# On the coordination non-innocence of antimony in nickel(II) complexes of the tetradentate *o*-$(Ph_2P)C_6H_4)_3Sb$ ligand

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## Supporting Information

**Table 1**. Crystal data, data collections, and structure refinements for **2** and **3**.

| | **2** | **3**•1.5$CHCl_3$ |
|---|---|---|
| Formula | $C_{54}H_{42}AsP_3$ | $C_{111}H_{87}Cl_9P_6Sb_2$ |
| Formula Weight | 858.70 | 2169.17 |
| Crystal Size (mm) | 0.30 x 0.21 x 0.04 | 0.45 x 0.37 x 0.28 |
| Crystal System | Triclinic | Triclinic |
| Space Group | P-1 | P-1 |
| *a* (Å) | 10.438(2) | 15.442(5) |
| *b* (Å) | 13.155(3) | 15.443(5) |
| *c* (Å) | 15.671(3) | 22.924(8) |
| $\alpha$ (°) | 102.724(14) | 89.098(18) |
| $\beta$ (°) | 90.398(14) | 87.977(18) |
| $\gamma$ (°) | 92.371(14) | 60.383(14) |
| V ($Å^3$) | 2097.0(7) | 4750(3) |
| Z | 2 | 2 |
| $\rho_{calc}$ ($g/cm^3$) | 1.360 | 1.517 |
| $\mu$ ($mm^{-1}$) | 0.963 | 0.974 |
| F(000) | 888 | 2196 |
| T (K) | 110(2) | 110(2) |
| *hkl* Range | -14 → 14 | -19 → 17 |
| | -18 → 18 | -19 → 19 |
| | -22 → 22 | -29 → 32 |
| Reflections collected | 42880 | 65695 |
| Unique reflections [Rint] | 12481 [0.0807] | 19868 [0.0489] |
| Reflns. used for refinement | 12481 | 19868 |
| Refined parameters | 523 | 1184 |
| GooF | 1.005 | 1.058 |
| R1[a], *w*R2[b] (all data) | 0.1084, 0.1654 | 0.0839, 0.2377 |
| $\rho_{fin}$ (max., min.) ($eA^{-3}$) | 2.352, -0.964 | 4.379, -2.737 |

[a]R1 = $\sum||F_o| - |F_c||/\sum|F_o|$. [b] *w*R2 $([w(F_o^2 - F_c^2)^2]/[\sum w(F_o^2)^2])^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (ap)^2 + bp]$; $p = (F_o^2 + 2F_c^2)/3$ with $a$ = 0.0823 for **2** and 0.1312 for **3**; and $b$ = 0.0000 for **2** and 49.1873 for **3**.

