# Electronic Supplementary Information

# Anion-controlled structural motif in one-dimensional coordination networks *via* cooperative weak noncovalent interactions

*Behrouz Notash, Nasser Safari* and Hamid Reza Khavasi*

*Chemistry Department, Shahid Beheshti University, G. C., Evin, Tehran 1983963113, Iran*

*To whom correspondence should be addressed

*Tel.: +98 21 29902886; Fax: +98 21 22431661*

*E-mail address: n-safari@cc.sbu.ac.ir (N. Safari)*

**Table S1.** Crystal data and structure refinement for **1.**

| | |
|---|---|
| Identification code | (**1**) |
| Empirical formula | $C_{22}H_{18}Cl_4Hg_2N_6$ |
| Formula weight | 909.40 |
| Temperature | 293(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | Monoclinic, $P2_1/c$ |
| Unit cell dimensions | *a* = 11.582(2) Å alpha = 90 [°]<br>*b* = 15.457(3) Å beta = 92.69(3) [°]<br>*c* = 14.730(3) Å gamma = 90 [°] |
| Volume | 2634.1(9) $Å^3$ |
| Z, Calculated density | 4, 2.293 $Mg/m^3$ |
| Absorption coefficient | 12.071 $mm^{-1}$ |
| F(000) | 1680 |
| Crystal size | 0.17 × 0.12 × 0.12 mm |
| Theta range for data collection | 1.76 to 29.27 [°] |
| Limiting indices | -15<=h<=15, -21<=k<=19, -15<=l<=20 |
| Reflections collected / unique | 20628 / 7103 [*R*(int) = 0.0671] |
| Completeness to theta = 29.27 | 98.8 % |
| Absorption correction | Numerical |
| Max. and min. transmission | 0.233 and 0.190 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 7103 / 0 / 307 |
| Goodness-of-fit on $F^2$ | 1.155 |
| Final *R* indices [I>2sigma(I)] | *R*1 = 0.0609, *wR*2 = 0.1001 |
| *R* indices (all data) | *R*1 = 0.1114, *wR*2 = 0.1133 |
| Largest diff. peak and hole | 1.730 and -1.790 e.$Å^{-3}$ |

**Table S2.** Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **1**. *U*(eq) is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

| | x | y | z | *U*(eq) |
|---|---|---|---|---|
| Hg(1) | -1472(1) | 1478(1) | 7768(1) | 47(1) |
| Hg(2) | 6871(1) | -3522(1) | 6662(1) | 45(1) |
| Cl(1) | -1469(4) | 1491(3) | 6178(2) | 87(1) |
| Cl(2) | -2549(2) | 1392(2) | 9088(2) | 55(1) |
| Cl(3) | 8006(2) | -3587(2) | 5376(2) | 53(1) |
| Cl(4) | 6894(3) | -3479(2) | 8276(2) | 64(1) |
| N(1) | 5657(6) | 5254(5) | 6440(5) | 37(2) |
| N(2) | 3230(7) | 4222(6) | 7499(6) | 46(2) |
| N(3) | -112(6) | 2599(6) | 8244(6) | 40(2) |
| N(4) | -166(6) | 272(5) | 8082(5) | 38(2) |
| N(5) | 2988(7) | -1439(7) | 7127(6) | 52(2) |
| N(6) | 5558(6) | -2388(6) | 6231(6) | 41(2) |
| C(1) | 4774(8) | 5076(7) | 6972(7) | 41(2) |
| C(2) | 5941(7) | 4667(6) | 5817(6) | 38(2) |
| C(3) | 5359(8) | 3893(7) | 5709(7) | 45(2) |
| C(4) | 4432(8) | 3733(6) | 6256(6) | 40(2) |
| C(5) | 4128(8) | 4339(6) | 6879(7) | 39(2) |
| C(6) | 2417(8) | 3708(6) | 7299(7) | 38(2) |
| C(7) | 1513(7) | 3497(8) | 7937(7) | 42(2) |
| C(8) | 1445(10) | 3895(8) | 8768(8) | 53(3) |
| C(9) | 580(10) | 3638(8) | 9329(8) | 56(3) |
| C(10) | -158(10) | 2999(8) | 9047(8) | 51(3) |
| C(11) | 726(8) | 2866(7) | 7694(7) | 42(2) |
| C(12) | 694(8) | 87(7) | 7543(7) | 44(2) |
| C(13) | -281(8) | -212(7) | 8822(6) | 38(2) |
| C(14) | 445(8) | -886(7) | 9046(7) | 44(2) |
| C(15) | 1333(8) | -1094(7) | 8477(7) | 40(2) |
| C(16) | 1457(7) | -593(7) | 7705(7) | 36(2) |
| C(17) | 2355(8) | -771(7) | 7070(7) | 42(2) |
| C(18) | 3877(8) | -1572(8) | 6513(7) | 45(2) |
| C(19) | 3997(11) | -1141(10) | 5701(9) | 74(4) |
| C(20) | 4906(12) | -1321(11) | 5155(10) | 84(5) |
| C(21) | 5688(8) | -1953(7) | 5477(7) | 46(3) |
| C(22) | 4666(8) | -2202(6) | 6736(7) | 37(2) |

**Table S3.** Bond lengths [Å] and angles [°] for **1**.

| | |
|---|---|
| Hg(1)-Cl(1) | 2.341(3) |
| Hg(1)-Cl(2) | 2.363(2) |
| Hg(1)-N(3) | 2.423(8) |
| Hg(1)-N(4) | 2.432(8) |
| Hg(2)-Cl(3) | 2.358(2) |
| Hg(2)-N(1)#1 | 2.372(7) |
| Hg(2)-Cl(4) | 2.378(3) |
| Hg(2)-N(6) | 2.387(9) |
| N(1)-C(2) | 1.342(12) |
| N(1)-C(1) | 1.346(11) |
| N(1)-Hg(2)#2 | 2.372(7) |
| N(2)-C(6) | 1.257(12) |
| N(2)-C(5) | 1.428(12) |
| N(3)-C(10) | 1.338(13) |
| N(3)-C(11) | 1.357(11) |
| N(4)-C(12) | 1.333(11) |
| N(4)-C(13) | 1.334(12) |
| N(5)-C(17) | 1.266(14) |
| N(5)-C(18) | 1.417(12) |
| N(6)-C(21) | 1.313(13) |
| N(6)-C(22) | 1.331(11) |
| C(1)-C(5) | 1.365(14) |
| C(1)-H(1) | 0.9300 |
| C(2)-C(3) | 1.378(14) |
| C(2)-H(2) | 0.9300 |
| C(3)-C(4) | 1.394(12) |
| C(3)-H(3) | 0.9300 |
| C(4)-C(5) | 1.369(13) |
| C(4)-H(4) | 0.9300 |
| C(6)-C(7) | 1.476(12) |
| C(6)-H(6) | 0.9300 |
| C(7)-C(11) | 1.371(15) |
| C(7)-C(8) | 1.376(16) |
| C(8)-C(9) | 1.386(14) |
| C(8)-H(8) | 0.9300 |
| C(9)-C(10) | 1.358(16) |
| C(9)-H(9) | 0.9300 |
| C(10)-H(10) | 0.9300 |
| C(11)-H(11) | 0.9300 |
| C(12)-C(16) | 1.387(14) |
| C(12)-H(12) | 0.9300 |
| C(13)-C(14) | 1.370(14) |
| C(13)-H(13) | 0.9300 |
| C(14)-C(15) | 1.394(13) |
| C(14)-H(14) | 0.9300 |
| C(15)-C(16) | 1.389(14) |
| C(15)-H(15) | 0.9300 |
| C(16)-C(17) | 1.457(12) |
| C(17)-H(17) | 0.9300 |

