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Supplementary Information for

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Formation of icosahedral C_{60} fullerene via migration of single sp atoms and annihilation of sp-atom pairs

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Contents

Calculated total energies ΔE (relative to the ground state position 1 with the minimal total energy), distance d between the two sp^2 atoms which are the nearest neighbors of the sp atom, and partition functions for all 47 nonequivalent positions of the sp atom.

Table S1. Calculated energies (in eV, relative to the ground state position 1 with the minimal total energy), distances d (in Å) between the two sp^2 atoms, which are the nearest neighbours of the sp atom, and partition functions q (ln(q) is given) of the 47 sp-atom postitions in the C_{58}-C_{2v} fullerene isomer instead of or above a common bond of sp^2-structure rings consisting of n and m atoms (see Figure 1). N_s is the number of sp-atom migration steps from the sp-atom position 1. Values of distances where the bond exists between the two sp^2 atoms which are the nearest neighbours of the sp atom are emphasized.

Sp-atom position	(n,m)	N_s	ΔE, eV	d, Å	ln(q)
1	(5,7)	0	0.00	2.35	46.43
2	(6,6)	2	0.96	2.38	46.86
3	(5,6)	1	1.19	2.28	46.66
4	(5,6)	2	1.30	2.28	46.58
5	(5,6)	3	1.35	2.25	46.64
6	(5,7)	1	1.41	2.30	46.73
7	(5,6)	3	1.41	2.22	46.66
8	(5,6)	4	1.42	2.23	46.59
9	(5,5)	1	1.58	2.21	46.59
10	(5,6)	3	1.68	2.25	46.67
11	(6,7)	1	1.70	2.35	47.13
12	(6,6)	3	1.73	2.25	46.93
13	(5,6)	4	1.76	2.22	46.72
14	(5,6)	4	1.82	2.21	46.66
15	(6,6)	4	1.82	2.34	47.14
16	(5,6)	2	1.84	_1.65_	46.71
17	(5,6)	3	1.84	_1.65_	46.71
18	(5,6)	5	1.89	2.23	46.72
19	(5,6)	2	1.94	2.19	46.71
20	(5,5)	2	1.96	2.13	46.64
21	(5,6)	5	1.96	2.24	46.76
22	(5,6)	6	2.00	2.18	46.70
23	(5,6)	6	2.00	2.22	46.66
24	(5,6)	5	2.02	2.21	46.69
25	(5,6)	7	2.02	2.20	46.68
26	(5,6)	6	2.03	2.23	46.72
27	(5,6)	5	2.04	2.21	46.69
28	(5,6)	4	2.04	2.23	46.77
29	(5,6)	7	2.06	2.20	46.69
30	(5,6)	5	2.06	2.20	46.72

31	(5,6)	4	2.07	2.18	46.72
32	(5,6)	7	2.07	2.20	46.71
33	(5,6)	2	2.13	2.02	47.02
34	(5,6)	8	2.15	2.21	46.73
35	(6,6)	5	2.17	2.11	46.93
36	(5,6)	7	2.20	2.11	46.89
37	(6,6)	3	2.23	2.35	46.79
38	(6,6)	6	2.26	<u>1.57</u>	47.15
39	(6,6)	4	2.26	<u>1.64</u>	46.95
40	(5,6)	5	2.27	2.20	46.99
41	(6,6)	5	2.30	<u>1.63</u>	46.95
42	(6,6)	6	2.32	<u>1.61</u>	47.13
43	(6,6)	6	2.37	<u>1.58</u>	47.02
44	(6,6)	9	2.38	<u>1.61</u>	47.07
45	(5,6)	4	2.48	2.10	46.91
46	(6,7)	2	2.50	2.28	47.01
47	(6,6)	3	2.65	2.05	47.07

Calculated barriers for sp-atom migration.

Table S2. Calculated barriers E_m (in eV) for sp-atom migration from position k to position l (see Figure 1).

$k \to l$	E_m, eV
$31 \to 10$	1.99
$10 \to 2$	1.95
$2 \to 11$	2.23
$11 \to 1$	1.34
$7 \to 20$	1.75
$20 \to 3$	0.97
$3 \to 1$	1.77
$11 \to 3$	1.20
average	1.65 ± 0.13