**Further Characterization of Film 9**

An ellipsometry measurement was performed on a Gaertner L117C ellipsometer using 633 nm light. Scanning electron micrograms were obtained on an Amray 1830 SEM at an accelerating potential of 20 KV. Conductivity (1.1 mOhm-cm) was obtained from 4-point resistivity measurements using a Jandel 4-point meter.

The ellipsometry measurement[S1] indicated that the thickness of film **9** was fairly uniform, giving an average of 2170 Å. Scanning electron microscopy (SEM) showed that film **9** was smooth (Figure S5). No pattern was observed in powder X-ray diffraction of film **9**, indicating that the film was amorphous. Film **9** also passed the "Scotch tape test," showing good adhesion of the film to the Si substrate. The conductivity test indicated that film **9** was conductive.

**Reference**

S1. (a) Al-Douri, A. A. J.; Heavens, O. S. *Thin Solid Films* **1983**, *100*, 273. (b) Bendavid, A.; Martin, P. J.; Netterfield, R. P; Kinder, T. J. *Surf. Interface Anal.* **1996**, *24*, 627.

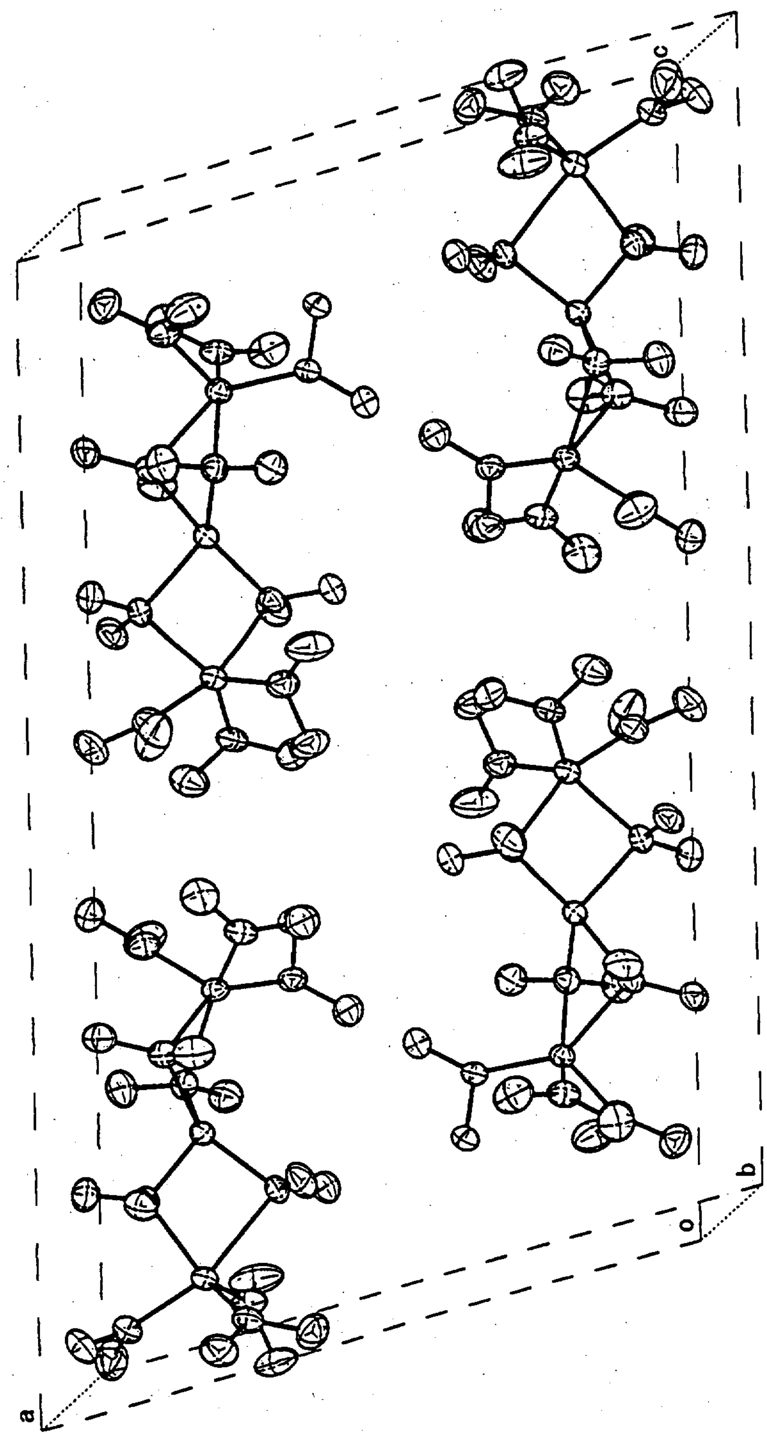



**Figure S1** Packing diagram of 1.

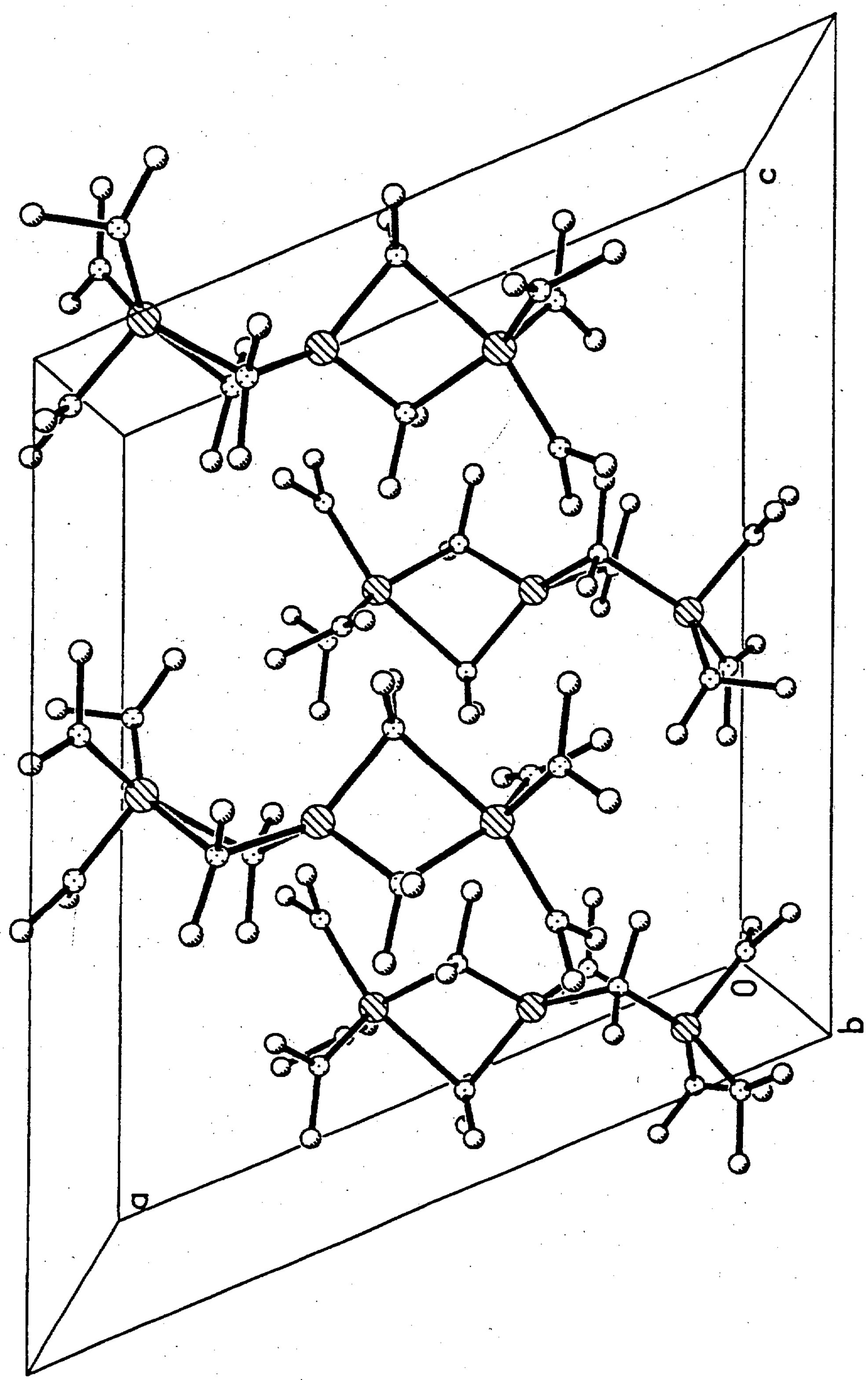



**Figure S2** Packing diagram of 2.

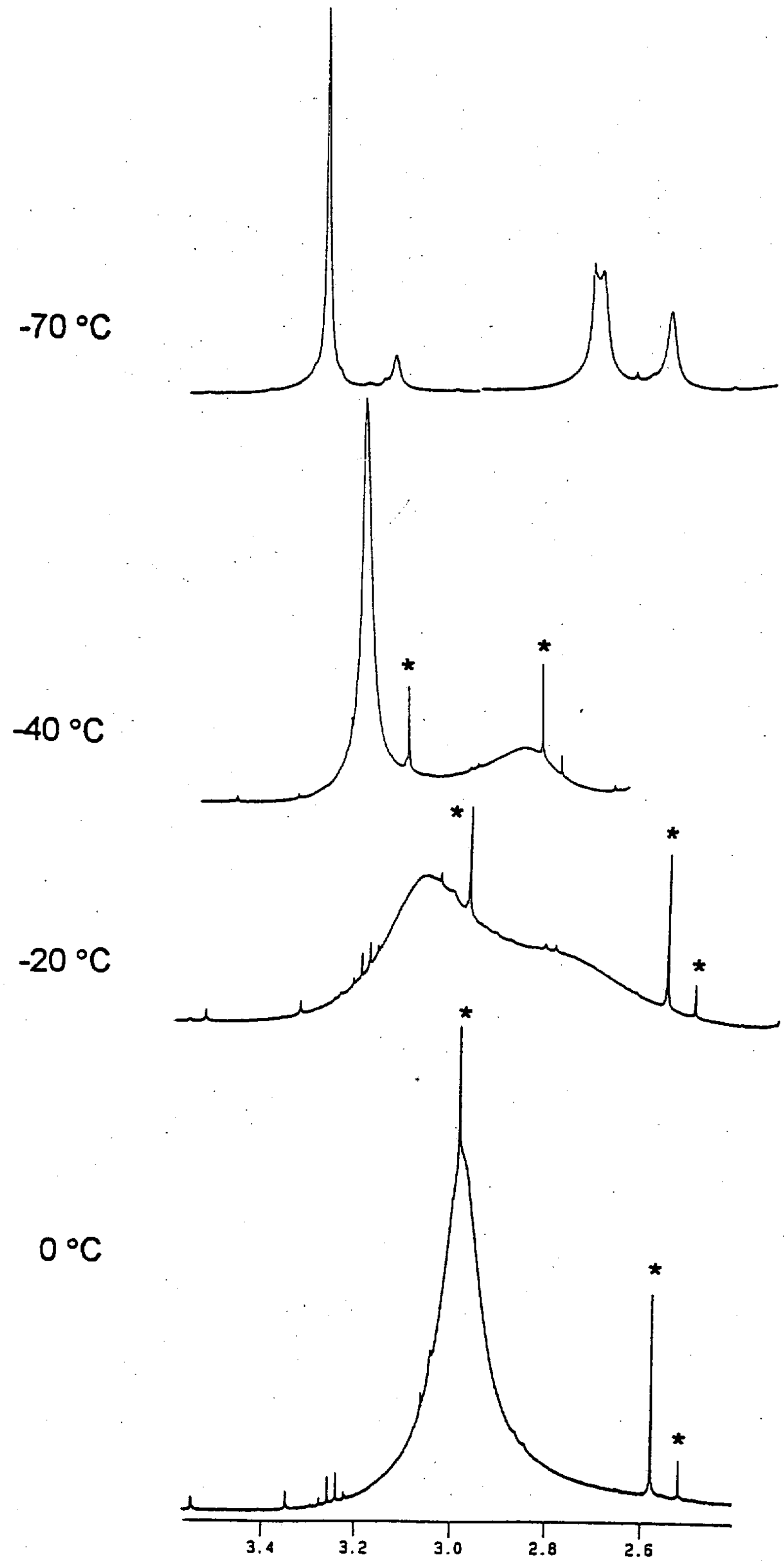



**Figure S3** Variable temperature $^{1}H$ NMR spectra of **1**. (* Impurity)

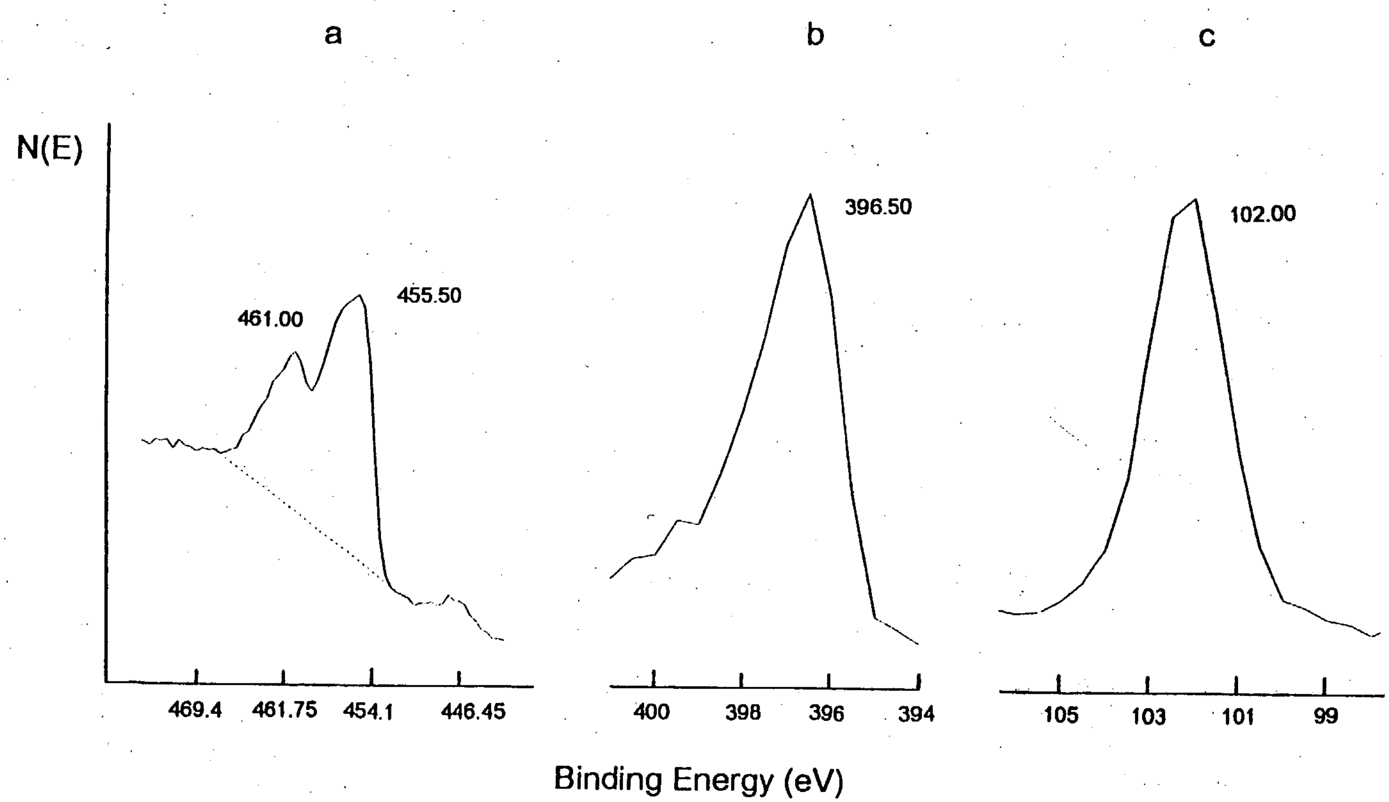



**Figure S4** XPS of film **9** after sputtering: (a) Ti $2p_{3/2}$; (b) N $1s$; (c) Si $2p$.

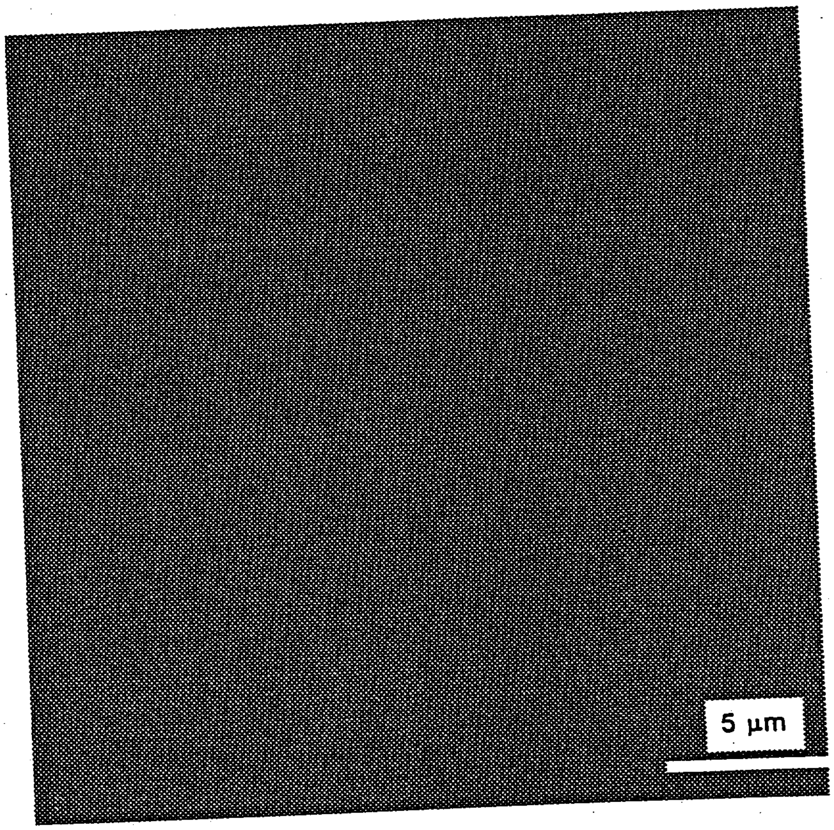
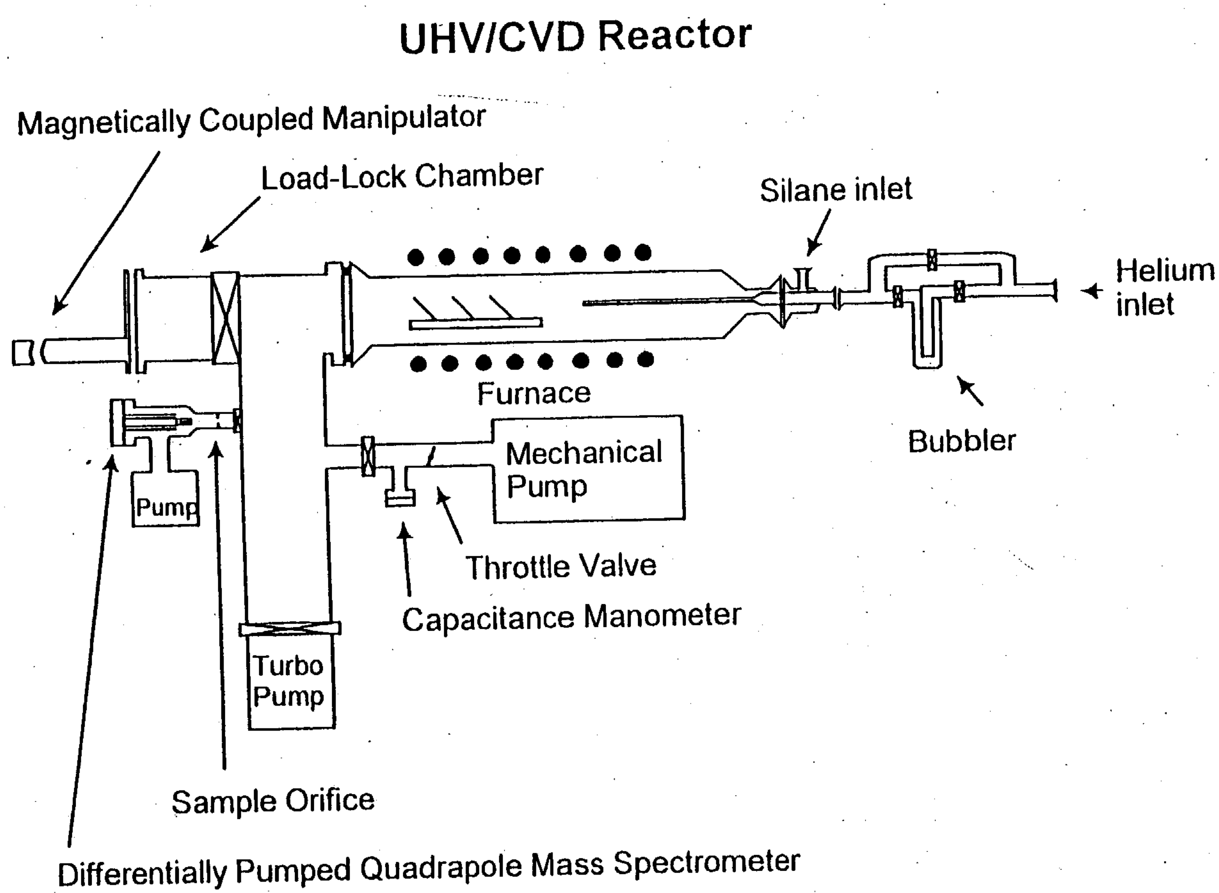
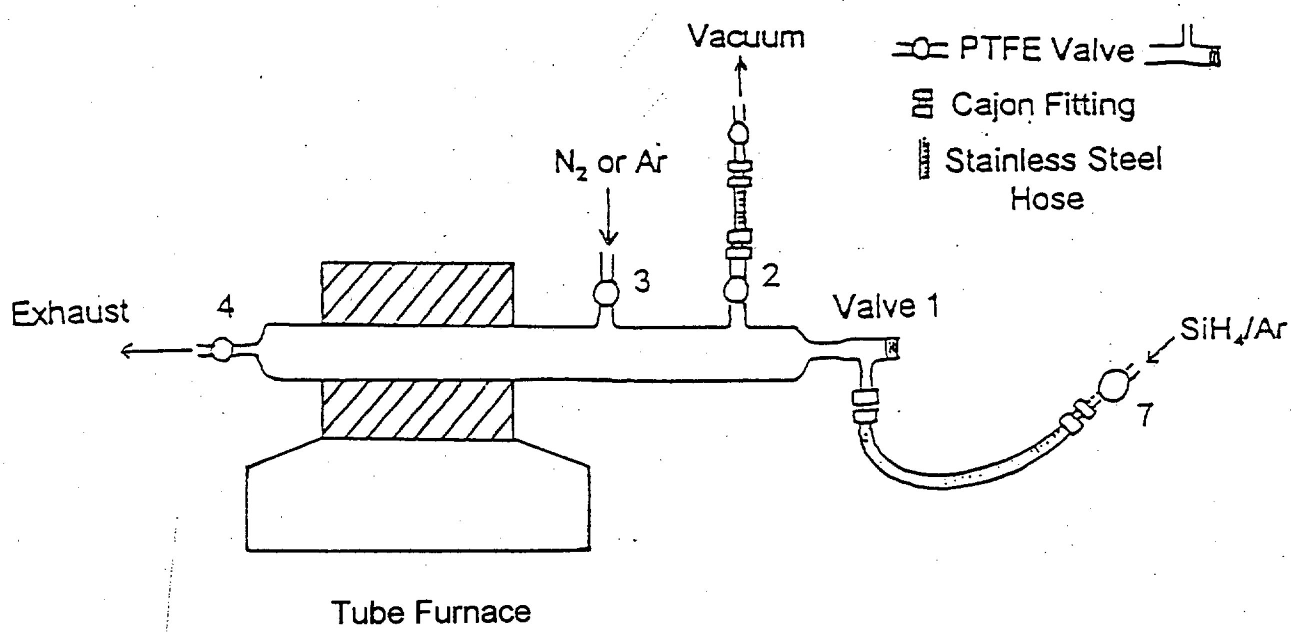