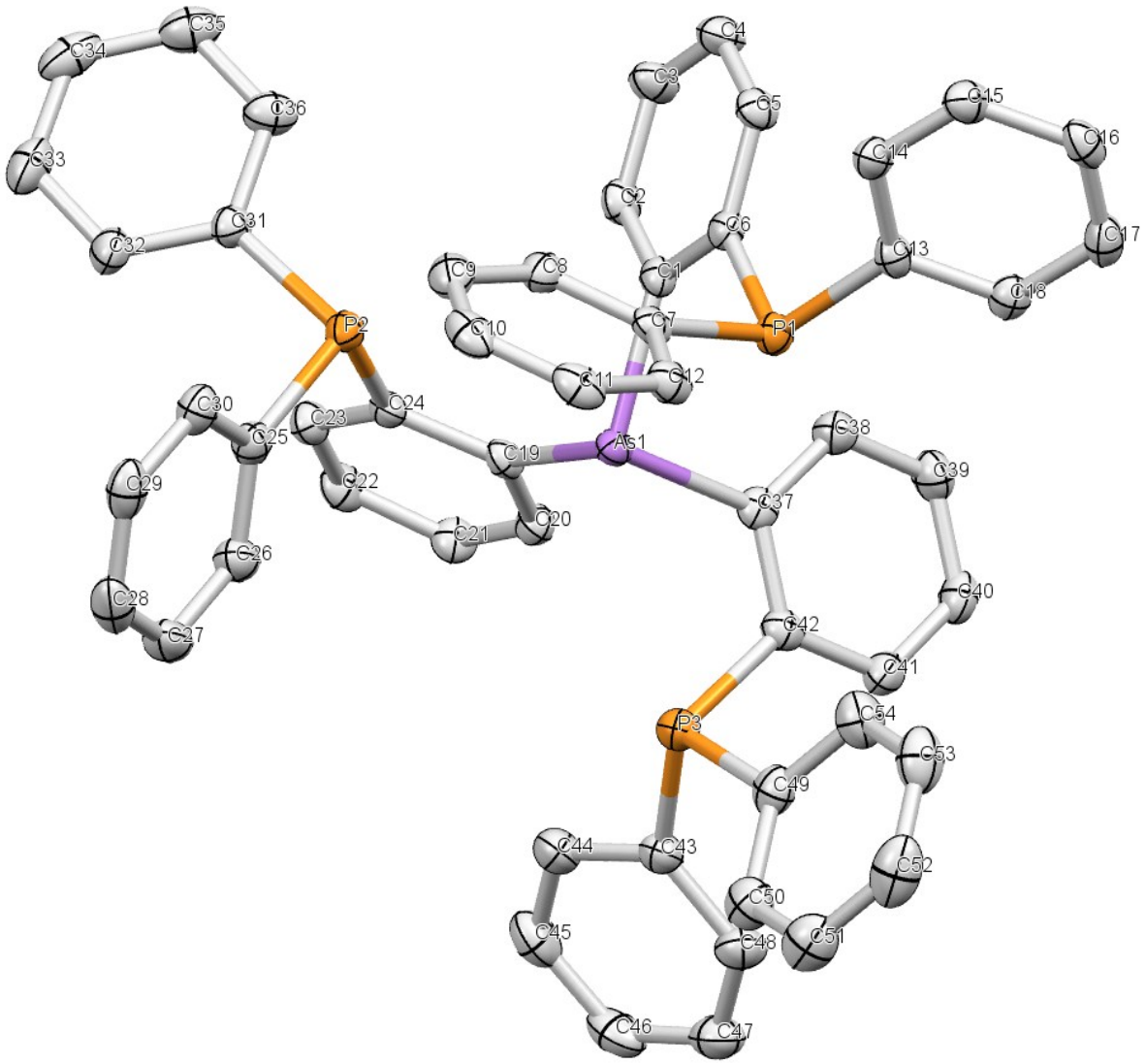


**Figure 1.** ORTEP view of 2 showing the two independent molecules. Solvent molecules and hydrogen atoms are omitted for clarity. Ellipsoids are drawn at the 50% probability level.

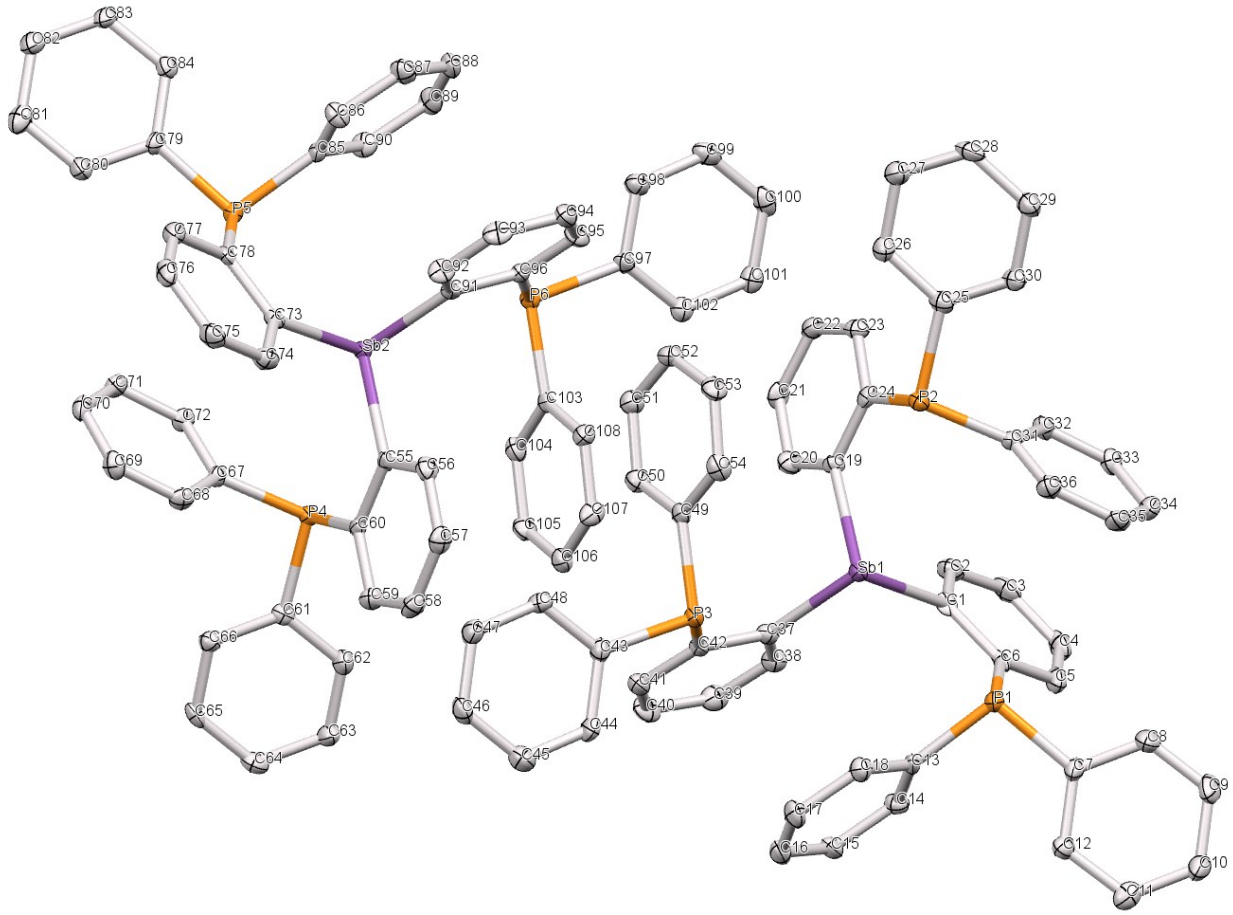


**Figure 2.** ORTEP view of 3 showing the two independent molecules. Solvent molecules and hydrogen atoms are omitted for clarity. Ellipsoids are drawn at the 50% probability level.

| Table 2. Bond lengths [Å] and angles [°] for 2 | |
|---|---|
| **Bond lengths** | |
| As(1)-C(1) | 1.964(3) |
| As(1)-C(37) | 1.972(3) |
| As(1)-C(19) | 1.982(3) |
| P(1)-C(7) | 1.822(3) |
| P(1)-C(13) | 1.833(3) |
| P(1)-C(6) | 1.843(3) |
| P(2)-C(25) | 1.831(3) |
| P(2)-C(24) | 1.834(3) |
| P(2)-C(31) | 1.843(3) |
| P(3)-C(49) | 1.818(3) |
| P(3)-C(43) | 1.821(4) |
| P(3)-C(42) | 1.844(3) |
| C(1)-C(2) | 1.394(4) |
| C(1)-C(6) | 1.409(4) |
| C(2)-C(3) | 1.385(4) |
| C(2)-H(2) | 0.9500 |
| C(3)-C(4) | 1.379(5) |
| C(3)-H(3) | 0.9500 |
| C(4)-C(5) | 1.382(4) |
| C(4)-H(4) | 0.9500 |
| C(5)-C(6) | 1.392(4) |
| C(5)-H(5) | 0.9500 |
| C(7)-C(8) | 1.387(4) |
| C(7)-C(12) | 1.398(4) |
| C(8)-C(9) | 1.392(5) |
| C(8)-H(8) | 0.9500 |
| C(9)-C(10) | 1.387(5) |
| C(9)-H(9) | 0.9500 |
| C(10)-C(11) | 1.371(5) |
| C(10)-H(10) | 0.9500 |
| C(11)-C(12) | 1.374(5) |
| C(11)-H(11) | 0.9500 |
| C(12)-H(12) | 0.9500 |
| C(13)-C(14) | 1.386(5) |
| C(13)-C(18) | 1.390(4) |
| C(14)-C(15) | 1.392(4) |
| C(14)-H(14) | 0.9500 |
| C(15)-C(16) | 1.396(5) |
| C(15)-H(15) | 0.9500 |
| C(16)-C(17) | 1.345(5) |
| C(16)-H(16) | 0.9500 |
| C(17)-C(18) | 1.401(4) |
| C(17)-H(17) | 0.9500 |
| C(18)-H(18) | 0.9500 |
