**Table I.** Positional and Thermal Parameters and Their Estimated Standard Deviations for Potassium Selenotrithionate[a]

| atom | $x$ | $y$ | $z$ | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|
| Se | 0.874 03 (4) | 0.168 12 (6) | 0.200 90 (2) | 228 (2) | 456 (3) | 279 (2) | 78 (2) | 78 (1) | 0 (2) |
| S(1) | 0.661 32 (9) | 0.290 83 (13) | 0.090 46 (5) | 268 (4) | 218 (5) | 205 (4) | 12 (3) | 56 (3) | 5 (3) |
| S(2) | 0.808 87 (9) | 0.239 82 (15) | 0.326 47 (5) | 239 (4) | 297 (5) | 203 (4) | −10 (4) | 37 (3) | −8 (3) |
| O(1) | 0.539 71 (25) | 0.231 5 (4) | 0.122 88 (16) | 212 (13) | 405 (15) | 360 (14) | 6 (11) | 47 (11) | 101 (11) |
| O(2) | 0.664 25 (31) | 0.164 2 (5) | 0.010 18 (16) | 559 (18) | 483 (17) | 228 (12) | 91 (14) | 70 (12) | −93 (11) |
| O(3) | 0.676 39 (28) | 0.530 1 (4) | 0.081 92 (16) | 500 (16) | 217 (14) | 435 (14) | 12 (12) | 182 (13) | 74 (11) |
| O(4) | 0.734 23 (29) | 0.455 8 (4) | 0.313 00 (15) | 508 (15) | 241 (13) | 342 (13) | 9 (12) | 199 (12) | −16 (10) |
| O(5) | 0.709 42 (27) | 0.057 9 (4) | 0.329 70 (16) | 430 (14) | 260 (13) | 322 (12) | −38 (11) | 155 (11) | 29 (10) |
| O(6) | 0.950 16 (31) | 0.234 5 (6) | 0.402 21 (18) | 332 (16) | 991 (24) | 260 (13) | 10 (16) | −43 (12) | −14 (15) |
| K(1) | 0.220 67 (9) | 0.235 20 (13) | 0.032 67 (5) | 290 (4) | 309 (4) | 244 (4) | 7 (3) | 38 (3) | 16 (3) |
| K(2) | 0.446 88 (9) | 0.278 13 (13) | 0.319 12 (5) | 323 (4) | 254 (4) | 379 (4) | 7 (3) | 91 (3) | 17 (3) |

[a] The form of the anisotropic thermal parameter is $\exp[-2\pi^2(U_{11}h^2a^{*2} + \ldots + U_{23}klb^*c^*)/10000]$.

**Table II.** Bond Distances (Å) and Angles (Deg) for Selenotrithionate

(a) Bond Distances

| | | | |
|---|---|---|---|
| Se–S(1) | 2.2566 (8) | S(2)–O(4) | 1.4448 (26) |
| Se–S(2) | 2.2567 (10) | S(2)–O(5) | 1.4474 (27) |
| S(1)–O(1) | 1.4515 (29) | S(2)–O(6) | 1.4361 (24) |
| S(1)–O(2) | 1.4495 (29) | | |
| S(1)–O(3) | 1.4385 (25) | | |

(b) Bond Angles

| | | | |
|---|---|---|---|
| S(1)–Se–S(2) | 97.896 (34) | Se–S(2)–O(4) | 108.23 (11) |
| Se–S(1)–O(1) | 106.09 (9) | Se–S(2)–O(5) | 105.36 (11) |
| Se–S(1)–O(2) | 101.01 (11) | Se–S(2)–O(6) | 103.11 (14) |
| Se–S(1)–O(3) | 107.19 (9) | O(4)–S(2)–O(5) | 111.91 (16) |
| O(1)–S(1)–O(2) | 114.66 (16) | O(4)–S(2)–O(6) | 114.13 (18) |
| O(1)–S(1)–O(3) | 112.79 (17) | O(5)–S(2)–O(6) | 113.19 (17) |
| O(2)–S(1)–O(3) | 113.78 (16) | | |

