

## 符合独立五元环规则的 $C_{100}(417)Cl_{28}$ 形成机理的密度泛函理论研究

尹凡华, 谭凯\*

厦门大学化学化工学院, 福建省理论与计算重点实验室, 福建 厦门 361005

## Density Functional Theory Study on the Formation Mechanism of Isolated-Pentagon-Rule $C_{100}(417)Cl_{28}$

YIN Fanhua, TAN Kai\*

Fujian Provincial Key Laboratory of Theoretical and Computational Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, Fujian Province, P. R. China

\*Corresponding author. Email: ktan@xmu.edu.cn; Tel: +86-592-2182826.

表 S1 C<sub>100</sub> IPR 异构体的相对能量( $E_r$  单位  $\text{kJ}\cdot\text{mol}^{-1}$ ), HOMO-LUMO 能隙( $\Delta$  单位  $\text{eV}$ )<sup>a</sup>

Table S1 Relative energies ( $E_r$  in  $\text{kJ}\cdot\text{mol}^{-1}$ ) of the C<sub>100</sub> IPR fullerene isomers, HOMO-LUMO gap ( $\Delta$  in  $\text{eV}$ )<sup>a</sup>.

Rank(B3LYP/6-31G*/PM3)	FM: Sym	$\Delta$	$E_r$			
			B3LYP/6-31G*	PM3 <sup>1,2</sup>	AM1 <sup>1,3</sup>	PBE1PBE/6-311G* <sup>4</sup>
1/1	449:D <sub>2</sub>	1.20	0.00	0.00	0.00	0.00
2/9	425:C <sub>1</sub>	1.32	2.93	38.07	38.07	0.04
3/3	442:C <sub>2</sub>	1.20	5.72	26.36	27.20	1.09
4/28	173:C <sub>1</sub>	1.09	9.74	62.34		5.02
5/4	440:C <sub>2</sub>	1.19	10.83	28.45	27.20	9.00
6/7	426:C <sub>1</sub>	1.30	17.40	31.38	35.98	
7/67	448:C <sub>2</sub>	1.01	18.30	83.26		
8/17	382:C <sub>1</sub>	1.35	19.41	49.37		
9/148	253:C <sub>1</sub>	0.99	22.54	108.78		
10/57	95:C <sub>1</sub>	1.39	22.54	76.15		
11/38	427:C <sub>1</sub>	1.05	24.41	65.69		
12/25	384:C <sub>1</sub>	1.28	24.88	60.67		
13/139	248:C <sub>1</sub>	1.14	28.45	104.60		
14/40	303:C <sub>1</sub>	1.33	28.63	66.11		
15/15	232:C <sub>1</sub>	1.34	30.58	48.53		
16/10	174:C <sub>2</sub>	0.86	30.83	41.84	41.84	
17/2	18:C <sub>2</sub>	1.87	30.95	20.92	20.08	
18/16	380:C <sub>1</sub>	1.05	31.31	48.53		
19/35	321:T	0.80	31.47	64.43		
20/121	441:C <sub>1</sub>	0.74	31.58	100.42		
21/56	383:C <sub>1</sub>	1.32	32.35	75.31		
22/11	216:C <sub>1</sub>	1.42	32.63	43.10		
23/13	424:C <sub>1</sub>	1.33	33.03	48.12		
24/37	432:D <sub>2</sub>	1.43	33.04	65.69		
25/50	357:C <sub>1</sub>	0.92	33.73	71.96		
26/12	445:D <sub>2</sub>	1.53	33.89	44.77	54.81	
27/39	414:C <sub>s</sub>	1.26	35.86	66.11		
281/64	254:C <sub>1</sub>	0.98	35.88	116.73		
29/48	71:C <sub>1</sub>	1.28	36.06	71.55		
30/58	412:C <sub>1</sub>	1.07	36.94	76.57		
31/34	431:D <sub>2</sub>	1.46	37.19	64.02		
32/29	344:C <sub>1</sub>	1.29	37.47	62.76		
33/80	260:C <sub>1</sub>	1.01	37.86	86.61		
34/127	323:C <sub>1</sub>	1.00	38.47	102.51		
35/5	148:C <sub>1</sub>	1.58	39.02	30.96	35.15	
36/109	322:C <sub>3</sub>	0.65	40.52	97.07		
37/69	308:C <sub>1</sub>	1.29	41.09	84.10		
38/53	214:C <sub>1</sub>	1.19	41.36	73.22		
39/150	172:C <sub>1</sub>	1.01	41.73	109.62		
40/66	77:C <sub>1</sub>	1.15	43.41	82.84		
41/23	149:C <sub>2</sub>	1.50	43.52	58.58		

