Understanding ligand flexibility and photoluminescence through bonding modes of ortho-anthraquinone inorganic-organic frameworks

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Contents

1 Thermal analysis

Thermogravimetric analysis conducted in air is shown in Figure 1. Results were consistent in all samples with the degree of hydration determined by single-crystal diffraction. The ligand H_2AQDC shows a small degradation step at 250°C and then a full decomposition with zero residue at 375°C. It is significantly less stable than the hybrid framework structures. The isostructural CaAQDC and MnAQDC both show a few unresolved dehydration steps from 20°C to 150°C. The CaAQDC structure is then stable on heating to 480°C where it undergoes a weight loss on conversion to $CaCO_3$. A second decomposition step beginning at 650°C indicates a conversion to calcium(II) oxide. An initial dehydration occurs in ZnAQDC between 20°C and 100°C. A broad decomposition step from 350°C to 520°C ending at 19% of the initial mass indicates a transformation to zinc(II) oxide. The initial dehydration steps in CdAQDC occur at 100°C and 160°C, indicating the loss of 3 and 1 water molecule, respectively. This is followed by a decomposition to cadmium(II) oxide beginning at 350°C and ending at 550°C. The decomposition steps in MnAQDC are overlapping and a broad weight loss beginning at 400°C and ending at 525°C indicates a conversion to manganese(II) oxide. NiAQDC similarly

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goes through dehydration steps up to 150°C, followed by a decomposition between 380°C and 450°C to nickel(II) oxide. Decomposition data is summarized in Table 1.

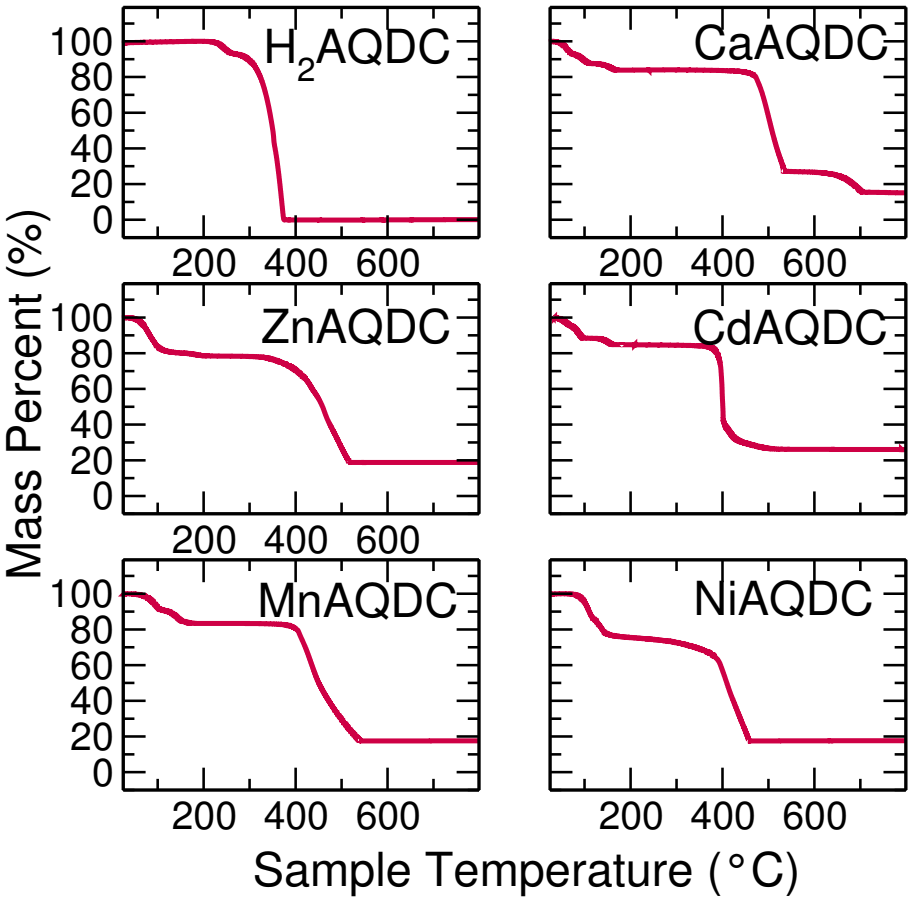

Figure 1 Thermogravimetric analysis of H_2AQDC, CaAQDC, ZnAQDC, CdAQDC, MnAQDC, and NiAQDC.

Table 1 Thermogravimetric analysis of anthraquinone frameworks

Compound	Initial Mass ($g \cdot mol^{-1}$)	Final Mass Percent (%)	Observed final mass ($g \cdot mol^{-1}$)	Decomposition product	Ideal decomposition mass ($g \cdot mol^{-1}$)	Error (%)
H_2AQDC	268.23	0	0	None	0	≈0
CaAQDC	406.35	15.0	60.95	CaO	56.08	8.7
ZnAQDC	431.64	18.8	81.15	ZnO	81.41	0.3
CdAQDC	478.67	26.0	124.45	CdO	128.41	3.1
MnAQDC	421.21	17.5	73.71	MnO	70.94	3.9
NiAQDC	479.03	17.6	84.31	NiO	74.69	12.8

2 Crystallographic details

2.1 Structure determination methods

All structures were determined using single crystal X-ray diffraction. CaAQDC, ZnAQDC, MnAQDC, and NiAQDC were collected at UCSB, Department of Chemistry and Biochemistry using MoKα radiation. CdAQDC was collected at University of Southampton on a Bruker Apex II diffractometer with a rotating anode source.

Table 2 Anthraquinone single crystal solution and structure data. Dimensionality is given as inorganic connectivity and the metal-oxygen-metal connectivity, as desribed in Cheetham et al., Chem. *Chem. Comm.*, 2006, **60**, 4780-4795.

	CaAQDC	MnAQDC	NiAQDC	ZnAQDC
Formula	$CaC_{16}H_{10}O_8{\cdot}2H_2O$	$MnC_{16}H_{10}O_8{\cdot}2H_2O$	$NiC_{16}H_{16}O_{11}{\cdot}2H_2O$	$ZnC_{16}H_{10}O_8{\cdot}2H_2O$
MW (g/mol)	406.35	421.21	479.03	431.64
Crystal System	Triclinic	Triclinic	Monoclinic	Triclinic
Space Group	$P\bar{1}$	$P\bar{1}$	$P21/c$	$P\bar{1}$
a (Å)	5.960(2)	5.799(2)	16.308(3)	7.629(2)
b (Å)	7.634(3)	7.477(3)	7.410(1)	7.843(2)
c (Å)	18.603(7)	18.493(7)	16.183(3)	15.045(5)
α (°)	90.145(6)	89.639(6)	90	91.409(6)
β (°)	95.804(6)	85.173(6)	106.064(4)	95.784(5)
γ (°)	97.105(6)	83.485(7)	90	115.160(5)
V (Å^3)	835.5(6)	793.8(5)	1879.2(7)	808.4(4)
Z	2	2	4	2
μ (mm^{-1})	0.433	0.891	1.104	1.578
ρ (g·cm^{-2})		1.762	1.693	1.773
Measurement Temp (K)	298	298	298	298
Radiation Source	Mo$K\alpha$	Mo$K\alpha$	Mo$K\alpha$	Mok_α
Radiation λ (Å)	0.71073	0.71073	0.71073	0.71073
Scan Mode	Omega	Omega	Omega	Omega
Absorption Correction	SADABS	SADABS	SADABS	SADABS
Solution Method	SHELX, $\lvert F\rvert^2$	SHELX, $\lvert F\rvert^2$	SHELX, $\lvert F\rvert^2$	SHELX, $\lvert F\rvert^2$
2θ Range (°)	2.97-29.36	2.21-25.68	1.30-26.02	2.73-26.02
data/parameters/restraints	3224/270/12	2965/274/12	3675/313/21	3124/269/12
R1/wR2 [I>2σ(I)]	5.00%/10.35%	8.06%/18.26%	6.22%/12.84%	6.63%/10.36%
R1/wR2 (all data)	8.75%/11.80%	13.59%/20.93%	11.31%/15.87%	16.81%/13.45%
Goodness of Fit	0.817	1.041	1.083	0.947
dimensionality	I^0O^2	I^0O^2	I^0O^0	I^0O^1
hydration	2 bound, 2 pore-space	2 bound, 2 pore-space	5-bound, 2 pore-space	2-bound, 2 pore-space

2.2 Powder X-ray diffraction

Data for CaAQDC, ZnAQDC, CdAQDC, MnAQDC, and NiAQDC were collected at the Advanced Photon Source synchrotron X-ray beamline 11-BM. The high flux and sharp wavelength distribution reveal impurity phases that would be otherwise invisible using a standard laboratory source X-ray diffractometer. Data for CaAQDC, MnAQDC and NiAQDC were collected using synchrotron radiation with a wavelength (λ) of 0.458 Å. Data for ZnAQDC were collected using 0.413 Å synchrotron radiation. Data for CdAQDC were collected on a Bruker D8 with CuKα. Figures 2, 3, 4, 4, 5, and 6, show Rietveld refinements of the structures determined by single crystal to the powder X-ray diffraction data. A summary of the refined crystal parameters and refinement statistics is shown in Table 3.

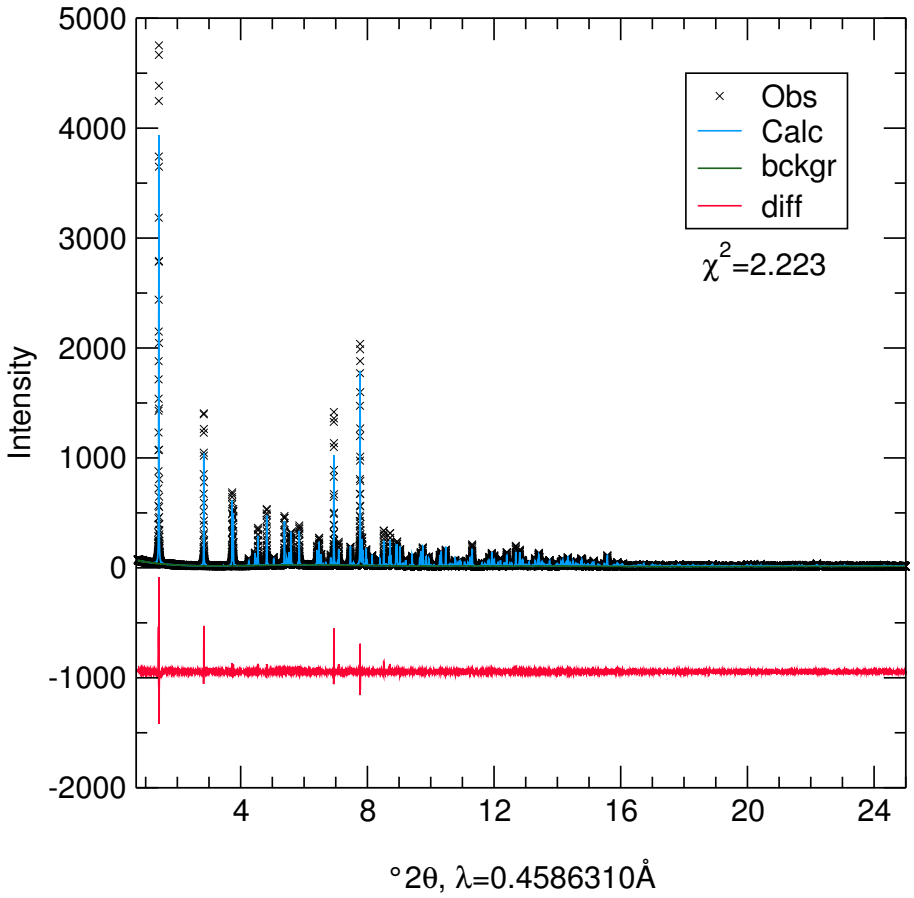

Figure 2 Synchrotron powder diffraction data for CaAQDC and Rietveld refinement of the model initially determined by single crystal experiment.

Table 3 Structure and refinement parameters from powder X-ray diffraction data

Compound	CaAQDC	ZnAQDC	CdAQDC	MnAQDC	NiAQDC
Formula	$CaC_{16}H_{14}O_{10}$	$ZnC_{16}H_{14}O_{10}$	$CdC_{16}H_{14}O_{10}$	$MnC_{16}H_{14}O_{10}$	$NiC_{16}H_{20}O_{13}$
Crystal System	triclinic	triclinic	triclinic	triclinic	monoclinic
Space Group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	$P2_1/c$
a (Å)	5.80099(6)	7.654318(10)	5.8644(7)	5.80099(6)	16.30970(15)
b (Å)	7.48853(6)	7.865764(12)	7.5272(6)	7.48853(6)	7.41339(5)
c (Å)	18.53285(17)	15.096604(20)	18.5553(13	18.53285(17)	16.19017(15))
α (°)	89.7232(11)	91.41250(10)	90.938(14)	89.7232(11)	90.0
β (°)	85.1458(9)	95.76910(10)	94.882(11)	85.1458(9)	106.1139(7)
γ (°)	83.5310(8)	115.10700(10)	95.868(12)	83.5310(8)	90.0
Volume (Å^3)	797.080(10)	816.5880(10)	811.57(11)	797.080(10)	1880.649(23)
Observations	49149	48501	1749	49199	48199
Variables	21	20	72	85	24
wRp	11.55%	9.87%	21.77%	10.75%	9.31%
Rp	9.73%	8.04%	22.73%	9.09%	8.03%
χ^2	2.223	1.607	43.93	1.403	1.468

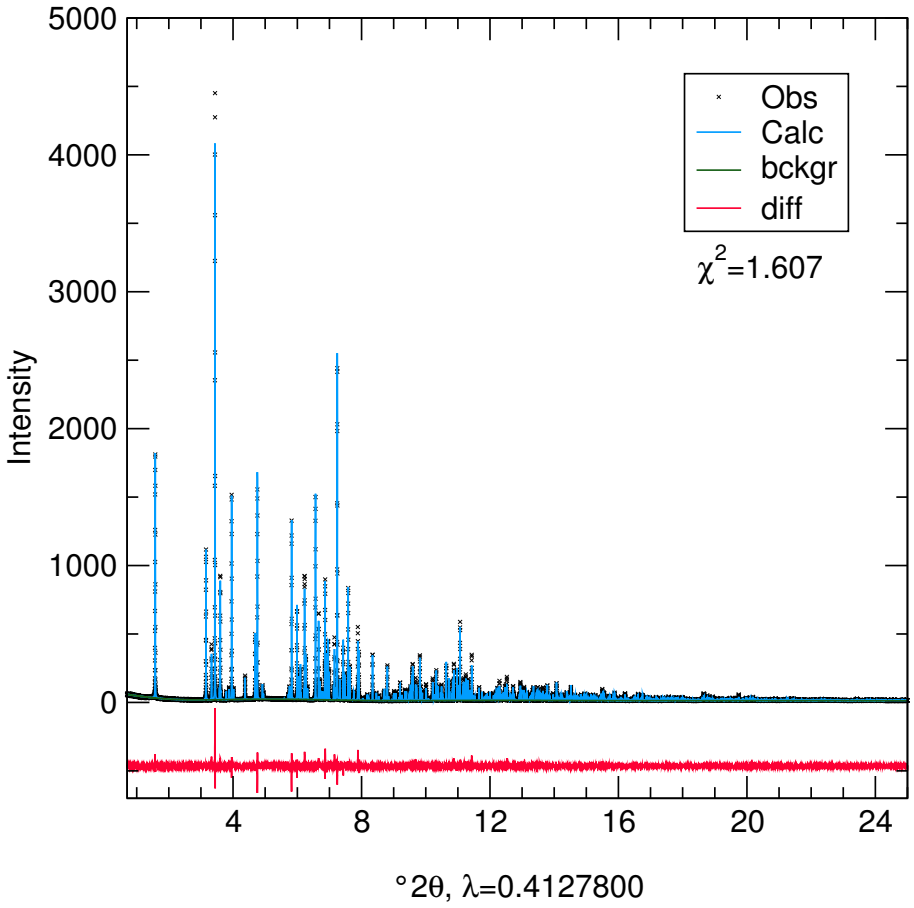

Figure 3 Synchrotron powder diffraction data for ZnAQDC and Rietveld refinement of the model initially determined by single crystal experiment.

