SUPPLEMENTARY MATERIAL

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S-1. Problems with the Z10 structure

The structure of Z10 is not completely satisfactory. The data for the sample were collected 14th in the series of 55 unit cell determinations that eventually comprised the overall data set.. The data showed an allotwinn between Z6 and Z10 with roughly equal sizes of the two components of the twin. A set of data was collected but with the expectation that an untwined crystal of Z10 would be found. This never happened. The original set of data, collected in 2002, has been lost somewhere between then and now.A set of 564 reflections contained 300 belonging to Z10, 53 belonging to Z6 and 158 belonging to both as will as 51 that could not be indexed. This corresponds to a Z6 sample about 75% the size of the Z10 sample.The structure was solved using all the Z10 data and gave a reasonable structure coopered to the Z2, Z4, and Z6 results. However about half the data contained intensity contributed by the Z6 component. The values for R1 and wR2 were both larger than they would be for a satisfactory structure. A referee pointed out that a difference Fourier map showed disordered molecules with the end-for-end disorder along the pseudo two-fold axis.This was found in the difference maps for molecule 2 and, less pronounced, for molecule 4.Results of refining the end-for-end disorder.

| Refinement | R1 | wR2 |
|---|---|---|
| No end-for end-disorder | 0.114 | 0.338 |
| side-to-side disorder end-for-end disorderin molecule 4 | 0.107 | 0.337 |
| the fractions of end-for-end disorder were 0.009 and 0.032 compared to the side-to-side disorder of 0.525 and 0.432end-for-end disorder for molecules 2 and 4 | 0.107 | 0.332 |

the end-for-end disorder refined to -0.003 and -0.009. I.e. the least-squares result was no end-for-end disorder, even though the difference map seemed to indicate it.These results suggest to us that the disorder found in the difference maps is a consequence of the contributions from the Z6 component. The question of end-for-end disorder is an open one.

Table S-2. Comparison of bond distances (A) among the four polymorphs

| distance | Z2 | Z4 | Z6 | Z10 |
|---|---|---|---|---|
| N1-O1 | 1.236(2) | 1.242(2) | 1.241(2) | 1.245(2) |
| N1-O2 | 1.456(2) | 1.448(2) | 1.442(2) | 1.434(2) |
| N2-O2 | 1.381(2) | 1.380(2) | 1.381(2) | 1.379(2) |
| C1-N1 | 1.331(3) | 1.338(3) | 1.338(2) | 1.335(3) |
| C2-N2 | 1.333(3) | 1.342(3) | 1.340(2) | 1.334(3) |
| C1-C2 | 1.417(3) | 1.401(2) | 1.401(2) | 1.406(2) |
| C2-C3 | 1.414(3) | 1.417(3) | 1.418(2) | 1.415(3) |
| C3-C4 | 1.367(3) | 1.373(4) | 1.370(3) | 1.366(3) |
| C4-C5 | 1.466(2) | 1.462(2) | 1.463(2) | 1.466(2) |
| C5-C6 | 1.363(3) | 1.357(4) | 1.361(3) | 1.368(3) |
| C6-C1 | 1.414(3) | 1.409(2) | 1.410(2) | 1.411(3) |
| C4-C7 | 1.500(3) | 1.503(5) | 1.497(3) | 1.499(4) |
| C5-C8 | 1.514(3) | 1.505(4) | 1.512(3) | 1.507(4) |

Table S-3. Degrees of disorder

| | |
|---|---|
| Z2 | |
| Molecule 1 | 0.893(2)/0.107(2) |
| Z4 | |
| Molecule 1 | 0.567(2)/0.433(2) |
| Molecule 2 | 0.631(2)/0.369(2) |
| Z6 | |
| Molecule 1 | 0.766(2)/0.234(2) |
| Molecule 2 | 0.502(2)/0.498(2) |
| Molecule 3 | 0.566(2)/0.434(2) |
| Z10 | |
| Molecule 1 | 0.546(2)/0.454(2) |
| Molecule 2 | 0.619(3)/0.381(3) |
| Molecule 3 | 0.598(3)/0.402(3) |
| Molecule 4 | 0.545(2)/0.455(2) |
| Molecule 5 | 0.810(3)/0.190(3) |

S-4. Determination of the twin laws

$A_1$ is the orientation matrix of component 1 of the twin.

