

## Supporting Information

### Guest-Induced Topological Polymorphism of Pseudo-Cubic Hydrogen Bond Networks - Robust and Adaptable Supramolecular Synthons -

Tetsuharu Yuge, Ichiro Hisaki, Mikiji Miyata\*, and Norimitsu Tohnai\*

*Department of Material and Life Science, Graduate School of Engineering, Osaka University, 2-1 Yamadaoka, Suita, Osaka 565-0871, Japan*

#### General Methods

**IR spectroscopic analysis.** FT-IR spectra of **1** in a KBr pellet were recorded using a Horiba FT-720 spectrometer.

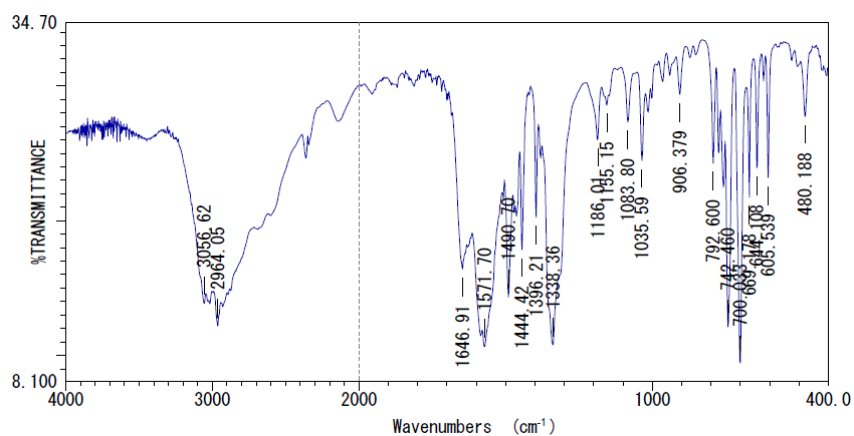


Fig. S1 FT-IR spectra of **1** with C1 topology.

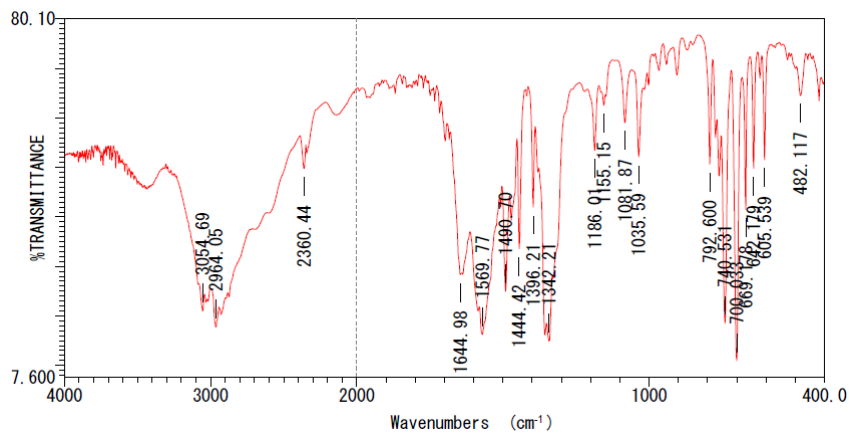


Fig. S2 FT-IR spectra of **1** with Cs topology.

Table S1 Crystallographic data of primary ammonium triphenylacetates

|                                          | 1                                                                 | 1·toluene                                                                                       | 2                                                             | 2·benzene                                                                                   |
|------------------------------------------|-------------------------------------------------------------------|-------------------------------------------------------------------------------------------------|---------------------------------------------------------------|---------------------------------------------------------------------------------------------|
| formula                                  | 4(C <sub>24</sub> H <sub>27</sub> O <sub>2</sub> N <sub>1</sub> ) | 8(C <sub>24</sub> H <sub>27</sub> O <sub>2</sub> N <sub>1</sub> ) C <sub>7</sub> H <sub>8</sub> | C <sub>24</sub> H <sub>27</sub> O <sub>2</sub> N <sub>1</sub> | C <sub>24</sub> H <sub>27</sub> O <sub>2</sub> N <sub>1</sub> C <sub>3</sub> H <sub>3</sub> |
| Mw                                       | 1445.93                                                           | 2984.00                                                                                         | 361.48                                                        | 400.53                                                                                      |
| crystal system                           | monoclinic                                                        | trigonal                                                                                        | monoclinic                                                    | tetragonal                                                                                  |
| space group                              | P2 <sub>1</sub> /n (#14)                                          | R-3c (#167)                                                                                     | C2/c (#15)                                                    | I-4 (#82)                                                                                   |
| Z                                        | 4                                                                 | 6                                                                                               | 16                                                            | 8                                                                                           |
| a[Å]                                     | 13.9624(4)                                                        | 20.7677(6)                                                                                      | 24.3976(4)                                                    | 17.623                                                                                      |
| b[Å]                                     | 24.9353(7)                                                        |                                                                                                 | 14.4444(3)                                                    | 17.623                                                                                      |
| c[Å]                                     | 23.7426(7)                                                        | 70.979(2)                                                                                       | 24.3798(4)                                                    | 15.181                                                                                      |
| α[°]                                     | 90                                                                | 90                                                                                              | 90                                                            | 90                                                                                          |
| β[°]                                     | 92.140(2)                                                         | 90                                                                                              | 94.7956(8)                                                    | 90                                                                                          |
| γ[°]                                     | 90                                                                | 120                                                                                             | 90                                                            | 90                                                                                          |
| V[Å <sup>3</sup> ]                       | 8269.4(4)                                                         | 26511.5(14)                                                                                     | 8561.6(3)                                                     | 4714.4                                                                                      |
| T[K]                                     | 213                                                               | 213                                                                                             | 213                                                           | 213                                                                                         |
| ρ <sub>calcd</sub> [Mg m <sup>-3</sup> ] | 1.163                                                             | 1.121                                                                                           | 1.122                                                         | 1.129                                                                                       |
| 2θ <sub>max</sub>                        | 136.4                                                             | 136.4                                                                                           | 136.4                                                         | -                                                                                           |
| μ (Cu-Kα) [cm <sup>-1</sup> ]            | 5.73                                                              | 5.504                                                                                           | 5.532                                                         | -                                                                                           |
| GOF                                      | 1.89                                                              | 1.900                                                                                           | 1.224                                                         | -                                                                                           |
| total / unique reflections               | 57903 / 14728                                                     | 83491 / 5399                                                                                    | 32425 / 7704                                                  | -                                                                                           |
| reflections included in refinement       | 5121                                                              | 2207                                                                                            | 3492                                                          | -                                                                                           |
| residual electron density                | 0.70 / -0.56                                                      | 0.67 / -0.38                                                                                    | 0.33 / -0.42                                                  | -                                                                                           |
| Max / Min [e/Å <sup>3</sup> ]            |                                                                   |                                                                                                 |                                                               |                                                                                             |
| reflections / parameters                 | 9.00                                                              | 15.29                                                                                           | 15.79                                                         | -                                                                                           |
| R <sup>1</sup> [a] / wR <sup>2</sup> [b] | 0.148 / 0.294                                                     | 0.1395 / 0.3228                                                                                 | 0.0758 / 0.2294                                               | -                                                                                           |
| reference                                | CCDC-632005 (ref. 14)                                             | CCDC-XXXXXX                                                                                     | CCDC- 659622                                                  | IRUOUH (ref. 10d)                                                                           |