| | |
|---|---|
| C(18)-C(22) | 1.366(14) |
| C(18)-C(19) | 1.382(17) |
| C(19)-C(20) | 1.383(15) |
| C(19)-H(19) | 0.9300 |
| C(20)-C(21) | 1.400(18) |
| C(20)-H(20) | 0.9300 |
| C(21)-H(21) | 0.9300 |
| C(22)-H(22) | 0.9300 |
| Cl(1)-Hg(1)-Cl(2) | 148.13(13) |
| Cl(1)-Hg(1)-N(3) | 104.6(2) |
| Cl(2)-Hg(1)-N(3) | 99.4(2) |
| Cl(1)-Hg(1)-N(4) | 99.6(2) |
| Cl(2)-Hg(1)-N(4) | 98.52(19) |
| N(3)-Hg(1)-N(4) | 95.9(3) |
| Cl(3)-Hg(2)-N(1)#1 | 101.8(2) |
| Cl(3)-Hg(2)-Cl(4) | 145.51(10) |
| N(1)#1-Hg(2)-Cl(4) | 97.9(2) |
| Cl(3)-Hg(2)-N(6) | 101.0(2) |
| N(1)#1-Hg(2)-N(6) | 100.5(3) |
| Cl(4)-Hg(2)-N(6) | 102.8(2) |
| C(2)-N(1)-C(1) | 118.5(8) |
| C(2)-N(1)-Hg(2)#2 | 118.1(6) |
| C(1)-N(1)-Hg(2)#2 | 123.0(7) |
| C(6)-N(2)-C(5) | 119.3(9) |
| C(10)-N(3)-C(11) | 116.5(9) |
| C(10)-N(3)-Hg(1) | 122.3(6) |
| C(11)-N(3)-Hg(1) | 121.2(7) |
| C(12)-N(4)-C(13) | 118.2(9) |
| C(12)-N(4)-Hg(1) | 121.8(7) |
| C(13)-N(4)-Hg(1) | 120.0(6) |
| C(17)-N(5)-C(18) | 120.8(10) |
| C(21)-N(6)-C(22) | 119.0(9) |
| C(21)-N(6)-Hg(2) | 120.2(6) |
| C(22)-N(6)-Hg(2) | 120.7(7) |
| N(1)-C(1)-C(5) | 122.6(9) |
| N(1)-C(1)-H(1) | 118.7 |
| C(5)-C(1)-H(1) | 118.7 |
| N(1)-C(2)-C(3) | 122.1(8) |
| N(1)-C(2)-H(2) | 119.0 |
| C(3)-C(2)-H(2) | 119.0 |
| C(2)-C(3)-C(4) | 118.2(9) |
| C(2)-C(3)-H(3) | 120.9 |
| C(4)-C(3)-H(3) | 120.9 |
| C(5)-C(4)-C(3) | 119.7(9) |
| C(5)-C(4)-H(4) | 120.2 |
| C(3)-C(4)-H(4) | 120.2 |
| C(1)-C(5)-C(4) | 118.8(9) |
| C(1)-C(5)-N(2) | 116.9(9) |
| C(4)-C(5)-N(2) | 124.1(9) |
| N(2)-C(6)-C(7) | 122.4(10) |
| N(2)-C(6)-H(6) | 118.8 |
| C(7)-C(6)-H(6) | 118.8 |
| C(11)-C(7)-C(8) | 119.0(9) |
| C(11)-C(7)-C(6) | 118.3(10) |
| C(8)-C(7)-C(6) | 122.7(10) |

| | |
|---|---|
| C(7)-C(8)-C(9) | 118.4(11) |
| C(7)-C(8)-H(8) | 120.8 |
| C(9)-C(8)-H(8) | 120.8 |
| C(10)-C(9)-C(8) | 119.3(11) |
| C(10)-C(9)-H(9) | 120.4 |
| C(8)-C(9)-H(9) | 120.4 |
| N(3)-C(10)-C(9) | 123.7(9) |
| N(3)-C(10)-H(10) | 118.2 |
| C(9)-C(10)-H(10) | 118.2 |
| N(3)-C(11)-C(7) | 123.1(10) |
| N(3)-C(11)-H(11) | 118.5 |
| C(7)-C(11)-H(11) | 118.5 |
| N(4)-C(12)-C(16) | 123.3(10) |
| N(4)-C(12)-H(12) | 118.4 |
| C(16)-C(12)-H(12) | 118.4 |
| N(4)-C(13)-C(14) | 122.6(9) |
| N(4)-C(13)-H(13) | 118.7 |
| C(14)-C(13)-H(13) | 118.7 |
| C(13)-C(14)-C(15) | 119.5(10) |
| C(13)-C(14)-H(14) | 120.3 |
| C(15)-C(14)-H(14) | 120.3 |
| C(16)-C(15)-C(14) | 118.2(10) |
| C(16)-C(15)-H(15) | 120.9 |
| C(14)-C(15)-H(15) | 120.9 |
| C(12)-C(16)-C(15) | 118.2(8) |
| C(12)-C(16)-C(17) | 120.2(10) |
| C(15)-C(16)-C(17) | 121.6(9) |
| N(5)-C(17)-C(16) | 122.7(10) |
| N(5)-C(17)-H(17) | 118.6 |
| C(16)-C(17)-H(17) | 118.6 |
| C(22)-C(18)-C(19) | 117.3(9) |
| C(22)-C(18)-N(5) | 116.6(10) |
| C(19)-C(18)-N(5) | 126.0(10) |
| C(18)-C(19)-C(20) | 121.1(12) |
| C(18)-C(19)-H(19) | 119.4 |
| C(20)-C(19)-H(19) | 119.4 |
| C(19)-C(20)-C(21) | 116.1(12) |
| C(19)-C(20)-H(20) | 121.9 |
| C(21)-C(20)-H(20) | 121.9 |
| N(6)-C(21)-C(20) | 123.1(9) |
| N(6)-C(21)-H(21) | 118.4 |
| C(20)-C(21)-H(21) | 118.4 |
| N(6)-C(22)-C(18) | 123.1(10) |
| N(6)-C(22)-H(22) | 118.4 |
| C(18)-C(22)-H(22) | 118.4 |

Symmetry transformations used to generate equivalent atoms:
#1 x,y-1,z  #2 x,y+1,z

**Table S4.** Selected bond length (Å) and bond angles (º) for **1**[a]

| | | | |
|---|---|---|---|
| Hg(1)−N(3) | 2.423(8) | Hg(2)−N(1)$^{\#1}$ | 2.372(7 |
| Hg(1)−N(4) | 2.432(8) | Hg(2)−N(6) | 2.387(9 |
| Hg(1)−Cl(1) | 2.341(3) | Hg(2)−Cl(3) | 2.358(2 |
| Hg(1)−Cl(2) | 2.363(2) | Hg(2)−Cl(4) | 2.378(3 |
| C(6)−N(2) | 1.257(12) | C(17)−N(5) | 1.266(1 |
| Cl(1)−Hg(1)−Cl(2) | 148.13(13) | Cl(3)−Hg(2)−Cl(4) | 145.51( |
| N(3)−Hg(1)−N(4) | 95.9(3) | N(6)−Hg(2)−N(1)$^{\#1}$ | 100.5(3 |
| Cl(1)−Hg(1)−N(3) | 104.6(2) | Cl(3)−Hg(2)−N(6) | 101.0(2 |
| Cl(2)−Hg(1)−N(3) | 99.4(2) | Cl(4)−Hg(2)−N(6) | 102.8(2 |
| Cl(1)−Hg(1)−N(4) | 99.6(2) | Cl(3)−Hg(2)−N(1)$^{\#1}$ | 101.8(2 |
| Cl(2)−Hg(1)−N(4) | 98.52(19) | Cl(4)−Hg(2)−N(1)$^{\#1}$ | 97.9(2) |