**Figure S5** SEM of film **9** (thickness = 2170 Å).




**Scheme S1.** Hot wall horizontal CVD apparatus for deposition of Ti-Si-N thin film **9**.




**Scheme S2.** Schematic diagram of a reaction manifold for the reactions of $Ti(NMe_2)_4$ with $SiH_4$ to give powders **7-8**.

Table S1. Crystal data and structure refinement for 1.

| | |
|---|---|
| Identification code | b |
| Empirical formula | $C_{20}H_{62}N_{10}Zr_3$ |
| Formula weight | 716.46 |
| Temperature | 173(2) K |
| Wavelength | 0.71073 Å |
| Crystal system | Monoclinic |
| Space group | $P2_1/c$ |
| Unit cell dimensions | $a$ = 15.475(3) Å alpha = 90° |
| | $b$ = 8.613(2) Å beta = 106.310(10)° |
| | $c$ = 26.154(4) Å gamma = 90° |
| Volume, Z | 3345.7(11) $Å^3$, 4 |
| Density (calculated) | 1.422 $Mg/m^3$ |
| Absorption coefficient | 0.941 $mm^{-1}$ |
| F(000) | 1488 |
| Crystal size | 0.40 x 0.40 x 0.20 mm |
| θ range for data collection | 1.62 to 22.55° |
| Limiting indices | $0 \le h \le 16$, $0 \le k \le 9$, $-28 \le l \le 27$ |
| Reflections collected | 4589 |
| Independent reflections | 4397 ($R_{int}$ = 0.0382) |
| Completeness to θ = 22.55° | 100.0 % |
| Max. and min. transmission | 0.8341 and 0.7045 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 4397 / 0 / 326 |
| Goodness-of-fit on $F^2$ | 1.117 |
| Final R indices [$I>2\sigma(I)$] | R1 = 0.0314, wR2 = 0.0801 |
| R indices (all data) | R1 = 0.0447, wR2 = 0.0926 |
| Largest diff. peak and hole | 0.407 and -0.746 $eÅ^{-3}$ |

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

