Electronic Supplementary Information

Direct Detection of the Mercury–Nitrogen Bond in the Thymine–Hg^{II}–Thymine Base-pair with ^{199}Hg NMR Spectroscopy

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Experimental section

NMR measurement

The NMR sample of the thymidine-Hg^{II}-thymidine complex was prepared as described in the reference 24, except for the use of uniformly ^{15}N-labeled thymidine (Cambridge Isotope Laboratory, Inc., MA, USA, Catalog #: NLM-3901-0, Lot # PR-20710, isotope enrichment: 99.2%). The NMR sample solution contained 25 mM thymidine-Hg^{II}-thymidine complex in deuterated dimethyl sulfoxide (DMSO-d6). A 1-dimensional (1D) ^{199}Hg NMR spectrum (71.667 MHz for ^{199}Hg frequency) was recorded under the natural abundance on a Bruker AVANCE III HD 400 spectrometer equipped with 5mm BBFO probehead for double resonance experiments, which can be tuned to ^{1}H and multiple nuclei (^{19}F and ^{31}P to ^{15}N) at 25 °C with 2048 complex points for a spectral width of 14,124.294 Hz. 960,000 scans were averaged. A 1D ^{199}Hg NMR spectrum (71.667 MHz for ^{199}Hg frequency) with ^{15}N-decoupling was recorded under the natural abundance on a Bruker AVANCE III HD 400 spectrometer equipped with 5 mm TBI probehead for triple resonance experiments, which can be tuned to ^{1}H, ^{15}N and multiple heteronuclei (^{31}P to ^{109}Ag) at 25 °C with 2048 complex points for a spectral width of 14,124.294 Hz. 119,504 scans were averaged. One-dimensional ^{15}N NMR spectra (81.093695 MHz for ^{15}N frequency) were recorded on a Bruker AVANCE-I 800 spectrometer equipped with 5 mm TXI Cryogenic probehead for triple resonance experiments, which can be tuned to ^{1}H, ^{13}C and ^{15}N at 25 °C with 8192 complex points for a spectral width of 9,765.625 Hz, and 152,000 scans were averaged. The ^{199}Hg NMR chemical shift was referenced to dimethylmercury at 0 ppm, using 1 M $HgCl_2$ in DMSO-d6 as the secondary reference (-1501 ppm).[55] The ^{15}N NMR chemical shift was calibrated by indirect referencing using the chemical shift ratio of ^{15}N to ^{1}H.[S1]

Theoretical calculations of NMR parameters

The NMR parameters ($^{1}J(^{199}Hg,^{15}N)$, $^{2}J(^{15}N,^{15}N)$, and $\delta(^{199}Hg)$) for the thymidine-Hg^{II}-thymidine complex were calculated using relativistic density functional theory (DFT) as implemented in the Amsterdam Density Functional (ADF 2012a) (Amsterdam Density Functional package)[47-49], based on geometries obtained from optimizations with the Gaussian 09.A02 code.[S2] The propeller-twist angle dependency of NMR parameters were also examined, by generating rotamers of the T–Hg^{II}–T base-pair around the N3-Hg^{II}-N3 axis with different propeller-twist angles by 30° (Table S5 and Supporting Appendix in ESI†).

Geometries were optimized using the B3LYP/cc-pVTZ method, using the polarizable continuum (PCM) model to treat account for implicit solvation in DMSO, and a relativistic effective core potential (ECP)[S3] for the mercury atom augmented as was described in reference 11. Stationary points were subject to vibrational analyses to verify that they are proper equilibrium structures. The NMR parameters were calculated at the B3LYP/TZ2P level, employing the large slater-type-orbital basis set TZ2P, ZORA-SO for explicit relativistic effects, and the conductor-like screening model (COSMO) for simulating the effect of solvation in DMSO. The *J*-couplings were calculated as a sum of the "Fermi contact" + "spin-dipole coupling" (FC+SD), diamagnetic spin-orbit (DSO), and paramagnetic spin-orbit (PSO) contributions. The ^{199}Hg NMR shielding values were calculated as a sum of diamagnetic, paramagnetic, and spin-orbit contributions. The same method was employed in the calculations of the dimethylmercury reference molecule.

The ^{199}Hg chemical shift was calculated with respect to dimethylmercury using the following equation[18,S4]:

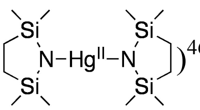
$$\delta(^{199}\mathrm{Hg}) \cong \sigma(^{199}\mathrm{Hg})_{\mathrm{Ref}} - \sigma(^{199}\mathrm{Hg})$$

where $\sigma(^{199}\mathrm{Hg})_{\mathrm{Ref}}$ is the ^{199}Hg NMR shielding calculated for dimethylmercury ($\sigma(^{199}\mathrm{Hg})_{\mathrm{Ref}}$ = 8923.3 ppm) and $\sigma(^{199}\mathrm{Hg})$ is the ^{199}Hg NMR shielding constants for thymidine-Hg$^{\mathrm{II}}$-thymidine. For $\sigma(^{199}\mathrm{Hg})$, the rotation around the N-Hg$^{\mathrm{II}}$-N axis of thymidine-Hg$^{\mathrm{II}}$-thymidine was also considered, and the $\sigma(^{199}\mathrm{Hg})$ values from the respective rotamers were averaged (Table 1; For details, see Table S5 in ESI†).

Theoretical NMR parameters ($^{1}J_{\mathrm{HgN}}$ and $\delta(^{199}\mathrm{Hg})$) for $(\mathrm{Me_3Si})_2$N-Hg$^{\mathrm{II}}$-N$(\mathrm{SiMe_3})_2$ were calculated using the same calculation procedure as was used for the thymidine-Hg$^{\mathrm{II}}$-thymidine calculation, with the COSMO implicit solvent corresponding to toluene employed.

Supporting Discussion

Regarding the hybridization state of the nitrogen atoms in $(\mathrm{Me_3Si})_2$N-Hg$^{\mathrm{II}}$-N$(\mathrm{SiMe_3})_2$, sp^2-like planar structure of the nitrogen atoms was suggested from the electron diffraction study.[19] This suggestion is supported by Bent's rule (*Original proposal: Atomic s character concentrates in orbitals directed toward electropositive substituents.*[45]). Since silicon and Hg$^{\mathrm{II}}$ are more electropositive than carbon, *s*-characters of N-Si and N-Hg$^{\mathrm{II}}$ bonds in $(\mathrm{Me_3Si})_2$N-Hg$^{\mathrm{II}}$-N$(\mathrm{SiMe_3})_2$ increase, and the central nitrogen atoms become more sp^2-like. Therefore, in this sense, the hybridization state of the nitrogen atoms in $(\mathrm{Me_3Si})_2$N-Hg$^{\mathrm{II}}$-N$(\mathrm{SiMe_3})_2$ can be regarded as approximately sp^2.

However, this sp^2-like nature of the nitrogen atoms seems to be different from a canonical sp^2-hybridization. In fact, the ^{14}N chemical shift ($\delta_{^{14}\mathrm{N}}$ = 66.2 ppm ($\cong \delta_{^{15}\mathrm{N}}$)) of a Hg-linked nitrogen of a closely related compound ([–{(CH$_2$)(CH$_3$)$_2$Si}$_2$N]$_2$Hg in Table S1 = )[46] is deviated from a standard range of ^{14}N chemical shifts of sp^2-hybridized nitrogen atoms (Table S1). For example, the canonical sp^2-hybridized nitrogen in $(t\text{-Bu})_2$Si=**N**-Si$(t\text{-Bu})_3$ resonates at 146.2 ppm,[S5] which is far from the $\delta_{^{14}\mathrm{N}}$ = 66.2 ppm ($\cong \delta_{^{15}\mathrm{N}}$) in [–{(CH$_2$)(CH$_3$)$_2$Si}$_2$N]$_2$Hg[46] (Table S1). In the past, it was thought that the empty *d*-orbitals of silicon might interact with the *p*-electrons of nitrogen to stabilized the planar structure of the nitrogen atom, but such evidence has not been found to date.[S6]

It may be possible for the nitrogen atoms in $(\mathrm{Me_3Si})_2$N-Hg$^{\mathrm{II}}$-N$(\mathrm{SiMe_3})_2$ to be classified as sp^2-like nitrogen, but this structural feature seem to be of a rather enforced nature (non-canonical one). Therefore, spectroscopic features could also retain some sp^3-like nature for the nitrogen atoms in the Si_2N-Hg^{II}-NSi_2 linkage. This might be the reason why $|^{1}J(^{199}Hg,^{15}N)|$, $\delta_{^{15}N}$, and $\delta_{^{199}Hg}$ of T-Hg^{II}-T were considerably different from those of $(Me_3Si)_2N$-Hg^{II}-$N(SiMe_3)_2$ and $[\{(CH_2)(CH_3)_2Si\}_2N]_2Hg$. Therefore, we should consider that T-Hg^{II}-T and $(Me_3Si)_2N$-Hg^{II}-$N(SiMe_3)_2$ belong to distinct structural categories, and their spectroscopic data should be classified distinctively.

