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Supporting Information

Solution and Solid-State Structural Studies of Epoxide Adducts of Cadmium Phenoxides. Chemistry Relevant to Epoxide Activation for Ring-Opening Reactions.

by

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X-ray Crystallography

A Bausch and Lomb 10x microscope was used to identify suitable colorless crystals of **1-5** and **7** from a representative sample of crystals of the same habit. The representative crystal was coated in a cryogenic protectant (i.e. mineral oil, paratone, or apezeon grease), and was then fixed to a glass fiber, which in turn was fashioned to a copper mounting pin. The mounted crystals were then placed in a cold nitrogen stream (Oxford) maintained at 110 K on a Bruker SMART 1000 three circle goniometer.

Crystal data and details of data collection for the complexes are provided in Table 1. The X-ray data were collected on a Bruker CCD diffractometer and covered more than a hemisphere of reciprocal space by a combination of three sets of

exposures; each exposure set had a different φ angle for the crystal orientation and each exposure covered 0.3° in ω. The crystal-to-detector distance was 4.9 cm. Crystal decay was monitored by repeating the data collection for 50 initial frames at the end of the data set and analyzing the duplicate reflections; crystal decay was negligible. The space group was determined based on systematic absences and intensity statistics.[8]

The structures were solved by direct methods. Full-matrix least-squares anisotropic refinement for all non-hydrogen atoms yielded R(F) and $wR(F^2)$ values as indicated in Table 1 at convergence. Hydrogen atoms were place in idealized positions with isotropic thermal parameters fixed 1.2 or 1.5 times the value of the attached atom. Neutral atom scattering factors and anomalous scattering factors were taken from the International Tables for X-ray Crystallography Vol. C.

For the title compound, data reduction: SAINTPLUS (Bruker[9]); program(s) used to solve the structure: SHELXS-96 (Sheldrick[10]); program(s) used to refine the structure: SHELXL-97 (Sheldrick[11]); program(s) used for molecular graphics: SHELXTL version 5.0 (Bruker[12]); software used to prepare material for publication: SHELXTL version 5.0 (Bruker[12]).

Table 1. Crystallographic Data for Complexes **1-5** and **7**.

	1	2	3	4	5	
al Formula	$C_{58}H_{88}O_4Cl_4Cd_2$	$C_{73}H_{54}Cl_2O_4Cd_2$	$C_{40}H_{62}O_4Cd$	$C_{48}H_{74}O_4Cd$	$C_{42}H_{62}O_4Cd$	$C_{42}H$
	1215.88	1290.89	718.89	827.47	743.32	6
System	Monoclinic	Triclinic	Monoclinic	Monoclinic	Triclinic	Tr
roup	P2(1)/n	P-1	P2(1)/n	P2(1)/n	P-1	
	2917(3)	2816.8(12)	1848.7(3)	2143.7(13)	1899.1(9)	187
	2	2	2	2	2	
	14.162(8)	12.645(3)	10.1968(8)	10.090(4)	9.786(3)	9.
	11.658(6)	15.071(4)	12.2084(10)	12.399(4)	9.844(3)	9.
	17.887(9)	17.494(4)	14.8543(12)	17.135(6)	23.110(6)	22.
	--	106.562(5)	--	--	88.846(7)	87.
	98.998(9)	109.931(4)	91.314(2)	90.103(7)	78.319(6)	78
	--	102.478(5)	--	--	61.004(5)	60
	110(2)	110(2)	110(2)	110(2)	110(2)	1
), g/cm^3	1.384	1.522	1.291	1.282	1.300	
coeff, mm^{-1}	0.955	0.903	0.727	0.551	0.614	
[I > 2σ(I)]	2.89	5.43	5.25	6.69	6.52	
	6.43	8.29	14.29	16.25	12.99	

[a] $R = \Sigma||F_o| - |F_c||/\Sigma F_o$. $Rw = \{[\Sigma w(F_o^2 - F_c^2)^2/[\Sigma w(F_o^2)^2]\}^{1/2}$