

Tetra- μ_3 -tert-butoxo-tetrakis[ethylzinc(II)]

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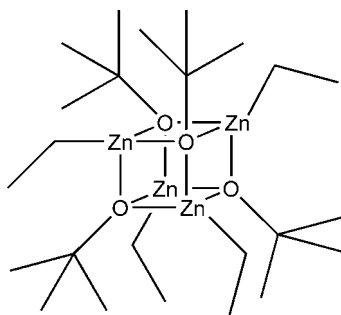
Received 21 August 2007; accepted 27 August 2007

 Key indicators: single-crystal X-ray study; $T = 220$ K; mean $\sigma(\text{C}-\text{C}) = 0.013$ Å; disorder in main residue; R factor = 0.061; wR factor = 0.169; data-to-parameter ratio = 19.2.

In the structure of the title compound, $[\text{Zn}_4(\text{C}_2\text{H}_5)_4(\text{C}_4\text{H}_9\text{O})_4]$, the Zn and O atoms form a distorted cubic arrangement with each Zn atom carrying an ethyl substituent. A tert-butyl group is bound to each of the O atoms. Coordination about the Zn and O atoms is distorted tetrahedral. Three of the four ethyl substituents are disordered over two positions; the site occupancy factors are *ca* 0.56 and 0.44. There are no significant close contacts in the crystal structure.

Related literature

For background on zinc oxide films, see: Delahoy & Cherny (1996); Dimova-Malinovska (2005); Beek *et al.* (2005). Structures of a number of related tetrakis(μ_3 -alkyloxo)tetraalkyl-tetrazinc complexes have been reported previously: Bond *et al.* (2001); Boyle *et al.* (2004); Charette *et al.* (2001); Herrmann *et al.* (1992); Olmstead *et al.* (1991); Polarz *et al.* (2005); Shearer & Spencer (1980).



Experimental

Crystal data

 $[\text{Zn}_4(\text{C}_2\text{H}_5)_4(\text{C}_4\text{H}_9\text{O})_4]$
 $M_r = 670.17$
 Triclinic, $P\bar{1}$
 $a = 10.0097$ (3) Å

 $b = 10.1372$ (3) Å
 $c = 17.7908$ (7) Å
 $\alpha = 94.740$ (2)°
 $\beta = 101.120$ (2)°

 $\gamma = 113.086$ (2)°
 $V = 1604.25$ (9) Å³
 $Z = 2$
 Mo $K\alpha$ radiation

 $\mu = 2.98$ mm⁻¹
 $T = 220$ (2) K
 $0.23 \times 0.07 \times 0.02$ mm

Data collection

 Nonius KappaCCD diffractometer
 Absorption correction: multi-scan
 (SORTAV; Blessing, 1995)
 $T_{\min} = 0.808$, $T_{\max} = 0.985$

 13938 measured reflections
 5615 independent reflections
 4047 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.068$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.061$
 $wR(F^2) = 0.169$
 $S = 1.06$
 5615 reflections
 293 parameters

 21 restraints
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.63$ e Å⁻³
 $\Delta\rho_{\min} = -0.70$ e Å⁻³

Data collection: COLLECT (Nonius, 1998); cell refinement: SCALEPACK (Otwinowski & Minor, 1997); data reduction: SCALEPACK and DENZO (Otwinowski & Minor, 1997); program(s) used to solve structure: SIR92 (Altomare *et al.*, 1993); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXL97, enCIFer (Allen *et al.*, 2004) and PLATON (Spek, 2003).

The authors thank Dr John Davies, University of Cambridge, for the X-ray data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2516).

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supplementary materials

Acta Cryst. (2007). E63, m2444 [doi:10.1107/S1600536807042018]

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Comment

Zinc oxide films show promise in a wide variety of optoelectronic devices such as photovoltaics (Delahoy & Cherny, 1996) and sensors (Dimova-Malinovska 2005) due to their electrical conductivity and transparency. While purely inorganic sol-gel, electrochemical or CVD techniques are often employed to make zinc oxide films, another technique is to use organozinc compounds that hydrolyse before or after film deposition. For instance, composite films of zinc oxide have been produced by the spincoating and subsequent hydrolysis of THF solutions of diethyl zinc (Beek *et al.*, 2005). The THF solvent was apparently able to stabilize the otherwise reactive organozinc in order to form good films. In an attempt to use *t*-butanol as a solvent for zinc oxide thin film deposition with diethyl zinc, we found that large needles of the partially alcoholized zinc title compound, (I), crystallized out after a few minutes.

In the structure of (I) (Fig 1) each Zn atom carries an ethyl substituent and binds to three *t*-butoxo O atoms. The resulting tetrameric unit is a distorted cube with the Zn and O atoms in distorted tetrahedral arrangements and Zn—O distances in the range 2.084 (4) Å to 2.055 (4) Å [mean 2.073 (6) Å]. This compares with a mean value of 2.07 (2) Å for the 11 other cubic tetrakis(μ_3 -alkyloxo)tetra-alkyl-tetrazinc complexes reported previously (Bond *et al.*, 2001; Herman *et al.*, 1992; Polarz *et al.*, 2005 and Shearer & Spencer, 1980; Boyle *et al.*, 2004). In the crystal structure of (I) there are no significant close contacts with the shortest intermolecular C62 \cdots H32Dⁱ ($i = x, y - 1, z$) distance being 3.02 Å.

Experimental

A solution of diethyl zinc in toluene (1 ml, 15 wt%) was added to dry *t*-butanol (10 ml) at 303 K. After several minutes, colourless needles of (I) started to form, and the reaction appeared complete after 30 minutes. The crystal was mounted for X-ray data collection immersed in the reaction solvent.

Refinement

The atoms of the ethyl groups bound to three of the four Zn atoms are disordered over two positions. The C atoms of these disordered groups were refined with common isotropic displacement parameters. The occupancy factor of the major disorder component refined to 0.559 (9). All H-atoms were positioned geometrically and refined using a riding model with C—H = 0.98 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for CH₂ groups and C—H = 0.97 Å, $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for CH₃ groups.

Figures

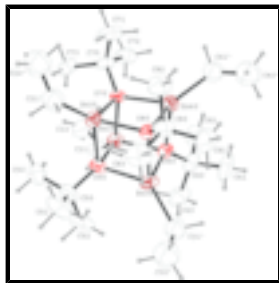


Fig. 1. The structure of (I) with displacement ellipsoids drawn at the 30% probability level for the non-hydrogen atoms. For clarity, only the principal disorder components of the disordered Zn bound ethyl groups are shown.

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$M_r = 670.17$

Triclinic, *PT*

Hall symbol: -P 1

$a = 10.0097$ (3) Å

$b = 10.1372$ (3) Å

$c = 17.7908$ (7) Å

$\alpha = 94.740$ (2)°

$\beta = 101.120$ (2)°

$\gamma = 113.086$ (2)°

$V = 1604.25$ (9) Å³

$Z = 2$

$F_{000} = 704$

$D_x = 1.387$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 13011 reflections

$\theta = 1.0$ – 25.0 °

$\mu = 2.98$ mm⁻¹

$T = 220$ (2) K

Needle, colourless

$0.23 \times 0.07 \times 0.02$ mm

Data collection

Nonius KappaCCD
diffractometer

Radiation source: fine-focus sealed tube

$T = 220$ (2) K

Thin-slice ω and ϕ scans

Absorption correction: multi-scan
(SORTAV; Blessing, 1995)

$T_{\min} = 0.808$, $T_{\max} = 0.985$

13938 measured reflections

5615 independent reflections

4047 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.068$

$\theta_{\text{max}} = 25.1$ °

$\theta_{\text{min}} = 3.5$ °

$h = -11 \rightarrow 11$

$k = -12 \rightarrow 12$

$l = -19 \rightarrow 21$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.061$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$wR(F^2) = 0.169$	$w = 1/[\sigma^2(F_o^2) + (0.0757P)^2 + 2.8014P]$
$S = 1.06$	where $P = (F_o^2 + 2F_c^2)/3$
5615 reflections	$(\Delta/\sigma)_{\max} = 0.001$
293 parameters	$\Delta\rho_{\max} = 0.63 \text{ e } \text{\AA}^{-3}$
21 restraints	$\Delta\rho_{\min} = -0.70 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. Three of the four ethyl groups are disordered, each over two sites. Common, isotropic displacement parameters were applied to the carbon atoms in all four of these groups.

