Supplementary Material (ESI) for Chemical Communications


# Supplementary Information

## Crystallographic characterization and identification of a minor isomer of $C_{84}$ fullerene

*Lars Epple, Konstantin Amsharov, Kalin Simeonov, Ina Dix and Martin Jansen*

Table S1. C-C bond lenghts [Å] in $C_{84}$(14) according to experimental data and DFT calculation (B3LYP-631G).

| C-C Bond | C-C bond length, Å | | | | Deviation, Å | |
|---|---|---|---|---|---|---|
| | X-Ray | X-Ray | X-Ray Avarage | DFT | from Cs symmetry | from calculated values |
| 1-2 | 1.377 | 1.379 | 1.378 | 1.391 | 0.002 | -0.0130 |
| 1-6 | 1.435 | 1.430 | 1.433 | 1.436 | 0.005 | -0.0035 |
| 1-9 | 1.433 | 1.456 | 1.445 | 1.455 | 0.023 | -0.0105 |
| 2-3 | 1.421 | 1.408 | 1.415 | 1.429 | 0.013 | -0.0145 |
| 2-12 | 1.459 | 1.459 | 1.459 | 1.462 | 0 | -0.0030 |
| 3-4 | 1.411 | 1.427 | 1.419 | 1.421 | 0.016 | -0.0020 |
| 3-14 | 1.463 | 1.451 | 1.457 | 1.461 | 0.012 | -0.0040 |
| 4-5 | 1.469 | 1.453 | 1.461 | 1.473 | 0.016 | -0.0120 |
| 4-17 | 1.467 | 1.449 | 1.458 | 1.468 | 0.018 | -0.0100 |
| 5-6 | 1.404 | 1.414 | 1.409 | 1.414 | 0.010 | -0.0050 |
| 5-20 | 1.463 | 1.472 | 1.468 | 1.474 | 0.009 | -0.0065 |
| 6-7 | 1.460 | 1.456 | 1.458 | 1.462 | 0.004 | -0.0040 |
| 7-8 | 1.426 | 1.437 | 1.432 | 1.439 | 0.011 | -0.0075 |
| 7-22 | 1.395 | 1.408 | 1.402 | 1.406 | 0.013 | -0.0045 |
| 8-9 | 1.433 | 1.437 | 1.435 | 1.444 | 0.004 | -0.0090 |
| 8-25 | 1.420 | 1.416 | 1.418 | 1.431 | 0.004 | -0.0130 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 9-10 | 1.383 | 1.382 | 1.383 | 1.383 | 0,001 | 0 |
| 10-11 | 1.447 | 1.453 | 1.450 | 1.462 | 0.006 | -0.0120 |
| 10-27 | 1.436 | 1.438 | 1.437 | 1.451 | -0.002 | -0.0140 |
| 11-12 | 1.368 | 1.374 | 1.371 | 1.380 | 0.006 | -0.0090 |
| 11-29 | 1.442 | 1.440 | 1.441 | 1.441 | 0.002 | 0 |
| 12-13 | 1.433 | 1.422 | 1.428 | 1.442 | 0.011 | -0.0145 |
| 13-14 | 1.445 | 1.450 | 1.448 | 1.449 | 0.005 | -0.0015 |
| 13-31 | 1.422 | 1.416 | 1.419 | 1.427 | 0.006 | -0.0080 |
| 14-15 | 1.341 | 1.349 | 1.345 | 1.364 | 0.008 | -0.0190 |
| 15-16 | 1.446 | 1.454 | 1.450 | 1.450 | 0.008 | 0 |
| 15-33 | 1.438 | 1.438 | 1.438 | 1.443 | 0 | -0.0050 |
| 16-17 | 1.412 | 1.424 | 1.418 | 1.428 | 0.012 | -0.0100 |
| 16-35 | 1.416 | 1.416 | 1.416 | 1.431 | 0 | -0.0150 |