[a] Symmetry code: #1: x, y–1, z

**Table S5.** Anisotropic displacement parameters ($Å^2 \times 10^3$) for **1**.
The anisotropic displacement factor exponent takes the form:
$-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

| | *U*11 | *U*22 | *U*33 | *U*23 | *U*13 | *U*12 |
|---|---|---|---|---|---|---|
| Hg(1) | 44(1) | 52(1) | 46(1) | 6(1) | 15(1) | 2(1) |
| Hg(2) | 42(1) | 41(1) | 52(1) | -7(1) | 17(1) | -2(1) |
| Cl(1) | 132(3) | 82(2) | 47(2) | 8(2) | 18(2) | 7(3) |
| Cl(2) | 41(1) | 69(2) | 56(1) | 15(2) | 27(1) | 6(1) |
| Cl(3) | 42(1) | 63(2) | 56(1) | -8(1) | 14(1) | -1(1) |
| Cl(4) | 87(2) | 58(2) | 48(1) | -6(2) | 24(1) | 2(2) |
| N(1) | 34(4) | 37(4) | 39(4) | -2(3) | 5(3) | -7(3) |
| N(2) | 43(4) | 49(6) | 48(5) | -3(4) | 16(4) | -3(4) |
| N(3) | 34(4) | 45(5) | 40(4) | 12(4) | 4(3) | 2(3) |
| N(4) | 37(4) | 41(5) | 38(4) | -9(3) | 10(3) | -2(3) |
| N(5) | 37(4) | 59(6) | 62(5) | -3(5) | 13(4) | 14(4) |
| N(6) | 37(4) | 43(5) | 44(5) | -10(4) | 15(3) | 1(3) |
| C(1) | 36(5) | 41(6) | 45(5) | 2(4) | 13(4) | 0(4) |
| C(2) | 33(4) | 43(5) | 40(5) | 5(4) | 7(4) | -2(4) |
| C(3) | 42(5) | 43(5) | 51(6) | -7(5) | 10(4) | -1(4) |
| C(4) | 36(4) | 39(6) | 45(5) | -2(4) | 4(4) | -11(4) |
| C(5) | 34(4) | 40(5) | 44(5) | 9(5) | 6(4) | 5(4) |
| C(6) | 35(4) | 38(6) | 42(5) | 3(4) | 10(4) | 1(4) |
| C(7) | 35(4) | 41(5) | 52(5) | 16(5) | 12(4) | 1(5) |
| C(8) | 58(6) | 48(6) | 55(7) | 4(5) | 10(5) | -12(5) |
| C(9) | 70(7) | 56(8) | 45(6) | -9(6) | 23(5) | -15(6) |
| C(10) | 54(6) | 54(7) | 47(6) | 2(5) | 16(5) | -12(5) |
| C(11) | 31(4) | 42(6) | 54(6) | 6(5) | 15(4) | 8(4) |
| C(12) | 40(5) | 48(6) | 46(6) | 0(5) | 17(4) | 2(4) |
| C(13) | 34(4) | 43(6) | 36(5) | -2(4) | 3(4) | -3(4) |
| C(14) | 46(5) | 45(6) | 41(5) | -5(4) | 11(4) | -7(4) |
| C(15) | 40(5) | 40(5) | 42(5) | -10(4) | 0(4) | 2(4) |
| C(16) | 23(4) | 37(5) | 49(5) | -12(4) | 11(3) | -4(4) |
| C(17) | 34(4) | 43(6) | 48(6) | -5(4) | 7(4) | -2(4) |
| C(18) | 34(4) | 47(6) | 55(6) | -11(5) | 10(4) | -1(4) |
| C(19) | 62(7) | 97(11) | 64(8) | 15(7) | 20(6) | 37(7) |
| C(20) | 80(9) | 99(12) | 76(9) | 21(8) | 48(7) | 31(8) |
| C(21) | 33(5) | 59(7) | 48(6) | -9(5) | 16(4) | 7(4) |
| C(22) | 40(5) | 35(5) | 39(5) | -11(4) | 14(4) | -1(4) |

**Table S6.** Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for **1.**

| | x | y | z | *U*(eq) |
|---|---|---|---|---|
| H(1) | 4596 | 5470 | 7422 | 49 |
| H(2) | 6549 | 4787 | 5446 | 46 |
| H(3) | 5579 | 3489 | 5282 | 54 |
| H(4) | 4022 | 3217 | 6197 | 48 |
| H(6) | 2385 | 3450 | 6727 | 45 |
| H(8) | 1967 | 4326 | 8949 | 64 |
| H(9) | 506 | 3900 | 9891 | 67 |
| H(10) | -728 | 2830 | 9435 | 61 |
| H(11) | 767 | 2609 | 7125 | 50 |
| H(12) | 786 | 431 | 7034 | 53 |
| H(13) | -879 | -87 | 9201 | 45 |
| H(14) | 347 | -1203 | 9574 | 53 |
| H(15) | 1829 | -1554 | 8611 | 48 |
| H(17) | 2469 | -379 | 6605 | 50 |
| H(19) | 3458 | -723 | 5519 | 89 |
| H(20) | 4994 | -1038 | 4605 | 100 |
| H(21) | 6329 | -2071 | 5142 | 56 |
| H(22) | 4577 | -2518 | 7266 | 45 |

**Table S7.** Torsion angles [°] for **1.**

| | |
|---|---|
| Cl(1)-Hg(1)-N(3)-C(10) | 156.0(8) |
| Cl(2)-Hg(1)-N(3)-C(10) | -2.7(8) |
| N(4)-Hg(1)-N(3)-C(10) | -102.4(8) |
| Cl(1)-Hg(1)-N(3)-C(11) | -22.6(7) |
| Cl(2)-Hg(1)-N(3)-C(11) | 178.7(7) |
| N(4)-Hg(1)-N(3)-C(11) | 79.0(7) |
| Cl(1)-Hg(1)-N(4)-C(12) | 31.1(8) |
| Cl(2)-Hg(1)-N(4)-C(12) | -175.2(8) |
| N(3)-Hg(1)-N(4)-C(12) | -74.8(8) |
| Cl(1)-Hg(1)-N(4)-C(13) | -150.6(7) |
| Cl(2)-Hg(1)-N(4)-C(13) | 3.1(7) |
| N(3)-Hg(1)-N(4)-C(13) | 103.5(7) |

| | |
|---|---|
| Cl(3)-Hg(2)-N(6)-C(21) | -5.6(8) |
| N(1)#1-Hg(2)-N(6)-C(21) | -110.0(8) |
| Cl(4)-Hg(2)-N(6)-C(21) | 149.2(8) |
| Cl(3)-Hg(2)-N(6)-C(22) | 172.5(7) |
| N(1)#1-Hg(2)-N(6)-C(22) | 68.1(8) |
| Cl(4)-Hg(2)-N(6)-C(22) | -32.6(8) |
| C(2)-N(1)-C(1)-C(5) | -2.7(15) |
| Hg(2)#2-N(1)-C(1)-C(5) | -175.4(7) |
| C(1)-N(1)-C(2)-C(3) | -0.1(14) |
| Hg(2)#2-N(1)-C(2)-C(3) | 173.0(8) |
| N(1)-C(2)-C(3)-C(4) | 1.4(15) |
| C(2)-C(3)-C(4)-C(5) | -0.1(15) |
| N(1)-C(1)-C(5)-C(4) | 4.0(15) |
| N(1)-C(1)-C(5)-N(2) | 178.8(9) |
| C(3)-C(4)-C(5)-C(1) | -2.5(15) |
| C(3)-C(4)-C(5)-N(2) | -176.9(10) |
| C(6)-N(2)-C(5)-C(1) | 159.9(10) |
| C(6)-N(2)-C(5)-C(4) | -25.5(15) |
| C(5)-N(2)-C(6)-C(7) | 174.7(9) |
| N(2)-C(6)-C(7)-C(11) | -173.7(10) |
| N(2)-C(6)-C(7)-C(8) | 4.9(16) |
| C(11)-C(7)-C(8)-C(9) | 0.2(17) |
| C(6)-C(7)-C(8)-C(9) | -178.5(10) |
| C(7)-C(8)-C(9)-C(10) | 0.8(19) |
| C(11)-N(3)-C(10)-C(9) | -0.4(17) |
| Hg(1)-N(3)-C(10)-C(9) | -179.0(9) |
| C(8)-C(9)-C(10)-N(3) | -1(2) |
| C(10)-N(3)-C(11)-C(7) | 1.4(15) |
| Hg(1)-N(3)-C(11)-C(7) | -179.9(7) |
| C(8)-C(7)-C(11)-N(3) | -1.3(16) |
| C(6)-C(7)-C(11)-N(3) | 177.4(9) |
| C(13)-N(4)-C(12)-C(16) | 1.4(15) |
| Hg(1)-N(4)-C(12)-C(16) | 179.7(7) |
| C(12)-N(4)-C(13)-C(14) | 0.0(14) |
| Hg(1)-N(4)-C(13)-C(14) | -178.4(7) |
| N(4)-C(13)-C(14)-C(15) | -1.2(15) |
| C(13)-C(14)-C(15)-C(16) | 1.0(14) |
| N(4)-C(12)-C(16)-C(15) | -1.4(15) |
| N(4)-C(12)-C(16)-C(17) | 178.2(9) |
| C(14)-C(15)-C(16)-C(12) | 0.2(14) |
| C(14)-C(15)-C(16)-C(17) | -179.4(9) |
| C(18)-N(5)-C(17)-C(16) | -177.9(9) |
| C(12)-C(16)-C(17)-N(5) | -171.7(10) |
| C(15)-C(16)-C(17)-N(5) | 7.9(15) |
| C(17)-N(5)-C(18)-C(22) | 166.5(10) |
| C(17)-N(5)-C(18)-C(19) | -15.5(18) |
| C(22)-C(18)-C(19)-C(20) | -2(2) |
| N(5)-C(18)-C(19)-C(20) | 179.7(13) |
| C(18)-C(19)-C(20)-C(21) | 0(2) |
| C(22)-N(6)-C(21)-C(20) | -2.5(18) |
| Hg(2)-N(6)-C(21)-C(20) | 175.6(11) |
| C(19)-C(20)-C(21)-N(6) | 3(2) |
| C(21)-N(6)-C(22)-C(18) | -0.6(15) |
| Hg(2)-N(6)-C(22)-C(18) | -178.8(7) |
| C(19)-C(18)-C(22)-N(6) | 3.0(17) |
| N(5)-C(18)-C(22)-N(6) | -178.8(9) |

