Supporting Information for

Local Structure in the Disordered Solid Solution of *cis*- and *trans*-Perinones

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IUPAC name for *cis*-perinone:
3,10,17,24-tetraazaoctacyclo[13.13.2.0^{2},^{10}.0^{4},^{9}.0^{12},^{29}.0^{17},^{25}.0^{18},^{23}.0^{26},^{30}]triaconta-1(28),2,4(9),5,7,12,14,18(23),19,21,24,26,29-tridecaene-11,16-dione;
IUPAC name for *trans*-perinone:
3,10,17,24-tetraazaoctacyclo[13.13.2.0^{2},^{10}.0^{4},^{9}.0^{12},^{29}.0^{16},^{24}.0^{18},^{23}.0^{26},^{30}]triaconta-1(28),2,4(9),5,7,12,14,16,18(23),19,21,26,29-tridecaene-11,25-dione).

Table SI 1. Coordination sphere of a reference molecule.

	Molecular position	Symmetry operation [a)]
Reference molecule	0.5, 0.5, 0.5	*x*, *y*, *z*
Neighbouring molecule		
1	1.5, 1.5, 0.5	*x*+1, *y*+1, *z*
2	1.5, 2.5, 0.5	*x*+1, *y*+2, *z*
3	1.5, 0, 1	*x*+1, *y*-0.5, *z*+0.5
4	1.5, 1, 1	*x*+1, *y*+0.5, *z*+0.5
5	0.5, -1, 0	*x*, *y*-1.5, *z*-0.5
6	0.5, 0, 0	*x*, *y*-0.5, *z*-0.5
7	0.5, 1, 0	*x*, *y*+0.5, *z*-0.5
8	0.5, 2, 0	*x*, *y*+1.5, *z*-0.5
9	0.5, -0.5, 0.5	*x*, *y*-1, *z*
10	0.5, 1.5, 0.5	*x*, *y*+1, *z*
11	0.5, -1, 1	*x*, *y*-1.5, *z*+0.5
12	0.5, 0, 1	*x*, *y*-0.5, *z*+0.5
13	0.5, 1, 1	*x*, *y*+0.5, *z*+0.5
14	0.5, 2, 1	*x*, *y*+1.5, *z*+0.5
15	-0.5, 0, 0	*x*-1, *y*-0.5, *z*-0.5
16	-0.5, 1, 0	*x*-1, *y*+0.5, *z*-0.5
17	-0.5, -1.5, 0.5	*x*-1, *y*-2, *z*
18	-0.5, -0.5, 0.5	*x*-1, *y*-1, *z*

a) With regards to neighbourhoods, symmetry operations denote the translation between molecules, given with the standard setting of the unit cell with $Z = 2$ as reference.

Table SI 2: Calculated structures for the solid solution from DFT-D minimisations.

Structure	Z	SG [a]	a	b	c	α	β	γ	g_i	E_{rel} / kJ/mol [b]	p_i at 293 K / %
V.R. 14, experimental	**2**	***P* $2_1/c$**	**11.80**	**4.81**	**16.24**	**90.00**	**99.02**	**90.00**			
C T'	2	*P* 1	12.69	4.82	15.88	87.32	103.61	93.57	12	23.96	0.000
C T	2	*P* 1	12.15	4.77	16.05	89.33	99.64	89.83	12	12.78	0.258
c' = 2**c**$_0$: C' C T' T'	4	*P* 2_1	12.03	4.81	32.61	90	98.04	90	4	23.10	0.000
c' = 2**c**$_0$: C' C T T'	4	*P* 1	12.38	4.78	31.86	87.89	101.19	92.58	8	16.68	0.000
c' = 2**c**$_0$: C' C T T	4	*P* 2_1	12.11	4.77	31.79	90	99.46	90	4	10.88	3.149
c' = 2**c**$_0$: C C' T' T'	4	*P* 2_1	12.14	4.77	32.71	90	96.76	90	4	27.61	0.000
c' = 2**c**$_0$: C C' T T'	4	*P* 1	12.62	4.77	31.92	91.45	102.74	89.73	8	19.80	0.000
c' = 2**c**$_0$: C C' T T	4	*P* 2_1	12.2	4.74	32.17	90	100.3	90	4	11.92	0.255
c' = 2**c**$_0$: C C T' T'	4	*P* 1	12.02	4.81	32.83	90.12	97.2	89.86	8	25.80	0.000
c' = 2**c**$_0$: C C T' T	4	*P* 1	12.28	4.79	32.22	91.22	101.32	88.12	8	18.37	0.000
c' = 2**c**$_0$: C C T T'	4	*P* 1	12.35	4.78	31.97	88.71	100.64	91.91	8	19.45	0.000
c' = 2**c**$_0$: C C T T	4	*P* 1	11.87	4.77	32.68	86.24	97.82	92.07	8	11.36	1.319
c' = 2**c**$_0$: C T' C' T'	4	*P* 1	12.69	4.82	31.85	88.29	103.8	92.57	4	24.06	0.000
c' = 2**c**$_0$: C T' C' T	4	*P* 1	12.42	4.79	32.22	87.81	102.75	91.91	4	16.59	0.000
c' = 2**c**$_0$: C T C' T'	4	*P* 1	12.44	4.78	31.87	95.12	101.15	86.02	4	16.05	0.000
c' = 2**c**$_0$: C T C' T	4	*P* 1	12.28	4.76	31.83	89.94	100.01	89.39	4	12.00	0.232

c' = 2**c**$_0$: C T C T'	4	*P* 1	12.33	4.78	32.19	89.3	101.86	90.6	8	18.84	0.000
b' = 2**b**$_0$: C T' C' T'	4	*P* 1	12.66	9.54	16.46	98.48	104.04	84.82	4	21.49	0.000
b' = 2**b**$_0$: C T' C' T	4	*P* 1	12.96	9.34	16.35	94.78	103.98	86.78	4	20.12	0.000
b' = 2**b**$_0$: C T C' T'	4	*P* 1	12.67	9.49	16.08	92.84	103.13	87.54	4	19.47	0.000
b' = 2**b**$_0$: C T C' T	4	*P* 1	11.64	9.5	16.71	83.39	96.83	93.59	4	11.47	0.548
b' = 2**b**$_0$: C T C T'	4	*P* 1	12.58	9.55	16.05	92.34	102.53	87.84	8	20.25	0.000
b' = 2**b**$_0$: C T' T' C	4	*P c*	12.52	9.83	16.13	90	105.68	90	4	26.41	0.000
b' = 2**b**$_0$: C T T C	4	*P c*	11.93	9.61	16.22	90	99.67	90	4	12.51	0.251
b' = 2**b**$_0$: C' C' T T'	4	*P* 1	12.56	9.49	16.47	97.18	102.24	85.86	8	19.18	0.000
b' = 2**b**$_0$: C C' T' T	4	*P* 1	12.55	9.51	16.48	82.49	102.49	94.49	8	18.69	0.000
b' = 2**b**$_0$: C C' T' T'	4	*P* 1	12.74	9.65	16.06	89.02	105.4	90.72	8	25.12	0.000
b' = 2**b**$_0$: C C' T T	4	*P* 1	12.13	9.54	16.16	89.91	100.35	90.1	8	13.28	0.060
b' = 2**b**$_0$: C C' T T'	4	*P* 1	12.57	9.58	16.06	92.77	103.18	88.58	8	20.31	0.000
b' = 2**b**$_0$: C C T' T	4	*P* 1	12.49	9.52	16.46	82.74	102.12	94.26	8	19.50	0.000
b' = 2**b**$_0$: C C T' T'	4	*P c*	12.59	9.75	16.09	90	105.31	90	4	25.90	0.000
b' = 2**b**$_0$: C C T T	4	*P c*	12.17	9.52	16.26	90	100.38	90	4	14.02	0.006
a' = 2**a**$_0$: C C' T' T'	4	*P* 2$_1$	22.18	4.8	17.58	90	94.67	90	4	21.25	0.000
a' = 2**a**$_0$: C C' T T'	4	*P* 1	23.95	4.75	16.37	89.47	97.73	91.03	8	21.80	0.000
a' = 2**a**$_0$: C C' T T	4	*P* 2$_1$	23.83	4.75	16.07	90	96.33	90	4	13.05	0.068
a' = 2**a**$_0$: C C T' T'	4	*P c*	22.19	4.74	17.48	90	88.5	90	4	20.39	0.000

