8	0.1924
	217: <i>C</i> <sub>1</sub>	(3, 6, 9)	2	152.9	0.3276	245: <i>C</i> <sub>1</sub>	(4, 4, 10)	0	173.8	0.2348

234: <i>C</i> <sub>1</sub>	(4, 4, 10)	2	173.9	0.1993	238:C <sub>2</sub>	(2, 8, 8)	7	193.0	0.0397
190: <i>C</i> <sub>1</sub>	(3, 6, 9)	5	173.9	0.2466	197: <i>C</i> <sub>1</sub>	(4, 4, 10)	2	193.9	0.0957
$209:C_{I}$	(3, 6, 9)	4	174.9	0.4143	213: <i>C</i> <sub>1</sub>	(3, 6, 9)	4	194.2	0.1415
203:C <sub>1</sub>	(2, 8, 8)	7	174.9	0.2568	207: <i>C</i> <sub>1</sub>	(2, 8, 8)	6	194.2	0.0309
161: <i>C</i> <sub>2</sub>	(4, 4, 10)	0	175.2	0.1070	274: <i>C</i> <sub>2</sub>	(2, 8, 8)	8	194.3	0.1296
201: <i>C</i> <sub>1</sub>	(2, 8, 8)	6	175.3	0.1400	281: <i>C</i> <sub>1</sub>	(3, 6, 9)	3	195	0.3391
170:D <sub>2</sub>	(4, 4, 10)	2	175.6	0.2528	165: <i>C</i> <sub>1</sub>	(3, 6, 9)	4	195.2	0.1989
103: <i>C</i> <sub>2</sub>	(2, 8, 8)	10	175.7	0.0504	226: <i>C</i> <sub>1</sub>	(2, 8, 8)	6	195.3	0.0594
122: <i>C</i> <sub>1</sub>	(3, 6, 9)	5	176.6	0.1763	199: <i>C</i> <sub>s</sub>	(3, 6, 9)	5	195.5	0.3157
50: <i>C</i> <sub>2</sub>	(2, 8, 8)	7	176.8	0.0999	182: <i>D</i> <sub>2</sub>	(4, 4, 10)	0	196.1	0.1563
181: <i>C</i> <sub>1</sub>	(2, 8, 8)	6	176.8	0.2432	128: <i>C</i> <sub>1</sub>	(3, 6, 9)	4	196.5	0.0011
218: <i>C</i> <sub>1</sub>	(3, 6, 9)	3	176.9	0.2046	353:C <sub>s</sub>	(5, 2, 11)	0	197.3	0.4207
196: <i>C</i> 1	(4, 4, 10)	3	177.3	0.1637	271: <i>C</i> <sub>1</sub>	(4, 4, 10)	2	197.6	0.3692
253:D <sub>2</sub>	(4, 4, 10)	0	177.3	0.3783	313:D <sub>2</sub>	(4, 4, 10)	1	198.1	0.0527
$211:C_{I}$	(3, 6, 9)	5	178.4	0.2301	292: <i>C</i> <sub>1</sub>	(4, 4, 10)	1	198.1	0.1097
355:C <sub>1</sub>	(5, 2, 11)	0	178.5	0.0000	289:C <sub>2</sub>	(4, 4, 10)	2	198.9	0.3046
185: <i>C</i> <sub>1</sub>	(3, 6, 9)	3	179.0	0.1619	248:C <sub>1</sub>	(4, 4, 10)	1	199.3	0.3051
360: <i>C</i> <sub>s</sub>	(5, 2, 11)	0	179.2	0.1679	127: <i>C</i> <sub>1</sub>	(3, 6, 9)	4	200.6	0.0284
214: <i>C</i> <sub>1</sub>	(2, 8, 8)	9	180.2	0.1146	129: <i>C</i> <sub>s</sub>	(3, 6, 9)	4	200.8	0.0542
162: <i>C</i> <sub>s</sub>	(3, 6, 9)	5	181.6	0.1967	220: <i>C</i> <sub>1</sub>	(3, 6, 9)	4	201.5	0.1257
311:C <sub>2h</sub>	(4, 4, 10)	0	182.0	0.2947	243:C <sub>1</sub>	(3, 6, 9)	3	201.6	0.2373