$A_2$ is the orientation matrix of component 2 of the twin.

$A_1^{-1}$ and $A_2^{-2}$ are inverse matrices for $A_1$ and $A_2$.

$A_1^{-1}A_2$ gives the matrix to convert the indices of a reflection of component 2 to those of the overlapping reflection of component 1.

$A_1^{-1}A_2$ gives the corresponding transformation for component 1 to component 2.

This can be confirmed by picking any three sets of indices from the list produced by the program GEMINI (Sparks, 1999) and solving for the transformation matrix,

## S-5. Matrix conversions for the allotwins

| Twin law from Orientation matrices | | | Rational fraction approximation | | |
|---|---|---|---|---|---|
| **Z2/Z4** | | | | | |
| 1.998 | -0.006 | -0.010 | 2 | 0 | 0 |
| 0.972 | -1.003 | 0.013 | 1 | -1 | 0 |
| 0.961 | 0.036 | -0.999 | 1 | 0 | -1 |
| **Z2/Z6** | | | | | |
| -0.998 | 1.000 | -0.001 | -1 | 1 | 0 |
| 2.283 | 0.745 | 0.003 | 9/4 | 3/4 | 0 |
| 1.292 | 0.726 | -0.993 | 5/4 | 3/4 | -1 |
| **Z4/Z6** | | | | | |
| -0.005 | 0.998 | 0.002 | 0 | 1 | 0 |
| 0.740 | 0.172 | 0.764 | 3/4 | 1/6 | 3/4 |
| 1.741 | 0.168 | -0.238 | 7/4 | 1/6 | -1/6 |
| **Z6/Z10** | | | | | |
| -0.987 | 0.008 | -0.009 | -1 | 0 | 0 |
| -0.045 | -1.022 | 1.025 | 0 | -1 | 1 |
| -0.092 | 1.183 | 0.489 | 0 | 5/4 | 5/12 |

Legends for Supplementary figures

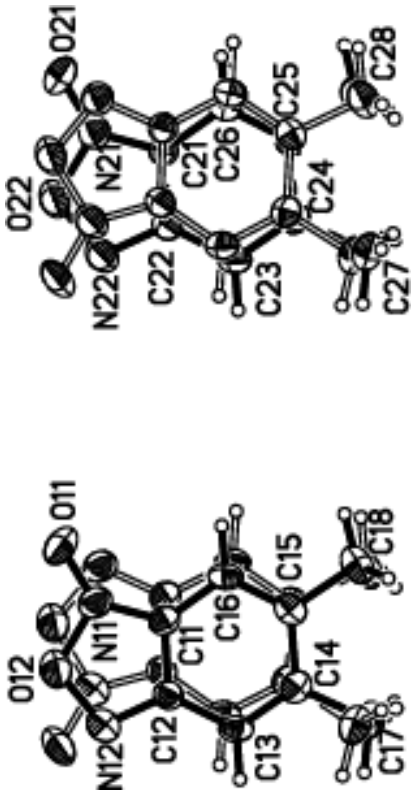



Fig. S-6 Thermal ellipsoids and labeling for molecules in Z4. Molecule 1: disorder 56.7(1)%/43.3(1)%. Molecule 2: disorder 63.1(1)%/36.9(1)%.