---

42/70	122:C <sub>1</sub>	1.33	44.03	84.10	
43/118	428:C <sub>1</sub>	0.82	44.47	99.16	
44/152	409:C <sub>1</sub>	1.01	44.59	110.46	
45/137	147:C <sub>1</sub>	1.13	45.04	104.18	
46/136	175:C <sub>1</sub>	1.19	45.30	104.18	
47/102	258:C <sub>1</sub>	0.95	46.34	94.14	
48/18	168:C <sub>1</sub>	1.07	46.71	51.04	
49/68	261:C <sub>1</sub>	0.89	48.00	84.10	
50/55	358:C <sub>1</sub>	1.07	49.32	75.31	
51/60	73:C <sub>1</sub>	1.37	50.02	76.99	
52/14	297:C <sub>1</sub>	1.51	51.19	48.53	55.23
53/241	439:C <sub>2</sub>	0.54	51.66	138.07	
54/46	170:C <sub>1</sub>	1.18	51.76	68.62	
55/65	313:C <sub>1</sub>	1.03	52.14	82.84	
56/24	89:C <sub>1</sub>	1.73	52.60	59.83	
57/77	371:C <sub>1</sub>	0.93	52.99	85.77	
58/84	103:C <sub>2</sub>	1.10	53.25	88.28	
59/43	256:C <sub>1</sub>	0.65	53.33	66.53	
60/113	374:C <sub>1</sub>	1.01	53.43	97.91	
61/204	430:C <sub>2</sub>	0.54	53.83	128.87	
62/147	118:C <sub>1</sub>	1.11	53.85	108.37	
63/21	446:C <sub>2</sub>	1.48	54.09	57.32	
64/155	127:C <sub>s</sub>	1.27	54.27	112.13	
65/126	362:C <sub>1</sub>	0.99	54.28	102.51	
66/106	373:C <sub>1</sub>	1.08	54.43	95.81	
67/19	444:C <sub>s</sub>	1.34	54.58	54.39	
68/20	415:C <sub>1</sub>	1.21	54.66	56.90	
69/47	163:C <sub>1</sub>	1.59	55.13	70.29	
70/26	422:C <sub>2</sub>	1.55	55.27	61.09	
71/36	423:C <sub>1</sub>	1.77	55.47	64.85	
72/151	377:C <sub>1</sub>	0.91	55.52	110.04	
73/33	419:C <sub>1</sub>	1.74	55.87	63.60	
74/202	249:C <sub>1</sub>	1.07	56.87	128.87	
75/116	219:C <sub>1</sub>	1.15	56.92	98.32	
76/203	242:C <sub>1</sub>	1.08	57.48	128.87	
77/128	402:C <sub>2</sub>	0.76	58.89	102.93	
78/85	210:C <sub>1</sub>	1.40	59.00	88.70	
79/237	255:C <sub>1</sub>	0.95	59.41	137.65	
80/221	363:C <sub>1</sub>	1.11	59.54	133.89	
81/30	144: C <sub>1</sub>	1.57	59.91	62.76	
82/184	134:C <sub>1</sub>	1.04	60.00	123.01	
83/62	167: C <sub>1</sub>	0.91	60.45	77.40	
84/41	354: C <sub>s</sub>	1.12	60.59	66.53	
85/105	218: C <sub>1</sub>	1.01	60.85	95.40	
86/260	369: C <sub>1</sub>	0.83	61.25	147.28	
87/54	408: C <sub>1</sub>	1.22	61.74	73.64	