224: <i>C</i> <sub>1</sub>	(3, 6, 9)	5	182.0	0.2711	193: <i>C</i> <sub>s</sub>	(3, 6, 9)	9	201.7	0.1453
131: <i>C</i> <sub>1</sub>	(3, 6, 9)	2	182.6	0.2278	225:C <sub>2</sub>	(4, 4, 10)	0	201.7	0.3637
$186:C_{I}$	(3, 6, 9)	3	183.7	0.0874	117: <i>C</i> <sub>1</sub>	(3, 6, 9)	3	202.2	0.1936
$166:C_1$	(4, 4, 10)	2	183.9	0.1201	293: <i>C</i> <sub>s</sub>	(4, 4, 10)	0	203.3	0.1125
143: <i>C</i> <sub>1</sub>	(3, 6, 9)	3	185.3	0.029	230: <i>C</i> <sub>1</sub>	(3, 6, 9)	6	203.4	0.0683
139: <i>C</i> <sub>s</sub>	(1, 10, 7)	13	185.4	0.0728	194: <i>C</i> <sub>1</sub>	(3, 6, 9)	6	204.3	0.0699
235: <i>C</i> <sub>s</sub>	(2, 8, 8)	10	185.7	0.2391	250: <i>C</i> <sub>2</sub>	(4, 4, 10)	0	204.4	0.0914
259:C <sub>2</sub>	(4, 4, 10)	1	186.0	0.3843	137: <i>C</i> <sub>1</sub>	(4, 4, 10)	1	204.5	0.2693
176: <i>C</i> <sub>1</sub>	(3, 6, 9)	3	186.0	0.2275	192: <i>C</i> <sub>1</sub>	(3, 6, 9)	4	204.6	0.0622
275:C <sub>1</sub>	(3, 6, 9)	5	186.2	0.1527	242: <i>C</i> <sub>1</sub>	(3, 6, 9)	4	205.5	0.0282
216: <i>C</i> <sub>s</sub>	(3, 6, 9)	4	187.2	0.0586	156: <i>C</i> <sub>2</sub>	(4, 4, 10)	1	206.2	0.3983
229: $C_s$	(2, 8, 8)	5	187.2	0.1146	115: <i>C</i> <sub>1</sub>	(3, 6, 9)	4	206.9	0.0293
354: <i>C</i> <sub>2</sub>	(5, 2, 11)	0	188.8	0.2454	237:C <sub>1</sub>	(3, 6, 9)	4	206.9	0.1695
$140:C_2$	(2, 8, 8)	11	189.9	0.0066	254:C <sub>2h</sub>	(4, 4, 10)	0	207.1	0.1452
278:D <sub>2</sub>	(4, 4, 10)	0	190.1	0.1531	301: <i>C</i> <sub>1</sub>	(3, 6, 9)	5	207.3	0.1062
121:D <sub>2</sub>	(2, 8, 8)	6	190.5	0.1796	303: <i>C</i> <sub>2</sub>	(2, 8, 8)	9	208.8	0.1816
187: <i>C</i> <sub>1</sub>	(4, 4, 10)	2	190.6	0.3605	227:C <sub>1</sub>	(3, 6, 9)	3	209.2	0.1614
249: <i>C</i> <sub>1</sub>	(4, 4, 10)	1	191.0	0.2364	272: <i>C</i> <sub>s</sub>	(3, 6, 9)	2	210.3	0.254
231: <i>C</i> <sub>1</sub>	(3, 6, 9)	6	191.1	0.0928	273:C <sub>1</sub>	(3, 6, 9)	4	211.3	0.2292
$252:C_2$	(4, 4, 10)	1	191.3	0.1785	221: <i>C</i> <sub>1</sub>	(2, 8, 8)	6	211.6	0.0527
$222:C_{I}$	(3, 6, 9)	3	191.5	0.0169	206: <i>C</i> <sub>1</sub>	(3, 6, 9)	5	212.4	0.1775
48: <i>C</i> <sub>1</sub>	(3, 6, 9)	5	191.8	0.1021	291: <i>C</i> <sub>s</sub>	(3, 6, 9)	4	216.6	0.0971
256:C <sub>1</sub>	(3, 6, 9)	4	192.1	0.0273	228:C <sub>1</sub>	(3, 6, 9)	5	217.6	0.2271