A symmetric selenotrithionate may be described by a Se–S bond distance, a S–Se–S bond angle, and the rotation of the $-SO_3$ from some arbitrary position. That arbitrary position could be the $C_{2v}$ conformation, wherein Se, the two S atoms, and two O atoms lie in a planar W, or it could be the $C_2$ conformation, wherein two oxygen atoms are in trans arrangement across the $SeS_2$ plane and are as far from the plane as possible. The choice of a reference conformation may reflect one's prejudice as to the conformation of "free" trithionate. Since the symmetry of $S_3O_6^{2-}$ in $K_2S_3O_6$[8] is $C_s$ and nearly $C_{2v}$, it might seem natural to describe the geometry of $SeS_2O_6^{2-}$ as distorted from $C_{2v}$ by approximately equal rotations of the $-SO_3$ groups around the Se–S bonds. However, an examination of the dihedral angles of the known polythionate anions reveals that in many cases the $-SO_3$ orientation conforms most nearly to the "trans $C_2$" conformation.

Thus, the selenotrithionate dianion appears as a Se atom coordinated by two $-SO_3$ groups at an angle of 97.90 (4)° and distances of 2.257 (1) Å. The dianion contains no crystallographic symmetry elements but displays approximate $C_2$ geometry. The orientation of the $-SO_3$ groups is distinctly different from that found for $S_3O_6^{2-}$, and the pentachalcogen chain O(3)–S(1)–Se–S(2)–O(5) bears a startling resemblence to the central pentachalcogen chain of the known trans pentathionate structures.

The Se–S bond length, 2.257 (1) Å, is short when compared to the corresponding distances in $Se_2S_2O_6^{2-}$[9] of 2.273 (2), 2.278 (2), 2.282 (4), and 2.295 (3) Å. There are several bond lengths for dibonded Se–dibonded S,[10-12] 2.180 (3), 2.181 (2), 2.178 (2), and 2.153 (4) Å, which should not be compared.

The bond angle at Se, 97.90 (4)°, might be compared to the bond angles at Se in the selenopentathionates,[10-12] 103.06 (11), 104.00 (8), and 104.9 (2)°, or to the average angle at dibonded Se listed by Abrahams,[13] 104°, or to the average angles at Se in the selenotetrathionates[9,14] which are of range 100.36 (11)–103.80 (7)°. With any of these comparisons, the S–Se–S bond angle in the present structure seems unusually small. It is tempting to speculate that the Se orbitals used in bonding to the two relatively electronegative $-SO_3$ groups are relatively high in p character.

The orientation of the $-SO_3$ groups is best illustrated by dihedral angles. The dihedral angle O(3)–S(1)–Se–S(2) is 84.9°, and the dihedral angle O(5)–S(2)–Se–S(1) is 78.2°. We expect these angles to be 90° in the "trans $C_2$" conformation and 60° or 120° in the $C_{2v}$ conformation. Curiously, in $Na^+$, $K^+$, and $NH_4^+$ salts of the polythionates, the corresponding angles are in the range 79–94° while in $Ba^{2+}$ and $Co(en)_2Cl_2^+$ salts, the corresponding angles are in the range 66–72°.[15] Thus, with current knowledge, there seem to be two reasonably well-delineated groups and the implication that it is the counterion which dictates $-SO_3$ orientation. We would prefer to believe that it is coincidences of packing geometry that dictate the $-SO_3$ orientation in the solid state.

**Acknowledgment.** The authors express gratitude to Professor Olav Foss of this department for stimulating discussions and guidance. V.J. thanks the Royal Norwegian Ministry of Foreign Affairs for a Norwegian Government Scholarship.

**Registry No.** $K_2SeS_2O_6$, 15099-06-6.

**Supplementary Material Available:** Listing of observed and calculated structure factors (8 pages). Ordering information is given on any current masthead page.

