**Table 13.** Bond Angles [deg] for **7c**•$SnCl_4$.

| bond angle | [deg] | bond angle | [deg] |
|---|---|---|---|
| C(19)-C(18)-H(18A) | 111.2 | H(14A)-C(14)-H(14B) | 109.5 |
| N(5)-C(18)-H(18A) | 111.2 | N(4)-C(14)-H(14C) | 109.5 |
| C(17)-C(18)-H(18A) | 111.2 | H(14A)-C(14)-H(14C) | 109.5 |
| N(6)-C(19)-C(18) | 108.1(11) | H(14B)-C(14)-H(14C) | 109.5 |
| N(6)-C(19)-C(20) | 102.2(12) | C(13)-N(4)-C(14) | 115.1(11) |
| C(18)-C(19)-C(20) | 117.2(14) | C(13)-N(4)-P(2) | 125.7(10) |
| N(6)-C(19)-H(19A) | 109.6 | C(14)-N(4)-P(2) | 119.1(9) |
| C(18)-C(19)-H(19A) | 109.6 | N(4)-C(13)-C(12) | 113.0(12) |
| C(20)-C(19)-H(19A) | 109.6 | N(4)-C(13)-H(13A) | 109.0 |
| C(21)-C(20)-C(19) | 103.1(14) | C(12)-C(13)-H(13A) | 109.0 |
| C(21)-C(20)-H(20A) | 111.1 | N(4)-C(13)-H(13B) | 109.0 |
| C(19)-C(20)-H(20A) | 111.1 | C(12)-C(13)-H(13B) | 109.0 |
| C(21)-C(20)-H(20B) | 111.1 | H(13A)-C(13)-H(13B) | 107.8 |
| C(19)-C(20)-H(20B) | 111.1 | C(11)-C(12)-C(13) | 112.6(16) |
| H(20A)-C(20)-H(20B) | 109.1 | C(11)-C(12)-H(12A) | 109.1 |
| C(20)-C(21)-C(22) | 109.3(16) | C(13)-C(12)-H(12A) | 109.1 |
| C(20)-C(21)-H(21A) | 109.8 | C(11)-C(12)-H(12B) | 109.1 |
| C(22)-C(21)-H(21A) | 109.8 | C(13)-C(12)-H(12B) | 109.1 |
| C(20)-C(21)-H(21B) | 109.8 | H(12A)-C(12)-H(12B) | 107.8 |
| C(22)-C(21)-H(21B) | 109.8 | Cl(7)-C(23)-Cl(5) | 108.2(9) |
| H(21A)-C(21)-H(21B) | 108.3 | Cl(7)-C(23)-Cl(6) | 108.4(9) |
| N(6)-C(22)-C(21) | 100.0(13) | Cl(5)-C(23)-Cl(6) | 108.1(9) |
| N(6)-C(22)-H(22A) | 111.8 | Cl(7)-C(23)-H(23) | 110.7 |
| C(21)-C(22)-H(22A) | 111.8 | Cl(5)-C(23)-H(23) | 110.7 |
| N(6)-C(22)-H(22B) | 111.8 | Cl(6)-C(23)-H(23) | 110.7 |
| C(21)-C(22)-H(22B) | 111.8 | Cl(10)-C(24)-Cl(9) | 108.3(9) |
| H(22A)-C(22)-H(22B) | 109.5 | Cl(10)-C(24)-Cl(8) | 108.2(9) |
| C(22)-N(6)-C(19) | 115.7(12) | Cl(9)-C(24)-Cl(8) | 108.9(9) |
| C(22)-N(6)-P(2) | 130.8(11) | Cl(10)-C(24)-H(24) | 110.5 |
| C(19)-N(6)-P(2) | 109.0(9) | Cl(9)-C(24)-H(24) | 110.5 |
| N(4)-C(14)-H(14A) | 109.5 | Cl(8)-C(24)-H(24) | 110.5 |
| N(4)-C(14)-H(14B) | 109.5 | Cl(12)-C(25)-Cl(11) | 108.7(9) |

**Table 13.** Bond Angles [deg] for **7c**•$SnCl_4$.

| bond angle | [deg] | bond angle | [deg] |
|---|---|---|---|
| Cl(12)-C(25)-Cl(13) | 109.1(9) | Cl(14)-C(26)-Cl(15) | 107.1(8) |
| Cl(11)-C(25)-Cl(13) | 108.2(8) | Cl(16)-C(26)-Cl(15) | 107.1(9) |
| Cl(12)-C(25)-H(25) | 110.3 | Cl(14)-C(26)-H(26) | 111.6 |
| Cl(11)-C(25)-H(25) | 110.3 | Cl(16)-C(26)-H(26) | 111.6 |
| Cl(13)-C(25)-H(25) | 110.3 | Cl(15)-C(26)-H(26) | 111.6 |
| Cl(14)-C(26)-Cl(16) | 107.5(9) | | |

