

unit, the phen,²² bpy,²² tren,^{5b} and DMEPA⁶ complexes show slight anisotropy in the high-field region. Complex 1 displays evidence of anisotropy in both high-field and low-field regions of the spectrum.

Concluding Remarks. The hexadentate ligand tpen has the appropriate geometry to span across an $\{\text{Mn}_2\text{O}_2\}^{3+}$ core, thus leaving open two syn-oriented coordination sites that are perpendicular to the Mn_2O_2 plane. The spectral, magnetic, and electrochemical properties of 1 are very similar to those of other species which contain the $\{\text{Mn}_2\text{O}_2\}^{3+}$ core. In compound 1, the syn-oriented coordination sites are occupied by a bridging acetate

ligand. Our current efforts are directed toward removing this acetate group so that water, hydroxide, and/or other substrate molecules may coordinate to the oxo-bridged dimer.

Acknowledgment. This work was supported by Grant No. GM 382751 from the National Institute of General Medical Sciences.

Supplementary Material Available: For $[\text{Mn}_2\text{O}_2(\text{O}_2\text{CCH}_3)(\text{tpen})](\text{ClO}_4)_2 \cdot 2\text{CH}_3\text{CN}$, a fully labeled ORTEP drawing (Figure S1), electronic and EPR spectra (Figures S2 and S3), plots of observed and calculated molar susceptibilities and moments as a function of temperature (Figure S4), and tables of crystal data and data collection parameters (Table S1), atomic positional parameters (Table S2), anisotropic thermal parameters (Table S3), and intramolecular bond distances and angles (Tables S4 and S5) (12 pages); a listing of observed and calculated structure factors (Table S6) (29 pages). Ordering information is given on any current masthead page.

(22) Cooper, S. R.; Dismukes, G. C.; Klein, M. P.; Calvin, M. J. *Am. Chem. Soc.* 1978, 100, 7248–7252.

Additions and Corrections

1990, Volume 29

N. Sreehari, Babu Varghese, and P. T. Manoharan*: Crystal and Molecular Structure of Dimeric Bis[*N,N*-di-*n*-propylidithiocarbamate]zinc(II) and the Study of Exchange-Coupled Copper(II)–Copper(II) Pairs in Its Lattice.

Pages 4011–4015. The space group of the title compound is $P2_1/c$ rather than $P2_1$. The structure solved in $P2_1/c$ has a final R value of 0.044 and $R_w = 0.047$. Side chains are found to have disorder.

We gratefully acknowledge the suggestions from Dr. Richard E. Marsh of the Beckman Institute at Caltech, Pasadena, CA.

Supplementary Material Available: Tables of fractional coordinates, anisotropic thermal parameters, bond lengths, bond angles, relevant torsion angles, and least-squares mean planes (5 pages); a listing of structure factors (9 pages). Ordering information is given on any current masthead page.—P. T. Manoharan

1991, Volume 30

Kimoon Kim,* Won S. Lee, Hee-Joon Kim, Sung-Hee Cho, Gregory S. Girolami,* Philip A. Gorlin, and Kenneth S. Suslick*: Synthesis and Structure of Transition-Metal Bis(porphyrinato) Complexes. Characterization of $\text{Zr}(\text{TPP})_2$ and $\text{Zr}(\text{OEP})_2$.

Pages 2653–2654. The crystal structure of $\text{Zr}(\text{TPP})_2$ was described incorrectly in space group $C2/c$ and should be in the orthorhombic space group $Fddd$. The lattice vectors $[100][010][102]$ define the new F -centered cell: $a' = 21.120(5) \text{ \AA}$, $b' = 21.286(6) \text{ \AA}$, $c' = 30.805(11) \text{ \AA}$, $V = 13901(7) \text{ \AA}^3$, $Z = 8$. The corresponding coordinate transformations are $x' = x - z/2 + 0.25$, $y' = y + 0.25$, and $z' = z/2$. Further refinement with the orthorhombic-averaged data improved the structure, notably the description of the disordered solvate molecule, which is best described as CH_2Cl_2 . The new formula of the crystal structure is $\text{Zr-N}_8\text{C}_{88}\text{H}_{156}\cdot\text{CH}_2\text{Cl}_2$ ($\text{fw} = 1401.63$), which is also consistent with the elemental analysis of the bulk material and measured density, as reported. The final residuals were $R_F = 0.058$ and $R_{wF} = 0.060$ for 226 variables and 966 independent reflections with $I > 3\sigma(I)$. This revision did not change the overall structure of the $\text{Zr}(\text{TPP})_2$ molecule, which now has exact 222 symmetry, and no changes in bond lengths or angles exceeded previous standard deviations. Revised versions of Tables II and III follow. We thank Dr. R. E. Marsh for bringing this issue to our attention.