Symmetry transformations used to generate equivalent atoms:
#1 x,y-1,z  #2 x,y+1,z

**Table S8.** Crystal data and structure refinement for **2.**

| | |
|---|---|
| Identification code | (**2**) |
| Empirical formula | $C_{22}H_{18}Br_4Hg_2N_6$ |
| Formula weight | 1087.21 |
| Temperature | 293(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | Triclinic, $P\bar{1}$ |
| Unit cell dimensions | *a* = 8.2037(16) Å alpha = 88.07(3) [°]<br>*b* = 11.926(2) Å beta = 82.43(3) [°]<br>*c* = 14.227(3) Å gamma = 87.89(3) [°] |
| Volume | 1378.3(5) $Å^3$ |
| Z, Calculated density | 2, 2.620 $Mg/m^3$ |
| Absorption coefficient | 16.945 $mm^{-1}$ |
| F(000) | 984 |
| Crystal size | 0.27 × 0.14 × 0.12 mm |
| Theta range for data collection | 1.71 to 29.28 [°] |
| Limiting indices | -10<=h<=11, -16<=k<=16, -19<=l<=18 |
| Reflections collected / unique | 15726 / 7422 [*R*(int) = 0.1031] |
| Completeness to theta = 29.28 | 98.6 % |
| Absorption correction | Numerical |
| Max. and min. transmission | 0.132 and 0.071 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 7422 / 0 / 308 |
| Goodness-of-fit on $F^2$ | 1.127 |
| Final *R* indices [I>2sigma(I)] | *R*1 = 0.0748, *wR*2 = 0.1744 |
| *R* indices (all data) | *R*1 = 0.1123, *wR*2 = 0.1947 |
| Extinction coefficient | 0.0023(3) |
| Largest diff. peak and hole | 3.391 and -1.936 $e.Å^{-3}$ |

**Table S9.** Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **2**. *U*(eq) is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

| | x | y | z | *U*(eq) |
|---|---|---|---|---|
| Hg(1) | 1326(1) | -1731(1) | 7218(1) | 48(1) |
| Hg(2) | -2029(1) | 6412(1) | 12541(1) | 49(1) |
| Br(1) | 3873(2) | -1851(2) | 8017(1) | 69(1) |
| Br(2) | -652(2) | -2963(1) | 6600(1) | 54(1) |
| Br(3) | 109(2) | 7536(1) | 13116(1) | 55(1) |
| Br(4) | -4604(2) | 6530(3) | 11809(2) | 91(1) |
| N(1) | 7307(13) | 5192(10) | 3883(8) | 44(2) |
| N(2) | 4422(14) | 1979(10) | 5247(8) | 46(2) |
| N(3) | 2051(14) | -527(10) | 5891(8) | 45(2) |
| N(4) | -421(15) | -493(11) | 8222(8) | 52(3) |
| N(5) | 41(19) | 1892(13) | 9680(9) | 62(3) |
| N(6) | -249(16) | 5106(10) | 11582(8) | 48(3) |
| C(1) | 6309(15) | 4318(10) | 3880(9) | 41(3) |
| C(2) | 7993(16) | 5320(12) | 4697(9) | 45(3) |
| C(3) | 7668(17) | 4606(13) | 5493(10) | 49(3) |
| C(4) | 6648(16) | 3733(12) | 5453(9) | 46(3) |
| C(5) | 5943(14) | 3565(10) | 4660(9) | 38(2) |
| C(6) | 4852(17) | 2671(10) | 4541(10) | 44(3) |
| C(7) | 3465(16) | 1022(11) | 5097(9) | 42(3) |
| C(8) | 3139(17) | 685(12) | 4220(9) | 46(3) |
| C(9) | 2222(18) | -266(11) | 4205(9) | 45(3) |
| C(10) | 1722(17) | -851(11) | 5036(10) | 45(3) |
| C(11) | 2921(17) | 394(12) | 5885(10) | 47(3) |
| C(12) | 196(19) | 327(11) | 8649(9) | 46(3) |
| C(13) | -2050(20) | -598(14) | 8299(10) | 56(4) |
| C(14) | -3130(20) | 120(20) | 8849(12) | 79(6) |
| C(15) | -2460(20) | 976(16) | 9316(12) | 63(4) |
| C(16) | -790(20) | 1073(12) | 9230(9) | 48(3) |
| C(17) | -704(18) | 2697(12) | 10088(9) | 46(3) |
| C(18) | 70(20) | 3521(11) | 10595(9) | 48(3) |
| C(19) | 1840(20) | 3541(14) | 10563(10) | 57(4) |
| C(20) | 2420(20) | 4369(16) | 11053(13) | 65(4) |
| C(21) | 1360(19) | 5131(14) | 11549(11) | 56(4) |
| C(22) | -888(17) | 4323(11) | 11088(9) | 44(3) |

**Table S10.** Bond lengths [Å] and angles [°] for **2**.

| | |
|---|---|
| Hg(1)-N(3) | 2.358(11) |
| Hg(1)-N(4) | 2.392(12) |
| Hg(1)-Br(2) | 2.4901(16) |
| Hg(1)-Br(1) | 2.5045(18) |
| Hg(2)-N(1)#1 | 2.378(11) |
| Hg(2)-N(6) | 2.422(13) |
| Hg(2)-Br(4) | 2.474(2) |
| Hg(2)-Br(3) | 2.4835(16) |
| N(1)-C(1) | 1.349(15) |
| N(1)-C(2) | 1.368(17) |
| N(1)-Hg(2)#2 | 2.378(11) |
| N(2)-C(6) | 1.299(16) |
| N(2)-C(7) | 1.446(16) |
| N(3)-C(11) | 1.332(17) |
| N(3)-C(10) | 1.351(16) |
| N(4)-C(12) | 1.318(16) |
| N(4)-C(13) | 1.336(19) |
| N(5)-C(17) | 1.24(2) |
| N(5)-C(16) | 1.424(19) |
| N(6)-C(21) | 1.316(19) |
| N(6)-C(22) | 1.349(17) |
| C(1)-C(5) | 1.411(17) |
| C(1)-H(1) | 0.9300 |
| C(2)-C(3) | 1.396(19) |
| C(2)-H(2) | 0.9300 |
| C(3)-C(4) | 1.366(18) |
| C(3)-H(3) | 0.9300 |
| C(4)-C(5) | 1.359(19) |
| C(4)-H(4) | 0.9300 |
| C(5)-C(6) | 1.446(17) |
| C(6)-H(6) | 0.9300 |
| C(7)-C(11) | 1.361(18) |
| C(7)-C(8) | 1.386(18) |
| C(8)-C(9) | 1.386(17) |
| C(8)-H(8) | 0.9300 |
| C(9)-C(10) | 1.375(18) |
| C(9)-H(9) | 0.9300 |
| C(10)-H(10) | 0.9300 |
| C(11)-H(11) | 0.9300 |
| C(12)-C(16) | 1.40(2) |
| C(12)-H(12) | 0.9300 |
| C(13)-C(14) | 1.39(2) |
| C(13)-H(13) | 0.9300 |
| C(14)-C(15) | 1.40(2) |
| C(14)-H(14) | 0.9300 |
| C(15)-C(16) | 1.37(2) |
| C(15)-H(15) | 0.9300 |
| C(17)-C(18) | 1.452(19) |
| C(17)-H(17) | 0.9300 |
| C(18)-C(22) | 1.368(19) |
| C(18)-C(19) | 1.44(2) |
| C(19)-C(20) | 1.36(2) |
| C(19)-H(19) | 0.9300 |
| C(20)-C(21) | 1.38(2) |
| C(20)-H(20) | 0.9300 |
| C(21)-H(21) | 0.9300 |