| C(19)-C(20) | 1.383(4) |
| C(19)-C(24) | 1.410(4) |
| C(20)-C(21) | 1.395(4) |
| C(20)-H(20) | 0.9500 |
| C(21)-C(22) | 1.378(5) |
| C(21)-H(21) | 0.9500 |
| C(22)-C(23) | 1.375(5) |
| C(22)-H(22) | 0.9500 |
| C(23)-C(24) | 1.394(4) |
| C(23)-H(23) | 0.9500 |
| C(25)-C(26) | 1.383(5) |
| C(25)-C(30) | 1.399(5) |
| C(26)-C(27) | 1.397(5) |
| C(26)-H(26) | 0.9500 |
| C(27)-C(28) | 1.381(5) |
| C(27)-H(27) | 0.9500 |
| C(28)-C(29) | 1.373(5) |
| C(28)-H(28) | 0.9500 |
| C(29)-C(30) | 1.387(5) |
| C(29)-H(29) | 0.9500 |
| C(30)-H(30) | 0.9500 |
| C(31)-C(32) | 1.388(4) |
| C(31)-C(36) | 1.392(4) |
| C(32)-C(33) | 1.389(5) |
| C(32)-H(32) | 0.9500 |
| C(33)-C(34) | 1.365(5) |
| C(33)-H(33) | 0.9500 |
| C(34)-C(35) | 1.378(5) |
| C(34)-H(34) | 0.9500 |
| C(35)-C(36) | 1.383(5) |
| C(35)-H(35) | 0.9500 |
| C(36)-H(36) | 0.9500 |
| C(37)-C(42) | 1.391(4) |
| C(37)-C(38) | 1.407(4) |
| C(38)-C(39) | 1.366(5) |
| C(38)-H(38) | 0.9500 |
| C(39)-C(40) | 1.384(5) |
| C(39)-H(39) | 0.9500 |
| C(40)-C(41) | 1.377(5) |
| C(40)-H(40) | 0.9500 |
| C(41)-C(42) | 1.394(4) |
| C(41)-H(41) | 0.9500 |
| C(43)-C(48) | 1.398(5) |
| C(43)-C(44) | 1.410(5) |
| C(44)-C(45) | 1.377(5) |
| C(44)-H(44) | 0.9500 |
| C(45)-C(46) | 1.388(6) |
| C(45)-H(45) | 0.9500 |
| C(46)-C(47) | 1.380(5) |
| C(46)-H(46) | 0.9500 |
| C(47)-C(48) | 1.369(5) |
| C(47)-H(47) | 0.9500 |
| C(48)-H(48) | 0.9500 |
| C(49)-C(54) | 1.396(5) |
| C(49)-C(50) | 1.410(5) |
| C(50)-C(51) | 1.376(5) |
| C(50)-H(50) | 0.9500 |
| C(51)-C(52) | 1.385(6) |
| C(51)-H(51) | 0.9500 |
| C(52)-C(53) | 1.372(6) |
| C(52)-H(52) | 0.9500 |
| C(53)-C(54) | 1.387(5) |
| C(53)-H(53) | 0.9500 |
| C(54)-H(54) | 0.9500 |
| **Angles** | |
| C(1)-As(1)-C(37) | 96.04(12) |