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Zn10	0.35356 (8)	0.28721 (8)	0.66335 (4)	0.0558 (2)	
Zn20	0.33809 (8)	0.13653 (8)	0.80705 (5)	0.0581 (2)	
Zn30	0.54499 (9)	0.11431 (9)	0.70330 (5)	0.0634 (3)	
Zn40	0.62433 (8)	0.40687 (8)	0.80647 (4)	0.0569 (2)	
C11	0.2445 (12)	0.3324 (13)	0.5710 (5)	0.111 (4)	
H11A	0.3213	0.3880	0.5452	0.133*	
H11B	0.1839	0.2387	0.5362	0.133*	
C12	0.1518 (14)	0.4034 (14)	0.5699 (6)	0.134 (5)	
H12A	0.1141	0.4110	0.5167	0.200*	
H12B	0.2076	0.5002	0.6008	0.200*	
H12C	0.0684	0.3491	0.5912	0.200*	
C21	0.203 (3)	-0.003 (3)	0.8655 (17)	0.095 (2)*	0.441 (9)
H21A	0.1783	-0.1023	0.8405	0.114*	0.441 (9)
H21B	0.2636	0.0109	0.9183	0.114*	0.441 (9)
C22	0.068 (3)	0.003 (3)	0.8727 (19)	0.140 (4)*	0.441 (9)
H22A	0.0062	-0.0852	0.8889	0.209*	0.441 (9)
H22B	0.0147	0.0115	0.8229	0.209*	0.441 (9)
H22C	0.0892	0.0867	0.9112	0.209*	0.441 (9)
C21'	0.216 (2)	0.039 (2)	0.8726 (13)	0.095 (2)*	0.559 (9)
H21C	0.1217	-0.0274	0.8358	0.114*	0.559 (9)
H21D	0.2624	-0.0228	0.8936	0.114*	0.559 (9)
C22'	0.168 (3)	0.084 (3)	0.9346 (13)	0.140 (4)*	0.559 (9)

supplementary materials

H22D	0.1186	0.0008	0.9580	0.209*	0.559 (9)
H22E	0.0988	0.1261	0.9159	0.209*	0.559 (9)
H22F	0.2541	0.1562	0.9731	0.209*	0.559 (9)
C31	0.583 (2)	-0.043 (3)	0.6554 (14)	0.095 (2)*	0.441 (9)
H31A	0.5468	-0.1255	0.6824	0.114*	0.441 (9)
H31B	0.5233	-0.0744	0.6015	0.114*	0.441 (9)
C32	0.733 (3)	-0.014 (4)	0.6544 (18)	0.140 (4)*	0.441 (9)
H32A	0.7652	0.0538	0.6192	0.209*	0.441 (9)
H32B	0.7392	-0.1039	0.6368	0.209*	0.441 (9)
H32C	0.7968	0.0285	0.7064	0.209*	0.441 (9)
C31'	0.656 (2)	0.0269 (19)	0.6527 (11)	0.095 (2)*	0.559 (9)
H31C	0.6278	0.0264	0.5968	0.114*	0.559 (9)
H31D	0.7630	0.0925	0.6711	0.114*	0.559 (9)
C32'	0.642 (3)	-0.116 (2)	0.6621 (14)	0.140 (4)*	0.559 (9)
H32D	0.6983	-0.1450	0.6310	0.209*	0.559 (9)
H32E	0.5367	-0.1834	0.6451	0.209*	0.559 (9)
H32F	0.6794	-0.1165	0.7164	0.209*	0.559 (9)
C41	0.764 (3)	0.586 (3)	0.8822 (14)	0.095 (2)*	0.441 (9)
H41A	0.7842	0.6631	0.8508	0.142*	0.441 (9)
H41B	0.7025	0.6025	0.9150	0.142*	0.441 (9)
C42	0.901 (3)	0.622 (3)	0.9333 (17)	0.140 (4)*	0.441 (9)
H42A	0.9554	0.7267	0.9454	0.209*	0.441 (9)
H42B	0.9578	0.5794	0.9098	0.209*	0.441 (9)
H42C	0.8845	0.5841	0.9808	0.209*	0.441 (9)
C41'	0.794 (2)	0.591 (2)	0.8590 (11)	0.095 (2)*	0.559 (9)
H41C	0.7961	0.6592	0.8228	0.142*	0.559 (9)
H41D	0.7630	0.6249	0.9032	0.142*	0.559 (9)
C42'	0.942 (2)	0.616 (3)	0.8881 (15)	0.140 (4)*	0.559 (9)
H42D	0.9985	0.7166	0.9142	0.209*	0.559 (9)
H42E	0.9839	0.5980	0.8456	0.209*	0.559 (9)
H42F	0.9476	0.5517	0.9247	0.209*	0.559 (9)
O50	0.3256 (5)	0.0832 (4)	0.6901 (2)	0.0569 (10)	
C50	0.2051 (10)	-0.0496 (8)	0.6407 (5)	0.087 (2)	
C51	0.2095 (14)	-0.1776 (10)	0.6775 (7)	0.133 (4)	
H51A	0.1862	-0.1714	0.7278	0.199*	
H51B	0.3087	-0.1758	0.6842	0.199*	
H51C	0.1363	-0.2676	0.6441	0.199*	
C52	0.2303 (13)	-0.0573 (11)	0.5584 (5)	0.123 (4)	
H52A	0.2310	0.0289	0.5382	0.184*	
H52B	0.1502	-0.1433	0.5248	0.184*	
H52C	0.3255	-0.0624	0.5601	0.184*	
C53	0.0588 (10)	-0.0402 (12)	0.6401 (7)	0.117 (3)	
H53A	0.0449	-0.0355	0.6926	0.176*	
H53B	-0.0227	-0.1255	0.6068	0.176*	
H53C	0.0596	0.0467	0.6206	0.176*	
O60	0.5792 (5)	0.3255 (5)	0.6893 (2)	0.0554 (10)	
C60	0.6733 (9)	0.4022 (10)	0.6402 (5)	0.083 (2)	
C61	0.8320 (10)	0.4144 (14)	0.6760 (7)	0.133 (4)	
H61A	0.8591	0.4503	0.7315	0.200*	

H61B	0.9033	0.4813	0.6518	0.200*
H61C	0.8333	0.3193	0.6671	0.200*
C62	0.6752 (12)	0.5518 (10)	0.6416 (6)	0.109 (3)
H62A	0.5743	0.5429	0.6214	0.164*
H62B	0.7393	0.6042	0.6096	0.164*
H62C	0.7133	0.6046	0.6947	0.164*
C63	0.6096 (12)	0.3108 (12)	0.5580 (5)	0.107 (3)
H63A	0.5051	0.2925	0.5401	0.160*
H63B	0.6181	0.2188	0.5590	0.160*
H63C	0.6655	0.3632	0.5229	0.160*
O70	0.3941 (4)	0.3452 (4)	0.7825 (2)	0.0483 (9)
C70	0.3316 (8)	0.4399 (8)	0.8144 (4)	0.0668 (18)
C71	0.3813 (12)	0.4622 (11)	0.9020 (5)	0.100 (3)
H71A	0.4896	0.5124	0.9184	0.149*
H71B	0.3488	0.3684	0.9188	0.149*
H71C	0.3373	0.5202	0.9251	0.149*
C72	0.3888 (11)	0.5799 (9)	0.7851 (5)	0.091 (3)
H72A	0.3690	0.5603	0.7288	0.137*
H72B	0.4959	0.6318	0.8072	0.137*
H72C	0.3388	0.6389	0.8002	0.137*
C73	0.1627 (9)	0.3624 (10)	0.7861 (5)	0.086 (2)
H73A	0.1342	0.3499	0.7298	0.129*
H73B	0.1175	0.4199	0.8084	0.129*
H73C	0.1282	0.2678	0.8019	0.129*
O80	0.5643 (5)	0.1904 (4)	0.8183 (2)	0.0527 (10)
C80	0.6518 (9)	0.1508 (8)	0.8808 (4)	0.0694 (19)
C81	0.8102 (9)	0.2040 (11)	0.8726 (5)	0.098 (3)
H81A	0.8113	0.1578	0.8229	0.147*
H81B	0.8698	0.1798	0.9144	0.147*
H81C	0.8519	0.3088	0.8754	0.147*
C82	0.6450 (11)	0.2222 (11)	0.9572 (4)	0.091 (3)
H82A	0.6920	0.3272	0.9614	0.136*
H82B	0.6974	0.1933	0.9999	0.136*
H82C	0.5412	0.1917	0.9592	0.136*
C83	0.5779 (12)	-0.0139 (10)	0.8734 (6)	0.099 (3)
H83A	0.5809	-0.0589	0.8238	0.148*
H83B	0.4745	-0.0443	0.8762	0.148*
H83C	0.6311	-0.0436	0.9153	0.148*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn10	0.0630 (5)	0.0626 (5)	0.0470 (4)	0.0363 (4)	0.0053 (3)	0.0042 (3)
Zn20	0.0594 (5)	0.0578 (5)	0.0626 (5)	0.0271 (4)	0.0198 (4)	0.0144 (4)
Zn30	0.0773 (6)	0.0697 (5)	0.0595 (5)	0.0495 (4)	0.0165 (4)	0.0029 (4)
Zn40	0.0526 (4)	0.0529 (4)	0.0584 (5)	0.0211 (3)	0.0034 (3)	0.0019 (3)
C11	0.148 (9)	0.158 (10)	0.062 (5)	0.115 (8)	-0.001 (5)	0.010 (6)
C12	0.170 (11)	0.211 (13)	0.078 (6)	0.149 (11)	0.008 (7)	0.032 (7)