**Table 14.** Torsional angles [deg] for **7c**•$SnCl_4$.

| torsional angle | [deg] | torsional angle | [deg] |
|---|---|---|---|
| O(2)-Sn(1)-O(1)-P(1) | 127.0(16) | C(7)-C(8)-N(2)-P(1) | -127.7(16) |
| Cl(4)-Sn(1)-O(1)-P(1) | -49.3(15) | C(4)-C(5)-N(2)-C(8) | -127.3(17) |
| Cl(2)-Sn(1)-O(1)-P(1) | 42.0(15) | C(6)-C(5)-N(2)-C(8) | -3.5(18) |
| Cl(1)-Sn(1)-O(1)-P(1) | -141.6(15) | C(4)-C(5)-N(2)-P(1) | 27.5(16) |
| Sn(1)-O(1)-P(1)-N(3) | -109.9(15) | C(6)-C(5)-N(2)-P(1) | 151.3(12) |
| Sn(1)-O(1)-P(1)-N(1) | 127.2(15) | O(1)-P(1)-N(2)-C(8) | -109.6(15) |
| Sn(1)-O(1)-P(1)-N(2) | 17.0(18) | N(3)-P(1)-N(2)-C(8) | 15.8(17) |
| O(1)-P(1)-N(1)-C(1) | 13.7(14) | N(1)-P(1)-N(2)-C(8) | 133.0(15) |
| N(3)-P(1)-N(1)-C(1) | -107.0(13) | O(1)-P(1)-N(2)-C(5) | 100.5(11) |
| N(2)-P(1)-N(1)-C(1) | 136.3(12) | N(3)-P(1)-N(2)-C(5) | -134.1(11) |
| O(1)-P(1)-N(1)-C(4) | -121.5(11) | N(1)-P(1)-N(2)-C(5) | -16.9(11) |
| N(3)-P(1)-N(1)-C(4) | 117.8(11) | O(1)-P(1)-N(3)-C(10) | 19.4(16) |
| N(2)-P(1)-N(1)-C(4) | 1.1(12) | N(1)-P(1)-N(3)-C(10) | 141.3(14) |
| C(4)-N(1)-C(1)-C(2) | 26.6(16) | N(2)-P(1)-N(3)-C(10) | -110.7(14) |
| P(1)-N(1)-C(1)-C(2) | -108.8(13) | O(1)-P(1)-N(3)-C(9) | -163.5(15) |
| N(1)-C(1)-C(2)-C(3) | -36.8(17) | N(1)-P(1)-N(3)-C(9) | -41.7(18) |
| C(1)-C(2)-C(3)-C(4) | 32.3(18) | N(2)-P(1)-N(3)-C(9) | 66.3(17) |
| C(1)-N(1)-C(4)-C(5) | -125.4(14) | C(9)-N(3)-C(10)-C(11) | 70(2) |
| P(1)-N(1)-C(4)-C(5) | 14.8(16) | P(1)-N(3)-C(10)-C(11) | -112.7(17) |
| C(1)-N(1)-C(4)-C(3) | -7.6(16) | N(3)-C(10)-C(11)-C(12) | 39(2) |
| P(1)-N(1)-C(4)-C(3) | 132.6(12) | O(1)-Sn(1)-O(2)-P(2) | 122.9(18) |
| C(2)-C(3)-C(4)-N(1) | -14.9(17) | Cl(2)-Sn(1)-O(2)-P(2) | -146.6(17) |
| C(2)-C(3)-C(4)-C(5) | 99.4(16) | Cl(3)-Sn(1)-O(2)-P(2) | -53.3(17) |
| N(1)-C(4)-C(5)-N(2) | -26.0(17) | Cl(1)-Sn(1)-O(2)-P(2) | 37.0(17) |
| C(3)-C(4)-C(5)-N(2) | -138.1(13) | Sn(1)-O(2)-P(2)-N(4) | -105.5(17) |
| N(1)-C(4)-C(5)-C(6) | -141.1(14) | Sn(1)-O(2)-P(2)-N(5) | 131.2(17) |
| C(3)-C(4)-C(5)-C(6) | 106.8(16) | Sn(1)-O(2)-P(2)-N(6) | 20(2) |
| N(2)-C(5)-C(6)-C(7) | -17.1(18) | O(2)-P(2)-N(5)-C(15) | 12.9(14) |
| C(4)-C(5)-C(6)-C(7) | 101(2) | N(4)-P(2)-N(5)-C(15) | -106.7(13) |
| C(5)-C(6)-C(7)-C(8) | 31(2) | N(6)-P(2)-N(5)-C(15) | 135.8(13) |
| C(6)-C(7)-C(8)-N(2) | -32(2) | O(2)-P(2)-N(5)-C(18) | -120.1(11) |
| C(7)-C(8)-N(2)-C(5) | 20.8(19) | N(4)-P(2)-N(5)-C(18) | 120.2(11) |