| 17-18 | 1.414 | 1.407 | 1.411 | 1.411 | 0.007 | 0 |
| 18-19 | 1.456 | 1.455 | 1.456 | 1.461 | 0,001 | -0.0055 |
| 18-37 | 1.423 | 1.418 | 1.421 | 1.436 | 0.005 | -0.0155 |
| 19-20 | 1.404 | 1.407 | 1.406 | 1.413 | 0.003 | -0.0075 |
| 19-39 | 1.447 | 1.423 | 1.435 | 1.438 | 0.024 | -0.0030 |
| 20-21 | 1.460 | 1.462 | 1.461 | 1.474 | 0.002 | -0.0130 |
| 21-22 | 1.471 | 1.463 | 1.467 | 1.468 | 0.008 | -0,0010 |
| 21-41 | 1.419 | 1.415 | 1.417 | 1.421 | 0.004 | -0.0040 |
| 22-23 | 1.422 | 1.415 | 1.419 | 1.429 | 0.007 | -0.0105 |
| 23-24 | 1.417 | 1.430 | 1.424 | 1.430 | 0.013 | -0.0065 |
| 23-43 | 1.432 | 1.443 | 1.438 | 1.444 | 0.011 | -0.0065 |
| 24-24 | 1.455 | -- | 1.455 | 1.459 | -- | -0.0040 |
| 24-25 | 1.408 | 1.405 | 1.407 | 1.415 | 0.003 | -0.0085 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 25-26 | 1.464 | 1.474 | 1.469 | 1.472 | 0.010 | -0.0030 |
| 26-26 | 1.470 | -- | 1.470 | 1.477 | -- | -0.0070 |
| 26-27 | 1.417 | 1.423 | 1.420 | 1.419 | 0.006 | 0,0010 |
| 27-28 | 1.436 | 1.439 | 1.438 | 1.433 | 0.003 | 0.0045 |
| 28-28 | 1.365 | -- | 1.365 | 1.368 | -- | -0.0030 |
| 28-29 | 1.442 | 1.445 | 1.444 | 1.449 | 0.003 | -0.0055 |
| 29-30 | 1.415 | 1.414 | 1.415 | 1.425 | 0,001 | -0.0105 |
| 30-30 | 1.472 | -- | 1.472 | 1.473 | -- | -0.0010 |
| 30-31 | 1.454 | 1.465 | 1.460 | 1.467 | 0.011 | -0.0075 |
| 31-32 | 1.472 | 1.461 | 1.467 | 1.471 | 0.011 | -0.0045 |
| 32-32 | 1.450 | -- | 1.450 | 1.464 | -- | -0.0140 |
| 32-33 | 1.410 | 1.426 | 1.418 | 1.425 | 0.016 | -0.0070 |
| 33-34 | 1.439 | 1.418 | 1.429 | 1.441 | 0.021 | -0.0125 |
| 34-34 | 1.361 | -- | 1.361 | 1.372 | -- | -0.0110 |
| 34-35 | 1.454 | 1.465 | 1.460 | 1.459 | 0.011 | 0 |
| 35-36 | 1.421 | 1.413 | 1.417 | 1.422 | 0.008 | -0.0050 |
| 36-36 | 1.454 | -- | 1.454 | 1.477 | -- | -0.0230 |
| 36-37 | 1.420 | 1.427 | 1.424 | 1.427 | 0.007 | -0.0035 |
| 37-38 | 1.438 | 1.445 | 1.442 | 1.450 | 0.007 | -0.0085 |
| 38-38 | 1.375 | -- | 1.375 | 1.386 | -- | -0.0110 |
| 38-39 | 1.453 | 1.447 | 1.450 | 1.456 | 0.006 | -0.0060 |
| 39-40 | 1.373 | 1.385 | 1.379 | 1.387 | 0.012 | -0.0080 |
| 40-40 | 1.449 | -- | 1.449 | 1.465 | -- | -0.0160 |
| 40-41 | 1.423 | 1.420 | 1.422 | 1.432 | 0.003 | -0.0105 |
| 41-42 | 1.444 | 1.458 | 1.451 | 1.462 | 0.014 | -0.0110 |
| 42-43 | 1.355 | -- | 1.355 | 1.367 | -- | -0.0120 |