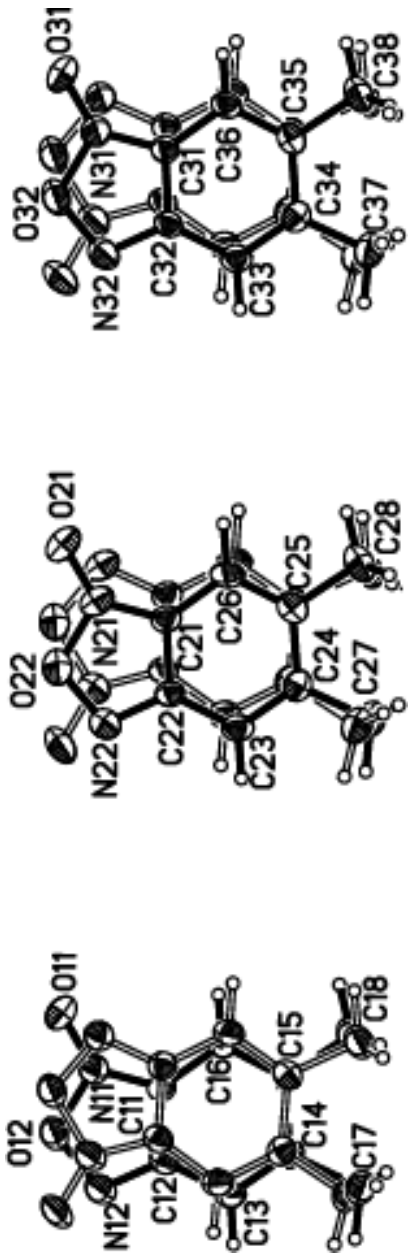



Fig. S-7 Thermal ellipsoids and labeling for molecules in Z6. Molecule 1: disorder 76.6(2)%/23.4(2)%. Molecule 2: disorder 50.2(1)%/49.8(1)%. Molecule 3: disorder 56.5(1)%/43.5(1)%.

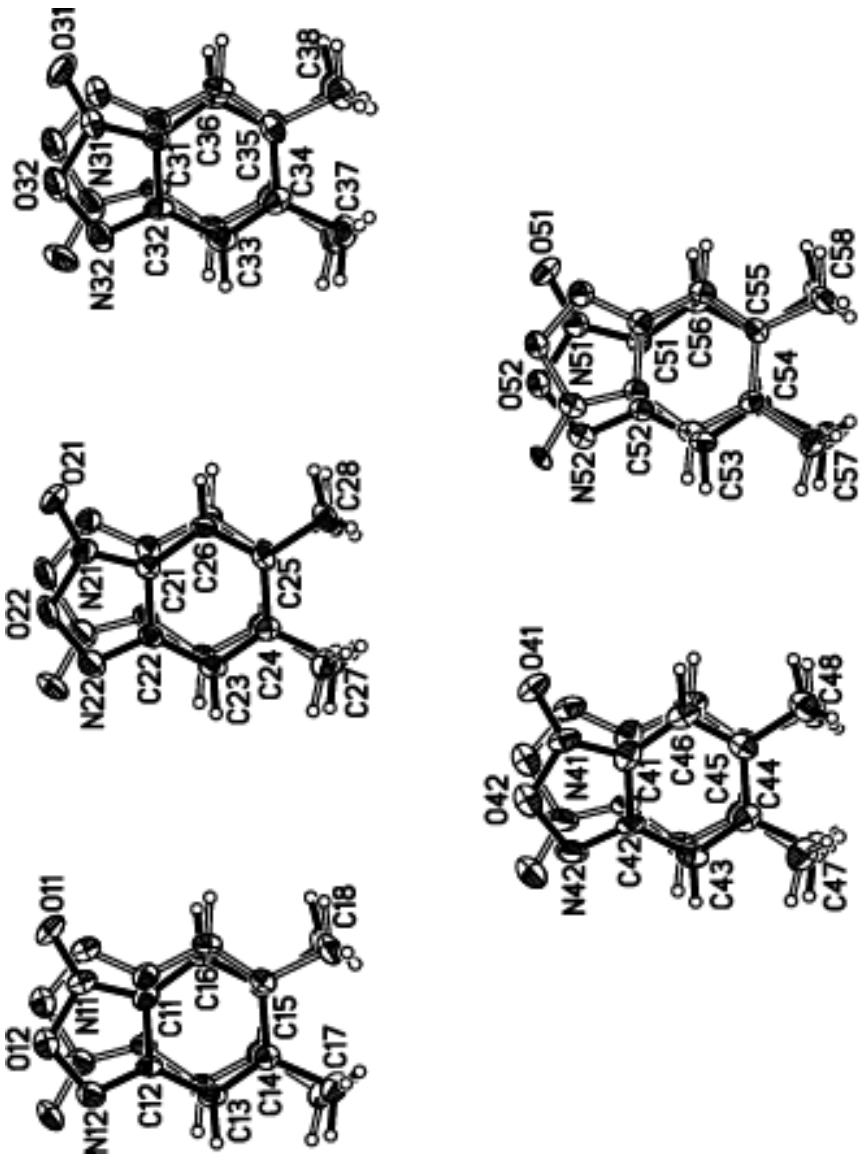



Fig. S-8 Thermal ellipsoids and labeling for molecules in Z10. Molecule 1: disorder 54.6(2)%/45.4(2)%. Molecule 2: disorder 61.9(3)%/38.1(3)%. Molecule 3: disorder 59.8(3)%/40.2(3)%.

