Supporting Information

Prediction of the crystal packing of Di-tetrazine-tetroxide (DTTO) Energetic Material

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Note: Originally we named the structure Tetrazino-tetrazine-tetraoxide (TTTO) but now it described as Di-tetrazine-tetroxide (DTTO). This is because most of the literature citations use DTTO.

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1 Structures obtained from classical Force Fields

Using classical Force Fields Dreiding and the Universal Force Field (UFF), we explore the structure of on the most stable isomers of DTTO we found: **c1** and **c2** would form stable packing structures.

We explore their packing in the 10 most common space groups for molecular crystals: P21/c, P-1, P212121, P21, C2/c, PBCA, C2, PNA21, PBCN and CC.

The space group symmetry was calculated within the atomistic simulation codes and also were corroborated at the beginning and at the end of the simulation with FINDSYM. [1]

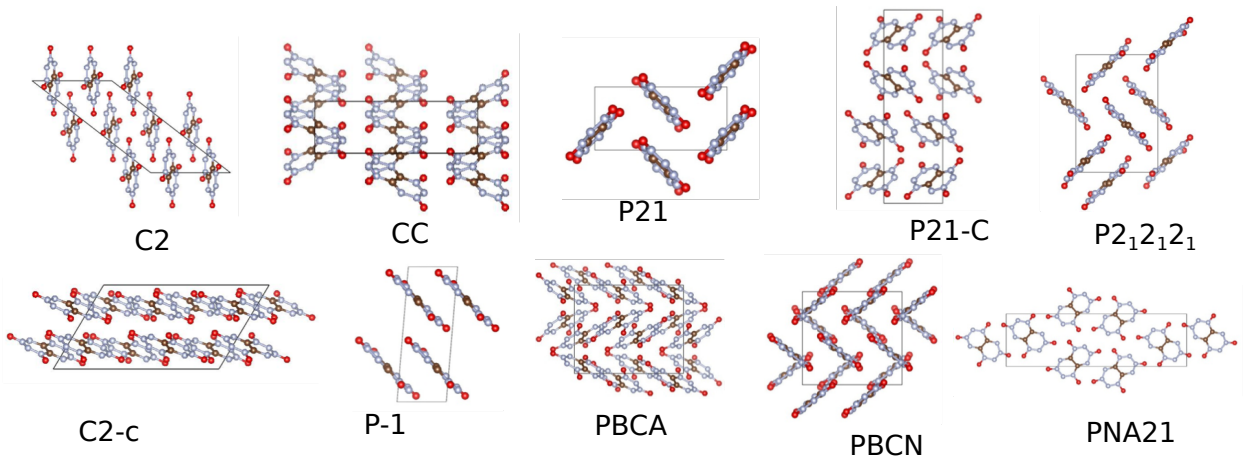


Figure S1: Dreiding FF structures for the 10 most common space groups for the **c1**-isomer

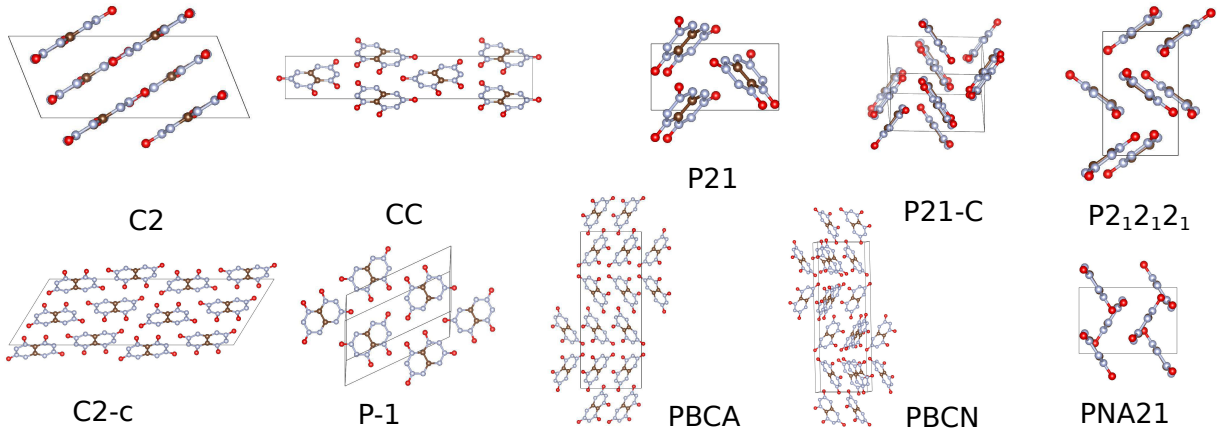


Figure S2: Dreiding FF structures for the 10 most common space groups for the **c2**-isomer

2 Relative Energies from FF vs QM

We show the relative energies (ΔE) with respect to the given force field and isomer in Table S1-S4. In general Dreiding and UFF give the same trends for this case. However the magnitude is different.

Table S1: Dreiding packing for **c1**

Space group	Formula	Rank	ΔE (kcal/mol)
DTTO alone	C2N8O4		
C2/c	C16N64O32	7	8.7
C2	C8N32O16	4	6.3
CC	C8N32O16	8	9.1
P-1	C4N16O8	2	3.0
P21/C	C8N32O16	**1**	**0.0**
P21	C4N16O8	3	3.2
P212121	C8N32O16	5	6.8
PBCA	C16N64O32	6	7.1
PBCN	C16N64O32	9	10.0
PNA21	C8N32O16	10	11.5

Table S2: UFF packing for **c1**

Space group	Formula	Rank	ΔE (kcal/mol)
DTTO alone	C2N8O4		
C2/c	C16N64O32	7	39.7
C2	C8N32O16	4	25.6
CC	C8N32O16	8	45.4
P-1	C4N16O8	3	10.0
P21/C	C8N32O16	**1**	**0.0**
P21	C4N16O8	2	9.7
P212121	C8N32O16	5	30.5
PBCA	C16N64O32	6	35.9
PBCN	C16N64O32	10	50.9
PNA21	C8N32O16	9	46.1

Table S3: Dreiding packing for **c2**

Space group	Formula	Rank	ΔE (kcal/mol)
DTTO alone	C2N8O4		
C2/c	C16N64O32	**1**	**0.0**
C2	C8N32O16	5	0.8
CC	C8N32O16	3	0.7
P-1	C4N16O8	6	1.3
P21/C	C8N32O16	8	2.5
P21	C4N16O8	10	3.9
P212121	C8N32O16	4	0.7
PBCA	C16N64O32	2	0.1
PBCN	C16N64O32	7	1.7
PNA21	C8N32O16	9	2.6

Table S4: UFF packing for **c2**

Space group	Formula	Rank	ΔE (kcal/mol)
DTTO alone	C2N8O4		
C2/c	C16N64O32	2	6.8
C2	C8N32O16	**1**	**0.0**
CC	C8N32O16	4	13.5
P-1	C4N16O8	7	25.9
P21/C	C8N32O16	10	35.9
P21	C4N16O8	6	23.2
P212121	C8N32O16	5	19.5
PBCA	C16N64O32	3	10.6
PBCN	C16N64O32	9	32.3
PNA21	C8N32O16	8	27.1

A direct comparison shows that the top 5 structures predicted by UFF and Dreiding are the top 5 predicted by QM. In other words, the trend can be captured by a general purpose Force Field such as Dreiding or UFF. This can be seen more clearly in Figure S3.

