through the nitrogen atom (Co-NS) and not through the sulfur atom. The oxidation of the Co-NS moiety with oxygen may lead to the formation of two possible products CoNSO⁻ (linear thiazate) or CoN(O)S⁻ (thionitro), which could be distinguished by IR spectrum.¹⁰ Thus the bands due to asymmetric, symmetric stretching, and bending modes of the coordinated thiazate group (NSO⁻) appear at 1160, 1060, and 565 cm⁻¹, respectively, and those of thiazate ion (linear NSO⁻ group) at 1270, 990, and 515 cm⁻¹, respectively. It is therefore presumed that the ligand NSO- in the cobalt complex is bonded not as thiazate but in the thionitro



form. The far-IR spectrum of (I) showed two bands at 355 and 390 cm⁻¹ assigned to ν (Co-Cl).

The complex was prepared a number of times. In each case the melting point of the compound was found in the range ± 2 °C. Under the experimental conditions the possibility of formation of a mixture of many geometrical isomers exists. However, the consistancy of the product suggests that it is one of the many possible isomers.

The reduction of trithiazyl trichloride to tetrasulfur tetranitride by iron¹¹ and copper¹² has been reported recently, but no one has used a complex for the reduction of (NSCl)₃. This novel route for the preparation of S_4N_4 is of importance since it is one of the most valuable starting materials for preparing other inorganic sulfur-nitrogen compounds.

Registry No. I, 80028-18-8; (NSCl)₃, 5964-00-1; CoH[P(OPh)₃]₄, 41089-90-1.

- (10) Armitage, D. A.; Brand, J. C. J. Chem. Soc., Chem. Commun. 1979, 1078. Pandey, K. K.; Agarwala, U. C. Indian J. Chem. 1981, 20, 906.
- (11) Banister, A. J.; Fielder, A. J.; Hey, R. G.; Smith, N. R. M. J. Chem. Soc., Dalton. Trans. 1980, 1457.
- (12) Berthen, M. P.; Vinneht, H.; Monteil, Y. Z. Naturforsch., B: Anorg. Chem., Org. Chem. 1980, 35, 329.

Contribution from the Gibbs Chemical Laboratories, Harvard University, Cambridge, Massachusetts 02138, and the Department of Chemistry, Brandeis University, Waltham, Massachusetts 02154

Boron Hydride Valence Structures. A Topological Approach

W. N. Lipscomb* and I. R. Epstein

Received September 18, 1981

We wish to correct two labeling errors in our previously published paper¹ having the above title and to make two ad-

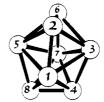


Figure 1. Numbering system for $B_8H_8^{2-}$ valence structures.

ditions, prompted by recent interest^{2,3} in these topological three-center bond structures.

For B_6H_{10} the doubly degenerate valence structure should be labeled as 1-2,2-6. For hypothetical $B_8H_8^{2-}$ of D_{4d} symmetry, the labeling should read 1-2,1-5,5-8. These errors arose from translation of the numbering system used in the computer program into the conventional numbering system of the publication.¹ The computer program itself produced correct results, and in particular yielded correctly both the number and the topology of these valence structures.

The first addition is the list of two-center, three-center valence structures for B_8H_8 of D_{2d} symmetry, which is connected as shown in Figure 1. We list here the type (a-e), two-center bonds, and number of equivalent structures (in parentheses) as follows: a, 12,47,48 (4); b, 12,48,67 (2); c, 12,48,78 (4); d, 23,26,56 (2); e 25,26,36 (2). Thus, there are 14 valence structures.

The second addition concerns $B_{12}H_{12}^{2-}$, for which we refer the reader to the publication by $Gielen^2$ Our program has selected 240 structures as follows: 20 of type 27_b⁺, 20 of type 27_{b}^{-} (both of C_{3} symmetry); 60 of type 31^{+} , 60 of type 31^{-} (both of C_1 symmetry); 20 of type 39 (of C_{3v} symmetry); and 30 of type 40⁺, 30 of type 40⁻ (both of C_2 symmetry). Gielen's paper contains a complete specification of the two-center and three-center bonds in these valence structures. Thus, our 240 structures correct the 5430 structures proposed by Gielen² and the 132 structures of an incomplete study supplied by us at the request of Aihara.³ Finally, in all of our valence structures the specification of locations of single bonds is sufficient to establish uniquely the positions of three-center bonds.

Acknowledgment. We thank the National Science Foundation, Grant No. CHE77-19899, for support and acknowledge the questions that were raised by M. Gielen, which led us to these corrections and additions.

Registry No. $B_8H_8^{2-}$, 12430-13-6; $B_{12}H_{12}^{2-}$, 12356-13-7.

- I. R. Epstein and W. N. Lipscomb, Inorg. Chem., 10, 1921 (1971).
 M. Gielen, Bull. Soc. Chim. Belg., 90, 501 (1981).
- (3) J. Aihara, J. Am. Chem. Soc., 100, 3339 (1978).

[•] To whom correspondence should be addressed at Harvard University.