Molecule 4: disorder 54.5(2)%/45.5(2)%. Molecule 5: disorder 81.0(3)%/19.0(3)%.

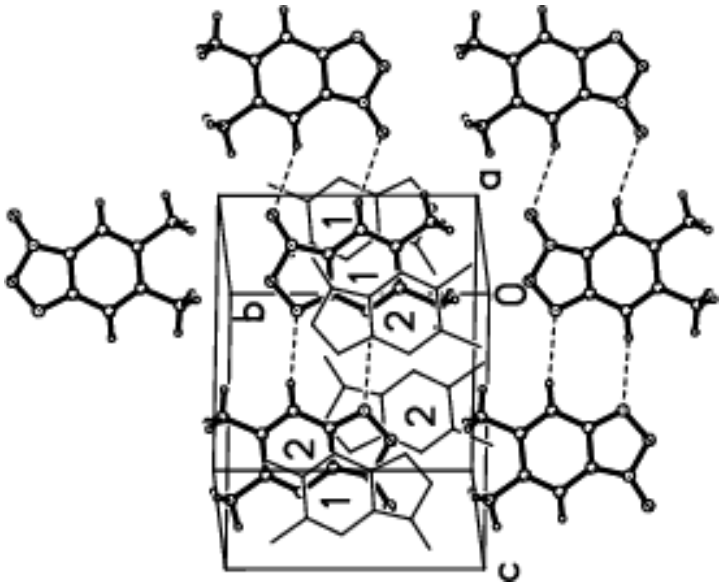



Fig. S-9 View of Z4 normal to the plane (1,0,1). The numbers indicate the independent molecules.

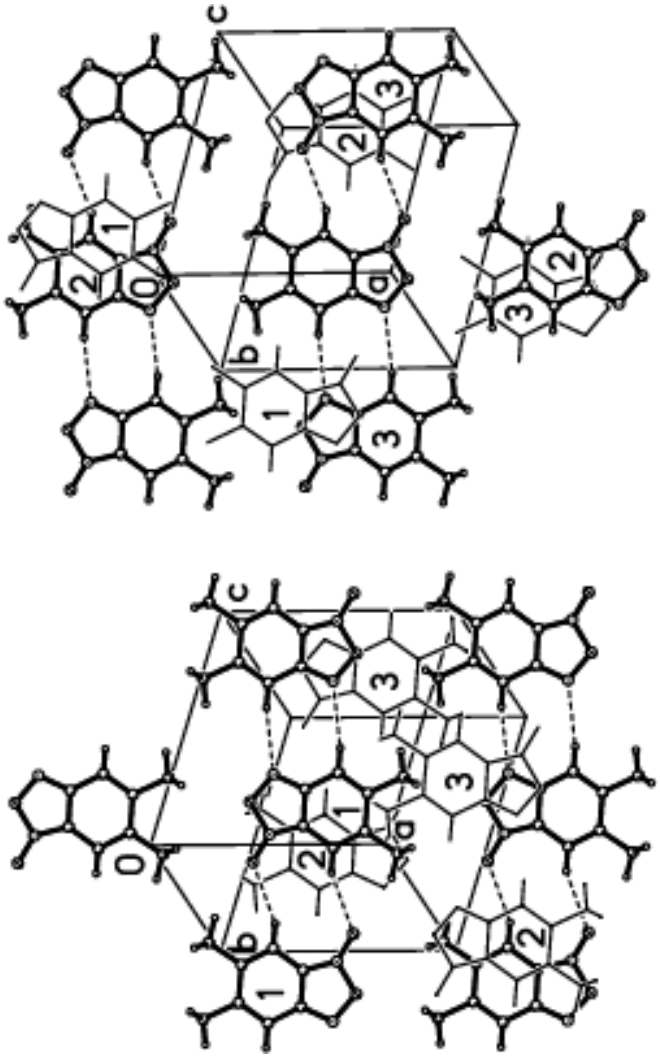
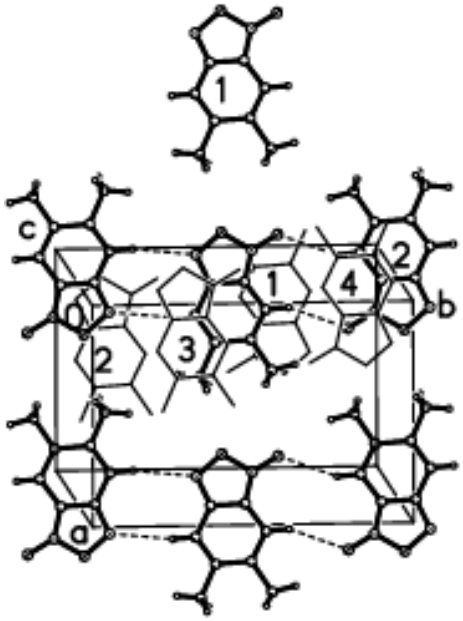
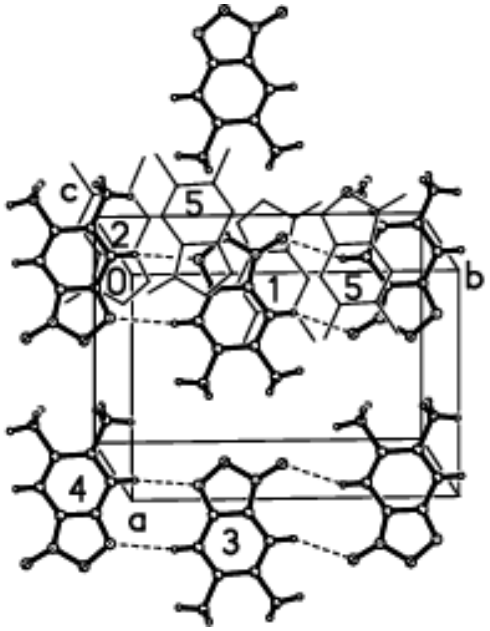



