10.1071/CH17187_AC

Australian Journal of Chemistry 2017, 70(9), 973-978

SUPPLEMENTARY MATERIAL

Transformation of Cadmium Tetracyanoquinodimethane (TCNQ) into a Cadmium Terephthalate Metal Organic Framework

Manzar Sohail[A,B], Farooq Ahmad Kiani[C,D], Vedapriya Pandarinathan[E], Safyan Akram Khan[A], Damien J. Carter[E], Roland De Marco[B,E,F], Alan M. Bond[G]

[A] Center of Excellence for Nanotechnology, King Fahd University of Petroleum and Minerals, Dhahran 31260, Saudi Arabia.

[B] Faculty of Science, Health and Education, University of the Sunshine Coast, 90 Sippy Downs Drive, Sippy Downs, Queensland 4556, Australia

[C] Interdisciplinary Center for Scientific Computing (IWR), Heidelberg University, Im Neuenheimer Feld-368, D-69120 Heidelberg, Germany

[D] Research Center for Modeling and Simulation (RCMS), National University of Sciences and Technology (NUST), Sector H-12, 44000 Islamabad, Pakistan.

[E] Nanochemistry Research Institute, Department of Chemistry, Curtin University, Perth, WA 6845, Australia

[F] School of Chemistry and Molecular Biosciences, The University of Queensland, Brisbane, Queensland 4072, Australia

[G] School of Chemistry, Monash University, Clayton, Victoria 3800, Australia

Corresponding Author: [*] E-mail:rdemarc1@usc.edu.au; Tel:+61 7 5430 2867; Fax: +61 7 5456 5544

Appendix S1: Cartesian coordinates of the structures optimized using B3LYP/6-31+G(d).

2a

C	1.223195	0.000000	-0.688345
C	-0.026545	0.000000	-0.001931
C	0.020888	0.000000	1.423172
C	1.216979	0.000000	2.104946
C	2.467250	0.000000	1.418432
C	2.419519	0.000000	-0.007031
C	-1.271091	0.000000	-0.715215
C	-2.511051	0.000000	-0.041227
N	-3.534136	0.000000	0.526661
C	3.711473	0.000000	2.126864
C	4.954325	0.000000	1.447066
N	5.974619	0.000000	0.873497
C	3.761697	0.000000	3.542575
N	3.789910	0.000000	4.712678
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N	-1.343402	0.000000	-3.301135
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H	1.211464	0.000000	3.191509
H	3.351377	0.000000	-0.565936
H	1.228048	0.000000	-1.774859
H	-5.251138	0.000000	1.380280
O	-6.142460	0.000000	1.822742

2b

C	0.776284	-1.182153	0.115683
C	1.555881	0.017826	0.090817
C	0.855177	1.263679	-0.110809
C	-0.493398	1.295896	-0.297659
C	-1.273389	0.086699	-0.315392
C	-0.581559	-1.150515	-0.052337
C	2.957220	0.000364	0.257892
C	3.673094	-1.212495	0.452797
N	4.259693	-2.210980	0.609269
C	-2.636882	0.106299	-0.615061
C	-3.332584	1.328160	-0.851941
N	-3.895115	2.326123	-1.073385
O	-2.321975	-0.453390	1.801246
C	-3.398907	-1.086898	-0.798239
N	-4.022561	-2.040521	-1.047667
C	3.734324	1.190617	0.231268
N	4.371159	2.170349	0.206601
H	-1.161036	-2.064749	-0.019117
H	1.274808	-2.128625	0.301422
H	1.424170	2.188658	-0.110250
H	-0.997292	2.245731	-0.449207
H	-2.471716	-0.690142	2.736986

2c

C	2.477942	0.001516	0.030877
C	1.243986	-0.291321	-0.616797
C	0.040641	-0.266027	0.067545
C	-0.010268	0.049685	1.438833
C	1.200294	0.341547	2.096149
C	2.406887	0.317959	1.417494
C	-1.331414	0.177558	2.155818
O	-1.822089	1.533033	2.030782
C	-1.212849	-0.148915	3.607408
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C	3.730719	-0.026541	-0.676863
C	3.785708	-0.343855	-2.052183
N	3.801227	-0.610531	-3.194642
C	-2.360527	-0.749559	1.599829
N	-3.203387	-1.431858	1.183413
C	4.947113	0.264655	-0.020505
N	5.942032	0.511149	0.550412
H	1.197684	0.590587	3.154910
H	3.323864	0.543987	1.954279
H	1.249969	-0.542592	-1.673633
H	-0.875531	-0.495633	-0.471819
H	-2.675968	1.607279	2.496811

2d

C	1.202006	0.867371	1.910596
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C	2.501655	0.031538	0.013990
C	1.301418	-0.567898	-0.499946
C	0.106568	-0.441765	0.154308
C	0.002169	0.296908	1.376563
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C	3.843304	-0.784855	-1.899003
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C	-1.594743	-1.203268	3.715350
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C	-2.448196	0.046585	1.408508
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H	1.145607	1.402199	2.852299
H	3.292993	1.190365	1.680420
H	1.352270	-1.128632	-1.428376
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H	-1.860430	1.052127	3.715020

2e

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C	0.183164	0.762248	0.000000
C	-1.074114	0.093444	0.000000
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O	-0.758019	2.964503	0.000000
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H	-2.125006	-1.762331	0.000000
H	2.198465	-2.002592	0.000000
H	2.333676	0.437446	0.000000
H	-1.203209	4.823333	0.000000

Table S1. Crystal data and structure refinement for $C_8H_{15}CdO_{9.50}$.