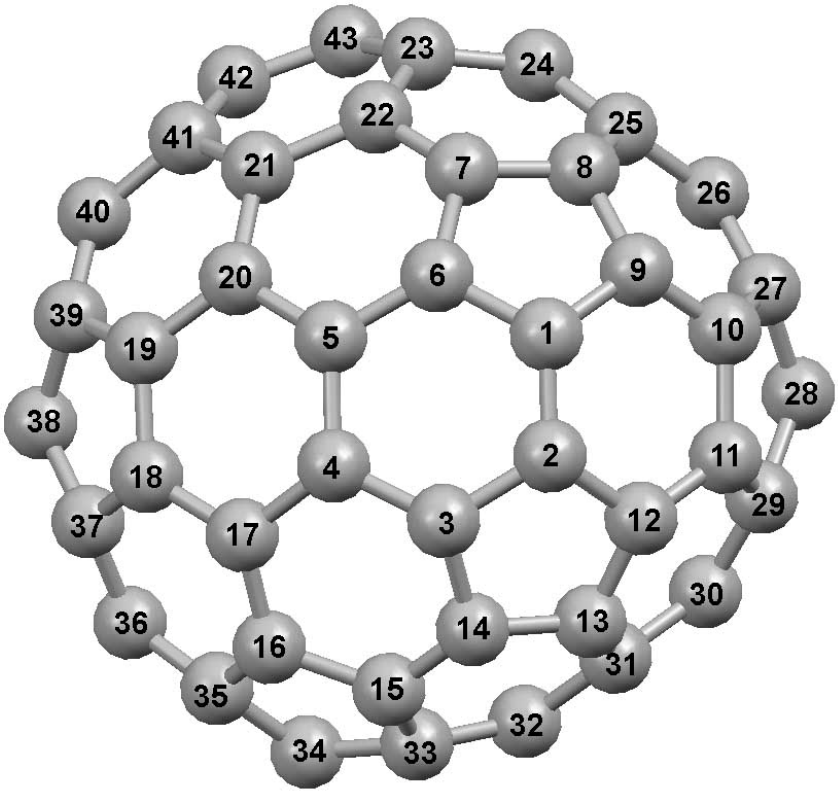


Fig S1. Numbering of symmetry-independent carbon atoms of $C_{84}$(14).