We also found $|^{1}J(^{199}Hg,^{15}N)|$ values for $N(sp^3)$-Hg^{II}-$N(sp^3)$ in Hg^{II}-CyDTA (365.7-395.5 Hz)[20] and $Hg^{II}(NHMe_2)Cl_2$ (14.7 Hz)[21]. Interestingly, their $|^{1}J(^{199}Hg,^{15}N)|$ values were strikingly smaller than that of T-Hg^{II}-T. Unfortunately, direct comparison with T-Hg^{II}-T is difficult, since coordination environments for these complexes are not defined, and *J*-coupling values are generally affected by the coordination number. We then considered measuring $|^{1}J(^{199}Hg,^{15}N)|$ values for the compounds with N(sp)–Hg^{II}–N(sp) and $N(sp^3)$–Hg^{II}–$N(sp^3)$ linkages by ourselves. However, we had to give up preparing such compounds and recording their NMR spectra, due to their possible toxicities. Therefore, the clear correlation between $|^{1}J(^{199}Hg,^{15}N)|$ values and N-hybridization is not demonstrated at this moment, unfortunately. However, it is interesting to note that the experimental $|^{1}J(^{199}Hg,^{15}N)|$ values available to date satisfy a prerequisite for the assumption that $|^{1}J(^{199}Hg,^{15}N)|$ values may also be correlated with the *s*-character of the corresponding nitrogen atoms in N-Hg^{II} bonds.

Supplementary references

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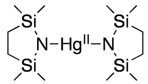
Table S1. Experimental NMR spectral parameters of the T-Hg^{II}-T pair and related works

Compounds	$\lvert ^{1}J_{HgN} \rvert$ (Hz)[a]	$\lvert ^{2}J_{NN} \rvert$ (Hz)[b]	$\delta_{^{199}Hg}$ (ppm)[c]	$\delta_{^{15}N}/\delta_{^{14}N}$ (ppm)[d]	N-hybrid.[e]	N-metal Bond
Thy-Hg^{II}-Thy	1047	2.4[f]	-1784[g]	184[h], 185.2 – 189.2[f]	sp^2	Covalent
$[\{(CH_3)_3Si\}_2N]_2Hg$	316.2[i]	–[j]	-992[k]	–	sp^3/sp^2	Covalent
$[\{(CH_2)(CH_3)_2Si\}_2N]_2Hg$ = 	–	–	–	66.2[l]	sp^3/sp^2	Covalent
$\{(CH_3)_3Si\}_2NH$	N.A.	N.A.	N.A.	27.2[m]	sp^3/sp^2	Metal-free
$(t\text{-Bu})_2Si{=}N\text{-}Si(t\text{-Bu})_3$	N.A.	N.A.	N.A.	146.2[n]	sp^2	Metal-free
Hg^{II}-CyDTA	365.7-395.5[o]	–	–	51.1[o]	sp^3	Coordination
Hg^{II}-$(NHMe_2)_2Cl_2$	14.7[p]	N.A.	-1298[p]	–	sp^3	Coordination
(9-Me-1-deazapurine)$_2$Hg	–	–	-1948[q]	–	sp^2	Coordination
$[Ru^{II}Cl(PPh_3)(BPM)_2]Cl$	N.A.	4.3[r]	N.A.	229.1 – 230.8[r]	sp^2	Coordination

–: Not reported. N.A.: Not applicable. $\{(CH_2)(CH_3)_2Si\}_2N^-$: 2,2,5,5-tetramethyl-2,5-disila-1-aza-cyclopentanide. *t*-Bu: *tert*-Butyl. CyDTA: *trans*-l,2-diaminocyclohexane-*NNN'N'*-tetraacetate. PPh_3: triphenylphosphine. BPM: bis(1-pyrazolyl)methane. [a] One-bond ^{15}N-^{199}Hg *J*-coupling (absolute value). [b] Two-bond ^{15}N-^{15}N *J*-coupling across metal cation (absolute value). [c] Mercury-199 NMR chemical shift with respect to dimethylmercury (CH_3HgCH_3) at 0 ppm. [d] Nitrogen-15 NMR chemical shift ($\delta_{^{15}N}$) or ^{14}N NMR chemical shift ($\delta_{^{14}N}$) with respect to liquid ammonia at 0 ppm. The $\delta_{^{15}N}$ and $\delta_{^{14}N}$ values are essentially the same except for the small isotope shift between ^{15}N and ^{14}N nuclei. [e] Hybridization states of nitrogen atoms. [f] Reference-6. [g] Mercury-199 chemical shift in this work ($\delta_{^{199}Hg}$ reference: $\delta_{^{199}Hg}$ = -1501 ppm for external 1.0 M $HgCl_2$ in dimethyl sulfoxide (DMSO) relative to dimethylmercury[55]) and reference-23. [h] This work (Figure S1). [i] Reference-19. [j] $^{2}J(^{15}N,^{14}N) < 9$ Hz was estimated from the line-broadening of ^{15}N resonance. [k] References-53: Mercury-199 chemical shift was referenced with $\delta_{^{199}Hg}$ = -2400 ppm for external 1.0 M $Hg(NO_3)_2$ in D_2O relative to dimethylmercury as described,[53] although the conversion with $\delta_{^{199}Hg}$ = 2430 ppm[S7] seems to be better. [l] References-46; Solvent: C_6D_6; Reported ^{14}N chemical shift (-310 ppm) was converted with $\delta_{^{14}N}$ = 376.2 ppm for external 2.0 M $NH_3\underline{N}O_3$ in D_2O relative to liquid ammonia (NH_3).[18] [m] Reference-S8; Solvent: C_6D_6; Reported ^{14}N chemical shift (-353 ppm) was converted with $\delta_{^{14}N}$ = 380.2 ppm for external neat $CH_3\underline{N}O_3$ relative to liquid ammonia (NH_3).[18] [n] Reference-S5; Solvent: C_6D_6; Reported ^{14}N chemical shift (-230 ppm) was converted with $\delta_{^{14}N}$ = 376.2 ppm for external 2.0 M $NH_3\underline{N}O_3$ in D_2O relative to liquid ammonia (NH_3)[18]. [o] Reference-20; Solvent: 10% D_2O/90% H_2O; Reported ^{15}N chemical shift (-329.1 ppm) was converted with $\delta_{^{15}N}$ = 380.2 ppm for external neat $CH_3\underline{N}O_3$ relative to liquid ammonia (NH_3).[18] [p] Reference-21; Solvent: DMSO; Mercury-199 chemical shift was referenced with $\delta_{^{199}Hg}$ = -1501 ppm for external 1.0 M $HgCl_2$ in DMSO relative to dimethylmercury.[55] [q] Reference-S9; Solvent: D_2O (pD 4.0). [r] Reference-S10; Solvent: CD_3OD; Reported ^{15}N chemical shift (-329.1 ppm) was converted with $\delta_{^{15}N}$ = 380.2 ppm for external neat $CH_3\underline{N}O_3$ relative to liquid ammonia (NH_3).[18]

Table S2. Experimental ^{199}Hg NMR spectral parameters of Hg^{II}-complexes

X-Hg^{II}-Y [Branch][a]	Coordination	$\delta_{^{199}Hg}$ (ppm)[b]	$\lvert {}^1J_{HgX} \rvert$ or $\lvert {}^1J_{CH} \rvert$ (Hz)[c]	$\lvert {}^1J_{HgY} \rvert$ (Hz)[c]
C(sp)-Hg^{II}-C(sp)	linear two-coordinate	-978 – -864[S11]	2493 – 2676[S11,S12]	N.A.
C(sp)-Hg^{II}-C(sp^2)	linear two-coordinate	-848 – -808[S11]	sp: 1502 – 1650[S11]	sp^2: 1691 – 1875[S11]
C(sp)-Hg^{II}-C(sp^3)	linear two-coordinate	-485 – -629[S11]	sp: 1134 – 1447[S11,S12]	sp^3: 1145 – 1245[S11,S12]
C(sp^2)-Hg^{II}-C(sp^2)	linear two-coordinate	-809 – -354[S3,S13-S16]	1044 – 1176[S12,S13,S15]	N.A.
C(sp^2)-Hg^{II}-C(sp^3)	linear two-coordinate	-392 – -237[S11,S17]	sp^2: 926, 970[S12]	sp^3: 817, 819[S12]
C(sp^3)-Hg^{II}-C(sp^3) [1°]	linear two-coordinate	-366 – +5.3[S3,S11,S13,S14,S18,S19]	549 – 760[S12,S13,S18,S20]	N.A.
C(sp^3)-Hg^{II}-C(sp^3) [2°]	linear two-coordinate	-640 – -597[S3,S13,S19]	636[S12,S13]	N.A.
C(sp^3)-Hg^{II}-C(sp^3) [3°]	linear two-coordinate	-838 – -826[S3,S13,S21]	628 – 652[S12,S13,S21,S22]	N.A.
N(sp^2)-Hg^{II}-C(sp^2)	linear two-coordinate	-1292 – -1191[16a,S16,S23]	N: –	C: 2361[S23]
N(sp^2)-Hg^{II}-C(sp^3)	linear two-coordinate	-1357 – -787[S23-S26]	N: –	C: 1491 – 1663[S23,S24]
N(sp^3)-Hg^{II}-N(sp^3) {Hg^{II}-CyDTA}	–	–	365.7–395.5[20]	N.A.
N(sp^3)-Hg^{II}-N(sp^3) {Hg^{II}-$(NHR^1R^2)_2Cl_2$}	possible tetrahedral[e]	-1200 – -1496[21]	14.7[21]	N.A.
$(R_3Si)_2N$-Hg^{II}-$N(SiR_3)_2$	linear two-coordinate	-992[53]	316.2[19]	N.A.
N(sp^2)-Hg^{II}-N(sp^2)	linear two-coordinate	-1948, -1784[S9,This work]	1050[This work]	N.A.
C(sp)-H {hydrocarbon}	N.A.	N.A.	$\lvert {}^1J_{CH} \rvert$: ~250[S27]	N.A.
C(sp^2)-H {hydrocarbon}	N.A.	N.A.	$\lvert {}^1J_{CH} \rvert$: ~160[S27]	N.A.
C(sp^3)-H {hydrocarbon}	N.A.	N.A.	$\lvert {}^1J_{CH} \rvert$: ~125[S27]	N.A.