204: <i>C</i> <sub>1</sub>	(3, 6, 9)	4	217.6	0.0808	304: <i>C</i> <sub>1</sub>	(3, 6, 9)	3	256.2	0.1834
255:C <sub>1</sub>	(4, 4, 10)	2	218.1	0.2174	212: <i>C</i> <sub>1</sub>	(4, 4, 10)	2	256.4	0.1998
80: <i>C</i> <sub>2</sub>	(4, 4, 10)	3	218.2	0.0921	261: <i>C</i> <sub>1</sub>	(4, 4, 10)	1	257.1	0.1120
$280:C_s$	(3, 6, 9)	4	218.5	0.1588	308: <i>C</i> <sub>1</sub>	(3, 6, 9)	3	259.2	0.2332
359:C <sub>s</sub>	(5, 2, 11)	0	218.7	0.3861	305: <i>C</i> <sub>1</sub>	(3, 6, 9)	5	260.2	0.1705
$263:C_s$	(3, 6, 9)	4	218.8	0.0905	322:C <sub>s</sub>	(2, 8, 8)	12	260.6	0.1714
205:C <sub>1</sub>	(3, 6, 9)	3	219.3	0.2384	$262:C_s$	(3, 6, 9)	5	260.7	0.2412
$202:C_{I}$	(2, 8, 8)	7	219.4	0.1277	264: <i>C</i> <sub>1</sub>	(4, 4, 10)	3	260.9	0.1675
135:C <sub>1</sub>	(3, 6, 9)	3	220.2	0.2036	361: <i>C</i> <sub>1</sub>	(5, 2, 11)	0	260.9	0.1221
$188:C_{I}$	(4, 4, 10)	2	220.3	0.3108	285:D <sub>2</sub>	(2, 8, 8)	6	266.0	0.0430
257:C <sub>s</sub>	(4, 4, 10)	1	221.1	0.3739	306: <i>C</i> <sub>2</sub>	(4, 4, 10)	0	266.1	0.0429
270: <i>C</i> <sub>1</sub>	(3, 6, 9)	6	221.4	0.0205	$258:C_2$	(4, 4, 10)	2	267.1	0.3473
236:C <sub>2h</sub>	(2, 8, 8)	8	222.3	0.1232	358: <i>C</i> <sub>1</sub>	(5, 2, 11)	0	268.4	0.3113
279:C <sub>1</sub>	(4, 4, 10)	2	225.1	0.0386	284:D <sub>2</sub>	(3, 6, 9)	4	273.2	0.2955
244: <i>C</i> 1	(3, 6, 9)	4	225.2	0.0557	307: <i>C</i> 1	(4, 4, 10)	3	273.6	0.3033
232:C <sub>1</sub>	(3, 6, 9)	4	225.8	0.1280	310: <i>C</i> <sub>1</sub>	(4, 4, 10)	1	274.1	0.1646
152: <i>C</i> <sub>2v</sub>	(3, 6, 9)	2	226.0	0.0096	290:D <sub>2</sub>	(4, 4, 10)	2	274.9	0.1815
195: <i>C</i> <sub>1</sub>	(3, 6, 9)	5	226.5	0.0555	343:C <sub>s</sub>	(5, 2, 11)	0	277.7	0.0286
294: <i>C</i> 1	(3, 6, 9)	4	226.6	0.1323	299: <i>C</i> <sub>1</sub>	(4, 4, 10)	3	280.2	0.1857
269: <i>C</i> <sub>1</sub>	(3, 6, 9)	4	228.3	0.1392	315: <i>C</i> <sub>1</sub>	(4, 4, 10)	5	280.2	0.0838
219: <i>C</i> <sub>1</sub>	(4, 4, 10)	1	228.5	0.0521	300: <i>C</i> <sub>2</sub>	(4, 4, 10)	5	282.8	0.1125
268:C <sub>1</sub>	(4, 4, 10)	1	229.3	0.1486	327: <i>C</i> <sub>1</sub>	(3, 6, 9)	5	283.3	0.1028
246: <i>C</i> <sub>1</sub>	(4, 4, 10)	2	229.9	0.2147	265: <i>C</i> <sub>1</sub>	(4, 4, 10)	3	283.5	0.1332
175:D <sub>2</sub>	(4, 4, 10)	2	231.7	0.1788	316: <i>C</i> <sub>1</sub>	(4, 4, 10)	0	283.5	0.2725
342: <i>C</i> <sub>s</sub>	(5, 2, 11)	0	232.1	0.0000	334:D <sub>2</sub>	(2, 8, 8)	8	283.6	0.1885
276: <i>C</i> <sub>s</sub>	(3, 6, 9)	5	234.3	0.2091	298: <i>C</i> <sub>1</sub>	(4, 4, 10)	3	284.3	0.2452