Identification code	1
Empirical formula	$C_8H_{15}CdO_{9.50}$
Formula weight	375.60
Temperature	100(2) K
Wavelength	0.71252 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 7.0630(10) Å
	b = 9.7000(10) Å
	c = 10.1060(10) Å
	α= 108.771(2)°
	β= 92.874(2)°
	γ = 107.702(2)°
Volume	616.04(12) $Å^3$
Z	2
Density (calculated)	2.025 Mg/m^3
Absorption coefficient	1.815 mm^{-1}
F(000)	374
Crystal size	0.02 x 0.004 x 0.004 mm^3
θ range for data collection	2.36 to 31.01°.
Index ranges	-10<=h<=10, -13<=k<=13, -14<=l<=14
Reflections collected	6343
Independent reflections	3347 [R(int) = 0.0689]
Completeness to θ = 25.35°	91.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3347 / 30 / 181
Goodness-of-fit on F^2	1.074
Final R indices [I>2σ(I)]	R_1 = 0.0652, wR_2 = 0.1611
R indices (all data)	R_1 = 0.0872, wR_2 = 0.1800
Largest diff. peak and hole	3.332 and -2.893 e.$Å^{-3}$

Table S2. Selected bond lengths [Å] and angles [°] for $C_8H_{15}CdO_{9.50}$.

Cd(1)-O(2)	2.285(6)
Cd(1)-O(1)	2.286(6)
Cd(1)-O(11)	2.329(4)
Cd(1)-O(3)	2.335(5)
Cd(1)-O(22)	2.350(5)
Cd(1)-O(21)	2.467(5)
Cd(1)-O(12)	2.481(6)
O(2)-Cd(1)-O(1)	169.9(2)
O(2)-Cd(1)-O(11)	89.18(19)
O(1)-Cd(1)-O(11)	87.68(18)
O(2)-Cd(1)-O(3)	80.4(2)
O(1)-Cd(1)-O(3)	95.3(2)
O(11)-Cd(1)-O(3)	136.3(2)
O(2)-Cd(1)-O(22)	97.8(2)
O(1)-Cd(1)-O(22)	91.0(2)
O(11)-Cd(1)-O(22)	137.43(18)
O(3)-Cd(1)-O(22)	86.2(2)
O(2)-Cd(1)-O(21)	88.6(2)
O(1)-Cd(1)-O(21)	100.7(2)
O(11)-Cd(1)-O(21)	84.09(17)
O(3)-Cd(1)-O(21)	137.27(18)
O(22)-Cd(1)-O(21)	54.39(16)
O(2)-Cd(1)-O(12)	87.4(2)
O(1)-Cd(1)-O(12)	83.0(2)
O(11)-Cd(1)-O(12)	54.17(17)
O(3)-Cd(1)-O(12)	82.83(19)
O(22)-Cd(1)-O(12)	166.94(17)
O(21)-Cd(1)-O(12)	138.09(16)

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CIF file

data_cdtcnq



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_publ_contact_author_address
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 Chemistry,
School of Biomedical, Biomolecular and Chemical Science,
M313, University of Western Australia,
Perth, WA 6009,
 Australia
;
_publ_contact_author_email            brian.skelton@uwa.edu.au
_publ_contact_author_fax               (+61)_08_6488_1118
_publ_contact_author_phone             (+61)_08_6488_7107



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Chemistry,
School of Biomedical, Biomolecular and Chemical Science,
M313, University of Western Australia,
Perth, WA 6009,
 Australia
;


_publ_section_references
;
Farrugia, L. J. (1999). J. Appl. Cryst. 32, 837-838.

Johnson, C. K. (1976). ORTEPII. Report ORNL-5138.
 Oak Ridge National Laboratory, Tennessee, USA.

Sheldrick, G. M. (2008). Acta Cryst. A64, 112-122.
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'-x, -y, -z'