–: Not reported. N.A.: Not applicable. CyDTA: *trans*-1,2-diaminocyclohexane-*NNN'N'*-tetraacetate. NHR^1R^2: secondary amine [a] Branching (degree of substitution) on sp^3-carbon are listed in brackets; 1°: primary carbon, 2°: secondary carbon, 3°: tertiary carbon. [b] Mercury-199 NMR chemical shift with respect to dimethylmercury (CH_3HgCH_3) as 0 ppm. Each range of $\delta_{^{199}Hg}$ includes solvent/concentration-dependent chemical shift perturbations. [c] One-bond $^{15}N/^{13}C-^{199}Hg$ or $^1H-^{13}C$ *J*-coupling (absolute value). Reference numbers are written in the parentheses beside the chemical shifts and *J*-coupling values are indicated as superscripts.

Table S3. Theoretical values of *J*-coupling and ^{199}Hg NMR chemical shift for the T-Hg^{II}-T pair

Compound	$^{1}J_{HgN}$ (Hz)^{a}	$^{2}J_{NN}$ (Hz)^{b}	$\delta(^{199}Hg)$ (ppm)^{c}	Ref.
T-Hg^{II}-T (*average*)^{d} [B3LYP/TZ2P]	-931	2.8	-1848	This work
T-Hg^{II}-T (*cis*)^{e} [BLYP/TZ2P]	-670	1.7	-1727	ref. 50
Experiment(Thy-Hg^{II}-Thy$^{\#}$; T-Hg^{II}-T in DNA*)	1050$^{\#}$	2.4*	-1784$^{\#}$	$^{\#}$ This work; * ref. 6 for $^{2}J_{NN}$

^{a} One-bond ^{199}Hg-^{15}N *J*-coupling. Experimental value is given as absolute value. ^{b} Two-bond ^{15}N-^{15}N *J*-coupling across Hg^{II} in the T-Hg^{II}-T pair. * Experimental value is given as absolute value. ^{c} Theoretical ^{199}Hg NMR chemical shift with respect to dimethylmercury at 0 ppm, as previously described.[50] Experimental chemical shift was reported with respect to dimethylmercury (0 ppm) by using 1.0 M $HgCl_2$ in dimethyl sulfoxide (DMSO-d6) as the secondary reference at -1501 ppm.[55] ^{d} The $^{1}J_{HgN}$, $^{2}J_{NN}$ and $\delta(^{199}Hg)$ values were averaged over those from rotamers around the N-Hg^{II}-N axis (see the footnote to Table S5 for the rotamers). Calculation with ADF 2012a considering relativistic effect. DMSO solvent was modeled implicitly with COSMO. ^{e} Calculations by Bagno and Saielli.[50]

Table S4. Decomposition of theoretical ^{15}N-^{199}Hg *J*-coupling.

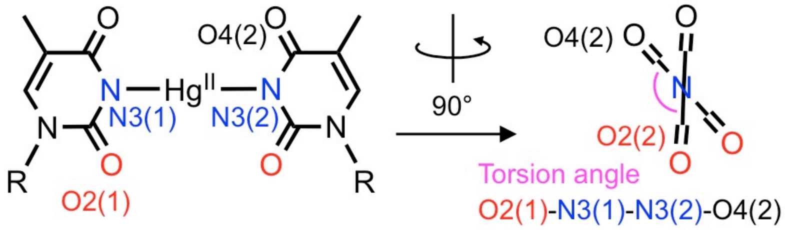
Compound	DSO (Hz)[a]	PSO (Hz)[b]	FC+SD (Hz)[c]	Total (Hz)
T-Hg^{II}-T (*average*)[d]	-0.053	10.727	-942.062	-931.388
$(Me_3Si)_2N$-Hg^{II}-$N(SiMe_3)_2$[e]	-0.058	17.246	-295.616	-278.383

[a] DSO: Diamagnetic spin-orbit coupling. [b] PSO: Paramagnetic spin-orbit coupling. [c] FC+SD: Mixed Fermi contact plus Spin-dipole coupling. All the calculations were performed with ADF 2012a. [d] The average values of DSO, PSO and FC+SD terms and $^1J_{NHg}$ coupling (For details see the footnote to Table S5). The DMSO solvent was modeled implicitly with COSMO. [e] Toluene solvent was modeled implicitly with COSMO.

Table S5. Theoretical $^1J_{NHg}$ $^2J_{NN}$ and δ (Hg) values for rotamers of thymidine-Hg^{II}-thymidine.

Torsion angle: O2(1)-N3(1)-N3(2)-O4(2) [O2(1)-N3(1)-N3(2)-O2(2)]	$^1J_{NHg}$	$^2J_{NN}$	δ (^{199}Hg)	σ (^{199}Hg)
180.0 [-0.88: cisoid]	-940.627	2.900	-1875.25	10798.58
210.0 [31.9]	-935.642	2.791	-1847.59	10770.92
240.0 [59.7]	-931.940	2.841	-1884.23	10807.56
270.0 [89.1]	-935.290	2.816	-1885.72	10809.05
300.0 [119.1]	-933.920	2.792	-1890.59	10813.92
330.0 [151.2]	-928.581	2.736	-1797.53	10720.86
0.0 [180.5: transoid]	-930.469	2.746	-1840.35	10763.68
30.0 [209.1]	-930.156	2.779	-1842.99	10766.32
60.0 [241.1]	-922.103	2.831	-1831.24	10754.57
90.0 [271.1]	-931.155	2.863	-1854.28	10777.61
120.0 [298.3]	-925.421	2.844	-1822.55	10745.88
150.0 [330.0]	-931.356	2.786	-1809.46	10732.79
Average[a]	-931.388	2.810	-1848.48	10771.81

[a] The averaged value of NMR parameters for rotation around the N3(1)-Hg^{II}-N3(2) bond was calculated employing the structures that were optimized with constrained torsion angle O2(1)-N3(1)-N3(2)-O4(2) rotation). The torsion angles for O2(1)-N3(1)-N3(2)-O2(2) are written in the parenthesis. The definition of the torsion angle O2(1)-N3(1)-N3(2)-O4(2) is as follows where R denotes ribose.