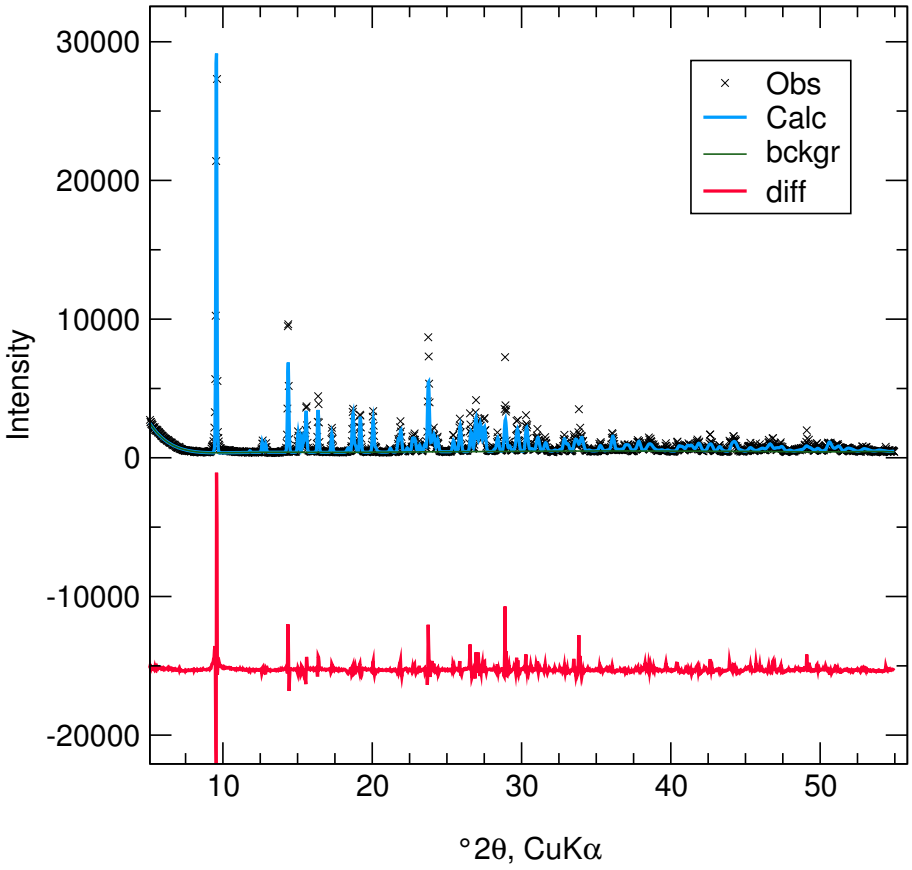

Figure 4 Powder diffraction data for CdAQDC and Rietveld refinement of the model initially determined by single crystal experiment.

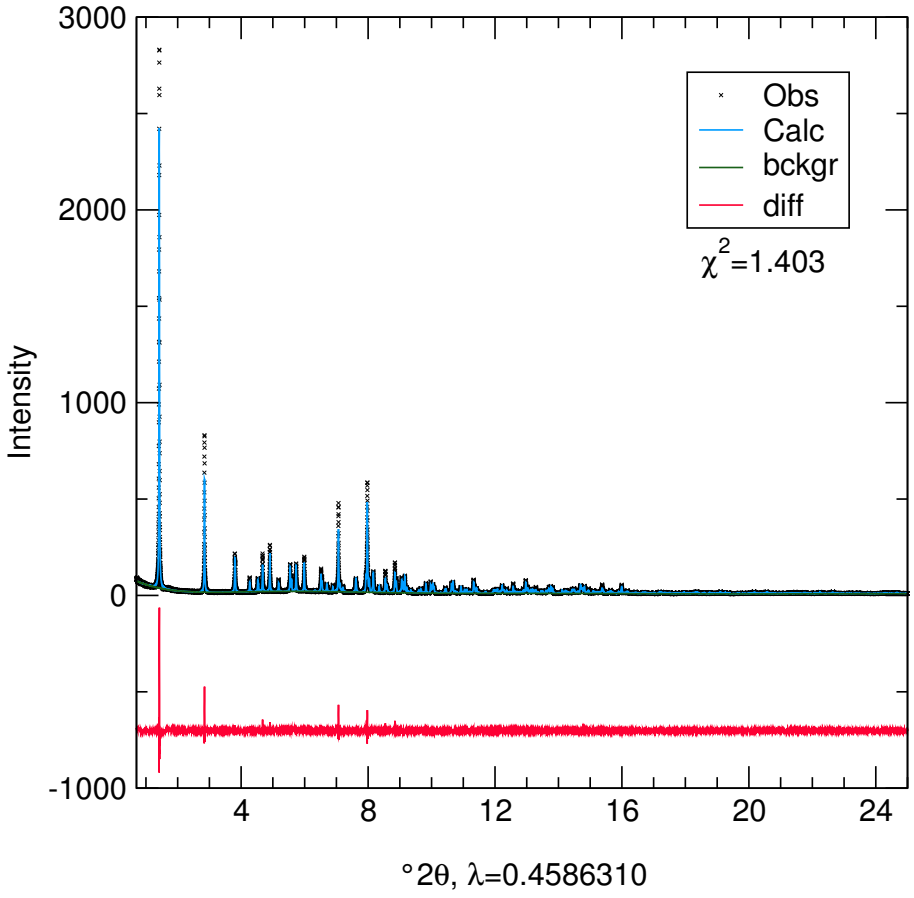

Figure 5 Synchrotron powder diffraction data for MnAQDC and Rietveld refinement of the model initially determined by single crystal experiment.

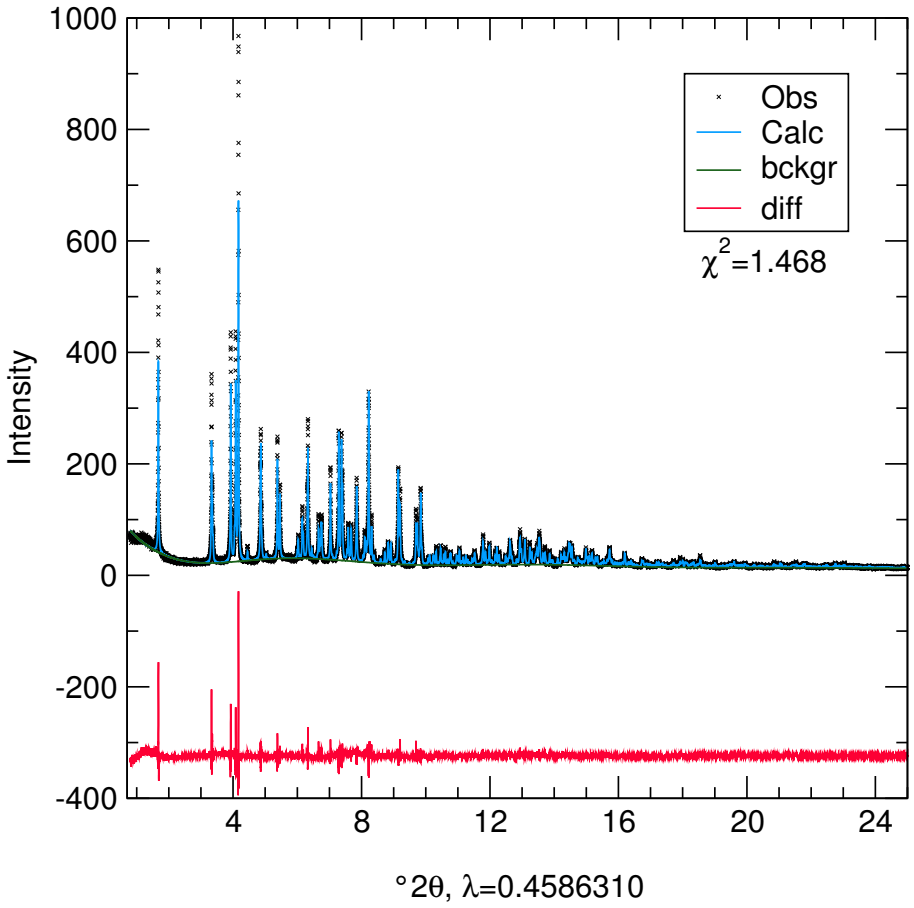

Figure 6 Synchrotron powder diffraction data for NiAQDC and Rietveld refinement of the model initially determined by single crystal experiment.

3 Crystallographic Tables

3.1 CaAQDC structure details

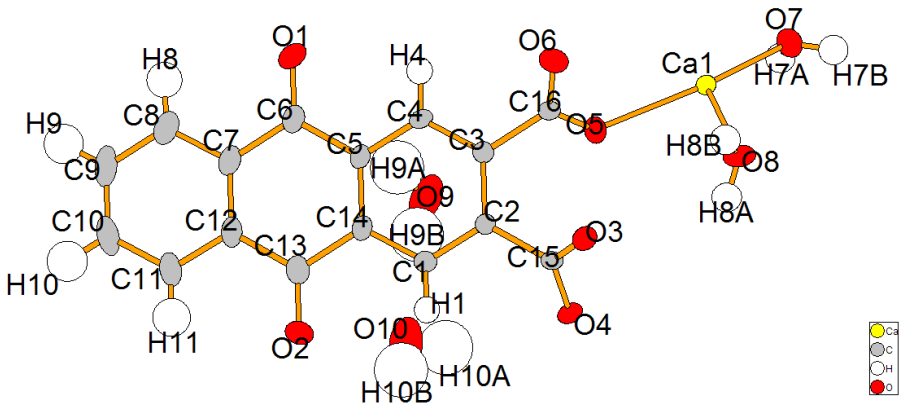

Figure 7 Asymmetric unit with atom numbers for CaAQDC.

Table 4 Crystal data and structure refinement for CaAQDC.

Parameter	Value
Empirical formula	$C_{16}H_{14}O_{10}Ca$
Formula weight	406.35 g·mol^{-1}
Collection Temperature	293(2) K
Wavelength	0.71073Å
Crystal system	Triclinic
Space Group	$P\bar{1}$
Unit cell dimensions	
a	5.81330(10)
b	7.4885(2)
c	18.6076(6)
α	90.4040(10)
β	95.523(2)
γ	95.088(2)
Volume	803.01(4)
Z	2
Calculated density	1.980 g/m^3
Absorption coefficient	1.419 mm^{-1}
F(000)	476
Crystal size	0.12×0.11×0.05 mm
Theta range for data collection	° to °
Limiting indices	$\leq h \leq$, $\leq k \leq$, $\leq l \leq$
Reflections collected / unique	/ [R(int) =]
Data Completeness	%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	and
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	/ /
Goodness-of-fit on F^2	0.
Final R indices [I>2sigma(I)]	R1 = 0.0, wR2 = 0.
R indices (all data)	R1 = 0.0, wR2 = 0.
Largest diff. peak and hole	0. and -0. e·Å^{-3}

Table 5 Crystal coordinates [Å] and equivalent isotropic displacement parameters [Å^2] for CaAQDC. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Ca(1)	0.01213(10)	0.26769(7)	1.04132(3)	0.01654(18)
C(1)	0.6884(5)	0.3306(4)	0.78485(17)	0.0226(7)
H(1)	0.8315	0.3957	0.7927	0.027
C(2)	0.5723(5)	0.2767(3)	0.84306(16)	0.0170(7)
C(3)	0.3530(5)	0.1825(4)	0.83117(17)	0.0180(7)
C(4)	0.2585(5)	0.1416(4)	0.76142(17)	0.0231(7)
H(4)	0.1142	0.0785	0.7536	0.028
C(5)	0.3768(5)	0.1938(4)	0.70275(17)	0.0240(7)
C(6)	0.2704(6)	0.1454(4)	0.62827(18)	0.0316(8)
C(7)	0.3997(6)	0.2041(4)	0.56716(18)	0.0315(8)
C(8)	0.3061(6)	0.1657(5)	0.49654(19)	0.0404(9)
H(8)	0.1591	0.1075	0.4879	0.049
C(9)	0.4297(7)	0.2134(5)	0.4390(2)	0.0505(11)
H(9)	0.3654	0.1874	0.3920	0.061
C(10)	0.6455(8)	0.2985(5)	0.4511(2)	0.0537(12)
H(10)	0.7287	0.3284	0.4123	0.064
C(11)	0.7407(7)	0.3403(5)	0.5206(2)	0.0463(10)
H(11)	0.8872	0.3997	0.5283	0.056
C(12)	0.6196(6)	0.2944(4)	0.57910(18)	0.0320(8)
C(13)	0.7244(6)	0.3457(5)	0.65262(19)	0.0350(9)
C(14)	0.5935(5)	0.2885(4)	0.71416(17)	0.0244(8)
C(15)	0.6889(5)	0.3018(4)	0.91869(17)	0.0168(7)
C(16)	0.2163(5)	0.1346(4)	0.89378(16)	0.0176(7)
O(1)	0.0841(4)	0.0587(4)	0.61889(14)	0.0555(8)
O(2)	0.9125(4)	0.4300(4)	0.66229(14)	0.0578(8)
O(3)	0.6881(3)	0.1670(2)	0.95728(11)	0.0231(5)
O(4)	0.7935(3)	0.4496(2)	0.93883(11)	0.0232(5)
O(5)	0.2042(3)	0.2595(3)	0.93706(11)	0.0261(5)
O(6)	0.1237(3)	-0.0191(3)	0.89812(12)	0.0290(6)
O(7)	-0.2439(4)	0.3960(3)	1.10960(14)	0.0285(6)
H(7A)	-0.251(5)	0.497(4)	1.0962(17)	0.034
H(7B)	-0.214(5)	0.385(4)	1.1575(19)	0.034
O(8)	0.3471(4)	0.1697(3)	1.09909(13)	0.0292(6)
H(8A)	0.472(6)	0.228(4)	1.0913(18)	0.035
H(8B)	0.350(6)	0.073(4)	1.0879(18)	0.035
O(9)	0.2223(7)	0.6670(5)	0.7472(2)	0.0962(16)
H(9A)	0.161(9)	0.582(7)	0.716(3)	0.115
H(9B)	0.348(9)	0.692(8)	0.744(3)	0.115
O(10)	0.6948(8)	0.8097(6)	0.7490(2)	0.0966(14)
H(10A)	0.690(10)	0.831(8)	0.790(3)	0.116
H(10B)	0.825(9)	0.765(8)	0.753(3)	0.116