$\mathbf{a}' = 2\mathbf{a}_0$: C C T' T	4	$P\,1$	24.65	4.79	15.96	91.6	101.21	87.65	8	17.86	0.000
$\mathbf{a}' = 2\mathbf{a}_0$: C C T T	4	$P\,c$	23.79	4.78	16.15	90	99.29	90	4	9.83	15.383
$\mathbf{a}' = 2\mathbf{a}_0$: C T' T' C'	4	$P\,2_1$	23.45	4.78	16.91	90	99.88	90	4	25.15	0.000
$\mathbf{a}' = 2\mathbf{a}_0$: C T' T' C	4	$P\,n$	22.02	4.84	17.5	90	94.98	90	4	22.07	0.000
$\mathbf{a}' = 2\mathbf{a}_0$: C T' T C'	4	$P\,1$	23.91	4.75	16.52	92.35	99.48	87.82	8	18.65	0.000
$\mathbf{a}' = 2\mathbf{a}_0$: C T T' C	4	$P\,1$	23.5	4.79	16.66	81.52	93.91	95.27	8	18.22	0.000
$\mathbf{a}' = 2\mathbf{a}_0$: C T T C	4	$P\,n$	24.5	4.77	15.92	90	99.89	90	4	14.15	0.007
$\mathbf{a}' = 2\mathbf{a}_0$: C T T C'	4	$P\,2_1$	24.07	4.75	15.99	90	99.97	90	4	8.74	78.346
$\mathbf{a}' = 2\mathbf{a}_0$: C' T C' T'	4	$P\,1$	25.23	4.73	15.95	90.1	102.75	89.87	8	16.63	0.000
$\mathbf{a}' = 2\mathbf{a}_0$: C T' C' T'	4	$P\,1$	24.5	4.75	16.34	92.92	99.35	87.75	4	25.68	0.000
$\mathbf{a}' = 2\mathbf{a}_0$: C T' C' T	4	$P\,1$	24.81	4.76	15.88	89.64	96.03	88.68	8	19.40	0.000
$\mathbf{a}' = 2\mathbf{a}_0$: C T C' T	4	$P\,1$	23.96	4.75	16.66	82.33	98.31	93.92	4	12.25	0.114

a) SG denotes the space-group of the optimized model; b) Lattice energies relative to the model T T, cf. § 3.3.

The disordered *cis*-isomer was found with a relative free energy of 14.02 kJ/mol at 473 K. The relative free energy of the solid solution was obtained with a value of 6.76 kJ/mol at 473 K, thus yielding a value lower than the average relative free energy of the isomers.
Thus, under the assumption of an idealized 1 : 1 mixture of isomers, the voluntary formation of the solid solution during synthesis arises from a slight advantage in the free energy, which is then extended further by an entropy contribution.

Table SI 3: *cis*-perinone: Lattice parameters and lattice energies of ordered models, optimized by force field calculations.

No.	Structure	Z	SG [a]	g_i	a	b	c	α	β	γ	Volume / Å^3	Volume per molecule / Å^3	E_{latt} / kJ/mol
experimental		**2**	***P* 2$_1$/*c***		**12.42**	**4.72**	**16.11**	**90.00**	**102.98**	**90.00**	920.89	460.44	
1	C C	2	*P c*	2	11.46	5.23	16.53	90.00	106.84	90.00	948.51	474.25	-229.608
2	C C'	2	*P* 2$_1$	2	11.91	5.00	16.32	90.00	105.78	90.00	936.00	468.00	-231.925
3	**a'** = 2**a**$_0$: C C C' C'	4	*P* 2$_1$/*c*	2	20.83	5.76	16.24	90.00	109.68	90.00	1835.91	458.98	-234.445
4	**a'** = 2**a**$_0$: C C' C' C	4	*P* 2$_1$/*n*	2	25.46	4.92	16.80	90.00	108.18	90.00	2000.33	500.08	-224.934
5	**a'** = 2**a**$_0$: C C C C'	4	*P* 1	8	20.53	5.10	17.69	89.42	96.34	90.63	1841.91	460.48	-229.190
6	**b'** = 2**b**$_0$: C C C' C'	4	*P c*	4	11.39	10.51	16.43	90.00	107.42	90.00	1876.65	469.16	-233.040
7	**b'** = 2**b**$_0$: C C C C'	4	*P* 1	8	11.48	10.43	16.44	89.73	107.10	90.11	1881.11	470.28	-231.762
8	**c'** = 2**c**$_0$: C C C' C'	4	*P* 2$_1$	4	11.49	5.19	32.84	90.00	106.39	90.00	1878.28	469.57	-232.144
9	**c'** = 2**c**$_0$: C C C C'	4	*P* 1	8	11.59	5.15	32.83	89.93	106.39	90.03	1881.85	470.46	-231.409
10	**a'** = 2**a**$_0$; **b'** = 2**b**$_0$: C C C' C'.C' C' C C	8	*C c*		25.38	10.32	16.50	90.00	112.39	90.00	3992.59	499.07	-223.655
11	**a'** = 2**a**$_0$; **c'** = 2**c**$_0$: C C C' C'.C' C' C C	8	B 2$_1$ [b]		26.10	4.92	33.10	90.00	110.12	90.00	3991.01	498.88	-223.848
12	**b'** = 2**b**$_0$; **c'** = 2**c**$_0$: C C C' C'.C' C' C C	8	*A* 1 [c]		11.37	10.56	32.82	90.34	107.66	89.44	3752.76	469.10	-233.129

a) SG denotes the space-group of the optimized model; b) non-standard setting of *P* 2$_1$, Z = 4; c) non-standard setting of *P* 1, Z = 4.