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Zr(2) | 2617(1) | 1210(1) | 2101(1) | 19(1) |
| Zr(3) | 2372(1) | 1170(1) | 3290(1) | 22(1) |
| Zr(1) | 2587(1) | 850(1) | 867(1) | 25(1) |
| N(3) | 3301(2) | 2495(4) | 2837(2) | 28(1) |
| N(1) | 3555(2) | 2012(4) | 1646(2) | 26(1) |
| N(4) | 2668(2) | -741(4) | 2609(1) | 25(1) |
| N(2) | 1585(2) | 1897(4) | 1417(2) | 27(1) |
| N(6) | 1744(3) | -977(5) | 593(2) | 37(1) |
| N(10) | 2176(3) | 3189(5) | 3668(2) | 32(1) |
| N(8) | 1112(2) | 273(5) | 3202(1) | 32(1) |
| N(9) | 3299(3) | -60(5) | 3877(2) | 32(1) |
| N(5) | 2147(3) | 2688(5) | 351(2) | 34(1) |
| N(7) | 3680(3) | 14(5) | 640(2) | 39(1) |
| C(2) | 3811(3) | 3636(6) | 1576(2) | 37(1) |
| C(7) | 1937(3) | -1893(6) | 2439(2) | 37(1) |
| C(17) | 4138(3) | 359(7) | 4264(2) | 43(1) |
| C(4) | 1383(4) | 3570(6) | 1385(2) | 45(1) |
| C(1) | 4380(3) | 1108(6) | 1870(2) | 39(1) |
| C(3) | 745(3) | 1014(7) | 1327(2) | 43(1) |
| C(9) | 1206(3) | 2978(7) | 79(2) | 51(2) |
| C(8) | 3527(3) | -1567(6) | 2751(2) | 39(1) |
| C(5) | 3024(4) | 4133(6) | 2733(2) | 44(1) |
| C(14) | 4454(4) | 894(8) | 587(2) | 59(2) |
| C(12) | 1357(4) | -1017(7) | 16(2) | 55(2) |
| C(16) | 998(4) | -212(8) | 3715(2) | 53(2) |
| C(6) | 4257(3) | 2448(6) | 3134(2) | 37(1) |
| C(19) | 2870(4) | 4052(6) | 4051(2) | 48(2) |
| C(10) | 2699(4) | 3734(6) | 137(2) | 48(2) |
| C(20) | 1320(4) | 3977(7) | 3574(2) | 56(2) |
| C(18) | 3111(4) | -1685(6) | 3969(2) | 54(2) |
| C(15) | 264(3) | 156(7) | 2792(2) | 47(2) |
| C(11) | 1480(5) | -2393(7) | 814(2) | 70(2) |
| C(13) | 3761(4) | -1550(8) | 458(3) | 75(2) |