Table 6 Anisotropic displacement parameters [Å^2] for CaAQDC. The anisotropic displacement factor exponent takes the form $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ca(1)	0.0188(3)	0.0138(3)	0.0161(4)	-0.0009(2)	0.0016(3)	-0.0014(2)
C(1)	0.0214(17)	0.0228(16)	0.022(2)	0.0011(14)	0.0020(15)	-0.0035(13)
C(2)	0.0194(16)	0.0149(14)	0.0163(18)	-0.0005(13)	0.0025(14)	-0.0004(12)
C(3)	0.0210(17)	0.0146(14)	0.0180(19)	-0.0006(13)	0.0032(14)	0.0001(12)
C(4)	0.0187(17)	0.0261(17)	0.022(2)	-0.0023(14)	-0.0020(15)	-0.0054(13)
C(5)	0.0258(18)	0.0289(17)	0.0158(19)	-0.0040(14)	0.0012(15)	-0.0016(14)
C(6)	0.037(2)	0.0362(19)	0.019(2)	-0.0021(16)	0.0017(17)	-0.0041(17)
C(7)	0.039(2)	0.0349(19)	0.019(2)	-0.0044(16)	0.0003(17)	0.0000(16)
C(8)	0.049(2)	0.047(2)	0.022(2)	-0.0017(18)	-0.0033(19)	-0.0008(18)
C(9)	0.074(3)	0.058(3)	0.018(2)	0.0016(19)	0.005(2)	0.003(2)
C(10)	0.074(3)	0.062(3)	0.024(2)	0.006(2)	0.020(2)	-0.006(2)
C(11)	0.054(3)	0.061(3)	0.021(2)	0.0003(19)	0.012(2)	-0.008(2)
C(12)	0.044(2)	0.0335(19)	0.017(2)	0.0007(15)	0.0055(17)	-0.0016(17)
C(13)	0.037(2)	0.044(2)	0.022(2)	0.0006(17)	0.0054(17)	-0.0042(18)
C(14)	0.0295(19)	0.0265(17)	0.0156(19)	-0.0011(14)	0.0017(15)	-0.0027(14)
C(15)	0.0114(16)	0.0189(16)	0.0199(19)	0.0000(14)	0.0013(13)	0.0014(12)
C(16)	0.0116(15)	0.0232(16)	0.0170(18)	0.0059(14)	-0.0032(13)	0.0014(13)
O(1)	0.0434(17)	0.084(2)	0.0285(17)	-0.0115(14)	-0.0019(13)	-0.0285(16)
O(2)	0.0439(17)	0.086(2)	0.0336(18)	-0.0059(15)	0.0104(14)	-0.0361(15)
O(3)	0.0278(12)	0.0184(11)	0.0212(13)	0.0041(10)	-0.0024(10)	-0.0009(9)
O(4)	0.0251(12)	0.0179(11)	0.0237(14)	-0.0039(9)	-0.0013(10)	-0.0057(9)
O(5)	0.0305(13)	0.0268(12)	0.0214(14)	-0.0045(10)	0.0079(10)	0.0014(10)
O(6)	0.0313(13)	0.0207(12)	0.0332(15)	0.0072(10)	0.0042(11)	-0.0054(10)
O(7)	0.0368(14)	0.0213(12)	0.0284(15)	0.0012(12)	0.0095(12)	0.0022(11)
O(8)	0.0237(13)	0.0200(12)	0.0416(17)	-0.0012(11)	-0.0010(12)	-0.0026(10)
O(9)	0.150(4)	0.081(3)	0.041(2)	-0.0071(18)	-0.004(3)	-0.041(3)
O(10)	0.128(4)	0.113(3)	0.045(2)	-0.001(2)	0.010(3)	0.000(3)

Table 7 Symmetry operations used in the following tables for CaAQDC.

	Operation
#1	'x,y,z'
#2	'-x,-y,-z'

Table 8 Bond Lengths [Å] for CaAQDC.

	Angle	Symm. op. atom 1	Symm. op. atom 3
Ca(1)-O(4)	2.329(2)	2	
Ca(1)-O(5)	2.354(2)		
Ca(1)-O(8)	2.374(2)		
Ca(1)-O(7)	2.378(2)		
Ca(1)-O(3)	2.405(2)	1	
Ca(1)-O(4)	2.687(2)	1	
Ca(1)-C(15)	2.867(3)	1	
Ca(1)-Ca(1)	3.8826(17)	2	
Ca(1)-Ca(1)	4.3434(19)	2	
Ca(1)-H(7A)	2.75(3)		
Ca(1)-H(8B)	2.72(3)		
C(1)-C(2)	1.380(4)		
C(1)-C(14)	1.398(4)		
C(1)-H(1)	0.9300		
C(2)-C(3)	1.408(4)		
C(2)-C(15)	1.506(4)		
C(3)-C(4)	1.380(4)		
C(3)-C(16)	1.508(4)		
C(4)-C(5)	1.391(4)		
C(4)-H(4)	0.9300		
C(5)-C(14)	1.396(4)		
C(5)-C(6)	1.490(4)		
C(6)-O(1)	1.217(4)		
C(6)-C(7)	1.477(5)		
C(7)-C(8)	1.390(5)		
C(7)-C(12)	1.399(5)		
C(8)-C(9)	1.384(5)		
C(8)-H(8)	0.9300		
C(9)-C(10)	1.364(5)		
C(9)-H(9)	0.9300		
C(10)-C(11)	1.377(5)		
C(10)-H(10)	0.9300		
C(11)-C(12)	1.388(5)		
C(11)-H(11)	0.9300		
C(12)-C(13)	1.476(5)		
C(13)-O(2)	1.218(4)		
C(13)-C(14)	1.486(4)		
C(15)-O(3)	1.256(3)		
C(15)-O(4)	1.257(3)		
C(15)-Ca(1)	2.867(3)	1	
C(16)-O(6)	1.240(3)		
C(16)-O(5)	1.260(3)		
O(3)-Ca(1)	2.405(2)	1	
O(4)-Ca(1)	2.329(2)	2	
O(4)-Ca(1)	2.687(2)	1	
O(6)-Ca(1)	2.311(2)	2	
O(7)-H(7A)	0.82(3)		
O(7)-H(7B)	0.90(3)		
O(8)-H(8A)	0.84(3)		
O(8)-H(8B)	0.77(3)		
O(9)-H(9A)	0.88(5)		
O(9)-H(9B)	0.76(5)		
O(10)-H(10A)	0.78(5)		
O(10)-H(10B)	0.88(5)		

Table 9 Bond Angles [°] for CaAQDC.

	Angle	Symm. op. atom 1	Symm. op. atom 3
O(4)-Ca(1)-O(8)	85.18(8)	2	
O(5)-Ca(1)-O(8)	83.50(8)		
O(6)-Ca(1)-O(7)	81.33(8)	2	
O(4)-Ca(1)-O(7)	79.80(8)	2	
O(5)-Ca(1)-O(7)	150.30(8)		
O(8)-Ca(1)-O(7)	120.75(9)		
O(6)-Ca(1)-O(3)	81.54(8)	2	1
O(4)-Ca(1)-O(3)	129.78(7)	2	1
O(5)-Ca(1)-O(3)	82.27(8)		1
O(8)-Ca(1)-O(3)	140.81(8)		1
O(7)-Ca(1)-O(3)	86.89(8)		1
O(6)-Ca(1)-O(4)	129.09(8)	2	1
O(4)-Ca(1)-O(4)	78.82(8)	2	1
O(5)-Ca(1)-O(4)	72.68(7)		1
O(8)-Ca(1)-O(4)	151.99(8)		1
O(7)-Ca(1)-O(4)	78.99(8)		1
O(3)-Ca(1)-O(4)	51.06(6)	1	1
O(6)-Ca(1)-C(15)	106.75(8)	2	1
O(4)-Ca(1)-C(15)	104.60(8)	2	1
O(5)-Ca(1)-C(15)	72.43(8)		1
O(8)-Ca(1)-C(15)	153.06(8)		1
O(7)-Ca(1)-C(15)	85.96(9)		1
O(3)-Ca(1)-C(15)	25.70(7)	1	1
O(4)-Ca(1)-C(15)	25.89(7)	1	1
O(6)-Ca(1)-Ca(1)	155.29(6)	2	2
O(4)-Ca(1)-Ca(1)	42.77(5)	2	2
O(5)-Ca(1)-Ca(1)	75.70(5)		2
O(8)-Ca(1)-Ca(1)	124.10(6)		2
O(7)-Ca(1)-Ca(1)	76.21(6)		2
O(3)-Ca(1)-Ca(1)	87.07(5)	1	2
O(4)-Ca(1)-Ca(1)	36.05(4)	1	2
C(15)-Ca(1)-Ca(1)	61.87(6)	1	2
O(6)-Ca(1)-Ca(1)	56.14(6)	2	2
O(4)-Ca(1)-Ca(1)	149.67(6)	2	2
O(5)-Ca(1)-Ca(1)	68.31(5)		2
O(8)-Ca(1)-Ca(1)	76.29(6)		2
O(7)-Ca(1)-Ca(1)	130.36(6)		2
O(3)-Ca(1)-Ca(1)	64.52(5)	1	2
O(4)-Ca(1)-Ca(1)	107.12(5)	1	2
C(15)-Ca(1)-Ca(1)	83.56(6)	1	2
Ca(1)-Ca(1)-Ca(1)	136.18(4)	2	2
O(6)-Ca(1)-H(7A)	97.6(7)	2	
O(4)-Ca(1)-H(7A)	67.6(7)	2	
O(5)-Ca(1)-H(7A)	134.8(7)		
O(8)-Ca(1)-H(7A)	127.3(7)		
O(7)-Ca(1)-H(7A)	16.4(6)		
O(3)-Ca(1)-H(7A)	87.3(7)	1	
O(4)-Ca(1)-H(7A)	66.7(7)	1	
C(15)-Ca(1)-H(7A)	79.3(7)	1	
Ca(1)-Ca(1)-H(7A)	59.9(7)	2	
Ca(1)-Ca(1)-H(7A)	142.5(7)	2	
O(6)-Ca(1)-H(8B)	68.2(7)	2	
O(4)-Ca(1)-H(8B)	99.6(7)	2	
O(5)-Ca(1)-H(8B)	78.9(7)		
O(8)-Ca(1)-H(8B)	15.5(7)		
O(7)-Ca(1)-H(8B)	129.0(7)		
O(3)-Ca(1)-H(8B)	125.3(7)	1	
O(4)-Ca(1)-H(8B)	151.6(7)	1	
C(15)-Ca(1)-H(8B)	140.7(7)	1	
Ca(1)-Ca(1)-H(8B)	135.1(7)	2	

Table 10 Continued: Bond Angles [°] for CaAQDC.

	Angle	Symm. op. atom 1	Symm. op. atom 3
Ca(1)-Ca(1)-H(8B)	60.8(7)	2	
H(7A)-Ca(1)-H(8B)	139.2(10)		
C(2)-C(1)-C(14)	120.8(3)		
C(2)-C(1)-H(1)	119.6		
C(14)-C(1)-H(1)	119.6		
C(1)-C(2)-C(3)	119.7(3)		
C(1)-C(2)-C(15)	120.0(3)		
C(3)-C(2)-C(15)	120.0(3)		
C(4)-C(3)-C(2)	119.6(3)		
C(4)-C(3)-C(16)	119.9(3)		
C(2)-C(3)-C(16)	120.5(3)		
C(3)-C(4)-C(5)	120.7(3)		
C(3)-C(4)-H(4)	119.6		
C(5)-C(4)-H(4)	119.6		
C(4)-C(5)-C(14)	119.9(3)		
C(4)-C(5)-C(6)	119.2(3)		
C(14)-C(5)-C(6)	120.9(3)		
O(1)-C(6)-C(7)	121.7(3)		
O(1)-C(6)-C(5)	120.5(3)		
C(7)-C(6)-C(5)	117.8(3)		
C(8)-C(7)-C(12)	118.9(3)		
C(8)-C(7)-C(6)	120.1(3)		
C(12)-C(7)-C(6)	121.0(3)		
C(9)-C(8)-C(7)	120.5(4)		
C(9)-C(8)-H(8)	119.7		
C(7)-C(8)-H(8)	119.7		
C(10)-C(9)-C(8)	120.2(4)		
C(10)-C(9)-H(9)	119.9		
C(8)-C(9)-H(9)	119.9		
C(9)-C(10)-C(11)	120.3(4)		
C(9)-C(10)-H(10)	119.8		
C(11)-C(10)-H(10)	119.8		
C(10)-C(11)-C(12)	120.5(4)		
C(10)-C(11)-H(11)	119.8		
C(12)-C(11)-H(11)	119.8		
C(11)-C(12)-C(7)	119.5(3)		
C(11)-C(12)-C(13)	119.0(3)		
C(7)-C(12)-C(13)	121.5(3)		
O(2)-C(13)-C(12)	121.0(3)		
O(2)-C(13)-C(14)	121.4(3)		
C(12)-C(13)-C(14)	117.6(3)		
C(5)-C(14)-C(1)	119.2(3)		
C(5)-C(14)-C(13)	121.2(3)		
C(1)-C(14)-C(13)	119.5(3)		
O(3)-C(15)-O(4)	123.1(3)		
O(3)-C(15)-C(2)	116.7(2)		
O(4)-C(15)-C(2)	120.0(3)		
O(3)-C(15)-Ca(1)	56.10(15)		1
O(4)-C(15)-Ca(1)	69.02(16)		1
C(2)-C(15)-Ca(1)	159.36(18)		1
O(6)-C(16)-O(5)	125.7(3)		
O(6)-C(16)-C(3)	118.9(3)		
O(5)-C(16)-C(3)	115.4(3)		
C(15)-O(3)-Ca(1)	98.20(17)		1
C(15)-O(4)-Ca(1)	171.8(2)		2
C(15)-O(4)-Ca(1)	85.09(17)		1
Ca(1)-O(4)-Ca(1)	101.18(8)	2	1
C(16)-O(5)-Ca(1)	130.90(19)		
C(16)-O(6)-Ca(1)	154.7(2)		2
Ca(1)-O(7)-H(7A)	108(2)		

Table 11 Continued: Bond Angles [°] for CaAQDC.

	Angle	Symm. op. atom 1	Symm. op. atom 3
Ca(1)-O(7)-H(7B)	113(2)		
H(7A)-O(7)-H(7B)	115(3)		
Ca(1)-O(8)-H(8A)	117(2)		
Ca(1)-O(8)-H(8B)	109(3)		
H(8A)-O(8)-H(8B)	108(3)		
H(9A)-O(9)-H(9B)	112(6)		
H(10A)-O(10)-H(10B)	97(6)		

3.2 ZnAQDC structure details

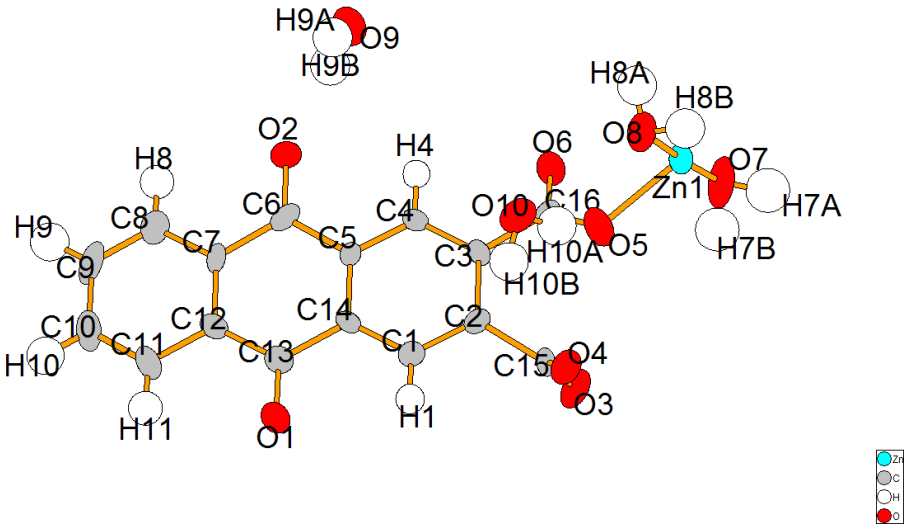

Figure 8 Asymmetric unit with atom numbers for ZnAQDC.

