Supplementary materials.

Details of vibrational calculations:

Cartesian DFT force field of $C_{60}Cl_{24}$ was transferred into redundant internal coordinate system, which included all chemical bonds and bond angles (totally 366 coordinates). Then internal force constants $F_{ij}^{DFT}$ were scaled through the following equation:

$$F_{ij}^{scaled} = t_i^{1/2} F_{ij}^{DFT} t_j^{1/2}$$

where $t_{i,j}$ are scaling factors for internal coordinates *i* and *j*, respectively. We introduced 6 scaling factors, one for each set of the chemically equivalent internal coordinates (see Table S1), and refined their values in the least square fitting of the calculated frequencies to the experimental values.

Table1 S1. Description of internal coordinates and values of scaling factors

| internal coordinate | scaling factor | description of the internal coordinates |
|---|---|---|
| q(C-C) | 1.0135 | ordinary C-C bonds: types a, b and c (Fig. 1) |
| q(C=C) | 1.0432 | double C=C bonds: types e and d (Fig. 1) |
| q(C-Cl) | 1.1894 | C-Cl bonds |
| $\gamma$(CC($sp^2$)C) | 1.0531 | angles between two C-C bonds with C-$sp^2$ atom in the vertex |
| $\gamma$(C(C$sp^3$)C) | 0.9076 | angles between two C-C bonds with C-$sp^3$ atom in the vertex |
| $\alpha$(CCCl) | 1.2937 | angles between C-Cl and ordinary C-C bonds |