

Au(1)···Au(3) distances range from 5.0 Å in the cis configuration,  $\phi = 0^\circ$ , to 6.7 Å in the trans configuration,  $\phi = 180^\circ$ , with a value of 5.8 Å for  $\phi = 90^\circ$ . The peak (3) in the RDF at 5.8 Å strongly supports the choice of  $\phi = 90^\circ$ .

Two possible gold-sulfur frameworks for the Myochrisin structure are indicated in Figure 2. Of the possibilities for cyclic structures only the closed hexamer of Figure 2 can satisfy Au-S = 2.30 Å, Au(1)···Au(2) = 3.35 Å, and Au(1)···Au(3) = 5.8 Å. For instance, a closed tetramer would have Au(1)···Au(3) = 4.6 Å, whereas a pentamer would have 5.2 Å for that distance. A heptameric structure is quite irregular with a variety of Au(1)···Au(3) type distances from 4.6 to 6.4 Å. Although an octamer can be symmetric, the Au(1)···Au(3) type distance becomes 6.2 Å. The one difficulty with the closed hexamer is that the Au(1)···Au(4) distance is predicted to be 6.7 Å, where no excess density is found in the RDF. Although there is only one distance of the type Au(1)···Au(4) for two of the types assigned to peaks 2 and 3, the absence of a noticeable peak at 6.7 Å makes it unlikely that a closed structure occurs. The open structure, as in the pentamer of Figure 2, solves the Au(1)···Au(4) problem by turning out rather than in. That structure yields a distance of 8.1 Å in agreement with peak 4. The open-chain structure can be composed of any number of units and still give distances in accord with peaks

1-4 in the RDF. For an open structure one additional ligand is required to end the chain as indicated in Figure 2. Preparations of the drug frequently contain "excess" ligand<sup>15</sup> and could satisfy the formula Au<sub>n</sub>(ligand)<sub>n+1</sub>. The length of the chain is currently a matter of conjecture; however, the work of Sadler<sup>16</sup> would suggest a hexamer as most likely in solution.

The use of WAXS and EXAFS as complementary tools is very promising. EXAFS defines the first coordination sphere most precisely, while WAXS can give information over more extended distances. The paired techniques should be extremely useful for studying cluster species.

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(15) Rudge, S. R.; Perrett, D.; Swannell, A. J.; Drury, P. L. *J. Rheumatol.* **1984**, *11*, 150.

(16) Isab. A. A.; Sadler, P. J. *J. Chem. Soc., Dalton Trans.* **1982**, 135.

## Additions and Corrections

**Molecular Mechanical Studies of Inclusion of Alkali Cations into Anisole Spherands** [*J. Am. Chem. Soc.* **1985**, *107*, 2212-2219]. PETER A. KOLLMAN,\* GEORGES WIPFF, and U. CHANDRA SINGH

Pages 2216 and 2217: The captions for Figures 3 and 4 were inadvertently reversed. Figure 3 corresponds to structure Li<sup>+</sup>/3b and Figure 4 to structure Li<sup>+</sup>/3a.

**Stereoselective Synthesis and Biological Activity of  $\beta$ - and  $\alpha$ -D-Arabinose 1,5-Diphosphate: Analogues of a Potent Metabolic Regulator** [*J. Am. Chem. Soc.* **1984**, *106*, 7851]. BRUCE E. MARYANOFF,\* ALLEN B. REITZ, GENE F. TUTWILER, STEPHEN J. BENKOVIC, PATRICIA A. BENKOVIC, and SIMON J. PILKIS

Page 7853: In the synthesis of known compound 5, "pyridine/HOAc" should read as "pyridine/Ac<sub>2</sub>O".

**Optimized Intermolecular Potential Functions for Amides and Peptides. Hydration of Amides** [*J. Am. Chem. Soc.* **1985**, *107*, 1489-1496]. WILLIAM L. JORGENSEN\* and CAROL J. SWENSON

Page 1495: The solute-water interaction energies in Table III for NMA and DMF are incorrect. The correct values are given below. No changes in the text are required.

atom	solute-water energy	
	NMA	DMF
N	-1.00	-0.87
C	-0.12	-0.84
O	-4.41	-4.68
H <sub>N</sub> trans	-3.80	
CH <sub>3</sub> cis	-0.34	-0.42
CH <sub>3</sub> trans		-0.38
CH <sub>3</sub> on C	-0.32	