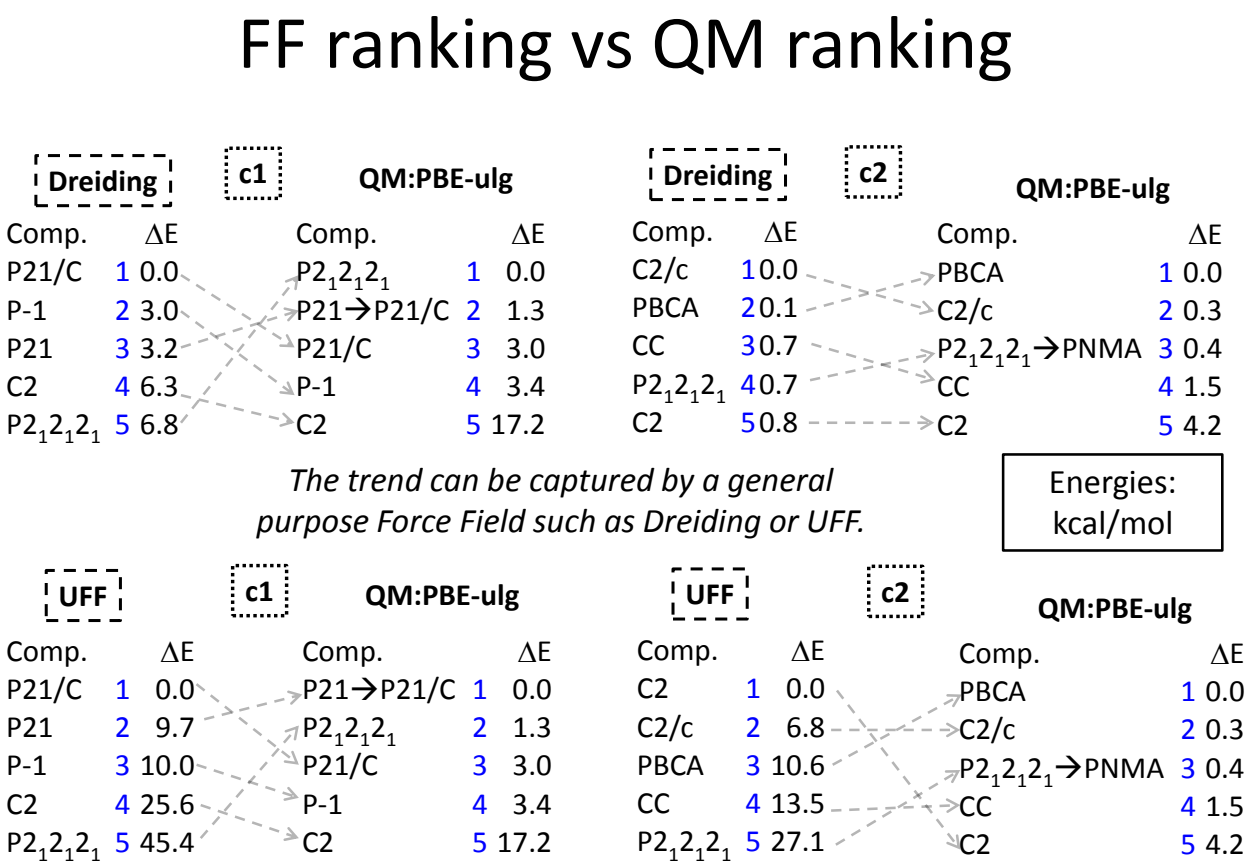


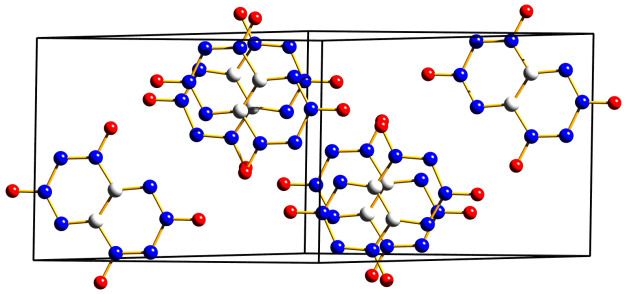
Figure S3: FF relative energies vs QM relative energies.

3 Structures obtained from periodic quantum mechanics (PBE-ulg)

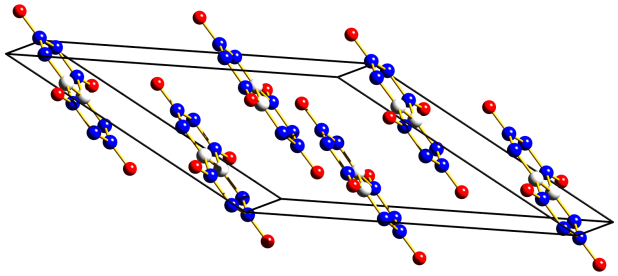
In the main text we discussed the top 5 structures obtained from the Force Field (FF) for configuration 1 and 2 of DTTO, which were further optimized with Quantum Mechanics at the DFT:PBE-ulg level. These structures are presented in the following section, first we present their representation followed by their coordinates. We present the space group with the Hermann-Mauguin alphanumeric code and in parenthesis we also show the space group sequential number(1-230).

3.1 DTTO configuration 1 (c1)

In general we the space group obtained from FF is maintained after QM optimization. There is only one case where we found that the QM minimization found a minimum with a more symmetrical space group. This case is the structure for which the FF packing procedure found $P21$ (4) and QM minimization found this structure transition to $P\,21/c$ (14). The FF procedure found this to be the 3rd most stable packing, however with the QM scheme this packing becomes the most stable packing for configuration 1 (c1) of DTTO.

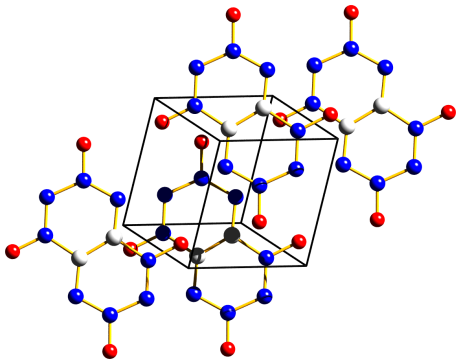


4.1: view 1

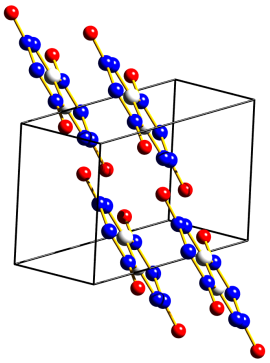


4.2: view 2

Figure S4: **c1**-DTTO: space group $C\,2/c$ (15)

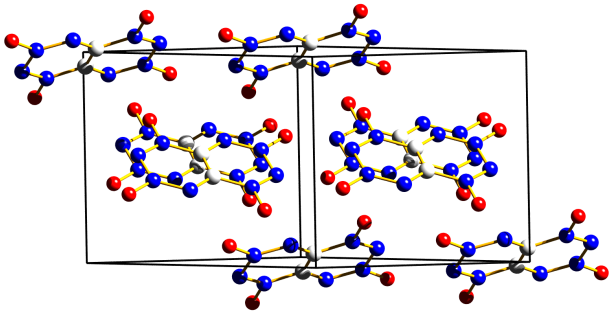


5.1: view 1

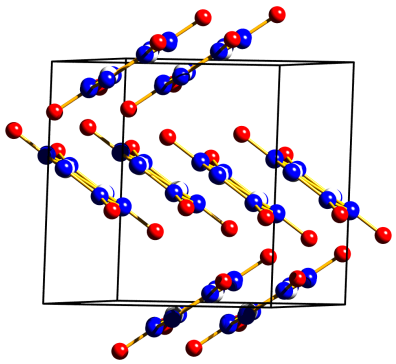


5.2: view 2

Figure S5: **c1**-DTTO: space group $P\,-1$ (2)

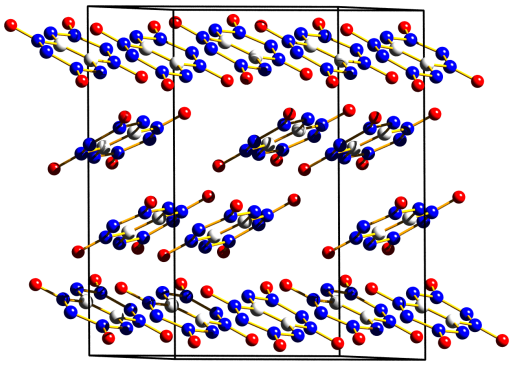


6.1: view 1

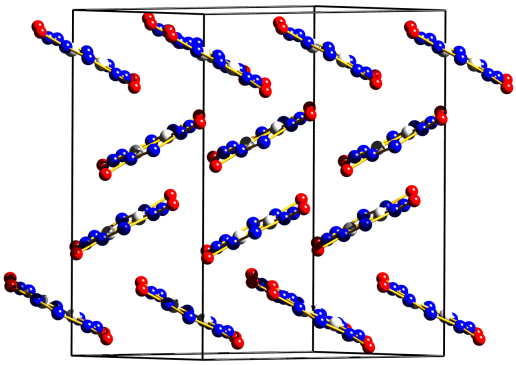


6.2: view 2

Figure S6: **c1**-DTTO: space group $P\,21/c$ (14) global minimum

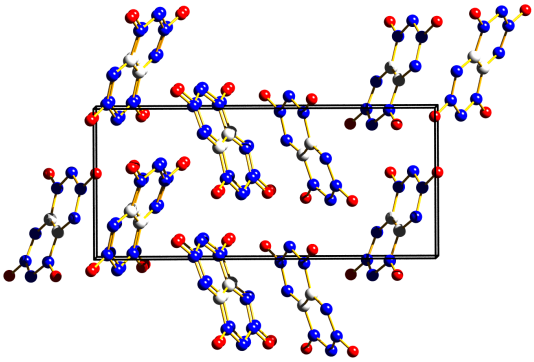


7.1: view 1

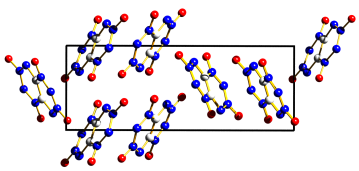


7.2: view 2

Figure S7: **c1**-DTTO: space group $P\,21/c$ (14) local minima



8.1: view 1



8.2: view 2

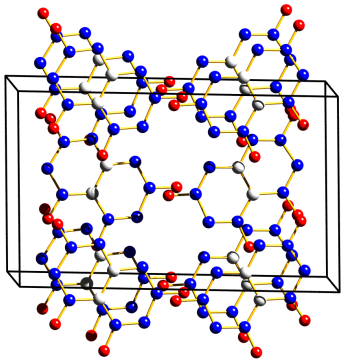
Figure S8: **c1**-DTTO: space group $P\,2_1\,2_1\,2_1$ (19)

3.2 DTTO configuration 2 (c2)

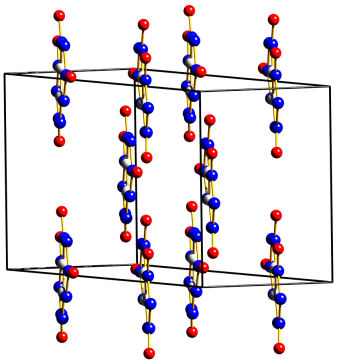
In a similar fashion as for c1, we found that for the configuration 2 (c2) of DTTO the symmetry from the structures obtained from FF is maintained after QM optimization.

There is only one exception for the cases studied. The structure obtained from the FF packing scheme with $P\,2_1\,2_1\,2_1$ (19) space group transition to $P\,n\,m\,a$ (62) space group after QM minimization. In the FF scheme (packing + minimization) the structure with $P\,2_1\,2_1\,2_1$ (19) space group ranks as the 4th, however after minimization with periodic DFT:PBE-ulg the structure becomes the 3rd most stable structure besides transition to a more symmetrical space group, $P\,n\,m\,a$ (62).