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

| | | | |
|---|---|---|---|
| Zr(2)-N(2) | 2.122(4) | Zr(2)-N(4) | 2.129(4) |
| Zr(2)-N(3) | 2.215(4) | Zr(2)-N(1) | 2.231(4) |
| Zr(2)-Zr(1) | 3.2296(8) | Zr(2)-Zr(3) | 3.2348(7) |
| Zr(2)-H(2) | 1.93(4) | Zr(2)-H(1) | 1.88(4) |
| Zr(3)-N(8) | 2.049(4) | Zr(3)-N(10) | 2.066(4) |
| Zr(3)-N(9) | 2.075(4) | Zr(3)-N(3) | 2.393(4) |
| Zr(3)-N(4) | 2.560(4) | Zr(3)-H(2) | 2.16(4) |
| Zr(1)-N(6) | 2.041(4) | Zr(1)-N(5) | 2.068(4) |
| Zr(1)-N(7) | 2.073(4) | Zr(1)-N(1) | 2.383(4) |
| Zr(1)-N(2) | 2.556(4) | Zr(1)-H(1) | 2.15(4) |
| N(3)-C(6) | 1.465(6) | N(3)-C(5) | 1.478(6) |
| N(1)-C(1) | 1.470(6) | N(1)-C(2) | 1.479(6) |
| N(4)-C(8) | 1.460(6) | N(4)-C(7) | 1.476(6) |
| N(2)-C(3) | 1.466(6) | N(2)-C(4) | 1.472(6) |
| N(6)-C(11) | 1.457(7) | N(6)-C(12) | 1.459(7) |
| N(10)-C(20) | 1.446(6) | N(10)-C(19) | 1.451(6) |
| N(8)-C(15) | 1.445(6) | N(8)-C(16) | 1.463(6) |
| N(9)-C(17) | 1.450(6) | N(9)-C(18) | 1.463(7) |
| N(5)-C(9) | 1.452(6) | N(5)-C(10) | 1.456(6) |
| N(7)-C(13) | 1.446(7) | N(7)-C(14) | 1.457(7) |
| C(2)-H(2A) | 0.9800 | C(2)-H(2B) | 0.9800 |
| C(2)-H(2C) | 0.9800 | C(7)-H(7A) | 0.9800 |
| C(7)-H(7B) | 0.9800 | C(7)-H(7C) | 0.9800 |
| C(17)-H(17A) | 0.9800 | C(17)-H(17B) | 0.9800 |
| C(17)-H(17C) | 0.9800 | C(4)-H(4A) | 0.9800 |
| C(4)-H(4B) | 0.9800 | C(4)-H(4C) | 0.9800 |
| C(1)-H(1A) | 0.9800 | C(1)-H(1B) | 0.9800 |
| C(1)-H(1C) | 0.9800 | C(3)-H(3A) | 0.9800 |
| C(3)-H(3B) | 0.9800 | C(3)-H(3C) | 0.9800 |
| C(9)-H(9A) | 0.9800 | C(9)-H(9B) | 0.9800 |
| C(9)-H(9C) | 0.9800 | C(8)-H(8A) | 0.9800 |
| C(8)-H(8B) | 0.9800 | C(8)-H(8C) | 0.9800 |
| C(5)-H(5A) | 0.9800 | C(5)-H(5B) | 0.9800 |
| C(5)-H(5C) | 0.9800 | C(14)-H(14A) | 0.9800 |
| C(14)-H(14B) | 0.9800 | C(14)-H(14C) | 0.9800 |
| C(12)-H(12A) | 0.9800 | C(12)-H(12B) | 0.9800 |
| C(12)-H(12C) | 0.9800 | C(16)-H(16A) | 0.9800 |
| C(16)-H(16B) | 0.9800 | C(16)-H(16C) | 0.9800 |
| C(6)-H(6A) | 0.9800 | C(6)-H(6B) | 0.9800 |
| C(6)-H(6C) | 0.9800 | C(19)-H(19A) | 0.9800 |
| C(19)-H(19B) | 0.9800 | C(19)-H(19C) | 0.9800 |
| C(10)-H(10A) | 0.9800 | C(10)-H(10B) | 0.9800 |
| C(10)-H(10C) | 0.9800 | C(20)-H(20A) | 0.9800 |
| C(20)-H(20B) | 0.9800 | C(20)-H(20C) | 0.9800 |
| C(18)-H(18A) | 0.9800 | C(18)-H(18B) | 0.9800 |
| C(18)-H(18C) | 0.9800 | C(15)-H(15A) | 0.9800 |
| C(15)-H(15B) | 0.9800 | C(15)-H(15C) | 0.9800 |
| C(11)-H(11A) | 0.9800 | C(11)-H(11B) | 0.9800 |
| C(11)-H(11C) | 0.9800 | C(13)-H(13A) | 0.9800 |
| C(13)-H(13B) | 0.9800 | C(13)-H(13C) | 0.9800 |

| | | | |
|---|---|---|---|
| N(2)-Zr(2)-N(4) | 129.29(14) | N(2)-Zr(2)-N(3) | 131.07(15) |
| N(4)-Zr(2)-N(3) | 85.87(14) | N(2)-Zr(2)-N(1) | 84.91(13) |
| N(4)-Zr(2)-N(1) | 131.42(14) | N(3)-Zr(2)-N(1) | 94.93(13) |
| N(2)-Zr(2)-Zr(1) | 52.21(10) | N(4)-Zr(2)-Zr(1) | 122.29(10) |
| N(3)-Zr(2)-Zr(1) | 141.80(9) | N(1)-Zr(2)-Zr(1) | 47.52(9) |
| N(2)-Zr(2)-Zr(3) | 123.36(10) | N(4)-Zr(2)-Zr(3) | 52.18(10) |
| N(3)-Zr(2)-Zr(3) | 47.71(9) | N(1)-Zr(2)-Zr(3) | 141.85(10) |
| Zr(1)-Zr(2)-Zr(3) | 170.480(18) | N(2)-Zr(2)-H(2) | 83.0(11) |
| N(4)-Zr(2)-H(2) | 76.7(12) | N(3)-Zr(2)-H(2) | 72.7(11) |
| N(1)-Zr(2)-H(2) | 149.4(12) | Zr(1)-Zr(2)-H(2) | 134.3(11) |
| Zr(3)-Zr(2)-H(2) | 40.4(11) | N(2)-Zr(2)-H(1) | 78.2(13) |
| N(4)-Zr(2)-H(1) | 82.7(13) | N(3)-Zr(2)-H(1) | 147.4(12) |
| N(1)-Zr(2)-H(1) | 70.9(13) | Zr(1)-Zr(2)-H(1) | 39.7(13) |
| Zr(3)-Zr(2)-H(1) | 134.5(13) | H(2)-Zr(2)-H(1) | 132.9(17) |
| N(8)-Zr(3)-N(10) | 96.20(16) | N(8)-Zr(3)-N(9) | 109.24(16) |
| N(10)-Zr(3)-N(9) | 103.84(15) | N(8)-Zr(3)-N(3) | 144.04(14) |
| N(10)-Zr(3)-N(3) | 91.42(14) | N(9)-Zr(3)-N(3) | 102.85(14) |
| N(8)-Zr(3)-N(4) | 91.74(14) | N(10)-Zr(3)-N(4) | 162.59(14) |
| N(9)-Zr(3)-N(4) | 87.99(14) | N(3)-Zr(3)-N(4) | 73.30(12) |
| N(8)-Zr(3)-Zr(2) | 105.13(10) | N(10)-Zr(3)-Zr(2) | 121.59(11) |
| N(9)-Zr(3)-Zr(2) | 118.25(11) | N(3)-Zr(3)-Zr(2) | 43.20(9) |
| N(4)-Zr(3)-Zr(2) | 41.07(8) | N(8)-Zr(3)-H(2) | 78.6(10) |
| N(10)-Zr(3)-H(2) | 102.4(10) | N(9)-Zr(3)-H(2) | 151.5(10) |
| N(3)-Zr(3)-H(2) | 65.4(10) | N(4)-Zr(3)-H(2) | 64.0(10) |
| Zr(2)-Zr(3)-H(2) | 35.4(10) | N(6)-Zr(1)-N(5) | 107.48(16) |
| N(6)-Zr(1)-N(7) | 97.10(17) | N(5)-Zr(1)-N(7) | 102.94(16) |
| N(6)-Zr(1)-N(1) | 144.17(15) | N(5)-Zr(1)-N(1) | 104.39(15) |
| N(7)-Zr(1)-N(1) | 91.28(14) | N(6)-Zr(1)-N(2) | 92.37(15) |
| N(5)-Zr(1)-N(2) | 87.52(13) | N(7)-Zr(1)-N(2) | 162.99(14) |
| N(1)-Zr(1)-N(2) | 72.96(12) | N(6)-Zr(1)-Zr(2) | 104.73(11) |
| N(5)-Zr(1)-Zr(2) | 119.26(11) | N(7)-Zr(1)-Zr(2) | 122.38(11) |
| N(1)-Zr(1)-Zr(2) | 43.68(9) | N(2)-Zr(1)-Zr(2) | 41.00(8) |
| N(6)-Zr(1)-H(1) | 80.3(11) | N(5)-Zr(1)-H(1) | 151.5(12) |
| N(7)-Zr(1)-H(1) | 103.2(11) | N(1)-Zr(1)-H(1) | 63.8(11) |
| N(2)-Zr(1)-H(1) | 64.5(11) | Zr(2)-Zr(1)-H(1) | 34.0(12) |
| C(6)-N(3)-C(5) | 108.8(4) | C(6)-N(3)-Zr(2) | 127.7(3) |
| C(5)-N(3)-Zr(2) | 105.8(3) | C(6)-N(3)-Zr(3) | 112.5(3) |
| C(5)-N(3)-Zr(3) | 111.3(3) | Zr(2)-N(3)-Zr(3) | 89.09(13) |
| C(1)-N(1)-C(2) | 108.5(4) | C(1)-N(1)-Zr(2) | 104.2(3) |
| C(2)-N(1)-Zr(2) | 126.5(3) | C(1)-N(1)-Zr(1) | 112.7(3) |
| C(2)-N(1)-Zr(1) | 114.7(3) | Zr(2)-N(1)-Zr(1) | 88.80(12) |
| C(8)-N(4)-C(7) | 108.4(4) | C(8)-N(4)-Zr(2) | 114.5(3) |
| C(7)-N(4)-Zr(2) | 116.9(3) | C(8)-N(4)-Zr(3) | 117.6(3) |
| C(7)-N(4)-Zr(3) | 111.7(3) | Zr(2)-N(4)-Zr(3) | 86.75(13) |
| C(3)-N(2)-C(4) | 109.6(4) | C(3)-N(2)-Zr(2) | 114.5(3) |
| C(4)-N(2)-Zr(2) | 114.7(3) | C(3)-N(2)-Zr(1) | 112.1(3) |
| C(4)-N(2)-Zr(1) | 117.8(3) | Zr(2)-N(2)-Zr(1) | 86.79(12) |
| C(11)-N(6)-C(12) | 108.2(4) | C(11)-N(6)-Zr(1) | 136.7(4) |
| C(12)-N(6)-Zr(1) | 114.7(3) | C(20)-N(10)-C(19) | 110.0(4) |
| C(20)-N(10)-Zr(3) | 124.3(3) | C(19)-N(10)-Zr(3) | 125.6(3) |