Supplementary Material Available: Revised tables of anisotropic thermal parameters, bond distances, bond angles, least-squares planes, and dihedral angles (4 pages); a revised listing of structure factors (5 pages). Ordering information is given on any current masthead page.

Table II'. Positional and Equivalent Isotropic Thermal Parameters for $\text{Zr}(\text{TPP})_2 \cdot \text{CH}_2\text{Cl}_2^{a,b}$

atom	<i>x</i>	<i>y</i>	<i>z</i>	$B_{\text{eq}}, \text{ \AA}^2$
Zr	-0.1250	0.3750	0.3750	2.49 (3)
Cl	0.1350 (9)	1.0088 (9)	0.6686 (6)	11.0 (5)*
N1	-0.2152 (3)	0.3454 (3)	0.3332 (2)	2.5 (2)
N2	-0.0938 (3)	0.2846 (3)	0.3337 (2)	2.7 (2)
C1	-0.2662 (3)	0.3825 (4)	0.3227 (3)	2.9 (2)
C2	-0.3163 (4)	0.3453 (4)	0.3049 (3)	3.5 (2)
C3	-0.2960 (4)	0.2859 (4)	0.3027 (3)	3.6 (2)
C4	-0.2336 (4)	0.2855 (4)	0.3198 (3)	3.0 (2)
C5	-0.1958 (4)	0.2318 (4)	0.3199 (3)	2.8 (2)
C6	-0.1309 (4)	0.2321 (3)	0.3261 (3)	2.8 (2)
C7	-0.0921 (4)	0.1782 (4)	0.3202 (3)	3.6 (2)
C8	-0.0317 (4)	0.1972 (4)	0.3223 (3)	3.2 (2)
C9	-0.0323 (4)	0.2638 (4)	0.3293 (3)	2.7 (2)
C10	0.0203 (4)	0.3016 (4)	0.3253 (3)	2.7 (2)
C21	-0.2272 (4)	0.1721 (4)	0.3042 (3)	3.3 (2)
C22	-0.2714 (4)	0.1423 (5)	0.3289 (3)	5.0 (3)
C23	-0.3030 (5)	0.0884 (5)	0.3125 (4)	6.2 (3)
C24	-0.2890 (5)	0.0682 (5)	0.2719 (4)	7.0 (3)
C25	-0.2451 (5)	0.0975 (5)	0.2469 (4)	6.4 (3)
C26	-0.2133 (4)	0.1496 (4)	0.2632 (3)	5.3 (3)
C27	0.0832 (4)	0.2714 (4)	0.3178 (3)	3.2 (2)
C28	0.0941 (4)	0.2320 (4)	0.2824 (3)	4.2 (2)
C29	0.1512 (4)	0.2033 (4)	0.2770 (3)	4.9 (3)
C30	0.2008 (5)	0.2143 (5)	0.3054 (4)	6.2 (3)
C31	0.1902 (5)	0.2554 (5)	0.3401 (3)	5.7 (3)
C32	0.1320 (4)	0.2829 (4)	0.3466 (3)	4.6 (2)
C33	0.125	0.975 (2)	0.625	11 (1)*

^aThe original numbering scheme is retained. ^bStarred values indicate atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as $(4/3)[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos \gamma)B(1,2) + ac(\cos \beta)B(1,3) + bc(\cos \alpha)B(2,3)]$.

Table III'. Selected Bond Lengths (Å) and Angles (deg) in $\text{Zr}(\text{TPP})_2 \cdot \text{CH}_2\text{Cl}_2^a$

	Zr–N1	2.390 (6)	Zr–N2	2.400 (6)
N1–Zr–N1'	114.8 (2)		N1–Zr–N1''	73.8 (2)
N1–Zr–N1'''	149.4 (2)		N1–Zr–N2	72.9 (2)
N1–Zr–N2'	74.0 (2)		N1–Zr–N2''	81.6 (2)
N1–Zr–N2'''	135.9 (2)		N2–Zr–N2'	116.0 (2)
N2–Zr–N2''	148.0 (2)		N2–Zr–N2'''	73.3 (2)

^aPrimed atoms are on the same porphyrin pyrrole ring, and double- and triple-primed atoms are on the other ring.

—Kimoon Kim, Gregory S. Girolami, and Kenneth S. Suslick