| C(1)-As(1)-C(19) | 100.33(12) |
| C(37)-As(1)-C(19) | 96.90(12) |
| C(7)-P(1)-C(13) | 101.61(14) |
| C(7)-P(1)-C(6) | 103.11(14) |
| C(13)-P(1)-C(6) | 104.80(14) |
| C(25)-P(2)-C(24) | 102.08(15) |
| C(25)-P(2)-C(31) | 101.74(14) |
| C(24)-P(2)-C(31) | 101.23(14) |
| C(49)-P(3)-C(43) | 103.84(16) |
| C(49)-P(3)-C(42) | 101.34(15) |
| C(43)-P(3)-C(42) | 102.22(15) |
| C(2)-C(1)-C(6) | 119.3(3) |
| C(2)-C(1)-As(1) | 123.2(2) |
| C(6)-C(1)-As(1) | 117.5(2) |
| C(3)-C(2)-C(1) | 120.9(3) |
| C(3)-C(2)-H(2) | 119.6 |
| C(1)-C(2)-H(2) | 119.6 |
| C(4)-C(3)-C(2) | 120.0(3) |
| C(4)-C(3)-H(3) | 120.0 |
| C(2)-C(3)-H(3) | 120.0 |
| C(3)-C(4)-C(5) | 119.7(3) |
| C(3)-C(4)-H(4) | 120.2 |
| C(5)-C(4)-H(4) | 120.2 |
| C(4)-C(5)-C(6) | 121.7(3) |
| C(4)-C(5)-H(5) | 119.2 |
| C(6)-C(5)-H(5) | 119.2 |
| C(5)-C(6)-C(1) | 118.5(3) |
| C(5)-C(6)-P(1) | 124.2(2) |
| C(1)-C(6)-P(1) | 117.3(2) |
| C(8)-C(7)-C(12) | 118.8(3) |
| C(8)-C(7)-P(1) | 124.0(2) |
| C(12)-C(7)-P(1) | 117.1(2) |
| C(7)-C(8)-C(9) | 120.3(3) |
| C(7)-C(8)-H(8) | 119.8 |
| C(9)-C(8)-H(8) | 119.8 |
| C(10)-C(9)-C(8) | 119.7(3) |
| C(10)-C(9)-H(9) | 120.1 |
| C(8)-C(9)-H(9) | 120.1 |
| C(11)-C(10)-C(9) | 120.2(3) |
| C(11)-C(10)-H(10) | 119.9 |
| C(9)-C(10)-H(10) | 119.9 |
| C(10)-C(11)-C(12) | 120.4(3) |
| C(10)-C(11)-H(11) | 119.8 |
| C(12)-C(11)-H(11) | 119.8 |
| C(11)-C(12)-C(7) | 120.7(3) |
| C(11)-C(12)-H(12) | 119.7 |
| C(7)-C(12)-H(12) | 119.7 |
| C(14)-C(13)-C(18) | 118.6(3) |
| C(14)-C(13)-P(1) | 123.0(2) |
| C(18)-C(13)-P(1) | 118.4(2) |
| C(13)-C(14)-C(15) | 120.7(3) |
| C(13)-C(14)-H(14) | 119.7 |
| C(15)-C(14)-H(14) | 119.7 |
| C(14)-C(15)-C(16) | 119.6(3) |
| C(14)-C(15)-H(15) | 120.2 |