As it was discussed in the main text the other structures maintain their symmetry through the QM minimization procedure, however their ranks changes, i.e. FF: $C\,2/c$ (15) changes from 1st to QM: 2nd; FF:$C\,c$ (9) changes from 3rd to QM: 4th; and FF:$P\,b\,c\,a$ (61) changes from 2nd to QM: 1st. [FF: $C2$ (5) does not change and remains in 5th also after QM.]

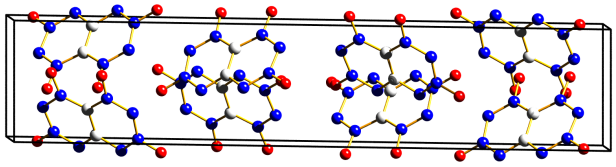


9.1: view 1

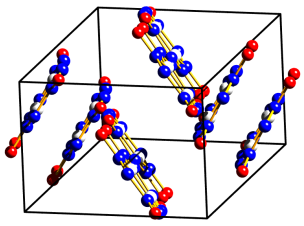


9.2: view 2

Figure S9: **c2**-DTTO: space group $C2$ (5)

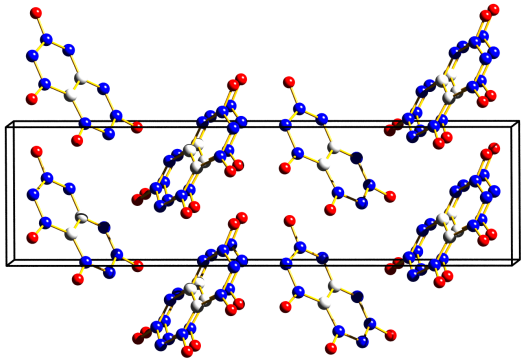


10.1: view 1

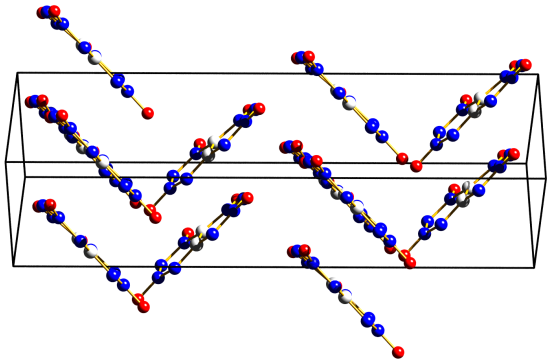


10.2: view 2

Figure S10: **c2**-DTTO: space group $C\,2/c$ (15)

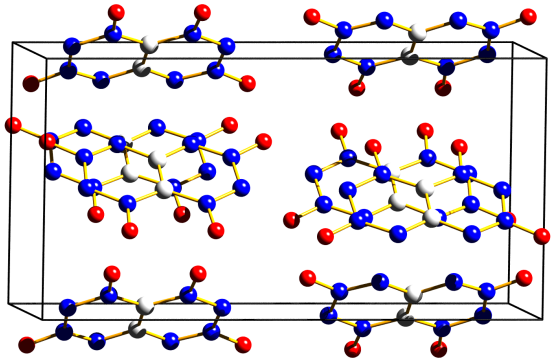


11.1: view 1

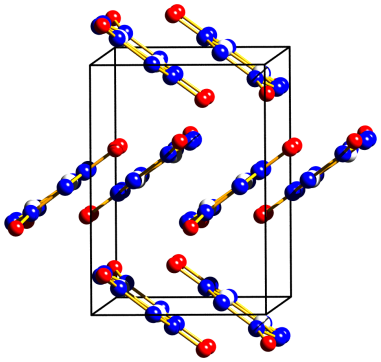


11.2: view 2

Figure S11: **c2**-DTTO: space group $C\,c$ (9)

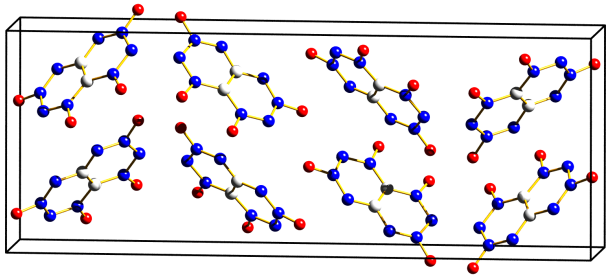


12.1: view 1

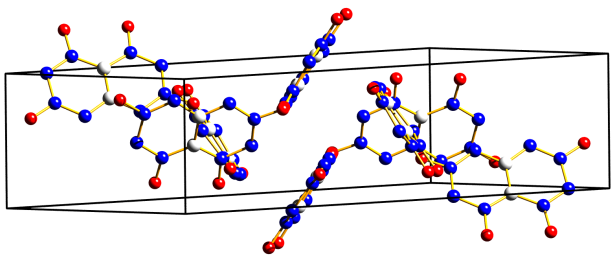


12.2: view 2

Figure S12: **c2**-DTTO: space group $P\,n\,m\,a$ (62)



13.1: view 1



13.2: view 2

Figure S13: **c2**-DTTO: space group $P\,b\,c\,a$ (61)

3.3 Coordinates for structures of DTTO configuration 1 (c1)

3.3.1 c1-DTTO: space group $C\,2/c$ (15)

```
_cell_length_a 10.6410
_cell_length_b  8.2460
_cell_length_c 12.4020
_cell_angle_alpha 90.000
_cell_angle_beta 150.686
_cell_angle_gamma 90.000
_cell_volume 532.8
_symmetry_int_tables_number 15
_symmetry_space_group_name_H-M 'C 1 2/c 1'

O1  0.2262  0.8020  0.7931
O2  0.7496  0.0969  0.9853
N3  0.8200  0.5365  0.0338
N4  0.0191  0.5450  0.1148
N5  0.0949  0.6977  0.1375
N6  0.9973  0.8390  0.0981
C7  0.6982  0.6789  0.9803
```

3.3.2 c1-DTTO: space group $P\,-1$ (2)

```
_cell_length_a  4.7720
_cell_length_b  4.8910
_cell_length_c  5.8990
_cell_angle_alpha 76.761
_cell_angle_beta 80.360
_cell_angle_gamma 88.774
_cell_volume 132.1
_symmetry_int_tables_number 2
_symmetry_space_group_name_H-M 'P -1'

O1 0.4166 -0.6873  0.8806
O2 0.9448 -0.9002  0.7376
N3 1.3542 -0.6572  0.3923
N4 0.5810 -0.5603  0.2323
N5 0.8231 -0.7036  0.1778
N6 0.8380 -0.9629  0.3041
C7 1.6159 -1.0838  0.4855
```

3.3.3 c1-DTTO: space group $P\,21/c$ (14) global minimum

```
_cell_length_a  7.4330
_cell_length_b  7.2890
_cell_length_c  8.8030
_cell_angle_alpha 90.000
_cell_angle_beta 146.295
_cell_angle_gamma 90.000
_cell_volume 264.7
_symmetry_int_tables_number 14
_symmetry_space_group_name_H-M 'P 1 21/c 1'

O1 -0.2675  0.3925 -0.3737
O2 -1.3838  0.7017 -0.6442
N3 -1.0978  0.5994 -0.6998
```

```
N4 -0.9994  0.5526 -0.7691
N5 -1.1613  0.4433 -0.9839
N6 -1.4616  0.3976 -1.1588
C7 -0.3985  0.9521 -0.3811
```

3.3.4 c1-DTTO: space group $P\,21/c$ (14) local minima

```
_cell_length_a 10.0500
_cell_length_b 13.7240
_cell_length_c  5.6880
_cell_angle_alpha 90.000
_cell_angle_beta 138.179
_cell_angle_gamma 90.000
_cell_volume 523.1
_symmetry_int_tables_number 14
_symmetry_space_group_name_H-M 'P 1 21/c 1'

O1  0.4972  0.2987  0.1032
O2  0.3969  0.4527  0.6375
O3  0.0389  0.4473  0.8389
O4  0.1469  0.2993  0.3048
N5  0.0314  0.3411  0.2891
N6  0.1022  0.3758  0.5838
N7  0.9661  0.4151  0.5576
N8  0.7717  0.4244  0.2676
N9  0.7664  0.3185  0.6758
N10 0.5715  0.3319  0.3831
N11 0.4422  0.3801  0.3545
N12 0.5113  0.4091  0.6536
C13 0.7116  0.1057  0.4792
C14 0.8285  0.1481  0.4626
```

3.3.5 c1-DTTO: space group $P\,2_1\,2_1\,2_1$ (19)

```
_cell_length_a                       18.12900
_cell_length_b                       5.39900
_cell_length_c                       6.93650
_cell_angle_alpha                    90
_cell_angle_beta                     90
_cell_angle_gamma                    90
_symmetry_space_group_name_H-M       'P 21 21 21'
_symmetry_Int_Tables_number          19

O1 0.24691  0.26434  0.587080
O2 0.10287  0.60352  0.587820
O3 0.99609  0.62793  0.954250
O4 0.13986  0.28753  0.955810
N1 0.11415  0.10639  0.041840
N2 0.06810  0.95599  0.946750
N3 0.04056  0.75533  0.046010
N4 0.05800  0.68834  0.226020
N5 0.18064  0.21252  0.321540
N6 0.20087  0.14045  0.496950
N7 0.17519  0.93387  0.595070
N8 0.12727  0.78751  0.503190
C1 0.60466  0.65750  0.687920
```

```
C2 0.63445  0.44348  0.764430
```