Table 12 Crystal data and structure refinement for ZnAQDC.

Parameter	Value
Empirical formula	$C_{16}H_{14}O_{10}Zn$
Formula weight	431.64 g·mol^{-1}
Collection Temperature	298(2) K
Wavelength	0.71073Å
Crystal system	Triclinic
Space Group	$P\bar{1}$
Unit cell dimensions	
a	7.629(2)Å
b	7.843(2)Å
c	15.045(5)Å
α	91.409(6)°
β	95.784(5)°
γ	115.160(5)°
Volume	808.4(4)Å^3
Z	2
Calculated density	1.773 g/m^3
Absorption coefficient	1.578 mm^{-1}
F(000)	440
Crystal size	0.5×0.3×0.2 mm
Theta range for data collection	2.73° to 26.02°
Limiting indices	$-9 \leq h \leq 9$, $-9 \leq k \leq 9$, $-18 \leq l \leq 17$
Reflections collected / unique	6709 / 3124 [R(int) = 0.0977]
Data Completeness	97.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.969 and 0.572
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3124 / 12 / 269
Goodness-of-fit on F^2	0.947
Final R indices [I>2sigma(I)]	R1 = 0.0663, wR2 = 0.1036
R indices (all data)	R1 = 0.1681, wR2 = 0.1345
Largest diff. peak and hole	0.532 and -0.490 e·Å^{-3}

Table 13 Crystal coordinates [Å] and equivalent isotropic displacement parameters [Å^2] for ZnAQDC. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Zn(1)	1.00224(13)	0.71567(12)	0.43583(6)	0.0321(3)
C(1)	0.9008(9)	0.8656(9)	0.8297(4)	0.0265(16)
H(1)	0.9023	0.9774	0.8528	0.032
C(2)	0.9614(9)	0.8605(8)	0.7463(4)	0.0231(15)
C(3)	0.9515(9)	0.6901(9)	0.7100(4)	0.0213(15)
C(4)	0.8839(9)	0.5326(8)	0.7589(4)	0.0237(16)
H(4)	0.8754	0.4186	0.7348	0.028
C(5)	0.8286(9)	0.5414(8)	0.8433(4)	0.0215(15)
C(6)	0.7657(9)	0.3700(9)	0.8928(5)	0.0278(17)
C(7)	0.7333(9)	0.3876(9)	0.9880(4)	0.0247(16)
C(8)	0.6905(9)	0.2335(10)	1.0390(5)	0.0341(18)
H(8)	0.6864	0.1217	1.0144	0.041
C(9)	0.6546(10)	0.2457(11)	1.1248(5)	0.046(2)
H(9)	0.6227	0.1414	1.1588	0.055
C(10)	0.6657(10)	0.4132(11)	1.1617(5)	0.043(2)
H(10)	0.6451	0.4215	1.2212	0.051
C(11)	0.7061(10)	0.5670(10)	1.1129(4)	0.0349(18)
H(11)	0.7094	0.6777	1.1385	0.042
C(12)	0.7425(9)	0.5566(9)	1.0243(4)	0.0257(16)
C(13)	0.7850(9)	0.7212(9)	0.9703(4)	0.0270(17)
C(14)	0.8382(9)	0.7101(9)	0.8794(4)	0.0227(15)
C(15)	1.0529(11)	1.0406(9)	0.6994(4)	0.0250(16)
C(16)	1.0076(9)	0.6701(9)	0.6195(4)	0.0277(17)
O(1)	0.7815(7)	0.8645(6)	1.0010(3)	0.0408(13)
O(2)	0.7409(7)	0.2174(6)	0.8583(3)	0.0422(13)
O(3)	1.2329(7)	1.1150(6)	0.7064(3)	0.0396(13)
O(4)	0.9402(6)	1.1011(6)	0.6594(3)	0.0331(12)
O(5)	0.9934(8)	0.7791(7)	0.5631(3)	0.0486(14)
O(6)	1.0715(7)	0.5510(6)	0.6052(3)	0.0426(13)
O(7)	1.2913(8)	0.7768(8)	0.4467(4)	0.0586(16)
H(7A)	1.368(9)	0.845(8)	0.408(3)	0.070
H(7B)	1.331(11)	0.884(6)	0.480(4)	0.070
O(8)	0.7033(8)	0.6485(7)	0.4203(3)	0.0468(14)
H(8A)	0.628(9)	0.538(4)	0.392(4)	0.056
H(8B)	0.706(10)	0.698(7)	0.368(2)	0.056
O(9)	0.5294(8)	0.0157(7)	0.6885(3)	0.0468(14)
H(9A)	0.429(6)	0.040(9)	0.697(4)	0.056
H(9B)	0.587(8)	0.079(9)	0.739(3)	0.056
O(10)	0.5388(7)	0.7237(6)	0.5788(4)	0.0462(14)
H(10A)	0.649(6)	0.782(8)	0.556(4)	0.055
H(10B)	0.579(9)	0.822(6)	0.618(3)	0.055

Table 14 Anisotropic displacement parameters [Å^2] for ZnAQDC. The anisotropic displacement factor exponent takes the form $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	0.0492(6)	0.0271(5)	0.0274(5)	0.0090(4)	0.0155(4)	0.0207(4)
C(1)	0.031(4)	0.022(4)	0.027(4)	0.002(3)	0.002(3)	0.011(3)
C(2)	0.020(4)	0.019(4)	0.026(4)	0.004(3)	-0.002(3)	0.006(3)
C(3)	0.035(4)	0.025(4)	0.013(4)	0.006(3)	0.002(3)	0.022(3)
C(4)	0.028(4)	0.022(4)	0.022(4)	-0.004(3)	0.003(3)	0.011(3)
C(5)	0.019(4)	0.021(4)	0.019(4)	0.003(3)	0.003(3)	0.002(3)
C(6)	0.020(4)	0.018(4)	0.043(5)	0.006(4)	0.005(3)	0.006(3)
C(7)	0.022(4)	0.027(4)	0.025(4)	0.011(3)	0.012(3)	0.008(3)
C(8)	0.032(4)	0.036(5)	0.033(5)	0.010(4)	0.001(4)	0.014(4)
C(9)	0.046(5)	0.045(6)	0.045(5)	0.034(4)	0.010(4)	0.015(4)
C(10)	0.036(5)	0.060(6)	0.024(4)	0.015(4)	0.003(4)	0.012(4)
C(11)	0.045(5)	0.045(5)	0.020(4)	0.004(4)	0.008(4)	0.022(4)
C(12)	0.022(4)	0.030(4)	0.024(4)	-0.005(3)	0.003(3)	0.010(3)
C(13)	0.030(4)	0.029(4)	0.026(4)	0.001(3)	0.001(3)	0.017(4)
C(14)	0.027(4)	0.023(4)	0.018(4)	-0.004(3)	0.003(3)	0.011(3)
C(15)	0.037(5)	0.026(4)	0.019(4)	0.009(3)	0.013(4)	0.018(4)
C(16)	0.026(4)	0.019(4)	0.032(4)	0.004(3)	0.009(3)	0.003(3)
O(1)	0.062(4)	0.035(3)	0.033(3)	0.003(2)	0.017(3)	0.025(3)
O(2)	0.067(4)	0.023(3)	0.036(3)	0.002(2)	0.012(3)	0.018(3)
O(3)	0.025(3)	0.038(3)	0.055(4)	0.019(3)	0.013(3)	0.010(3)
O(4)	0.034(3)	0.031(3)	0.046(3)	0.014(2)	0.011(2)	0.023(3)
O(5)	0.091(4)	0.052(3)	0.032(3)	0.015(2)	0.023(3)	0.054(3)
O(6)	0.059(4)	0.038(3)	0.042(3)	0.006(2)	0.028(3)	0.027(3)
O(7)	0.046(4)	0.077(4)	0.052(4)	0.039(3)	0.018(3)	0.022(3)
O(8)	0.050(4)	0.047(3)	0.049(4)	0.017(3)	0.022(3)	0.021(3)
O(9)	0.044(3)	0.059(4)	0.043(3)	0.003(3)	0.014(3)	0.026(3)
O(10)	0.037(3)	0.037(3)	0.057(4)	0.004(3)	0.007(3)	0.009(3)

Table 15 Symmetry operations used in the following tables for ZnAQDC.

	Operation
#1	'x,y,z'
#2	'-x,-y,-z'

Table 16 Bond Lengths [Å] for ZnAQDC.

	Angle	Symm. op. atom 1	Symm. op. atom 3
Zn(1)-O(6)	1.984(5)	2	
Zn(1)-O(4)	2.000(4)	2	
Zn(1)-O(7)	2.036(6)		
Zn(1)-O(8)	2.097(5)		
C(1)-C(14)	1.377(8)		
C(1)-C(2)	1.385(8)		
C(1)-H(1)	0.9300		
C(2)-C(3)	1.400(8)		
C(2)-C(15)	1.514(8)		
C(3)-C(4)	1.383(8)		
C(3)-C(16)	1.492(8)		
C(4)-C(5)	1.387(8)		
C(4)-H(4)	0.9300		
C(5)-C(14)	1.387(8)		
C(5)-C(6)	1.471(8)		
C(6)-O(2)	1.222(7)		
C(6)-C(7)	1.491(8)		
C(7)-C(8)	1.384(8)		
C(7)-C(12)	1.392(8)		
C(8)-C(9)	1.357(9)		
C(8)-H(8)	0.9300		
C(9)-C(10)	1.378(10)		
C(9)-H(9)	0.9300		
C(10)-C(11)	1.364(9)		
C(10)-H(10)	0.9300		
C(11)-C(12)	1.396(8)		
C(11)-H(11)	0.9300		
C(12)-C(13)	1.476(8)		
C(13)-O(1)	1.217(7)		
C(13)-C(14)	1.477(8)		
C(15)-O(3)	1.234(7)		
C(15)-O(4)	1.258(7)		
C(16)-O(6)	1.247(7)		
C(16)-O(5)	1.248(7)		
O(4)-Zn(1)	2.000(4)	2	
O(6)-Zn(1)	1.984(5)	2	
O(7)-H(7A)	0.89(2)		
O(7)-H(7B)	0.88(2)		
O(8)-H(8A)	0.88(2)		
O(8)-H(8B)	0.89(2)		
O(9)-H(9A)	0.88(2)		
O(9)-H(9B)	0.87(2)		
O(10)-H(10A)	0.88(2)		
O(10)-H(10B)	0.88(2)		

Table 17 Bond Angles [°] for ZnAQDC.

	Angle	Symm. op. atom 1	Symm. op. atom 3
O(6)-Zn(1)-O(7)	91.5(2)	2	
O(4)-Zn(1)-O(7)	85.67(19)	2	
O(5)-Zn(1)-O(8)	84.8(2)		
O(6)-Zn(1)-O(8)	87.24(19)	2	
O(4)-Zn(1)-O(8)	93.55(18)	2	
O(7)-Zn(1)-O(8)	178.1(2)		
C(14)-C(1)-C(2)	122.0(6)		
C(14)-C(1)-H(1)	119.0		
C(2)-C(1)-H(1)	119.0		
C(1)-C(2)-C(3)	119.0(6)		
C(1)-C(2)-C(15)	120.1(5)		
C(3)-C(2)-C(15)	120.7(6)		
C(4)-C(3)-C(2)	119.1(6)		
C(4)-C(3)-C(16)	118.3(5)		
C(2)-C(3)-C(16)	122.6(6)		
C(3)-C(4)-C(5)	121.2(6)		
C(3)-C(4)-H(4)	119.4		
C(5)-C(4)-H(4)	119.4		
C(4)-C(5)-C(14)	119.8(6)		
C(4)-C(5)-C(6)	118.1(6)		
C(14)-C(5)-C(6)	122.1(6)		
O(2)-C(6)-C(5)	122.1(6)		
O(2)-C(6)-C(7)	120.3(6)		
C(5)-C(6)-C(7)	117.6(5)		
C(8)-C(7)-C(12)	120.7(6)		
C(8)-C(7)-C(6)	119.3(6)		
C(12)-C(7)-C(6)	120.0(6)		
C(9)-C(8)-C(7)	120.0(7)		
C(9)-C(8)-H(8)	120.0		
C(7)-C(8)-H(8)	120.0		
C(8)-C(9)-C(10)	119.8(7)		
C(8)-C(9)-H(9)	120.1		
C(10)-C(9)-H(9)	120.1		
C(11)-C(10)-C(9)	121.6(7)		
C(11)-C(10)-H(10)	119.2		
C(9)-C(10)-H(10)	119.2		
C(10)-C(11)-C(12)	119.4(7)		
C(10)-C(11)-H(11)	120.3		
C(12)-C(11)-H(11)	120.3		
C(7)-C(12)-C(11)	118.6(6)		
C(7)-C(12)-C(13)	121.2(6)		
C(11)-C(12)-C(13)	120.1(6)		
O(1)-C(13)-C(12)	120.7(6)		
O(1)-C(13)-C(14)	120.8(6)		
C(12)-C(13)-C(14)	118.5(5)		
C(1)-C(14)-C(5)	118.9(6)		
C(1)-C(14)-C(13)	121.2(5)		
C(5)-C(14)-C(13)	119.8(6)		
O(3)-C(15)-O(4)	126.8(6)		
O(3)-C(15)-C(2)	115.6(6)		
O(4)-C(15)-C(2)	117.5(6)		
O(6)-C(16)-O(5)	123.8(6)		
O(6)-C(16)-C(3)	118.7(6)		
O(5)-C(16)-C(3)	117.5(6)		
C(15)-O(4)-Zn(1)	127.8(4)		2
C(16)-O(5)-Zn(1)	117.9(4)		
C(16)-O(6)-Zn(1)	144.5(5)		2
Zn(1)-O(7)-H(7A)	122(5)		
Zn(1)-O(7)-H(7B)	96(5)		
H(7A)-O(7)-H(7B)	86(2)		

Table 18 Continued: Bond Angles [°] for for ZnAQDC.

