

## Supporting information

### EXPERIMENTAL

#### Materials

B<sup>III</sup>SubPcCl (98%) was purchased from Aldrich. C<sub>60</sub> of 99.9 % purity was received from MTR Ltd. Sodium fluorenone ketyl was obtained as described.<sup>1</sup> Solvents were purified in argon atmosphere. *o*-Dichlorobenzene (C<sub>6</sub>H<sub>4</sub>Cl<sub>2</sub>) was distilled over CaH<sub>2</sub> under reduced pressure; hexane was distilled over Na/benzophenone. The solvents were degassed and stored in the glove box. All operations on the synthesis of **1** and the storage of crystals were carried out in a MBraun 150B-G glove box with controlled atmosphere and water and oxygen content less than 1 ppm. KBr pellets for IR- and UV-visible-NIR measurements were prepared in the glove box

#### General

UV-visible-NIR spectra were measured in KBr pellets on a Perkin Elmer Lambda 1050 spectrometer in the 250-2500 nm range. FT-IR spectra were obtained in KBr pellets with a Perkin-Elmer Spectrum 400 spectrometer (400-7800 cm<sup>-1</sup>). EPR spectra were recorded for sealed polycrystalline samples of **1** at 295 K with a JEOL JES-TE 200 X-band ESR spectrometer.

#### X-ray crystal structure determination

Crystal data of **1** at 100(2) K: C<sub>146</sub>H<sub>48</sub>B<sub>2</sub>Cl<sub>4</sub>N<sub>12</sub>O<sub>2</sub>, *M*<sub>r</sub> = 2165.38 g mol<sup>-1</sup>, black plate, monoclinic, *P* 2<sub>1</sub>, *a* = 15.4619(8), *b* = 16.9321(8), *c* = 19.6980(10) Å, β = 110.386(5)°, *V* = 4834.0(4) Å<sup>3</sup>, *Z* = 2, *d*<sub>calc</sub> = 1.488 g·cm<sup>-3</sup>, μ = 0.314 mm<sup>-1</sup>, *F*(000) = 2204, 2θ<sub>max</sub> = 69.50°, reflections measured 75952, unique reflections 21328, reflections with *I* > 2σ(*I*) = 16669, parameters refined 1708, restraints 2395, *R*<sub>1</sub> = 0.0808, *wR*<sub>2</sub> = 0.2045, G.O.F. = 1.005, CCDC 1046031.

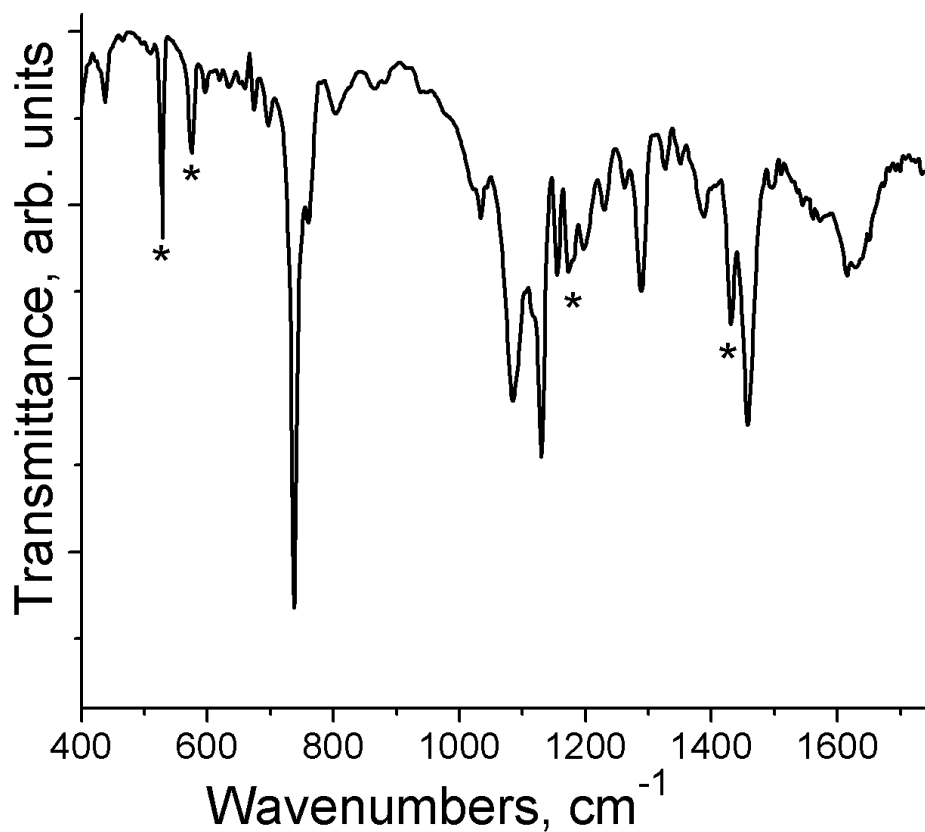
The intensity data for **1** were collected on a MAR225 CCD detector using synchrotron radiation at the BESSY storage ring, BL 14.2 (λ = 0.9050 Å, PSF of the Free University of Berlin, Germany). The structures were solved by direct method and refined by the full-matrix

least-squares method against  $F^2$  using SHELX-97 package.<sup>2</sup> Non-hydrogen atoms were anisotropically refined. Positions of hydrogen atoms were included into refinement in a riding mode. See .....for crystallographic data in CIF. Structure of **1** contains two orientations of the  $C_{60}$  molecule having 0.537(5)/0.463(5) occupancies. One of two solvent  $C_6H_4Cl_2$  molecules disordered between two orientations with the 0.660(6)/0.340(6) occupancies. To keep geometry of disordered  $C_{60}$  and one  $C_6H_4Cl_2$  molecules close to ideal one restraints were applied for the refinement of the crystal structures of **1**.