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 F^2^ > 2\s(F^2^) is used only for calculating R-factors(gt) etc. and is
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Cd Cd -0.776 1.211 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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C12 C 0.1014(10) 0.1581(7) 0.0635(6) 0.0135(12) Uani 1 1 d . . .
H12 H 0.1721 0.2661 0.1065 0.016 Uiso 1 1 calc R . .
C13 C 0.0079(10) 0.0966(7) -0.0777(6) 0.0120(11) Uani 1 1 d . . .
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C21 0.012(2) 0.013(2) 0.0063(19) 0.0050(16) -0.0003(16) 0.0060(16)
C22 0.022(3) 0.013(3) 0.012(3) 0.003(2) 0.005(2) 0.003(2)
C23 0.022(3) 0.019(3) 0.007(2) 0.000(2) 0.004(2) 0.005(3)
C2 0.022(3) 0.016(3) 0.005(2) 0.005(2) 0.003(2) 0.005(2)
O21 0.022(2) 0.022(2) 0.009(2) 0.0071(19) -0.0032(17) 0.0026(19)
O22 0.034(3) 0.012(2) 0.015(2) 0.0062(18) 0.000(2) 0.006(2)
O1 0.034(3) 0.023(3) 0.014(2) -0.001(2) 0.003(2) 0.001(2)
O2 0.020(2) 0.013(2) 0.030(3) 0.001(2) -0.001(2) 0.0010(19)
O3 0.057(4) 0.009(2) 0.017(2) 0.0036(19) 0.005(2) -0.001(2)
O4 0.031(3) 0.026(3) 0.034(3) 0.004(3) 0.006(3) 0.006(2)
O5 0.050(4) 0.018(3) 0.038(4) 0.007(2) 0.017(3) 0.010(3)
O6 0.035(7) 0.030(7) 0.034(7) 0.011(5) 0.003(5) 0.015(5)
O7 0.035(7) 0.027(6) 0.026(6) 0.011(5) 0.005(5) 0.010(5)


#------------------------------------------------------------------------
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#                   MOLECULAR GEOMETRY
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#------------------------------------------------------------------------
---#

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

```
;
loop_
    _geom_bond_atom_site_label_1
    _geom_bond_atom_site_label_2
    _geom_bond_distance
    _geom_bond_site_symmetry_2
    _geom_bond_publ_flag
Cd1 O2 2.285(6) . ?
Cd1 O1 2.286(6) . ?
Cd1 O11 2.329(4) . ?
Cd1 O3 2.335(5) . ?
Cd1 O22 2.350(5) . ?
Cd1 O21 2.467(5) . ?
Cd1 O12 2.481(6) . ?
C11 C13 1.390(8) 2 ?
C11 C12 1.395(9) . ?
C11 C1 1.493(9) . ?
C12 C13 1.394(8) . ?
C13 C11 1.390(8) 2 ?
C1 O11 1.250(9) . ?
C1 O12 1.271(8) . ?
C21 C23 1.394(9) 2_657 ?
C21 C22 1.395(9) . ?
C21 C2 1.497(9) . ?
C22 C23 1.378(10) . ?
C23 C21 1.394(9) 2_657 ?
C2 O21 1.248(8) . ?
C2 O22 1.291(8) . ?


loop_
    _geom_angle_atom_site_label_1
    _geom_angle_atom_site_label_2
    _geom_angle_atom_site_label_3
    _geom_angle
    _geom_angle_site_symmetry_1
    _geom_angle_site_symmetry_3
    _geom_angle_publ_flag
O2 Cd1 O1 169.9(2) . . ?
O2 Cd1 O11 89.18(19) . . ?
O1 Cd1 O11 87.68(18) . . ?
O2 Cd1 O3 80.4(2) . . ?
O1 Cd1 O3 95.3(2) . . ?
O11 Cd1 O3 136.3(2) . . ?
O2 Cd1 O22 97.8(2) . . ?
O1 Cd1 O22 91.0(2) . . ?
O11 Cd1 O22 137.43(18) . . ?
O3 Cd1 O22 86.2(2) . . ?
O2 Cd1 O21 88.6(2) . . ?
O1 Cd1 O21 100.7(2) . . ?
O11 Cd1 O21 84.09(17) . . ?
O3 Cd1 O21 137.27(18) . . ?
O22 Cd1 O21 54.39(16) . . ?
O2 Cd1 O12 87.4(2) . . ?
```

```
O1 Cd1 O12 83.0(2) . . ?
O11 Cd1 O12 54.17(17) . . ?
O3 Cd1 O12 82.83(19) . . ?
O22 Cd1 O12 166.94(17) . . ?
O21 Cd1 O12 138.09(16) . . ?
C13 C11 C12 119.7(5) 2 . ?
C13 C11 C1 120.5(6) 2 . ?
C12 C11 C1 119.7(5) . . ?
C13 C12 C11 120.3(5) . . ?
C11 C13 C12 120.0(6) 2 . ?
O11 C1 O12 121.0(6) . . ?
O11 C1 C11 119.5(6) . . ?
O12 C1 C11 119.6(6) . . ?
C1 O11 Cd1 96.2(4) . . ?
C1 O12 Cd1 88.6(4) . . ?
C23 C21 C22 119.2(6) 2_657 . ?
C23 C21 C2 120.1(6) 2_657 . ?
C22 C21 C2 120.7(6) . . ?
C23 C22 C21 120.0(6) . . ?
C22 C23 C21 120.8(6) . 2_657 ?
O21 C2 O22 120.4(6) . . ?
O21 C2 C21 120.5(6) . . ?
O22 C2 C21 119.0(6) . . ?
C2 O21 Cd1 90.4(4) . . ?
C2 O22 Cd1 94.7(4) . . ?
#===END
```