	Angle	Symm. op. atom 1	Symm. op. atom 3
Zn(1)-O(8)-H(8A)	115(5)		
Zn(1)-O(8)-H(8B)	94(5)		
H(8A)-O(8)-H(8B)	88(2)		
H(9A)-O(9)-H(9B)	88(2)		
H(10A)-O(10)-H(10B)	87(2)		

3.3 CdAQDC structure details

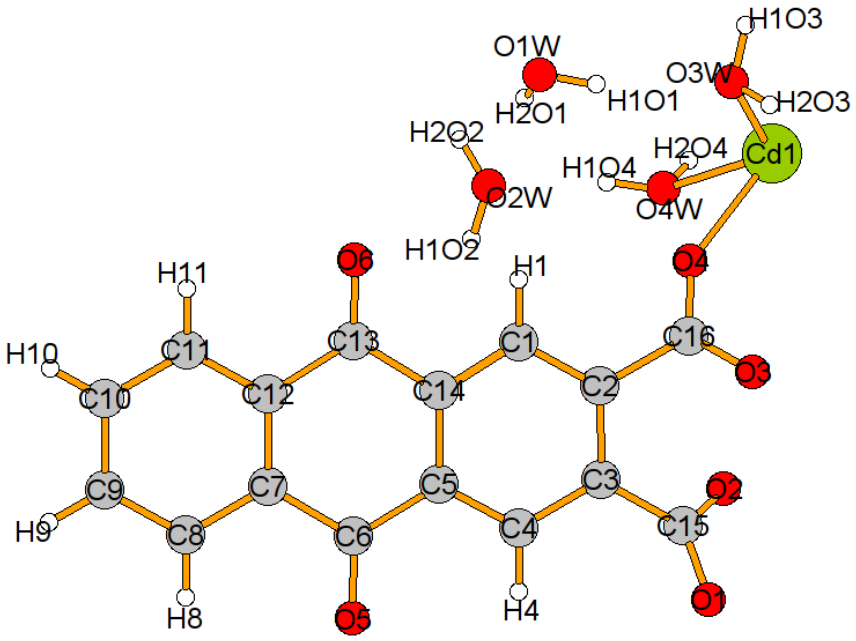

Figure 9 Asymmetric unit with atom numbers for CdAQDC.

Table 19 Crystal data and structure refinement for CdAQDC at 120 K.

Parameter	Value
Empirical formula	$C_{16}H_{14}O_{10}Cd$
Formula weight	478.67 g·mol^{-1}
Collection Temperature	298(2)
Wavelength	0.71073Å
Crystal system	Triclinic
Space Group	$P\bar{1}$
Unit cell dimensions	
a	5.8534(17)
b	7.504(2)
c	18.599(5)
α	91.10(2)
β	95.03(2)
γ	95.97(2)
Volume	809.1(4)
Z	2
Calculated density	1.965 g/m^3
Absorption coefficient	1.408 mm^{-1}
F(000)	476
Crystal size	0.5×0.3×0.2 mm
Theta range for data collection	2.97° to 26.53°
Limiting indices	$-7 \leq h \leq 7, -9 \leq k \leq 9, -20 \leq l \leq 23$
Reflections collected / unique	4197 / 3124 [R(int) = 0.0977]
Data Completeness	97.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.969 and 0.572
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4197 / 8 / 268
Goodness-of-fit on F^2	1.093
Final R indices [I>2sigma(I)]	R1 = 0.0500, wR2 = 0.1302
R indices (all data)	R1 = 0.0775, wR2 = 0.1659
Largest diff. peak and hole	0.64 and -0.37 e·Å^{-3}

Table 20 Crystal coordinates for CdAQDC [Å] and equivalent isotropic displacement parameters [Å^2]. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Cd(01)	0.99053(19)	-0.25420(12)	0.96143(3)	0.01586(18)
C(1)	1.7450(19)	-0.1492(13)	1.2392(5)	0.021(2)
C(2)	1.642(2)	-0.1890(14)	1.1690(5)	0.016(2)
C(3)	1.4224(19)	-0.2841(13)	1.1579(6)	0.015(2)
C(4)	1.308(2)	-0.3366(12)	1.2164(5)	0.022(2)
C(5)	1.4053(19)	-0.2937(13)	1.2865(5)	0.022(2)
C(6)	1.2777(19)	-0.3489(14)	1.3491(6)	0.025(2)
C(7)	1.3809(19)	-0.3006(15)	1.4221(5)	0.028(3)
C(8)	1.261(2)	-0.3407(16)	1.4811(7)	0.044(3)
C(9)	1.350(3)	-0.2960(18)	1.5500(5)	0.041(3)
C(10)	1.576(3)	-0.2115(18)	1.5613(7)	0.046(3)
C(11)	1.699(2)	-0.1663(15)	1.5044(5)	0.036(3)
C(12)	1.607(2)	-0.2052(16)	1.4337(5)	0.030(2)
C(13)	1.7355(19)	-0.1462(14)	1.3717(6)	0.027(2)
C(14)	1.6241(18)	-0.1980(13)	1.2969(5)	0.025(2)
C(15)	1.7791(18)	-0.1422(12)	1.1054(6)	0.017(2)
C(16)	1.3046(18)	-0.3126(15)	1.0832(6)	0.021(2)
O(1)	1.2113(13)	-0.4655(9)	1.0641(4)	0.0243(16)
O(2)	1.2934(13)	-0.1787(10)	1.0457(4)	0.0191(14)
O(3)	1.7889(14)	-0.2673(10)	1.0593(4)	0.0267(19)
O(4)	1.8691(13)	0.0153(9)	1.1005(4)	0.0286(18)
O(5)	1.0931(15)	-0.4391(11)	1.3408(4)	0.044(2)
O(6)	1.9180(16)	-0.0616(12)	1.3799(4)	0.047(2)
H(1)	1.8966	-0.0892	1.2467	0.025
H(4)	1.1605	-0.4033	1.2091	0.027
H(8)	1.1100	-0.4019	1.4736	0.052
H(9)	1.2609	-0.3213	1.5896	0.049
H(11)	1.8512	-0.1072	1.5131	0.044
H(10)	1.6443	-0.1857	1.6091	0.055
O(1W)	1.2476(16)	-0.3863(10)	0.8968(5)	0.0270(19)
H(1O1)	1.211(19)	-0.496(6)	0.907(6)	0.025
H(2O1)	1.348(14)	-0.298(10)	0.909(6)	0.025
O(2W)	0.6661(14)	-0.1619(10)	0.9025(5)	0.0217(18)
H(1O2)	0.631(19)	-0.056(6)	0.910(6)	0.025
H(2O2)	0.649(19)	-0.212(13)	0.861(2)	0.025
O(3W)	1.313(3)	0.192(2)	1.2479(6)	0.075(4)
H(1O3)	1.221(16)	0.100(9)	1.254(6)	0.025
H(2O3)	1.419(14)	0.248(14)	1.276(5)	0.025
O(4W)	1.790(3)	0.3314(18)	1.2490(6)	0.079(4)
H(1O4)	1.829(19)	0.430(8)	1.272(5)	0.025
H(2O4)	1.78(2)	0.362(13)	1.2051(19)	0.025

Table 21 Anisotropic displacement parameters for CdAQDC [Å^2]. The anisotropic displacement factor exponent takes the form $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cd(01)	0.0145(3)	0.0175(3)	0.0147(3)	0.0004(4)	0.0015(5)	-0.00233(19)
O(1W)	0.025(5)	0.030(4)	0.025(4)	-0.004(3)	0.007(4)	-0.008(4)
O(2W)	0.019(5)	0.016(3)	0.028(4)	-0.004(3)	0.000(3)	-0.004(3)
C(3)	0.008(5)	0.011(4)	0.026(6)	-0.004(4)	0.002(4)	-0.004(4)
C(7)	0.032(7)	0.033(6)	0.019(5)	0.007(5)	0.006(4)	-0.006(5)
C(2)	0.012(5)	0.024(5)	0.011(5)	-0.001(4)	0.003(4)	-0.003(4)
O(3)	0.023(5)	0.025(4)	0.031(4)	-0.016(3)	0.002(3)	-0.003(3)
O(4)	0.026(4)	0.026(4)	0.031(4)	0.010(3)	-0.001(3)	-0.010(3)
C(11)	0.046(8)	0.045(7)	0.016(5)	-0.003(5)	0.004(5)	-0.007(6)
C(15)	0.009(5)	0.015(5)	0.027(6)	0.006(4)	-0.001(4)	0.006(4)
C(10)	0.064(10)	0.052(7)	0.021(6)	0.004(6)	0.002(6)	0.006(7)
C(12)	0.034(6)	0.032(6)	0.020(5)	-0.004(5)	-0.003(6)	-0.003(5)
O(6)	0.040(5)	0.067(6)	0.024(4)	-0.009(4)	-0.002(4)	-0.027(5)
C(6)	0.024(6)	0.032(5)	0.019(5)	0.001(4)	0.008(4)	-0.005(4)
C(13)	0.027(6)	0.032(5)	0.020(5)	0.001(4)	0.001(4)	-0.004(5)
C(9)	0.049(9)	0.058(8)	0.013(5)	0.006(6)	0.010(6)	-0.010(6)
C(14)	0.025(7)	0.032(6)	0.017(5)	-0.010(4)	0.000(4)	-0.004(5)
C(1)	0.024(6)	0.018(5)	0.018(6)	-0.003(4)	-0.002(4)	-0.002(4)
C(4)	0.033(7)	0.017(5)	0.015(5)	0.001(4)	0.011(5)	-0.011(4)
O(5)	0.038(5)	0.062(5)	0.028(5)	0.003(4)	0.010(4)	-0.023(4)
C(5)	0.024(6)	0.029(5)	0.012(5)	-0.001(4)	0.000(4)	0.005(4)
C(8)	0.045(8)	0.045(7)	0.041(7)	0.001(6)	0.016(6)	-0.008(6)
O(2)	0.015(3)	0.021(3)	0.019(4)	0.000(3)	-0.003(3)	-0.006(3)
O(1)	0.028(4)	0.023(4)	0.021(4)	-0.012(3)	0.005(3)	-0.003(3)
O(3W)	0.096(11)	0.084(8)	0.044(6)	0.002(8)	0.024(8)	-0.018(7)
O(4W)	0.141(14)	0.059(6)	0.034(6)	-0.005(7)	0.020(8)	-0.020(8)
C(16)	0.013(6)	0.022(5)	0.024(6)	-0.012(5)	0.003(4)	-0.009(4)

Table 22 Symmetry operations used in the following tables.

	Operation
#1	'x,y,z'
#2	'-x,-y,-z'

Table 23 Bond Lengths for CdAQDC [Å].

	Angle	Symm. op. atom 1	Symm. op. atom 3
Cd(01)-O(4)	2.271(7)	2	
Cd(01)-O(2)	2.278(7)		
Cd(01)-O(2W)	2.286(8)		
Cd(01)-O(1W)	2.296(9)		
Cd(01)-O(1)	2.322(7)	2	
C(3)-C(4)	1.370(14)		
C(3)-C(2)	1.400(12)		
C(3)-C(16)	1.496(15)		
C(7)-C(8)	1.376(15)		
C(7)-C(12)	1.434(17)		
C(7)-C(6)	1.461(14)		
C(2)-C(1)	1.404(14)		
C(2)-C(15)	1.513(14)		
O(3)-C(15)	1.269(11)		
O(3)-Cd(01)	2.253(8)	1	
O(4)-C(15)	1.251(11)		
O(4)-Cd(01)	2.271(7)	2	
C(11)-C(10)	1.359(16)		
C(11)-C(12)	1.391(14)		
C(10)-C(9)	1.405(19)		
C(12)-C(13)	1.481(15)		
O(6)-C(13)	1.181(13)		
C(6)-O(5)	1.210(13)		
C(6)-C(5)	1.481(14)		
C(13)-C(14)	1.510(14)		
C(9)-C(8)	1.362(16)		
C(14)-C(1)	1.371(14)		
C(14)-C(5)	1.397(15)		
C(4)-C(5)	1.393(13)		
O(2)-C(16)	1.239(14)		
O(1)-C(16)	1.250(12)		
O(1)-Cd(01)	2.322(7)	2	

Table 24 Bond Angles for CdAQDC [°].

	Angle	Symm. op. atom 1	Symm. op. atom 3
O(4)-Cd(01)-O(2W)	76.9(3)	2	
O(2)-Cd(01)-O(2W)	145.4(3)		
O(3)-Cd(01)-O(1W)	146.3(3)	1	
O(4)-Cd(01)-O(1W)	80.0(3)	2	
O(2)-Cd(01)-O(1W)	86.3(3)		
O(2W)-Cd(01)-O(1W)	119.6(3)		
O(3)-Cd(01)-O(1)	82.6(3)	1	2
O(4)-Cd(01)-O(1)	137.8(3)	2	2
O(2)-Cd(01)-O(1)	128.2(3)		2
O(2W)-Cd(01)-O(1)	81.9(3)		2
O(1W)-Cd(01)-O(1)	79.6(3)		2
C(4)-C(3)-C(2)	119.2(10)		
C(4)-C(3)-C(16)	120.2(10)		
C(2)-C(3)-C(16)	120.3(10)		
C(8)-C(7)-C(12)	118.5(10)		
C(8)-C(7)-C(6)	120.8(11)		
C(12)-C(7)-C(6)	120.6(9)		
C(3)-C(2)-C(1)	120.5(10)		
C(3)-C(2)-C(15)	120.2(10)		
C(1)-C(2)-C(15)	119.1(10)		
C(15)-O(3)-Cd(01)	127.0(7)		1
C(15)-O(4)-Cd(01)	153.7(8)		2
C(10)-C(11)-C(12)	121.1(12)		
O(4)-C(15)-O(3)	124.5(10)		
O(4)-C(15)-C(2)	119.0(9)		
O(3)-C(15)-C(2)	116.5(9)		
C(11)-C(10)-C(9)	120.7(12)		
C(11)-C(12)-C(7)	118.3(10)		
C(11)-C(12)-C(13)	121.1(12)		
C(7)-C(12)-C(13)	120.6(9)		
O(5)-C(6)-C(7)	119.4(10)		
O(5)-C(6)-C(5)	121.0(10)		
C(7)-C(6)-C(5)	119.5(9)		
O(6)-C(13)-C(12)	121.7(10)		
O(6)-C(13)-C(14)	120.8(10)		
C(12)-C(13)-C(14)	117.4(9)		
C(8)-C(9)-C(10)	118.6(11)		
C(1)-C(14)-C(5)	120.8(9)		
C(1)-C(14)-C(13)	117.9(9)		
C(5)-C(14)-C(13)	121.3(9)		
C(14)-C(1)-C(2)	119.1(10)		
C(3)-C(4)-C(5)	121.0(10)		
C(4)-C(5)-C(14)	119.3(10)		
C(4)-C(5)-C(6)	120.2(10)		
C(14)-C(5)-C(6)	120.5(9)		
C(9)-C(8)-C(7)	122.6(12)		
C(16)-O(2)-Cd(01)	105.0(6)		
C(16)-O(1)-Cd(01)	173.5(7)		2
O(2)-C(16)-O(1)	123.9(10)		
O(2)-C(16)-C(3)	117.1(9)		
O(1)-C(16)-C(3)	118.8(10)		

3.4 CdAQDC at 120 K structure details

Table 25 Crystal data and structure refinement for CdAQDC at 120 K.