Table SI 4: *cis*-perinone: Probabilities of ordered models, optimized by force field calculations.

No.	Structure	Z	SG [a]	g_i	E_{latt} / kJ/mol /molecule	p_i at 293 K for **a'** = 2**a**$_0$ / % [b]	p_i at 293 K for **b'** = 2**b**$_0$ / % [b]	p_i at 293 K for **c'** = 2**c**$_0$ / % [b]	p_i at 293 K / % [c]
1	C C	2	$P\,c$	2	-229.608	0.04	0.13	0.40	0.03
2	C C'	2	$P\,2_1$	2	-231.925	1.57	6.03	17.83	1.19
3	**a'** = 2**a**$_0$: C C C' C'	4	$P\,2_1/c$	2	-234.445	98.33			74.76
4	**a'** = 2**a**$_0$: C C' C' C	4	$P\,2_1/n$	2	-224.934	0.0			0.0
5	**a'** = 2**a**$_0$: C C C C'	4	$P\,1$	8	-229.190	0.07			0.05
6	**b'** = 2**b**$_0$: C C C' C'	4	$P\,c$	4	-233.040		75.36		14.87
7	**b'** = 2**b**$_0$: C C C C'	4	$P\,1$	8	-231.762		18.48		3.65
8	**c'** = 2**c**$_0$: C C C' C'	4	$P\,2_1$	4	-232.144			51.17	3.41
9	**c'** = 2**c**$_0$: C C C C'	4	$P\,1$	8	-231.409			30.60	2.04

a) SG denotes the space-group of the optimized model; b) Probabilities calculated separately for each supercell setting;

c) Probabilities calculated for all models with $Z \leq 4$.

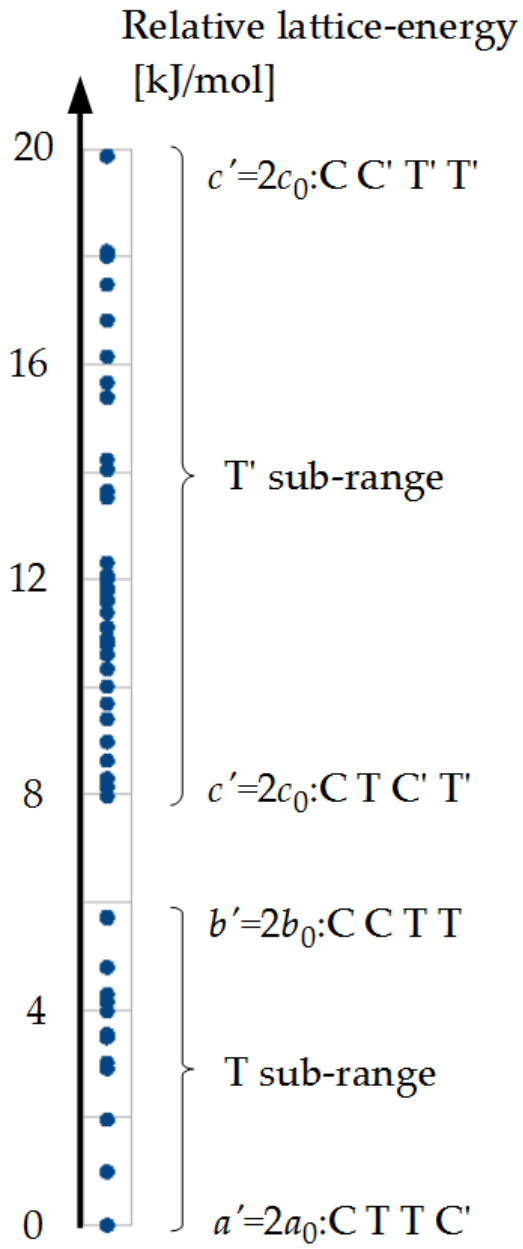


Figure SI 1: Energy sub-ranges from DFT-D minimisations.