supplementary materials

O50	0.066 (3)	0.042 (2)	0.056 (3)	0.023 (2)	0.004 (2)	-0.0074 (19)
C50	0.083 (6)	0.053 (4)	0.095 (6)	0.016 (4)	-0.003 (4)	-0.015 (4)
C51	0.152 (10)	0.052 (5)	0.155 (11)	0.018 (6)	0.013 (8)	-0.001 (6)
C52	0.153 (10)	0.100 (7)	0.078 (6)	0.044 (7)	-0.012 (6)	-0.039 (6)
C53	0.065 (5)	0.115 (8)	0.130 (9)	0.015 (5)	-0.004 (5)	-0.012 (7)
O60	0.060 (3)	0.063 (3)	0.053 (2)	0.031 (2)	0.022 (2)	0.018 (2)
C60	0.078 (5)	0.101 (6)	0.089 (6)	0.041 (5)	0.043 (4)	0.041 (5)
C61	0.068 (6)	0.189 (12)	0.152 (10)	0.042 (7)	0.058 (6)	0.063 (9)
C62	0.129 (8)	0.087 (7)	0.123 (8)	0.038 (6)	0.055 (7)	0.062 (6)
C63	0.130 (8)	0.148 (9)	0.069 (6)	0.072 (7)	0.050 (6)	0.032 (6)
O70	0.056 (2)	0.050 (2)	0.046 (2)	0.0334 (19)	0.0097 (18)	-0.0023 (18)
C70	0.081 (5)	0.070 (5)	0.071 (5)	0.053 (4)	0.023 (4)	0.006 (4)
C71	0.135 (8)	0.123 (8)	0.068 (5)	0.089 (7)	0.021 (5)	-0.007 (5)
C72	0.116 (7)	0.068 (5)	0.103 (7)	0.057 (5)	0.023 (5)	0.001 (5)
C73	0.086 (6)	0.112 (7)	0.099 (6)	0.074 (5)	0.036 (5)	0.025 (5)
O80	0.060 (2)	0.058 (3)	0.049 (2)	0.036 (2)	0.0082 (19)	0.009 (2)
C80	0.087 (5)	0.078 (5)	0.060 (4)	0.055 (4)	0.011 (4)	0.013 (4)
C81	0.084 (6)	0.132 (8)	0.098 (6)	0.073 (6)	0.003 (5)	0.026 (6)
C82	0.110 (7)	0.123 (7)	0.054 (5)	0.066 (6)	0.013 (4)	0.019 (5)
C83	0.137 (8)	0.087 (6)	0.101 (7)	0.072 (6)	0.029 (6)	0.043 (5)

Geometric parameters (Å, °)

Zn10—C11	1.981 (7)	C42—H42C	0.9700
Zn10—O70	2.069 (4)	C41'—C42'	1.387 (14)
Zn10—O50	2.084 (4)	C41'—H41C	0.9800
Zn10—O60	2.084 (4)	C41'—H41D	0.9800
Zn10—Zn20	3.0831 (10)	C42'—H42D	0.9700
Zn10—Zn40	3.0903 (10)	C42'—H42E	0.9700
Zn10—Zn30	3.0925 (10)	C42'—H42F	0.9700
Zn20—C21'	1.90 (2)	O50—C50	1.470 (9)
Zn20—C21	2.05 (3)	C50—C53	1.503 (12)
Zn20—O50	2.072 (4)	C50—C51	1.512 (13)
Zn20—O70	2.072 (4)	C50—C52	1.535 (13)
Zn20—O80	2.074 (4)	C51—H51A	0.9700
Zn20—Zn30	3.0852 (10)	C51—H51B	0.9700
Zn20—Zn40	3.0949 (11)	C51—H51C	0.9700
Zn30—C31	1.95 (2)	C52—H52A	0.9700
Zn30—C31'	1.967 (18)	C52—H52B	0.9700
Zn30—O50	2.055 (4)	C52—H52C	0.9700
Zn30—O80	2.070 (4)	C53—H53A	0.9700
Zn30—O60	2.075 (4)	C53—H53B	0.9700
Zn30—Zn40	3.0799 (11)	C53—H53C	0.9700
Zn40—C41'	1.96 (2)	O60—C60	1.454 (8)
Zn40—C41	1.98 (3)	C60—C62	1.507 (12)
Zn40—O60	2.071 (4)	C60—C63	1.535 (13)
Zn40—O80	2.077 (4)	C60—C61	1.545 (13)
Zn40—O70	2.081 (4)	C61—H61A	0.9700
C11—C12	1.378 (10)	C61—H61B	0.9700

C11—H11A	0.9800	C61—H61C	0.9700
C11—H11B	0.9800	C62—H62A	0.9700
C12—H12A	0.9700	C62—H62B	0.9700
C12—H12B	0.9700	C62—H62C	0.9700
C12—H12C	0.9700	C63—H63A	0.9700
C21—C22	1.409 (16)	C63—H63B	0.9700
C21—H21A	0.9800	C63—H63C	0.9700
C21—H21B	0.9800	O70—C70	1.467 (7)
C22—H22A	0.9700	C70—C72	1.488 (11)
C22—H22B	0.9700	C70—C71	1.511 (11)
C22—H22C	0.9700	C70—C73	1.515 (11)
C21'—C22'	1.390 (15)	C71—H71A	0.9700
C21'—H21C	0.9800	C71—H71B	0.9700
C21'—H21D	0.9800	C71—H71C	0.9700
C22'—H22D	0.9700	C72—H72A	0.9700
C22'—H22E	0.9700	C72—H72B	0.9700
C22'—H22F	0.9700	C72—H72C	0.9700
C31—C32	1.410 (15)	C73—H73A	0.9700
C31—H31A	0.9800	C73—H73B	0.9700
C31—H31B	0.9800	C73—H73C	0.9700
C32—H32A	0.9700	O80—C80	1.462 (8)
C32—H32B	0.9700	C80—C81	1.502 (11)
C32—H32C	0.9700	C80—C82	1.513 (10)
C31'—C32'	1.424 (14)	C80—C83	1.519 (11)
C31'—H31C	0.9800	C81—H81A	0.9700
C31'—H31D	0.9800	C81—H81B	0.9700
C32'—H32D	0.9700	C81—H81C	0.9700
C32'—H32E	0.9700	C82—H82A	0.9700
C32'—H32F	0.9700	C82—H82B	0.9700
C41—C42	1.378 (16)	C82—H82C	0.9700
C41—H41A	0.9800	C83—H83A	0.9700
C41—H41B	0.9800	C83—H83B	0.9700
C42—H42A	0.9700	C83—H83C	0.9700
C42—H42B	0.9700		
C11—Zn10—O70	135.1 (3)	H31C—C31'—H31D	106.9
C11—Zn10—O50	128.1 (4)	C31'—C32'—H32D	109.5
O70—Zn10—O50	83.44 (16)	C31'—C32'—H32E	109.5
C11—Zn10—O60	126.2 (4)	H32D—C32'—H32E	109.5
O70—Zn10—O60	83.43 (15)	C31'—C32'—H32F	109.5
O50—Zn10—O60	82.85 (17)	H32D—C32'—H32F	109.5
C11—Zn10—Zn20	147.8 (4)	H32E—C32'—H32F	109.5
O70—Zn10—Zn20	41.93 (11)	C42—C41—Zn40	133 (2)
O50—Zn10—Zn20	41.96 (11)	C42—C41—H41A	104.1
O60—Zn10—Zn20	85.60 (11)	Zn40—C41—H41A	104.1
C11—Zn10—Zn40	146.2 (4)	C42—C41—H41B	104.1
O70—Zn10—Zn40	42.01 (11)	Zn40—C41—H41B	104.1
O50—Zn10—Zn40	85.08 (12)	H41A—C41—H41B	105.5
O60—Zn10—Zn40	41.78 (11)	C42'—C41'—Zn40	128.3 (17)
Zn20—Zn10—Zn40	60.17 (2)	C42'—C41'—H41C	105.2