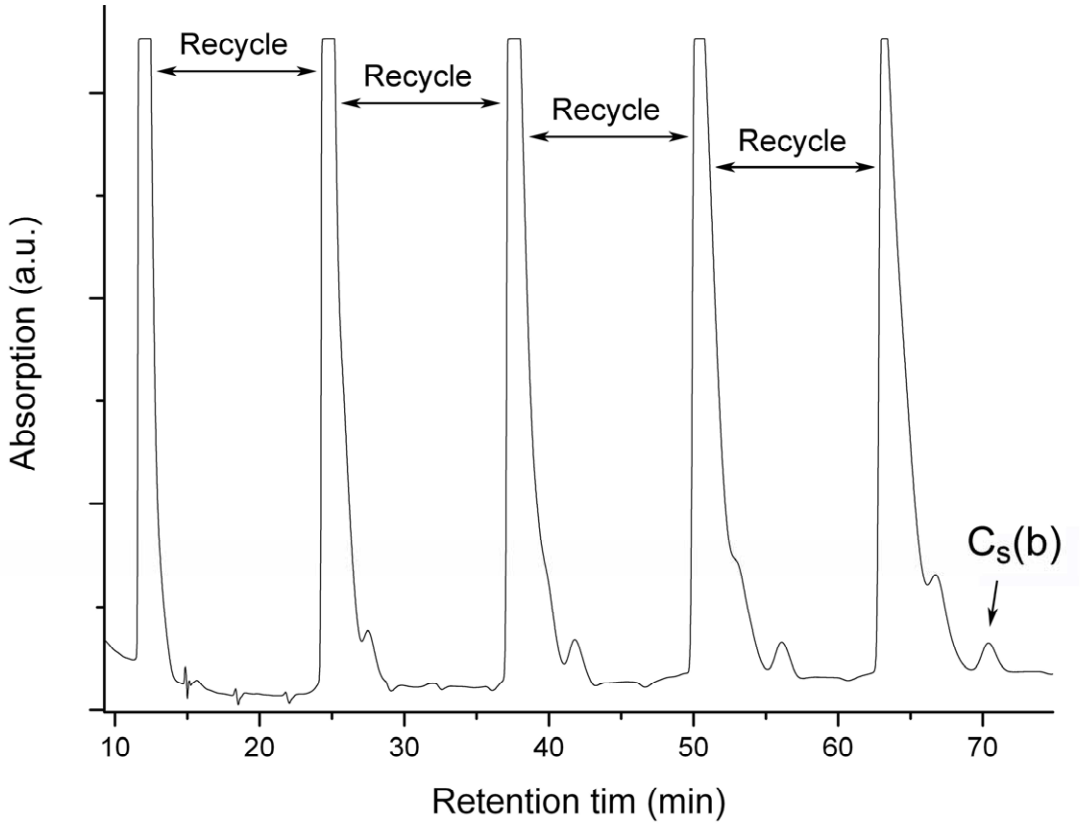


Fig S2. Recycling-phase HPLC profile of the $C_{84}$-containing fraction. Cosmosil *5PYE* column (10mm × 250mm), monitored at 290 nm with toluene as eluent.