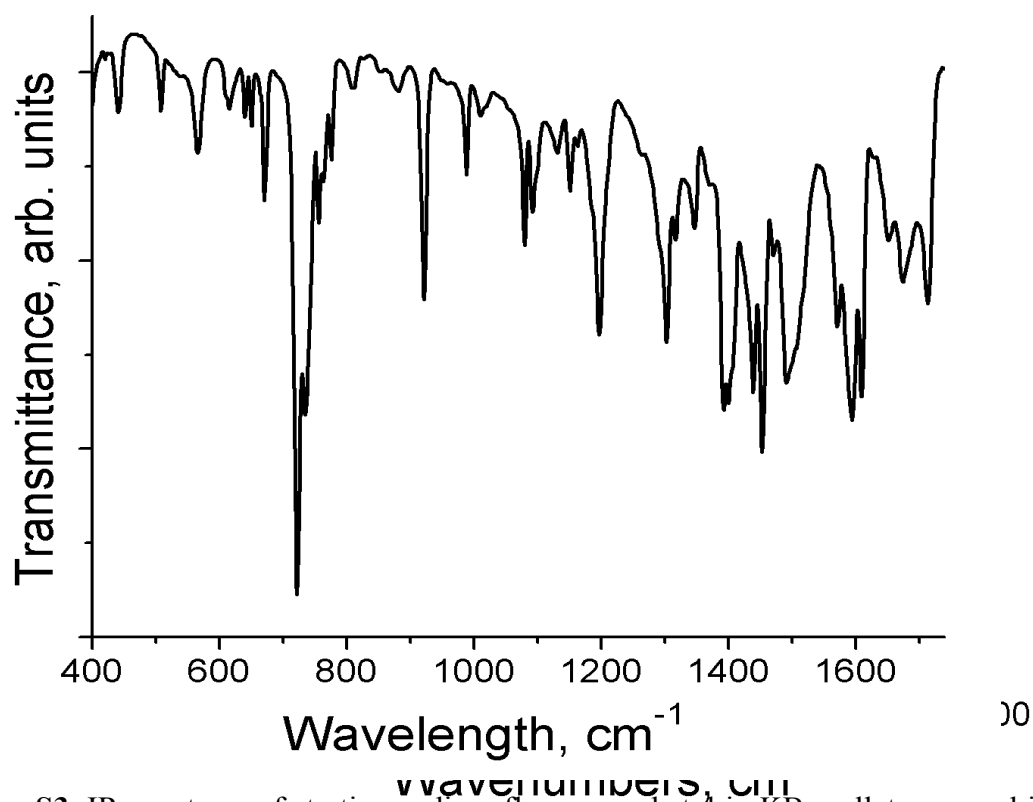
## IR- spectra.

**Table S1.** IR-spectra (cm<sup>-1</sup> in KBr) of starting compounds and complex **1**.

	B <sup>III</sup> SubPcCl	C <sub>60</sub>	(Na <sup>+</sup> )(Fluorenone <sup>-</sup> )	C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>	<b>1</b>
B <sup>III</sup> SubPc	444w 631w 697w 750vs 758m 797w 880w 951m 960m 1088w 1130s 1150w 1196w 1231m 1281s 1321w 1386m 1432s 1440s 1453s 1491w 2853w 2925w 3058w				437w* 596w 696w 737vs* 760m* 805w 881w 943w - 1084s* 1130s* 1154w* 1196w 1229w 1289w 1326w 1388w* 1431s* - 1457s* 1496w* 2850w 2920w 3058w*
C <sub>60</sub>		526s 576m 1182m 1429s			527m 575w 1181w 1431s*
Fluorenone <sup>-</sup>			439w 671w 723vs 735s 756w 922s 989m 1080m 1151w 1197w 1392m 1400m 1439m 1453s 1492m 1594s 1651m 1675m 1714m 3058w		437w* 673w - 737vs* 760m* - - 1084s* 1154w* 1196w* 1388w* - 1431s* 1457s* 1496w* - 1630m 3058w*
C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub>				657w 748s 1030m 1122m 1453m	657w 737vs* 1034w 1130s* 1457s*



**Figure S1.** IR-spectrum of complex **1** in KBr pellet prepared in anaerobic conditions. Absorption bands of C<sub>60</sub> are marked by asterisks.



**Figure S3.** IR-spectrum of starting sodium fluorenone ketyl in KBr pellet prepared in anaerobic conditions.  
**Figure S2.** IR-spectrum of starting B<sup>III</sup>SubPcCl in KBr pellet.