288:C <sub>1</sub>	(4, 4, 10)	2	234.7	0.2232	296: <i>C</i> <sub>s</sub>	(4, 4, 10)	2	291.1	0.2862
282:C <sub>1</sub>	(3, 6, 9)	3	234.9	0.1606	317: <i>C</i> <sub>1</sub>	(3, 6, 9)	5	294.9	0.1177
286: <i>C</i> 1	(3, 6, 9)	7	235.5	0.1983	351: <i>C</i> <sub>s</sub>	(5, 2, 11)	0	295.3	0.1942
362: <i>C</i> <sub>s</sub>	(5, 2, 11)	0	235.5	0.061	319: <i>C</i> <sub>1</sub>	(3, 6, 9)	5	295.4	0.2743
309: <i>C</i> 1	(3, 6, 9)	4	237.2	0.2158	328: <i>C</i> <sub>1</sub>	(4, 4, 10)	2	295.4	0.0329
295: <i>C</i> <sub>s</sub>	(4, 4, 10)	2	237.9	0.0887	314: <i>C</i> <sub>2</sub>	(4, 4, 10)	2	296.8	0.3688
267:C <sub>1</sub>	(4, 4, 10)	2	237.9	0.0937	266: <i>C</i> <sub>s</sub>	(4, 4, 10)	3	296.9	0.3336
247: <i>C</i> <sub>3</sub>	(3, 6, 9)	3	238.3	0.3872	344: <i>C</i> 1	(5, 2, 11)	0	298.2	0.2104
297:C <sub>2</sub>	(4, 4, 10)	0	240.6	0.294	318: <i>C</i> <sub>2</sub>	(4, 4, 10)	1	298.5	0.0286
287: <i>C</i> 1	(4, 4, 10)	2	242.7	0.2107	348: <i>C</i> 1	(5, 2, 11)	0	298.7	0.208
283:C <sub>1</sub>	(3, 6, 9)	4	246.9	0.194	337:C <sub>2</sub>	(4, 4, 10)	2	299.9	0.0117
277:C <sub>1</sub>	(2, 8, 8)	8	247.2	0.1294	321:C <sub>1</sub>	(4, 4, 10)	0	300.6	0.0361
149: <i>C</i> <sub>2</sub>	(4, 4, 10)	2	248.1	0.3693	331:C <sub>s</sub>	(4, 4, 10)	2	301.9	0.0546
312: <i>C</i> <sub>1</sub>	(3, 6, 9)	5	248.1	0.1707	345:C <sub>1</sub>	(5, 2, 11)	0	302.9	0.1762
260: <i>C</i> <sub>1</sub>	(3, 6, 9)	3	251.4	0.3315	329: <i>C</i> <sub>1</sub>	(4, 4, 10)	1	303.8	0.0288
233:C <sub>2</sub>	(4, 4, 10)	2	253.4	0.0827	346: <i>C</i> <sub>1</sub>	(5, 2, 11)	0	310.2	0.1086
302:D <sub>2</sub>	(2, 8, 8)	10	254.6	0.1512	332: <i>C</i> <sub>s</sub>	(4, 4, 10)	3	315.5	0.0763
198: <i>C</i> <sub>1</sub>	(4, 4, 10)	2	255.7	0.0683	320: <i>C</i> <sub>1</sub>	(3, 6, 9)	4	317.5	0.0896
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325:C <sub>1</sub>	(4, 4, 10)	2	317.8	0.1981	330:C <sub>1</sub>	(4, 4, 10)	1	331.9	0.1745
347:C <sub>2</sub>	(6, 0, 12)	0	319.8	0.2489	339: <i>C</i> <sub>1</sub>	(4, 4, 10)	2	338.3	0.183
336:C <sub>2</sub>	(4, 4, 10)	2	321.4	0.3297	326: <i>C</i> <sub>1</sub>	(4, 4, 10)	1	347.0	0.0792
323:C <sub>1</sub>	(3, 6, 9)	4	322.6	0.1485	349: <i>C</i> <sub>1</sub>	(5, 2, 11)	0	352.8	0.3553
324: <i>C</i> <sub>1</sub>	(4, 4, 10)	1	326.6	0.1004	352: <i>C</i> <sub>1</sub>	(5, 2, 11)	0	355.1	0.276
350:C <sub>2</sub>	(6, 0, 12)	0	326.8	0.2585	333:C <sub>2</sub>	(4, 4, 10)	1	377.0	0.1124
335:C <sub>1</sub>	(4, 4, 10)	0	328.9	0.2379	341:C <sub>2h</sub>	(4, 4, 10)	2	401.4	0.1618
338:C <sub>1</sub>	(4, 4, 10)	2	330.2	0.1475	340: <i>C</i> <sub>2</sub>	(4, 4, 10)	2	405.0	0.1727