3.4 Coordinates for structures of DTTO configuration 2 (c2)

3.4.1 c1-DTTO: space group $C2$ (5)

```
_cell_length_a  6.0340
_cell_length_b  8.6200
_cell_length_c 14.4100
_cell_angle_alpha 90.000
_cell_angle_beta 108.197
_cell_angle_gamma 90.000
_cell_volume 712.0
_symmetry_int_tables_number 5
_symmetry_space_group_name_H-M 'C 1 2 1'

N1  0.1965  0.9509  0.8529
N2  0.2525  0.0875  0.9007
N3  0.1817  0.2196  0.8457
N4  0.0497  0.2286  0.7521
N5  0.9945  0.8134  0.7020
N6  0.8709  0.8182  0.6067
N7  0.8223  0.9644  0.5652
N8  0.8691  0.0999  0.6111
C9  0.0670  0.9495  0.7540
C10 0.9951  0.0912  0.7062
O11 0.2504  0.3417  0.8899
O12 0.2656  0.8320  0.9008
O13 0.0358  0.6820  0.7395
O14 0.7224  0.9625  0.4765
```

3.4.2 c1-DTTO: space group $C\,2/c$ (15)

```
_cell_length_a 30.5990
_cell_length_b  5.4130
_cell_length_c  9.5830
_cell_angle_alpha 90.000
_cell_angle_beta 121.835
_cell_angle_gamma 90.000
_cell_volume 1348.5
_symmetry_int_tables_number 15
_symmetry_space_group_name_H-M 'C 1 2/c 1'

N1  0.1554  0.3695  0.4826
N2  0.1989  0.2509  0.5209
N3  0.2091  0.0338  0.6084
N4  0.1820  0.9359  0.6669
N5  0.0778  0.3885  0.4957
N6  0.0491  0.2900  0.5510
N7  0.0682  0.0813  0.6461
N8  0.1115  0.9618  0.6874
C9  0.1239  0.2775  0.5346
C10 0.1392  0.0611  0.6293
O11 0.2479  0.9251  0.6328
O12 0.1454  0.5605  0.3994
O13 0.0608  0.5776  0.4115
```

```
O14 0.0415  0.0003  0.6970
```

3.4.3 c1-DTTO: space group Cc (9)

```
_cell_length_a  5.9310
_cell_length_b 21.6090
_cell_length_c  5.3870
_cell_angle_alpha 90.000
_cell_angle_beta 88.567
_cell_angle_gamma 90.000
_cell_volume 690.2
_symmetry_int_tables_number 9
_symmetry_space_group_name_H-M 'C 1 c 1'

N1  0.2971  0.9272  0.7214
N2  0.4981  0.9523  0.6557
N3  0.6064  0.9277  0.4483
N4  0.5242  0.8861  0.2922
N5  0.0102  0.8491  0.6484
N6  0.9291  0.8045  0.5004
N7  0.0486  0.7929  0.2824
N8  0.2416  0.8189  0.2070
C9  0.2118  0.8784  0.5852
C10 0.3251  0.8611  0.3640
O11 0.7968  0.9487  0.4065
O12 0.1978  0.9500  0.9048
O13 0.8948  0.8616  0.8366
O14 0.9600  0.7541  0.1482
```

3.4.4 c1-DTTO: space group $Pnma$ (62)

```
_cell_length_a  5.5430
_cell_length_b 15.3780
_cell_length_c  7.9240
_cell_angle_alpha 90.000
_cell_angle_beta 90.000
_cell_angle_gamma 90.000
_cell_volume 675.4
_symmetry_int_tables_number 62
_symmetry_space_group_name_H-M 'P n m a'

N1 0.9387  0.3295  0.5598
N2 0.8404  0.4044  0.5052
N3 0.6418  0.3972  0.4008
N4 0.5282  0.3237  0.3572
O5 0.5656  0.4663  0.3454
O6 0.1189  0.3361  0.6518
C7 0.1590  0.7500  0.4881
C8 0.3666  0.7500  0.5893
```

3.4.5 c1-DTTO: space group $Pbca$ (61)

```
_cell_length_a                         25.54000
_cell_length_b                         5.43300
_cell_length_c                         9.68500
_cell_angle_alpha                      90
```

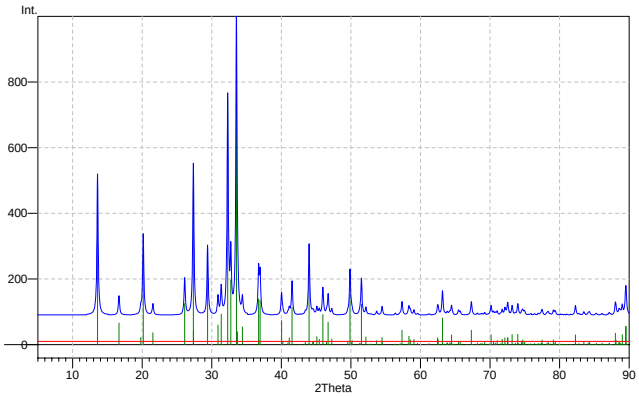
```
_cell_angle_beta                        90
_cell_angle_gamma                       90
_symmetry_space_group_name_H-M          'P b c a'
_symmetry_Int_Tables_number             61

N1   1.095850  0.117770  0.356090
N9   1.051590  0.000100  0.391960
N17  1.040920  0.783530  0.322700
N25  1.068020  0.685780  0.218880
N33  1.174470  0.134050  0.212760
N41  1.203250  0.035990  0.109370
N49  1.182320  0.834500  0.043310
N57  1.138790  0.713100  0.077740
C1   1.127300  0.026000  0.251190
C9   1.111410  0.810590  0.183080
O1   1.001620  0.675430  0.364430
O9   1.106410  0.307360  0.421930
O17  1.192470  0.320290  0.268590
O25  1.207650  0.761520  0.943290
```

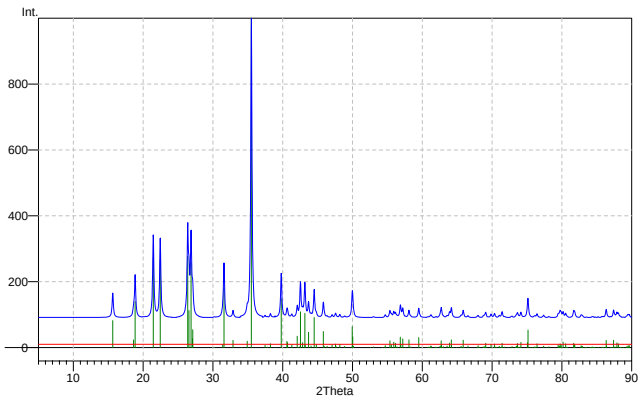
4 Simulation of the Powder X-ray of the most stable structures

Based on the structures obtained from periodic DFT:PBE-ulg we have simulated the PXRD in order to facilitate its identification when their synthesis is attained. The parameters used for the simulation of the PXRD are X-ray (laboratory) with wavelength of 1.5406 Åand we assumed a conventional laboratory X-ray diffractometers thus both Lorentz and polarization correction were applied. We report the first peaks for every PXRD in order to quickly identified the crystal packing using crystalline powder, instead of waiting to growth a single crystal. If further refinement is needed, the coordinates for the structures reported above should be used.

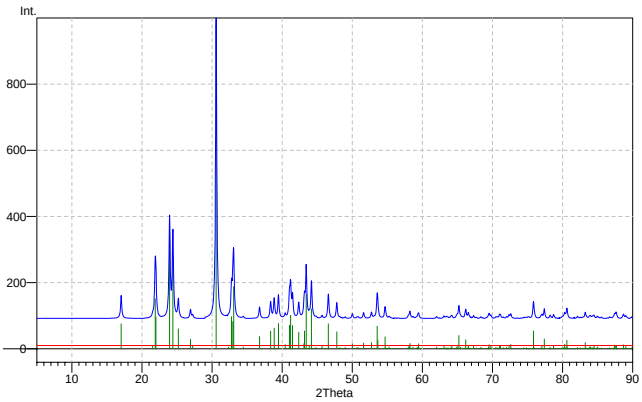
4.1 PXRD plot for c1-DTTO



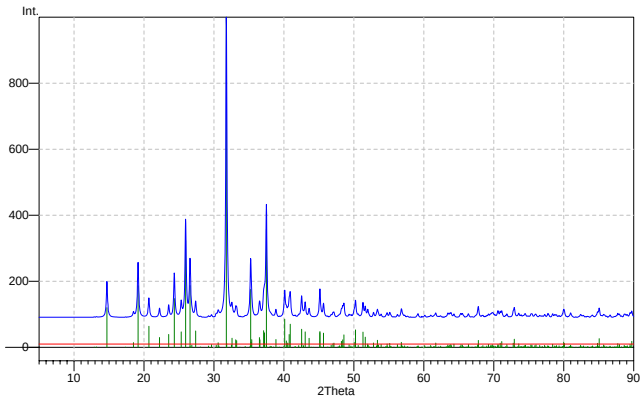
14.1: $C\,2/c$ (15)