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# Metal Binding to N(1) of 9-Methyladenine in the 1:1 Complex with Methylmercuric Nitrate

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A large body of structural data is now available concerning metal complexes with DNA bases, and the coordination sites normally used have been identified for all the bases. For N(9)-blocked adenine ligands, imidazolic nitrogen N(7) is considered as the primary target for most metal ions. This statement is supported by a number of crystal structures[1] as

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(1) Hodgson, D. J. *Prog. Inorg. Chem.* **1977**, *23*, 211.

well as results from spectroscopic and other techniques.[2] However, the acceptor properties of N(1) are not believed to be much weaker than those of N(7). Indeed, N(1) is the site occupied by $H^+$ ions in monoprotonated adenine rings, and many complexes have been prepared in which both N(1) and N(7) are involved in coordination. Metal binding to N(1) exclusively has been observed so far in only one crystal structure: the 9-methyladeninium salt of $[ZnCl_3(m^9Ade)]^-$ where $m^9Ade$ is 9-methyladenine.[3] This compound was isolated from a mixture containing the N(1),N(7)-coordinated compound $ZnCl_2(m^9Ade)$ as the major component.[4]

We have recently reported the crystal structure of a 1:2 complex of 9-methyladenine with $CH_3Hg^+$ in which mercury binds to two uncommon sites, that is, N(1) and the deprotonated amino group.[5] Since no previous structures of amino-bonded compounds were available, it was not clear whether N(1)-coordination was promoted by initial deprotonation and metalation of the amino group or N(1) should be recognized as the primary target in the case of $CH_3Hg^+$ ions. Selective coordination of $CH_3Hg^+$ to N(1) in adenosine was first proposed by Simpson on the basis of UV spectra,[6] and the same conclusion was reached more recently by Tobias and coworkers from Raman spectroscopy.[7] The present crystallographic study provides further evidence that $CH_3Hg^+$ ions, unlike many other metallic species studied so far, show a preference for N(1) as the first binding site in adenine rings.

## Experimental Section

**Crystal data**: $C_7H_{10}HgN_6O_3$; fw 426.8; triclinic, of space group $P\bar{1}$ with $a = 7.010$ (3) Å, $b = 7.432$ (3) Å, $c = 10.763$ (2) Å, $\alpha = 82.62$ (3)°, $\beta = 86.76$ (3)°, $\gamma = 87.39$ (4)°, $V = 554.8$ Å$^3$, $Z = 2$, $D_o = 2.52$ g cm$^{-3}$ (flotation in bromobenzene–bromoform), $D_c = 2.55$ g cm$^{-3}$; $\mu$(Mo K$\alpha$) = 138.7 cm$^{-1}$, $\lambda$(Mo K$\bar{\alpha}$) = 0.71069 Å (graphite monochromator), $T = 23$°C.

**Preparation.** The compound was prepared from a 1:1 mixture of 9-methyladenine and $CH_3HgNO_3$ in hot water. Crystals suitable for X-ray work formed overnight.

**Crystallographic Measurements.** The crystal used was needle-shaped with the following dimensions between pairs of opposite faces: 0.011 mm (101 and $\bar{1}0\bar{1}$), 0.095 mm ($10\bar{1}$ and $\bar{1}01$), and 0.45 mm (011 and $0\bar{1}\bar{1}$).

A set of precession photographs showed triclinic Laue symmetry with $P1$ or $P\bar{1}$ as possible space groups. The crystal was mounted on an Enraf-Nonius CAD4 diffractometer, and the cell parameters were determined from least-squares refinement of the setting angles for 25 centered reflections. Intensity data were collected by using the $\omega$–$2\theta$ scan technique. A fixed slit of 3.5 mm was used, and the scan range was $\omega = (0.70 + 0.35 \tan \theta)$° extended 25% on either side for background. Prescans at 10° min$^{-1}$ were made for each reflection. When net intensity $I$ was less than its standard deviation $\sigma(I)$, the reflection was labeled "weak" and not remeasured at lower speed. For accepted reflections, scan speed $S$ between 10 and 0.5° min$^{-1}$ was automatically selected to make $I/\sigma(I) = 100$, but scan time was limited to $\leq 120$ s. Three standard reflections used as a check on instrument and crystal stability showed only random fluctuation. Crystal orientation was checked every 100 reflections by recentering three axial reflections. If a difference >0.10° was found between any scattering vector and the direction deduced form the orientation matrix, a new matrix was defined.