| C(16)-C(15)-H(15) | 120.2 |
| C(17)-C(16)-C(15) | 120.1(3) |
| C(17)-C(16)-H(16) | 119.9 |
| C(15)-C(16)-H(16) | 119.9 |
| C(16)-C(17)-C(18) | 120.7(3) |
| C(16)-C(17)-H(17) | 119.6 |
| C(18)-C(17)-H(17) | 119.6 |
| C(13)-C(18)-C(17) | 120.3(3) |
| C(13)-C(18)-H(18) | 119.9 |
| C(17)-C(18)-H(18) | 119.9 |
| C(20)-C(19)-C(24) | 118.5(3) |
| C(20)-C(19)-As(1) | 120.9(2) |
| C(24)-C(19)-As(1) | 120.3(2) |
| C(19)-C(20)-C(21) | 121.0(3) |
| C(19)-C(20)-H(20) | 119.5 |
| C(21)-C(20)-H(20) | 119.5 |
| C(22)-C(21)-C(20) | 120.1(3) |
| C(22)-C(21)-H(21) | 119.9 |
| C(20)-C(21)-H(21) | 119.9 |
| C(23)-C(22)-C(21) | 119.7(3) |
| C(23)-C(22)-H(22) | 120.2 |
| C(21)-C(22)-H(22) | 120.2 |
| C(22)-C(23)-C(24) | 121.0(3) |
| C(22)-C(23)-H(23) | 119.5 |
| C(24)-C(23)-H(23) | 119.5 |
| C(23)-C(24)-C(19) | 119.7(3) |
| C(23)-C(24)-P(2) | 122.0(2) |
| C(19)-C(24)-P(2) | 118.4(2) |
| C(26)-C(25)-C(30) | 118.0(3) |
| C(26)-C(25)-P(2) | 124.8(3) |

| | |
|---|---|
| C(30)-C(25)-P(2) | 117.1(3) |
| C(25)-C(26)-C(27) | 120.9(3) |
| C(25)-C(26)-H(26) | 119.5 |
| C(27)-C(26)-H(26) | 119.5 |
| C(28)-C(27)-C(26) | 119.9(3) |
| C(28)-C(27)-H(27) | 120.0 |
| C(26)-C(27)-H(27) | 120.0 |
| C(29)-C(28)-C(27) | 119.9(3) |
| C(29)-C(28)-H(28) | 120.0 |
| C(27)-C(28)-H(28) | 120.0 |
| C(28)-C(29)-C(30) | 120.2(4) |
| C(28)-C(29)-H(29) | 119.9 |
| C(30)-C(29)-H(29) | 119.9 |
| C(29)-C(30)-C(25) | 121.0(3) |
| C(29)-C(30)-H(30) | 119.5 |
| C(25)-C(30)-H(30) | 119.5 |
| C(32)-C(31)-C(36) | 118.2(3) |
| C(32)-C(31)-P(2) | 124.2(2) |
| C(36)-C(31)-P(2) | 117.5(2) |
| C(31)-C(32)-C(33) | 120.7(3) |
| C(31)-C(32)-H(32) | 119.7 |
| C(33)-C(32)-H(32) | 119.7 |
| C(34)-C(33)-C(32) | 120.1(3) |
| C(34)-C(33)-H(33) | 120.0 |