**Table 14.** Torsional angles [deg] for **7c**•$SnCl_4$.

| torsional angle | [deg] | torsional angle | [deg] |
|---|---|---|---|
| N(6)-P(2)-N(5)-C(18) | 2.7(12) | C(18)-C(19)-N(6)-C(22) | -132.4(17) |
| C(18)-N(5)-C(15)-C(16) | 26.9(18) | C(20)-C(19)-N(6)-C(22) | -8(2) |
| P(2)-N(5)-C(15)-C(16) | -106.5(14) | C(18)-C(19)-N(6)-P(2) | 26.6(16) |
| N(5)-C(15)-C(16)-C(17) | -38.6(19) | C(20)-C(19)-N(6)-P(2) | 150.8(12) |
| C(15)-C(16)-C(17)-C(18) | 35(2) | O(2)-P(2)-N(6)-C(22) | -104.1(18) |
| C(15)-N(5)-C(18)-C(19) | -125.3(15) | N(4)-P(2)-N(6)-C(22) | 19.0(19) |
| P(2)-N(5)-C(18)-C(19) | 12.5(16) | N(5)-P(2)-N(6)-C(22) | 137.5(18) |
| C(15)-N(5)-C(18)-C(17) | -6.5(17) | O(2)-P(2)-N(6)-C(19) | 101.1(11) |
| P(2)-N(5)-C(18)-C(17) | 131.4(12) | N(4)-P(2)-N(6)-C(19) | -135.7(10) |
| C(16)-C(17)-C(18)-C(19) | 98.2(18) | N(5)-P(2)-N(6)-C(19) | -17.3(12) |
| C(16)-C(17)-C(18)-N(5) | -16.9(18) | O(2)-P(2)-N(4)-C(13) | 14.5(16) |
| N(5)-C(18)-C(19)-N(6) | -24.1(17) | N(5)-P(2)-N(4)-C(13) | 136.7(14) |
| C(17)-C(18)-C(19)-N(6) | -137.0(13) | N(6)-P(2)-N(4)-C(13) | -114.3(14) |
| N(5)-C(18)-C(19)-C(20) | -138.9(14) | O(2)-P(2)-N(4)-C(14) | -169.0(15) |
| C(17)-C(18)-C(19)-C(20) | 108.2(16) | N(5)-P(2)-N(4)-C(14) | -46.8(17) |
| N(6)-C(19)-C(20)-C(21) | 23.9(19) | N(6)-P(2)-N(4)-C(14) | 62.2(17) |
| C(18)-C(19)-C(20)-C(21) | 141.8(18) | C(14)-N(4)-C(13)-C(12) | 63(2) |
| C(19)-C(20)-C(21)-C(22) | -32(2) | P(2)-N(4)-C(13)-C(12) | -120.3(15) |
| C(20)-C(21)-C(22)-N(6) | 27(2) | C(10)-C(11)-C(12)-C(13) | 68(2) |
| C(21)-C(22)-N(6)-C(19) | -10(2) | N(4)-C(13)-C(12)-C(11) | 53(2) |
| C(21)-C(22)-N(6)-P(2) | -163.5(16) | | |

Symmetry transformations used to generate equivalent atoms:

**Crystal Preparation and Structure Refinement Summary for 7d•$SnCl_4$**

To a solution of **7d** (50 mg, 0.10 mmol) in 2.0 mL of $CH_2Cl_2$ at rt under nitrogen was added $SnCl_4$ (12 mL, 0.10 mmol, 1.0 equiv) with stirring and the mixture was filtered through glass wool to obtain a clear solution. The solution was then added to a small test tube (15 X 50 mm). The test tube was placed in a vessel (40 X 80 mm) which contained 2.0 mL of pentane. Slow diffusion of pentane at rt provided the single crystals suitable for X-ray analysis.

The data crystal was mounted using oil (Paratone-N, Exxon) to a thin glass fiber with the (0 0 1) scattering planes roughly normal to the spindles axis. Systematic conditions suggested the unambiguous space group. Structure was solved by direct methods (Sheldrick, 1998). Two-fold symmetry along the b-axis was imposed on the host molecule. A Fourier map less contributions from the host molecule revealed a water solvate disordered in five positions about the b-axis two-fold. Anisotropic displacement parameters for the disordered solvate atom positions were restrained to have similar symmetric values with an effective standard deviation of 0.02 \%A. No other restrains were imposed on the model. H atoms for the water solvate never surfaced and were not included in the proposed model. Methyl H atom positions, R-$CH_3$, were optimized by rotation about R-C bonds with idealized C-H, R-H and H-H distances. Remaining H atoms for the host molecule were included as fixed idealized contributors. H atom U's were assigned as 1.2 times Ueq of adjacent non-H atoms. The space group choice was confirmed by successful convergence of the full-matrix least-squares refinement on $F^2$ (Sheldrick, 1998). The highest peaks in the final difference Fourier map were in the vicinity of Sn and Cl atoms; the final map had no other significant features. A final analysis of variance between observed and calculated structure factors showed no dependence on amplitude or resolution.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Sheldrick, G. M. SHELX-97-2. **1998**, Program for crystal structure solution and refinement. Institute fur anorg chemie, Göttingen, Germany.