**Table I.** Refined Fractional Coordinates of $[CH_3Hg(m^9Ade)]NO_3$ ($\times 10^4$; for Hg $\times 10^5$)

| atom | $x$ | $y$ | $z$ |
|---|---|---|---|
| Hg(1) | 29968 (6) | 30671 (6) | 2458 (3) |
| N(1) | 1980 (13) | 2844 (11) | 2164 (8) |
| C(2) | 147 (15) | 3524 (15) | 2365 (10) |
| N(3) | −784 (13) | 3500 (13) | 3457 (8) |
| C(4) | 227 (14) | 2643 (14) | 4411 (9) |
| C(5) | 2047 (14) | 1901 (13) | 4326 (9) |
| C(6) | 2986 (14) | 2029 (14) | 3140 (9) |
| N(6) | 4761 (13) | 1347 (14) | 2925 (8) |
| N(7) | 2607 (13) | 1082 (12) | 5501 (8) |
| C(8) | 1109 (16) | 1407 (16) | 6256 (9) |
| N(9) | −373 (12) | 2357 (12) | 5643 (7) |
| C(11) | 4077 (19) | 3469 (20) | −1597 (11) |
| C(19) | −2263 (17) | 2900 (18) | 6191 (12) |
| N(10) | 1848 (13) | 8357 (13) | 205 (8) |
| O(1) | 1033 (16) | 6933 (13) | 464 (11) |
| O(2) | 1726 (18) | 9517 (13) | 949 (9) |
| O(3) | 2765 (16) | 8714 (19) | −786 (11) |

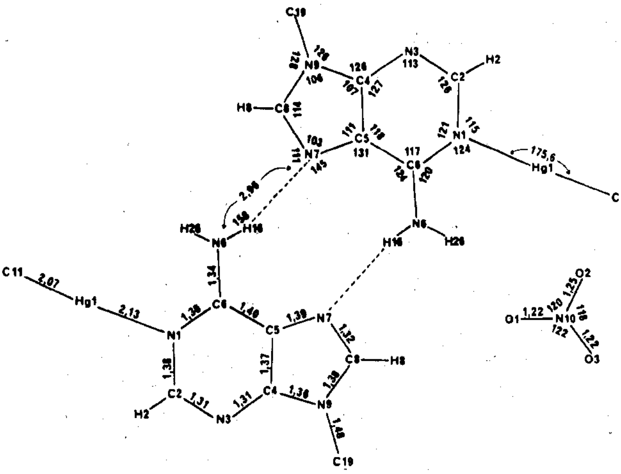

**Figure 1.** Interatomic distances and bond angles. The esd's are 0.015 Å and 0.5–1.0°, respectively, except for those involving mercury, 0.008 Å and 0.3°, respectively.

A total of 2340 independent reflections ($hkl$, $h\bar{k}l$, $\bar{h}kl$, and $\bar{h}\bar{k}l$; $2\theta \leq 54$°) were measured by using an Enraf-Nonius option NEEDLE, a procedure to measure intensity at the $\psi$ position where absorption is minimum. Net intensity $I$ was calculated from $I = (P - 2B)S$, where $P$ is the peak count and $B$ is the total background counted during half of the scanning time. The standard deviation was obtained from $\sigma^2(I) = (P + 4B)S^2 + (0.04I)^2$. A set of 1920 reflections with $I \geq 2.5\sigma(I)$ was retained for structure determination. An absorption correction was applied (Gaussian integration; grid $10 \times 10 \times 10$, program NRC-3 by F. R. Ahmed and P. Singh). Transmission factors ranged from 0.27 to 0.41. The data were finally corrected for $Lp$.