---

---

88/223	247: C <sub>1</sub>	1.06	61.81	133.89	
89/64	399:C <sub>1</sub>	1.04	61.87	79.08	
90/199	245: C <sub>1</sub>	0.98	62.12	127.61	
91/243	370:C <sub>1</sub>	0.79	62.86	139.75	
92/95	257:C <sub>1</sub>	0.95	63.12	91.21	
93/205	94:C <sub>1</sub>	1.44	63.37	129.29	
94/143	120:C <sub>1</sub>	1.11	64.20	105.86	
95/87	348:C <sub>1</sub>	1.34	64.21	89.12	
96/59	268:C <sub>1</sub>	1.09	64.77	76.57	
97/51	98:C <sub>2</sub>	1.49	65.13	72.80	
98/157	304:C <sub>2</sub>	1.54	65.59	112.97	
99/166	202:C <sub>1</sub>	1.04	65.70	117.15	
100/231	378:C <sub>2</sub>	0.78	65.73	135.98	
101/104	360:C <sub>1</sub>	1.01	65.88	95.40	
102/269	250:C <sub>1</sub>	0.79	65.99	150.21	
103/72	345:C <sub>s</sub>	1.24	66.36	84.52	
104/96	437:C <sub>1</sub>	0.96	67.08	92.47	
105/89	162:C <sub>1</sub>	1.11	67.17	89.54	
106/225	413:C <sub>2</sub>	1.21	67.32	134.72	
107/93	217:C <sub>1</sub>	1.14	67.69	90.37	
108/132	72:C <sub>1</sub>	1.37	67.70	103.76	
109/98	17:C <sub>1</sub>	1.08	68.02	93.30	
110/27	75:C <sub>1</sub>	1.08	68.32	61.92	
111/6	12:C <sub>1</sub>	1.42	68.39	31.38	31.80
112/32	286:C <sub>1</sub>	1.58	68.47	63.60	
113/156	434:C <sub>1</sub>	0.78	68.58	112.55	
114/259	416:C <sub>1</sub>	0.67	68.60	146.86	
115/134	436:C <sub>1</sub>	0.76	68.83	104.18	
116/75	397:C <sub>1</sub>	0.99	68.88	84.94	
117/42	151:C <sub>2</sub>	1.27	69.33	66.53	
118/78	152:C <sub>1</sub>	1.06	69.38	86.61	
119/117	183:C <sub>1</sub>	1.23	69.42	98.32	
120/208	243:C <sub>1</sub>	1.10	69.45	130.12	
121/86	320:C <sub>1</sub>	1.36	69.73	88.70	
122/163	350:C <sub>2</sub>	1.23	70.83	116.32	
123/97	353:C <sub>1</sub>	0.97	70.89	92.88	
124/176	309:C <sub>1</sub>	1.02	71.45	120.08	
125/119	129:C <sub>1</sub>	0.87	71.67	99.16	
126/63	417:C <sub>2v</sub>	1.85	71.97	78.24	
127/160	379:C <sub>1</sub>	0.85	72.42	116.32	
128/44	139:C <sub>2</sub>	1.30	72.73	66.94	
129/122	299:C <sub>1</sub>	1.27	73.41	100.83	
130/115	145:C <sub>1</sub>	1.43	73.68	98.32	
131/74	90:C <sub>s</sub>	1.78	73.77	84.94	
132/94	82:C <sub>1</sub>	1.66	74.10	91.21	
133/301	410:C <sub>1</sub>	0.87	74.29	163.59	

---

---

134/263	312:C <sub>1</sub>	0.94	74.86	147.28	
135/108	213:C <sub>1</sub>	0.74	75.37	96.65	
136/194	330:C <sub>2</sub>	0.83	75.84	125.10	
137/83	27:C <sub>1</sub>	1.27	76.05	87.86	
138/207	352:C <sub>1</sub>	1.04	76.68	129.70	
139/149	125:C <sub>1</sub>	1.51	76.71	109.62	
140/129	116:C <sub>1</sub>	1.06	76.79	103.34	
141/114	351:C <sub>1</sub>	1.39	76.96	97.91	
142/239	405:C <sub>1</sub>	0.67	76.98	138.07	
143/159	240:C <sub>1</sub>	1.06	77.08	115.90	
144/120	126:C <sub>s</sub>	1.48	77.10	100.00	
145/61	420:C <sub>1</sub>	1.58	77.15	76.99	
146/153	215:C <sub>1</sub>	1.12	77.30	111.29	
147/158	229:C <sub>1</sub>	1.08	77.48	113.80	
148/73	418:C <sub>1</sub>	1.61	77.70	84.52	
149/100	128:C <sub>1</sub>	0.87	78.52	94.14	
150/245	206:C <sub>1</sub>	1.00	78.59	140.16	
151/22	11:C <sub>1</sub>	1.55	78.60	58.16	
152/264	433:C <sub>2</sub>	0.47	78.62	147.70	
153/330	263:C <sub>1</sub>	0.94	79.08	172.38	
154/49	9:C <sub>1</sub>	1.06	79.41	71.96	
155/90	438:D <sub>2</sub>	1.33	79.66	90.37	
156/82	23:C <sub>2</sub>	1.53	79.76	87.86	
157/135	259:C <sub>1</sub>	0.93	79.83	104.18	
158/219	396:C <sub>2</sub>	0.85	80.13	133.89	
159/167	197:C <sub>1</sub>	0.97	80.74	117.99	
160/228	74:C <sub>1</sub>	1.09	80.78	135.98	
161/88	30:C <sub>1</sub>	1.42	81.19	89.12	
162/8	8:C <sub>2</sub>	1.33	81.19	36.82	35.98
163/189	150:C <sub>s</sub>	0.94	81.46	124.26	
164/371	252:C <sub>s</sub>	1.01	82.24	193.30	
165/154	336:C <sub>1</sub>	1.23	82.25	111.71	
166/190	123:C <sub>1</sub>	1.37	82.25	124.26	
167/261	204:C <sub>1</sub>	1.09	82.54	147.28	
168/196	119:C <sub>1</sub>	1.18	82.56	127.19	
169/183	233:C <sub>1</sub>	1.01	83.11	122.59	
170/181	124:C <sub>1</sub>	1.23	83.14	122.17	
171/103	86:C <sub>1</sub>	1.66	83.24	94.56	
172/247	220:C <sub>1</sub>	0.83	83.81	142.26	
173/303	376:C <sub>2</sub>	0.66	84.35	163.59	
174/71	33:C <sub>1</sub>	1.53	84.51	84.10	
175/91	421:C <sub>2</sub>	2.06	84.88	90.37	
176/182	346:C <sub>1</sub>	1.08	85.26	122.59	
177/31	58:C <sub>1</sub>	1.51	85.53	63.18	
178/171	97:C <sub>1</sub>	1.31	85.53	119.24	
179/138	100:C <sub>1</sub>	1.02	86.08	104.18	