Bruker AXS, Inc. **1998**, Madison, Wisconsin, USA.

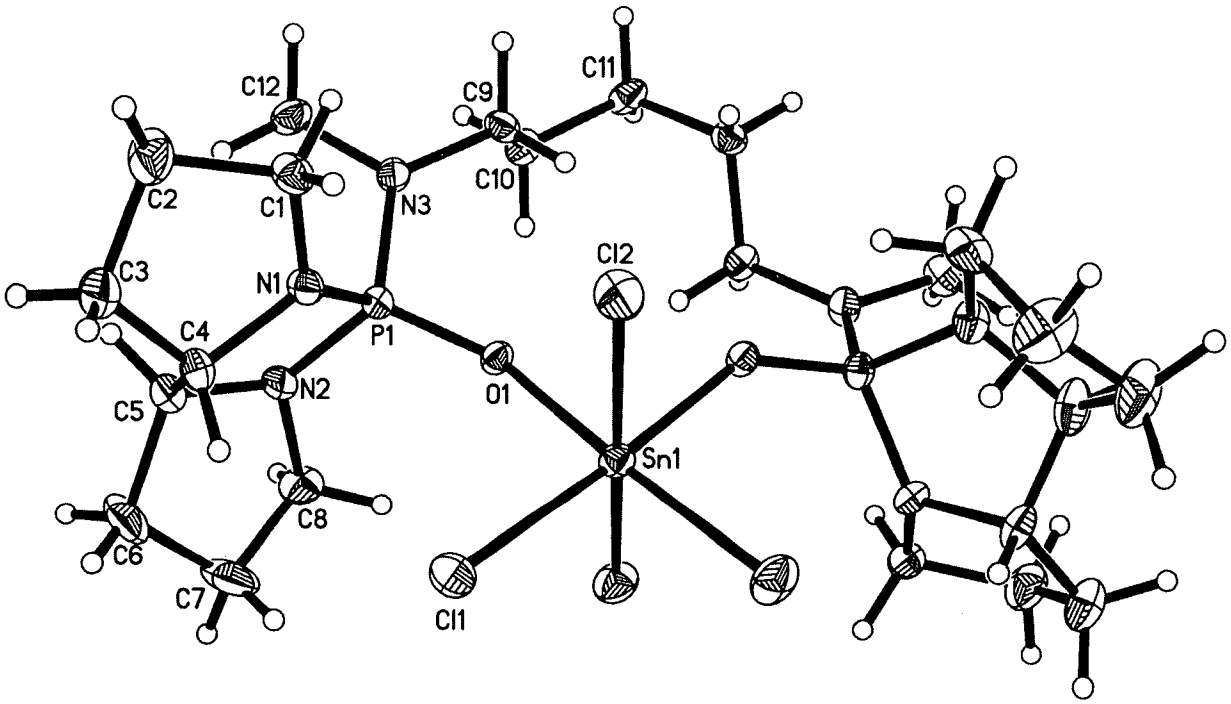


**Figure 3.** ORTEP representation **7d**•$SnCl_4$ (35% ellipsoids)

**Table 15.** Crystal data and structure refinement for **7d**•$SnCl_4$.

| | | |
|---|---|---|
| Empirical formula | C23 H46 Cl4 N6 O3 P2 Sn | |
| Formula weight | 777.09 | |
| Temperature | 193(2) K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Orthorhombic | |
| Space group | C 2 2 21 | |
| Unit cell dimensions | a = 14.898(3) Å | _alpha = 90°. |
| | b = 18.010(3) Å | _beta = 90°. |
| | c = 12.420(2) Å | _gamma = 90°. |
| Volume | 3332.6(10) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.549 $Mg/m^3$ | |
| Absorption coefficient | 1.218 $mm^{-1}$ | |
| F(000) | 1592 | |
| Crystal size | 0.26 x 0.06 x 0.03 $mm^3$ | |
| Theta range for data collection | 1.77 to 28.28°. | |
| Index ranges | -19<=h<=18, -23<=k<=23, -16<=l<=16 | |
| Reflections collected | 15641 | |
| Independent reflections | 4023 [R(int) = 0.0806] | |
| Completeness to theta = 28.28° | 98.6 % | |
| Absorption correction | Integration | |
| Max. and min. transmission | 0.9680 and 0.8267 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 4023 / 25 / 200 | |
| Goodness-of-fit on $F^2$ | 0.920 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0398, wR2 = 0.0612 | |
| R indices (all data) | R1 = 0.0766, wR2 = 0.0679 | |
| Absolute structure parameter | 0.00(3) | |
| Largest diff. peak and hole | 0.437 and -0.420 e.$Å^{-3}$ | |