| | |
|---|---|
| C(22)-H(22) | 0.9300 |
| N(3)-Hg(1)-N(4) | 100.5(4) |
| N(3)-Hg(1)-Br(2) | 101.3(3) |
| N(4)-Hg(1)-Br(2) | 103.2(3) |
| N(3)-Hg(1)-Br(1) | 103.4(3) |
| N(4)-Hg(1)-Br(1) | 101.9(3) |
| Br(2)-Hg(1)-Br(1) | 140.60(7) |
| N(1)#1-Hg(2)-N(6) | 97.5(4) |
| N(1)#1-Hg(2)-Br(4) | 103.1(3) |
| N(6)-Hg(2)-Br(4) | 104.8(3) |
| N(1)#1-Hg(2)-Br(3) | 100.1(3) |
| N(6)-Hg(2)-Br(3) | 98.9(3) |
| Br(4)-Hg(2)-Br(3) | 144.10(9) |
| C(1)-N(1)-C(2) | 116.3(11) |
| C(1)-N(1)-Hg(2)#2 | 123.0(9) |
| C(2)-N(1)-Hg(2)#2 | 120.7(8) |
| C(6)-N(2)-C(7) | 119.2(11) |
| C(11)-N(3)-C(10) | 115.9(12) |
| C(11)-N(3)-Hg(1) | 125.6(9) |
| C(10)-N(3)-Hg(1) | 118.0(8) |
| C(12)-N(4)-C(13) | 120.0(14) |
| C(12)-N(4)-Hg(1) | 120.9(10) |
| C(13)-N(4)-Hg(1) | 118.9(10) |
| C(17)-N(5)-C(16) | 122.1(15) |
| C(21)-N(6)-C(22) | 118.6(13) |
| C(21)-N(6)-Hg(2) | 120.7(9) |
| C(22)-N(6)-Hg(2) | 120.7(10) |
| N(1)-C(1)-C(5) | 123.7(12) |
| N(1)-C(1)-H(1) | 118.1 |
| C(5)-C(1)-H(1) | 118.1 |
| N(1)-C(2)-C(3) | 122.5(11) |
| N(1)-C(2)-H(2) | 118.7 |
| C(3)-C(2)-H(2) | 118.7 |
| C(4)-C(3)-C(2) | 118.9(12) |
| C(4)-C(3)-H(3) | 120.6 |
| C(2)-C(3)-H(3) | 120.6 |
| C(5)-C(4)-C(3) | 120.9(13) |
| C(5)-C(4)-H(4) | 119.6 |
| C(3)-C(4)-H(4) | 119.6 |
| C(4)-C(5)-C(1) | 117.7(11) |
| C(4)-C(5)-C(6) | 125.5(12) |
| C(1)-C(5)-C(6) | 116.9(12) |
| N(2)-C(6)-C(5) | 119.5(12) |
| N(2)-C(6)-H(6) | 120.2 |
| C(5)-C(6)-H(6) | 120.2 |
| C(11)-C(7)-C(8) | 119.0(12) |
| C(11)-C(7)-N(2) | 116.0(12) |
| C(8)-C(7)-N(2) | 124.9(12) |
| C(7)-C(8)-C(9) | 117.2(12) |
| C(7)-C(8)-H(8) | 121.4 |
| C(9)-C(8)-H(8) | 121.4 |
| C(10)-C(9)-C(8) | 119.9(12) |
| C(10)-C(9)-H(9) | 120.0 |
| C(8)-C(9)-H(9) | 120.0 |
| N(3)-C(10)-C(9) | 122.9(12) |
| N(3)-C(10)-H(10) | 118.6 |
| C(9)-C(10)-H(10) | 118.6 |
| N(3)-C(11)-C(7) | 125.0(13) |
| N(3)-C(11)-H(11) | 117.5 |
| C(7)-C(11)-H(11) | 117.5 |

| | |
|---|---|
| N(4)-C(12)-C(16) | 122.5(14) |
| N(4)-C(12)-H(12) | 118.7 |
| C(16)-C(12)-H(12) | 118.7 |
| N(4)-C(13)-C(14) | 121.6(15) |
| N(4)-C(13)-H(13) | 119.2 |
| C(14)-C(13)-H(13) | 119.2 |
| C(13)-C(14)-C(15) | 118.0(16) |
| C(13)-C(14)-H(14) | 121.0 |
| C(15)-C(14)-H(14) | 121.0 |
| C(16)-C(15)-C(14) | 119.7(15) |
| C(16)-C(15)-H(15) | 120.1 |
| C(14)-C(15)-H(15) | 120.1 |
| C(15)-C(16)-C(12) | 118.1(13) |
| C(15)-C(16)-N(5) | 125.1(14) |
| C(12)-C(16)-N(5) | 116.9(14) |
| N(5)-C(17)-C(18) | 124.1(15) |
| N(5)-C(17)-H(17) | 118.0 |
| C(18)-C(17)-H(17) | 118.0 |
| C(22)-C(18)-C(19) | 119.1(13) |
| C(22)-C(18)-C(17) | 119.2(14) |
| C(19)-C(18)-C(17) | 121.6(13) |
| C(20)-C(19)-C(18) | 116.0(15) |
| C(20)-C(19)-H(19) | 122.0 |
| C(18)-C(19)-H(19) | 122.0 |
| C(19)-C(20)-C(21) | 121.2(16) |
| C(19)-C(20)-H(20) | 119.4 |
| C(21)-C(20)-H(20) | 119.4 |
| N(6)-C(21)-C(20) | 122.7(14) |
| N(6)-C(21)-H(21) | 118.6 |
| C(20)-C(21)-H(21) | 118.6 |
| N(6)-C(22)-C(18) | 122.3(14) |
| N(6)-C(22)-H(22) | 118.9 |
| C(18)-C(22)-H(22) | 118.9 |

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y,z+1  #2 x+1,y,z-1

**Table S11.** Selected bond length (Å) and bond angles (°) for **2**[a]

| | | | |
|---|---|---|---|
| Hg(1)−N(3) | 2.358(1 | Hg(2)−N(1)#1 | 2.378(1 |
| Hg(1)−N(4) | 2.392(1 | Hg(2)−N(6) | 2.422(1 |
| Hg(1)−Br(1) | 2.5045( | Hg(2)−Br(3) | 2.4835( |
| Hg(1)−Br(2) | 2.4901( | Hg(2)−Br(4) | 2.474(2) |
| C(6)−N(2) | 1.299(1 | C(17)−N(5) | 1.24(2) |
| Br(1)−Hg(1)−Br(2) | 140.60( | Br(3)−Hg(2)− | 144.10( |
| N(3)−Hg(1)−N(4) | 100.5(4 | N(6)−Hg(2)− | 97.5(4) |
| Br(1)−Hg(1)−N(3) | 103.4(3 | Br(3)−Hg(2)− | 98.9(3) |
| Br(2)−Hg(1)−N(3) | 101.3(3 | Br(4)−Hg(2)− | 104.8(3) |
| Br(1)−Hg(1)−N(4) | 101.9(3 | Br(3)−Hg(2)− | 100.1(3) |
| Br(2)−Hg(1)−N(4) | 103.2(3 | Br(4)−Hg(2)− | 103.1(3) |