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C11—Zn10—Zn30	139.6 (3)	Zn40—C41'—H41C	105.2
O70—Zn10—Zn30	85.28 (10)	C42'—C41'—H41D	105.2
O50—Zn10—Zn30	41.31 (12)	Zn40—C41'—H41D	105.2
O60—Zn10—Zn30	41.86 (12)	H41C—C41'—H41D	105.9
Zn20—Zn10—Zn30	59.94 (2)	C41'—C42'—H42D	109.5
Zn40—Zn10—Zn30	59.76 (2)	C41'—C42'—H42E	109.5
C21'—Zn20—C21	10.8 (11)	H42D—C42'—H42E	109.5
C21'—Zn20—O50	131.8 (7)	C41'—C42'—H42F	109.5
C21—Zn20—O50	122.8 (8)	H42D—C42'—H42F	109.5
C21'—Zn20—O70	129.5 (6)	H42E—C42'—H42F	109.5
C21—Zn20—O70	139.6 (7)	C50—O50—Zn30	119.6 (4)
O50—Zn20—O70	83.65 (15)	C50—O50—Zn20	121.9 (5)
C21'—Zn20—O80	128.2 (7)	Zn30—O50—Zn20	96.74 (18)
C21—Zn20—O80	126.1 (7)	C50—O50—Zn10	120.3 (4)
O50—Zn20—O80	82.95 (16)	Zn30—O50—Zn10	96.68 (18)
O70—Zn20—O80	83.41 (15)	Zn20—O50—Zn10	95.78 (16)
C21'—Zn20—Zn10	146.1 (7)	O50—C50—C53	107.7 (7)
C21—Zn20—Zn10	146.4 (8)	O50—C50—C51	107.5 (7)
O50—Zn20—Zn10	42.26 (11)	C53—C50—C51	109.6 (9)
O70—Zn20—Zn10	41.85 (10)	O50—C50—C52	108.6 (7)
O80—Zn20—Zn10	85.65 (11)	C53—C50—C52	110.7 (9)
C21'—Zn20—Zn30	145.0 (6)	C51—C50—C52	112.5 (8)
C21—Zn20—Zn30	134.9 (7)	C50—C51—H51A	109.5
O50—Zn20—Zn30	41.43 (12)	C50—C51—H51B	109.5
O70—Zn20—Zn30	85.42 (10)	H51A—C51—H51B	109.5
O80—Zn20—Zn30	41.85 (11)	C50—C51—H51C	109.5
Zn10—Zn20—Zn30	60.18 (2)	H51A—C51—H51C	109.5
C21'—Zn20—Zn40	143.1 (7)	H51B—C51—H51C	109.5
C21—Zn20—Zn40	150.8 (8)	C50—C52—H52A	109.5
O50—Zn20—Zn40	85.15 (12)	C50—C52—H52B	109.5
O70—Zn20—Zn40	41.92 (11)	H52A—C52—H52B	109.5
O80—Zn20—Zn40	41.82 (11)	C50—C52—H52C	109.5
Zn10—Zn20—Zn40	60.03 (2)	H52A—C52—H52C	109.5
Zn30—Zn20—Zn40	59.78 (3)	H52B—C52—H52C	109.5
C31—Zn30—C31'	23.8 (7)	C50—C53—H53A	109.5
C31—Zn30—O50	117.8 (7)	C50—C53—H53B	109.5
C31'—Zn30—O50	137.0 (6)	H53A—C53—H53B	109.5
C31—Zn30—O80	131.8 (7)	C50—C53—H53C	109.5
C31'—Zn30—O80	133.0 (6)	H53A—C53—H53C	109.5
O50—Zn30—O80	83.45 (16)	H53B—C53—H53C	109.5
C31—Zn30—O60	137.6 (8)	C60—O60—Zn40	121.5 (5)
C31'—Zn30—O60	117.0 (5)	C60—O60—Zn30	121.6 (4)
O50—Zn30—O60	83.77 (16)	Zn40—O60—Zn30	95.96 (16)
O80—Zn30—O60	83.70 (16)	C60—O60—Zn10	119.4 (4)
C31—Zn30—Zn40	156.2 (7)	Zn40—O60—Zn10	96.10 (16)
C31'—Zn30—Zn40	135.4 (6)	Zn30—O60—Zn10	96.05 (17)
O50—Zn30—Zn40	85.81 (11)	O60—C60—C62	109.1 (7)
O80—Zn30—Zn40	42.12 (11)	O60—C60—C63	107.7 (7)
O60—Zn30—Zn40	41.96 (11)	C62—C60—C63	112.2 (8)

C31—Zn30—Zn20	135.3 (7)	O60—C60—C61	106.2 (7)
C31'—Zn30—Zn20	157.2 (5)	C62—C60—C61	110.1 (9)
O50—Zn30—Zn20	41.84 (12)	C63—C60—C61	111.2 (8)
O80—Zn30—Zn20	41.95 (11)	C60—C61—H61A	109.5
O60—Zn30—Zn20	85.69 (11)	C60—C61—H61B	109.5
Zn40—Zn30—Zn20	60.26 (2)	H61A—C61—H61B	109.5
C31—Zn30—Zn10	140.0 (7)	C60—C61—H61C	109.5
C31'—Zn30—Zn10	138.9 (5)	H61A—C61—H61C	109.5
O50—Zn30—Zn10	42.01 (12)	H61B—C61—H61C	109.5
O80—Zn30—Zn10	85.47 (11)	C60—C62—H62A	109.5
O60—Zn30—Zn10	42.09 (11)	C60—C62—H62B	109.5
Zn40—Zn30—Zn10	60.09 (2)	H62A—C62—H62B	109.5
Zn20—Zn30—Zn10	59.88 (2)	C60—C62—H62C	109.5
C41'—Zn40—C41	15.8 (8)	H62A—C62—H62C	109.5
C41'—Zn40—O60	123.3 (6)	H62B—C62—H62C	109.5
C41—Zn40—O60	138.5 (7)	C60—C63—H63A	109.5
C41'—Zn40—O80	134.2 (6)	C60—C63—H63B	109.5
C41—Zn40—O80	128.9 (7)	H63A—C63—H63B	109.5
O60—Zn40—O80	83.66 (16)	C60—C63—H63C	109.5
C41'—Zn40—O70	131.4 (6)	H63A—C63—H63C	109.5
C41—Zn40—O70	120.7 (7)	H63B—C63—H63C	109.5
O60—Zn40—O70	83.49 (15)	C70—O70—Zn10	120.0 (4)
O80—Zn40—O70	83.15 (16)	C70—O70—Zn20	120.9 (4)
C41'—Zn40—Zn30	142.4 (6)	Zn10—O70—Zn20	96.22 (16)
C41—Zn40—Zn30	153.2 (7)	C70—O70—Zn40	121.1 (4)
O60—Zn40—Zn30	42.08 (12)	Zn10—O70—Zn40	96.26 (15)
O80—Zn40—Zn30	41.96 (11)	Zn20—O70—Zn40	96.35 (15)
O70—Zn40—Zn30	85.42 (10)	O70—C70—C72	108.5 (6)
C41'—Zn40—Zn10	140.0 (6)	O70—C70—C71	107.2 (5)
C41—Zn40—Zn10	143.4 (7)	C72—C70—C71	111.7 (7)
O60—Zn40—Zn10	42.12 (11)	O70—C70—C73	107.4 (6)
O80—Zn40—Zn10	85.43 (11)	C72—C70—C73	110.6 (7)
O70—Zn40—Zn10	41.73 (10)	C71—C70—C73	111.3 (7)
Zn30—Zn40—Zn10	60.16 (2)	C70—C71—H71A	109.5
C41'—Zn40—Zn20	151.1 (5)	C70—C71—H71B	109.5
C41—Zn40—Zn20	135.5 (7)	H71A—C71—H71B	109.5
O60—Zn40—Zn20	85.52 (12)	C70—C71—H71C	109.5
O80—Zn40—Zn20	41.76 (11)	H71A—C71—H71C	109.5
O70—Zn40—Zn20	41.72 (11)	H71B—C71—H71C	109.5
Zn30—Zn40—Zn20	59.95 (3)	C70—C72—H72A	109.5
Zn10—Zn40—Zn20	59.80 (2)	C70—C72—H72B	109.5
C12—C11—Zn10	127.3 (7)	H72A—C72—H72B	109.5
C12—C11—H11A	105.5	C70—C72—H72C	109.5
Zn10—C11—H11A	105.5	H72A—C72—H72C	109.5
C12—C11—H11B	105.5	H72B—C72—H72C	109.5
Zn10—C11—H11B	105.5	C70—C73—H73A	109.5
H11A—C11—H11B	106.1	C70—C73—H73B	109.5
C11—C12—H12A	109.5	H73A—C73—H73B	109.5
C11—C12—H12B	109.5	C70—C73—H73C	109.5