**Table 16.** Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2 x\ 10^3$). U(eq) is defined as one third of the trace of the orthogonalized $U^{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Sn(1) | 5000 | 3206(1) | 2500 | 23(1) |
| Cl(1) | 3862(1) | 2283(1) | 2218(1) | 41(1) |
| Cl(2) | 4698(1) | 3316(1) | 4380(1) | 38(1) |
| P(1) | 3102(1) | 4256(1) | 2453(1) | 22(1) |
| O(1) | 4072(2) | 4066(1) | 2255(2) | 23(1) |
| N(1) | 2517(2) | 3743(2) | 3269(3) | 24(1) |
| N(2) | 2458(2) | 4118(2) | 1400(3) | 29(1) |
| N(3) | 3095(2) | 5110(2) | 2874(3) | 26(1) |
| C(1) | 2292(3) | 3875(3) | 4388(3) | 31(1) |
| C(2) | 1280(3) | 3808(3) | 4410(4) | 46(1) |
| C(3) | 1068(3) | 3232(3) | 3565(3) | 43(1) |
| C(4) | 1824(3) | 3289(2) | 2720(3) | 33(1) |
| C(5) | 1621(3) | 3707(3) | 1682(4) | 40(1) |
| C(6) | 1441(3) | 3226(4) | 680(4) | 57(2) |
| C(7) | 2304(4) | 3206(3) | 80(4) | 57(2) |
| C(8) | 2760(3) | 3934(3) | 310(3) | 36(1) |
| C(9) | 3901(3) | 5541(2) | 3121(3) | 25(1) |
| C(10) | 4174(3) | 6063(2) | 2218(3) | 27(1) |
| C(11) | 5000 | 6526(3) | 2500 | 32(1) |
| C(12) | 2239(3) | 5523(2) | 2833(3) | 32(1) |
| O(2) | 500(20) | 5170(20) | 540(30) | 170(17) |
| O(3) | 70(30) | 5664(17) | 1830(30) | 139(9) |
| O(4) | 0 | 5350(30) | 2500 | 118(11) |

**Table 17.** Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **7d**•$SnCl_4$. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{23}$ | $U^{13}$ | $U^{12}$ |
|---|---|---|---|---|---|---|
| Sn(1) | 24(1) | 18(1) | 27(1) | 0 | 3(1) | 0 |
| Cl(1) | 38(1) | 27(1) | 60(1) | -6(1) | 2(1) | -8(1) |
| Cl(2) | 40(1) | 48(1) | 27(1) | 3(1) | 6(1) | -7(1) |
| P(1) | 20(1) | 22(1) | 25(1) | -4(1) | -1(1) | 0(1) |
| O(1) | 19(2) | 18(1) | 32(2) | -1(1) | 3(1) | 1(1) |
| N(1) | 25(2) | 23(2) | 23(2) | -2(2) | 4(2) | -6(2) |
| N(2) | 27(2) | 36(2) | 23(2) | -8(2) | -1(2) | -2(2) |
| N(3) | 22(2) | 18(2) | 38(2) | -4(2) | -2(2) | 2(2) |
| C(1) | 34(3) | 35(3) | 23(2) | 0(2) | -1(2) | -7(2) |
| C(2) | 36(3) | 62(4) | 39(3) | 3(3) | 8(2) | -10(3) |
| C(3) | 31(3) | 53(3) | 45(3) | -9(3) | 7(2) | -9(3) |
| C(4) | 24(2) | 32(2) | 43(3) | -7(2) | 3(2) | -10(2) |
| C(5) | 27(3) | 50(3) | 41(3) | -19(3) | -1(2) | -5(3) |
| C(6) | 48(3) | 82(4) | 40(3) | -25(4) | -4(2) | -28(4) |
| C(7) | 76(4) | 52(3) | 44(3) | -27(3) | 5(3) | -19(4) |
| C(8) | 43(3) | 51(3) | 15(2) | -3(2) | 1(2) | 6(3) |
| C(9) | 27(3) | 22(2) | 26(2) | -6(2) | 0(2) | -5(2) |
| C(10) | 29(2) | 25(2) | 28(3) | 4(2) | 1(2) | 4(2) |
| C(11) | 30(3) | 19(3) | 46(3) | 0 | 14(4) | 0 |
| C(12) | 33(3) | 26(2) | 36(3) | -4(2) | 2(2) | 9(2) |
| O(2) | 180(20) | 150(20) | 180(20) | 15(17) | 1(16) | -1(17) |
| O(3) | 115(12) | 159(15) | 143(16) | 10(12) | -9(15) | 21(13) |
| O(4) | 84(13) | 125(17) | 145(18) | 0 | 3(16) | 0 |