**Structure Determination.** The structure was solved by the heavy-atom method and refined by full-matrix least squares in the early stages. The function minimized was $\sum w(|F_o| - |F_c|)^2$. The centrosymmetric space group $P\bar{1}$ was first assumed, and this choice was later confirmed by successful refinement. Mercury was easily located from a three-dimensional Patterson synthesis. The remaining nonhydrogen atoms were found on the Fourier map phased on mercury. Isotropic refinement with unit weights converged to $R = \sum||F_o| - |F_c||/\sum|F_o| = 0.097$. Refinement was continued by using the block-diagonal approximation. Anisotropic temperature factors were defined for all nonhydrogen atoms. H(2), H(8), H(16), and H(26) were fixed at their calculated positions (on the assumption of $sp^2$ hybridization for the amino group; C–H = 0.95 Å, N–H = 0.87 Å) with temperature factors $B = 4.0$ Å$^2$. Hydrogen parameters were not refined. The hydrogens of the methyl groups were not located. Individual weights based on counting statistics $w = 1/\sigma(F)$ were applied in the last least-squares cycles. Anisotropic refinement of all nonhydrogen atoms and of the scale factor converged to $R = 0.041$ and $R_w = [\sum w(|F_o| - |F_c|)^2/\sum w|F_o|^2]^{1/2} = 0.055$. General background in the final $\Delta F$ map was <0.7 e Å$^{-3}$ except for a few peaks of ~1.5 e Å$^{-3}$ near mercury. There were no indications from the map that the space group could be $P1$ instead of $P\bar{1}$.

The form factors used were those of Cromer and Waber,[8] except

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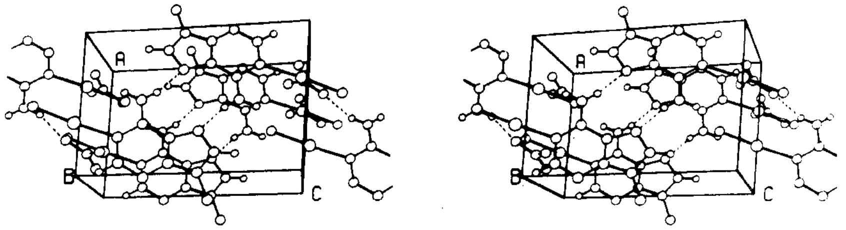

**Figure 2.** Stereoscopic view of the unit cell of $[CH_3Hg(m^9Ade)]NO_3$. Mercury and hydrogen are represented by large and small spheres, respectively. Ligand atoms can be identified by reference to Figure 1. Methyl hydrogen atoms were not found.

for the case of hydrogen.[9] Anomalous dispersion terms $f'$ and $f''$ were used for Hg.[10]

The refined coordinates are listed in Table I. Anisotropic temperature factors and hydrogen coordinates are given as supplementary material.

## Description of the Structure

The structure consists of an uncoordinated nitrate ion and a $[CH_3Hg(m^9Ade)]^+$ complex in which mercury is bonded to N(1). Interatomic distances and bond angles are shown in Figure 1.

Mercury exhibits the common linear coordination, forming normal bonds with N(1) of the pyrimidine ring (Hg–N = 2.13 (1) Å) and a methyl group (Hg–C = 2.07 (1) Å). Deviation from linearity (C–Hg–N = 175.6 (4)°) is significant but within the range that may reasonably be ascribed to packing forces. The significant difference between Hg(1)–N(1)–C(2) (115 (1)°) and Hg(1)–N(1)–C(6) (124 (1)°) may be related to steric effects of H(26) (see Discussion), but crystal packing might also be responsible for such a small departure (4.5°) from the bisecting position.

Ligand geometry is as usual.[11] Because of the high esd's, no significant differences in bond lengths or angles can be detected from either neutral or N(1)-protonated adenine rings. Least-squares planes calculated through individual rings indicate that they are planar within 0.013 Å ($1.5\sigma$), and a dihedral angle of 1.9° is found between the two rings. The amino and the methyl groups are part of their respective planes within 0.026 Å ($2\sigma$), but mercury is found at 0.12 Å above the six-membered ring.

The $NO_3^-$ ion has the expected trigonal-planar structure (Figure 1) with three normal N–O bond lengths.[12]