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H12A—C12—H12B	109.5	H73A—C73—H73C	109.5
C11—C12—H12C	109.5	H73B—C73—H73C	109.5
H12A—C12—H12C	109.5	C80—O80—Zn30	119.9 (4)
H12B—C12—H12C	109.5	C80—O80—Zn20	121.7 (4)
C22—C21—Zn20	121 (2)	Zn30—O80—Zn20	96.21 (17)
C22—C21—H21A	107.2	C80—O80—Zn40	120.7 (4)
Zn20—C21—H21A	107.2	Zn30—O80—Zn40	95.92 (16)
C22—C21—H21B	107.2	Zn20—O80—Zn40	96.42 (16)
Zn20—C21—H21B	107.2	O80—C80—C81	108.7 (6)
H21A—C21—H21B	106.8	O80—C80—C82	107.5 (5)
C22'—C21'—Zn20	134.9 (17)	C81—C80—C82	111.1 (7)
C22'—C21'—H21C	103.4	O80—C80—C83	107.3 (6)
Zn20—C21'—H21C	103.4	C81—C80—C83	112.0 (7)
C22'—C21'—H21D	103.4	C82—C80—C83	109.9 (7)
Zn20—C21'—H21D	103.4	C80—C81—H81A	109.5
H21C—C21'—H21D	105.3	C80—C81—H81B	109.5
C21'—C22'—H22D	109.5	H81A—C81—H81B	109.5
C21'—C22'—H22E	109.5	C80—C81—H81C	109.5
H22D—C22'—H22E	109.5	H81A—C81—H81C	109.5
C21'—C22'—H22F	109.5	H81B—C81—H81C	109.5
H22D—C22'—H22F	109.5	C80—C82—H82A	109.5
H22E—C22'—H22F	109.5	C80—C82—H82B	109.5
C32—C31—Zn30	118 (2)	H82A—C82—H82B	109.5
C32—C31—H31A	107.9	C80—C82—H82C	109.5
Zn30—C31—H31A	107.9	H82A—C82—H82C	109.5
C32—C31—H31B	107.9	H82B—C82—H82C	109.5
Zn30—C31—H31B	107.9	C80—C83—H83A	109.5
H31A—C31—H31B	107.2	C80—C83—H83B	109.5
C32'—C31'—Zn30	119.8 (17)	H83A—C83—H83B	109.5
C32'—C31'—H31C	107.4	C80—C83—H83C	109.5
Zn30—C31'—H31C	107.4	H83A—C83—H83C	109.5
C32'—C31'—H31D	107.4	H83B—C83—H83C	109.5
Zn30—C31'—H31D	107.4		
C11—Zn10—Zn20—C21'	-9.9 (12)	C31—Zn30—C31'—C32'	-28 (2)
O70—Zn10—Zn20—C21'	92.8 (11)	O50—Zn30—C31'—C32'	-70 (2)
O50—Zn10—Zn20—C21'	-97.9 (11)	O80—Zn30—C31'—C32'	70 (2)
O60—Zn10—Zn20—C21'	177.9 (11)	O60—Zn30—C31'—C32'	178.0 (16)
Zn40—Zn10—Zn20—C21'	142.8 (11)	Zn40—Zn30—C31'—C32'	130.2 (17)
Zn30—Zn10—Zn20—C21'	-147.0 (11)	Zn20—Zn30—C31'—C32'	4(3)
C11—Zn10—Zn20—C21	9.6 (14)	Zn10—Zn30—C31'—C32'	-135.0 (15)
O70—Zn10—Zn20—C21	112.4 (13)	C41'—Zn40—C41—C42	-76 (4)
O50—Zn10—Zn20—C21	-78.4 (13)	O60—Zn40—C41—C42	-94 (3)
O60—Zn10—Zn20—C21	-162.6 (13)	O80—Zn40—C41—C42	40 (3)
Zn40—Zn10—Zn20—C21	162.3 (13)	O70—Zn40—C41—C42	147 (3)
Zn30—Zn10—Zn20—C21	-127.5 (13)	Zn30—Zn40—C41—C42	-19 (4)
C11—Zn10—Zn20—O50	88.0 (6)	Zn10—Zn40—C41—C42	-164 (2)
O70—Zn10—Zn20—O50	-169.3 (2)	Zn20—Zn40—C41—C42	97 (3)
O60—Zn10—Zn20—O50	-84.2 (2)	C41—Zn40—C41'—C42'	113 (5)
Zn40—Zn10—Zn20—O50	-119.31 (18)	O60—Zn40—C41'—C42'	-82 (2)

Zn30—Zn10—Zn20—O50	-49.13 (18)	O80—Zn40—C41'—C42'	35 (2)
C11—Zn10—Zn20—O70	-102.8 (5)	O70—Zn40—C41'—C42'	164.6 (16)
O50—Zn10—Zn20—O70	169.3 (2)	Zn30—Zn40—C41'—C42'	-29 (2)
O60—Zn10—Zn20—O70	85.1 (2)	Zn10—Zn40—C41'—C42'	-135.2 (17)
Zn40—Zn10—Zn20—O70	49.95 (16)	Zn20—Zn40—C41'—C42'	102 (2)
Zn30—Zn10—Zn20—O70	120.13 (16)	C31—Zn30—O50—C50	-4.7 (10)
C11—Zn10—Zn20—O80	172.3 (5)	C31'—Zn30—O50—C50	13.2 (9)
O70—Zn10—Zn20—O80	-84.97 (19)	O80—Zn30—O50—C50	-138.9 (5)
O50—Zn10—Zn20—O80	84.3 (2)	O60—Zn30—O50—C50	136.7 (5)
O60—Zn10—Zn20—O80	0.09 (16)	Zn40—Zn30—O50—C50	178.8 (5)
Zn40—Zn10—Zn20—O80	-35.02 (11)	Zn20—Zn30—O50—C50	-132.8 (6)
Zn30—Zn10—Zn20—O80	35.16 (11)	Zn10—Zn30—O50—C50	130.6 (6)
C11—Zn10—Zn20—Zn30	137.1 (5)	C31—Zn30—O50—Zn20	128.1 (8)
O70—Zn10—Zn20—Zn30	-120.13 (16)	C31'—Zn30—O50—Zn20	145.9 (7)
O50—Zn10—Zn20—Zn30	49.13 (18)	O80—Zn30—O50—Zn20	-6.16 (16)
O60—Zn10—Zn20—Zn30	-35.07 (12)	O60—Zn30—O50—Zn20	-90.50 (17)
Zn40—Zn10—Zn20—Zn30	-70.18 (3)	Zn40—Zn30—O50—Zn20	-48.41 (12)
C11—Zn10—Zn20—Zn40	-152.7 (5)	Zn10—Zn30—O50—Zn20	-96.66 (18)
O70—Zn10—Zn20—Zn40	-49.95 (16)	C31—Zn30—O50—Zn10	-135.2 (8)
O50—Zn10—Zn20—Zn40	119.31 (18)	C31'—Zn30—O50—Zn10	-117.4 (7)
O60—Zn10—Zn20—Zn40	35.11 (12)	O80—Zn30—O50—Zn10	90.50 (17)
Zn30—Zn10—Zn20—Zn40	70.18 (3)	O60—Zn30—O50—Zn10	6.16 (16)
C21'—Zn20—Zn30—C31	15.8 (15)	Zn40—Zn30—O50—Zn10	48.25 (12)
C21—Zn20—Zn30—C31	9.4 (15)	Zn20—Zn30—O50—Zn10	96.66 (18)
O50—Zn20—Zn30—C31	-82.1 (10)	C21'—Zn20—O50—C50	1.0 (10)
O70—Zn20—Zn30—C31	-167.7 (10)	C21—Zn20—O50—C50	8.6 (10)
O80—Zn20—Zn30—C31	107.1 (10)	O70—Zn20—O50—C50	-138.5 (5)
Zn10—Zn20—Zn30—C31	-132.3 (9)	O80—Zn20—O50—C50	137.4 (5)
Zn40—Zn20—Zn30—C31	157.1 (9)	Zn10—Zn20—O50—C50	-131.3 (6)
C21'—Zn20—Zn30—C31'	-2(2)	Zn30—Zn20—O50—C50	131.3 (6)
C21—Zn20—Zn30—C31'	-8.4 (19)	Zn40—Zn20—O50—C50	179.4 (5)
O50—Zn20—Zn30—C31'	-99.9 (16)	C21'—Zn20—O50—Zn30	-130.3 (9)
O70—Zn20—Zn30—C31'	174.5 (16)	C21—Zn20—O50—Zn30	-122.7 (8)
O80—Zn20—Zn30—C31'	89.3 (16)	O70—Zn20—O50—Zn30	90.27 (17)
Zn10—Zn20—Zn30—C31'	-150.1 (16)	O80—Zn20—O50—Zn30	6.15 (16)
Zn40—Zn20—Zn30—C31'	139.3 (16)	Zn10—Zn20—O50—Zn30	97.4 (2)
C21'—Zn20—Zn30—O50	97.9 (12)	Zn40—Zn20—O50—Zn30	48.15 (12)
C21—Zn20—Zn30—O50	91.5 (12)	C21'—Zn20—O50—Zn10	132.2 (8)
O70—Zn20—Zn30—O50	-85.6 (2)	C21—Zn20—O50—Zn10	139.9 (8)
O80—Zn20—Zn30—O50	-170.8 (2)	O70—Zn20—O50—Zn10	-7.18 (16)
Zn10—Zn20—Zn30—O50	-50.22 (17)	O80—Zn20—O50—Zn10	-91.30 (17)
Zn40—Zn20—Zn30—O50	-120.80 (17)	Zn30—Zn20—O50—Zn10	-97.4 (2)
C21'—Zn20—Zn30—O80	-91.3 (12)	Zn40—Zn20—O50—Zn10	-49.29 (13)
C21—Zn20—Zn30—O80	-97.7 (12)	C11—Zn10—O50—C50	-5.1 (7)
O50—Zn20—Zn30—O80	170.8 (2)	O70—Zn10—O50—C50	139.6 (5)
O70—Zn20—Zn30—O80	85.2 (2)	O60—Zn10—O50—C50	-136.3 (5)
Zn10—Zn20—Zn30—O80	120.60 (17)	Zn20—Zn10—O50—C50	132.4 (6)
Zn40—Zn20—Zn30—O80	50.03 (17)	Zn40—Zn10—O50—C50	-178.2 (5)
C21'—Zn20—Zn30—O60	-176.6 (12)	Zn30—Zn10—O50—C50	-130.1 (6)