**Table 18.** Hydrogen coordinates (x $10^4$) and isotropic displacement parameters ($Å^2$x $10^3$).

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1A) | 2487 | 4375 | 4619 | 37 |
| H(1B) | 2575 | 3499 | 4861 | 37 |
| H(2A) | 1069 | 3645 | 5128 | 55 |
| H(2B) | 994 | 4289 | 4232 | 55 |
| H(3A) | 477 | 3334 | 3231 | 51 |
| H(3B) | 1054 | 2730 | 3888 | 51 |
| H(4) | 2067 | 2784 | 2552 | 39 |
| H(5) | 1115 | 4063 | 1797 | 47 |
| H(6A) | 1255 | 2719 | 892 | 68 |
| H(6B) | 962 | 3449 | 232 | 68 |
| H(7A) | 2194 | 3149 | -701 | 69 |
| H(7B) | 2679 | 2786 | 330 | 69 |
| H(8A) | 3421 | 3882 | 283 | 44 |
| H(8B) | 2572 | 4320 | -212 | 44 |
| H(9A) | 4402 | 5195 | 3270 | 30 |
| H(9B) | 3793 | 5835 | 3782 | 30 |
| H(10A) | 3668 | 6401 | 2055 | 33 |
| H(10B) | 4301 | 5769 | 1563 | 33 |
| H(11) | 5147 | 6850 | 1881 | 38 |
| H(12A) | 2155 | 5796 | 3508 | 38 |
| H(12B) | 1741 | 5173 | 2736 | 38 |
| H(12C) | 2251 | 5873 | 2230 | 38 |

**Table 19.** Bond lengths [Å] for **7d**•$SnCl_4$.

| bond | [Å] | bond | [Å] |
|---|---|---|---|
| Sn(1)-O(1)#1 | 2.098(2) | C(4)-C(5) | 1.524(6) |
| Sn(1)-O(1) | 2.098(2) | C(4)-H(4) | 1.0000 |
| Sn(1)-Cl(2) | 2.3863(11) | C(5)-C(6) | 1.540(6) |
| Sn(1)-Cl(2)#1 | 2.3863(11) | C(5)-H(5) | 1.0000 |
| Sn(1)-Cl(1)#1 | 2.4008(11) | C(6)-C(7) | 1.485(6) |
| Sn(1)-Cl(1) | 2.4008(11) | C(6)-H(6A) | 0.9900 |
| P(1)-O(1) | 1.505(3) | C(6)-H(6B) | 0.9900 |
| P(1)-N(3) | 1.623(3) | C(7)-C(8) | 1.506(6) |
| P(1)-N(1) | 1.626(3) | C(7)-H(7A) | 0.9900 |
| P(1)-N(2) | 1.641(4) | C(7)-H(7B) | 0.9900 |
| N(1)-C(1) | 1.449(5) | C(8)-H(8A) | 0.9900 |
| N(1)-C(4) | 1.483(5) | C(8)-H(8B) | 0.9900 |
| N(2)-C(8) | 1.464(5) | C(9)-C(10) | 1.519(5) |
| N(2)-C(5) | 1.492(6) | C(9)-H(9A) | 0.9900 |
| N(3)-C(9) | 1.463(5) | C(9)-H(9B) | 0.9900 |
| N(3)-C(12) | 1.478(5) | C(10)-C(11) | 1.526(4) |
| C(1)-C(2) | 1.513(6) | C(10)-H(10A) | 0.9900 |
| C(1)-H(1A) | 0.9900 | C(10)-H(10B) | 0.9900 |
| C(1)-H(1B) | 0.9900 | C(11)-C(10)#1 | 1.526(4) |
| C(2)-C(3) | 1.509(6) | C(11)-H(11) | 0.9900 |
| C(2)-H(2A) | 0.9900 | C(12)-H(12A) | 0.9800 |
| C(2)-H(2B) | 0.9900 | C(12)-H(12B) | 0.9800 |
| C(3)-C(4) | 1.544(5) | C(12)-H(12C) | 0.9800 |
| C(3)-H(3A) | 0.9900 | O(2)-O(2)#2 | 1.48(7) |
| C(3)-H(3B) | 0.9900 | O(3)-O(3)#3 | 1.68(8) |