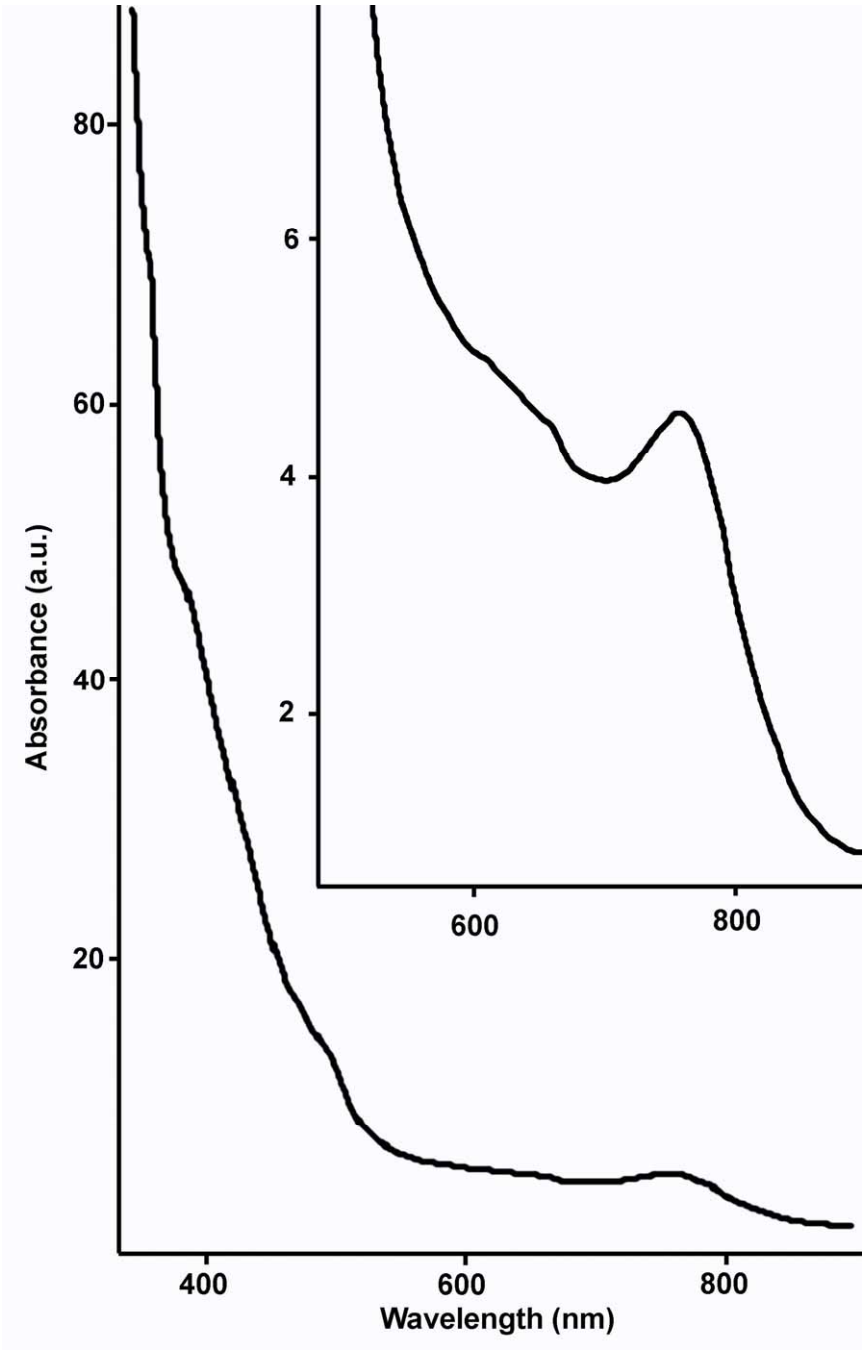


Fig S3. UV/VIS absorption spectra of $C_{84}$(14) in toluene solution.

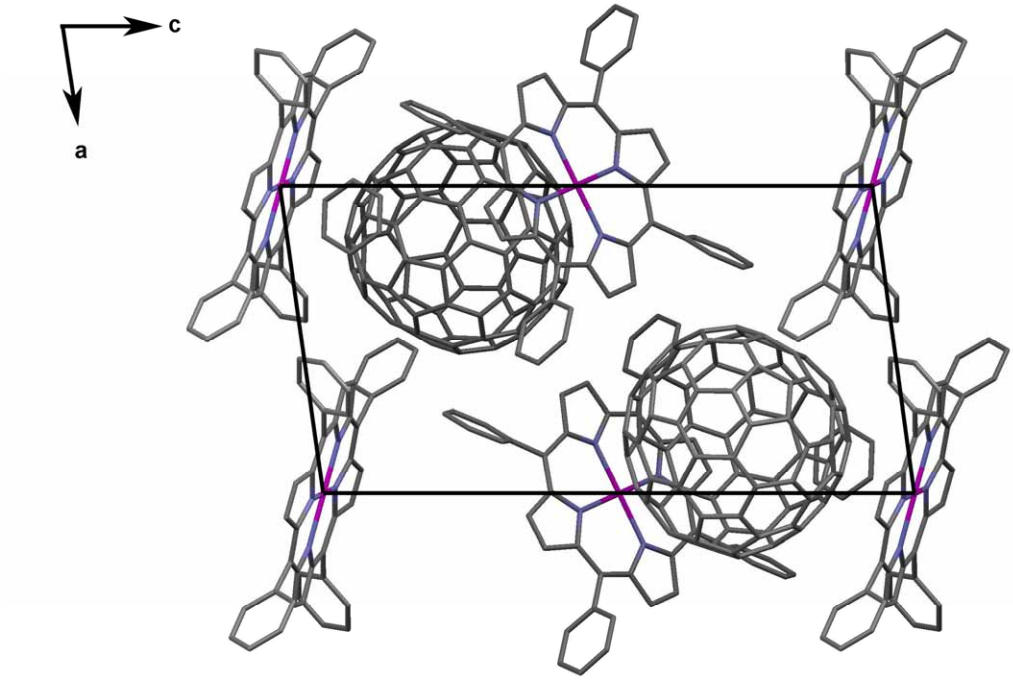


Fig S4. Projection of $C_{84}$ (14) ·AgTPP·$C_6H_6$ onto [010] plane.