---

---

180/45	287:C <sub>s</sub>	1.54	86.15	68.20
181/234	317:C <sub>1</sub>	0.64	86.30	137.24
182/287	251:C <sub>1</sub>	0.78	87.72	159.83
183/130	398:C <sub>1</sub>	1.08	87.77	103.34
184/110	83:C <sub>1</sub>	1.76	88.17	97.07
185/187	368:C <sub>1</sub>	0.91	88.36	123.85
186/131	67:D <sub>2</sub>	0.96	88.79	103.76
187/141	180:C <sub>1</sub>	1.27	89.37	105.44
188/124	84:C <sub>1</sub>	1.59	89.52	100.83
189/81	87:C <sub>1</sub>	1.50	90.51	87.03
190/99	88:C <sub>1</sub>	2.01	91.12	93.72
191/76	132:C <sub>2</sub>	1.39	91.41	85.77
192/195	311:C <sub>1</sub>	1.10	91.98	127.19
193/112	298:C <sub>1</sub>	1.55	92.13	97.91
194/52	273:C <sub>2</sub>	1.54	93.41	72.80
195/140	269:C <sub>1</sub>	1.17	94.61	105.02
196/145	143:C <sub>1</sub>	1.88	95.32	106.27
197/248	230:C <sub>1</sub>	1.11	95.41	143.09
198/209	276:C <sub>1</sub>	0.94	95.42	130.12
199/275	121:C <sub>1</sub>	1.03	95.59	152.30
200/198	366:C <sub>1</sub>	0.98	95.67	127.61
201/162	361:C <sub>1</sub>	0.88	96.54	116.32
202/246	96:C <sub>1</sub>	1.37	97.13	141.00
203/101	10:C <sub>1</sub>	0.94	97.25	94.14
204/133	28:C <sub>1</sub>	1.05	97.36	103.76
205/318	305:C <sub>1</sub>	1.08	97.82	167.78
206/201	165:C <sub>1</sub>	1.10	98.10	128.45
207/213	443:C <sub>2</sub>	1.29	98.30	132.63
208/339	201:C <sub>1</sub>	0.93	98.44	174.89
209/253	278:C <sub>1</sub>	1.11	98.55	146.02
210/296	385:C <sub>1</sub>	0.78	98.62	162.76
211/168	192:C <sub>1</sub>	1.05	98.75	118.41
212/313	300:C <sub>1</sub>	1.08	98.95	166.10
213/285	133:C <sub>1</sub>	1.13	99.12	159.83
214/257	325:C <sub>1</sub>	0.73	99.18	146.86
215/125	164:C <sub>1</sub>	1.50	99.82	102.09
216/254	386:C <sub>1</sub>	0.86	100.06	146.44
217/355	372:C <sub>2</sub>	0.59	100.18	184.93
218/334	228:C <sub>1</sub>	0.81	100.80	173.64
219/165	81:C <sub>1</sub>	1.43	101.13	116.73
220/284	171:C <sub>1</sub>	0.90	101.94	159.41
221/220	76:C <sub>1</sub>	1.05	103.55	133.89
222/230	115:C <sub>2</sub>	0.86	104.55	135.98
223/107	272:C <sub>1</sub>	1.64	104.79	95.81
224/177	400:C <sub>1</sub>	1.10	105.35	120.92
225/169	389:C <sub>1</sub>	1.27	105.82	119.24