| C(32)-C(33)-H(33) | 120.0 |
| C(33)-C(34)-C(35) | 120.3(3) |
| C(33)-C(34)-H(34) | 119.8 |
| C(35)-C(34)-H(34) | 119.8 |
| C(34)-C(35)-C(36) | 119.8(4) |
| C(34)-C(35)-H(35) | 120.1 |
| C(36)-C(35)-H(35) | 120.1 |
| C(35)-C(36)-C(31) | 120.8(3) |
| C(35)-C(36)-H(36) | 119.6 |
| C(31)-C(36)-H(36) | 119.6 |
| C(42)-C(37)-C(38) | 118.4(3) |
| C(42)-C(37)-As(1) | 119.3(2) |
| C(38)-C(37)-As(1) | 122.2(2) |
| C(39)-C(38)-C(37) | 121.7(3) |
| C(39)-C(38)-H(38) | 119.2 |
| C(37)-C(38)-H(38) | 119.2 |
| C(38)-C(39)-C(40) | 119.4(3) |
| C(38)-C(39)-H(39) | 120.3 |
| C(40)-C(39)-H(39) | 120.3 |
| C(41)-C(40)-C(39) | 120.1(3) |
| C(41)-C(40)-H(40) | 120.0 |
| C(39)-C(40)-H(40) | 120.0 |
| C(40)-C(41)-C(42) | 121.0(3) |
| C(40)-C(41)-H(41) | 119.5 |
| C(42)-C(41)-H(41) | 119.5 |
| C(37)-C(42)-C(41) | 119.4(3) |
| C(37)-C(42)-P(3) | 118.3(2) |
| C(41)-C(42)-P(3) | 122.3(2) |
| C(48)-C(43)-C(44) | 118.3(3) |
| C(48)-C(43)-P(3) | 125.9(3) |
| C(44)-C(43)-P(3) | 115.8(3) |
| C(45)-C(44)-C(43) | 120.9(3) |
| C(45)-C(44)-H(44) | 119.6 |
| C(43)-C(44)-H(44) | 119.6 |
| C(44)-C(45)-C(46) | 119.4(4) |
| C(44)-C(45)-H(45) | 120.3 |
| C(46)-C(45)-H(45) | 120.3 |
| C(47)-C(46)-C(45) | 120.3(4) |
| C(47)-C(46)-H(46) | 119.9 |
| C(45)-C(46)-H(46) | 119.9 |
| C(48)-C(47)-C(46) | 120.7(4) |
| C(48)-C(47)-H(47) | 119.7 |
| C(46)-C(47)-H(47) | 119.7 |
| C(47)-C(48)-C(43) | 120.4(3) |
| C(47)-C(48)-H(48) | 119.8 |
| C(43)-C(48)-H(48) | 119.8 |
| C(54)-C(49)-C(50) | 117.4(3) |
| C(54)-C(49)-P(3) | 121.2(3) |
| C(50)-C(49)-P(3) | 120.5(3) |
| C(51)-C(50)-C(49) | 120.8(4) |
| C(51)-C(50)-H(50) | 119.6 |
| C(49)-C(50)-H(50) | 119.6 |
| C(50)-C(51)-C(52) | 120.7(4) |
| C(50)-C(51)-H(51) | 119.7 |