A packing pattern is given in Figure 2. The complex cations are grouped as planar dimeric units by means of a pair of H bonds between N(7) and the amino groups. This type of pairing is common for adenine and involves strong N(6)–H(6)···N(7) hydrogen bonds. The N(6)–N(7) distance (2.96 (1) Å) is on the short side of the range 2.88–3.38 Å proposed by Stout and Jensen[13] for N–H···N bonds. The angles are C(6)–N(6)–N(7) = 133 (1)° and C(5)–N(7)–N(6) = 151(7)°. Such dimers form layers at distances of ~3.5 Å as usually found in this type of compounds. Atom O(3) of the nitrate ion is strongly hydrogen bonded to the remaining hydrogen of the amino group: N(6)–O(3) = 2.80 (1) Å, C(6)–N(6)–O(3) = 134 (1)°, and N(10)–O(3)–N(6) = 166(1)°. There are very long contacts between mercury and oxygen atoms from different nitrate ions: Hg–O(1) ($\bar{x}$, 1 − $y$, $\bar{z}$) = 2.97 (1) Å, Hg–O(2) ($x$, 1 − $y$, $z$) = 2.82 (1) Å. They make a contribution to crystal stabilization by weak ionic interactions.

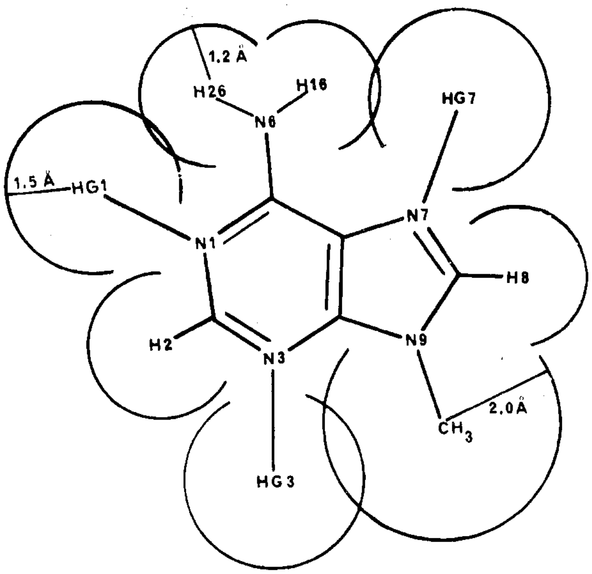

**Figure 3.** Steric effects in the binding of mercury to 9-methyladenine. Ring geometry is from ref 11, and Hg–N = 2.10 Å.

## Discussion

The present crystal structure supports earlier spectroscopic studies [6,7] pointing to N(1)-coordination of $CH_3Hg^+$ in N(9)-substituted adenine rings. It is noteworthy that there appears to be no evidence yet for a 1:1 $CH_3Hg^+$ complex with N(7) only, even though the latter site is favored with most metal ions.[2] Position N(7) was found to be occupied, simultaneously with N(9), in the 2:1 $CH_3Hg$–adenine complex,[5] but it is very likely that the acceptor capability N(7) would have in the free ligand is enhanced when H(9) is displaced by the first $CH_3Hg^+$ ion. Thus, it appears that in N(9)-blocked adenine, N(1) is the first binding position.

The availability of the various basic sites of the adenine ring has been discussed by other workers.[14,15] They examined three major factors: (i) intrinsic basicity of the donor atom, (ii) steric effects due to exocyclic groups, and (iii) repulsive or attractive interactions between exocyclic groups and other ligands in the coordination sphere. It is interesting to apply those considerations to $CH_3Hg^+$, a unique Lewis acid in which mercury commonly possesses linear two-coordination, leaving only one position available. As a result, the coordination sphere is devoid of other ligands to interact with exocyclic groups, which makes effect iii inoperative in the present case. For an examination of steric effects, a scale drawing of a 9-methyladenine molecule (Figure 3) was generated from the normal geometry of adenine.[11] Mercury was assumed to coordinate along the supposed lone-pair direction (symmetrically with respect to the two nearby N–C bonds), and accepted values

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(9) Stewart, R. F.; Davidson, E. R.; Simpson, W. T. *J. Chem. Phys.* **1965**, *42*, 3175.

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(14) Clarke, M. J. *J. Am. Chem. Soc.* **1978**, *100*, 5068.

(15) Marzilli, L. G.; Kistenmacher, T. J. *Acc. Chem. Res.* **1977**, *10*, 146.

of the van der Waals radii for light atoms[16] and for mercury[17] were used.