Fig. S-10 View of Z6 normal to the plane (0,1,1). The numbers indicate the independent molecules. Left: layer of molecules 1. Right: layer of molecules 2 and 3.


1
c
2
1
4
0
b
2
3
a


c
5
2
0
1
5
b
4
a
3

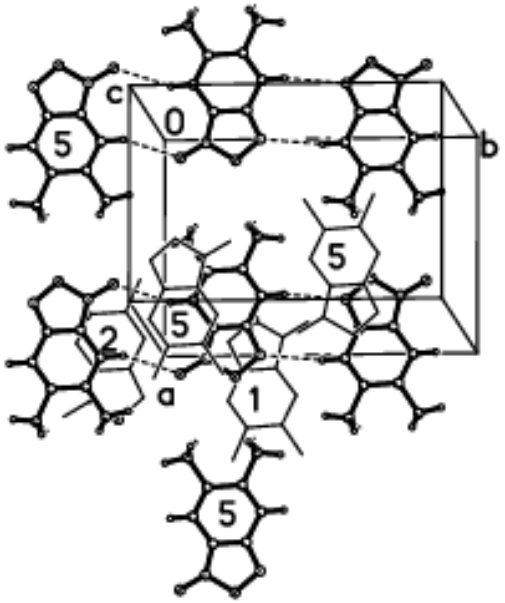

c
0
5
b
5
5
2
a
1
5

Fig. S-11  View of Z10 normal to the plane (0,0,1).  The numbers indicate the independent molecules.  Left: layer of molecules 1 and 2.  Center:  layer of molecules 3 and 4.  Right: layer of molecules 5.

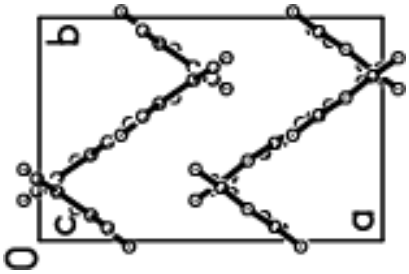



Fig. S-12.  Dimethylphthalic anhydride viewed down the c axis.  It is clear that there are no ribbons nor layers present.