| | |
|---|---|
| C(15)-N(8)-C(16) | 109.9(4) |
| C(16)-N(8)-Zr(3) | 111.1(3) |
| C(17)-N(9)-Zr(3) | 133.4(3) |
| C(9)-N(5)-C(10) | 108.7(4) |
| C(10)-N(5)-Zr(1) | 127.1(3) |
| C(13)-N(7)-Zr(1) | 124.8(4) |
| N(1)-C(2)-H(2A) | 109.5 |
| H(2A)-C(2)-H(2B) | 109.5 |
| H(2A)-C(2)-H(2C) | 109.5 |
| N(4)-C(7)-H(7A) | 109.5 |
| H(7A)-C(7)-H(7B) | 109.5 |
| H(7A)-C(7)-H(7C) | 109.5 |
| N(9)-C(17)-H(17A) | 109.5 |
| H(17A)-C(17)-H(17B) | 109.5 |
| H(17A)-C(17)-H(17C) | 109.5 |
| N(2)-C(4)-H(4A) | 109.5 |
| H(4A)-C(4)-H(4B) | 109.5 |
| H(4A)-C(4)-H(4C) | 109.5 |
| N(1)-C(1)-H(1A) | 109.5 |
| H(1A)-C(1)-H(1B) | 109.5 |
| H(1A)-C(1)-H(1C) | 109.5 |
| N(2)-C(3)-H(3A) | 109.5 |
| H(3A)-C(3)-H(3B) | 109.5 |
| H(3A)-C(3)-H(3C) | 109.5 |
| N(5)-C(9)-H(9A) | 109.5 |
| H(9A)-C(9)-H(9B) | 109.5 |
| H(9A)-C(9)-H(9C) | 109.5 |
| N(4)-C(8)-H(8A) | 109.5 |
| H(8A)-C(8)-H(8B) | 109.5 |
| H(8A)-C(8)-H(8C) | 109.5 |
| N(3)-C(5)-H(5A) | 109.5 |
| H(5A)-C(5)-H(5B) | 109.5 |
| H(5A)-C(5)-H(5C) | 109.5 |
| N(7)-C(14)-H(14A) | 109.5 |
| H(14A)-C(14)-H(14B) | 109.5 |
| H(14A)-C(14)-H(14C) | 109.5 |
| N(6)-C(12)-H(12A) | 109.5 |
| H(12A)-C(12)-H(12B) | 109.5 |
| H(12A)-C(12)-H(12C) | 109.5 |
| N(8)-C(16)-H(16A) | 109.5 |
| H(16A)-C(16)-H(16B) | 109.5 |
| H(16A)-C(16)-H(16C) | 109.5 |
| N(3)-C(6)-H(6A) | 109.5 |
| H(6A)-C(6)-H(6B) | 109.5 |
| H(6A)-C(6)-H(6C) | 109.5 |
| N(10)-C(19)-H(19A) | 109.5 |
| H(19A)-C(19)-H(19B) | 109.5 |
| H(19A)-C(19)-H(19C) | 109.5 |
| N(5)-C(10)-H(10A) | 109.5 |
| H(10A)-C(10)-H(10B) | 109.5 |
| H(10A)-C(10)-H(10C) | 109.5 |
| N(10)-C(20)-H(20A) | 109.5 |
| C(15)-N(8)-Zr(3) | 138.3(3) |
| C(17)-N(9)-C(18) | 107.7(4) |
| C(18)-N(9)-Zr(3) | 118.8(3) |
| C(9)-N(5)-Zr(1) | 123.5(3) |
| C(13)-N(7)-C(14) | 107.7(5) |
| C(14)-N(7)-Zr(1) | 127.3(4) |
| N(1)-C(2)-H(2B) | 109.5 |
| N(1)-C(2)-H(2C) | 109.5 |
| H(2B)-C(2)-H(2C) | 109.5 |
| N(4)-C(7)-H(7B) | 109.5 |
| N(4)-C(7)-H(7C) | 109.5 |
| H(7B)-C(7)-H(7C) | 109.5 |
| N(9)-C(17)-H(17B) | 109.5 |
| N(9)-C(17)-H(17C) | 109.5 |
| H(17B)-C(17)-H(17C) | 109.5 |
| N(2)-C(4)-H(4B) | 109.5 |
| N(2)-C(4)-H(4C) | 109.5 |
| H(4B)-C(4)-H(4C) | 109.5 |
| N(1)-C(1)-H(1B) | 109.5 |
| N(1)-C(1)-H(1C) | 109.5 |
| H(1B)-C(1)-H(1C) | 109.5 |
| N(2)-C(3)-H(3B) | 109.5 |
| N(2)-C(3)-H(3C) | 109.5 |
| H(3B)-C(3)-H(3C) | 109.5 |
| N(5)-C(9)-H(9B) | 109.5 |
| N(5)-C(9)-H(9C) | 109.5 |
| H(9B)-C(9)-H(9C) | 109.5 |
| N(4)-C(8)-H(8B) | 109.5 |
| N(4)-C(8)-H(8C) | 109.5 |
| H(8B)-C(8)-H(8C) | 109.5 |
| N(3)-C(5)-H(5B) | 109.5 |
| N(3)-C(5)-H(5C) | 109.5 |
| H(5B)-C(5)-H(5C) | 109.5 |
| N(7)-C(14)-H(14B) | 109.5 |
| N(7)-C(14)-H(14C) | 109.5 |
| H(14B)-C(14)-H(14C) | 109.5 |
| N(6)-C(12)-H(12B) | 109.5 |
| N(6)-C(12)-H(12C) | 109.5 |
| H(12B)-C(12)-H(12C) | 109.5 |
| N(8)-C(16)-H(16B) | 109.5 |
| N(8)-C(16)-H(16C) | 109.5 |
| H(16B)-C(16)-H(16C) | 109.5 |
| N(3)-C(6)-H(6B) | 109.5 |
| N(3)-C(6)-H(6C) | 109.5 |
| H(6B)-C(6)-H(6C) | 109.5 |
| N(10)-C(19)-H(19B) | 109.5 |
| N(10)-C(19)-H(19C) | 109.5 |
| H(19B)-C(19)-H(19C) | 109.5 |
| N(5)-C(10)-H(10B) | 109.5 |
| N(5)-C(10)-H(10C) | 109.5 |
| H(10B)-C(10)-H(10C) | 109.5 |
| N(10)-C(20)-H(20B) | 109.5 |

| | | | |
|---|---|---|---|
| H(20A)-C(20)-H(20B) | 109.5 | N(10)-C(20)-H(20C) | 109.5 |
| H(20A)-C(20)-H(20C) | 109.5 | H(20B)-C(20)-H(20C) | 109.5 |
| N(9)-C(18)-H(18A) | 109.5 | N(9)-C(18)-H(18B) | 109.5 |
| H(18A)-C(18)-H(18B) | 109.5 | N(9)-C(18)-H(18C) | 109.5 |
| H(18A)-C(18)-H(18C) | 109.5 | H(18B)-C(18)-H(18C) | 109.5 |
| N(8)-C(15)-H(15A) | 109.5 | N(8)-C(15)-H(15B) | 109.5 |
| H(15A)-C(15)-H(15B) | 109.5 | N(8)-C(15)-H(15C) | 109.5 |
| H(15A)-C(15)-H(15C) | 109.5 | H(15B)-C(15)-H(15C) | 109.5 |
| N(6)-C(11)-H(11A) | 109.5 | N(6)-C(11)-H(11B) | 109.5 |
| H(11A)-C(11)-H(11B) | 109.5 | N(6)-C(11)-H(11C) | 109.5 |
| H(11A)-C(11)-H(11C) | 109.5 | H(11B)-C(11)-H(11C) | 109.5 |
| N(7)-C(13)-H(13A) | 109.5 | N(7)-C(13)-H(13B) | 109.5 |
| H(13A)-C(13)-H(13B) | 109.5 | N(7)-C(13)-H(13C) | 109.5 |
| H(13A)-C(13)-H(13C) | 109.5 | H(13B)-C(13)-H(13C) | 109.5 |