[a] Symmetry code: #1: x-1,y,z+1

**Table S12.** Anisotropic displacement parameters ($Å^2 \times 10^3$) for **2**.
The anisotropic displacement factor exponent takes the form:
$-2\,pi^2\,[\,h^2\,a^{*2}\,U11 + ... + 2\,h\,k\,a^*\,b^*\,U12\,]$

| | *U*11 | *U*22 | *U*33 | *U*23 | *U*13 | *U*12 |
|---|---|---|---|---|---|---|
| Hg(1) | 55(1) | 48(1) | 41(1) | -5(1) | -1(1) | -15(1) |
| Hg(2) | 50(1) | 50(1) | 49(1) | -4(1) | -6(1) | -13(1) |
| Br(1) | 54(1) | 103(1) | 53(1) | -7(1) | -7(1) | -24(1) |
| Br(2) | 61(1) | 44(1) | 59(1) | -6(1) | -11(1) | -14(1) |
| Br(3) | 64(1) | 45(1) | 60(1) | -3(1) | -14(1) | -19(1) |
| Br(4) | 51(1) | 152(2) | 73(1) | 4(1) | -14(1) | -12(1) |
| N(1) | 36(5) | 44(6) | 47(6) | -3(5) | 8(4) | -5(5) |
| N(2) | 44(6) | 45(6) | 47(6) | -4(5) | -2(5) | -4(5) |
| N(3) | 52(6) | 42(6) | 39(5) | -2(4) | -1(4) | -6(5) |
| N(4) | 49(6) | 59(7) | 45(6) | -8(5) | 5(5) | -15(6) |
| N(5) | 75(9) | 63(8) | 48(7) | -15(6) | -10(6) | 7(7) |
| N(6) | 62(7) | 40(6) | 42(6) | 2(5) | -6(5) | -6(5) |
| C(1) | 35(6) | 36(6) | 50(7) | 4(5) | 1(5) | -10(5) |
| C(2) | 39(6) | 48(7) | 51(7) | -7(6) | -8(5) | -18(6) |
| C(3) | 46(7) | 56(8) | 45(7) | -3(6) | -6(5) | -7(6) |
| C(4) | 42(7) | 50(7) | 41(6) | 2(5) | 10(5) | -13(6) |
| C(5) | 33(6) | 35(6) | 44(6) | -5(5) | 6(5) | 1(5) |
| C(6) | 56(8) | 31(6) | 44(7) | 2(5) | -4(5) | -5(6) |
| C(7) | 41(6) | 43(7) | 41(6) | -5(5) | 4(5) | -6(6) |
| C(8) | 49(7) | 47(7) | 43(7) | 9(5) | -9(5) | -14(6) |
| C(9) | 59(8) | 36(6) | 42(6) | 1(5) | -5(6) | -14(6) |
| C(10) | 47(7) | 39(6) | 51(7) | -3(5) | -10(5) | -7(6) |
| C(11) | 45(7) | 44(7) | 50(7) | -3(6) | -1(5) | -2(6) |
| C(12) | 63(8) | 38(6) | 38(6) | -5(5) | -8(6) | -12(6) |
| C(13) | 63(9) | 60(9) | 45(7) | -7(6) | -13(6) | 0(8) |
| C(14) | 51(9) | 129(18) | 59(10) | -39(11) | -1(7) | -9(10) |
| C(15) | 49(8) | 72(11) | 69(10) | -37(9) | -6(7) | 11(8) |
| C(16) | 69(9) | 42(7) | 34(6) | -8(5) | -7(6) | -4(7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(17) | 46(7) | 46(7) | 43(7) | -5(5) | 6(5) | -7(6) |
| C(18) | 67(9) | 37(6) | 39(6) | 0(5) | 0(6) | -6(6) |
| C(19) | 64(9) | 61(9) | 44(7) | -8(6) | 8(6) | -1(8) |
| C(20) | 48(8) | 69(11) | 76(11) | -14(9) | -4(7) | -4(8) |
| C(21) | 53(8) | 61(9) | 56(8) | -19(7) | -7(6) | -13(7) |
| C(22) | 44(7) | 39(6) | 45(7) | -7(5) | 9(5) | -9(6) |

**Table S13.** Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for **2.**

| | x | y | z | *U*(eq) |
|---|---|---|---|---|
| H(1) | 5836 | 4205 | 3333 | 49 |
| H(2) | 8704 | 5904 | 4722 | 54 |
| H(3) | 8137 | 4723 | 6040 | 58 |
| H(4) | 6434 | 3248 | 5977 | 55 |
| H(6) | 4462 | 2591 | 3963 | 53 |
| H(8) | 3520 | 1081 | 3664 | 55 |
| H(9) | 1946 | -508 | 3633 | 54 |
| H(10) | 1131 | -1497 | 5009 | 54 |
| H(11) | 3178 | 627 | 6464 | 56 |
| H(12) | 1329 | 410 | 8559 | 55 |
| H(13) | -2470 | -1164 | 7976 | 67 |
| H(14) | -4261 | 33 | 8905 | 95 |
| H(15) | -3149 | 1475 | 9683 | 76 |
| H(17) | -1831 | 2778 | 10069 | 55 |
| H(19) | 2535 | 3020 | 10228 | 69 |
| H(20) | 3544 | 4421 | 11053 | 78 |
| H(21) | 1803 | 5685 | 11873 | 67 |
| H(22) | -2021 | 4328 | 11082 | 53 |

**Table S14.** Torsion angles [°] for **2.**

| | |
|---|---|
| N(4)-Hg(1)-N(3)-C(11) | 64.5(12) |
| Br(2)-Hg(1)-N(3)-C(11) | 170.4(11) |
| Br(1)-Hg(1)-N(3)-C(11) | -40.5(12) |
| N(4)-Hg(1)-N(3)-C(10) | -123.2(10) |
| Br(2)-Hg(1)-N(3)-C(10) | -17.3(11) |
| Br(1)-Hg(1)-N(3)-C(10) | 131.7(10) |
| N(3)-Hg(1)-N(4)-C(12) | -72.6(11) |
| Br(2)-Hg(1)-N(4)-C(12) | -176.9(10) |
| Br(1)-Hg(1)-N(4)-C(12) | 33.7(11) |
| N(3)-Hg(1)-N(4)-C(13) | 103.2(11) |
| Br(2)-Hg(1)-N(4)-C(13) | -1.1(12) |
| Br(1)-Hg(1)-N(4)-C(13) | -150.5(11) |
| N(1)#1-Hg(2)-N(6)-C(21) | -98.1(12) |
| Br(4)-Hg(2)-N(6)-C(21) | 156.2(11) |
| Br(3)-Hg(2)-N(6)-C(21) | 3.4(12) |
| N(1)#1-Hg(2)-N(6)-C(22) | 80.4(10) |
| Br(4)-Hg(2)-N(6)-C(22) | -25.3(10) |
| Br(3)-Hg(2)-N(6)-C(22) | -178.1(9) |
| C(2)-N(1)-C(1)-C(5) | 0.8(19) |
| Hg(2)#2-N(1)-C(1)-C(5) | 177.9(9) |
| C(1)-N(1)-C(2)-C(3) | -1(2) |
| Hg(2)#2-N(1)-C(2)-C(3) | -178.4(11) |
| N(1)-C(2)-C(3)-C(4) | 1(2) |
| C(2)-C(3)-C(4)-C(5) | -1(2) |
| C(3)-C(4)-C(5)-C(1) | 0(2) |
| C(3)-C(4)-C(5)-C(6) | 179.8(14) |
| N(1)-C(1)-C(5)-C(4) | 0(2) |
| N(1)-C(1)-C(5)-C(6) | -179.9(13) |
| C(7)-N(2)-C(6)-C(5) | -174.0(12) |
| C(4)-C(5)-C(6)-N(2) | 3(2) |
| C(1)-C(5)-C(6)-N(2) | -177.4(13) |
| C(6)-N(2)-C(7)-C(11) | -173.8(13) |
| C(6)-N(2)-C(7)-C(8) | 9(2) |
| C(11)-C(7)-C(8)-C(9) | 2(2) |
| N(2)-C(7)-C(8)-C(9) | 178.9(14) |
| C(7)-C(8)-C(9)-C(10) | -2(2) |
| C(11)-N(3)-C(10)-C(9) | -1(2) |
| Hg(1)-N(3)-C(10)-C(9) | -174.0(11) |
| C(8)-C(9)-C(10)-N(3) | 2(2) |
| C(10)-N(3)-C(11)-C(7) | 1(2) |
| Hg(1)-N(3)-C(11)-C(7) | 173.4(11) |
| C(8)-C(7)-C(11)-N(3) | -2(2) |
| N(2)-C(7)-C(11)-N(3) | -178.7(13) |
| C(13)-N(4)-C(12)-C(16) | 3(2) |
| Hg(1)-N(4)-C(12)-C(16) | 179.2(10) |
| C(12)-N(4)-C(13)-C(14) | -2(2) |
| Hg(1)-N(4)-C(13)-C(14) | -178.0(14) |
| N(4)-C(13)-C(14)-C(15) | 1(3) |
| C(13)-C(14)-C(15)-C(16) | -1(3) |
| C(14)-C(15)-C(16)-C(12) | 2(3) |
| C(14)-C(15)-C(16)-N(5) | -179.0(17) |
| N(4)-C(12)-C(16)-C(15) | -3(2) |
| N(4)-C(12)-C(16)-N(5) | 177.5(13) |
| C(17)-N(5)-C(16)-C(15) | -10(2) |