As noted previously,[14,15] the methyl group at N(9) is a serious barrier to metal binding to N(3). Indeed, in the bisecting position, mercury would overlap appreciably with the methyl group, and the closeness of H(2) would make it impossible to cancel the overlap by moving the metal in that direction. Steric hindrance is obviously less severe at positions N(1) and N(7), but it is difficult to determine which position is sterically favored. The extent of amino hydrogen–metal overlap is marginally smaller for N(1). However, since small departures from bisecting positions are probably not detrimental to bond strength, the larger gap between H(8) and Hg(7) than between H(2) and Hg(1) would tend to favor the former site. Consequently, direct steric effects with the exocyclic groups are not expected to create major differences between N(1) and N(7).

This leaves factor i (intrinsic basicity) as the determining effect. Also consistent with this conclusion is the fact that $H^+$, the least bulky Lewis acid, also reacts with N(1). Furthermore, since the hard $H^+$ ion and the soft $CH_3Hg^+$ ion both interact with N(1) in the first place, appreciable difference in softness between N(1) and N(7) has to be ruled out. The present results reinforce previous conclusions that stabilizing or repulsive effects between the amino group and other ligands in the coordination sphere may play a determining role.

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**Registry No.** $[CH_3Hg(m^9Ade)]NO_3$, 72827-58-8; $CH_3HgNO_3$, 2374-27-8.

**Supplementary Material Available:** Listings of temperature factors, observed and calculated structure factors, and hydrogen coordinates (11 pages). Ordering information is given on any current masthead page.

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Contribution from the Materials and Molecular Research
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# Structure of Di-μ-aquo-bis(dioxobis(nitrato)uranium(VI))-Diimidazole, $[UO_2(NO_3)_2(H_2O)]_2\cdot 2C_3H_4N_2$, a Water-Bridged Dimer of Uranyl Nitrate

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While a large number of uranium complexes have been postulated as dimers, trimers, or polymers, relatively few of them have been corroborated by X-ray crystallography. Several of these compounds are connected by oxygen-containing bridging units such as carboxylates or hydroxy groups; uranyl acetate dihydrate, for example, is a dimer with both bridging and terminal acetate groups.[2] Uranyl oxalate trihydrate[3] contains bridging, coordinated oxalate groups (with both coordinated and uncoordinated hydrogen-bonded water molecules) that contribute to the formation of a pentagonal-bipyramidal structure. Hydrogen bonding also plays a role in the dimerization of uranyl complexes involving thiocarboxylic-like donor centers.[4,5] Dimeric, trimeric, and tetrameric complexes of uranium(IV) have recently been reported.[6-9]

One of the reasons for interest in the coordination properties of imidazole is the important role its derivatives play in coordinating transition-metal ions in biological systems.[10] Presumably, for example, three of the four ligands of cobalt(II) in carbonic anhydrase are nitrogen donors, most likely imidazole nitrogens of histidine residues.[11] Important systems containing imidazole as a ligand include hemoglobin which has $Fe^{2+}$ attached octahedrally with the four nitrogens of heme, a histidine molecule, and either a water or oxygen molecule also coordinated;[12] myoglobin,[12b] histidine deaminase,[13] cytochrome *c*,[14] and cytochrome oxidase[15] are other examples.

In forming chemical systems with metal ions, imidazole, which is somewhat more basic than pyridine and slightly more acidic than pyrrole, can exist in several forms.[10] First, the pyridine-like nitrogen (N(3)) possesses a pair of electrons for coordination with metal ions, thus effectively acting as a monodentate ligand. Second, the N(3) nitrogen can be protonated in acidic solutions to form the imidazolium cation which forms salts with metal ions such as the uranyl ion.[16] Third, the neutral imidazole can undergo deprotonization in strongly basic solutions to form the imidazolate anion which possesses two equivalent nitrogen coordination sites and is thus a potential bridging ligand.[10]

Imidazole, however, also participates in the formation of hydrogen bonds in a number of systems,[10] and it is this property which is utilized in still another mode of bonding in the compound $[UO_2(NO_3)_2(H_2O)]\cdot 2C_3H_4N_2$ which is reported here. The molecules of imidazole act as secondary ligands in the complex, since they are not directly bonded to the uranium species but are hydrogen bonded to the bridging water molecules.

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