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for **1**.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [ (ha^*)^2 U_{11} + \ldots + 2hka^*b^*U_{12} ]$

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Zr(2) | 19(1) | 20(1) | 20(1) | 0(1) | 7(1) | 0(1) |
| Zr(3) | 24(1) | 23(1) | 19(1) | 0(1) | 7(1) | -3(1) |
| Zr(1) | 25(1) | 31(1) | 21(1) | 0(1) | 9(1) | 0(1) |
| N(3) | 31(2) | 25(2) | 28(2) | -1(2) | 11(2) | -10(2) |
| N(1) | 21(2) | 30(2) | 28(2) | 1(2) | 8(2) | -2(2) |
| N(4) | 26(2) | 23(2) | 28(2) | 4(2) | 8(2) | -2(2) |
| N(2) | 23(2) | 32(2) | 28(2) | 7(2) | 11(2) | 6(2) |
| N(6) | 46(3) | 36(3) | 27(2) | -3(2) | 10(2) | -10(2) |
| N(10) | 42(2) | 31(2) | 25(2) | -2(2) | 15(2) | 2(2) |
| N(8) | 30(2) | 44(3) | 22(2) | -1(2) | 10(2) | -10(2) |
| N(9) | 39(2) | 31(2) | 25(2) | 4(2) | 8(2) | 0(2) |
| N(5) | 37(2) | 43(3) | 27(2) | 4(2) | 15(2) | 0(2) |
| N(7) | 34(2) | 53(3) | 31(2) | -7(2) | 12(2) | 7(2) |
| C(2) | 38(3) | 38(3) | 38(3) | -4(2) | 17(2) | -11(2) |
| C(7) | 41(3) | 33(3) | 37(3) | -6(2) | 10(2) | -4(2) |
| C(17) | 36(3) | 49(3) | 39(3) | 1(3) | 5(2) | 10(3) |
| C(4) | 42(3) | 44(3) | 55(4) | 1(3) | 24(3) | 13(3) |
| C(1) | 27(3) | 49(3) | 39(3) | 3(3) | 6(2) | 0(2) |
| C(3) | 29(3) | 62(4) | 40(3) | 3(3) | 14(2) | -6(3) |
| C(9) | 43(3) | 64(4) | 41(3) | 16(3) | 7(3) | 2(3) |
| C(8) | 39(3) | 32(3) | 49(3) | -1(3) | 14(3) | 5(2) |
| C(5) | 63(4) | 27(3) | 43(3) | 5(2) | 17(3) | -11(3) |
| C(14) | 41(3) | 90(5) | 57(4) | 7(4) | 29(3) | 11(3) |
| C(12) | 69(4) | 62(4) | 30(3) | -6(3) | 5(3) | -22(3) |
| C(16) | 41(3) | 89(5) | 29(3) | 3(3) | 12(3) | -27(3) |
| C(6) | 36(3) | 42(3) | 33(3) | -6(2) | 13(2) | -17(2) |
| C(19) | 55(4) | 29(3) | 58(4) | -13(3) | 16(3) | -3(3) |
| C(10) | 58(4) | 48(4) | 43(3) | 14(3) | 23(3) | 4(3) |
| C(20) | 59(4) | 58(4) | 47(4) | -4(3) | 11(3) | 25(3) |
| C(18) | 74(4) | 38(3) | 42(3) | 12(3) | 6(3) | 1(3) |
| C(15) | 33(3) | 70(4) | 37(3) | 3(3) | 11(2) | -12(3) |
| C(11) | 116(6) | 51(4) | 40(4) | -8(3) | 20(4) | -35(4) |
| C(13) | 51(4) | 86(5) | 78(5) | -38(4) | 2(3) | 23(4) |

Table S5. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$ x $10^3$) for **1**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(2A) | 4150 | 4062 | 1922 | 55 |
| H(2B) | 3266 | 4257 | 1431 | 55 |
| H(2C) | 4185 | 3666 | 1330 | 55 |
| H(7A) | 2060 | -2578 | 2168 | 56 |
| H(7B) | 1364 | -1355 | 2289 | 56 |
| H(7C) | 1902 | -2512 | 2747 | 56 |
| H(17A) | 4095 | 136 | 4624 | 64 |
| H(17B) | 4253 | 1469 | 4233 | 64 |
| H(17C) | 4632 | -244 | 4197 | 64 |
| H(4A) | 961 | 3810 | 1038 | 67 |
| H(4B) | 1941 | 4158 | 1428 | 67 |
| H(4C) | 1113 | 3858 | 1669 | 67 |
| H(1A) | 4747 | 1111 | 1620 | 58 |
| H(1B) | 4220 | 37 | 1932 | 58 |
| H(1C) | 4722 | 1573 | 2208 | 58 |
| H(3A) | 411 | 1382 | 1571 | 64 |
| H(3B) | 885 | -91 | 1391 | 64 |
| H(3C) | 378 | 1161 | 958 | 64 |
| H(9A) | 1067 | 4074 | 118 | 76 |
| H(9B) | 826 | 2327 | 235 | 76 |
| H(9C) | 1089 | 2727 | -300 | 76 |
| H(8A) | 3547 | -2284 | 3045 | 59 |
| H(8B) | 4021 | -818 | 2861 | 59 |
| H(8C) | 3589 | -2154 | 2442 | 59 |
| H(5A) | 3067 | 4661 | 3071 | 66 |
| H(5B) | 2400 | 4176 | 2507 | 66 |
| H(5C) | 3419 | 4648 | 2551 | 66 |
| H(14A) | 5009 | 381 | 791 | 89 |
| H(14B) | 4432 | 1947 | 725 | 89 |
| H(14C) | 4441 | 945 | 211 | 89 |
| H(12A) | 1534 | -1982 | -126 | 83 |
| H(12B) | 1578 | -128 | -145 | 83 |
| H(12C) | 699 | -968 | -70 | 83 |
| H(16A) | 543 | 442 | 3804 | 79 |
| H(16B) | 1572 | -105 | 3992 | 79 |
| H(16C) | 803 | -1299 | 3693 | 79 |
| H(6A) | 4612 | 2971 | 2928 | 55 |
| H(6B) | 4453 | 1365 | 3196 | 55 |
| H(6C) | 4346 | 2976 | 3477 | 55 |

| | | | | |
|---|---|---|---|---|
| H(19A) | 2852 | 5142 | 3941 | 71 |
| H(19B) | 3461 | 3611 | 4068 | 71 |
| H(19C) | 2766 | 3986 | 4403 | 71 |
| H(10A) | 2586 | 3543 | -246 | 72 |
| H(10B) | 3336 | 3551 | 318 | 72 |
| H(10C) | 2545 | 4812 | 194 | 72 |
| H(20A) | 1161 | 4070 | 3910 | 83 |
| H(20B) | 854 | 3381 | 3318 | 83 |
| H(20C) | 1365 | 5015 | 3430 | 83 |
| H(18A) | 3623 | -2331 | 3950 | 80 |
| H(18B) | 2569 | -2023 | 3696 | 80 |
| H(18C) | 3015 | -1790 | 4322 | 80 |
| H(15A) | 60 | -926 | 2760 | 70 |
| H(15B) | 342 | 506 | 2452 | 70 |
| H(15C) | -186 | 808 | 2888 | 70 |
| H(11A) | 822 | -2441 | 728 | 105 |
| H(11B) | 1738 | -2394 | 1202 | 105 |
| H(11C) | 1702 | -3297 | 662 | 105 |
| H(13A) | 3733 | -1530 | 79 | 112 |
| H(13B) | 3266 | -2187 | 509 | 112 |
| H(13C) | 4337 | -1994 | 663 | 112 |
| H(2) | 1720(30) | 1690(50) | 2462(15) | 19(11) |
| H(1) | 2700(30) | -330(50) | 1606(17) | 30(12) |

Table S6. Crystal data and structure refinement for **2**.