| | |
|---|---|
| C(17)-N(5)-C(16)-C(12) | 168.6(14) |
| C(16)-N(5)-C(17)-C(18) | 176.9(12) |
| N(5)-C(17)-C(18)-C(22) | -174.6(15) |
| N(5)-C(17)-C(18)-C(19) | 8(2) |
| C(22)-C(18)-C(19)-C(20) | 1(2) |
| C(17)-C(18)-C(19)-C(20) | 178.8(14) |
| C(18)-C(19)-C(20)-C(21) | 0(3) |
| C(22)-N(6)-C(21)-C(20) | -2(2) |
| Hg(2)-N(6)-C(21)-C(20) | 176.6(13) |
| C(19)-C(20)-C(21)-N(6) | 0(3) |
| C(21)-N(6)-C(22)-C(18) | 3(2) |
| Hg(2)-N(6)-C(22)-C(18) | -175.2(10) |
| C(19)-C(18)-C(22)-N(6) | -3(2) |
| C(17)-C(18)-C(22)-N(6) | 179.3(12) |

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y,z+1  #2 x+1,y,z-1

**Table S15.** Crystal data and structure refinement for **3.**

| | |
|---|---|
| Identification code | (**3**) |
| Empirical formula | $C_{11}H_9HgI_2N_3$ |
| Formula weight | 637.60 |
| Temperature | 293(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | Monoclinic, $P2_1/n$ |
| Unit cell dimensions | $a$ = 8.6931(17) Å alpha = 90 [°]<br>$b$ = 12.727(3) Å beta = 93.54(3) [°]<br>$c$ = 13.158(3) Å gamma = 90 [°] |
| Volume | 1453.0(6) $Å^3$ |
| Z, Calculated density | 4, 2.915 $Mg/m^3$ |
| Absorption coefficient | 14.825 $mm^{-1}$ |
| F(000) | 1128 |
| Crystal size | 0.12 × 0.12 × 0.10 mm |
| Theta range for data collection | 2.23 to 29.23 [°] |
| Limiting indices | -11<=h<=11, -17<=k<=17, -17<=l<=18 |
| Reflections collected / unique | 11016 / 3909 [$R$(int) = 0.0893] |
| Completeness to theta = 29.23 | 99.2 % |
| Absorption correction | Numerical |
| Max. and min. transmission | 0.225 and 0.193 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 3909 / 0 / 155 |
| Goodness-of-fit on $F^2$ | 1.172 |
| Final $R$ indices [I>2sigma(I)] | $R1$ = 0.0793, $wR2$ = 0.1845 |
| $R$ indices (all data) | $R1$ = 0.1007, $wR2$ = 0.1978 |
| Extinction coefficient | 0.0022(4) |
| Largest diff. peak and hole | 4.112 and -5.039 $e.Å^{-3}$ |

**Table S16.** Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **3**. *U*(eq) is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

| | x | y | z | *U*(eq) |
|---|---|---|---|---|
| Hg(1) | 2532(1) | 7273(1) | 3589(1) | 48(1) |
| I(1) | 4675(1) | 7436(1) | 2248(1) | 60(1) |
| I(2) | -218(1) | 6412(1) | 3691(1) | 79(1) |
| N(3) | 3998(13) | 6561(9) | 5073(8) | 48(2) |
| C(11) | 3369(17) | 6307(12) | 5931(11) | 54(3) |
| C(10) | 5528(15) | 6342(10) | 5054(9) | 42(2) |
| N(2) | 3908(14) | 5298(11) | 8479(9) | 54(3) |
| C(7) | 4083(15) | 5886(10) | 6771(10) | 46(3) |
| C(6) | 3268(18) | 5677(13) | 7700(10) | 53(3) |
| C(9) | 6375(15) | 5925(12) | 5854(12) | 52(3) |
| C(8) | 5664(15) | 5696(11) | 6711(11) | 48(3) |
| C(1) | 3131(16) | 4184(11) | 9830(10) | 46(3) |
| C(5) | 3067(14) | 5160(11) | 9341(10) | 46(3) |
| C(4) | 2249(19) | 5982(11) | 9752(11) | 55(3) |
| N(1) | 2382(11) | 3998(8) | 10662(8) | 41(2) |
| C(2) | 1581(15) | 4767(11) | 11077(11) | 49(3) |
| C(3) | 1533(19) | 5765(13) | 10661(12) | 59(4) |

**Table S17.** Bond lengths [Å] and angles [°] for **3**.

| | |
|---|---|
| Hg(1)-N(1)#1 | 2.405(10) |
| Hg(1)-N(3) | 2.440(12) |
| Hg(1)-I(2) | 2.6404(12) |
| Hg(1)-I(1) | 2.6518(12) |
| N(3)-C(11) | 1.325(17) |
| N(3)-C(10) | 1.360(17) |
| C(11)-C(7) | 1.34(2) |
| C(11)-H(11) | 0.9300 |
| C(10)-C(9) | 1.35(2) |
| C(10)-H(10) | 0.9300 |
| N(2)-C(6) | 1.234(18) |
| N(2)-C(5) | 1.397(16) |
| C(7)-C(8) | 1.402(18) |
| C(7)-C(6) | 1.475(17) |
| C(6)-H(6) | 0.9300 |
| C(9)-C(8) | 1.351(19) |
| C(9)-H(9) | 0.9300 |
| C(8)-H(8) | 0.9300 |
| C(1)-N(1) | 1.329(14) |
| C(1)-C(5) | 1.399(18) |
| C(1)-H(1) | 0.9300 |
| C(5)-C(4) | 1.392(19) |
| C(4)-C(3) | 1.409(19) |
| C(4)-H(4) | 0.9300 |
| N(1)-C(2) | 1.338(16) |
| N(1)-Hg(1)#2 | 2.405(10) |
| C(2)-C(3) | 1.38(2) |
| C(2)-H(2) | 0.9300 |
| C(3)-H(3) | 0.9300 |
| N(1)#1-Hg(1)-N(3) | 90.5(4) |
| N(1)#1-Hg(1)-I(2) | 111.3(2) |
| N(3)-Hg(1)-I(2) | 103.6(3) |
| N(1)#1-Hg(1)-I(1) | 101.3(2) |
| N(3)-Hg(1)-I(1) | 102.0(3) |
| I(2)-Hg(1)-I(1) | 137.87(5) |
| C(11)-N(3)-C(10) | 114.9(11) |
| C(11)-N(3)-Hg(1) | 123.3(9) |
| C(10)-N(3)-Hg(1) | 121.7(8) |
| N(3)-C(11)-C(7) | 127.1(13) |
| N(3)-C(11)-H(11) | 116.4 |
| C(7)-C(11)-H(11) | 116.4 |
| C(9)-C(10)-N(3) | 123.5(11) |
| C(9)-C(10)-H(10) | 118.3 |
| N(3)-C(10)-H(10) | 118.3 |
| C(6)-N(2)-C(5) | 119.4(12) |
| C(11)-C(7)-C(8) | 115.3(12) |
| C(11)-C(7)-C(6) | 122.1(12) |
| C(8)-C(7)-C(6) | 122.5(12) |