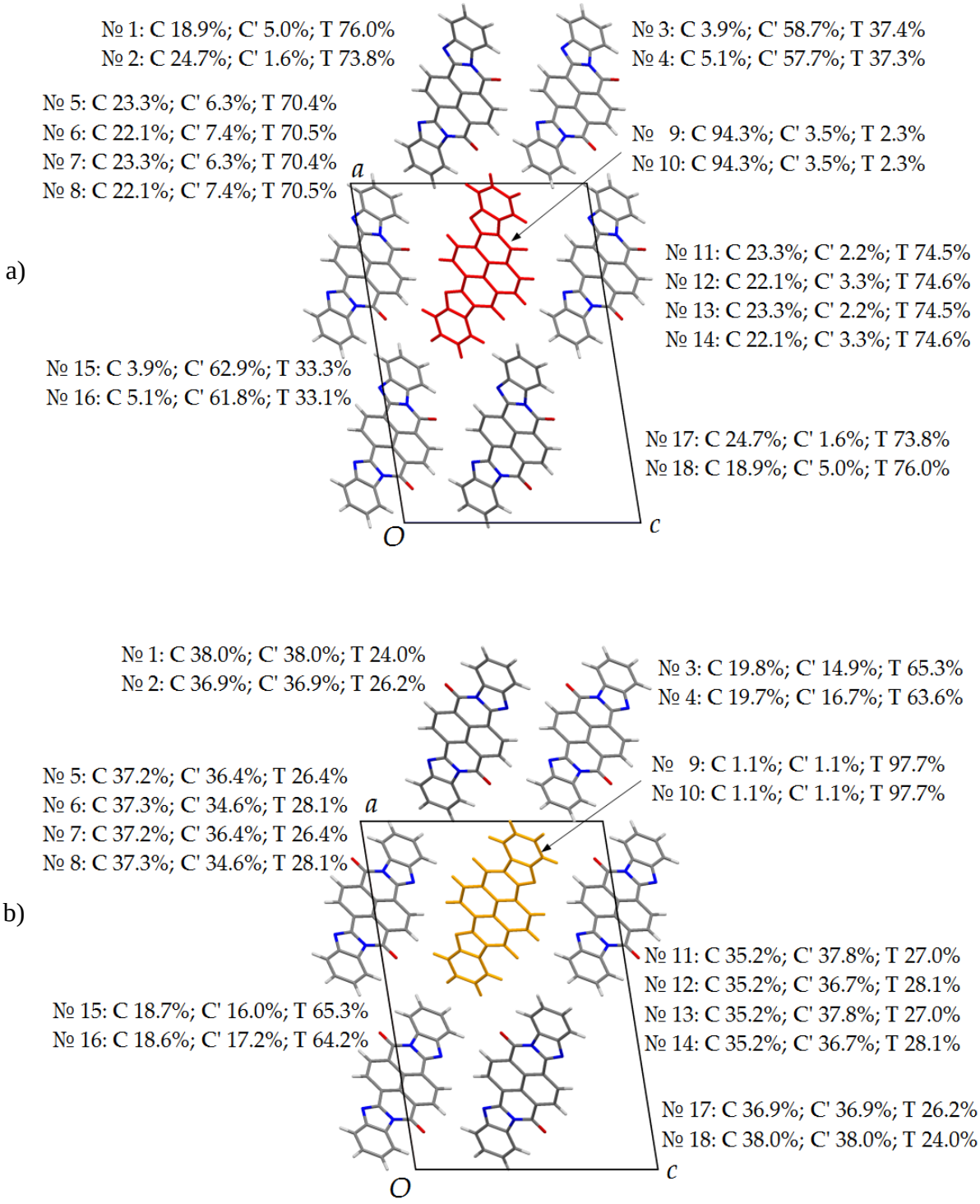
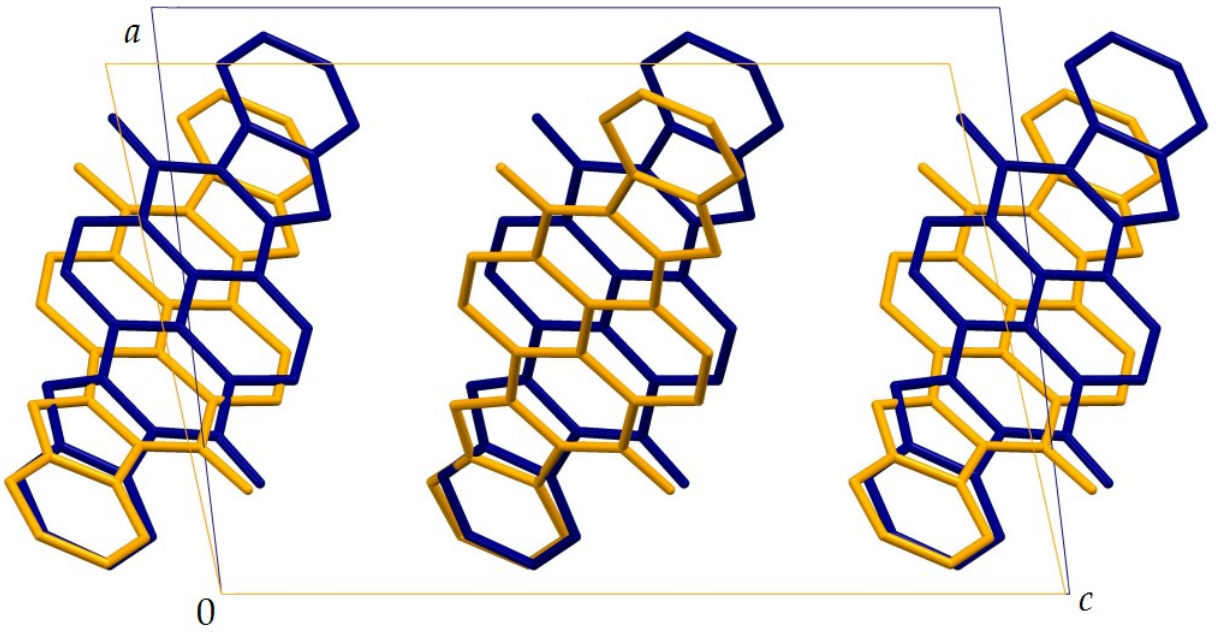


Figure SI 2: Neighbourhood frequencies calculated from the polytype approximation.

Frequencies calculated from DFT-D1 minimizations for the synthesis temperature of approx. 473 K. a) With regard to a *cis*-perinone molecule; b) with regard to a *trans*-perinone molecule.

a)



b)

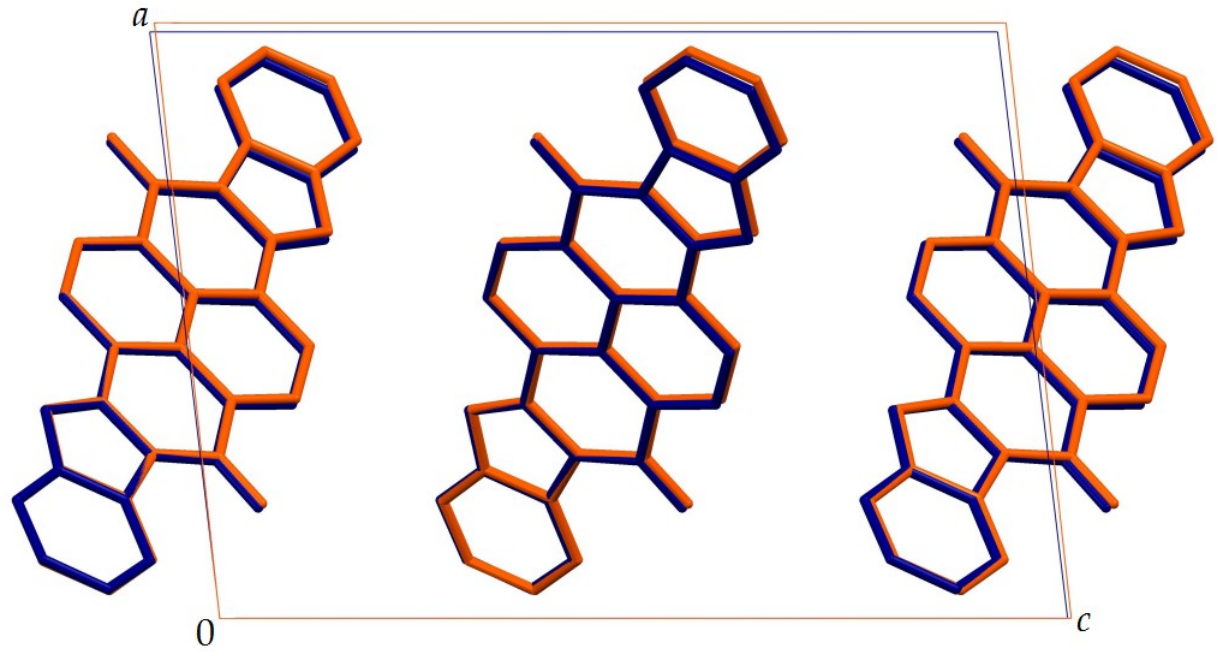


Figure SI 3: Comparison of geometry optimisations of the model T T.

a) Experimental structure (blue) vs. force field final geometry (yellow).

b) Experimental structure (blue) vs. DFT-D1 final geometry (orange).