---

---

226/79	3:C <sub>1</sub>	1.54	106.04	86.61
227/312	277:C <sub>1</sub>	0.88	106.94	166.10
228/210	391:C <sub>1</sub>	1.08	106.96	130.54
229/274	34:C <sub>2</sub>	0.75	107.08	151.46
230/175	404:C <sub>1</sub>	0.84	107.36	120.08
231/111	271:C <sub>2</sub>	1.44	107.40	97.49
232/174	101:C <sub>1</sub>	1.02	107.97	119.66
233/144	29:C <sub>1</sub>	1.34	108.06	106.27
234/282	265:C <sub>1</sub>	0.81	108.48	158.16
235/286	381:C <sub>2</sub>	0.53	109.58	159.83
236/229	355:C <sub>1</sub>	1.29	109.77	135.98
237/375	411:C <sub>2</sub>	0.85	109.88	196.65
238/235	26:C <sub>1</sub>	0.94	109.99	137.24
239/242	224:C <sub>1</sub>	1.26	110.57	138.91
240/123	57:C <sub>1</sub>	1.03	110.65	100.83
241/262	349:C <sub>1</sub>	1.14	110.73	147.28
242/179	146:C <sub>1</sub>	1.49	110.74	121.75
243/251	367:C <sub>1</sub>	1.02	110.85	144.77
244/192	235:C <sub>1</sub>	1.08	111.00	125.10
245/335	231:C <sub>1</sub>	0.77	111.47	174.05
246/300	182:C <sub>1</sub>	0.80	112.39	163.59
247/340	429:C <sub>2</sub>	0.56	112.80	176.56
248/233	356:C <sub>s</sub>	1.47	113.20	136.82
249/306	153:C <sub>1</sub>	0.89	113.63	165.27
250/344	236:C <sub>1</sub>	1.01	114.50	179.08
251/232	91:C <sub>1</sub>	1.37	114.55	136.40
252/359	340:C <sub>1</sub>	0.82	114.75	188.28
253/215	337:C <sub>1</sub>	0.83	114.79	133.05
254/299	264:C <sub>1</sub>	0.80	114.86	162.76
255/173	15:C <sub>s</sub>	0.69	115.18	119.66
256/226	403:C <sub>1</sub>	0.83	115.37	135.14
257/280	178:C <sub>1</sub>	1.10	116.23	156.90
258/224	78:C <sub>1</sub>	1.37	116.45	134.31
259/216	407:C <sub>1</sub>	1.27	116.59	133.47
260/369	176:C <sub>1</sub>	0.94	116.60	192.46
261/349	110:C <sub>1</sub>	1.02	117.09	180.75
262/252	169:C <sub>1</sub>	1.04	117.37	145.18
263/278	70:C <sub>1</sub>	1.17	117.82	155.64
264/345	239:C <sub>1</sub>	0.81	118.34	179.49
265/146	142:C <sub>2</sub>	1.61	118.62	106.69
266/170	49:C <sub>1</sub>	1.70	119.10	119.24
267/314	316:C <sub>1</sub>	0.71	119.11	166.52
268/336	310:C <sub>2</sub>	1.04	120.57	174.05
269/258	211:C <sub>1</sub>	0.87	120.95	146.86
270/240	179:C <sub>1</sub>	1.04	121.37	138.07
271/186	186:C <sub>1</sub>	1.54	121.41	123.85