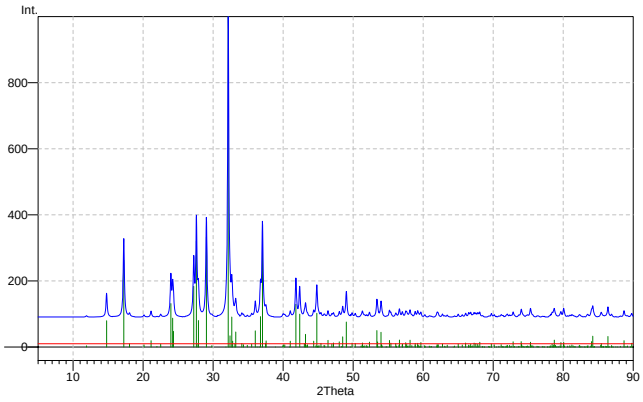
14.2: $P\,-1$ (2)



14.3: $P\,21/c$ (14) global minimum



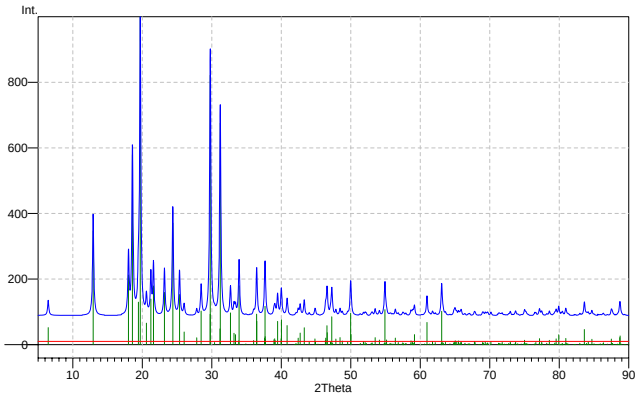
14.4: $P\,21/c$ (14) local minima



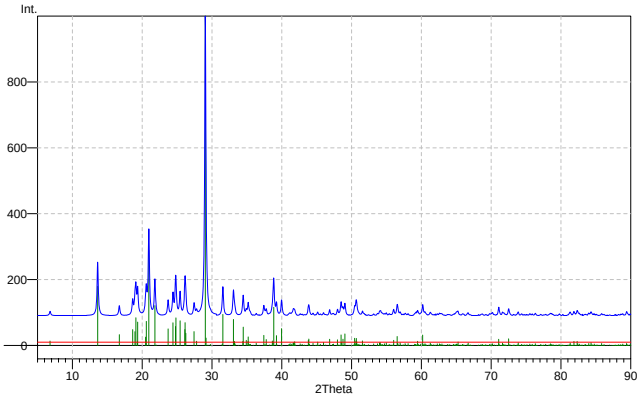
14.5: $P\,2_1\,2_1\,2_1$ (19)

Figure S14: PXRD for configuration 1 of DTTO with space group $C\,2/c$ (15), $P\,-1$ (2), $P\,21/c$ (14) and $P\,2_1\,2_1\,2_1$ (19)

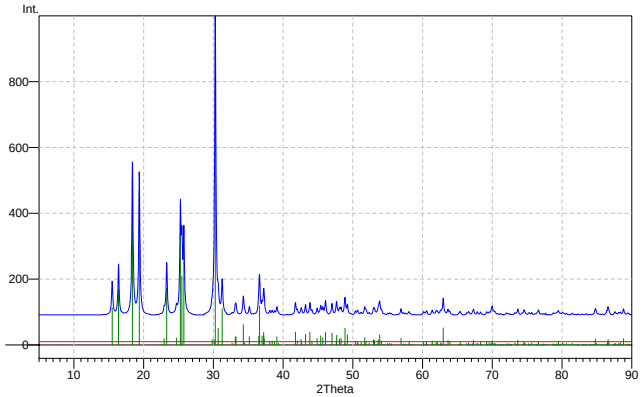
4.2 PXRD plot for c2-DTTO



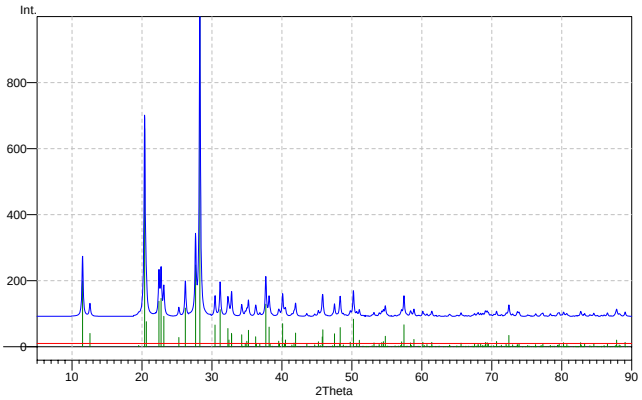
15.1: $C2$ (5)



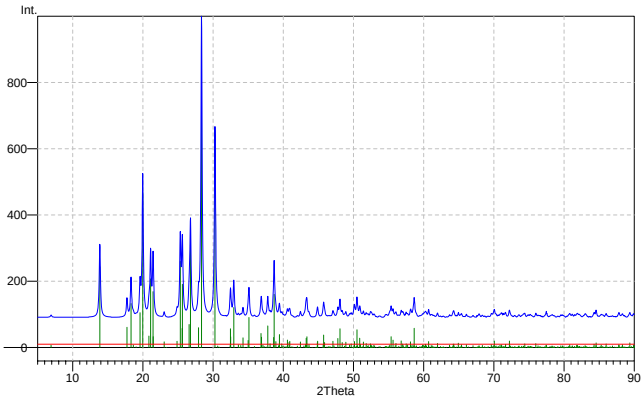
15.2: $C\,2/c$ (15)



15.3: $C\,c$ (9)



15.4: $P\,n\,m\,a$ (62)



15.5: $P\,b\,c\,a$ (61)

Figure S15: PXRD for configuration 2 of DTTO with space group $C2$ (5), $C\,2/c$ (15), $C\,c$ (9), $P\,n\,m\,a$ (62) and $P\,b\,c\,a$ (61)

4.3 First peaks PXRD data for c1-DTTO

Table S5: Table of reflexion parameters of the PXRD for c1-DTTO with space group $C\,2/c$ (15)

No.	2Theta[°]	d-spacing [Å]	Int.	F	h	k	l	Mult.
1	13.576	6.517	439227.62	39.580	-1	-1	1	4
2	16.656	5.3183	60554.11	25.600	-2	0	2	2
3	19.794	4.4817	19916.31	12.400	-1	1	2	4
4	20.145	4.4044	251764.4	44.890	1	1	0	4
5	21.536	4.123	33320.52	24.750	0	2	0	2
6	26.103	3.411	115198.28	39.800	0	2	1	4
7	27.348	3.2585	433146.17	81.080	-2	-2	2	4
8	27.359	3.2572	37927.89	24.000	-3	-1	3	4
9	29.396	3.036	218200.78	87.890	0	0	2	2
10	30.785	2.9021	485.93	3.080	-3	1	4	4
11	30.892	2.8923	54736.33	32.830	-2	2	3	4
12	31.356	2.8505	85730.12	41.750	-2	-2	1	4
13	31.48	2.8396	283.29	2.410	-3	-1	2	4
14	32.285	2.7706	689476.39	122.180	-1	1	3	4
15	32.731	2.7338	181510.06	63.630	1	1	1	4
16	33.542	2.6695	922796.87	208.350	-2	0	4	2
17	33.65	2.6612	852.87	4.490	-1	-3	1	4
18	33.677	2.6592	36158.3	41.420	-4	0	4	2
19	34.401	2.6049	49544.28	49.620	2	0	0	2
20	36.732	2.4447	128502.08	60.710	0	2	2	4
21	36.746	2.4438	7383.6	14.560	-1	3	2	4
22	36.946	2.4311	124817.95	60.220	1	3	0	4
23	40.033	2.2504	67630.61	48.440	-3	1	5	4
24	40.212	2.2408	8796.67	17.560	-2	2	4	4
25	40.327	2.2347	202.05	2.670	-4	-2	4	4
26	40.949	2.2022	5350.67	13.970	2	2	0	4

Table S6: Table of reflexion parameters of the PXRD for c1-DTTO with space group $P\,-1$ (2)

No.	2Theta[°]	d-spacing [Å]	Int.	F	h	k	l	Mult.
1	15.640	5.6616	6737.49	8.01	0	0	1	2
2	18.625	4.7603	1914.51	5.11	0	1	0	2
3	18.850	4.7039	11515.20	12.68	1	0	0	2
4	21.448	4.1396	22536.48	20.27	0	1	1	2
5	22.448	3.9575	21837.13	20.92	1	0	1	2
6	26.380	3.3759	22782.17	25.31	-1	1	0	2
7	26.561	3.3532	9238.89	16.24	-1	0	1	2
8	26.859	3.3167	21266.34	24.93	1	1	0	2
9	27.068	3.2915	2197.01	8.08	0	-1	1	2
10	27.111	3.2865	4438.17	11.50	1	1	1	2
11	30.220	2.9551	58.70	1.48	-1	1	1	2
12	31.396	2.8470	727.88	5.45	1	-1	1	2
13	31.580	2.8308	14725.14	24.66	0	0	2	2
14	32.879	2.7219	1795.32	8.99	0	1	2	2
15	34.102	2.6270	23.95	1.08	1	0	2	2

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Table S6 – *Continued from previous page*

No.	2Theta[°]	d-spacing [Å]	Int.	F	h	k	l	Mult.
16	34.908	2.5682	1565.87	8.96	-1	-1	1	2
17	35.503	2.5265	82267.30	66.18	1	1	2	2
18	37.460	2.3989	531.84	5.64	0	2	1	2
19	37.766	2.3801	105.19	2.53	0	2	0	2
20	38.236	2.3519	925.20	7.62	2	0	0	2
21	38.903	2.3132	26.62	1.32	2	0	1	2
22	39.781	2.2641	12194.30	28.89	-1	0	2	2
23	40.602	2.2202	1525.73	10.45	0	-1	2	2
24	40.687	2.2158	1196.75	9.28	-1	1	2	2