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C21—Zn20—Zn30—O60	177.0 (11)	C11—Zn10—O50—Zn30	125.0 (4)
O50—Zn20—Zn30—O60	85.5 (2)	O70—Zn10—O50—Zn30	-90.31 (17)
O70—Zn20—Zn30—O60	-0.13 (16)	O60—Zn10—O50—Zn30	-6.14 (16)
O80—Zn20—Zn30—O60	-85.4 (2)	Zn20—Zn10—O50—Zn30	-97.5 (2)
Zn10—Zn20—Zn30—O60	35.24 (12)	Zn40—Zn10—O50—Zn30	-48.10 (12)
Zn40—Zn20—Zn30—O60	-35.33 (12)	C11—Zn10—O50—Zn20	-137.5 (4)
C21'—Zn20—Zn30—Zn40	-141.3 (12)	O70—Zn10—O50—Zn20	7.20 (17)
C21—Zn20—Zn30—Zn40	-147.7 (11)	O60—Zn10—O50—Zn20	91.36 (17)
O50—Zn20—Zn30—Zn40	120.80 (17)	Zn40—Zn10—O50—Zn20	49.40 (13)
O70—Zn20—Zn30—Zn40	35.20 (11)	Zn30—Zn10—O50—Zn20	97.5 (2)
O80—Zn20—Zn30—Zn40	-50.03 (16)	Zn30—O50—C50—C53	-178.2 (6)
Zn10—Zn20—Zn30—Zn40	70.58 (3)	Zn20—O50—C50—C53	60.9 (8)
C21'—Zn20—Zn30—Zn10	148.1 (12)	Zn10—O50—C50—C53	-59.1 (9)
C21—Zn20—Zn30—Zn10	141.7 (11)	Zn30—O50—C50—C51	63.7 (9)
O50—Zn20—Zn30—Zn10	50.22 (17)	Zn20—O50—C50—C51	-57.1 (9)
O70—Zn20—Zn30—Zn10	-35.37 (11)	Zn10—O50—C50—C51	-177.2 (6)
O80—Zn20—Zn30—Zn10	-120.60 (17)	Zn30—O50—C50—C52	-58.3 (8)
Zn40—Zn20—Zn30—Zn10	-70.58 (3)	Zn20—O50—C50—C52	-179.1 (6)
C11—Zn10—Zn30—C31	-20.0 (13)	Zn10—O50—C50—C52	60.9 (8)
O70—Zn10—Zn30—C31	161.4 (11)	C41'—Zn40—O60—C60	0.4 (9)
O50—Zn10—Zn30—C31	76.0 (11)	C41—Zn40—O60—C60	6.3 (12)
O60—Zn10—Zn30—C31	-113.1 (11)	O80—Zn40—O60—C60	-139.7 (5)
Zn20—Zn10—Zn30—C31	126.0 (11)	O70—Zn40—O60—C60	136.5 (5)
Zn40—Zn10—Zn30—C31	-163.1 (11)	Zn30—Zn40—O60—C60	-133.1 (5)
C11—Zn10—Zn30—C31'	16.9 (11)	Zn10—Zn40—O60—C60	130.2 (5)
O70—Zn10—Zn30—C31'	-161.7 (9)	Zn20—Zn40—O60—C60	178.4 (5)
O50—Zn10—Zn30—C31'	112.9 (9)	C41'—Zn40—O60—Zn30	133.5 (7)
O60—Zn10—Zn30—C31'	-76.2 (9)	C41—Zn40—O60—Zn30	139.4 (10)
Zn20—Zn10—Zn30—C31'	162.9 (9)	O80—Zn40—O60—Zn30	-6.58 (16)
Zn40—Zn10—Zn30—C31'	-126.2 (9)	O70—Zn40—O60—Zn30	-90.37 (17)
C11—Zn10—Zn30—O50	-96.0 (6)	Zn10—Zn40—O60—Zn30	-96.77 (19)
O70—Zn10—Zn30—O50	85.4 (2)	Zn20—Zn40—O60—Zn30	-48.50 (12)
O60—Zn10—Zn30—O50	170.8 (2)	C41'—Zn40—O60—Zn10	-129.8 (7)
Zn20—Zn10—Zn30—O50	49.99 (17)	C41—Zn40—O60—Zn10	-123.9 (10)
Zn40—Zn10—Zn30—O50	120.86 (17)	O80—Zn40—O60—Zn10	90.19 (17)
C11—Zn10—Zn30—O80	178.7 (6)	O70—Zn40—O60—Zn10	6.39 (16)
O70—Zn10—Zn30—O80	0.19 (17)	Zn30—Zn40—O60—Zn10	96.77 (19)
O50—Zn10—Zn30—O80	-85.2 (2)	Zn20—Zn40—O60—Zn10	48.27 (12)
O60—Zn10—Zn30—O80	85.6 (2)	C31—Zn30—O60—C60	-11.2 (11)
Zn20—Zn10—Zn30—O80	-35.25 (12)	C31'—Zn30—O60—C60	4.0 (8)
Zn40—Zn10—Zn30—O80	35.62 (12)	O50—Zn30—O60—C60	-136.3 (5)
C11—Zn10—Zn30—O60	93.1 (6)	O80—Zn30—O60—C60	139.6 (5)
O70—Zn10—Zn30—O60	-85.4 (2)	Zn40—Zn30—O60—C60	133.0 (6)
O50—Zn10—Zn30—O60	-170.8 (2)	Zn20—Zn30—O60—C60	-178.3 (5)
Zn20—Zn10—Zn30—O60	-120.86 (17)	Zn10—Zn30—O60—C60	-130.2 (6)
Zn40—Zn10—Zn30—O60	-49.99 (17)	C31—Zn30—O60—Zn40	-144.3 (10)
C11—Zn10—Zn30—Zn40	143.1 (6)	C31'—Zn30—O60—Zn40	-129.0 (7)
O70—Zn10—Zn30—Zn40	-35.42 (11)	O50—Zn30—O60—Zn40	90.66 (17)
O50—Zn10—Zn30—Zn40	-120.86 (17)	O80—Zn30—O60—Zn40	6.60 (16)