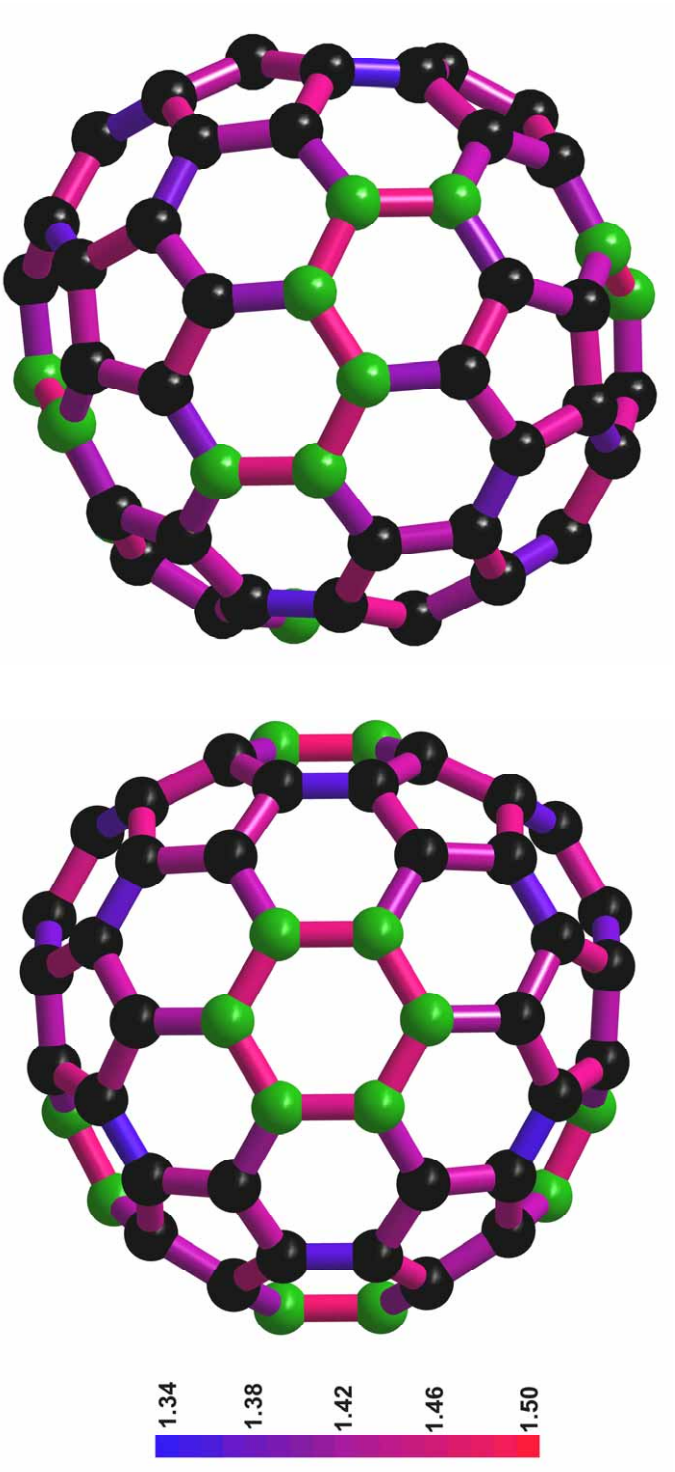


Fig S5. Bond length distribution in $C_{84}$ (14). The shortest bonds correspond to the bonds between two pentagons in the pyracylene fragments, the longest ones between carbon atoms which are not involved in pentagons (green labeled). (C-C distances in Å).