Parameter	Value
Empirical formula	$C_{16}H_{14}O_{10}Cd$
Formula weight	478.67 g·mol^{-1}
Collection Temperature	120(2) K
Wavelength	0.71073Å
Crystal system	Triclinic
Space Group	$P\bar{1}$
Unit cell dimensions	
a	5.629(2)Å
b	7.843(2)Å
c	15.045(5)Å
α	91.409(6)°
β	95.784(5)°
γ	115.160(5)°
Volume	808.4(4)Å^3
Z	2
Calculated density	1.773 g/m^3
Absorption coefficient	1.578 mm^{-1}
F(000)	440
Crystal size	0.5×0.3×0.2 mm
Theta range for data collection	2.73° to 26.02°
Limiting indices	$-9 \leq h \leq 9$, $-9 \leq k \leq 9$, $-18 \leq l \leq 17$
Reflections collected / unique	6709 / 3124 [R(int) = 0.0977]
Data Completeness	97.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.969 and 0.572
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3124 / 12 / 269
Goodness-of-fit on F^2	0.947
Final R indices [I>2sigma(I)]	R1 = 0.0663, wR2 = 0.1036
R indices (all data)	R1 = 0.1681, wR2 = 0.1345
Largest diff. peak and hole	0.532 and -0.490 e·Å^{-3}

Table 26 Crystal coordinates [Å] and equivalent isotropic displacement parameters [Å^2] for CdAQDC at 120 K. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
C(1)	0.2451(9)	0.3545(7)	0.2399(3)	0.0086(10)
H(1)	0.3925	0.4211	0.2475	0.010
C(2)	0.1479(10)	0.3110(7)	0.1701(3)	0.0059(10)
C(3)	-0.0710(10)	0.2155(8)	0.1580(3)	0.0067(10)
C(4)	-0.1879(10)	0.1615(8)	0.2176(3)	0.0101(11)
H(4)	-0.3346	0.0939	0.2101	0.012
C(5)	-0.0935(9)	0.2049(8)	0.2875(3)	0.0089(10)
C(6)	-0.2248(10)	0.1506(8)	0.3493(3)	0.0105(11)
C(7)	-0.1178(10)	0.2030(8)	0.4233(3)	0.0109(11)
C(8)	-0.2464(11)	0.1602(9)	0.4820(3)	0.0160(12)
H(8)	-0.3988	0.1021	0.4740	0.019
C(9)	-0.1489(12)	0.2037(9)	0.5522(3)	0.0154(13)
H(9)	-0.2352	0.1747	0.5920	0.019
C(10)	0.0750(11)	0.2895(8)	0.5641(3)	0.0144(11)
H(10)	0.1420	0.3169	0.6119	0.017
C(11)	0.1999(11)	0.3348(8)	0.5054(3)	0.0127(11)
H(11)	0.3518	0.3940	0.5132	0.015
C(12)	0.1023(10)	0.2933(8)	0.4352(3)	0.0106(11)
C(13)	0.2359(10)	0.3522(8)	0.3735(3)	0.0099(11)
C(14)	0.1266(10)	0.3005(7)	0.2990(3)	0.0087(11)
C(15)	-0.1923(9)	0.1884(7)	0.0840(3)	0.0055(9)
C(16)	0.2818(9)	0.3608(7)	0.1058(3)	0.0068(10)
Cd(1)	0.51077(6)	0.75432(5)	0.038627(16)	0.00503(15)
O(5)	-0.4139(8)	0.0636(7)	0.3407(2)	0.0176(9)
O(1)	-0.2870(7)	0.0361(5)	0.0638(2)	0.0119(8)
O(2)	-0.2016(7)	0.3272(5)	0.0451(2)	0.0093(8)
O(6)	0.4228(7)	0.4392(7)	0.3822(2)	0.0169(9)
O(1W)	0.8131(10)	0.6946(8)	0.2489(3)	0.0290(12)
O(3)	0.2899(7)	0.2353(6)	0.0603(2)	0.0099(8)
O(2W)	0.2927(9)	0.8333(7)	0.2473(3)	0.0225(11)
O(4)	0.3769(7)	0.5170(5)	0.1046(2)	0.0106(8)
O(3W)	0.8407(7)	0.6631(6)	0.0977(2)	0.0090(8)
O(4W)	0.2534(7)	0.8844(5)	0.1025(2)	0.0089(8)
H(1O1)	0.815(13)	0.666(10)	0.2049(13)	0.011
H(1O2)	0.164(7)	0.780(9)	0.256(4)	0.011
H(1O3)	0.962(8)	0.733(8)	0.093(4)	0.011
H(1O4)	0.260(13)	0.893(10)	0.1481(7)	0.011
H(2O1)	0.686(7)	0.742(10)	0.250(4)	0.011
H(2O2)	0.360(12)	0.920(7)	0.273(4)	0.011
H(2O3)	0.857(13)	0.572(6)	0.072(3)	0.011
H(2O4)	0.255(13)	0.980(6)	0.078(3)	0.011

Table 27 Anisotropic displacement parameters [Å^2] for CdAQDC at 120 K. The anisotropic displacement factor exponent takes the form $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	0.006(2)	0.006(2)	0.014(3)	0.000(2)	0.002(2)	-0.0005(19)
C(2)	0.009(2)	0.002(2)	0.008(2)	0.0008(19)	0.004(2)	0.0020(19)
C(3)	0.010(2)	0.008(3)	0.004(2)	0.0009(19)	0.0045(19)	0.003(2)
C(4)	0.010(3)	0.007(3)	0.014(3)	0.001(2)	0.007(2)	-0.0003(19)
C(5)	0.009(3)	0.008(3)	0.010(3)	-0.001(2)	0.001(2)	0.003(2)
C(6)	0.012(3)	0.012(3)	0.008(3)	0.001(2)	0.004(2)	0.001(2)
C(7)	0.010(3)	0.009(3)	0.013(3)	0.002(2)	0.002(2)	-0.001(2)
C(8)	0.017(3)	0.017(3)	0.014(3)	0.002(2)	0.004(2)	-0.002(2)
C(9)	0.021(3)	0.020(3)	0.006(2)	0.003(2)	0.004(2)	0.001(3)
C(10)	0.019(3)	0.014(3)	0.010(3)	-0.002(2)	0.002(2)	0.002(2)
C(11)	0.014(3)	0.012(3)	0.011(3)	0.000(2)	-0.001(2)	0.000(2)
C(12)	0.011(3)	0.012(3)	0.010(2)	0.000(2)	0.005(2)	0.002(2)
C(13)	0.009(2)	0.010(3)	0.011(3)	0.000(2)	0.005(2)	0.000(2)
C(14)	0.011(3)	0.006(3)	0.009(2)	0.0016(18)	0.001(2)	0.006(2)
C(16)	0.004(2)	0.006(2)	0.010(2)	0.0033(19)	0.0008(19)	0.0023(18)
Cd(1)	0.0040(2)	0.0047(2)	0.0066(2)	-0.00121(19)	0.00160(18)	-0.00003(13)
O(5)	0.011(2)	0.027(3)	0.013(2)	-0.0010(18)	0.0023(16)	-0.0082(17)
O(1)	0.0089(18)	0.0059(19)	0.020(2)	-0.0025(16)	0.0019(16)	-0.0044(15)
O(2)	0.0080(18)	0.0089(19)	0.0105(19)	0.0019(15)	-0.0024(15)	0.0006(15)
O(6)	0.011(2)	0.027(3)	0.011(2)	-0.0031(18)	0.0000(16)	-0.0055(18)
O(1W)	0.031(3)	0.033(3)	0.022(3)	-0.002(2)	0.003(2)	0.001(2)
O(3)	0.0104(18)	0.0098(19)	0.0099(19)	0.0009(14)	0.0033(15)	0.0008(15)
O(2W)	0.030(3)	0.023(3)	0.013(2)	-0.0060(19)	0.004(2)	-0.010(2)
O(4)	0.0134(19)	0.0057(18)	0.0128(19)	-0.0004(15)	0.0045(15)	-0.0018(15)
O(3W)	0.0052(17)	0.0066(19)	0.015(2)	-0.0022(15)	-0.0002(15)	0.0006(14)
O(4W)	0.0094(18)	0.0059(18)	0.013(2)	-0.0020(15)	0.0067(15)	0.0018(15)

Table 28 Symmetry operations used in the following tables.

	Operation
#1	'x,y,z'
#2	'-x,-y,-z'

Table 29 Bond Lengths [Å] for CdAQDC at 120 K.

	Angle	Symm. op. atom 1	Symm. op. atom 3
C(1)-C(14)	1.397(8)		
C(2)-C(3)	1.401(7)		
C(2)-C(16)	1.519(7)		
C(3)-C(4)	1.400(7)		
C(3)-C(15)	1.489(7)		
C(4)-C(5)	1.387(8)		
C(5)-C(14)	1.406(8)		
C(5)-C(6)	1.479(8)		
C(6)-O(5)	1.223(7)		
C(6)-C(7)	1.490(8)		
C(7)-C(12)	1.390(8)		
C(7)-C(8)	1.404(8)		
C(8)-C(9)	1.397(9)		
C(9)-C(10)	1.396(9)		
C(10)-C(11)	1.396(8)		
C(11)-C(12)	1.394(8)		
C(12)-C(13)	1.495(7)		
C(13)-O(6)	1.213(7)		
C(13)-C(14)	1.500(8)		
C(15)-O(1)	1.260(7)		
C(15)-O(2)	1.272(7)		
C(16)-O(4)	1.250(7)		
C(16)-O(3)	1.268(7)		
Cd(1)-O(3)	2.266(4)	2	
Cd(1)-O(4W)	2.277(4)		
Cd(1)-O(3W)	2.278(4)		
Cd(1)-O(4)	2.289(4)		
Cd(1)-O(2)	2.299(4)	2	
Cd(1)-O(1)	2.344(4)	1	
O(1)-Cd(1)	2.344(4)	1	
O(2)-Cd(1)	2.299(4)	2	
O(3)-Cd(1)	2.266(4)	2	

Table 30 Bond Angles [°] for CdAQDC at 120 K.

	Angle	Symm. op. atom 1	Symm. op. atom 3
C(4)-C(3)-C(2)	118.7(5)		
C(4)-C(3)-C(15)	119.4(5)		
C(2)-C(3)-C(15)	121.6(5)		
C(5)-C(4)-C(3)	121.3(5)		
C(4)-C(5)-C(14)	119.6(5)		
C(4)-C(5)-C(6)	119.9(5)		
C(14)-C(5)-C(6)	120.6(5)		
O(5)-C(6)-C(5)	121.7(5)		
O(5)-C(6)-C(7)	120.5(5)		
C(5)-C(6)-C(7)	117.9(5)		
C(12)-C(7)-C(8)	119.9(5)		
C(12)-C(7)-C(6)	121.9(5)		
C(8)-C(7)-C(6)	118.2(5)		
C(9)-C(8)-C(7)	119.7(6)		
C(10)-C(9)-C(8)	120.3(6)		
C(9)-C(10)-C(11)	119.7(5)		
C(12)-C(11)-C(10)	120.1(6)		
C(7)-C(12)-C(11)	120.3(5)		
C(7)-C(12)-C(13)	121.0(5)		
C(11)-C(12)-C(13)	118.7(5)		
O(6)-C(13)-C(12)	122.4(5)		
O(6)-C(13)-C(14)	120.8(5)		
C(12)-C(13)-C(14)	116.8(5)		
C(1)-C(14)-C(5)	119.7(5)		
C(1)-C(14)-C(13)	118.5(5)		
C(5)-C(14)-C(13)	121.8(5)		
O(1)-C(15)-O(2)	123.4(5)		
O(1)-C(15)-C(3)	120.2(5)		
O(2)-C(15)-C(3)	116.3(5)		
O(4)-C(16)-O(3)	127.3(5)		
O(4)-C(16)-C(2)	117.3(5)		
O(3)-C(16)-C(2)	115.4(5)		
O(3)-Cd(1)-O(4W)	146.89(15)	2	
O(3)-Cd(1)-O(3W)	85.43(15)	2	
O(4W)-Cd(1)-O(3W)	119.42(14)		
O(3)-Cd(1)-O(4)	131.11(14)	2	
O(4W)-Cd(1)-O(4)	78.98(14)		
O(3W)-Cd(1)-O(4)	76.69(15)		
O(3)-Cd(1)-O(2)	82.69(16)	2	2
O(4W)-Cd(1)-O(2)	86.58(15)		2
O(3W)-Cd(1)-O(2)	144.67(15)		2
O(4)-Cd(1)-O(2)	86.44(15)		2
O(3)-Cd(1)-O(1)	83.26(15)	2	1
O(4W)-Cd(1)-O(1)	79.81(15)		1
O(3W)-Cd(1)-O(1)	81.22(15)		1
O(4)-Cd(1)-O(1)	136.25(16)		1
O(2)-Cd(1)-O(1)	129.78(15)	2	1
C(15)-O(1)-Cd(1)	173.0(4)		1
C(15)-O(2)-Cd(1)	102.4(3)		2
C(16)-O(3)-Cd(1)	127.0(4)		2
C(16)-O(4)-Cd(1)	148.8(4)		

3.5 MnAQDC structure details

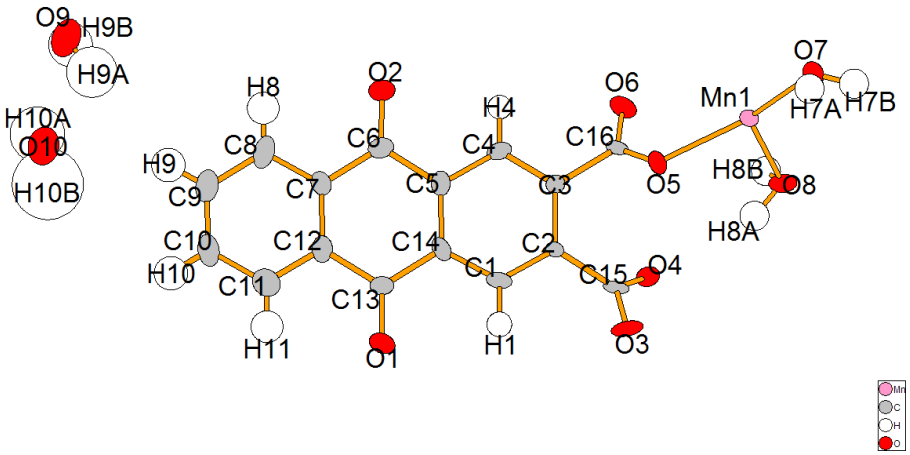

Figure 10 Asymmetric unit with atom numbers for MnAQDC.

Table 31 Crystal data and structure refinement for MnAQDC.