O60—Zn10—Zn30—Zn40	49.99 (17)	Zn20—Zn30—O60—Zn40	48.69 (12)
Zn20—Zn10—Zn30—Zn40	-70.87 (3)	Zn10—Zn30—O60—Zn40	96.81 (18)
C11—Zn10—Zn30—Zn20	-146.0 (6)	C31—Zn30—O60—Zn10	118.9 (10)
O70—Zn10—Zn30—Zn20	35.44 (11)	C31'—Zn30—O60—Zn10	134.2 (7)
O50—Zn10—Zn30—Zn20	-49.99 (17)	O50—Zn30—O60—Zn10	-6.15 (16)
O60—Zn10—Zn30—Zn20	120.86 (17)	O80—Zn30—O60—Zn10	-90.22 (17)
Zn40—Zn10—Zn30—Zn20	70.87 (3)	Zn40—Zn30—O60—Zn10	-96.81 (18)
C31—Zn30—Zn40—C41'	18 (2)	Zn20—Zn30—O60—Zn10	-48.13 (12)
C31'—Zn30—Zn40—C41'	-3.7 (12)	C11—Zn10—O60—C60	5.0 (7)
O50—Zn30—Zn40—C41'	-169.7 (9)	O70—Zn10—O60—C60	-138.0 (5)
O80—Zn30—Zn40—C41'	105.4 (9)	O50—Zn10—O60—C60	137.8 (5)
O60—Zn30—Zn40—C41'	-84.4 (9)	Zn20—Zn10—O60—C60	179.9 (5)
Zn20—Zn30—Zn40—C41'	155.2 (9)	Zn40—Zn10—O60—C60	-131.6 (6)
Zn10—Zn30—Zn40—C41'	-134.6 (9)	Zn30—Zn10—O60—C60	131.7 (6)
C31—Zn30—Zn40—C41	-4(2)	C11—Zn10—O60—Zn40	136.6 (4)
C31'—Zn30—Zn40—C41	-25.8 (17)	O70—Zn10—O60—Zn40	-6.43 (16)
O50—Zn30—Zn40—C41	168.1 (16)	O50—Zn10—O60—Zn40	-90.61 (17)
O80—Zn30—Zn40—C41	83.2 (16)	Zn20—Zn10—O60—Zn40	-48.51 (12)
O60—Zn30—Zn40—C41	-106.6 (16)	Zn30—Zn10—O60—Zn40	-96.68 (18)
Zn20—Zn30—Zn40—C41	133.0 (16)	C11—Zn10—O60—Zn30	-126.7 (4)
Zn10—Zn30—Zn40—C41	-156.7 (16)	O70—Zn10—O60—Zn30	90.25 (17)
C31—Zn30—Zn40—O60	102.3 (18)	O50—Zn10—O60—Zn30	6.07 (16)
C31'—Zn30—Zn40—O60	80.7 (7)	Zn20—Zn10—O60—Zn30	48.18 (12)
O50—Zn30—Zn40—O60	-85.3 (2)	Zn40—Zn10—O60—Zn30	96.68 (18)
O80—Zn30—Zn40—O60	-170.2 (2)	Zn40—O60—C60—C62	-58.9 (8)
Zn20—Zn30—Zn40—O60	-120.40 (17)	Zn30—O60—C60—C62	179.7 (6)
Zn10—Zn30—Zn40—O60	-50.16 (17)	Zn10—O60—C60—C62	60.4 (8)
C31—Zn30—Zn40—O80	-87.5 (18)	Zn40—O60—C60—C63	179.0 (5)
C31'—Zn30—Zn40—O80	-109.1 (7)	Zn30—O60—C60—C63	57.6 (7)
O50—Zn30—Zn40—O80	84.9 (2)	Zn10—O60—C60—C63	-61.7 (7)
O60—Zn30—Zn40—O80	170.2 (2)	Zn40—O60—C60—C61	59.8 (9)
Zn20—Zn30—Zn40—O80	49.80 (16)	Zn30—O60—C60—C61	-61.7 (9)
Zn10—Zn30—Zn40—O80	120.04 (17)	Zn10—O60—C60—C61	179.0 (6)
C31—Zn30—Zn40—O70	-172.3 (18)	C11—Zn10—O70—C70	1.3 (7)
C31'—Zn30—Zn40—O70	166.1 (7)	O50—Zn10—O70—C70	-138.5 (5)
O50—Zn30—Zn40—O70	0.02 (16)	O60—Zn10—O70—C70	138.0 (5)
O80—Zn30—Zn40—O70	-84.8 (2)	Zn20—Zn10—O70—C70	-131.3 (5)
O60—Zn30—Zn40—O70	85.4 (2)	Zn40—Zn10—O70—C70	131.6 (5)
Zn20—Zn30—Zn40—O70	-35.04 (11)	Zn30—Zn10—O70—C70	-180.0 (4)
Zn10—Zn30—Zn40—O70	35.19 (11)	C11—Zn10—O70—Zn20	132.6 (5)
C31—Zn30—Zn40—Zn10	152.5 (18)	O50—Zn10—O70—Zn20	-7.20 (16)
C31'—Zn30—Zn40—Zn10	130.9 (7)	O60—Zn10—O70—Zn20	-90.72 (17)
O50—Zn30—Zn40—Zn10	-35.17 (12)	Zn40—Zn10—O70—Zn20	-97.12 (17)
O80—Zn30—Zn40—Zn10	-120.04 (17)	Zn30—Zn10—O70—Zn20	-48.69 (11)
O60—Zn30—Zn40—Zn10	50.16 (17)	C11—Zn10—O70—Zn40	-130.2 (5)
Zn20—Zn30—Zn40—Zn10	-70.24 (3)	O50—Zn10—O70—Zn40	89.92 (17)
C31—Zn30—Zn40—Zn20	-137.3 (18)	O60—Zn10—O70—Zn40	6.40 (16)
C31'—Zn30—Zn40—Zn20	-158.9 (7)	Zn20—Zn10—O70—Zn40	97.12 (17)
O50—Zn30—Zn40—Zn20	35.06 (12)	Zn30—Zn10—O70—Zn40	48.43 (11)

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O80—Zn30—Zn40—Zn20	-49.80 (16)	C21'—Zn20—O70—C70	-3.1 (10)
O60—Zn30—Zn40—Zn20	120.40 (17)	C21—Zn20—O70—C70	2.7 (14)
Zn10—Zn30—Zn40—Zn20	70.24 (3)	O50—Zn20—O70—C70	137.9 (4)
C11—Zn10—Zn40—C41'	2.0 (10)	O80—Zn20—O70—C70	-138.5 (4)
O70—Zn10—Zn40—C41'	-102.1 (9)	Zn10—Zn20—O70—C70	130.7 (5)
O50—Zn10—Zn40—C41'	172.2 (9)	Zn30—Zn20—O70—C70	179.5 (4)
O60—Zn10—Zn40—C41'	87.5 (9)	Zn40—Zn20—O70—C70	-132.3 (5)
Zn20—Zn10—Zn40—C41'	-152.0 (8)	C21'—Zn20—O70—Zn10	-133.8 (9)
Zn30—Zn10—Zn40—C41'	137.6 (8)	C21—Zn20—O70—Zn10	-128.0 (13)
C11—Zn10—Zn40—C41	27.1 (12)	O50—Zn20—O70—Zn10	7.24 (17)
O70—Zn10—Zn40—C41	-77.0 (11)	O80—Zn20—O70—Zn10	90.84 (16)
O50—Zn10—Zn40—C41	-162.7 (11)	Zn30—Zn20—O70—Zn10	48.83 (11)
O60—Zn10—Zn40—C41	112.5 (11)	Zn40—Zn20—O70—Zn10	97.04 (17)
Zn20—Zn10—Zn40—C41	-126.9 (11)	C21'—Zn20—O70—Zn40	129.2 (9)
Zn30—Zn10—Zn40—C41	162.6 (11)	C21—Zn20—O70—Zn40	135.0 (13)
C11—Zn10—Zn40—O60	-85.5 (5)	O50—Zn20—O70—Zn40	-89.79 (17)
O70—Zn10—Zn40—O60	170.4 (2)	O80—Zn20—O70—Zn40	-6.20 (15)
O50—Zn10—Zn40—O60	84.8 (2)	Zn10—Zn20—O70—Zn40	-97.04 (17)
Zn20—Zn10—Zn40—O60	120.59 (17)	Zn30—Zn20—O70—Zn40	-48.21 (11)
Zn30—Zn10—Zn40—O60	50.10 (17)	C41'—Zn40—O70—C70	-7.8 (9)
C11—Zn10—Zn40—O80	-171.1 (5)	C41—Zn40—O70—C70	6.7 (9)
O70—Zn10—Zn40—O80	84.83 (19)	O60—Zn40—O70—C70	-137.3 (4)
O50—Zn10—Zn40—O80	-0.83 (16)	O80—Zn40—O70—C70	138.4 (4)
O60—Zn10—Zn40—O80	-85.6 (2)	Zn30—Zn40—O70—C70	-179.5 (4)
Zn20—Zn10—Zn40—O80	34.99 (11)	Zn10—Zn40—O70—C70	-130.8 (5)
Zn30—Zn10—Zn40—O80	-35.50 (11)	Zn20—Zn40—O70—C70	132.2 (5)
C11—Zn10—Zn40—O70	104.1 (5)	C41'—Zn40—O70—Zn10	123.0 (7)
O50—Zn10—Zn40—O70	-85.7 (2)	C41—Zn40—O70—Zn10	137.5 (8)
O60—Zn10—Zn40—O70	-170.4 (2)	O60—Zn40—O70—Zn10	-6.44 (16)
Zn20—Zn10—Zn40—O70	-49.84 (16)	O80—Zn40—O70—Zn10	-90.80 (16)
Zn30—Zn10—Zn40—O70	-120.33 (16)	Zn30—Zn40—O70—Zn10	-48.68 (12)
C11—Zn10—Zn40—Zn30	-135.6 (5)	Zn20—Zn40—O70—Zn10	-97.00 (17)
O70—Zn10—Zn40—Zn30	120.33 (16)	C41'—Zn40—O70—Zn20	-140.0 (7)
O50—Zn10—Zn40—Zn30	34.67 (12)	C41—Zn40—O70—Zn20	-125.5 (8)
O60—Zn10—Zn40—Zn30	-50.10 (17)	O60—Zn40—O70—Zn20	90.56 (16)
Zn20—Zn10—Zn40—Zn30	70.49 (3)	O80—Zn40—O70—Zn20	6.20 (15)
C11—Zn10—Zn40—Zn20	153.9 (5)	Zn30—Zn40—O70—Zn20	48.32 (11)
O70—Zn10—Zn40—Zn20	49.84 (16)	Zn10—Zn40—O70—Zn20	97.00 (17)
O50—Zn10—Zn40—Zn20	-35.82 (12)	Zn10—O70—C70—C72	-59.0 (7)
O60—Zn10—Zn40—Zn20	-120.59 (17)	Zn20—O70—C70—C72	-178.5 (5)
Zn30—Zn10—Zn40—Zn20	-70.49 (3)	Zn40—O70—C70—C72	60.7 (7)
C21'—Zn20—Zn40—C41'	-4.7 (16)	Zn10—O70—C70—C71	-179.8 (5)
C21—Zn20—Zn40—C41'	-18.7 (18)	Zn20—O70—C70—C71	60.8 (7)
O50—Zn20—Zn40—C41'	177.2 (12)	Zn40—O70—C70—C71	-60.0 (7)
O70—Zn20—Zn40—C41'	91.3 (12)	Zn10—O70—C70—C73	60.5 (7)
O80—Zn20—Zn40—C41'	-97.9 (12)	Zn20—O70—C70—C73	-59.0 (6)
Zn10—Zn20—Zn40—C41'	141.2 (12)	Zn40—O70—C70—C73	-179.8 (4)
Zn30—Zn20—Zn40—C41'	-148.0 (12)	C31—Zn30—O80—C80	16.6 (10)
C21'—Zn20—Zn40—C41	-8.7 (14)	C31'—Zn30—O80—C80	-15.7 (9)