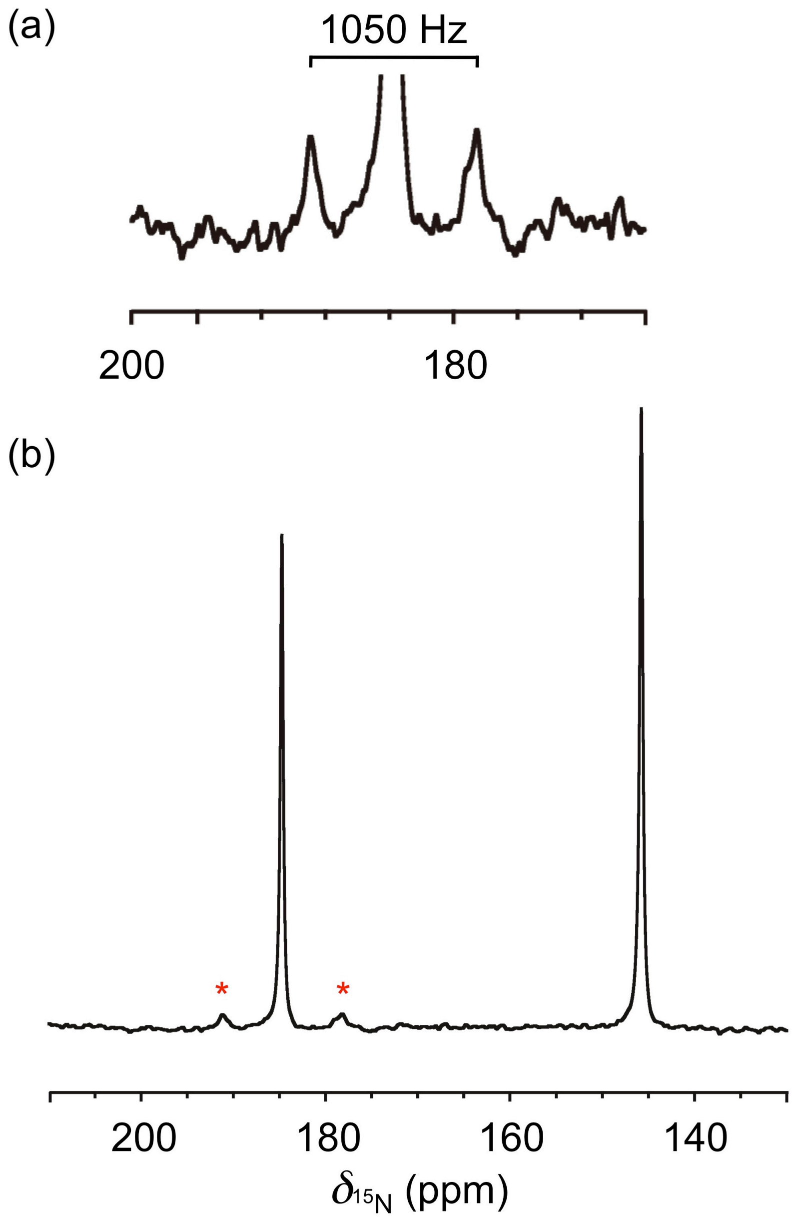


Figure S1. One-dimensional ^{15}N NMR spectrum of thymidine-Hg^{II}-thymidine complex (25 mM in DMSO-d6). (a) A doublet resonance of N3 due to the ^{15}N3-^{199}Hg linkage observed as satellite peaks ($^{1}J(^{199}$Hg,^{15}N): 1050 Hz). (b) All ^{15}N signals in ^{15}N-labeled thymidine. Satellite peaks of N3 due to $^{1}J(^{199}$Hg,^{15}N) are highlighted with red asterisks.

Supporting Appendix Cartesian coordinates of computed molecules:

Thymidine-Hg^{II}-thymidine (torsion angle O2(1)-N3(1)-N3(2)-O4(2): 0°)

O	-7.35468100	6.29222600	0.98571200
C	-6.46557100	5.24191500	1.33911000
C	-5.66322300	5.51119600	2.62276100
O	-4.47790500	4.72655100	2.46650800
C	-4.09062700	4.75436600	1.08572600
C	-5.36329700	5.10423000	0.28656800
C	-6.36890600	5.12757100	3.89948100
N	-3.47496500	3.47535200	0.76324100
C	-4.23723900	2.33068000	0.76919100
C	-3.72945800	1.10552200	0.55086900
C	-2.29261000	1.00026400	0.31651500
N	-1.56298000	2.17267500	0.34157300
C	-2.08981100	3.41308600	0.56664900
O	-1.39939300	4.43167900	0.59322500
N	2.74122700	1.86646000	-0.09812600
C	3.26663200	0.62566600	-0.32399100
N	4.64999500	0.56170500	-0.51384000
C	5.42373000	1.69637900	-0.46892500
C	4.91718000	2.92234900	-0.24723800
C	3.47614400	3.03520600	-0.05016000
C	5.27411000	-0.73180900	-0.77155700
O	6.37341500	-0.89317100	0.12440900
C	7.37407300	-1.73628000	-0.48037600
C	6.90821300	-2.00322500	-1.93059600
C	5.87454700	-0.91061500	-2.16467200
C	8.73810600	-1.08107600	-0.39650200
O	2.57316200	-0.39107300	-0.37025700
O	2.92111000	4.12151500	0.15153100
C	5.76208300	4.15787600	-0.19121900
O	6.24211500	-3.26023700	-2.05725500
O	-1.73753600	-0.08439800	0.10945300
C	-4.56329700	-0.13856900	0.54983100
H	8.72456300	-0.11614800	-0.91445200
O	9.07991200	-0.91881100	0.97622000
H	7.40235400	-2.67941400	0.07200000
H	4.50536400	-1.47409900	-0.57702600

H	6.48162800	1.53048100	-0.60370500
H	6.81146200	3.92011300	-0.36025700
H	5.67268300	4.65241100	0.77780900
H	5.44728200	4.88311500	-0.94378400
H	6.35858200	0.00922500	-2.49190500
H	5.13782700	-1.20238700	-2.90909000
H	7.73994700	-1.94612900	-2.63539000
O	-5.59621200	5.57356800	5.01052300
H	-7.35826800	5.59827900	3.90161000
H	-5.40940300	6.57822600	2.65600200
H	-3.31145600	5.49468800	0.93739700
H	-5.28814300	2.47891400	0.96808500
H	-5.60912600	0.09274100	0.74736300
H	-4.21686500	-0.84365900	1.30754900
H	-4.49964800	-0.65335600	-0.41053200
H	-5.59397100	4.36716300	-0.47791200
H	-5.23420800	6.06634700	-0.20721500
H	-7.01850700	4.30443400	1.44722200
Hg	0.58937800	2.02013100	0.12112900
H	-6.50458800	4.04146400	3.92304800
H	6.87559000	-3.96428300	-1.88131700
H	9.45996300	-1.72964500	-0.90473000
H	-8.18555900	6.17115900	1.45619100
H	9.93330300	-0.47701200	1.02469800
H	-6.05410300	5.32085100	5.81815700

Thymidine-Hg^{II}-thymidine (torsion angle O2(1)-N3(1)-N3(2)-O4(2): 30°)

O	-7.36991100	6.03906500	0.22263000
C	-6.49216600	5.11715400	0.85377000
C	-5.80062200	5.67788000	2.10785400
O	-4.57760600	4.94100400	2.20030300
C	-4.09161100	4.68287500	0.87745600
C	-5.30826800	4.80527900	-0.06370400
C	-6.59050500	5.52081000	3.38366400
N	-3.43409600	3.38249200	0.88529300
C	-4.16334600	2.25748200	1.19187200
C	-3.62130100	1.03151700	1.29208600
C	-2.18336500	0.90876300	1.07685900
N	-1.49457100	2.06258200	0.75932200

C	-2.05331300	3.30654700	0.67410400
O	-1.38989400	4.31274400	0.42161100
N	2.80107400	1.73668700	0.29984100
C	3.28881200	0.56628900	-0.21257100
N	4.66977700	0.50253900	-0.41736800
C	5.48154100	1.56619800	-0.10772900
C	5.01661200	2.71632700	0.41095000
C	3.58056800	2.82556200	0.64215600
C	5.24897500	-0.71122900	-0.98976300
O	6.38345400	-1.08646000	-0.21042200
C	7.36832800	-1.72696600	-1.04691500
C	6.80861600	-1.69212000	-2.48581800
C	5.77511700	-0.57715000	-2.41806500
C	8.71264400	-1.03896800	-0.91115700
O	2.56587600	-0.39092700	-0.49331600
O	3.06976900	3.84393400	1.12198600
C	5.90298100	3.87210900	0.76010200
O	6.12036900	-2.89721600	-2.82307600
O	-1.59135100	-0.17163100	1.17431800
C	-4.41725600	-0.19109900	1.63061600
H	8.63048000	0.01045900	-1.21354000
O	9.14372500	-1.14785200	0.44134700
H	7.46860800	-2.76334500	-0.71449800
H	4.47195800	-1.46721900	-0.92671700
H	6.53304400	1.40268800	-0.28613300
H	6.94363300	3.64846300	0.52910200
H	5.83059600	4.11775700	1.82118000
H	5.61284300	4.76912200	0.20998800
H	6.25200900	0.39264600	-2.55849600
H	4.99687500	-0.69630500	-3.16782600
H	7.59351200	-1.48890600	-3.21676000
O	-5.92578000	6.21834100	4.43318900
H	-7.59386300	5.93021000	3.22162900
H	-5.58878900	6.74127800	1.94121700
H	-3.31517300	5.39583100	0.62055300
H	-5.21610100	2.42603400	1.36244400
H	-5.46940700	0.05432600	1.76850000
H	-4.04890500	-0.65720600	2.54618400
H	-4.33903500	-0.94191400	0.84226400

H	-5.45912000	3.91232000	-0.66464700
H	-5.16631100	5.64494200	-0.74270000
H	-7.03418700	4.20340100	1.11376400
Hg	0.64504000	1.91344500	0.51659700
H	-6.68810500	4.45551600	3.61685500
H	6.75825100	-3.61853600	-2.85167500
H	9.41865400	-1.53287900	-1.58760300
H	-8.22902700	6.00129800	0.65475500
H	9.98196000	-0.68371500	0.52927200
H	-6.43858600	6.11011300	5.24019400

Thymidine-Hg^{II}-thymidine (torsion angle O2(1)-N3(1)-N3(2)-O4(2): 60°)