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

**Table 20.** Bond Angles [deg] for **7d**•$SnCl_4$:

| bond angle | [deg] | bond angle | [deg] |
|---|---|---|---|
| O(1)#1-Sn(1)-O(1) | 84.87(13) | N(1)-C(1)-H(1A) | 111.1 |
| O(1)#1-Sn(1)-Cl(2) | 85.48(8) | C(2)-C(1)-H(1A) | 111.1 |
| O(1)-Sn(1)-Cl(2) | 87.49(8) | N(1)-C(1)-H(1B) | 111.1 |
| O(1)#1-Sn(1)-Cl(2)#1 | 87.49(8) | C(2)-C(1)-H(1B) | 111.1 |
| O(1)-Sn(1)-Cl(2)#1 | 85.48(8) | H(1A)-C(1)-H(1B) | 109.0 |
| Cl(2)-Sn(1)-Cl(2)#1 | 170.48(6) | C(3)-C(2)-C(1) | 104.5(4) |
| O(1)#1-Sn(1)-Cl(1)#1 | 91.40(7) | C(3)-C(2)-H(2A) | 110.8 |
| O(1)-Sn(1)-Cl(1)#1 | 176.23(7) | C(1)-C(2)-H(2A) | 110.8 |
| Cl(2)-Sn(1)-Cl(1)#1 | 92.75(4) | C(3)-C(2)-H(2B) | 110.8 |
| Cl(2)#1-Sn(1)-Cl(1)#1 | 93.84(4) | C(1)-C(2)-H(2B) | 110.8 |
| O(1)#1-Sn(1)-Cl(1) | 176.23(7) | H(2A)-C(2)-H(2B) | 108.9 |
| O(1)-Sn(1)-Cl(1) | 91.40(7) | C(2)-C(3)-C(4) | 106.0(4) |
| Cl(2)-Sn(1)-Cl(1) | 93.84(4) | C(2)-C(3)-H(3A) | 110.5 |
| Cl(2)#1-Sn(1)-Cl(1) | 92.75(4) | C(4)-C(3)-H(3A) | 110.5 |
| Cl(1)#1-Sn(1)-Cl(1) | 92.33(6) | C(2)-C(3)-H(3B) | 110.5 |
| O(1)-P(1)-N(3) | 105.91(15) | C(4)-C(3)-H(3B) | 110.5 |
| O(1)-P(1)-N(1) | 119.16(17) | H(3A)-C(3)-H(3B) | 108.7 |
| N(3)-P(1)-N(1) | 109.48(18) | N(1)-C(4)-C(5) | 104.7(3) |
| O(1)-P(1)-N(2) | 113.41(17) | N(1)-C(4)-C(3) | 103.3(3) |
| N(3)-P(1)-N(2) | 113.34(18) | C(5)-C(4)-C(3) | 117.6(4) |
| N(1)-P(1)-N(2) | 95.58(18) | N(1)-C(4)-H(4) | 110.2 |
| P(1)-O(1)-Sn(1) | 140.99(15) | C(5)-C(4)-H(4) | 110.2 |
| C(1)-N(1)-C(4) | 111.8(3) | C(3)-C(4)-H(4) | 110.2 |
| C(1)-N(1)-P(1) | 129.0(3) | N(2)-C(5)-C(4) | 106.2(3) |
| C(4)-N(1)-P(1) | 113.6(3) | N(2)-C(5)-C(6) | 103.6(4) |
| C(8)-N(2)-C(5) | 111.2(4) | C(4)-C(5)-C(6) | 116.1(4) |
| C(8)-N(2)-P(1) | 126.2(3) | N(2)-C(5)-H(5) | 110.2 |
| C(5)-N(2)-P(1) | 112.1(3) | C(4)-C(5)-H(5) | 110.2 |
| C(9)-N(3)-C(12) | 116.6(3) | C(6)-C(5)-H(5) | 110.2 |
| C(9)-N(3)-P(1) | 124.4(3) | C(7)-C(6)-C(5) | 105.6(4) |
| C(12)-N(3)-P(1) | 118.1(3) | C(7)-C(6)-H(6A) | 110.6 |
| N(1)-C(1)-C(2) | 103.5(3) | C(5)-C(6)-H(6A) | 110.6 |

**Table 20.** Bond Angles [deg] for **7d**•$SnCl_4$.

| bond angle | [deg] | bond angle | [deg] |
|---|---|---|---|
| C(7)-C(6)-H(6B) | 110.6 | N(3)-C(9)-H(9B) | 108.9 |
| C(5)-C(6)-H(6B) | 110.6 | C(10)-C(9)-H(9B) | 108.9 |
| H(6A)-C(6)-H(6B) | 108.8 | H(9A)-C(9)-H(9B) | 107.8 |
| C(6)-C(7)-C(8) | 105.9(4) | C(9)-C(10)-C(11) | 112.6(3) |
| C(6)-C(7)-H(7A) | 110.6 | C(9)-C(10)-H(10A) | 109.1 |
| C(8)-C(7)-H(7A) | 110.6 | C(11)-C(10)-H(10A) | 109.1 |
| C(6)-C(7)-H(7B) | 110.6 | C(9)-C(10)-H(10B) | 109.1 |
| C(8)-C(7)-H(7B) | 110.6 | C(11)-C(10)-H(10B) | 109.1 |
| H(7A)-C(7)-H(7B) | 108.7 | H(10A)-C(10)-H(10B) | 107.8 |
| N(2)-C(8)-C(7) | 103.5(4) | C(10)-C(11)-C(10)#1 | 113.9(4) |
| N(2)-C(8)-H(8A) | 111.1 | C(10)-C(11)-H(11) | 108.8 |
| C(7)-C(8)-H(8A) | 111.1 | C(10)#1-C(11)-H(11) | 108.8 |
| N(2)-C(8)-H(8B) | 111.1 | N(3)-C(12)-H(12A) | 109.5 |
| C(7)-C(8)-H(8B) | 111.1 | N(3)-C(12)-H(12B) | 109.5 |
| H(8A)-C(8)-H(8B) | 109.0 | H(12A)-C(12)-H(12B) | 109.5 |
| N(3)-C(9)-C(10) | 113.2(3) | N(3)-C(12)-H(12C) | 109.5 |
| N(3)-C(9)-H(9A) | 108.9 | H(12A)-C(12)-H(12C) | 109.5 |
| C(10)-C(9)-H(9A) | 108.9 | H(12B)-C(12)-H(12C) | 109.5 |