---

---

272/255	32:C <sub>1</sub>	1.13	121.45	146.44
273/161	56:C <sub>1</sub>	0.99	121.46	116.32
274/305	447:C <sub>s</sub>	0.92	121.75	164.85
275/180	46:C <sub>1</sub>	1.12	121.77	122.17
276/323	395:D <sub>2d</sub>	0.62	121.86	169.87
277/290	435:C <sub>2</sub>	0.80	122.32	161.08
278/317	203:C <sub>1</sub>	0.94	122.47	167.36
279/316	333:C <sub>1</sub>	0.86	122.59	166.94
280/322	334:C <sub>1</sub>	0.73	122.83	169.45
281/188	208:C <sub>s</sub>	1.33	122.83	123.85
282/236	207:C <sub>1</sub>	0.91	123.04	137.24
283/185	294:C <sub>s</sub>	1.41	123.08	123.43
284/178	50:C <sub>1</sub>	1.70	123.54	121.75
285/268	130:C <sub>2</sub>	1.15	123.65	149.79
286/193	200:C <sub>1</sub>	1.03	123.68	125.10
287/272	135:C <sub>1</sub>	0.76	123.89	150.62
288/373	359:C <sub>1</sub>	0.76	123.99	194.97
289/218	241:C <sub>1</sub>	1.07	123.99	133.89
290/212	16:C <sub>2</sub>	0.90	124.10	132.63
291/266	43:C <sub>1</sub>	0.96	124.12	148.95
292/307	335:C <sub>1</sub>	1.06	124.66	165.27
293/289	226:C <sub>1</sub>	0.98	124.70	160.25
294/191	282:C <sub>1</sub>	1.70	124.75	124.68
295/142	7:C <sub>1</sub>	1.68	124.86	105.44
296	54:C <sub>1</sub>	1.01	125.09	161.08
297/270	401:C <sub>1</sub>	0.53	125.31	150.21
298/217	246:C <sub>1</sub>	0.74	125.94	133.47
299/197	199:C <sub>1</sub>	1.70	125.97	127.61
300/227	238:C <sub>1</sub>	0.74	126.17	135.98
301/92	1:D <sub>3d</sub>	2.19	126.76	90.37
302/244	79:C <sub>1</sub>	1.60	126.85	139.75
303/352	222:C <sub>1</sub>	0.59	127.17	182.84
304/277	160:C <sub>1</sub>	0.81	127.23	154.39
305/211	288:C <sub>1</sub>	0.99	127.34	131.80
306/271	65:C <sub>1</sub>	1.04	127.55	150.21
307/294	184:C <sub>1</sub>	0.79	127.56	161.92
308/319	332:C <sub>1</sub>	0.91	127.94	168.62
309/293	223:C <sub>1</sub>	0.93	128.47	161.08
310/325	106:C <sub>1</sub>	1.08	130.46	170.71
311/297	69:C <sub>1</sub>	1.22	130.96	162.76
312/377	341:C <sub>1</sub>	0.72	131.28	199.16
313/387	112:C <sub>1</sub>	1.00	131.37	203.76
314/265	388:C <sub>s</sub>	1.28	132.52	147.70
315/405	364:C <sub>2</sub>	0.92	133.16	225.10
316/288	301:C <sub>1</sub>	0.85	133.73	160.25
317/302	318:C <sub>2</sub>	0.66	133.75	163.59

---



---

318/311	198:C <sub>1</sub>	0.87	134.15	166.10
319/273	270:C <sub>1</sub>	0.99	134.64	151.46
320/249	279:C <sub>1</sub>	1.31	135.12	143.09
321/320	237:C <sub>1</sub>	0.72	135.18	169.03
322/200	406:D <sub>2</sub>	1.56	135.28	128.45
323/291	329:C <sub>1</sub>	0.82	135.62	161.08
324/276	375:C <sub>1</sub>	0.84	136.39	153.55
325/270	296:C <sub>1</sub>	0.95	137.60	150.21
326/321	195:C <sub>1</sub>	0.76	137.62	169.45
327/392	221:C <sub>3</sub>	0.56	137.73	210.04
328/304	99:C <sub>2</sub>	0.63	138.04	164.43
329/329	137:C <sub>1</sub>	0.92	138.47	171.96
330/382	108:C <sub>1</sub>	1.00	139.02	202.09
331/361	314:C <sub>1</sub>	0.95	139.25	188.70
332/376	205:C <sub>1</sub>	0.86	139.99	197.48
333/250	138:C <sub>1</sub>	1.10	140.05	143.93
334/381	113:C <sub>1</sub>	0.79	140.49	201.25
335/214	31:C <sub>1</sub>	1.64	140.74	132.63
336/351	193:C <sub>1</sub>	0.73	140.87	182.84
337/256	102:C <sub>1</sub>	0.97	140.94	146.86
338/347	284:C <sub>1</sub>	1.03	140.96	179.91
339/403	262:C <sub>1</sub>	0.66	141.89	223.43
340/310	157:C <sub>1</sub>	1.12	142.30	165.69
341/283	85:C <sub>s</sub>	1.48	142.42	158.99
342/354	166:C <sub>1</sub>	0.99	142.46	184.10
343/328	196:C <sub>1</sub>	0.94	142.57	171.96
344/409	117:C <sub>2</sub>	0.77	143.09	227.19
345/395	450:D <sub>5</sub>	0.68	143.37	214.22
346/383	136:C <sub>1</sub>	1.00	143.61	202.09
347/308	188:C <sub>1</sub>	1.04	143.65	165.27
348/222	290:C <sub>s</sub>	1.65	143.83	133.89
349/172	275:C <sub>1</sub>	0.76	143.85	119.66
350/394	244:C <sub>s</sub>	0.82	144.13	210.87
351/309	387:C <sub>2</sub>	1.03	144.43	165.69
352/389	21:C <sub>1</sub>	0.78	144.94	205.02
353/366	267:C <sub>1</sub>	0.80	144.95	190.37
354/279	38:C <sub>s</sub>	0.97	146.29	155.64
355/396	194:C <sub>1</sub>	0.77	146.46	214.22
356/367	225:C <sub>1</sub>	0.96	147.15	191.63
357/358	44:C <sub>1</sub>	0.90	148.05	187.44
358/378	39:C <sub>s</sub>	0.95	148.98	199.58
359/398	315:C <sub>1</sub>	0.77	149.08	216.73
360/331	291:C <sub>s</sub>	0.87	150.60	172.80
361/238	51:C <sub>1</sub>	1.60	150.69	138.07
362/206	4:C <sub>2</sub>	0.88	150.96	129.29
363/327	209:C <sub>s</sub>	0.87	151.46	171.54