- Original .cif file of the crystal structure of *trans*-perinone determined by single crystal analysis at room temperature (Paulus & Kunstmann, 1978)

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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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N01 N 0.2789(6) 0.4910(16) 0.4423(4) 0.0411(19) Uani 1 1 d . . .
N02 N 0.3528(6) 0.6027(17) 0.3242(4) 0.047(2) Uani 1 1 d . . .
C01 C 0.2711(7) 0.3647(19) 0.5188(5) 0.043(2) Uani 1 1 d . . .
C02 C 0.3660(7) 0.1492(18) 0.5421(5) 0.036(2) Uani 1 1 d . . .
C03 C 0.4553(6) 0.1025(19) 0.4876(5) 0.038(2) Uani 1 1 d . . .
C04 C 0.4580(7) 0.2448(17) 0.4119(5) 0.035(2) Uani 1 1 d . . .
C05 C 0.3659(7) 0.449(2) 0.3899(5) 0.042(2) Uani 1 1 d . . .
C06 C 0.2523(7) 0.7653(19) 0.3313(5) 0.041(2) Uani 1 1 d . . .
C07 C 0.2024(8) 0.6997(19) 0.4048(5) 0.041(2) Uani 1 1 d . . .
C08 C 0.1017(8) 0.826(2) 0.4256(6) 0.053(3) Uani 1 1 d . . .
H08A H 0.0686 0.7748 0.4730 0.063 Uiso 1 1 calc R . .
C09 C 0.0539(8) 1.031(2) 0.3722(6) 0.051(3) Uani 1 1 d . . .
H09A H -0.0106 1.1270 0.3851 0.061 Uiso 1 1 calc R . .
C10 C 0.1016(8) 1.095(2) 0.2987(6) 0.058(3) Uani 1 1 d . . .
H10A H 0.0652 1.2256 0.2624 0.069 Uiso 1 1 calc R . .
C11 C 0.2011(7) 0.970(2) 0.2785(6) 0.050(3) Uani 1 1 d . . .
H11A H 0.2330 1.0212 0.2306 0.060 Uiso 1 1 calc R . .
C12 C 0.3680(7) 0.008(2) 0.6149(5) 0.044(2) Uani 1 1 d . . .
H12A H 0.3114 0.0412 0.6496 0.052 Uiso 1 1 calc R . .
C13 C 0.4549(8) -0.1898(19) 0.6387(5) 0.043(2) Uani 1 1 d . . .
H13A H 0.4543 -0.2851 0.6888 0.052 Uiso 1 1 calc R . .

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N01 0.048(4) 0.049(5) 0.028(3) -0.008(4) 0.010(3) -0.005(4)
N02 0.046(5) 0.057(5) 0.037(4) -0.002(4) 0.004(3) -0.004(4)
C01 0.043(5) 0.056(6) 0.031(5) -0.008(5) 0.005(4) -0.005(5)
C02 0.039(5) 0.044(6) 0.027(4) -0.010(4) 0.005(3) -0.004(5)
C03 0.030(4) 0.058(7) 0.025(4) -0.003(4) 0.006(3) -0.009(4)
C04 0.041(5) 0.040(6) 0.025(4) -0.010(4) 0.008(4) -0.008(5)
C05 0.047(6) 0.060(6) 0.021(4) 0.001(5) 0.002(4) -0.008(5)
C06 0.044(5) 0.041(6) 0.036(5) -0.005(5) -0.003(4) 0.005(5)
C07 0.048(5) 0.040(6) 0.034(5) -0.007(4) 0.004(4) 0.003(5)
C08 0.048(6) 0.068(7) 0.042(5) -0.011(5) 0.009(4) 0.002(6)
C09 0.047(6) 0.052(7) 0.053(6) -0.001(5) 0.003(4) 0.023(5)
C10 0.045(6) 0.074(8) 0.049(5) 0.007(6) -0.012(4) -0.001(6)
C11 0.037(5) 0.060(7) 0.049(5) 0.008(5) -0.004(4) -0.002(5)
C12 0.039(5) 0.059(6) 0.035(5) 0.011(5) 0.015(4) 0.010(6)
C13 0.064(6) 0.038(6) 0.031(4) 0.001(4) 0.013(4) -0.010(5)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix. The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only

used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
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N02 C06 1.431(11) . ?
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N01 C01 C02 113.2(7) . . ?

C12 C02 C03 120.2(8) . . ?
C12 C02 C01 119.4(7) . . ?
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C04 C03 C02 122.6(8) . . ?
C04 C03 C03 118.7(9) . 3_656 ?
C02 C03 C03 118.7(9) . 3_656 ?
C03 C04 C13 120.4(8) . 3_656 ?
C03 C04 C05 116.5(7) . . ?
C13 C04 C05 123.2(7) 3_656 . ?
N02 C05 N01 112.7(8) . . ?
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N01 C05 C04 120.7(7) . . ?
C11 C06 C07 118.6(8) . . ?
C11 C06 N02 129.8(8) . . ?
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C08 C07 N01 134.9(8) . . ?
C06 C07 N01 102.2(7) . . ?
C09 C08 C07 116.8(8) . . ?
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C10 C11 C06 118.6(9) . . ?
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C06 C11 H11A 120.7 . . ?
C02 C12 C13 120.9(8) . . ?
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C07 N01 C01 C02 -179.9(7) . . . . ?
O01 C01 C02 C12 -3.7(13) . . . . ?

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O01 C01 C02 C03 178.1(8) . . . . ?
N01 C01 C02 C03 2.5(11) . . . . ?
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C01 C02 C03 C04 -1.2(12) . . . . ?
C12 C02 C03 C03 1.2(14) . . . 3_656 ?
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C06 N02 C05 C04 -179.9(8) . . . . ?
C01 N01 C05 N02 -177.6(8) . . . . ?
C07 N01 C05 N02 -0.8(10) . . . . ?
C01 N01 C05 C04 3.4(13) . . . . ?
C07 N01 C05 C04 -179.8(7) . . . . ?
C03 C04 C05 N02 179.6(9) . . . . ?
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C03 C04 C05 N01 -1.6(11) . . . . ?
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C05 N02 C06 C11 178.2(9) . . . . ?
C05 N02 C06 C07 -1.1(10) . . . . ?
C11 C06 C07 C08 1.9(13) . . . . ?
N02 C06 C07 C08 -178.7(8) . . . . ?
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N01 C07 C08 C09 178.3(9) . . . . ?
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C09 C10 C11 C06 2.8(14) . . . . ?
C07 C06 C11 C10 -1.9(13) . . . . ?
N02 C06 C11 C10 178.9(9) . . . . ?
C03 C02 C12 C13 -1.1(14) . . . . ?
C01 C02 C12 C13 -179.3(8) . . . . ?
C02 C12 C13 C04 0.3(14) . . . 3_656 ?

