

**Supplementary material for the manuscript**

**“Effective magnetic coupling with strong spin frustration in  $(\text{Ph}_3\text{MeP}^+)(\text{C}_{60}^{\bullet-})$  and reversible  $\text{C}_{60}^{\bullet-}$  dimerization in  $(\text{Ph}_3\text{MeP}^+)(\text{C}_{60}^{\bullet-})\cdot\text{C}_6\text{H}_5\text{CN}$  . Effect of solvent on structure and properties” by**

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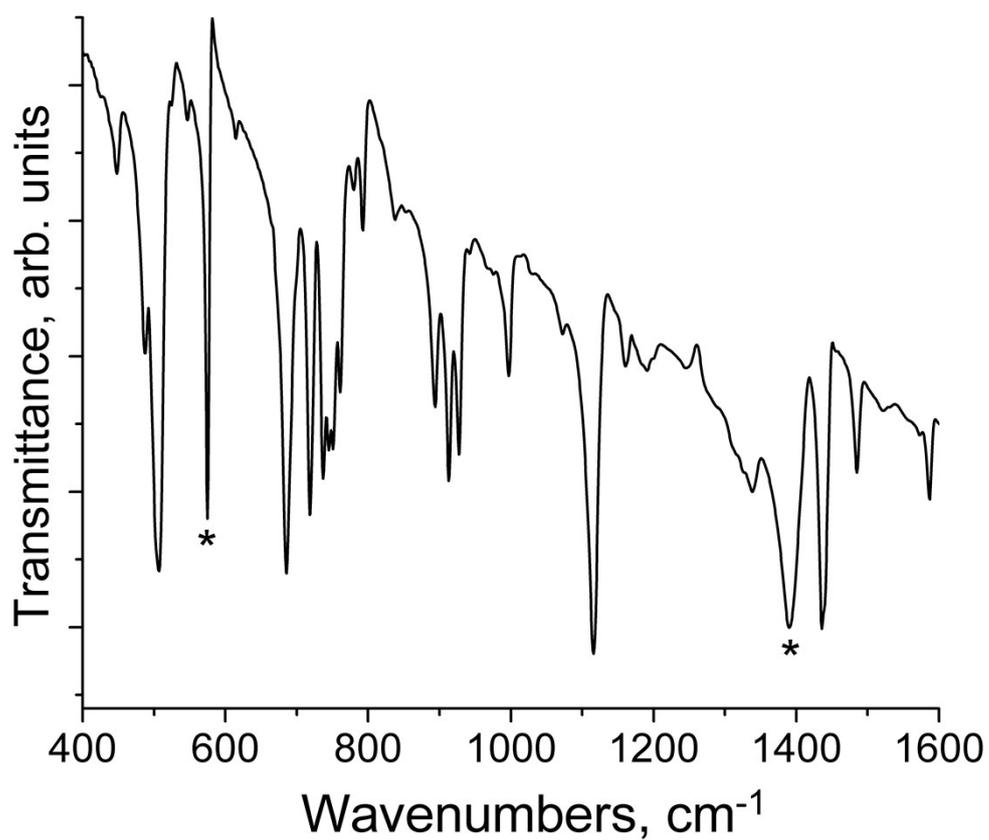
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## IR- spectra.

| Components                       | Ph <sub>3</sub> MePBr | C <sub>60</sub> | C <sub>6</sub> H <sub>5</sub> CN | (Ph <sub>3</sub> MeP <sup>+</sup> )(C <sub>60</sub> <sup>•-</sup> ) (1) | (Ph <sub>3</sub> MeP <sup>+</sup> )(C <sub>60</sub> <sup>•-</sup> )·C <sub>6</sub> H <sub>5</sub> CN (2) |       |
|----------------------------------|-----------------------|-----------------|----------------------------------|---|--|-------|
| Ph <sub>3</sub> MeP <sup>+</sup> | 432m                  |                 |                                  | 446w  | 447w   |       |
|                                  | 488w                  |                 |                                  | 488m  | 488m   |       |
|                                  | 506s sp               |                 |                                  | 506s*   | 507s*  |       |
|                                  | 514s sp               |                 |                                  | -   | -  |       |
|                                  | 567m                  |                 |                                  | 575s*   | 575s*  |       |
|                                  | 684s sp               |                 |                                  | 686s  | 686s*  |       |
|                                  | 692s sp               |                 |                                  | -   | -  |       |
|                                  | 696s sp               |                 |                                  | -   | -  |       |
|                                  | 718s                  |                 |                                  | 716s  | 718s   |       |
|                                  | -                     |                 |                                  | 735m  | 736m   |       |
|                                  | 743s                  |                 |                                  | 746m  | 745m   |       |
|                                  | 751s                  |                 |                                  | 751m  | 751m*  |       |
|                                  | 762s                  |                 |                                  | 760m  | 761m   |       |
|                                  | 903s sp               |                 |                                  | -   | -  |       |
|                                  | 911s sp               |                 |                                  | 912m  | 913m   |       |
|                                  | 927m                  |                 |                                  | 927m  | 927m   |       |
|                                  | 997w                  |                 |                                  | 998w  | 997w   |       |
|                                  | 1117s                 |                 |                                  | 1116s   | 1116s  |       |
|                                  | 1340w                 |                 |                                  | 1340w   | 1338w  |       |
|                                  | 1437s                 |                 |                                  | 1437s   | 1436s*   |       |
|                                  | 1486w                 |                 |                                  | 1485w   | 1485w  |       |
|                                  | 1587w                 |                 |                                  | 1586w   | 1587w  |       |
|                                  | 1630w                 |                 |                                  | -   | -  |       |
|                                  | 2879w                 |                 |                                  | 2873w   | 2871w  |       |
|                                  | 2917w                 |                 |                                  | 2915w   | 2912w  |       |
|                                  | 2935w                 |                 |                                  | -   | -  |       |
|                                  | 3054w                 |                 |                                  | 3054w   | 3053w  |       |
|                                  | C <sub>60</sub>       |                 | 526s                             |   | 506s*  | 507s* |
|                                  |                       |                 | 576m                             |   | 575s*  | 575s* |
|                                  |                       |                 | 1182m                            |   | -  | -     |
|                                  |                       | 1429s           |                                  | 1391s   | 1390s  |       |
| C <sub>6</sub> H <sub>5</sub> CN |                       |                 | 554w                             |   | -  |       |
|                                  |                       |                 | 686w                             |   | 686s*  |       |
|                                  |                       |                 | 754s                             |   | 751m*  |       |
|                                  |                       |                 | 1445w                            |   | 1435s*   |       |
|                                  |                       |                 | 2235w                            |   | 2223w  |       |