Table S7: Table of reflexion parameters of the PXRD for c1-DTTO with space group $P\,21/c$ (14) global minimum

No.	2Theta[°]	d-spacing [Å]	Int.	F	h	k	l	Mult.
1	17.026	5.2036	24642.06	11.81	-1	-1	1	4
2	21.527	4.1247	2533.13	6.82	1	0	0	2
3	21.885	4.0579	49564.67	21.71	0	1	1	4
4	21.981	4.0405	31407.61	24.55	-1	0	2	2
5	23.930	3.7156	107571.70	49.64	-2	0	2	2
6	24.404	3.6445	91597.64	46.76	0	2	0	2
7	24.782	3.5898	127.63	1.25	1	1	0	4
8	25.180	3.5339	19711.34	15.85	-1	1	2	4
9	26.912	3.3103	9301.36	11.68	-2	-1	2	4
10	27.232	3.2722	3220.71	6.96	-1	-2	1	4
11	30.580	2.9211	327842.06	79.47	0	2	1	4
12	32.338	2.7662	1574.49	5.85	-2	-1	1	4
13	32.765	2.7311	31608.96	26.58	1	2	0	4
14	32.962	2.7152	26800.94	24.64	-2	1	3	4
15	33.074	2.7063	61548.07	37.47	-1	2	2	4
16	34.443	2.6018	1580.39	6.28	-2	-2	2	4
17	36.767	2.4425	12037.17	26.31	0	0	2	2
18	38.348	2.3453	17437.35	23.45	-3	-1	3	4
19	38.855	2.3159	20307.11	25.68	0	1	2	4
20	38.931	2.3115	720.06	4.85	-2	-2	1	4
21	38.969	2.3094	401.25	3.62	-1	-3	1	4
22	39.464	2.2816	24916.99	28.94	-2	2	3	4
23	40.424	2.2295	4053.00	16.95	-3	0	2	2
24	40.520	2.2245	15.41	0.74	1	1	1	4

Table S8: Table of reflexion parameters of the PXRD for c1-DTTO with space group $P\,21/c$ (14) local minima

No.	2Theta[°]	d-spacing [Å]	Int.	F	h	k	l	Mult.
1	12.891	6.8620	729.27	2.16	0	2	0	2
2	13.201	6.7014	1058.62	2.67	1	0	0	2
3	14.699	6.0218	139159.98	24.15	1	1	0	4
4	17.375	5.0997	604.30	1.89	-1	1	1	4

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Table S8 – *Continued from previous page*

No.	2Theta[°]	d-spacing [Å]	Int.	F	h	k	l	Mult.
5	18.491	4.7944	16306.47	10.46	1	2	0	4
6	19.147	4.6317	216074.22	39.46	-2	-1	1	4
7	20.696	4.2883	73800.79	24.99	-1	2	1	4
8	22.214	3.9987	34347.93	18.35	-2	-2	1	4
9	23.528	3.7783	45183.10	22.35	1	3	0	4
10	24.328	3.6558	171017.84	45.03	0	1	1	4
11	25.316	3.5152	54149.88	26.42	-1	3	1	4
12	25.948	3.4310	375119.37	100.94	0	4	0	2
13	26.581	3.3507	216768.21	78.71	2	0	0	2
14	26.584	3.3503	2100.52	5.48	-2	-3	1	4
15	26.836	3.3195	7150.54	10.21	0	2	1	4
16	27.377	3.2551	57261.06	29.51	2	1	0	4
17	28.098	3.1732	1124.32	4.25	-3	-1	1	4
18	29.219	3.0540	4267.91	8.64	1	4	0	4
19	29.646	3.0109	9108.15	12.81	2	2	0	4
20	30.317	2.9458	7193.29	11.66	-3	-2	1	4
21	30.594	2.9198	15930.64	17.53	0	3	1	4
22	30.699	2.9100	4816.44	9.67	-1	4	1	4
23	31.770	2.8144	1159143.11	155.69	-2	-4	1	4
24	31.818	2.8102	13496.70	23.80	-3	0	2	2
25	32.496	2.7531	8432.07	13.61	-3	1	2	4
26	32.576	2.7465	31933.54	37.55	-2	0	2	2
27	33.113	2.7032	26346.68	24.55	2	3	0	4
28	33.241	2.6931	23369.34	23.22	-2	1	2	4
29	33.722	2.6557	524.18	3.53	-3	-3	1	4
30	34.459	2.6006	2983.37	8.63	-3	2	2	4
31	35.167	2.5498	4081.88	10.32	-2	2	2	4
32	35.245	2.5444	203130.33	72.95	0	4	1	4
33	35.308	2.5400	17954.82	21.73	1	5	0	4
34	35.394	2.5340	26867.45	26.65	1	1	1	4
35	36.493	2.4602	34181.37	43.97	-4	0	2	2
36	36.568	2.4553	26441.16	27.41	-1	5	1	4
37	37.095	2.4216	58234.00	41.32	-4	-1	2	4
38	37.223	2.4136	50969.96	38.80	1	2	1	4
39	37.487	2.3972	8932.77	16.37	2	4	0	4
40	37.489	2.3971	413684.36	111.41	-2	-5	1	4
41	37.531	2.3945	2664.40	8.95	-3	3	2	4
42	38.035	2.3639	3519.17	10.44	-3	-4	1	4
43	38.190	2.3547	3157.04	9.93	-2	3	2	4
44	38.485	2.3373	1063.91	8.22	-1	0	2	2
45	38.856	2.3159	27482.15	29.87	-4	-2	2	4
46	39.061	2.3041	74.52	1.56	-1	1	2	4
47	39.360	2.2873	509.73	5.84	0	6	0	2
48	39.936	2.2557	1854.05	8.00	-4	-1	1	4
49	40.112	2.2462	98792.61	58.68	1	3	1	4
50	40.344	2.2338	22248.25	39.63	3	0	0	2
51	40.537	2.2236	14947.09	23.09	0	5	1	4
52	40.750	2.2125	44895.07	40.26	-1	2	2	4
53	40.898	2.2048	81162.97	54.35	3	1	0	4

Table S9: Table of reflexion parameters of the PXRD for c1-DTTO with space group $P\,2_1\,2_1\,2_1$ (19)

No.	2Theta[°]	d-spacing [Å]	Int.	F	h	k	l	Mult.
1	11.914	7.4225	4210.50	4.80	2	0	0	2
2	14.782	5.9880	91625.47	19.71	1	0	1	4
3	17.238	5.1401	302225.16	41.89	1	1	0	4
4	18.057	4.9087	11132.08	8.43	2	0	1	4
5	20.128	4.4081	7283.80	7.63	2	1	0	4
6	21.131	4.2010	21938.40	13.92	0	1	1	4
7	21.971	4.0422	1891.88	3.01	1	1	1	8
8	22.508	3.9470	9478.34	9.77	3	0	1	4
9	23.959	3.7113	151571.68	59.00	4	0	0	2
10	24.216	3.6723	100406.64	34.34	3	1	0	4
11	24.326	3.6560	54652.16	18.00	2	1	1	8
12	27.233	3.2720	211559.40	79.78	0	0	2	2
13	27.609	3.2282	369387.11	75.63	4	0	1	4
14	27.836	3.2025	8995.98	8.42	3	1	1	8
15	27.900	3.1953	92315.00	38.23	1	0	2	4
16	29.037	3.0727	383189.07	81.28	4	1	0	4
17	29.818	2.9940	4488.24	9.05	2	0	2	4
18	31.829	2.8092	25.41	0.73	0	1	2	4
19	32.157	2.7814	1152720.35	111.23	4	1	1	8
20	32.410	2.7602	38863.56	20.60	1	1	2	8
21	32.662	2.7395	104508.79	68.12	0	2	0	2
22	32.787	2.7293	20153.05	21.24	3	0	2	4
23	33.106	2.7037	11053.23	15.90	5	0	1	4
24	33.229	2.6940	52200.48	34.68	1	2	0	4
25	34.098	2.6273	12375.69	12.28	2	1	2	8
26	34.326	2.6104	8065.71	14.12	5	1	0	4
27	34.882	2.5700	5731.11	12.12	2	2	0	4
28	35.496	2.5270	9572.74	15.96	0	2	1	4
29	36.023	2.4912	56387.15	27.84	1	2	1	8
30	36.280	2.4742	6.63	0.61	6	0	0	2
31	36.583	2.4543	61.23	1.32	4	0	2	4
32	36.759	2.4430	106002.29	39.02	3	1	2	8
33	37.048	2.4246	357425.40	72.28	5	1	1	8
34	37.495	2.3967	12478.27	19.35	3	2	0	4
35	37.569	2.3922	21349.84	17.94	2	2	1	8
36	38.883	2.3143	192.72	2.50	6	0	1	4
37	39.950	2.2549	3488.01	10.98	6	1	0	4
38	40.031	2.2505	7661.42	11.53	3	2	1	8
39	40.230	2.2399	7424.74	11.41	4	1	2	8
40	40.912	2.2041	193.89	2.66	4	2	0	4

4.4 First peaks PXRD data for c2-DTTO

Table S10: Table of reflexion parameters of the PXRD for c1-DTTO with space group $C2$ (5)

No.	2Theta[°]	d-spacing [Å]	Int.	F	h	k	l	Mult.
1	6.451	13.6893	67463.64	10.36	0	0	1	2

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Table S10 – *Continued from previous page*