O	-7.35213400	5.53719300	-0.34942500
C	-6.44662400	4.84782400	0.50109500
C	-5.71625100	5.76052100	1.49996800
O	-4.49130800	5.07480700	1.77676200
C	-4.04634700	4.42297900	0.58018600
C	-5.29213700	4.26626100	-0.31710300
C	-6.46472200	6.01279100	2.78517500
N	-3.38816900	3.18029900	0.96006800
C	-4.11476200	2.18859100	1.57723000
C	-3.57613300	1.03077200	1.99654500
C	-2.14466900	0.83626600	1.78823300
N	-1.45165000	1.87104300	1.19241900
C	-2.00860900	3.04547800	0.77336100
O	-1.34258600	3.94091400	0.25230800
N	2.82720300	1.48912500	0.74379300
C	3.27638700	0.48238600	-0.06209700
N	4.65545000	0.40385800	-0.25121200
C	5.49981100	1.32935400	0.31050400
C	5.06744200	2.33610200	1.09285600
C	3.63477700	2.43516400	1.34429700
C	5.18071500	-0.65504600	-1.12063400
O	6.40714300	-1.12643200	-0.57648600
C	7.32170300	-1.48386900	-1.63475600
C	6.57062500	-1.23159800	-2.95754200
C	5.51052200	-0.21933400	-2.54811900
C	8.61232400	-0.69474100	-1.52158300
O	2.51693900	-0.31993600	-0.60896600

O	3.14500300	3.31971900	2.05690700
C	5.99059500	3.34098000	1.71101600
O	5.89406400	-2.39981100	-3.42230300
O	-1.56351300	-0.19949800	2.12898000
C	-4.37048600	-0.04672900	2.66801900
H	8.40818000	0.37766100	-1.60912700
O	9.22052100	-0.99673000	-0.27019200
H	7.54875000	-2.54716100	-1.52848900
H	4.42997100	-1.44052500	-1.11364400
H	6.54638800	1.17251300	0.10181700
H	7.02509400	3.14047300	1.43531300
H	5.91563100	3.32882400	2.79989300
H	5.73977700	4.35388700	1.39036000
H	5.92593300	0.78831400	-2.54785500
H	4.64615800	-0.24247300	-3.20679400
H	7.23773800	-0.84752400	-3.73155400
O	-5.76909300	6.99892800	3.54269900
H	-7.47431600	6.35740200	2.53524100
H	-5.50993600	6.71898100	1.00769900
H	-3.27879100	5.01864500	0.09718300
H	-5.16338400	2.40590400	1.71353100
H	-5.41611200	0.24224100	2.76493400
H	-3.97801300	-0.25988400	3.66402900
H	-4.32127200	-0.98041600	2.10499800
H	-5.46101600	3.23603300	-0.61951700
H	-5.17310500	4.86371800	-1.21986200
H	-6.97323900	4.05934300	1.04630700
Hg	0.69030600	1.68534300	0.97258300
H	-6.55040100	5.07403000	3.34212700
H	6.55086600	-3.05962000	-3.66966600
H	9.26367900	-0.98508400	-2.35298000
H	-8.20098500	5.61917600	0.09653700
H	10.02007800	-0.46783800	-0.18807100
H	-6.25588800	7.15278700	4.35833100

Thymidine-Hg^{II}-thymidine (torsion angle O2(1)-N3(1)-N3(2)-O4(2): 90°)

O	-7.55963500	4.92749400	-0.52240300
C	-6.55383700	4.49470200	0.38257800
C	-5.75021500	5.64298600	1.01371800

O	-4.48515500	5.05751800	1.33396100
C	-4.14910400	4.09557200	0.32486300
C	-5.47411300	3.71051100	-0.36559600
C	-6.37048300	6.23444200	2.25535200
N	-3.43380000	3.00041500	0.96568800
C	-4.08706500	2.20522500	1.87824500
C	-3.48083700	1.22720300	2.57234400
C	-2.05360000	1.02243500	2.34702100
N	-1.43739200	1.84699300	1.42514700
C	-2.06082800	2.84982200	0.73814600
O	-1.46119000	3.58586400	-0.04553200
N	2.83174700	1.43551900	0.89509600
C	3.25491600	0.64264300	-0.13345800
N	4.63350600	0.58659300	-0.35112000
C	5.50266000	1.30248500	0.43697800
C	5.09719900	2.08771900	1.45127700
C	3.66362600	2.17934300	1.70799500
C	5.14479800	-0.22638900	-1.44914600
O	6.19227100	-1.05723300	-0.95225400
C	7.08992700	-1.38873000	-2.02998500
C	6.67971800	-0.50921900	-3.23708000
C	5.77719800	0.54286800	-2.60704800
C	8.52685000	-1.18613900	-1.59643100
O	2.47378700	0.01257800	-0.84719000
O	3.19466700	2.88744700	2.60598600
C	6.04625400	2.86355200	2.31205800
O	5.90194100	-1.23435600	-4.19062400
O	-1.41108400	0.15714800	2.95210500
C	-4.19565000	0.36375200	3.56552000
H	8.68491300	-0.14380500	-1.30005700
O	8.80621500	-2.07216200	-0.51733300
H	6.94290500	-2.44174900	-2.28591600
H	4.30390400	-0.82432400	-1.78957700
H	6.54653900	1.17367100	0.19497100
H	7.07634100	2.70686400	1.99481700
H	5.96001000	2.56817300	3.35933800
H	5.83115500	3.93276300	2.26853200
H	6.36950100	1.37624200	-2.23008200
H	5.04467100	0.92396800	-3.31440600

H	7.55142500	-0.06752300	-3.72360300
O	-5.63037300	7.38928700	2.64061400
H	-7.41043600	6.49687300	2.03062000
H	-5.62263900	6.43159300	0.26172600
H	-3.44393000	4.52822800	-0.37693800
H	-5.13565200	2.42435000	2.01195800
H	-5.24919200	0.63265200	3.62902200
H	-3.75438000	0.46149200	4.55901900
H	-4.12437400	-0.69065800	3.29282600
H	-5.64903800	2.63787500	-0.36589200
H	-5.45895800	4.04606300	-1.40165900
H	-6.99978000	3.88426100	1.17322900
Hg	0.70198200	1.63933400	1.15856800
H	-6.37087700	5.48156300	3.05016900
H	6.45821200	-1.91087800	-4.59166500
H	9.17448600	-1.39900800	-2.45392100
H	-8.34748700	5.16735200	-0.02413400
H	9.71454200	-1.92672000	-0.23522500
H	-6.03263500	7.75584700	3.43411200

Thymidine-Hg^{II}-thymidine (torsion angle O2(1)-N3(1)-N3(2)-O4(2): 120°)

O	-7.47621400	4.33114000	-0.94204800
C	-6.54342100	4.13374500	0.11195700
C	-5.83871700	5.42407900	0.56368000
O	-4.58302000	4.98000500	1.08310000
C	-4.12021100	3.89142200	0.27387000
C	-5.37686800	3.26709000	-0.37033900
C	-6.58128500	6.20870300	1.61657100
N	-3.33809500	3.00169900	1.11968400
C	-3.94701400	2.36094600	2.17266500
C	-3.28632000	1.57003800	3.03547100
C	-1.85062700	1.40812400	2.83626600
N	-1.27824900	2.07671100	1.77352400
C	-1.95906500	2.88161900	0.90346700
O	-1.41178200	3.47097800	-0.02806400
N	2.95428400	1.50563100	1.17067900
C	3.26989200	0.93820500	-0.03161900
N	4.62898000	0.75461400	-0.29714300
C	5.58239400	1.10881800	0.62789000

C	5.28232500	1.64657300	1.82350200
C	3.87347700	1.86105300	2.13736500
C	5.03269600	0.15650600	-1.56384300
O	5.88218900	-0.95770300	-1.29055600
C	6.76048900	-1.17596400	-2.41133700
C	6.57839200	0.03307900	-3.36180400
C	5.85182700	1.05071800	-2.49205300
C	8.18503100	-1.36092400	-1.93157600
O	2.41107000	0.60899300	-0.85036400
O	3.49953100	2.33677200	3.21461800
C	6.32248100	2.02005400	2.83441500
O	5.73008900	-0.27808600	-4.46791700
O	-1.15604000	0.70729400	3.58052100
C	-3.95126300	0.86927900	4.17977300
H	8.51241100	-0.47329800	-1.38017500
O	8.23978500	-2.52196500	-1.10893200
H	6.44032000	-2.08698700	-2.92488200
H	4.11299600	-0.16723200	-2.04299700
H	6.60009900	0.90153000	0.33462700
H	7.32301800	1.80783900	2.45997700
H	6.17987200	1.47072000	3.76675400
H	6.26546700	3.08129000	3.08320200
H	6.56752400	1.64157000	-1.92107800
H	5.23625200	1.72319900	-3.08450000
H	7.53896100	0.40763800	-3.72077200
O	-5.92062500	7.45398100	1.82313600
H	-7.60824200	6.36731900	1.26897100
H	-5.68065600	6.05835800	-0.31756600
H	-3.42897500	4.25649800	-0.47875900
H	-5.00681100	2.54269200	2.27019900
H	-5.01887400	1.08375500	4.20091100
H	-3.51874700	1.17680600	5.13355000
H	-3.81814000	-0.21170300	4.10865400
H	-5.49643000	2.21768500	-0.11417800
H	-5.31232200	3.34000800	-1.45489100
H	-7.04123200	3.67133100	0.96880000
Hg	0.86610500	1.83864900	1.54259100
H	-6.61883000	5.62302900	2.54088600
H	6.16763800	-0.93926100	-5.01512000