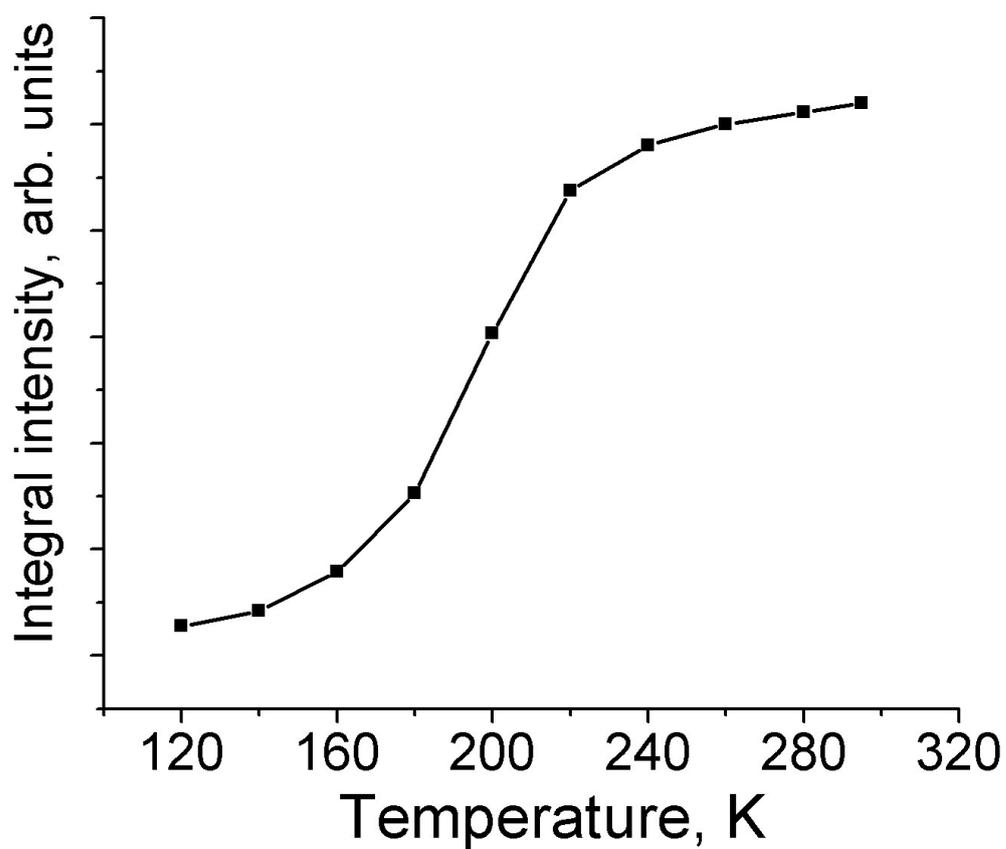
**Table S1.** IR-spectra (cm<sup>-1</sup> in KBr) of starting compounds and salts **1** and **2**.

\* Bands are overlapped, w-weak intensity, m – middle intensity, s – strong intensity, sp – split bands



**Fig. S1.** IR-spectrum of **2** measured in KBr pellet prepared in anaerobic conditions. Absorption bands of C<sub>60</sub> are marked by asterisks. Salt **1** has similar IR-spectrum.

EPR spectrum of salt 2.



**Fig. S2.** Temperature dependence of integral intensity of EPR signal of salt 2 in the 120-295 K range.