| | |
|---|---|
| Identification code | 2 |
| Empirical formula | $C_{20}H_{62}Hf_3N_{10}$ |
| Formula weight | 978.27 |
| Temperature | 173(2) K |
| Wavelength | 0.71073 Å |
| Crystal system | Monoclinic |
| Space group | $P2_1/c$ |
| Unit cell dimensions | $a$ = 14.5901(4) Å alpha = 90° |
| | $b$ = 14.8647(5) Å beta = 113.5665(13)° |
| | $c$ = 17.0738(3) Å gamma = 90° |
| Volume, Z | 3394.05(19) $Å^3$, 4 |
| Density (calculated) | 1.914 $g/cm^3$ |
| Absorption coefficient | 9.176 $mm^{-1}$ |
| F(000) | 1872 |
| Crystal size | 0.35 x 0.20 x 0.08 mm |
| $\theta$ range for data collection | 1.52 to 28.21° |
| Limiting indices | $-19 \le h \le 17$, $0 \le k \le 19$, $0 \le l \le 22$ |
| Reflections collected | 19538 |
| Independent reflections | 7792 ($R_{int}$ = 0.0637) |
| Completeness to $\theta$ = 28.21° | 93.1 % |
| Absorption correction | Empirical from DIFABS |
| Max. and min. transmission | 1.000 and 0.275 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 7792 / 0 / 318 |
| Goodness-of-fit on $F^2$ | 1.281 |
| Final R indices [$I>2\sigma(I)$] | R1 = 0.0639, wR2 = 0.1524 |
| R indices (all data) | R1 = 0.0763, wR2 = 0.1556 |
| Largest diff. peak and hole | 2.848 and -2.946 $eÅ^{-3}$ |

Table S7. Atomic coordinates [ x $10^4$] and equivalent isotropic displacement parameters [$Å^2$ x $10^3$] for 2. U(eq) is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Hf(1) | 4123.1(3) | 7642.9(3) | 3398.6(3) | 19(1) |
| Hf(2) | 6528.6(3) | 7673.2(3) | 4210.8(3) | 17(1) |
| Hf(3) | 8894.4(3) | 7460.0(3) | 5270.0(3) | 19(1) |
| N(1) | 5398(7) | 8521(7) | 3230(6) | 23(2) |
| N(2) | 5523(7) | 7753(7) | 4855(6) | 23(2) |
| N(3) | 7798(7) | 8554(6) | 4319(5) | 18(2) |
| N(4) | 7459(7) | 6586(7) | 4128(6) | 22(2) |
| N(5) | 3335(7) | 8621(7) | 3736(7) | 26(2) |
| N(6) | 3635(8) | 6424(8) | 3694(7) | 27(2) |
| N(7) | 3307(7) | 7584(8) | 2074(6) | 27(2) |
| N(8) | 9129(8) | 6447(7) | 6154(7) | 27(2) |
| N(9) | 9836(8) | 7146(9) | 4670(6) | 29(2) |
| N(10) | 9614(7) | 8455(8) | 6151(7) | 28(2) |
| C(1) | 5616(9) | 8232(11) | 2477(8) | 32(3) |
| C(2) | 5235(9) | 9493(9) | 3217(9) | 30(3) |
| C(3) | 5558(9) | 6960(10) | 5382(7) | 30(3) |
| C(4) | 5656(12) | 8582(11) | 5384(9) | 44(4) |
| C(5) | 7671(11) | 9366(9) | 4757(9) | 32(3) |
| C(6) | 8097(9) | 8830(10) | 3630(8) | 30(3) |
| C(7) | 7246(10) | 5727(10) | 4471(10) | 37(3) |
| C(8) | 7538(12) | 6391(12) | 3307(9) | 43(4) |
| C(9) | 3222(10) | 8595(12) | 4556(9) | 40(3) |
| C(10) | 2732(11) | 9358(11) | 3198(10) | 42(3) |
| C(11) | 3992(11) | 5513(10) | 3767(12) | 44(4) |
| C(12) | 2656(13) | 6426(13) | 3754(15) | 60(5) |
| C(13) | 2736(14) | 6786(12) | 1647(10) | 52(4) |
| C(14) | 3121(10) | 8286(11) | 1450(8) | 37(3) |
| C(15) | 8608(10) | 6041(14) | 6633(10) | 48(4) |
| C(16) | 10212(10) | 6205(12) | 6616(10) | 42(4) |
| C(17) | 10440(10) | 7741(13) | 4376(10) | 43(4) |
| C(18) | 10039(11) | 6233(12) | 4509(11) | 44(4) |
| C(19) | 10126(11) | 9268(11) | 6041(11) | 40(3) |
| C(20) | 9597(14) | 8482(12) | 7009(10) | 48(4) |

Table S8. Bond lengths [Å] and angles [°] for 2.

| | | | |
|---|---|---|---|
| Hf(1)-N(5) | 2.073(10) | Hf(1)-N(6) | 2.081(10) |
| Hf(1)-N(7) | 2.094(9) | Hf(1)-N(1) | 2.383(10) |
| Hf(1)-N(2) | 2.514(9) | Hf(1)-Hf(2) | 3.2173(6) |
| Hf(2)-N(4) | 2.151(9) | Hf(2)-N(2) | 2.160(9) |
| Hf(2)-N(3) | 2.215(9) | Hf(2)-N(1) | 2.215(10) |
| Hf(2)-Hf(3) | 3.2085(6) | Hf(3)-N(8) | 2.062(11) |
| Hf(3)-N(9) | 2.069(10) | Hf(3)-N(10) | 2.071(11) |
| Hf(3)-N(3) | 2.400(9) | Hf(3)-N(4) | 2.571(10) |
| N(1)-C(2) | 1.463(17) | N(1)-C(1) | 1.504(15) |
| N(2)-C(3) | 1.471(16) | N(2)-C(4) | 1.493(18) |
| N(3)-C(6) | 1.467(14) | N(3)-C(5) | 1.470(15) |
| N(4)-C(8) | 1.481(16) | N(4)-C(7) | 1.489(18) |
| N(5)-C(10) | 1.474(18) | N(5)-C(9) | 1.473(17) |
| N(6)-C(11) | 1.439(19) | N(6)-C(12) | 1.472(17) |
| N(7)-C(14) | 1.438(18) | N(7)-C(13) | 1.465(19) |
| N(8)-C(15) | 1.452(17) | N(8)-C(16) | 1.499(17) |
| N(9)-C(18) | 1.44(2) | N(9)-C(17) | 1.472(18) |
| N(10)-C(19) | 1.472(17) | N(10)-C(20) | 1.475(17) |
| | | | |
| N(5)-Hf(1)-N(6) | 105.1(4) | N(5)-Hf(1)-N(7) | 101.0(4) |
| N(6)-Hf(1)-N(7) | 97.1(4) | N(5)-Hf(1)-N(1) | 101.3(4) |
| N(6)-Hf(1)-N(1) | 149.9(4) | N(7)-Hf(1)-N(1) | 91.5(4) |
| N(5)-Hf(1)-N(2) | 90.1(4) | N(6)-Hf(1)-N(2) | 92.2(4) |
| N(7)-Hf(1)-N(2) | 163.1(4) | N(1)-Hf(1)-N(2) | 73.7(3) |
| N(5)-Hf(1)-Hf(2) | 120.1(3) | N(6)-Hf(1)-Hf(2) | 109.1(3) |
| N(7)-Hf(1)-Hf(2) | 121.1(3) | N(1)-Hf(1)-Hf(2) | 43.5(2) |
| N(2)-Hf(1)-Hf(2) | 42.1(2) | N(4)-Hf(2)-N(2) | 130.5(4) |
| N(4)-Hf(2)-N(3) | 85.5(4) | N(2)-Hf(2)-N(3) | 129.9(4) |
| N(4)-Hf(2)-N(1) | 132.6(4) | N(2)-Hf(2)-N(1) | 84.4(4) |
| N(3)-Hf(2)-N(1) | 94.1(3) | N(4)-Hf(2)-Hf(3) | 53.0(3) |
| N(2)-Hf(2)-Hf(3) | 121.0(2) | N(3)-Hf(2)-Hf(3) | 48.4(2) |
| N(1)-Hf(2)-Hf(3) | 142.2(3) | N(4)-Hf(2)-Hf(1) | 124.7(3) |
| N(2)-Hf(2)-Hf(1) | 51.3(2) | N(3)-Hf(2)-Hf(1) | 140.9(2) |
| N(1)-Hf(2)-Hf(1) | 47.8(3) | Hf(3)-Hf(2)-Hf(1) | 169.717(19) |
| N(8)-Hf(3)-N(9) | 104.4(4) | N(8)-Hf(3)-N(10) | 95.9(4) |
| N(9)-Hf(3)-N(10) | 106.1(4) | N(8)-Hf(3)-N(3) | 149.4(4) |
| N(9)-Hf(3)-N(3) | 102.3(4) | N(10)-Hf(3)-N(3) | 90.9(4) |
| N(8)-Hf(3)-N(4) | 91.9(4) | N(9)-Hf(3)-N(4) | 90.6(4) |
| N(10)-Hf(3)-N(4) | 159.1(4) | N(3)-Hf(3)-N(4) | 73.1(3) |
| N(8)-Hf(3)-Hf(2) | 108.1(3) | N(9)-Hf(3)-Hf(2) | 121.4(3) |
| N(10)-Hf(3)-Hf(2) | 117.3(3) | N(3)-Hf(3)-Hf(2) | 43.6(2) |
| N(4)-Hf(3)-Hf(2) | 41.9(2) | C(2)-N(1)-C(1) | 111.0(10) |
| C(2)-N(1)-Hf(2) | 129.9(8) | C(1)-N(1)-Hf(2) | 97.8(8) |
| C(2)-N(1)-Hf(1) | 114.3(8) | C(1)-N(1)-Hf(1) | 112.8(7) |
| Hf(2)-N(1)-Hf(1) | 88.7(3) | C(3)-N(2)-C(4) | 109.1(10) |
| C(3)-N(2)-Hf(2) | 113.7(8) | C(4)-N(2)-Hf(2) | 113.7(9) |
| C(3)-N(2)-Hf(1) | 111.6(7) | C(4)-N(2)-Hf(1) | 120.6(8) |
| Hf(2)-N(2)-Hf(1) | 86.6(3) | C(6)-N(3)-C(5) | 108.4(10) |
| C(6)-N(3)-Hf(2) | 127.3(8) | C(5)-N(3)-Hf(2) | 104.8(7) |
| C(6)-N(3)-Hf(3) | 113.7(7) | C(5)-N(3)-Hf(3) | 113.4(7) |
| Hf(2)-N(3)-Hf(3) | 88.0(3) | C(8)-N(4)-C(7) | 108.2(11) |

| | | | | |
|---|---|---|---|---|
| H(16A) | 10605 | 6512 | 6347 | 63 |
| H(16B) | 10292 | 5553 | 6589 | 63 |
| H(16C) | 10444 | 6394 | 7215 | 63 |
| H(17A) | 11142 | 7554 | 4638 | 64 |
| H(17B) | 10379 | 8362 | 4541 | 64 |
| H(17C) | 10201 | 7702 | 3753 | 64 |
| H(18A) | 9818 | 6140 | 3893 | 66 |
| H(18B) | 9679 | 5820 | 4733 | 66 |
| H(18C) | 10759 | 6117 | 4793 | 66 |
| H(19A) | 9839 | 9799 | 6196 | 61 |
| H(19B) | 10040 | 9316 | 5443 | 61 |
| H(19C) | 10840 | 9229 | 6409 | 61 |
| H(20A) | 10271 | 8364 | 7441 | 72 |
| H(20B) | 9135 | 8023 | 7048 | 72 |
| H(20C) | 9375 | 9077 | 7107 | 72 |