H	8.82932400	-1.47421900	-2.81019900
H	-8.31789500	4.60974800	-0.56751600
H	9.14382600	-2.62869600	-0.79734300
H	-6.39865000	7.94089200	2.50162200

Thymidine-Hg^{II}-thymidine (torsion angle O2(1)-N3(1)-N3(2)-O4(2): 150°)

O	-7.49117300	3.75695500	-1.03189900
C	-6.60952600	3.81883300	0.08210300
C	-5.85829200	5.15832900	0.19769500
O	-4.62763700	4.82264000	0.84376600
C	-4.19209000	3.56810400	0.30997500
C	-5.47385400	2.80233500	-0.08420300
C	-6.58479300	6.21910300	0.98604900
N	-3.34961200	2.92027500	1.30288200
C	-3.87532000	2.58806600	2.52961600
C	-3.15385300	2.01394600	3.50793000
C	-1.74451200	1.74155900	3.24059600
N	-1.25658400	2.10899400	2.00313700
C	-1.99769600	2.70058100	1.01862800
O	-1.51802600	3.02167200	-0.06877300
N	2.91245600	1.40534600	1.13831600
C	3.28945300	1.15514200	-0.15173200
N	4.65040000	0.89931900	-0.36266100
C	5.53747300	0.88011100	0.68714900
C	5.17809000	1.12905300	1.95837800
C	3.77229400	1.41436400	2.21894500
C	5.11388200	0.57191800	-1.70307800
O	5.69708100	-0.73319400	-1.67422400
C	6.65881600	-0.84998700	-2.73919000
C	6.84413900	0.57072400	-3.32847100
C	6.20714100	1.47039700	-2.27741400
C	7.94140700	-1.46551500	-2.21905100
O	2.49415500	1.15703500	-1.09076700
O	3.34594900	1.64978000	3.35494600
C	6.14594200	1.10831100	3.10125600
O	6.11697100	0.74491200	-4.54547500
O	-1.00445400	1.20903700	4.07398900
C	-3.72899600	1.65147400	4.84233300
H	8.34952900	-0.85144300	-1.40961400

O	7.65899200	-2.78588200	-1.76581400
H	6.24218900	-1.50515500	-3.50969900
H	4.22811200	0.58236900	-2.33171800
H	6.55415700	0.63249100	0.42293300
H	7.15217700	0.87640400	2.75481700
H	5.85808800	0.36489300	3.84676800
H	6.17135200	2.07234700	3.61250500
H	6.93558300	1.73048300	-1.51082100
H	5.81626300	2.38642900	-2.71357400
H	7.89888600	0.80413600	-3.48619800
O	-5.88453600	7.45393900	0.86490600
H	-7.60096000	6.30895600	0.58624200
H	-5.66142900	5.53091500	-0.81555500
H	-3.55250800	3.73324200	-0.55158500
H	-4.91875400	2.83217700	2.66187000
H	-4.78309500	1.92012900	4.89806500
H	-3.20004500	2.16101800	5.64966300
H	-3.63581200	0.58073300	5.03242000
H	-5.62212500	1.91137800	0.52037400
H	-5.42106700	2.49271700	-1.12656000
H	-7.16296500	3.63004600	1.00577300
Hg	0.82814600	1.74910900	1.57454900
H	-6.65477500	5.90486200	2.03247100
H	6.49286200	0.16340300	-5.21516900
H	8.66981300	-1.48136800	-3.03708100
H	-8.32480700	4.17536100	-0.79437100
H	8.46818200	-3.16113000	-1.40501700
H	-6.35655900	8.12020400	1.37399400

Thymidine-Hg^{II}-thymidine (torsion angle O2(1)-N3(1)-N3(2)-O4(2): 180°)

O	-7.84619500	3.23335300	-0.54510100
C	-6.78809300	3.54978900	0.34999900
C	-6.06774600	4.86770600	0.01421500
O	-4.74612900	4.68848000	0.52855800
C	-4.35864500	3.33247200	0.27524600
C	-5.66647300	2.51277700	0.23109300
C	-6.69449800	6.09843300	0.62010000
N	-3.40005300	2.93668500	1.29464000
C	-3.79083700	2.87917000	2.61224200

C	-2.95386600	2.55972900	3.61416300
C	-1.56328700	2.27015700	3.27289500
N	-1.21232600	2.36139100	1.93956800
C	-2.07079200	2.69568400	0.93143700
O	-1.70884100	2.77673400	-0.24244800
N	2.92309400	1.36899200	1.07751300
C	3.39801800	1.34456900	-0.20142800
N	4.72184100	0.92157200	-0.36624600
C	5.47693800	0.53291200	0.71536100
C	5.01619000	0.54828300	1.97837400
C	3.64189700	0.98976800	2.19337400
C	5.27936700	0.82486100	-1.70769900
O	5.69031000	-0.52590100	-1.93106400
C	6.74980700	-0.55072100	-2.90579100
C	7.16543200	0.92128500	-3.14815500
C	6.52876200	1.66024300	-1.97819300
C	7.88462900	-1.42991800	-2.42227800
O	2.71289700	1.67978800	-1.16819200
O	3.12821100	1.02399000	3.31709300
C	5.83956100	0.12235100	3.15484800
O	6.60094500	1.44666000	-4.35048000
O	-0.72797200	1.95987500	4.12852200
C	-3.38236600	2.49366500	5.04769500
H	8.26692700	-1.05528600	-1.46704300
O	7.40133500	-2.76309900	-2.29111200
H	6.35231500	-0.96868100	-3.83519000
H	4.47283200	1.09690000	-2.38264700
H	6.47336100	0.19257300	0.47858000
H	6.83834700	-0.18017900	2.84293700
H	5.37323900	-0.71398600	3.67877500
H	5.93554900	0.93235700	3.88007000
H	7.19472100	1.65047400	-1.11622900
H	6.29985000	2.69285200	-2.23031300
H	8.25134000	1.03247000	-3.16472200
O	-6.04620100	7.25640000	0.10151800
H	-7.75995700	6.10343400	0.36461100
H	-6.03641400	4.97618500	-1.07736000
H	-3.82302000	3.27124400	-0.66683000
H	-4.82792200	3.11896400	2.79386400

H	-4.43982300	2.73379500	5.14982100
H	-2.80950700	3.19114200	5.66147200
H	-3.21325300	1.49833300	5.46223100
H	-5.70903000	1.75840700	1.01231900
H	-5.75574600	2.00464000	-0.72768100
H	-7.16642500	3.59328500	1.37486600
Hg	0.84321600	1.97083900	1.37368200
H	-6.60315600	6.04877800	1.71002000
H	6.97652500	0.97271700	-5.10033300
H	8.69452600	-1.37889600	-3.15813700
H	-8.64424600	3.68990300	-0.26060600
H	8.11548200	-3.31116400	-1.95146600
H	-6.45052100	8.03315300	0.50036700

Thymidine-Hg^{II}-thymidine (torsion angle O2(1)-N3(1)-N3(2)-O4(2): 210°)

O	-7.93048000	2.74437300	-0.08116600
C	-6.82071400	3.31248700	0.60235000
C	-6.19857900	4.51623000	-0.12743700
O	-4.82736700	4.51103000	0.27954500
C	-4.39698800	3.14873200	0.35703700
C	-5.66129100	2.31265900	0.65486800
C	-6.83005200	5.84488700	0.20460800
N	-3.34109100	3.06187500	1.35598700
C	-3.60200400	3.43739400	2.65274000
C	-2.68218000	3.39036600	3.63230300
C	-1.35063500	2.90439200	3.28570900
N	-1.13613300	2.53745500	1.97264700
C	-2.07067500	2.61381000	0.97921700
O	-1.82621600	2.30041400	-0.18580900
N	2.75285900	0.85593200	1.06902700
C	3.30740400	1.08490800	-0.15882500
N	4.60207300	0.59461100	-0.35727000
C	5.25887100	-0.09175900	0.63548400
C	4.72248900	-0.32189300	1.84733500
C	3.38617200	0.20217900	2.10743700
C	5.27075200	0.85048400	-1.62793200
O	5.79140400	-0.38017500	-2.12722000
C	6.92044400	-0.10855600	-2.98071700
C	7.25878700	1.39327800	-2.80906600