<sup>[a]</sup> Heat of formation obtained at AM1 level, units in kilocalories per mole; band gap calculated at the HMO level, in units of  $|\beta|$ , where  $\beta$  is the Hückel resonance integral. <sup>[b]</sup> Numbering convention of isomers recommended in ref 41. <sup>[c]</sup> Ring Index: number of four-, five-, and six- membered rings. <sup>[d]</sup> PA: number of pentagon adjacency.

Table S2 Relative energies of the most stable  $C_{32}$  fullerene isomers<sup>[a]</sup>

label:sym	<u>B3LYP/6-31G(d)</u>	<u>B3LYP/6-311G(d, p)</u>	<u>PBE1PBE/6-311G(d, p)</u>	<u>HF/6-311G(d, p)</u>
<b>32</b> :D <sub>4d</sub>	0	0	0	0
<b>1</b> : <i>D</i> <sub>3</sub>	4.17	2.93	2.42	11.11
<b>5</b> : <i>C</i> <sub>s</sub>	10.21	9.63	9.54	16.24

<sup>[a]</sup> Relative energy units in kilocalories per mole.



Fig. S1 Transition state of rearrangement between 32 and 5 (TS1-A). Bond lengths (in Å) obtained at PBE1PBE/6-31G(d) level of theory.



**Fig. S2** Plot of the intrinsic reaction coordinate (in  $amu^{-1/2}$  Bohr) versus energy (in kcal mol<sup>-1</sup>, relative to **32**, starting from TS1-A as computed at the PBE1PBE/6-31G(d) level of theory.



Fig. S3 Transition states of rearrangement between 5 and 1 (TS2-Aa and TS2-Ab). Bond lengths (in Å) obtained at PBE1PBE/6-31G(d) level of theory.



