Supplementary Information

Crystal chemistry of diarylethene photochromic switches

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Network topology analysis for $[Fe^{II}(\mathbf{16o})_2\{Ag(CN)_2\}_2\{Ag(CN)\}_2]$.

Systre input file for $[Fe^{II}(\mathbf{16o})_2\{Ag(CN)_2\}_2\{Ag(CN)\}_2]$.

```
CRYSTAL
  NAME DAEFeAgCN
  GROUP Pbcn
  CELL 26.6944 10.2893 20.4517 90 90 90
  NODE 1 6 0.5000  1.0000  1.0000
EDGE 1 0.5000  2.0000  1.0000
EDGE 1 0.5000  1.0000  1.5000
EDGE 1 0.5000  0.0000  1.0000
EDGE 1 0.5000  1.0000  0.5000
EDGE 1 1.2266   0.8837   0.8506
EDGE 1 -0.2266   1.1163   1.1494
  NODE 2 3  1.2266   0.8837   0.8506
EDGE 2 0.5000  1.0000  1.0000
EDGE 2 1.2734   1.3837   0.8506
EDGE 2 1.2734   0.3837   0.8506
END
```

Systre output file for $[Fe^{II}(\mathbf{16o})_2\{Ag(CN)_2\}_2\{Ag(CN)\}_2]$.

```
Structure #1 - "DAEFeAgCN".
   Input structure described as 3-periodic.
   Given space group is Pbcn.
   12 nodes and 24 edges in repeat unit as given.
   Structure is not connected.
   Processing components separately.
   ==========
   Processing component 1:
      multiplicity = 3
   Input structure described as 3-periodic.
   Given space group is P1.
   12 nodes and 24 edges in repeat unit as given.
   Ideal repeat unit smaller than given (6 vs 24 edges).
   Point group has 8 elements.
   2 kinds of node.
   Equivalences for non-unique nodes:
      V2 --> V1
      V4 --> V3
      V5 --> V3
      V6 --> V3
      V7 --> V3
      V8 --> V3
      V9 --> V3
      V10 --> V3
      V11 --> V1
      V12 --> V1

   Coordination sequences:
      Node V3:    3 9 26 59 103 154 215 285 364 453
      Node V1:    6 20 44 76 118 170 230 300 380 468

   TD10 = 1719
   Ideal space group is Cmmm.
   Ideal group or setting differs from given (Cmmm vs P1).
   Structure is new for this run.
```

```
   Relaxed cell parameters:
       a = 5.70263, b = 1.00771, c = 1.00959
       alpha = 90.0000, beta = 90.0000, gamma = 90.0000
   Cell volume: 5.80169
   Relaxed positions:
      Node V3:    0.32515 0.00000 0.00000
      Node V1:    0.00000 0.50000 0.00000
   Edges:
      0.00000 0.50000 0.00000  <->  0.00000 1.50000 0.00000
      0.00000 0.50000 0.00000  <->  0.00000 0.50000 1.00000
      0.32515 0.00000 0.00000  <->  0.50000 -0.00000 -0.00000
      0.32515 0.00000 0.00000  <->  0.17485 0.50000 0.00000
   Edge centers:
      0.00000 1.00000 0.00000
      0.00000 0.50000 0.50000
      0.41258 -0.00000 -0.00000
      0.25000 0.25000 0.00000
   Edge statistics: minimum = 0.99427, maximum = 1.00959, average = 1.00000
   Angle statistics: minimum = 60.89624, maximum = 180.00000, average =
111.42857
   Shortest non-bonded distance = 1.00771
   Degrees of freedom: 4
   Finished component 1.
 ==========

Finished structure #1 - "DAEFeAgCN".
```

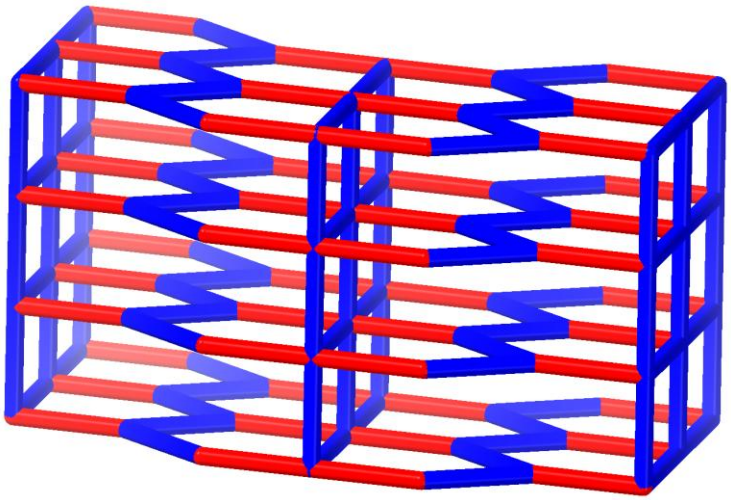

Figure S1 The most symmetric form of the 3,6-network in $[Fe^{II}(\mathbf{16o})_2\{Ag(CN)_2\}_2\{Ag(CN)\}_2$. Red linkers are placed where the DAE linker is placed in this coordination polymer.