C21—Zn20—Zn40—C41	-22.7 (17)	O50—Zn30—O80—C80	138.4 (5)
O50—Zn20—Zn40—C41	173.2 (10)	O60—Zn30—O80—C80	-137.2 (5)
O70—Zn20—Zn40—C41	87.3 (10)	Zn40—Zn30—O80—C80	-130.6 (5)
O80—Zn20—Zn40—C41	-101.9 (10)	Zn20—Zn30—O80—C80	132.2 (5)
Zn10—Zn20—Zn40—C41	137.2 (10)	Zn10—Zn30—O80—C80	-179.5 (5)
Zn30—Zn20—Zn40—C41	-152.0 (10)	C31—Zn30—O80—Zn20	-115.6 (9)
C21'—Zn20—Zn40—O60	178.7 (10)	C31'—Zn30—O80—Zn20	-148.0 (8)
C21—Zn20—Zn40—O60	164.7 (14)	O50—Zn30—O80—Zn20	6.15 (16)
O50—Zn20—Zn40—O60	0.66 (16)	O60—Zn30—O80—Zn20	90.56 (17)
O70—Zn20—Zn40—O60	-85.24 (19)	Zn40—Zn30—O80—Zn20	97.14 (17)
O80—Zn20—Zn40—O60	85.5 (2)	Zn10—Zn30—O80—Zn20	48.32 (12)
Zn10—Zn20—Zn40—O60	-35.39 (11)	C31—Zn30—O80—Zn40	147.3 (9)
Zn30—Zn20—Zn40—O60	35.44 (11)	C31'—Zn30—O80—Zn40	114.9 (8)
C21'—Zn20—Zn40—O80	93.3 (11)	O50—Zn30—O80—Zn40	-90.99 (17)
C21—Zn20—Zn40—O80	79.2 (14)	O60—Zn30—O80—Zn40	-6.58 (16)
O50—Zn20—Zn40—O80	-84.8 (2)	Zn20—Zn30—O80—Zn40	-97.14 (17)
O70—Zn20—Zn40—O80	-170.7 (2)	Zn10—Zn30—O80—Zn40	-48.82 (12)
Zn10—Zn20—Zn40—O80	-120.89 (17)	C21'—Zn20—O80—C80	2.0 (9)
Zn30—Zn20—Zn40—O80	-50.06 (17)	C21—Zn20—O80—C80	-11.3 (11)
C21'—Zn20—Zn40—O70	-96.0 (11)	O50—Zn20—O80—C80	-137.1 (5)
C21—Zn20—Zn40—O70	-110.1 (14)	O70—Zn20—O80—C80	138.5 (5)
O50—Zn20—Zn40—O70	85.90 (19)	Zn10—Zn20—O80—C80	-179.5 (4)
O80—Zn20—Zn40—O70	170.7 (2)	Zn30—Zn20—O80—C80	-131.0 (5)
Zn10—Zn20—Zn40—O70	49.86 (15)	Zn40—Zn20—O80—C80	132.3 (5)
Zn30—Zn20—Zn40—O70	120.68 (15)	C21'—Zn20—O80—Zn30	133.1 (8)
C21'—Zn20—Zn40—Zn30	143.3 (10)	C21—Zn20—O80—Zn30	119.7 (10)
C21—Zn20—Zn40—Zn30	129.3 (13)	O50—Zn20—O80—Zn30	-6.10 (16)
O50—Zn20—Zn40—Zn30	-34.78 (12)	O70—Zn20—O80—Zn30	-90.49 (16)
O70—Zn20—Zn40—Zn30	-120.68 (15)	Zn10—Zn20—O80—Zn30	-48.50 (12)
O80—Zn20—Zn40—Zn30	50.06 (17)	Zn40—Zn20—O80—Zn30	-96.70 (18)
Zn10—Zn20—Zn40—Zn30	-70.82 (3)	C21'—Zn20—O80—Zn40	-130.2 (8)
C21'—Zn20—Zn40—Zn10	-145.9 (10)	C21—Zn20—O80—Zn40	-143.6 (9)
C21—Zn20—Zn40—Zn10	-159.9 (13)	O50—Zn20—O80—Zn40	90.60 (17)
O50—Zn20—Zn40—Zn10	36.05 (12)	O70—Zn20—O80—Zn40	6.21 (15)
O70—Zn20—Zn40—Zn10	-49.86 (15)	Zn10—Zn20—O80—Zn40	48.21 (12)
O80—Zn20—Zn40—Zn10	120.89 (17)	Zn30—Zn20—O80—Zn40	96.70 (18)
Zn30—Zn20—Zn40—Zn10	70.82 (3)	C41'—Zn40—O80—C80	5.2 (9)
O70—Zn10—C11—C12	-9.6 (16)	C41—Zn40—O80—C80	-14.8 (10)
O50—Zn10—C11—C12	116.0 (12)	O60—Zn40—O80—C80	136.7 (4)
O60—Zn10—C11—C12	-131.8 (12)	O70—Zn40—O80—C80	-139.1 (4)
Zn20—Zn10—C11—C12	57.9 (16)	Zn30—Zn40—O80—C80	130.1 (5)
Zn40—Zn10—C11—C12	-76.4 (15)	Zn10—Zn40—O80—C80	179.0 (4)
Zn30—Zn10—C11—C12	172.5 (10)	Zn20—Zn40—O80—C80	-132.9 (5)
C21'—Zn20—C21—C22	55 (6)	C41'—Zn40—O80—Zn30	-124.9 (8)
O50—Zn20—C21—C22	-93 (2)	C41—Zn40—O80—Zn30	-144.9 (9)
O70—Zn20—C21—C22	30 (3)	O60—Zn40—O80—Zn30	6.59 (16)
O80—Zn20—C21—C22	160 (2)	O70—Zn40—O80—Zn30	90.76 (16)
Zn10—Zn20—C21—C22	-42 (3)	Zn10—Zn40—O80—Zn30	48.88 (12)
Zn30—Zn20—C21—C22	-145 (2)	Zn20—Zn40—O80—Zn30	96.95 (19)

supplementary materials

Zn40—Zn20—C21—C22	106 (3)	C41'—Zn40—O80—Zn20	138.2 (8)
C21—Zn20—C21'—C22'	179 (9)	C41—Zn40—O80—Zn20	118.1 (9)
O50—Zn20—C21'—C22'	-144 (2)	O60—Zn40—O80—Zn20	-90.36 (17)
O70—Zn20—C21'—C22'	-21 (3)	O70—Zn40—O80—Zn20	-6.19 (15)
O80—Zn20—C21'—C22'	96 (3)	Zn30—Zn40—O80—Zn20	-96.95 (19)
Zn10—Zn20—C21'—C22'	-81 (3)	Zn10—Zn40—O80—Zn20	-48.08 (12)
Zn30—Zn20—C21'—C22'	154 (2)	Zn30—O80—C80—C81	59.5 (7)
Zn40—Zn20—C21'—C22'	38 (3)	Zn20—O80—C80—C81	179.6 (5)
C31'—Zn30—C31—C32	22 (2)	Zn40—O80—C80—C81	-59.1 (7)
O50—Zn30—C31—C32	170.8 (19)	Zn30—O80—C80—C82	180.0 (5)
O80—Zn30—C31—C32	-82 (2)	Zn20—O80—C80—C82	-59.9 (7)
O60—Zn30—C31—C32	58 (3)	Zn40—O80—C80—C82	61.3 (7)
Zn40—Zn30—C31—C32	-18 (4)	Zn30—O80—C80—C83	-61.8 (7)
Zn20—Zn30—C31—C32	-140.9 (19)	Zn20—O80—C80—C83	58.3 (7)
Zn10—Zn30—C31—C32	123.6 (19)	Zn40—O80—C80—C83	179.5 (5)

Fig. 1