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- Original .cif file of the solid solution (single crystal data)

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 'H'  'H'   0.0000   0.0000
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 'N'  'N'   0.0061   0.0033
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 '-x, -y, -z'
 'x, -y-1/2, z-1/2'

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_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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_atom_sites_solution_secondary   difmap
_atom_sites_solution_hydrogens   geom
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_refine_ls_extinction_method     SHELXL
_refine_ls_extinction_coef       0.014(4)
_refine_ls_extinction_expression
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C02 C 0.3742(7) 0.4798(14) 0.6108(5) 0.083(2) Uani 1 1 d . . .
C03 C 0.4577(5) 0.3976(11) 0.4863(5) 0.0629(19) Uani 1 1 d . . .
C04 C 0.4581(7) 0.2611(13) 0.4100(5) 0.072(2) Uani 1 1 d . . .
C05 C 0.5392(7) 0.3182(14) 0.3623(5) 0.082(2) Uani 1 1 d . . .
C06 C 0.2827(8) 0.1381(16) 0.5105(6) 0.092(3) Uani 1 1 d . . .
C07 C 0.3672(7) 0.0533(13) 0.3844(6) 0.080(2) Uani 1 1 d . . .
H02 H 0.310(4) 0.440(10) 0.647(3) 0.07(2) Uiso 1 1 d . . .
H05 H 0.549(4) 0.245(11) 0.305(3) 0.08(2) Uiso 1 1 d . . .
N1 N 0.2862(6) 0.0035(11) 0.4353(5) 0.085(2) Uani 1 1 d . A .
N2 N 0.3602(6) -0.0900(12) 0.3169(4) 0.099(2) Uani 1 1 d . A .
O1 O 0.2048(5) 0.0747(11) 0.5519(4) 0.118(2) Uani 1 1 d . A .
C08 C 0.1954(16) -0.194(3) 0.4118(12) 0.041(5) Uiso 0.54(2) 1 d P A 1
C09 C 0.2424(17) -0.263(3) 0.3320(14) 0.047(5) Uiso 0.54(2) 1 d P A 1
C10 C 0.1882(15) -0.450(3) 0.2842(13) 0.067(5) Uiso 0.54(2) 1 d P A 1
H10 H 0.2153 -0.4894 0.2347 0.100 Uiso 0.54(2) 1 calc PR A 1
C11 C 0.0968(15) -0.592(3) 0.2997(17) 0.060(5) Uiso 0.54(2) 1 d P A 1
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C12 C 0.056(3) -0.529(4) 0.3726(17) 0.068(7) Uiso 0.54(2) 1 d P A 1
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C13 C 0.101(2) -0.317(6) 0.431(2) 0.103(11) Uiso 0.54(2) 1 d P A 1
H13 H 0.0682 -0.2693 0.4772 0.155 Uiso 0.54(2) 1 calc PR A 1
C081 C 0.236(2) -0.211(6) 0.388(2) 0.026(9) Uiso 0.29(2) 1 d P A 2
C091 C 0.281(3) -0.231(6) 0.3102(18) 0.049(9) Uiso 0.29(2) 1 d P A 2
C101 C 0.224(2) -0.438(4) 0.2538(16) 0.051(8) Uiso 0.29(2) 1 d P A 2
H101 H 0.2527 -0.4801 0.2051 0.077 Uiso 0.29(2) 1 calc PR A 2
C111 C 0.131(3) -0.571(6) 0.2713(19) 0.064(9) Uiso 0.29(2) 1 d P A 2
H111 H 0.0921 -0.6885 0.2307 0.096 Uiso 0.29(2) 1 calc PR A 2
C121 C 0.091(3) -0.548(6) 0.340(3) 0.040(9) Uiso 0.29(2) 1 d P A 2
H121 H 0.0340 -0.6752 0.3476 0.060 Uiso 0.29(2) 1 calc PR A 2
C131 C 0.123(3) -0.339(6) 0.410(2) 0.041(9) Uiso 0.29(2) 1 d P A 2
H131 H 0.0852 -0.2977 0.4550 0.062 Uiso 0.29(2) 1 calc PR A 2
C082 C 0.208(5) -0.179(10) 0.380(4) 0.029(16) Uiso 0.173(14) 1 d P A 3
C092 C 0.163(4) -0.153(8) 0.471(3) 0.073(15) Uiso 0.173(14) 1 d P A 3
C102 C 0.054(4) -0.306(8) 0.470(3) 0.079(14) Uiso 0.173(14) 1 d P A 3
H102 H 0.0109 -0.2747 0.5125 0.119 Uiso 0.173(14) 1 calc PR A 3
C112 C 0.017(3) -0.491(7) 0.409(2) 0.045(11) Uiso 0.173(14) 1 d P A 3
H112 H -0.0395 -0.6189 0.4175 0.068 Uiso 0.173(14) 1 calc PR A 3
C122 C 0.054(7) -0.495(14) 0.347(6) 0.08(3) Uiso 0.173(14) 1 d P A 3
H122 H 0.0154 -0.5745 0.2986 0.124 Uiso 0.173(14) 1 calc PR A 3
C132 C 0.170(4) -0.358(8) 0.353(3) 0.057(13) Uiso 0.173(14) 1 d P A 3
H132 H 0.2202 -0.4602 0.3262 0.086 Uiso 0.173(14) 1 calc PR A 3

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C02 0.100(6) 0.058(5) 0.087(6) 0.011(5) 0.003(5) 0.000(5)

C03 0.080(6) 0.044(4) 0.059(5) 0.011(4) -0.007(4) 0.001(3)
C04 0.102(6) 0.047(4) 0.060(6) 0.003(4) -0.012(4) 0.012(5)
C05 0.114(7) 0.060(5) 0.065(6) -0.001(4) -0.007(5) 0.004(5)
C06 0.108(7) 0.060(6) 0.098(8) 0.018(5) -0.016(6) 0.009(6)
C07 0.103(6) 0.041(5) 0.081(6) 0.005(5) -0.036(6) -0.002(4)
N1 0.104(5) 0.051(4) 0.085(5) 0.016(4) -0.026(5) -0.003(4)
N2 0.138(6) 0.050(3) 0.088(5) -0.023(3) -0.048(4) 0.007(4)
O1 0.122(5) 0.092(4) 0.134(5) 0.017(4) -0.007(4) -0.013(4)

_geom_special_details
;
All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
;

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C02 H02 1.05(5) . ?
C03 C04 1.403(8) . ?
C03 C03 1.422(11) 3_666 ?
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C04 C07 1.476(8) . ?
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C06 O1 1.258(8) . ?
C06 N1 1.389(9) . ?
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N1 C08 1.438(17) . ?
N1 C082 1.47(5) . ?
N1 C092 1.81(5) . ?
N2 C091 1.15(4) . ?
N2 C09 1.67(2) . ?
O1 C092 1.72(4) . ?
C08 C13 1.34(3) . ?
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C10 H10 0.9300 . ?
C11 C12 1.38(3) . ?
C11 H11 0.9300 . ?
C12 C13 1.44(3) . ?
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C111 C121 1.28(6) . ?
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C121 C131 1.53(6) . ?
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C131 H131 0.9300 . ?
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C05 C02 H02 120(3) 3_666 . ?
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C02 C05 H05 110(3) 3_666 . ?
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- Cif file of the energetically most favourable local structure of *cis*-perinone (**a**' = 2**a**$_0$: C C C' C')