---

---

364/333	140:C <sub>1</sub>	1.10	151.95	173.64
365/337	191:C <sub>1</sub>	1.11	152.69	174.47
366/362	306:C <sub>1</sub>	1.06	153.29	189.12
367/324	187:C <sub>1</sub>	1.29	153.30	170.71
368/386	327:C <sub>1</sub>	0.70	153.90	203.34
369/400	177:C <sub>1</sub>	0.98	154.45	217.57
370/390	93:C <sub>s</sub>	1.45	155.94	208.36
371/370	339:C <sub>1</sub>	0.92	157.11	192.88
372/346	154:C <sub>1</sub>	0.74	158.12	179.49
373/353	274:C <sub>1</sub>	0.79	160.06	183.68
374/356	62:C <sub>1</sub>	0.87	161.06	184.93
375/332	328:C <sub>1</sub>	0.97	161.30	173.64
376/425	342:C <sub>1</sub>	0.57	162.75	245.18
377/418	394:C <sub>s</sub>	0.75	162.83	231.38
378/364	212:C <sub>2</sub>	0.96	163.06	189.54
379/281	66:C <sub>2</sub>	1.38	164.02	157.32
380/267	13:C <sub>2</sub>	1.75	165.59	149.37
381/298	47:C <sub>1</sub>	1.72	166.09	162.76
382/380	343:C <sub>2</sub>	1.08	166.23	200.83
383/315	92:C <sub>1</sub>	1.45	166.43	166.52
384/391	114:C <sub>1</sub>	1.18	166.86	210.04
385/341	52:C <sub>1</sub>	1.19	168.01	176.98
386/413	307:C <sub>1</sub>	0.96	168.06	229.28
387/379	5:C <sub>2</sub>	1.07	168.94	200.41
388/295	41:C <sub>2</sub>	1.11	170.06	162.34
389/397	234:C <sub>1</sub>	0.98	170.71	215.06
390/326	80:C <sub>1</sub>	1.73	171.52	171.54
391/402	105:C <sub>1</sub>	1.10	171.67	221.75
392/348	289:C <sub>1</sub>	1.10	172.86	180.33
393/374	25:C <sub>s</sub>	1.56	173.23	195.81
394/342	280:C <sub>1</sub>	1.12	173.53	178.66
395/407	302:C <sub>1</sub>	0.93	173.60	225.52
396/357	42:C <sub>1</sub>	0.83	174.33	185.35
397/417	326:C <sub>2</sub>	0.74	175.11	230.12
398/414	181:C <sub>1</sub>	0.85	175.13	229.28
399/423	68:C <sub>1</sub>	0.81	176.45	241.42
400/343	156:C <sub>1</sub>	1.07	176.48	179.08
401/426	63:C <sub>1</sub>	0.93	176.82	246.86
402/360	292:C <sub>1</sub>	0.98	177.72	188.70
403/415	107:C <sub>1</sub>	1.08	178.72	229.70
404/433	331:C <sub>1</sub>	0.91	181.33	260.24
405/372	40:C <sub>1</sub>	1.24	181.66	193.30
406/401	393:C <sub>1</sub>	1.06	182.28	217.99
407/416	155:C <sub>1</sub>	0.86	182.31	229.70
408/436	104:C <sub>1</sub>	0.99	182.51	269.03
409/368	14:C <sub>s</sub>	0.76	187.03	192.05