Parameter	Value
Empirical formula	$C_{16}H_{14}O_{10}Mn$
Formula weight	421.21 g·mol^{-1}
Collection Temperature	293(2) K
Wavelength	0.71073Å
Crystal system	Triclinic
Space Group	$P\bar{1}$
Unit cell dimensions	
a	5.799(2)Å
b	7.477(3)Å
c	18.493(7)Å
α	89.639(6)°
β	85.173(6)°
γ	83.485(7)°
Volume	793.8(5)Å^3
Z	2
Calculated density	1.762 g/m^3
Absorption coefficient	0.891 mm^{-1}
F(000)	430
Crystal size	0.1×0.08×0.02 mm
Theta range for data collection	2.21° to 25.68°
Limiting indices	$-7 \leq h \leq 7$, $-9 \leq k \leq 8$, $-22 \leq l \leq 22$
Reflections collected / unique	6413 / 2965 [R(int) = 0.0777]
Data Completeness	98.8%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.982 and 0.918
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2965 / 12 / 274
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0806, wR2 = 0.1826
R indices (all data)	R1 = 0.1359, wR2 = 0.2093
Largest diff. peak and hole	1.242 and -0.554 e·Å^{-3}

Table 32 Crystal coordinates [Å] and equivalent isotropic displacement parameters [Å^2] for MnAQDC. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Mn(1)	0.48607(17)	0.75368(14)	1.04047(6)	0.0157(3)
C(1)	-0.1858(12)	0.8437(10)	0.7845(4)	0.0238(17)
H(1)	-0.3318	0.9100	0.7907	0.029
C(2)	-0.0732(10)	0.7944(8)	0.8436(3)	0.0130(14)
C(3)	0.1443(11)	0.6930(9)	0.8355(4)	0.0167(15)
C(4)	0.2459(12)	0.6461(9)	0.7671(4)	0.0219(16)
H(4)	0.3920	0.5797	0.7617	0.026
C(5)	0.1272(12)	0.6992(10)	0.7050(4)	0.0232(16)
C(6)	0.2343(12)	0.6450(10)	0.6314(4)	0.0266(17)
C(7)	0.1067(13)	0.7054(10)	0.5682(4)	0.0274(18)
C(8)	0.2026(15)	0.6631(12)	0.4990(4)	0.040(2)
H(8)	0.3522	0.6031	0.4919	0.048
C(9)	0.0753(17)	0.7102(12)	0.4391(4)	0.044(2)
H(9)	0.1408	0.6829	0.3922	0.053
C(10)	-0.1457(16)	0.7964(12)	0.4501(4)	0.044(2)
H(10)	-0.2318	0.8257	0.4106	0.053
C(11)	-0.2430(15)	0.8408(12)	0.5200(4)	0.040(2)
H(11)	-0.3932	0.8998	0.5271	0.048
C(12)	-0.1170(14)	0.7975(11)	0.5787(4)	0.0303(18)
C(13)	-0.2257(12)	0.8534(10)	0.6513(4)	0.0284(18)
C(14)	-0.0919(12)	0.7991(10)	0.7148(4)	0.0228(16)
C(15)	-0.1978(11)	0.8308(9)	0.9189(4)	0.0208(16)
C(16)	0.2806(11)	0.6410(9)	0.9002(4)	0.0177(15)
O(1)	-0.4161(9)	0.9432(9)	0.6593(3)	0.0493(17)
O(2)	0.4233(9)	0.5537(9)	0.6248(3)	0.0514(18)
O(3)	-0.2845(8)	0.9862(7)	0.9338(3)	0.0301(13)
O(4)	-0.2148(8)	0.6984(6)	0.9577(3)	0.0231(12)
O(5)	0.2932(8)	0.7686(6)	0.9444(2)	0.0220(11)
O(6)	0.3677(8)	0.4840(7)	0.9050(3)	0.0286(12)
H(7A)	0.741(14)	0.992(3)	1.095(4)	0.040(12)
H(7B)	0.718(13)	0.890(9)	1.1482(12)	0.040(12)
O(7)	0.7431(9)	0.8749(7)	1.1006(3)	0.0245(12)
H(8A)	0.056(10)	0.699(8)	1.067(3)	0.040(12)
H(8B)	0.164(12)	0.541(4)	1.077(4)	0.040(12)
O(8)	0.1720(8)	0.6512(7)	1.0946(3)	0.0281(13)
H(9A)	0.608(16)	0.882(13)	0.281(5)	0.12(5)
H(9B)	0.637(17)	0.728(9)	0.257(6)	0.09(5)
O(9)	0.7141(14)	0.8246(11)	0.2474(4)	0.064(2)
H(10A)	0.18(2)	0.564(5)	0.242(8)	0.14(6)
H(10B)	0.040(7)	0.69(2)	0.259(11)	0.24(10)
O(10)	0.1933(14)	0.6813(12)	0.2471(4)	0.065(2)

Table 33 Anisotropic displacement parameters [Å^2] for MnAQDC. The anisotropic displacement factor exponent takes the form $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn(1)	0.0152(6)	0.0141(6)	0.0174(6)	-0.0010(4)	-0.0031(4)	0.0017(4)
C(1)	0.017(4)	0.021(4)	0.032(4)	-0.003(3)	-0.005(3)	0.007(3)
C(2)	0.013(3)	0.011(3)	0.015(3)	0.002(3)	-0.002(3)	0.002(3)
C(3)	0.018(3)	0.015(4)	0.017(4)	-0.001(3)	-0.001(3)	-0.002(3)
C(4)	0.021(4)	0.016(4)	0.026(4)	0.003(3)	0.005(3)	0.006(3)
C(5)	0.030(4)	0.024(4)	0.017(4)	0.001(3)	-0.003(3)	-0.006(3)
C(6)	0.022(4)	0.026(4)	0.030(4)	-0.003(3)	0.001(3)	0.002(3)
C(7)	0.030(4)	0.032(5)	0.020(4)	0.006(3)	-0.005(3)	0.001(4)
C(8)	0.046(5)	0.053(6)	0.020(4)	-0.002(4)	0.004(4)	-0.011(4)
C(9)	0.064(6)	0.041(5)	0.023(5)	0.005(4)	-0.001(4)	0.007(5)
C(10)	0.057(6)	0.050(6)	0.023(5)	0.004(4)	-0.010(4)	0.007(5)
C(11)	0.037(5)	0.044(6)	0.038(5)	0.002(4)	-0.008(4)	0.001(4)
C(12)	0.035(4)	0.035(5)	0.020(4)	-0.001(3)	-0.004(3)	-0.001(4)
C(13)	0.021(4)	0.034(5)	0.028(4)	-0.008(4)	-0.004(3)	0.009(3)
C(14)	0.027(4)	0.023(4)	0.020(4)	0.001(3)	-0.010(3)	0.000(3)
C(15)	0.012(3)	0.016(4)	0.033(4)	-0.005(3)	-0.006(3)	0.007(3)
C(16)	0.008(3)	0.021(4)	0.023(4)	0.007(3)	-0.001(3)	0.001(3)
O(1)	0.034(3)	0.074(5)	0.033(3)	-0.003(3)	-0.009(3)	0.027(3)
O(2)	0.034(3)	0.080(5)	0.033(3)	-0.008(3)	-0.003(3)	0.026(3)
O(3)	0.017(3)	0.022(3)	0.048(3)	-0.015(2)	0.003(2)	0.006(2)
O(4)	0.021(3)	0.022(3)	0.025(3)	0.000(2)	0.002(2)	0.001(2)
O(5)	0.025(3)	0.025(3)	0.018(3)	-0.001(2)	-0.009(2)	-0.002(2)
O(6)	0.026(3)	0.024(3)	0.035(3)	0.004(2)	-0.010(2)	0.004(2)
O(7)	0.030(3)	0.022(3)	0.022(3)	0.000(2)	-0.007(2)	0.000(2)
O(8)	0.021(3)	0.025(3)	0.037(3)	-0.002(2)	0.000(2)	0.004(2)
O(9)	0.085(5)	0.062(5)	0.038(4)	-0.003(4)	0.004(4)	0.012(5)
O(10)	0.073(5)	0.074(6)	0.046(4)	-0.009(4)	-0.006(4)	0.000(4)

Table 34 Symmetry operations used in the following tables for MnAQDC.

	Operation
#1	'x,y,z'
#2	'-x,-y,-z'

Table 35 Bond Lengths [Å] for MnAQDC.

	Angle	Symm. op. atom 1	Symm. op. atom 3
Mn(1)-O(5)	2.174(5)		
Mn(1)-O(3)	2.185(5)	2	
Mn(1)-O(7)	2.208(5)		
Mn(1)-O(8)	2.215(5)		
Mn(1)-O(4)	2.218(5)	1	
C(1)-C(2)	1.348(9)		
C(1)-C(14)	1.383(9)		
C(1)-H(1)	0.9300		
C(2)-C(3)	1.393(9)		
C(2)-C(15)	1.526(9)		
C(3)-C(4)	1.380(9)		
C(3)-C(16)	1.513(9)		
C(4)-C(5)	1.420(9)		
C(4)-H(4)	0.9300		
C(5)-C(14)	1.397(10)		
C(5)-C(6)	1.486(10)		
C(6)-O(2)	1.221(8)		
C(6)-C(7)	1.477(10)		
C(7)-C(8)	1.376(10)		
C(7)-C(12)	1.397(10)		
C(8)-C(9)	1.403(11)		
C(8)-H(8)	0.9300		
C(9)-C(10)	1.368(12)		
C(9)-H(9)	0.9300		
C(10)-C(11)	1.393(11)		
C(10)-H(10)	0.9300		
C(11)-C(12)	1.375(11)		
C(11)-H(11)	0.9300		
C(12)-C(13)	1.476(10)		
C(13)-O(1)	1.224(8)		
C(13)-C(14)	1.492(10)		
C(15)-O(4)	1.227(8)		
C(15)-O(3)	1.236(8)		
C(16)-O(6)	1.229(8)		
C(16)-O(5)	1.272(8)		
O(3)-Mn(1)	2.185(5)	2	
O(4)-Mn(1)	2.218(5)	1	
O(6)-Mn(1)	2.162(5)	2	
O(7)-H(7A)	0.88(2)		
O(7)-H(7B)	0.89(2)		
O(8)-H(8A)	0.91(2)		
O(8)-H(8B)	0.89(2)		
O(9)-H(9A)	0.90(2)		
O(9)-H(9B)	0.90(2)		
O(10)-H(10A)	0.89(2)		
O(10)-H(10B)	0.89(2)		

Table 36 Bond Angles [°] for MnAQDC.

	Angle	Symm. op. atom 1	Symm. op. atom 3
O(5)-Mn(1)-O(7)	145.88(19)		
O(3)-Mn(1)-O(7)	81.38(19)	2	
O(6)-Mn(1)-O(8)	77.69(19)	2	
O(5)-Mn(1)-O(8)	84.82(19)		
O(3)-Mn(1)-O(8)	82.25(19)	2	
O(7)-Mn(1)-O(8)	122.9(2)		
O(6)-Mn(1)-O(4)	86.14(18)	2	1
O(5)-Mn(1)-O(4)	81.69(18)		1
O(3)-Mn(1)-O(4)	127.04(19)	2	1
O(7)-Mn(1)-O(4)	83.24(18)		1
O(8)-Mn(1)-O(4)	145.60(19)		1
C(2)-C(1)-C(14)	122.3(6)		
C(2)-C(1)-H(1)	118.9		
C(14)-C(1)-H(1)	118.9		
C(1)-C(2)-C(3)	119.9(6)		
C(1)-C(2)-C(15)	119.4(6)		
C(3)-C(2)-C(15)	120.3(6)		
C(4)-C(3)-C(2)	120.0(6)		
C(4)-C(3)-C(16)	118.4(6)		
C(2)-C(3)-C(16)	121.5(6)		
C(3)-C(4)-C(5)	119.9(6)		
C(3)-C(4)-H(4)	120.0		
C(5)-C(4)-H(4)	120.0		
C(14)-C(5)-C(4)	118.7(6)		
C(14)-C(5)-C(6)	121.3(6)		
C(4)-C(5)-C(6)	119.9(6)		
O(2)-C(6)-C(7)	122.1(7)		
O(2)-C(6)-C(5)	119.7(7)		
C(7)-C(6)-C(5)	118.2(6)		
C(8)-C(7)-C(12)	119.8(7)		
C(8)-C(7)-C(6)	120.2(7)		
C(12)-C(7)-C(6)	119.9(6)		
C(7)-C(8)-C(9)	120.2(8)		
C(7)-C(8)-H(8)	119.9		
C(9)-C(8)-H(8)	119.9		
C(10)-C(9)-C(8)	119.5(8)		
C(10)-C(9)-H(9)	120.3		
C(8)-C(9)-H(9)	120.3		
C(9)-C(10)-C(11)	120.5(8)		
C(9)-C(10)-H(10)	119.7		
C(11)-C(10)-H(10)	119.7		
C(12)-C(11)-C(10)	120.0(8)		
C(12)-C(11)-H(11)	120.0		
C(10)-C(11)-H(11)	120.0		
C(11)-C(12)-C(7)	119.9(7)		
C(11)-C(12)-C(13)	117.7(7)		
C(7)-C(12)-C(13)	122.4(7)		
O(1)-C(13)-C(12)	121.7(7)		
O(1)-C(13)-C(14)	121.0(6)		
C(12)-C(13)-C(14)	117.3(6)		
C(1)-C(14)-C(5)	119.2(6)		
C(1)-C(14)-C(13)	120.3(6)		
C(5)-C(14)-C(13)	120.5(6)		
O(4)-C(15)-O(3)	125.9(7)		
O(4)-C(15)-C(2)	115.9(6)		
O(3)-C(15)-C(2)	118.1(6)		
O(6)-C(16)-O(5)	126.8(6)		
O(6)-C(16)-C(3)	118.3(6)		
O(5)-C(16)-C(3)	114.9(6)		
C(15)-O(3)-Mn(1)	171.8(5)		2

Table 37 Continued: Bond Angles [°] for for MnAQDC.

	Angle	Symm. op. atom 1	Symm. op. atom 3
C(15)-O(4)-Mn(1)	109.9(4)		1
C(16)-O(5)-Mn(1)	126.5(4)		
C(16)-O(6)-Mn(1)	156.0(5)		2
Mn(1)-O(7)-H(7A)	114(5)		
Mn(1)-O(7)-H(7B)	120(5)		
H(7A)-O(7)-H(7B)	90(4)		
Mn(1)-O(8)-H(8A)	103(5)		
Mn(1)-O(8)-H(8B)	108(5)		
H(8A)-O(8)-H(8B)	91(4)		
H(9A)-O(9)-H(9B)	85(4)		
H(10A)-O(10)-H(10B)	86(4)		

3.6 NiAQDC structure details

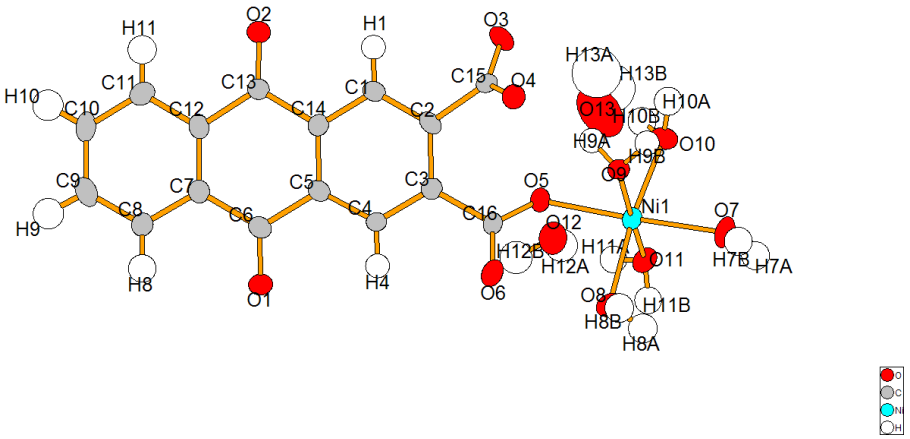

Figure 11 Asymmetric unit with atom numbers for NiAQDC.

Table 38 Crystal data and structure refinement for NiAQDC.