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_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 2_1/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,y+1/2,-z+1/2
3 -x,-y,-z
4 x,-y+1/2,z+1/2
_cell_length_a 23.370085679832300
_cell_length_b 4.979560725803978
_cell_length_c 16.301278876602467
_cell_angle_alpha 90.000000000000000
_cell_angle_beta 102.271056857926411
_cell_angle_gamma 90.000000000000000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.238911607319675 0.410904306948197 0.947647896282949
C2 C 0.282215365909055 0.609053561355139 0.978696940392374
C3 C 0.325958477740339 0.668601978999994 0.932373466308432
C4 C 0.325970640930803 0.536313621422572 0.857217961204792
C5 C 0.283483322661475 0.342155376957877 0.826587899083748
C6 C 0.240743881568783 0.277477550886735 0.871023217732327
C7 C 0.194622119262325 0.353109783330347 0.993419585852713
C8 C 0.194481530532477 0.488275567717863 1.068386673129877
C9 C 0.237089459265253 0.681451766586774 1.099072775914313
C10 C 0.280606742940692 0.743874796968109 1.055298190632424
C11 C 0.324997542580484 0.942764577046028 1.084871561479878
C12 C 0.371902854413788 0.873327335857415 0.962336202501360
C13 C 0.197498497668999 0.066756936871740 0.836797499228760
C14 C 0.151217060059367 0.153582941675877 0.959373162411851
N15 N 0.368327733710770 0.995829687348968 1.038460752627107
N16 N 0.155960635493048 0.016292336529748 0.885257975195714
N17 N 0.105565842025939 0.073931036122102 0.988526611240839
N18 N 0.331122654040682 1.093375107184434 1.152616328038115
O19 O 0.410185112570936 0.936520928768101 0.924392353318108
O20 O 0.196963914964340 -0.058348723034537 0.771423157339819
C21 C 0.379769615152025 1.253651799788242 1.152884925622049
C22 C 0.404393259294924 1.196803226297580 1.082278701507970
C23 C 0.078328936441645 -0.122675123586650 0.933030194213191
C24 C 0.109321499816841 -0.165022260605768 0.868058951773614
C25 C 0.453843390580742 1.329324927339978 1.067768843335164
C26 C 0.477380014131409 1.529130160728694 1.125461178188248
C27 C 0.452963408903433 1.589754480453384 1.195119949889738
C28 C 0.404473958020728 1.451637543070318 1.210542153794100
```

C29 C 0.027704012654146 -0.271860648341514 0.934186899402621
C30 C 0.010839150530334 -0.464787915395245 0.871695949809063
C31 C 0.043033641581158 -0.508551853555030 0.809160036651656
C32 C 0.092836921383575 -0.357564789633325 0.805485962116189
H33 H 0.160893790122220 0.441385629337548 1.103390288317889
H34 H 0.236624144288904 0.782681671146975 1.158119017912312
H35 H 0.283495008946456 0.243225044134490 0.766991063871122
H36 H 0.359335192314379 0.584896402229269 0.821992544292909
H37 H 0.473257822246871 1.277516158993790 1.014998425947976
H38 H 0.515961976931118 1.640096971398766 1.116964531277518
H39 H 0.473053127022651 1.745745006053061 1.238603433472439
H40 H 0.386780693820838 1.494792614698562 1.265835111402980
H41 H 0.002212547063842 -0.238357307912255 0.981933964644627
H42 H -0.028234546006638 -0.585362304086581 0.871067656699047
H43 H 0.028451564926801 -0.661846560695096 0.761720102921029
H44 H 0.117442836196440 -0.387833382909238 0.756629877967557
#END

- Cif file of the Model TT' for hypothetically disordered *trans*-perinone

```
data_tt9
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 12.144705876003712
_cell_length_b 4.808604676815349
_cell_length_c 16.028286005334188
_cell_angle_alpha 85.926825784070900
_cell_angle_beta 97.291461496496879
_cell_angle_gamma 95.369995730818019
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.449218189806679 -0.740546431184854 -0.086349654782226
C2 C 0.456089001506954 -0.910050137557065 -0.009425879785954
C3 C 0.622673772891784 -1.096685396721892 -0.048864517941092
C4 C 0.613598718552994 -0.928092294674564 -0.123242857172713
C5 C 0.527712123367229 -0.750878965377475 -0.142089689922988
C6 C 0.358859320161740 -0.562322579763638 -0.103810653921640
N7 N 0.282493390806877 -0.559162436404381 -0.044783575720547
C8 C 0.285683802980264 -0.717390983380657 0.032742918951659
C9 C 0.205922870615056 -0.369160725172401 -0.078461070549524
C10 C 0.242023919176033 -0.266974581568400 -0.156763478009453
N11 N 0.336399717907858 -0.390553654615001 -0.170534179420808
C12 C 0.183573303044229 -0.066585312365965 -0.207506035128285
C13 C 0.089770889571555 0.022133922442864 -0.178829310811503
C14 C 0.054367608699814 -0.084509159374065 -0.101601015034937
C15 C 0.112217814897953 -0.281309325957348 -0.049441133542650
O16 O 0.216828991221404 -0.694922301205392 0.081498916768145
H17 H 0.520764954740541 -0.622777218985078 -0.200939772336109
H18 H 0.674340771598117 -0.937972136520338 -0.167108000236493
H19 H 0.913533455450048 -1.637271229590398 -0.010718265160244
H20 H 1.020891322862270 -1.985617576011560 0.082428803825891
H21 H 0.957585420537737 -2.177145872425474 0.216966817058051
H22 H 0.788547145705003 -2.017139904996451 0.267050013156022
C23 C 0.643297078780393 -0.329578731934779 0.487219189078454
C24 C 0.539063600184374 -0.397261797209675 0.519495343204493
C25 C 0.488478279833628 -0.735211160209140 0.410206726597802
C26 C 0.589676418355286 -0.659876999776087 0.378715997938397
C27 C 0.666701947994976 -0.458947470981685 0.417042563579671
C28 C 0.721681034773414 -0.126428599754162 0.529799520965883
N29 N 0.690667138014842 0.007274064287044 0.597490222756143
C30 C 0.588089248523247 -0.042939988409010 0.629893585761011
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C31 C 0.781773375396477 0.191378046886841 0.625430030398772
C32 C 0.863988168822129 0.153119447344338 0.572578834054311
N33 N 0.823714470787166 -0.041997664262037 0.513758139943594
C34 C 0.968962123237080 0.302373930143656 0.584347605273196
C35 C 0.986955395023549 0.493013835184750 0.647233821137230
C36 C 0.904174736617682 0.531448825336453 0.698470162492165
C37 C 0.799872001885999 0.380014410740271 0.689024780831115
O38 O 0.566646143723625 0.093711001967529 0.687006214143374
H39 H 0.746144698015738 -0.402408014372632 0.392765588619091
H40 H 0.607362446425254 -0.757403179626914 0.323024067860332
H41 H 0.263677330117772 -1.409381054295914 0.271165921585232
H42 H 0.078114612623521 -1.681732130575318 0.252754950484742
H43 H -0.066868057025133 -1.617261994049610 0.342732696843897
H44 H -0.033461803436400 -1.266636711717674 0.454265651685228
#END