IRC starting from TS2-Ab

**Fig. S4** Plot of the intrinsic reaction coordinate (in  $amu^{-1/2}$  Bohr) versus energy (in kcal mol<sup>-1</sup>, relative to **32**, starting from TS2-Aa and TS2-Ab as computed at the PBE1PBE/6-31G(d) level of theory.



Fig. S5 Transition state of rearrangement between 32 and 5 (TS1-B1). Bond lengths (in Å) obtained at PBE1PBE/6-31G(d) level of theory.



**Fig. S6** Plot of the intrinsic reaction coordinate (in  $amu^{-1/2}$  Bohr) versus energy (in kcal mol<sup>-1</sup>, relative to **32**, starting from TS1-B1 as computed at the PBE1PBE/6-31G(d) level of theory.



Fig. S7 Transition state of rearrangement between 5 and 1 (TS2-B1c). Bond lengths (in Å) obtained at PBE1PBE/6-31G(d) level of theory.



**Fig. S8** Plot of the intrinsic reaction coordinate (in  $amu^{-1/2}$  Bohr) versus energy (in kcal mol<sup>-1</sup>, relative to **32**, starting from TS2-B1c as computed at the PBE1PBE/6-31G(d) level of theory.



Fig. S9 Transition state of rearrangement between 5 and 1 (TS2-B1d). Bond lengths (in Å) obtained at PBE1PBE/6-31G(d) level of theory.



**Fig. S10** Plot of the intrinsic reaction coordinate (in  $\text{amu}^{-1/2}$  Bohr) versus energy (in kcal mol<sup>-1</sup>, relative to **32**, starting from TS2-B1d as computed at the PBE1PBE/6-31G(d) level of theory.



Fig. S11 Transition state of rearrangement between 32 and 5 (TS1-B2). Bond lengths (in Å) obtained at PBE1PBE/6-31G(d) level of theory.



**Fig. S12** Plot of the intrinsic reaction coordinate (in  $\text{amu}^{-1/2}$  Bohr) versus energy (in kcal mol<sup>-1</sup>, relative to **32**, starting from TS1-B2 as computed at the PBE1PBE/6-31G(d) level of theory.



Fig. S13 Transition state of rearrangement between 5 and 1 (TS2-B2e). Bond lengths (in Å) obtained at PBE1PBE/6-31G(d) level of theory.



**Fig. S14** Plot of the intrinsic reaction coordinate (in  $\text{amu}^{-1/2}$  Bohr) versus energy (in kcal  $\text{mol}^{-1}$ , relative to **32**, starting from TS2-B2e as computed at the PBE1PBE/6-31G(d) level of theory.



Fig. S15 Transition state of rearrangement between 5 and 1 (TS2-B2f). Bond lengths (in Å) obtained at PBE1PBE/6-31G(d) level of theory.



**Fig. S16** Plot of the intrinsic reaction coordinate (in  $\text{amu}^{-1/2}$  Bohr) versus energy (in kcal mol<sup>-1</sup>, relative to **32**, starting from TS2-B2f as computed at the PBE1PBE/6-31G(d) level of theory.



Scheme S1. The GSWT relationship and transition states (TS1-A, TS2-Aa and TS2-Ab) between  $32:D_{4d}$ ,  $5:C_s$  and  $1:D_3$  of concerted reaction mechanism. Relative energies of structures (in kcal mol<sup>-1</sup>) at PBE1PBE/6-31G(d) level of theory.



**Scheme S2.** The GSWT relationship and transition states (TS1-B1, TS2-B1c and TS2-B1d) between  $32:D_{4d}$ ,  $5:C_s$  and  $1:D_3$  of stepwise reaction mechanism. Relative energies of structures (in kcal mol<sup>-1</sup>) obtained at PBE1PBE/6-31G(d) level of theory.



**Scheme S3.** The GSWT relationship and transition states (TS1-B2, TS2-B2e and TS2-B2f) between **32**: $D_{4d}$ , **5**: $C_s$  and **1**: $D_3$  of stepwise reaction mechanism. Relative energies of structures (in kcal mol<sup>-1</sup>) obtained at PBE1PBE/6-31G(d) level of theory.