Parameter	Value
Empirical formula	$C_{16}H_{20}O_{13}Ni$
Formula weight	479.03 g·mol^{-1}
Collection Temperature	293(2) K
Wavelength	0.71073Å
Crystal system	Monoclinic
Space Group	$P2_1/c$
Unit cell dimensions	
a	16.308(3)Å
b	7.4101(15)Å
c	16.183(3)Å
α	90°
β	106.064(4)°
γ	90°
Volume	1879.2(7)Å^3
Z	4
Calculated density	1.693 g/m^3
Absorption coefficient	1.104 mm^{-1}
F(000)	992
Crystal size	0.4×0.35×0.25 mm
Theta range for data collection	1.30° to 26.02°
Limiting indices	$-20 \leq h \leq 20$, $-9 \leq k \leq 8$, $-19 \leq l \leq 19$
Reflections collected / unique	13851 / 3675 [R(int) = 0.0809]
Data Completeness	99.7%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.758 and 0.648
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3675 / 21 / 313
Goodness-of-fit on F^2	1.083
Final R indices [I>2sigma(I)]	R1 = 0.0622, wR2 = 0.1284
R indices (all data)	R1 = 0.1131, wR2 = 0.1587
Largest diff. peak and hole	0.625 and -0.509 e·Å^{-3}

Table 39 Crystal coordinates [Å] and equivalent isotropic displacement parameters [Å^2] for NiAQDC. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
O(3)	0.3620(2)	1.0703(5)	0.5594(2)	0.0339(9)
C(6)	-0.0149(3)	0.7478(8)	0.3714(3)	0.0266(12)
Ni(1)	0.41465(4)	1.08704(9)	0.28644(4)	0.0211(2)
C(1)	0.1960(3)	0.8873(7)	0.5244(3)	0.0228(12)
H(1)	0.2192	0.9086	0.5829	0.027
C(2)	0.2458(3)	0.9082(7)	0.4685(3)	0.0223(11)
C(3)	0.2102(3)	0.8826(7)	0.3801(3)	0.0217(11)
C(4)	0.1257(3)	0.8320(7)	0.3496(3)	0.0223(11)
H(4)	0.1022	0.8152	0.2909	0.027
C(5)	0.0751(3)	0.8057(7)	0.4051(3)	0.0218(12)
C(7)	-0.0637(3)	0.7056(7)	0.4348(3)	0.0242(12)
C(8)	-0.1458(3)	0.6364(7)	0.4058(4)	0.0297(13)
H(8)	-0.1691	0.6108	0.3478	0.036
C(9)	-0.1925(3)	0.6058(8)	0.4637(4)	0.0370(15)
H(9)	-0.2477	0.5604	0.4442	0.044
C(10)	-0.1584(3)	0.6419(8)	0.5503(4)	0.0366(15)
H(10)	-0.1907	0.6222	0.5886	0.044
C(11)	-0.0758(3)	0.7074(8)	0.5798(4)	0.0320(14)
H(11)	-0.0522	0.7301	0.6381	0.038
C(12)	-0.0284(3)	0.7389(7)	0.5218(3)	0.0219(11)
C(13)	0.0593(3)	0.8127(7)	0.5559(3)	0.0239(12)
C(14)	0.1112(3)	0.8343(7)	0.4934(3)	0.0217(11)
C(15)	0.3405(3)	0.9430(7)	0.5080(3)	0.0235(12)
C(16)	0.2631(3)	0.9131(7)	0.3180(3)	0.0223(11)
O(1)	-0.0493(2)	0.7385(7)	0.2946(2)	0.0484(12)
O(2)	0.0881(2)	0.8531(6)	0.6308(2)	0.0399(11)
O(4)	0.3915(2)	0.8319(5)	0.4891(2)	0.0277(9)
O(5)	0.3129(2)	1.0467(5)	0.3335(2)	0.0245(8)
O(6)	0.2528(2)	0.8092(5)	0.2562(3)	0.0407(11)
O(7)	0.5246(2)	1.1090(5)	0.2472(3)	0.0307(9)
H(7A)	0.537(3)	1.171(6)	0.206(3)	0.037
H(7B)	0.556(3)	1.020(5)	0.236(3)	0.037
O(8)	0.3649(2)	0.9207(6)	0.1827(2)	0.0325(9)
H(8A)	0.384(3)	0.965(6)	0.142(3)	0.039
H(8B)	0.396(3)	0.825(4)	0.181(3)	0.039
O(9)	0.4747(2)	0.8762(5)	0.3663(2)	0.0236(8)
H(9A)	0.457(3)	0.880(7)	0.411(2)	0.028
H(9B)	0.5268(13)	0.889(7)	0.395(3)	0.028
O(10)	0.4699(2)	1.2703(5)	0.3803(2)	0.0311(9)
H(10A)	0.505(3)	1.247(7)	0.4305(19)	0.037
H(10B)	0.438(3)	1.334(7)	0.405(3)	0.037
O(11)	0.3562(2)	1.3107(5)	0.2178(2)	0.0283(9)
H(11A)	0.307(2)	1.347(7)	0.224(3)	0.034
H(11B)	0.335(3)	1.309(8)	0.1631(13)	0.034
O(12)	0.2201(2)	1.4402(6)	0.2615(3)	0.0405(10)
H(12A)	0.203(3)	1.550(4)	0.245(4)	0.049
H(12B)	0.1655(17)	1.407(7)	0.245(4)	0.049
O(13)	0.3566(4)	1.4826(9)	0.4210(5)	0.095(2)
H(13A)	0.385(6)	1.446(11)	0.475(3)	0.114
H(13B)	0.362(6)	1.592(5)	0.445(5)	0.114

Table 40 Anisotropic displacement parameters [Å^2] for NiAQDC. The anisotropic displacement factor exponent takes the form $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni(1)	0.0197(3)	0.0237(4)	0.0216(4)	0.0018(3)	0.0084(3)	0.0009(3)
C(1)	0.019(2)	0.028(3)	0.020(3)	-0.003(2)	0.003(2)	0.001(2)
C(2)	0.016(2)	0.022(3)	0.026(3)	-0.004(2)	0.002(2)	0.000(2)
C(3)	0.019(2)	0.024(3)	0.022(3)	0.001(2)	0.006(2)	0.002(2)
C(4)	0.019(2)	0.031(3)	0.016(3)	0.000(2)	0.004(2)	-0.002(2)
C(5)	0.018(2)	0.023(3)	0.022(3)	0.000(2)	0.002(2)	0.001(2)
C(6)	0.022(3)	0.033(3)	0.024(3)	-0.006(3)	0.005(2)	-0.003(2)
C(7)	0.021(3)	0.027(3)	0.025(3)	-0.001(2)	0.007(2)	-0.001(2)
C(8)	0.026(3)	0.040(4)	0.025(3)	-0.003(3)	0.010(2)	-0.006(2)
C(9)	0.025(3)	0.040(4)	0.045(4)	-0.003(3)	0.008(3)	-0.010(3)
C(10)	0.026(3)	0.048(4)	0.040(4)	0.005(3)	0.016(3)	-0.006(3)
C(11)	0.026(3)	0.047(4)	0.023(3)	0.002(3)	0.008(2)	0.004(3)
C(12)	0.017(2)	0.020(3)	0.029(3)	0.001(2)	0.007(2)	0.002(2)
C(13)	0.019(2)	0.032(3)	0.020(3)	0.002(2)	0.003(2)	0.000(2)
C(14)	0.019(2)	0.026(3)	0.021(3)	0.001(2)	0.007(2)	0.002(2)
C(15)	0.021(2)	0.035(3)	0.015(3)	0.001(3)	0.005(2)	-0.001(2)
C(16)	0.019(2)	0.028(3)	0.020(3)	0.005(3)	0.006(2)	-0.001(2)
O(1)	0.028(2)	0.095(4)	0.021(2)	-0.005(2)	0.0060(18)	-0.017(2)
O(2)	0.029(2)	0.067(3)	0.023(2)	-0.007(2)	0.0075(18)	-0.014(2)
O(3)	0.0202(18)	0.047(2)	0.034(2)	-0.019(2)	0.0062(16)	-0.0078(18)
O(4)	0.0182(17)	0.038(2)	0.027(2)	0.0031(18)	0.0062(16)	0.0058(16)
O(5)	0.0236(18)	0.026(2)	0.027(2)	-0.0031(16)	0.0119(16)	-0.0047(15)
O(6)	0.049(3)	0.046(3)	0.035(2)	-0.017(2)	0.027(2)	-0.024(2)
O(7)	0.030(2)	0.028(2)	0.040(2)	0.0080(19)	0.0214(18)	0.0029(17)
O(8)	0.032(2)	0.043(2)	0.024(2)	-0.001(2)	0.0110(16)	0.0072(19)
O(9)	0.0191(17)	0.032(2)	0.0195(19)	-0.0019(17)	0.0059(15)	0.0014(16)
O(10)	0.030(2)	0.035(2)	0.025(2)	-0.0061(19)	0.0032(17)	0.0016(18)
O(11)	0.0252(19)	0.036(2)	0.025(2)	0.0085(19)	0.0097(17)	0.0088(17)
O(12)	0.032(2)	0.043(3)	0.047(3)	0.008(2)	0.013(2)	0.0079(19)
O(13)	0.071(4)	0.066(4)	0.146(6)	-0.052(4)	0.027(4)	0.004(3)

Table 41 Symmetry operations used in the following tables for NiAQDC.

	Operation
#1	'x,y,z'
#2	'-x,y+1/2,-z+1/2'
#3	'-x,-y,-z'
#4	'x,-y-1/2,z-1/2'

Table 42 Bond Lengths [Å] for NiAQDC.

	Angle	Symm. op. atom 1	Symm. op. atom 3
C(6)-O(1)	1.217(6)		
C(6)-C(5)	1.481(7)		
C(6)-C(7)	1.494(7)		
Ni(1)-O(5)	2.031(3)		
Ni(1)-O(10)	2.050(4)		
Ni(1)-O(8)	2.060(4)		
Ni(1)-O(7)	2.068(3)		
Ni(1)-O(11)	2.074(4)		
Ni(1)-O(9)	2.090(4)		
C(1)-C(2)	1.382(7)		
C(1)-C(14)	1.391(6)		
C(1)-H(1)	0.9300		
C(2)-C(3)	1.401(7)		
C(2)-C(15)	1.521(6)		
C(3)-C(4)	1.381(6)		
C(3)-C(16)	1.512(6)		
C(4)-C(5)	1.391(7)		
C(4)-H(4)	0.9300		
C(5)-C(14)	1.402(7)		
C(7)-C(12)	1.388(7)		
C(7)-C(8)	1.389(7)		
C(8)-C(9)	1.380(7)		
C(8)-H(8)	0.9300		
C(9)-C(10)	1.383(8)		
C(9)-H(9)	0.9300		
C(10)-C(11)	1.386(7)		
C(10)-H(10)	0.9300		
C(11)-C(12)	1.390(7)		
C(11)-H(11)	0.9300		
C(12)-C(13)	1.488(7)		
C(13)-O(2)	1.209(6)		
C(13)-C(14)	1.496(7)		
C(15)-O(4)	1.266(6)		
C(16)-O(6)	1.236(6)		
C(16)-O(5)	1.260(6)		
O(7)-H(7A)	0.878(19)		
O(7)-H(7B)	0.877(19)		
O(8)-H(8A)	0.866(19)		
O(8)-H(8B)	0.877(19)		
O(9)-H(9A)	0.855(19)		
O(9)-H(9B)	0.856(19)		
O(10)-H(10A)	0.871(19)		
O(10)-H(10B)	0.873(19)		
O(11)-H(11A)	0.874(19)		
O(11)-H(11B)	0.858(19)		
O(12)-H(12A)	0.88(2)		
O(12)-H(12B)	0.89(2)		
O(13)-H(13A)	0.91(2)		
O(13)-H(13B)	0.89(2)		

Table 43 Bond Angles [°] for NiAQDC.

	Angle	Symm. op. atom 1	Symm. op. atom 3
O(5)-Ni(1)-O(8)	92.22(14)		
O(10)-Ni(1)-O(8)	173.33(16)		
O(5)-Ni(1)-O(7)	174.29(15)		
O(10)-Ni(1)-O(7)	86.24(15)		
O(8)-Ni(1)-O(7)	88.65(15)		
O(5)-Ni(1)-O(11)	90.91(14)		
O(10)-Ni(1)-O(11)	84.84(16)		
O(8)-Ni(1)-O(11)	91.30(16)		
O(7)-Ni(1)-O(11)	94.72(14)		
O(5)-Ni(1)-O(9)	87.12(13)		
O(10)-Ni(1)-O(9)	90.13(15)		
O(8)-Ni(1)-O(9)	93.92(15)		
O(7)-Ni(1)-O(9)	87.19(14)		
O(11)-Ni(1)-O(9)	174.49(14)		
C(2)-C(1)-C(14)	120.1(5)		
C(2)-C(1)-H(1)	120.0		
C(14)-C(1)-H(1)	120.0		
C(1)-C(2)-C(3)	120.1(4)		
C(1)-C(2)-C(15)	117.2(4)		
C(3)-C(2)-C(15)	122.5(4)		
C(4)-C(3)-C(2)	119.4(4)		
C(4)-C(3)-C(16)	120.0(4)		
C(2)-C(3)-C(16)	120.5(4)		
C(3)-C(4)-C(5)	121.3(5)		
C(3)-C(4)-H(4)	119.3		
C(5)-C(4)-H(4)	119.3		
C(4)-C(5)-C(14)	118.7(4)		
C(4)-C(5)-C(6)	120.5(5)		
C(14)-C(5)-C(6)	120.8(4)		
C(12)-C(7)-C(8)	119.9(5)		
C(12)-C(7)-C(6)	120.6(4)		
C(8)-C(7)-C(6)	119.4(5)		
C(9)-C(8)-C(7)	119.6(5)		
C(9)-C(8)-H(8)	120.2		
C(7)-C(8)-H(8)	120.2		
C(8)-C(9)-C(10)	120.8(5)		
C(8)-C(9)-H(9)	119.6		
C(10)-C(9)-H(9)	119.6		
C(9)-C(10)-C(11)	119.8(5)		
C(9)-C(10)-H(10)	120.1		
C(11)-C(10)-H(10)	120.1		
C(10)-C(11)-C(12)	119.7(5)		
C(10)-C(11)-H(11)	120.2		
C(12)-C(11)-H(11)	120.2		
C(7)-C(12)-C(11)	120.2(4)		
C(7)-C(12)-C(13)	121.8(4)		
C(11)-C(12)-C(13)	118.0(5)		
O(2)-C(13)-C(12)	121.9(5)		
O(2)-C(13)-C(14)	121.1(4)		
C(12)-C(13)-C(14)	117.0(5)		
C(1)-C(14)-C(5)	120.4(4)		
C(1)-C(14)-C(13)	118.5(5)		
C(5)-C(14)-C(13)	121.1(4)		
O(3)-C(15)-O(4)	125.0(5)		
O(3)-C(15)-C(2)	118.3(4)		
O(4)-C(15)-C(2)	116.5(5)		
O(6)-C(16)-O(5)	125.9(4)		
O(6)-C(16)-C(3)	118.0(4)		
O(5)-C(16)-C(3)	116.0(5)		
C(16)-O(5)-Ni(1)	126.1(3)		

Table 44 Continued: Bond Angles [°] for NiAQDC.

	Angle	Symm. op. atom 1	Symm. op. atom 3
Ni(1)-O(7)-H(7A)	132(3)		
Ni(1)-O(7)-H(7B)	127(3)		
H(7A)-O(7)-H(7B)	89(2)		
Ni(1)-O(8)-H(8A)	104(4)		
Ni(1)-O(8)-H(8B)	114(4)		
H(8A)-O(8)-H(8B)	88(2)		
Ni(1)-O(9)-H(9A)	107(3)		
Ni(1)-O(9)-H(9B)	119(4)		
H(9A)-O(9)-H(9B)	93(2)		
Ni(1)-O(10)-H(10A)	127(4)		
Ni(1)-O(10)-H(10B)	120(4)		
H(10A)-O(10)-H(10B)	90(2)		
Ni(1)-O(11)-H(11A)	119(3)		
Ni(1)-O(11)-H(11B)	123(4)		
H(11A)-O(11)-H(11B)	90(2)		
H(12A)-O(12)-H(12B)	87(2)		
H(13A)-O(13)-H(13B)	84(2)		