- Cif file of the energetically most favourable local structure of the solid solution (**a**' = 2**a**$_0$: C T T C')

```
data_perinone_2a_cttc9
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 2_1'
_symmetry_Int_Tables_number 4
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,y+1/2,-z
_cell_length_a 24.072206474901105
_cell_length_b 4.755126293835786
_cell_length_c 15.988658794721909
_cell_angle_alpha 90.000000000000000
_cell_angle_beta 99.970332856241924
_cell_angle_gamma 90.000000000000000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.763767357439654 0.741868829966062 0.863973425971031
C2 C 0.762707446070285 0.601220949009218 0.785131945445267
C3 C 0.719689166034712 0.399259450593804 0.758329892270802
C4 C 0.678218947294980 0.346161509346387 0.809824954461295
C5 C 0.680764256676308 0.486776607323314 0.886674759218660
C6 C 0.723363496714793 0.681855018201313 0.914046436792437
C7 C 0.719354353487025 0.253967554843954 0.680417194566428
C8 C 0.760278070730506 0.310863597411663 0.630978139077683
C9 C 0.802015704588153 0.511647698663993 0.657179024413026
C10 C 0.803822154111714 0.656533705377545 0.733172987257197
C11 C 0.807834586566734 0.944420764359716 0.889501211408784
N12 N 0.847103634624637 1.000539626943142 0.836118198477566
C13 C 0.848797542616177 0.866876991710646 0.758105655235662
C14 C 0.632259563677047 0.141994614429170 0.783697557124829
N15 N 0.634022356079005 0.007493499735395 0.706001635687925
C16 C 0.675476239144324 0.050052796008970 0.655279622955766
C17 C 0.883564716035090 1.205216359462387 0.877279070887247
C18 C 0.863688164560745 1.257857051133653 0.954341905189140
N19 N 0.816818319261994 1.094750019055692 0.959658964278510
N20 N 0.668300195301003 -0.112048652057800 0.587537219347636
C21 C 0.620417698241528 -0.269025901693941 0.591712681605397
C22 C 0.597589808230197 -0.197798460760661 0.664982311620766
C23 C 0.890954084286228 1.453615745863446 1.012677320380139
C24 C 0.936835496835646 1.596076132039160 0.990950765502990
C25 C 0.955518424984312 1.545115788897488 0.913715499157511
C26 C 0.929608819619928 1.346657201795433 0.855332835555528
C27 C 0.548682067602904 -0.321287035461667 0.683413231080207
C28 C 0.523787351053609 -0.527079871295174 0.626868976271360
C29 C 0.546583678239098 -0.603649133860611 0.554857509300234
C30 C 0.594637612002838 -0.474686364988351 0.535549655467242
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O31 O 0.885314407347685 0.927194612852173 0.716055840251422
O32 O 0.595044535597846 0.086448026457062 0.825071965248393
H33 H 0.725027437423287 0.785326997319413 0.975081877330311
H34 H 0.649273021431787 0.442885150476086 0.926134522068612
H35 H 0.530762661075051 -0.258362385363025 0.738221484400282
H36 H 0.485229417728280 -0.629108304936276 0.637928808438006
H37 H 0.525485974978993 -0.764523278364753 0.512605680116411
H38 H 0.611080276329105 -0.530049292832058 0.478456217528933
H39 H 0.759593895581961 0.199930154564293 0.571380617896800
H40 H 0.833595795573021 0.556182212050659 0.617901108692989
H41 H 0.944238556443129 1.304745696196145 0.796067551268934
H42 H 0.991457906448902 1.663763765793017 0.899548122165318
H43 H 0.958961103094911 1.750573609719278 1.034559336087528
H44 H 0.877204253785413 1.492448947681591 1.073050145166011
C45 C 0.765483666008123 -0.117617169032799 0.288233916711593
C46 C 0.721781544198471 0.080392997508251 0.260522690432118
C47 C 0.679142337397766 0.124945655240152 0.310524992644719
C48 C 0.680691072967051 -0.020978474182100 0.386111133884641
C49 C 0.723569394333598 -0.215592259818801 0.413381473669011
C50 C 0.765330510687145 -0.266563694483506 0.365242426850761
C51 C 0.808484537650723 -0.160291558494823 0.238574264596524
C52 C 0.806952255257487 -0.012447560516764 0.163002053798502
C53 C 0.763931493671910 0.180046798993631 0.135537486673515
C54 C 0.721811939564652 0.229737530129288 0.183461102967114
C55 C 0.677300307186453 0.429213147950136 0.157540532527746
C56 C 0.632745401411858 0.328411841784978 0.284021680007878
C57 C 0.809244519742700 -0.478672284660012 0.395534308511943
C58 C 0.852664044569261 -0.357577324457894 0.269309971911464
N59 N 0.635005863039939 0.466344259925965 0.207380213592868
N60 N 0.850394341909360 -0.509064177000895 0.344385160402404
N61 N 0.897362645764162 -0.420544994611619 0.235971830068302
N62 N 0.670176707257019 0.593113307267269 0.090258423279835
O63 O 0.595099158690753 0.378892352351860 0.325041674764551
O64 O 0.810625036668398 -0.621230629281251 0.460170796271162
C65 C 0.621602341067714 0.745873904449118 0.093709132701576
C66 C 0.598265029883877 0.670626189960969 0.166137809015544
C67 C 0.926893101153415 -0.618539969351487 0.290136608559488
C68 C 0.898205419735430 -0.681158597244135 0.358173889181807
C69 C 0.548723620993098 0.789376639109508 0.183741249430767
C70 C 0.523613997760064 0.994882135153803 0.127190605404112
C71 C 0.546826666149630 1.075044238728774 0.055933043417777
C72 C 0.595576291906728 0.950433992561426 0.037437534726443
C73 C 0.978515425094798 -0.747392096688818 0.285994742820903
C74 C 0.999248365263539 -0.941257037580000 0.348954092447130
C75 C 0.969406943420326 -1.006686399778796 0.414601538290182
C76 C 0.918311517253205 -0.876126437845175 0.421098906236551
H77 H 0.839474296496168 -0.048375731947596 0.124772472713222
H78 H 0.763139606508661 0.289847907089330 0.075696893932025
H79 H 0.724417304921344 -0.326091249687337 0.473133627172829
H80 H 0.648361431839550 0.017310523830691 0.424516430903621
H81 H 0.530410910106441 0.723047976541683 0.237858298662989
H82 H 0.484550098127213 1.093215608281959 0.137612581579430
H83 H 0.525533695212959 1.235079374611824 0.013535196569222

H84 H 0.612308598054275 1.007716549464548 -0.019247083808380
H85 H 1.002070086618175 -0.692705596239087 0.236131757435487
H86 H 1.039474083056238 -1.044456539145547 0.347645441475210
H87 H 0.986737688616388 -1.161121557876317 0.462278925702246
H88 H 0.895702099234095 -0.921853594677351 0.472692732731262
#END