| | |
|---|---|
| N(2)-C(6)-C(7) | 123.0(13) |
| N(2)-C(6)-H(6) | 118.5 |
| C(7)-C(6)-H(6) | 118.5 |
| C(8)-C(9)-C(10) | 118.6(12) |
| C(8)-C(9)-H(9) | 120.7 |
| C(10)-C(9)-H(9) | 120.7 |
| C(9)-C(8)-C(7) | 120.6(13) |
| C(9)-C(8)-H(8) | 119.7 |
| C(7)-C(8)-H(8) | 119.7 |
| N(1)-C(1)-C(5) | 122.0(12) |
| N(1)-C(1)-H(1) | 119.0 |
| C(5)-C(1)-H(1) | 119.0 |
| C(4)-C(5)-N(2) | 121.7(13) |
| C(4)-C(5)-C(1) | 119.7(12) |
| N(2)-C(5)-C(1) | 118.5(12) |
| C(5)-C(4)-C(3) | 116.5(13) |
| C(5)-C(4)-H(4) | 121.8 |
| C(3)-C(4)-H(4) | 121.8 |
| C(1)-N(1)-C(2) | 120.0(11) |
| C(1)-N(1)-Hg(1)#2 | 119.7(8) |
| C(2)-N(1)-Hg(1)#2 | 120.3(8) |
| N(1)-C(2)-C(3) | 121.0(12) |
| N(1)-C(2)-H(2) | 119.5 |
| C(3)-C(2)-H(2) | 119.5 |
| C(2)-C(3)-C(4) | 120.8(13) |
| C(2)-C(3)-H(3) | 119.6 |
| C(4)-C(3)-H(3) | 119.6 |

Symmetry transformations used to generate equivalent atoms:
#1 -x+1/2,y+1/2,-z+3/2  #2 -x+1/2,y-1/2,-z+3/2

**Table S18.** Selected bond length (Å) and bond angles (°) for **3**[a]

| | | | |
|---|---|---|---|
| Hg(1)−N(3) | 2.440(12 | Hg(1)−N(1)$^{\#1}$ | 2.405(1 |
| Hg(1)−I(1) | 2.6518(1 | Hg(1)−I(2) | 2.6404( |
| C(6)−N(2) | 1.234(18 | C(5)−N(2) | 1.397(1 |
| I(1)−Hg(1)−I(2) | 137.87(5 | N(3)−Hg(1)− | 90.5(4) |
| N(3)−Hg(1)−I(1) | 102.0(3) | N(3)−Hg(1)−I( | 103.6(3) |
| I(1)−Hg(1)−N(1)$^{\#1}$ | 101.3(2) | I(2)−Hg(1)−N( | 111.3(2) |

[a] Symmetry code: #1: -x+1/2, y+1/2, -z+3/2.

**Table S19.** Anisotropic displacement parameters (Å$^2$ × 10$^3$) for **3**.
The anisotropic displacement factor exponent takes the form:
-2 pi$^2$ [ h$^2$ a*$^2$ *U*11 + ... + 2 h k a* b* *U*12 ]

| | *U*11 | *U*22 | *U*33 | *U*23 | *U*13 | *U*12 |
|---|---|---|---|---|---|---|
| Hg(1) | 47(1) | 54(1) | 43(1) | 1(1) | 15(1) | -1(1) |
| I(1) | 60(1) | 72(1) | 52(1) | -4(1) | 28(1) | -3(1) |
| I(2) | 51(1) | 79(1) | 110(1) | -3(1) | 27(1) | -13(1) |
| N(3) | 49(6) | 53(6) | 43(6) | 1(5) | 9(5) | 4(5) |
| C(11) | 49(7) | 64(8) | 52(7) | 14(6) | 15(6) | 24(6) |
| C(10) | 48(6) | 46(6) | 34(6) | -3(5) | 7(5) | -4(5) |
| N(2) | 51(6) | 70(7) | 42(6) | 5(5) | 15(5) | 0(6) |
| C(7) | 43(6) | 49(6) | 46(6) | 2(5) | 3(5) | 4(5) |
| C(6) | 60(8) | 67(8) | 32(6) | 8(6) | 11(5) | 13(6) |
| C(9) | 37(6) | 60(8) | 58(8) | -6(6) | 1(5) | 0(5) |
| C(8) | 44(6) | 53(7) | 48(7) | -10(6) | 0(5) | 1(5) |
| C(1) | 52(7) | 50(6) | 37(6) | 5(5) | 17(5) | 8(5) |
| C(5) | 38(6) | 51(6) | 48(7) | 3(5) | 6(5) | -2(5) |
| C(4) | 74(9) | 45(6) | 46(7) | 0(5) | 9(7) | 5(6) |
| N(1) | 37(5) | 45(5) | 43(5) | 2(4) | 11(4) | -2(4) |
| C(2) | 44(6) | 57(7) | 46(7) | -11(6) | 12(5) | -3(5) |
| C(3) | 65(9) | 63(8) | 52(8) | -3(7) | 18(7) | 13(7) |

**Table S20.** Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for **3.**

| | x | y | z | *U*(eq) |
|---|---|---|---|---|
| H(11) | 2318 | 6433 | 5955 | 65 |
| H(10) | 6017 | 6485 | 4461 | 51 |
| H(6) | 2224 | 5837 | 7698 | 63 |
| H(9) | 7423 | 5798 | 5813 | 62 |
| H(8) | 6229 | 5411 | 7268 | 58 |
| H(1) | 3716 | 3649 | 9565 | 55 |
| H(4) | 2178 | 6638 | 9443 | 66 |
| H(2) | 1048 | 4629 | 11654 | 58 |
| H(3) | 1022 | 6300 | 10985 | 71 |

**Table S21.** Torsion angles [°] for **3.**

| | |
|---|---|
| N(1)#1-Hg(1)-N(3)-C(11) | 81.2(12) |
| I(2)-Hg(1)-N(3)-C(11) | -30.9(12) |
| I(1)-Hg(1)-N(3)-C(11) | -177.1(11) |
| N(1)#1-Hg(1)-N(3)-C(10) | -102.5(10) |
| I(2)-Hg(1)-N(3)-C(10) | 145.4(9) |
| I(1)-Hg(1)-N(3)-C(10) | -0.8(10) |
| C(10)-N(3)-C(11)-C(7) | 2(2) |
| Hg(1)-N(3)-C(11)-C(7) | 178.1(12) |
| C(11)-N(3)-C(10)-C(9) | -2(2) |
| Hg(1)-N(3)-C(10)-C(9) | -178.5(10) |
| N(3)-C(11)-C(7)-C(8) | 0(2) |
| N(3)-C(11)-C(7)-C(6) | 177.4(15) |
| C(5)-N(2)-C(6)-C(7) | 177.6(14) |
| C(11)-C(7)-C(6)-N(2) | -179.5(16) |
| C(8)-C(7)-C(6)-N(2) | -2(2) |
| N(3)-C(10)-C(9)-C(8) | 1(2) |
| C(10)-C(9)-C(8)-C(7) | 0(2) |
| C(11)-C(7)-C(8)-C(9) | 0(2) |
| C(6)-C(7)-C(8)-C(9) | -178.3(14) |
| C(6)-N(2)-C(5)-C(4) | -53(2) |
| C(6)-N(2)-C(5)-C(1) | 130.6(17) |
| N(1)-C(1)-C(5)-C(4) | 3(2) |
| N(1)-C(1)-C(5)-N(2) | 179.0(12) |
| N(2)-C(5)-C(4)-C(3) | -175.8(14) |
| C(1)-C(5)-C(4)-C(3) | 0(2) |
| C(5)-C(1)-N(1)-C(2) | -2(2) |
| C(5)-C(1)-N(1)-Hg(1)#2 | 177.3(11) |
| C(1)-N(1)-C(2)-C(3) | -1(2) |
| Hg(1)#2-N(1)-C(2)-C(3) | 179.3(12) |
| N(1)-C(2)-C(3)-C(4) | 4(2) |
| C(5)-C(4)-C(3)-C(2) | -4(2) |

Symmetry transformations used to generate equivalent atoms:
#1 -x+1/2,y+1/2,-z+3/2 #2 -x+1/2,y-1/2,-z+3/2