No.	2Theta[°]	d-spacing [Å]	Int.	F	h	k	l	Mult.
2	12.924	6.8447	451450.21	53.98	0	0	2	2
3	18.006	4.9225	276755.57	41.92	-1	-1	1	4
4	18.574	4.7732	754219.58	71.45	1	1	0	4
5	19.437	4.5631	168524.92	50.05	0	0	3	2
6	19.700	4.5029	1302605.29	99.77	-1	-1	2	4
7	20.591	4.3100	85105.12	37.76	0	2	0	2
8	21.230	4.1817	180910.59	40.18	1	1	1	4
9	21.599	4.1111	233165.63	46.44	0	2	1	4
10	23.183	3.8337	207304.26	47.14	-1	1	3	4
11	24.386	3.6472	482671.60	75.84	0	2	2	4
12	25.352	3.5103	198915.16	50.72	1	1	2	4
13	26.015	3.4223	50006.26	36.95	0	0	4	2
14	27.826	3.2036	27020.66	20.63	-1	1	4	4
15	28.463	3.1333	133317.55	46.93	0	2	3	4
16	29.762	2.9994	120364.28	66.14	-2	0	1	2
17	29.775	2.9982	1069788.15	197.28	-2	0	2	2
18	30.392	2.9387	8211.78	12.49	1	1	3	4
19	31.181	2.8661	62347.61	50.05	2	0	0	2
20	31.217	2.8629	879242.55	188.17	-2	0	3	2
21	32.682	2.7379	126035.98	74.86	0	0	5	2
22	33.194	2.6968	45047.67	32.18	-1	1	5	4
23	33.406	2.6802	39408.57	30.31	0	2	4	4
24	33.869	2.6445	14973.67	26.82	2	0	1	2
25	33.924	2.6404	233469.46	106.10	-2	0	4	2
26	34.588	2.5912	577.58	3.81	-1	-3	1	4
27	34.901	2.5687	2867.02	8.57	1	3	0	4
28	35.541	2.5239	1136.04	5.51	-1	-3	2	4
29	36.020	2.4914	16509.50	21.30	1	1	4	4
30	36.451	2.4629	120923.74	58.40	1	3	1	4
31	36.466	2.4619	92684.54	51.15	-2	-2	1	4
32	36.476	2.4613	872.41	4.96	-2	-2	2	4
33	37.588	2.3910	25685.66	39.37	2	0	2	2
34	37.658	2.3867	20278.26	35.06	-2	0	5	2
35	37.660	2.3866	152044.26	67.88	2	2	0	4
36	37.675	2.3857	31471.46	30.90	-1	3	3	4
37	37.690	2.3848	20819.32	25.14	-2	-2	3	4
38	38.940	2.3110	19229.43	25.05	0	2	5	4
39	39.049	2.3049	23162.69	27.58	-1	1	6	4
40	39.111	2.3013	16277.08	23.16	1	3	2	4
41	39.464	2.2816	92337.73	78.79	0	0	6	2
42	39.966	2.2540	22760.26	28.05	2	2	1	4
43	40.014	2.2515	98580.04	58.46	-2	-2	4	4
44	40.834	2.2081	75767.50	52.42	-1	3	4	4

Table S11: Table of reflexion parameters of the PXRD for c1-DTTO with space group $C\,2/c$ (15)

No.	2Theta[°]	d-spacing [Å]	Int.	F	h	k	l	Mult.
1	6.795	12.9980	114347.99	14.21	2	0	0	2
2	13.614	6.4990	1547408.40	105.36	4	0	0	2

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Table S11 – *Continued from previous page*

No.	2Theta[°]	d-spacing [Å]	Int.	F	h	k	l	Mult.
3	16.716	5.2993	282337.19	39.23	1	1	0	4
4	18.628	4.7594	413588.91	75.05	-4	0	2	2
5	18.959	4.6772	360107.18	50.42	-1	1	1	4
6	19.087	4.6460	726201.03	101.98	-2	0	2	2
7	19.319	4.5909	100311.16	27.13	3	1	0	4
8	19.346	4.5845	611263.04	67.08	-3	1	1	4
9	20.482	4.3327	216215.34	59.85	6	0	0	2
10	20.585	4.3112	629998.12	102.70	-6	0	2	2
11	20.945	4.2379	2493405.63	147.08	1	1	1	4
12	21.816	4.0707	1043381.23	140.37	0	0	2	2
13	21.987	4.0394	10520.10	10.05	-5	-1	1	4
14	23.709	3.7497	432144.27	69.67	5	1	0	4
15	24.406	3.6442	592756.98	118.96	-8	0	2	2
16	24.764	3.5924	496790.92	78.19	3	1	1	4
17	24.828	3.5832	720878.73	94.45	-3	1	2	4
18	25.427	3.5002	645334.21	91.63	-5	1	2	4
19	26.109	3.4102	415619.44	75.62	-1	1	2	4
20	26.143	3.4059	596769.25	128.32	2	0	2	2
21	26.239	3.3936	318732.21	66.57	-7	-1	1	4
22	27.425	3.2495	362977.45	105.28	8	0	0	2
23	27.792	3.2075	108530.14	41.28	-7	-1	2	4
24	29.038	3.0726	8638191.85	385.93	1	1	2	4
25	29.138	3.0623	193458.86	57.97	7	1	0	4
26	29.415	3.0341	8106.52	16.95	-10	0	2	2
27	29.759	2.9997	27223.92	22.24	5	1	1	4
28	31.464	2.8410	34271.28	37.47	4	0	2	2
29	31.505	2.8374	1449.10	5.46	-9	-1	1	4
30	31.557	2.8328	812090.73	129.38	-9	-1	2	4
31	32.521	2.7510	39.81	0.94	-5	1	3	4
32	33.071	2.7065	680088.29	176.14	0	2	0	2
33	33.219	2.6948	53136.96	34.98	3	1	2	4
34	33.224	2.6944	103312.83	48.79	-7	1	3	4
35	33.301	2.6883	38974.12	30.04	-3	1	3	4
36	33.802	2.6497	144.61	1.86	2	2	0	4
37	34.422	2.6033	106243.67	51.42	-2	2	1	4
38	34.473	2.5996	480284.49	154.85	10	0	0	2
39	34.906	2.5683	131810.88	58.15	0	2	1	4
40	35.167	2.5499	104863.48	73.95	-12	0	2	2
41	35.189	2.5483	223383.95	76.37	9	1	0	4
42	35.330	2.5385	23263.33	24.75	-9	1	3	4
43	35.348	2.5372	16248.51	20.70	-4	-2	1	4
44	35.477	2.5283	28664.40	27.60	-1	1	3	4
45	35.497	2.5269	19108.93	22.55	7	1	1	4
46	35.914	2.4985	4847.91	11.50	4	2	0	4
47	36.338	2.4703	55269.42	39.35	-11	-1	2	4
48	36.752	2.4435	3278.49	9.70	2	2	1	4
49	37.422	2.4012	84261.38	70.97	6	0	2	2
50	37.422	2.4012	179663.24	73.28	-11	-1	1	4
51	37.593	2.3907	1510.01	6.75	-6	-2	1	4
52	37.600	2.3902	25302.87	39.09	-6	0	4	2
53	37.773	2.3797	154414.49	97.07	-8	0	4	2
54	38.224	2.3527	11967.18	19.36	-4	2	2	4

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Table S11 – *Continued from previous page*

No.	2Theta[°]	d-spacing [Å]	Int.	F	h	k	l	Mult.
55	38.463	2.3386	5614.47	13.35	-2	2	2	4
56	38.640	2.3283	115935.58	60.98	-11	-1	3	4
57	38.732	2.3230	96565.36	78.92	-4	0	4	2
58	38.844	2.3166	998480.21	180.01	1	1	3	4
59	39.215	2.2954	27994.36	30.46	6	2	0	4
60	39.236	2.2943	255990.33	130.34	-10	0	4	2
61	39.273	2.2922	22675.46	27.46	-6	2	2	4
62	39.796	2.2633	180.39	2.49	4	2	1	4
63	39.970	2.2538	439863.02	123.33	0	2	2	4
64	40.973	2.2010	11465.70	20.47	-8	-2	1	4

Table S12: Table of reflexion parameters of the PXRD for c1-DTTO with space group $C\,c$ (9)

No.	2Theta[°]	d-spacing [Å]	Int.	F	h	k	l	Mult.
1	8.177	10.8045	72.67	0.43	0	2	0	2
2	15.485	5.7178	203916.96	30.83	1	1	0	4
3	16.395	5.4022	303762.34	56.42	0	4	0	2
4	18.393	4.8198	927882.28	78.46	0	2	1	4
5	19.375	4.5777	853927.97	79.41	1	3	0	4
6	22.386	3.9683	1890.96	4.34	1	1	1	4
7	22.939	3.8739	33688.39	18.79	-1	1	1	4
8	23.304	3.8140	313185.82	58.25	0	4	1	4
9	24.700	3.6015	38319.30	30.63	0	6	0	2
10	25.270	3.5216	609513.99	88.47	1	3	1	4
11	25.484	3.4925	377620.09	70.26	1	5	0	4
12	25.764	3.4551	471611.80	79.43	-1	3	1	4
13	29.820	2.9937	28979.93	23.00	0	6	1	4
14	30.121	2.9646	28890.58	32.82	2	0	0	2
15	30.271	2.9501	1807332.36	184.56	1	5	1	4
16	30.691	2.9107	91579.37	42.16	-1	5	1	4
17	31.262	2.8589	198058.89	63.25	2	2	0	4
18	32.679	2.7381	9355.60	14.42	1	7	0	4
19	33.139	2.7011	42195.95	43.97	0	8	0	2
20	33.246	2.6927	46024.80	46.08	0	0	2	2
21	34.294	2.6127	111241.73	52.40	0	2	2	4
22	34.482	2.5990	11680.32	17.08	2	4	0	4
23	35.154	2.5507	45744.02	34.52	2	2	1	4
24	35.888	2.5003	1551.46	6.50	-2	-2	1	4
25	36.511	2.4590	47562.00	36.69	1	1	2	4
26	36.616	2.4522	213390.55	77.97	1	7	1	4
27	36.972	2.4294	48194.45	37.45	-1	7	1	4
28	37.210	2.4144	68261.19	44.88	0	8	1	4
29	37.221	2.4137	50283.91	38.54	-1	1	2	4
30	37.282	2.4099	33928.89	31.71	0	4	2	4
31	38.084	2.3610	21512.70	25.85	2	4	1	4
32	38.426	2.3408	22180.23	26.51	1	3	2	4
33	38.770	2.3208	18541.93	24.48	-2	-4	1	4
34	39.106	2.3016	44089.71	38.11	-1	3	2	4
35	39.333	2.2889	8479.61	16.82	2	6	0	4