C	6.47827700	1.78339800	-1.56116400
C	8.07166800	-1.03038300	-2.63672400
O	2.72075200	1.69666600	-1.05210100
O	2.82840000	0.07721900	3.20408600
C	5.43640000	-1.07739400	2.92577300
O	6.76721000	2.18207900	-3.89348800
O	-0.44109600	2.81403900	4.11760100
C	-2.96748000	3.80362500	5.04324700
H	8.35933100	-0.89465300	-1.58880500
O	7.66968400	-2.37336200	-2.88671700
H	6.61914200	-0.29182200	-4.01601400
H	4.50573200	1.24499500	-2.29073600
H	6.23880900	-0.45474900	0.36532400
H	6.41822400	-1.40501800	2.58665200
H	4.86707800	-1.95665000	3.23284500
H	5.56713900	-0.46106300	3.81696000
H	7.06457300	1.57982700	-0.66561100
H	6.20305900	2.83528100	-1.56830300
H	8.33277200	1.54872500	-2.68978800
O	-6.29427400	6.84520900	-0.65664100
H	-7.91341100	5.75439500	0.06783100
H	-6.27081400	4.33958000	-1.20790700
H	-3.93644600	2.84828100	-0.57882500
H	-4.60574300	3.79216500	2.83289100
H	-3.99868500	4.13745600	5.15022800
H	-2.30838900	4.61535200	5.35638200
H	-2.79883800	2.97701600	5.73580200
H	-5.59654600	1.79740300	1.60986400
H	-5.80510700	1.56203900	-0.12068700
H	-7.11779500	3.61124200	1.61113100
Hg	0.79841000	1.70665900	1.49084800
H	-6.63633100	6.08261600	1.25568300
H	7.23744300	1.93068300	-4.69580700
H	8.92696600	-0.75573500	-3.26374500
H	-8.72659100	3.23099600	0.15484100
H	8.39702000	-2.95594400	-2.64718200
H	-6.70326300	7.68710100	-0.43327200

Thymidine-Hg^{II}-thymidine (torsion angle O2(1)-N3(1)-N3(2)-O4(2): 240°)

O	-8.05843200	2.63689200	0.34368400
C	-6.89596500	3.29112300	0.83663300
C	-6.20242300	4.18312400	-0.20972400
O	-4.82543100	4.17734700	0.17323300
C	-4.50653000	2.84940100	0.60349100
C	-5.81272400	2.26186100	1.18064500
C	-6.71775700	5.59898300	-0.26734800
N	-3.38572400	2.92927500	1.52643600
C	-3.52092500	3.63053800	2.70169600
C	-2.51869400	3.78993900	3.58352500
C	-1.22928300	3.18914000	3.25760300
N	-1.13920800	2.49940100	2.06559000
C	-2.16068900	2.35274900	1.17098500
O	-2.03031700	1.74433000	0.10914600
N	2.71763800	0.73735600	1.10993400
C	3.34618700	1.18034300	-0.02174100
N	4.61335400	0.64747000	-0.28035000
C	5.17242900	-0.28711300	0.55752000
C	4.55960600	-0.73822900	1.66578900
C	3.24146000	-0.19753500	1.98176200
C	5.34342900	1.08879900	-1.46237400
O	5.73668500	-0.06126500	-2.21076100
C	6.91145400	0.25084800	-2.98369600
C	7.41084800	1.63444300	-2.49649700
C	6.64559900	1.84128300	-1.19631300
C	7.94087600	-0.85024300	-2.83776500
O	2.84618200	2.01007700	-0.78319700
O	2.60998100	-0.55313400	2.98315400
C	5.16638800	-1.76292900	2.57409300
O	7.03988400	2.68423500	-3.39109700
O	-0.24794700	3.28412100	4.00290700
C	-2.66901100	4.55220500	4.86381700
H	8.21426300	-0.96905500	-1.78410700
O	7.39399800	-2.05561400	-3.36295700
H	6.62092600	0.32500200	-4.03560000
H	4.64629600	1.69887100	-2.02958400
H	6.13960100	-0.65483500	0.25060400
H	6.14650700	-2.07180500	2.21307300
H	4.53175000	-2.64787000	2.64838900

H	5.27967400	-1.37212000	3.58689000
H	7.18282900	1.38962400	-0.36301900
H	6.49014700	2.89587800	-0.98226400
H	8.49178000	1.63736200	-2.34393200
O	-6.12728000	6.26577900	-1.37927700
H	-7.80803200	5.56324100	-0.37004000
H	-6.32075300	3.71372100	-1.19456600
H	-4.14997800	2.26295200	-0.23772100
H	-4.49664900	4.06194400	2.86801900
H	-3.68219100	4.93729500	4.97096900
H	-1.97441400	5.39321600	4.90489300
H	-2.44771500	3.91981600	5.72549200
H	-5.74257500	2.07438500	2.24898600
H	-6.04809500	1.31834000	0.69134100
H	-7.15080800	3.88967000	1.71520400
Hg	0.77345000	1.60826600	1.57977700
H	-6.47850500	6.10800000	0.67206000
H	7.50929700	2.56072500	-4.22322700
H	8.83833000	-0.55451100	-3.39207400
H	-8.80595300	3.24017000	0.40560200
H	8.04073900	-2.75791000	-3.24351500
H	-6.46345300	7.16701700	-1.40487100

Thymidine-Hg^{II}-thymidine (torsion angle O2(1)-N3(1)-N3(2)-O4(2): 270°)

O	-8.13360100	2.44003000	1.02328100
C	-6.90871600	3.13970100	1.19646800
C	-6.38560500	3.79762600	-0.09212500
O	-4.96791500	3.85044200	0.08651700
C	-4.55767500	2.65324400	0.75763200
C	-5.78629700	2.16135900	1.55354200
C	-6.92468900	5.18209300	-0.35176400
N	-3.37694500	2.96312600	1.55009000
C	-3.46457300	3.88630400	2.56572300
C	-2.41179400	4.26299200	3.31204200
C	-1.11687700	3.66259600	3.00715500
N	-1.07596100	2.74982200	1.97197400
C	-2.15218300	2.37219600	1.22136300
O	-2.06503200	1.55268700	0.30681300
N	2.74612200	0.91841500	1.03118400

C	3.56478900	1.47682900	0.09145000
N	4.75814000	0.79240100	-0.17421100
C	5.05124300	-0.39053600	0.46153800
C	4.24691900	-0.95085700	1.38244600
C	3.00208300	-0.26120800	1.69923100
C	5.65958600	1.30422700	-1.19552300
O	5.81762900	0.30300000	-2.20296200
C	7.06811300	0.51273000	-2.88399400
C	7.86214900	1.55090800	-2.05013600
C	7.08333400	1.62092600	-0.74260800
C	7.79183300	-0.80528900	-3.06154900
O	3.29296200	2.52393900	-0.49526400
O	2.19091200	-0.69975300	2.52393800
C	4.56519900	-2.24360000	2.06869700
O	7.83490500	2.84986200	-2.64354300
O	-0.09248600	3.94885200	3.63721000
C	-2.51093400	5.26228700	4.42306100
H	7.96906000	-1.26782500	-2.08496100
O	7.00061100	-1.65022800	-3.89133200
H	6.85821900	0.93609100	-3.87074200
H	5.17341000	2.18638400	-1.60263600
H	5.97501600	-0.85649800	0.15424500
H	5.52092100	-2.64016800	1.72853700
H	3.79378600	-2.99125000	1.87511000
H	4.61147700	-2.11331400	3.15140100
H	7.44297400	0.86458200	-0.04599800
H	7.17101800	2.59800900	-0.27374600
H	8.89502800	1.23250100	-1.89680700
O	-6.51037300	5.61017000	-1.64580700
H	-8.01797000	5.14286500	-0.28728800
H	-6.63531100	3.14590500	-0.93878800
H	-4.23360800	1.91313600	0.03291100
H	-4.44857400	4.30225400	2.72277300
H	-3.53230500	5.62444700	4.53190900
H	-1.85854000	6.11816100	4.24120700
H	-2.19744600	4.82471200	5.37262200
H	-5.59426600	2.11303800	2.62229800
H	-6.07016000	1.16438200	1.22012900
H	-7.02069400	3.90042500	1.97415400

Hg	0.83515500	1.85193600	1.49558100
H	-6.55959700	5.86148700	0.42525100
H	8.30968700	2.81636300	-3.48114000
H	8.76324200	-0.60182300	-3.52525100
H	-8.86204000	3.06648300	1.08143800
H	7.45379700	-2.49409900	-3.98228200
H	-6.85302900	6.49690700	-1.79513800

Thymidine-Hg^{II}-thymidine (torsion angle O2(1)-N3(1)-N3(2)-O4(2): 300°)