---

---

410/363	6: $C_1$	1.07	190.98	189.54
411/384	131: $C_1$	1.09	192.01	202.51
412/435	109: $C_1$	0.95	192.88	268.61
413/427	227: $C_1$	0.90	194.43	248.53
414/393	185: $C_1$	0.93	194.54	210.87
415/412	365: $C_1$	0.79	196.59	228.45
416/408	159: $C_2$	1.03	196.94	227.19
417/424	59: $C_1$	0.78	199.55	242.67
418/419	283: $C_1$	0.97	200.17	231.38
419/420	20: $C_1$	0.63	200.52	233.05
420/350	2: $D_2$	1.75	201.22	180.75
421/399	158: $C_1$	0.86	201.94	217.15
422/388	60: $C_1$	1.48	205.91	204.60
423/428	141: $C_1$	0.91	206.27	249.78
424/422	161: $C_1$	0.86	208.40	235.98
425/432	111: $C_1$	1.01	209.18	259.83
426/385	55: $C_1$	1.71	209.95	202.92
427/406	45: $C_1$	1.01	210.34	225.52
428/404	61: $C_1$	1.10	213.91	224.26
429/411	281: $C_1$	0.91	215.47	228.45
430/439	266: $C_3$	0.64	215.55	277.82
431/365	37: $C_2$	1.14	217.85	189.95
432/421	53: $C_1$	1.03	219.51	235.14
433/410	392: $C_2$	1.05	221.07	228.45
434/440	324: $C_1$	0.96	221.81	284.51
435/434	22: $C_1$	0.88	225.93	264.85
436/430	319: $C_5$	0.84	228.81	257.32
437/429	19: $C_1$	0.64	228.86	256.06
438/445	338: $C_2$	0.88	239.90	313.38
439/431	189: $C_1$	0.78	240.61	258.15
440/444	347: $C_{2v}$	0.71	243.81	308.36
441/449	295: $C_{2v}$	0.87	249.96	337.65
442/441	35: $C_2$	0.53	256.77	297.90
443/437	24: $C_1$	0.82	260.39	271.12
444/442	190: $C_2$	1.14	263.45	298.32
445/438	64: $C_5$	1.75	267.76	272.38
446/447	293: $C_2$	0.65	271.44	318.82
447/446	48: $C_5$	0.87	297.05	317.98
448/448	390: $D_2$	0.76	298.50	321.33
449/443	285: $C_5$	0.66	302.31	303.34
450/450	36: $C_{2v}$	0.97	322.11	385.76

---

<sup>a</sup> FM:sym is Fullerene Fowler-Manolopoulos code: symmetry<sup>5</sup>

表 S2 C<sub>100</sub>(417)与 C<sub>2</sub> 反应生成的 C<sub>102</sub> 异构体的相对能量( $E_r$  单位 kJ·mol<sup>-1</sup>), HOMO-LUMO 能隙( $\Delta$  单位 eV)

Table S2 The relative energy ( $E_r$  in kJ·mol<sup>-1</sup>), HOMO-LUMO gap ( $\Delta$  in eV) of C<sub>102</sub> isomers formed by C<sub>100</sub> (417) and C<sub>2</sub> reaction.

Isomer	$\Delta$	$E_r$	Isomer	$\Delta$	$E_r$
C <sub>102</sub> (NC-177)	1.15	118.55	C <sub>102</sub> (NC-185)	1.07	207.09
C <sub>102</sub> (NC-178)	1.24	15.77	C <sub>102</sub> (NC-186)	1.17	27.21
C <sub>102</sub> (NC-179)	1.23	25.70	C <sub>102</sub> (NC)	1.43	-30.93
C <sub>102</sub> (NC-180)	1.04	256.43	C <sub>102</sub> (NC-188)	1.09	139.70
C <sub>102</sub> (NC-181)	1.34	127.57	C <sub>102</sub> (NC-189)	1.24	18.07
C <sub>102</sub> (NC-182)	1.23	29.21	C <sub>102</sub> (NC-190)	1.24	181.65
C <sub>102</sub> (NC-183)	1.47	58.06	<sup>#334408</sup> C <sub>102</sub>	1.13	0.00
C <sub>102</sub> (NC-184)	1.31	74.58			

## References

- (1) Zhao, X.; Goto, H.; Slanina, Z. *J. Chem. Phys.* **2004**, *306*, 93. doi: 10.1016/j.chemphys.2004.07.019
- (2) Cai, W.; Xu, L.; Shao, N.; Shao, X.; Guo, Q. *J. Chem. Phys.* **2005**, *122*, 184318. doi: org/10.1063/1.1891706
- (3) Yoshida, M.; Gotō, H.; Hirose, Y.; Zhao, X.; Ōsawa, E. *Electron. J. Theo. Chem.* **1996**, *1*, 163. doi: 10.1002/ejtc
- (4) Shao, N.; Gao, Y.; Yoo, S.; An, W.; Zeng, X. C. *J. Phys. Chem. A* **2006**, *110*, 7672. doi: 10.1021/jp0624092
- (5) Fowler P. *DE Manolopoulos An atlas of fullerenes*; Oxford University Press: Oxford. 1995.