Table S9. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 2. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [ $(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$ ]

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Hf(1) | 15(1) | 24(1) | 18(1) | -1(1) | 6(1) | -2(1) |
| Hf(2) | 14(1) | 22(1) | 16(1) | 0(1) | 6(1) | -2(1) |
| Hf(3) | 14(1) | 23(1) | 20(1) | 1(1) | 6(1) | -1(1) |
| N(1) | 22(5) | 31(5) | 8(4) | 4(4) | 0(3) | -5(4) |
| N(2) | 20(5) | 40(6) | 9(4) | -1(4) | 7(3) | -7(4) |
| N(3) | 15(4) | 24(5) | 13(4) | 5(3) | 5(3) | 4(3) |
| N(4) | 12(4) | 28(5) | 25(5) | -7(4) | 8(4) | 2(4) |
| N(5) | 21(5) | 22(5) | 38(6) | -10(4) | 16(4) | -3(4) |
| N(6) | 24(5) | 31(6) | 32(5) | -6(4) | 17(4) | -12(4) |
| N(7) | 13(4) | 41(6) | 14(4) | 3(4) | -7(3) | 3(4) |
| N(8) | 29(5) | 20(5) | 34(6) | 1(4) | 14(5) | 2(4) |
| N(9) | 21(5) | 50(7) | 22(5) | -3(5) | 13(4) | -1(5) |
| N(10) | 19(5) | 35(6) | 27(5) | 2(4) | 7(4) | -6(4) |
| C(1) | 17(5) | 57(9) | 22(5) | -4(6) | 8(5) | -4(6) |
| C(2) | 21(6) | 30(6) | 34(6) | 0(5) | 5(5) | -1(5) |
| C(3) | 19(5) | 48(8) | 18(5) | 13(5) | 4(4) | -2(5) |
| C(4) | 47(9) | 43(9) | 31(7) | -14(6) | 6(6) | -1(7) |
| C(5) | 37(7) | 28(7) | 34(7) | -10(5) | 15(6) | 1(5) |
| C(6) | 22(6) | 38(7) | 32(6) | 11(5) | 14(5) | -3(5) |
| C(7) | 17(6) | 36(7) | 46(8) | 3(6) | 0(6) | -1(5) |
| C(8) | 44(8) | 57(10) | 26(7) | -19(7) | 12(6) | -8(7) |
| C(9) | 26(7) | 63(10) | 36(7) | -4(7) | 17(6) | 8(6) |
| C(10) | 29(7) | 39(8) | 45(8) | 3(7) | 2(6) | 15(6) |
| C(11) | 35(8) | 33(7) | 65(10) | 5(7) | 21(7) | -5(6) |
| C(12) | 38(9) | 52(10) | 104(16) | -15(10) | 43(10) | -19(8) |
| C(13) | 64(11) | 47(9) | 34(7) | -9(7) | 7(7) | -26(8) |
| C(14) | 30(7) | 53(9) | 24(6) | 2(6) | 7(5) | 0(6) |
| C(15) | 21(6) | 76(12) | 40(8) | 22(8) | 6(6) | -8(7) |
| C(16) | 28(7) | 52(9) | 46(8) | 15(7) | 14(6) | 12(6) |
| C(17) | 21(6) | 71(11) | 45(8) | -2(8) | 21(6) | -4(7) |
| C(18) | 33(7) | 52(9) | 51(9) | -10(7) | 21(7) | 2(7) |
| C(19) | 27(7) | 43(8) | 52(9) | 0(7) | 17(7) | -12(6) |
| C(20) | 71(11) | 47(9) | 32(7) | -9(7) | 27(8) | -12(8) |

Table S10. Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$ x $10^3$) for 2.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1A) | 4985 | 8153 | 1977 | 48 |
| H(1B) | 5983 | 7661 | 2609 | 48 |
| H(1C) | 6021 | 8692 | 2355 | 48 |
| H(2A) | 5234 | 9683 | 3766 | 45 |
| H(2B) | 4590 | 9642 | 2757 | 45 |
| H(2C) | 5772 | 9805 | 3119 | 45 |
| H(3A) | 6171 | 6976 | 5905 | 45 |
| H(3B) | 5550 | 6412 | 5060 | 45 |
| H(3C) | 4975 | 6963 | 5531 | 45 |
| H(4A) | 5107 | 8628 | 5574 | 65 |
| H(4B) | 5654 | 9111 | 5041 | 65 |
| H(4C) | 6294 | 8549 | 5883 | 65 |
| H(5A) | 8319 | 9664 | 5044 | 49 |
| H(5B) | 7405 | 9197 | 5180 | 49 |
| H(5C) | 7203 | 9777 | 4337 | 49 |
| H(6A) | 7627 | 9283 | 3273 | 44 |
| H(6B) | 8091 | 8306 | 3280 | 44 |
| H(6C) | 8772 | 9086 | 3877 | 44 |
| H(7A) | 6654 | 5442 | 4039 | 56 |
| H(7B) | 7123 | 5850 | 4985 | 56 |
| H(7C) | 7821 | 5322 | 4617 | 56 |
| H(8A) | 8055 | 5935 | 3397 | 65 |
| H(8B) | 7716 | 6943 | 3086 | 65 |
| H(8C) | 6894 | 6167 | 2894 | 65 |
| H(9A) | 3470 | 9160 | 4865 | 60 |
| H(9B) | 3607 | 8090 | 4899 | 60 |
| H(9C) | 2515 | 8520 | 4448 | 60 |
| H(10A) | 2046 | 9319 | 3163 | 63 |
| H(10B) | 2725 | 9309 | 2623 | 63 |
| H(10C) | 3024 | 9937 | 3449 | 63 |
| H(11A) | 4031 | 5254 | 4307 | 66 |
| H(11B) | 4658 | 5508 | 3754 | 66 |
| H(11C) | 3532 | 5156 | 3288 | 66 |
| H(12A) | 2233 | 5953 | 3385 | 90 |
| H(12B) | 2334 | 7012 | 3569 | 90 |
| H(12C) | 2749 | 6314 | 4347 | 90 |
| H(13A) | 2020 | 6928 | 1406 | 78 |
| H(13B) | 2869 | 6296 | 2062 | 78 |
| H(13C) | 2936 | 6601 | 1187 | 78 |
| H(14A) | 3354 | 8093 | 1011 | 55 |
| H(14B) | 3480 | 8831 | 1729 | 55 |
| H(14C) | 2402 | 8411 | 1182 | 55 |
| H(15A) | 8446 | 5415 | 6453 | 71 |
| H(15B) | 7989 | 6375 | 6524 | 71 |
| H(15C) | 9036 | 6061 | 7244 | 71 |

| | | | |
|---|---|---|---|
| C(8)-N(4)-Hf(2) | 119.9(9) | C(7)-N(4)-Hf(2) | 112.5(8) |
| C(8)-N(4)-Hf(3) | 118.0(8) | C(7)-N(4)-Hf(3) | 111.7(8) |
| Hf(2)-N(4)-Hf(3) | 85.1(3) | C(10)-N(5)-C(9) | 110.2(11) |
| C(10)-N(5)-Hf(1) | 127.4(9) | C(9)-N(5)-Hf(1) | 122.1(9) |
| C(11)-N(6)-C(12) | 108.9(12) | C(11)-N(6)-Hf(1) | 133.9(9) |
| C(12)-N(6)-Hf(1) | 116.8(11) | C(14)-N(7)-C(13) | 108.5(11) |
| C(14)-N(7)-Hf(1) | 128.9(9) | C(13)-N(7)-Hf(1) | 122.4(9) |
| C(15)-N(8)-C(16) | 106.5(11) | C(15)-N(8)-Hf(3) | 138.1(9) |
| C(16)-N(8)-Hf(3) | 113.1(8) | C(18)-N(9)-C(17) | 107.7(11) |
| C(18)-N(9)-Hf(3) | 122.4(9) | C(17)-N(9)-Hf(3) | 129.8(10) |
| C(19)-N(10)-C(20) | 108.4(12) | C(19)-N(10)-Hf(3) | 129.0(9) |
| C(20)-N(10)-Hf(3) | 122.4(9) | | |

Symmetry transformations used to generate equivalent atoms: