Supporting Information

Isolation of C_{102} fractions

The fullerene soot was synthesized by a Krätschmer-Huffman DC-arc discharging method with undoped graphite rod under the condition of 400 mbar He. The as-produced soot was Soxhlet-extracted by CS_2 for 24 h. The fullerene mixture was subjected to HPLC separation in toluene using a preparative 5PYE column (20 × 250 mm, Nacalai Tesque, Japan; flow rate 15.0 ml/min; injection volume 15 ml; toluene as eluent). The fraction eluted between 44 and 47 min (fraction **A**) was further separated with a semi-preparative Buckyprep column (10 × 250 mm, Nacalai Tesque, Japan; flow rate 5.0 ml/min; injection volume 5 ml; toluene as eluent) and the main fraction (**A-3**) was subjected to recycling HPLC separation with a semi-preparative Buckyprep-M column (10 × 250 mm, Nacalai Tesque, Japan; flow rate 5.0 ml/min; injection volume 5 ml; toluene as eluent) (see Fig. S1). Each of four fractions collected after eight separation cycles contains C_{102} as the main component according to MALDI-TOF mass spectrometry. The first of four C_{102} fractions (**A-3-1**), which did not show any noticeable contamination with other fullerenes (see Fig. S2), was used as the starting material for chlorination.

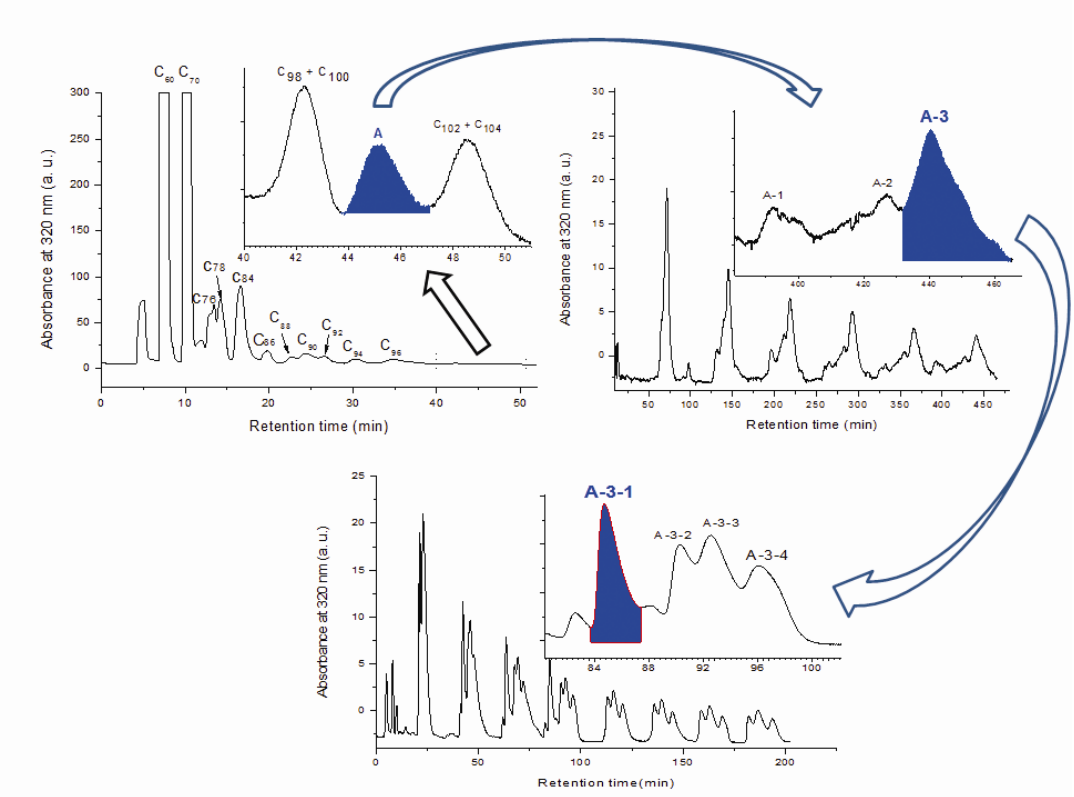

Fig. S1. Three-step HPLC isolation of a compositionally pure C_{102} fraction (fraction **A-3-1**) used for chlorination (see text).

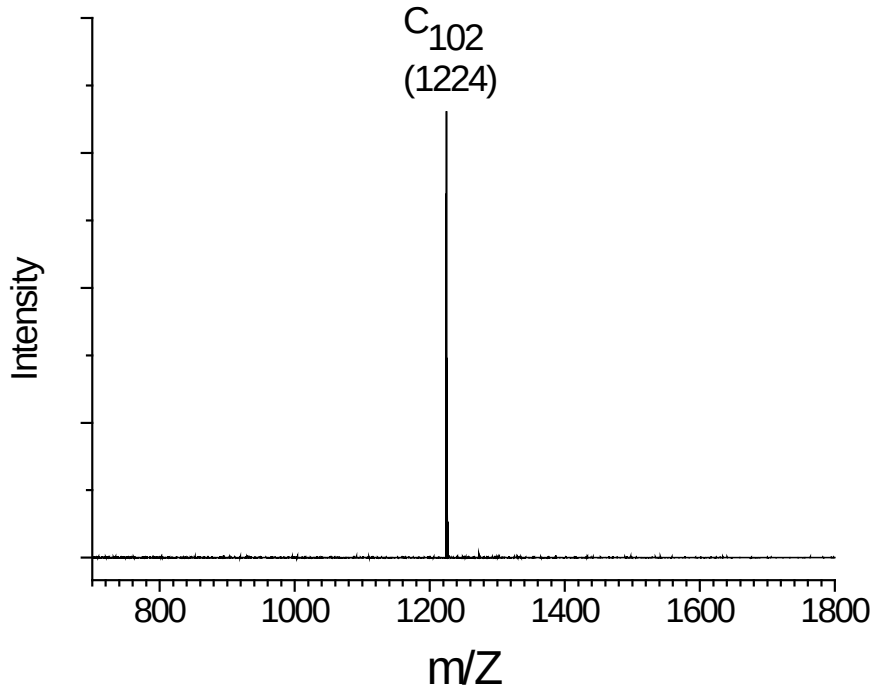

Fig. S2. MALDI TOF mass spectrum of subfraction **A-3-1**.

The estimation of the extremely low amount C_{102} used in our chlorination experiments could not be done by direct sample weighing. Instead, we estimated the C_{102} content by the following rough procedure. First, HPLC trace of the mixture solution of the known amount of the fullerene soot extract was analyzed by integrating all chromatographic peaks, providing information about the relative content of fraction **A** (see Fig. S1). Then, it was recalculated to the absolute amount with the assumption that the extinction coefficients of fullerenes at the wavelength of 320 nm (the wavelength used in HPLC detection) are approximately the same. This assumption was supported at least for the case of C_{60} and C_{70} fullerenes, which possess very close extinction coefficients determined at the same conditions in the separate quantitative experiments. The amount of the subfraction A-3-1 was calculated by integrating the corresponding HPLC subfractions and multiplying by the number of runs.

Numbering of C_{102} isomers

Theoretical calculations of relative stability of IPR C_{102} isomers were reported in the literature using two different numbering systems.[S1-S3] The numbering in ref. S1 and S2 is based on the sequence in the output of the generation program in ref. S4 (PentHex Puzzles). A more usual way of fullerene numbering uses the spiral algorithm of ref. S5. The correspondence of isomer numbers for fifteen IPR C_{102} isomers, which were considered in refs. S1 and S2, according to the numbering systems in refs. S4 and S5 is given below.

Numbering according to ref. S4: 32, 34, 369, 371, 409, 451, 452, 453, 562, 570, 598, 606, 611, and 616.

Numbering according to ref. S5: 530, 583, 73, 20, 554, 141, 581, 1, 251, 303, 93, 372, 567, and 552.

The use of different numbering systems in the literature resulted in some contradictions concerning the lists of most stable C_{102} fullerenes. In the present work, we use the numbering system proposed in ref. S5.

Most stable IPR C_{102} isomers

In the first step, formation energy of all 616 IPR isomers of C_{102} fullerene were calculated at the semiempirical level of theory (AM1). Most stable isomers within 120 kJ mol^{-1} were then recalculated at the DFT level of theory using the PRIRODA code [S6] and a PBE exchange-correlation functional [S7] with a built-in TZ2P basis set. Fifty most stable C_{102} IPR fullerenes are presented in Table S1.