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Table S12 – *Continued from previous page*

No.	2Theta[°]	d-spacing [Å]	Int.	F	h	k	l	Mult.
36	40.502	2.2255	1469.45	7.23	1	9	0	4

Table S13: Table of reflexion parameters of the PXRD for c1-DTTO with space group $P\,n\,m\,a$ (62)

No.	2Theta[°]	d-spacing [Å]	Int.	F	h	k	l	Mult.
1	11.499	7.6890	387419.79	44.43	0	2	0	2
2	12.557	7.0439	78221.57	15.43	0	1	1	4
3	19.528	4.5420	7529.26	7.52	1	0	1	4
4	20.371	4.3560	1284113.69	72.52	1	1	1	8
5	20.620	4.3040	147049.19	35.14	0	3	1	4
6	22.422	3.9620	267535.68	73.14	0	0	2	2
7	22.720	3.9107	284181.61	38.21	1	2	1	8
8	23.117	3.8445	178530.05	61.68	0	4	0	2
9	25.267	3.5219	54147.41	26.37	0	2	2	4
10	26.193	3.3995	227285.78	39.68	1	3	1	8
11	27.653	3.2233	480622.90	86.42	1	0	2	4
12	28.266	3.1547	1943089.27	125.76	1	1	2	8
13	30.037	2.9726	451.34	2.05	1	2	2	8
14	30.437	2.9344	127661.45	34.89	1	4	1	8
15	31.169	2.8672	218216.06	66.18	0	5	1	4
16	32.274	2.7715	106844.53	67.99	2	0	0	2
17	32.423	2.7591	39773.12	29.48	0	4	2	4
18	32.795	2.7286	78372.41	29.63	1	3	2	8
19	32.809	2.7276	72280.91	40.25	2	1	0	4
20	34.249	2.6161	70346.25	41.61	2	0	1	4
21	34.368	2.6073	3323.89	9.08	2	2	0	4
22	34.423	2.6032	1925.99	6.92	0	1	3	4
23	34.756	2.5790	20029.18	15.95	2	1	1	8
24	34.981	2.5630	32003.66	40.62	0	6	0	2
25	35.212	2.5467	96474.02	35.51	1	5	1	8
26	36.242	2.4767	58345.37	28.50	2	2	1	8
27	36.343	2.4700	19103.07	16.36	1	4	2	8
28	36.838	2.4380	15382.55	21.07	2	3	0	4
29	37.695	2.3845	250062.12	87.14	1	0	3	4
30	38.163	2.3563	115550.77	42.46	1	1	3	8
31	38.304	2.3480	15477.19	22.07	0	3	3	4
32	38.607	2.3302	3153.34	7.10	2	3	1	8
33	39.538	2.2775	32367.64	23.37	1	2	3	8
34	39.655	2.2710	15986.11	23.31	2	0	2	4
35	40.074	2.2482	1835.25	7.99	2	4	0	4
36	40.103	2.2466	135438.95	48.57	2	1	2	8
37	40.375	2.2321	17277.15	17.48	1	6	1	8
38	40.508	2.2251	39728.14	26.60	1	5	2	8

Table S14: Table of reflexion parameters of the PXRD for c1-DTTO with space group $P\,b\,c\,a$ (61)

No.	2Theta[°]	d-spacing [Å]	Int.	F	h	k	l	Mult.
1	6.916	12.7700	36379.50	8.16	2	0	0	2
2	13.858	6.3850	1331158.03	99.50	4	0	0	2
3	17.727	4.9993	332928.78	45.25	2	1	0	4
4	18.306	4.8425	724682.69	97.58	0	0	2	2
5	18.635	4.7577	38500.08	16.20	1	0	2	4
6	19.034	4.6589	10412.62	6.09	1	1	1	8
7	19.590	4.5279	573119.49	65.80	2	0	2	4
8	19.971	4.4424	2555114.11	100.22	2	1	1	8
9	20.852	4.2567	187792.24	56.82	6	0	0	2
10	21.090	4.2092	1132863.56	99.85	3	0	2	4
11	21.445	4.1403	921321.95	64.79	3	1	1	8
12	21.458	4.1378	177251.84	40.21	4	1	0	4
13	23.032	3.8584	92102.71	31.21	4	0	2	4
14	23.360	3.8051	1258.94	2.62	4	1	1	8
15	24.856	3.5793	101862.20	25.13	1	1	2	8
16	25.323	3.5143	1421181.26	135.40	5	0	2	4
17	25.590	3.4783	313331.61	45.45	2	1	2	8
18	25.623	3.4739	1043132.01	83.05	5	1	1	8
19	26.581	3.3507	379391.21	73.63	6	1	0	4
20	26.771	3.3274	1698021.89	110.97	3	1	2	8
21	27.884	3.1971	263.11	2.04	6	0	2	4
22	27.925	3.1925	326027.51	101.71	8	0	0	2
23	28.158	3.1666	2723.44	4.69	6	1	1	8
24	28.348	3.1458	5468744.53	211.64	4	1	2	8
25	30.265	2.9508	3465522.22	180.67	5	1	2	8
26	30.656	2.9140	24655.70	21.85	7	0	2	4
27	30.907	2.8909	4648.00	6.77	7	1	1	8
28	32.423	2.7591	30350.81	18.21	1	1	3	8
29	32.468	2.7554	308537.34	58.15	6	1	2	8
30	32.503	2.7525	175669.88	62.12	8	1	0	4
31	32.946	2.7165	658788.95	172.65	0	2	0	2
32	33.002	2.7120	4219.15	6.92	2	1	3	8
33	33.596	2.6654	43553.44	32.06	8	0	2	4
34	33.705	2.6570	3.11	0.27	2	2	0	4
35	33.828	2.6476	2036.15	4.94	8	1	1	8
36	33.947	2.6387	32787.53	19.89	3	1	3	8
37	34.256	2.6156	158674.44	62.51	0	2	1	4
38	34.441	2.6020	793.55	3.14	1	2	1	8
39	34.911	2.5680	9.76	0.35	7	1	2	8
40	34.990	2.5624	115258.24	38.55	2	2	1	8
41	35.108	2.5540	494609.62	160.31	10	0	0	2
42	35.232	2.5453	1499.37	4.43	4	1	3	8
43	35.889	2.5002	14201.29	13.91	3	2	1	8
44	35.897	2.4997	6597.24	13.41	4	2	0	4
45	36.676	2.4484	632.23	4.25	9	0	2	4
46	36.827	2.4386	230082.23	57.61	5	1	3	8
47	36.891	2.4346	169282.02	49.51	9	1	1	8
48	37.101	2.4213	37141.52	46.67	0	0	4	2
49	37.115	2.4204	4.62	0.26	4	2	1	8
50	37.274	2.4104	16059.51	21.81	1	0	4	4
51	37.556	2.3929	9408.92	11.90	8	1	2	8

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Table S14 – *Continued from previous page*

No.	2Theta[°]	d-spacing [Å]	Int.	F	h	k	l	Mult.
52	37.787	2.3789	354842.67	104.09	2	0	4	4
53	37.947	2.3692	2008.45	7.87	0	2	2	4
54	38.116	2.3591	59836.96	30.52	1	2	2	8
55	38.620	2.3294	163950.33	51.25	2	2	2	8
56	38.630	2.3289	27291.40	29.58	3	0	4	4
57	38.643	2.3281	46.21	0.86	5	2	1	8
58	38.700	2.3248	877017.85	118.80	6	1	3	8
59	38.935	2.3114	96173.06	56.01	10	1	0	4
60	39.314	2.2899	28564.75	30.86	6	2	0	4
61	39.448	2.2824	213060.83	59.81	3	2	2	8
62	39.784	2.2639	58851.11	44.88	4	0	4	4
63	39.874	2.2591	12581.00	20.80	10	0	2	4
64	40.074	2.2482	20238.49	18.76	10	1	1	8
65	40.375	2.2322	11953.32	14.54	9	1	2	8
66	40.444	2.2285	6161.46	10.46	6	2	1	8
67	40.583	2.2212	121846.13	46.68	4	2	2	8
68	40.819	2.2089	82183.21	38.59	7	1	3	8
69	40.927	2.2033	100308.10	42.76	1	1	4	8

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[1] H. Stokes and D. M. Hatch, "Findsym: Program for identifying the space group symmetry of a crystal," *Journal of Applied Crystallography*, vol. 38, pp. 237–238, 2005.