Additions and Corrections

1975, Volume 14

P. R. Robinson, E. O. Schlemper,* and R. Kent Murmann*: Characterization and Structures of Two Protonated Tetracyanomolybdenum(IV) Oxy Ions.

Page 2039. Table XI. Selected Interionic Distances Less Than 3.5 Å for $[Cr(en)_3][MoO(OH)(CN)_4]\cdot H_2O$

Distance	Value, Å	Distance	Value, Å
O(1)-N(4)	2.945 (6)	O(2)[a]-N(1)	2.87 (1)
O(1)-N(5)	2.871 (7)	N(2)-N(3)	3.097 (8)
O(2)[a]-N(1)	3.04 (1)	N(1)-N(3)	3.436 (9)
N(2)-N(3)	3.493 (8)	N(4)-O(2)[a]	3.061 (9)
N(2)-N(5)	2.964 (8)	N(4)-O(2)[a]	3.088 (9)

[a] O(2) is the disordered water which has half occupancy at each site. These sites are separated by 1.226 Å.

E. O. Schlemper

Author Index to Volume 14, 1975.

Page 3154. The index should contain the following entry: Mathur, M. A. Trends in the proton nuclear magnetic resonance spectra of some amine-haloboranes. Steric effects. 2874—M. A. Mathur

1976, Volume 15

G. L. Robbins and R. E. Tapscott*: Tartrate-Bridged Chromium(III) Complexes. Synthesis and Characterization.

Page 155. The names given for the bis(tartrato(3−)) complexes should all read "dichromium(III)" rather than "dichromate(III)".—R. E. Tapscott

Roman Osman, Patrick Coffey, and John R. Van Wazer*: Use of Pseudopotential Theory to Study Molecular Structure. II. A NOCOR (Neglect of Core Orbitals) Calculation of the P_4 and P_2 Molecules and Their Interconversion.

Page 291. With respect to Figure 5, Professor Roald Hoffmann of Cornell University has correctly pointed out that π_g orbitals of the P_2 pair of molecules must correlate with an $a_2 + b_1 + e$ set of orbitals in the D_{2d} symmetry group corresponding to the deformed P_4 molecule and that the π_u must correlate with an $a_1 + b_2 + e$ set. Since the single-determinant SCF computations on which this figure was based were not restrained as to orbital symmetries (i.e., symmetry blocked), it turned out that there was increasing "forbidden" mixing of the molecular orbitals as the P_4 molecule was pulled apart so that the assigned D_{2d} irreducible representations presented in Figure 5 apply only to the far left-hand side of the diagram. This mixing was probably due to the loss of some of the integrals as their values fell below an arbitrary cut-off point. Because of the forbidden mixing, the calculated curve labeled $7b_2^*$ converts completely to an orbital of b_1 symmetry as the far right-hand side of the diagram is reached and likewise the curve labeled $2b_1$ converts to b_2 symmetry. Had symmetry blocking been employed in the calculations, the $7b_2^*$ orbital would have connected with the $2\pi_u$. Consequently, the $P_4 \rightarrow 2P_2$ reaction represents a "forbidden" transition in the sense that, for the ground-state structures, the highest occupied molecular orbital of one molecule correlates with the lowest unoccupied orbital of the other. This means that the enthalpy of activation presented on page 290 for this process is only an upper limit since a multi-determinant calculation would be needed to obtain a more realistic description of the transition state.—John R. Van Wazer