Table S1. Fifty most stable IPR C_{102} fullerenes

No.	Canonical spiral code according to ref. S5	Formation energy, HA	E_{rel}, kJ mol^{-1}
603	566666566566656665666566666656666565665666656666656656	-3883.66929	0.0
371	566666565665666666666666566656565665665666666566656	-3883.66373	14.6
418	5666665656666666666656566566656566566566566666666665	-3883.66126	21.1
214	56666656566566666665666565666666666666565666566565	-3883.66055	23.0
377	566666565665666666666666566566566565665666656666566	-3883.66029	23.6
614	566666566566666665666656565666666566666565656666566656	-3883.65946	25.8
578	566666566566566666566666666666665656565665665666566566	-3883.65903	26.9
607	566666566566656666566566566666666666665656565656666	-3883.65815	29.3
606	566666566566656665666656666666566666566566565665666	-3883.65793	29.8
400	566666565665666666656656656566666666666656565656	-3883.65775	30.3
600	566666566566566666666666566566565656566566566666566666	-3883.65724	31.6
376	5666665656656666666666665666566565656566566566566566	-3883.65712	32.0
347	566666565665666666666665656565665656666656666566656	-3883.65710	32.0
594	5666665665665666666666665666565656565666566666666566566	-3883.65677	32.9
375	566666565665666666666666566566565656566566666666666565	-3883.65633	34.0
598	566666566566566666666666566656656565666566566656666	-3883.65624	34.3
45	5666665656566566666666666666666656665656565665666665	-3883.65593	35.1
615	566666566566666666566565656666656666665656666656665	-3883.65580	35.4
361	566666565665666666666665666656656566565666656666566	-3883.65559	36.0
611	566666566566666665666565665666666666656656656656666566	-3883.65535	36.6
579	566666566566566666666566666566566666656666656656656	-3883.65510	37.3
427	566666566565656666666666656566666656666656566665665	-3883.65441	39.1

602	566666566566566666666666665665665665665666566566566	-3883.65439	39.1
374	5666665665665666666666666566566566565665666666566566	-3883.65432	39.3
326	56666656566566666666666656566565665666666666656656566	-3883.65398	40.2
601	566666566566566666666666665665665665665666566566566	-3883.65350	41.5
582	5666665665665666666666656566565666566666665666656656	-3883.65328	42.0
612	566666566566666656665665656666666666665656566566665	-3883.65314	42.4
525	5666665665656666666666656566656665666566566566665665	-3883.65275	43.4
405	56666656566656666666656666665656656656566666665665666	-3883.65271	43.5
19	56666656565656666666666666666666656565656566656656	-3883.65258	43.9
328	5666665656656666666666656566565666566666665666656656	-3883.65257	43.9
592	566666566566566666666666566566566566666656656656566	-3883.65250	44.1
523	5666665665656666666666656566566566666656566665666656	-3883.65233	44.5
435	56666656656565666666666666666566566566565656656665666	-3883.65217	44.95
610	566666566566566666666656666566565666656666666566565	-3883.65216	45.0
360	5666665656656666666666656666566565666565656656666666	-3883.65206	45.2
096	56666656565666666666656566666666666666656565665656	-3883.65203	45.3
34	566666565656656666666666666566666566656666566566566	-3883.65200	45.4
550	5666665665656666666666666566565666656566666566566665666	-3883.65199	45.4
605	566666566566566566566566666666566666566566666566566	-3883.65157	46.5
35	5666665656566566666666666666566666566656666566566665	-3883.65147	46.8
331	56666656566566666666666656566566566566666656666656656	-3883.65146	46.8
488	566666566566566666566666566666666566566566566566566	-3883.65133	47.2
17	56666656565656666666666666666666656565665656666656	-3883.65110	47.8
332	56666656566566666666666656566566566666666656565656666	-3883.65101	48.0
165	566666565665666666566666566666666566566566566566566	-3883.65074	48.7
245	5666665656656666666666656656656566666666666656565666	-3883.64973	51.4
316	566666565665666666666656666656656665656566656666566	-3883.64879	53.8
43	5666665656566566666666666666666656566565656666666565	-3883.64876	53.9

Isomer 552 (616 according to the numbering system in ref. S4) has a relative formation energy of 55.7 kJ mol^{-1}.

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