O	-8.24245100	2.85470900	1.77499000
C	-6.91845500	3.33558000	1.59187300
C	-6.52172300	3.51622500	0.11779100
O	-5.09907400	3.36472600	0.10841600
C	-4.71935900	2.40328800	1.10282400
C	-5.90814200	2.29598600	2.07885200
C	-6.89956100	4.85369000	-0.46986900
N	-3.45952600	2.84097000	1.69115700
C	-3.41840100	4.01297200	2.40927900
C	-2.28512600	4.53350800	2.91072700
C	-1.04089400	3.82148800	2.64232500
N	-1.12597800	2.66364800	1.89612800
C	-2.28631600	2.12797600	1.41475800
O	-2.31501500	1.07592500	0.77669100
N	2.64769100	0.74353700	0.90683800
C	3.56819200	1.42292000	0.16087700
N	4.74908300	0.73351200	-0.14562700
C	4.93565900	-0.56559800	0.26324500
C	4.03291100	-1.24456400	0.99183900
C	2.79595100	-0.55797000	1.34468000
C	5.75580300	1.37500400	-0.97778500
O	5.93783900	0.58624700	-2.15639600
C	7.25483600	0.82173600	-2.68697800
C	8.03510000	1.61681000	-1.60927600
C	7.15320700	1.49161300	-0.37319400
C	7.90865300	-0.49133700	-3.06406100
O	3.39245800	2.57868900	-0.22401800
O	1.90433700	-1.10671200	2.00311000
C	4.23592600	-2.66082500	1.43453000
O	8.13610200	3.00411100	-1.93369500

O	0.05332500	4.22565100	3.05148000
C	-2.24672800	5.80312100	3.70404100
H	7.96985100	-1.14442900	-2.18726700
O	7.14479900	-1.09930700	-4.10101700
H	7.16033600	1.43932000	-3.58499100
H	5.35324300	2.35253000	-1.22814400
H	5.86118600	-1.01792100	-0.05808500
H	5.19915300	-3.04063400	1.09646600
H	3.45180300	-3.31120600	1.04262500
H	4.19589700	-2.74166900	2.52229700
H	7.40806300	0.59102700	0.18389600
H	7.25884800	2.35050300	0.28506100
H	9.03010600	1.19775300	-1.44773800
O	-6.63712800	4.84131700	-1.87007400
H	-7.96445100	5.02662300	-0.27697900
H	-6.99085800	2.71662300	-0.46850900
H	-4.50029700	1.45085800	0.63192900
H	-4.37094900	4.50207000	2.54689100
H	-3.24477800	6.22547900	3.81264800
H	-1.60760000	6.54631400	3.22400000
H	-1.83523600	5.63142300	4.70033000
H	-5.61213300	2.43973500	3.11454400
H	-6.36264800	1.30968000	1.99532000
H	-6.78947600	4.28299300	2.12322900
Hg	0.74575700	1.70310600	1.38597400
H	-6.32751700	5.64052300	0.03250100
H	8.68731800	3.09823800	-2.71812800
H	8.92843900	-0.27959800	-3.40364500
H	-8.85264400	3.59827700	1.74167500
H	7.54769400	-1.94624300	-4.31587500
H	-6.87297900	5.70236500	-2.22916000

Thymidine-Hg^{II}-thymidine (torsion angle O2(1)-N3(1)-N3(2)-O4(2): 330°)

O	-8.11766600	2.87360100	2.74163300
C	-6.90061400	3.38000400	2.21103100
C	-6.77715800	3.22390000	0.68606600
O	-5.36845600	3.16504600	0.44847500
C	-4.75451700	2.44409400	1.52500000
C	-5.71710000	2.55707600	2.72627700

C	-7.38532300	4.35076100	-0.11104800
N	-3.42130200	2.99141200	1.72991400
C	-3.27710300	4.28834400	2.16473400
C	-2.08482500	4.89585100	2.29514200
C	-0.89621000	4.13253600	1.93090800
N	-1.08825500	2.83614800	1.49967600
C	-2.30487300	2.23177400	1.36009800
O	-2.42664000	1.08270100	0.93750600
N	2.42296300	0.69759800	0.20840500
C	3.50240100	1.41353100	-0.22675900
N	4.64182500	0.67735900	-0.56231800
C	4.66487500	-0.69017500	-0.43811800
C	3.60995000	-1.40496700	-0.00686900
C	2.39954800	-0.67588300	0.35058500
C	5.84198900	1.39039900	-0.99683100
O	6.38678900	0.71814600	-2.12942900
C	7.81950400	0.88428000	-2.15611800
C	8.19893700	1.64216400	-0.86344700
C	6.97914400	1.43384000	0.02208600
C	8.50782700	-0.45944300	-2.28952300
O	3.49563500	2.64161400	-0.31562900
O	1.38409200	-1.24413900	0.76881400
C	3.62988400	-2.89732500	0.11877900
O	8.33730600	3.04613300	-1.08500800
O	0.24315300	4.60721100	1.99058600
C	-1.93257800	6.30719500	2.77242200
H	8.24381800	-1.10400000	-1.44443700
O	8.11432000	-1.04965100	-3.52408900
H	8.07146300	1.49562300	-3.02649500
H	5.51265400	2.39083300	-1.26271100
H	5.59037200	-1.15756800	-0.73737800
H	4.59772600	-3.30019000	-0.17662100
H	2.86103300	-3.35556200	-0.50608000
H	3.42607100	-3.20764000	1.14524300
H	7.04881600	0.48281300	0.54991700
H	6.86408100	2.23150400	0.75176800
H	9.11015400	1.24030500	-0.41627900
O	-7.35698400	4.01179100	-1.49462900
H	-8.41570200	4.49811900	0.23120500

H	-7.24975200	2.27749600	0.39493900
H	-4.60014600	1.40962800	1.23595500
H	-4.19941100	4.80150500	2.39237200
H	-2.90289600	6.75213800	2.98867200
H	-1.43000700	6.92214200	2.02380400
H	-1.32360800	6.35314500	3.67722700
H	-5.24386800	2.99599900	3.60069300
H	-6.07668800	1.56746400	3.00425900
H	-6.78671000	4.43409900	2.47968300
Hg	0.65671600	1.76387100	0.84974300
H	-6.82431400	5.27085400	0.08222400
H	9.10329000	3.19518400	-1.64978000
H	9.59004000	-0.29178700	-2.26358500
H	-8.79994800	3.54725500	2.65751400
H	8.53200100	-1.91370200	-3.59235900
H	-7.74159900	4.73993200	-1.99248900

$(Me_3Si)_2N\text{-}Hg^{II}\text{-}N(SiMe_3)_2$:

Hg	-1.47224800	-2.84503100	-0.02576500
N	0.60429800	-2.70698900	0.05404900
N	-3.54531700	-3.02007900	-0.16227300
Si	1.28832900	-1.60293200	1.21822200
Si	1.50128200	-3.75368800	-1.02104100
Si	-4.33550500	-1.89807900	-1.24449900
Si	-4.33440800	-4.06501400	0.99325800
C	3.01388800	-2.87745600	-1.75029700
C	2.08683800	-5.32765700	-0.14523300
C	0.44501500	-4.31061500	-2.49396700
C	2.81135300	-2.33320800	2.07554900
C	1.79282000	0.03479200	0.41255600
C	0.03160100	-1.20461500	2.57730200
C	-3.08916000	-4.75278000	2.24277000
C	-5.65795300	-3.14714700	1.99154200
C	-5.14782000	-5.55399300	0.15395100
C	-3.25838600	-1.59311100	-2.77038500
C	-6.00006000	-2.55869200	-1.85639700
C	-4.64365500	-0.22003800	-0.41951600
H	0.49568100	-0.56595800	3.33284500
H	-0.84251400	-0.66823600	2.20158300

H	-0.31523000	-2.10796500	3.08326900
H	2.54505900	-0.11790900	-0.36301700
H	0.93393800	0.52295000	-0.05324500
H	2.20948100	0.72629200	1.14883800
H	3.21342900	-1.61341700	2.79247100
H	2.55823100	-3.24269000	2.62339400
H	3.61205300	-2.57741900	1.37655400
H	3.55098900	-3.56002400	-2.41327900
H	2.71696900	-2.00786800	-2.33955800
H	3.71899100	-2.54001500	-0.99001600
H	2.76548800	-5.10491100	0.67920500
H	1.24050500	-5.88299000	0.26504600
H	2.61130500	-5.98860900	-0.83961900
H	1.05995600	-4.90297000	-3.17563300
H	-0.39894200	-4.93838300	-2.19943900
H	0.05383900	-3.46207900	-3.05888100
H	-3.70845700	0.24029900	-0.09242200
H	-5.13005600	0.47585500	-1.10740100
H	-5.28352900	-0.32131800	0.45898600
H	-6.71007200	-2.73330600	-1.04724800
H	-6.45079300	-1.82816100	-2.53239400
H	-5.88157600	-3.49239900	-2.40806500
H	-2.30934100	-1.11107600	-2.52385900
H	-3.03378600	-2.52673200	-3.28988300
H	-3.77685300	-0.93752900	-3.47384500
H	-2.31484800	-5.36040900	1.76928900
H	-2.59966100	-3.96236600	2.81573000
H	-3.60827400	-5.39609700	2.95735100
H	-6.44331300	-2.73001400	1.35975200
H	-6.13642200	-3.82493300	2.70256100
H	-5.21864900	-2.32529300	2.56056000
H	-4.41162600	-6.13652400	-0.40385800
H	-5.60124100	-6.21394400	0.89760900
H	-5.93081400	-5.25440800	-0.54323800