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

**Table 21.** Torsional angles [deg] for **7d**•$SnCl_4$.

| torsional angle | [deg] | torsional angle | [deg] |
|---|---|---|---|
| N(3)-P(1)-O(1)-Sn(1) | 137.1(2) | P(1)-N(1)-C(1)-C(2) | 125.9(4) |
| N(1)-P(1)-O(1)-Sn(1) | 13.3(3) | N(1)-C(1)-C(2)-C(3) | 33.0(5) |
| N(2)-P(1)-O(1)-Sn(1) | -98.0(3) | C(1)-C(2)-C(3)-C(4) | -29.0(5) |
| O(1)#1-Sn(1)-O(1)-P(1) | -144.5(3) | C(1)-N(1)-C(4)-C(5) | 131.1(4) |
| Cl(2)-Sn(1)-O(1)-P(1) | -58.9(2) | P(1)-N(1)-C(4)-C(5) | -24.9(4) |
| Cl(2)#1-Sn(1)-O(1)-P(1) | 127.6(3) | C(1)-N(1)-C(4)-C(3) | 7.4(5) |
| Cl(1)#1-Sn(1)-O(1)-P(1) | -152.7(11) | P(1)-N(1)-C(4)-C(3) | -148.6(3) |
| Cl(1)-Sn(1)-O(1)-P(1) | 34.9(2) | C(2)-C(3)-C(4)-N(1) | 13.8(5) |
| O(1)-P(1)-N(1)-C(1) | 99.2(4) | C(2)-C(3)-C(4)-C(5) | -101.0(5) |
| N(3)-P(1)-N(1)-C(1) | -22.9(4) | C(8)-N(2)-C(5)-C(4) | 124.6(4) |
| N(2)-P(1)-N(1)-C(1) | -140.1(4) | P(1)-N(2)-C(5)-C(4) | -22.8(4) |
| O(1)-P(1)-N(1)-C(4) | -109.9(3) | C(8)-N(2)-C(5)-C(6) | 1.8(5) |
| N(3)-P(1)-N(1)-C(4) | 128.1(3) | P(1)-N(2)-C(5)-C(6) | -145.6(3) |
| N(2)-P(1)-N(1)-C(4) | 10.9(3) | N(1)-C(4)-C(5)-N(2) | 28.3(4) |
| O(1)-P(1)-N(2)-C(8) | -8.6(4) | C(3)-C(4)-C(5)-N(2) | 142.3(4) |
| N(3)-P(1)-N(2)-C(8) | 112.2(4) | N(1)-C(4)-C(5)-C(6) | 142.8(4) |
| N(1)-P(1)-N(2)-C(8) | -133.8(4) | C(3)-C(4)-C(5)-C(6) | -103.2(5) |
| O(1)-P(1)-N(2)-C(5) | 132.8(3) | N(2)-C(5)-C(6)-C(7) | 17.9(6) |
| N(3)-P(1)-N(2)-C(5) | -106.3(3) | C(4)-C(5)-C(6)-C(7) | -98.1(5) |
| N(1)-P(1)-N(2)-C(5) | 7.7(3) | C(5)-C(6)-C(7)-C(8) | -30.8(6) |
| O(1)-P(1)-N(3)-C(9) | -6.8(4) | C(5)-N(2)-C(8)-C(7) | -20.3(5) |
| N(1)-P(1)-N(3)-C(9) | 122.9(3) | P(1)-N(2)-C(8)-C(7) | 121.5(4) |
| N(2)-P(1)-N(3)-C(9) | -131.7(3) | C(6)-C(7)-C(8)-N(2) | 31.3(5) |
| O(1)-P(1)-N(3)-C(12) | 162.5(3) | C(12)-N(3)-C(9)-C(10) | -69.9(4) |
| N(1)-P(1)-N(3)-C(12) | -67.9(3) | P(1)-N(3)-C(9)-C(10) | 99.4(4) |
| N(2)-P(1)-N(3)-C(12) | 37.5(3) | N(3)-C(9)-C(10)-C(11) | 178.3(3) |
| C(4)-N(1)-C(1)-C(2) | -25.4(5) | C(9)-C(10)-C(11)-C(10)#1 | 58.1(3) |

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1/2 #2 x,-y+1,-z #3 -x,y,-z+1/2

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