| C(52)-C(51)-H(51) | 119.7 |
| C(53)-C(52)-C(51) | 119.5(4) |
| C(53)-C(52)-H(52) | 120.3 |
| C(51)-C(52)-H(52) | 120.3 |
| C(52)-C(53)-C(54) | 120.5(4) |
| C(52)-C(53)-H(53) | 119.7 |
| C(54)-C(53)-H(53) | 119.7 |
| C(53)-C(54)-C(49) | 121.1(4) |
| C(53)-C(54)-H(54) | 119.5 |
| C(49)-C(54)-H(54) | 119.5 |

| Table 3. Bond lengths [Å] and angles [°] for 3•1.5$CHCl_3$ | |
|---|---|
| **Bond lengths** | |
| Sb(1)-C(37) | 2.157(6) |
| Sb(1)-C(19) | 2.165(6) |
| Sb(1)-C(1) | 2.189(6) |
| Sb(2)-C(91) | 2.154(6) |
| Sb(2)-C(55) | 2.160(6) |
| Sb(2)-C(73) | 2.180(6) |
| Cl(1)-C(109) | 1.761(7) |
| Cl(2)-C(109) | 1.759(8) |
| Cl(3)-C(109) | 1.760(8) |
| Cl(4)-C(110) | 1.743(7) |
| Cl(5)-C(110) | 1.747(6) |
| Cl(6)-C(110) | 1.746(7) |
| P(1)-C(13) | 1.822(6) |
| P(1)-C(7) | 1.831(6) |
| P(1)-C(6) | 1.849(7) |
| P(2)-C(25) | 1.821(7) |
| P(2)-C(31) | 1.836(6) |
| P(2)-C(24) | 1.839(7) |
| P(3)-C(43) | 1.821(6) |
| P(3)-C(49) | 1.830(6) |
| P(3)-C(42) | 1.860(7) |
| P(4)-C(61) | 1.833(6) |
| P(4)-C(60) | 1.836(6) |
| P(4)-C(67) | 1.841(6) |
| P(5)-C(85) | 1.824(6) |
| P(5)-C(79) | 1.826(6) |
| P(5)-C(78) | 1.840(7) |
| P(6)-C(97) | 1.821(6) |
| P(6)-C(103) | 1.829(6) |
| P(6)-C(96) | 1.854(6) |
| C(1)-C(2) | 1.388(9) |
| C(1)-C(6) | 1.409(9) |
| C(2)-C(3) | 1.395(10) |
| C(2)-H(2) | 0.9300 |
| C(3)-C(4) | 1.383(11) |
| C(3)-H(3) | 0.9300 |
| C(4)-C(5) | 1.378(11) |
| C(4)-H(4) | 0.9300 |
| C(5)-C(6) | 1.402(9) |
| C(5)-H(5) | 0.9300 |
| C(7)-C(8) | 1.389(9) |
| C(7)-C(12) | 1.397(9) |
| C(8)-C(9) | 1.367(10) |
| C(8)-H(8) | 0.9300 |
| C(9)-C(10) | 1.395(11) |
| C(9)-H(9) | 0.9300 |
| C(10)-C(11) | 1.367(10) |
| C(10)-H(10) | 0.9300 |
| C(11)-C(12) | 1.392(9) |
| C(11)-H(11) | 0.9300 |
| C(12)-H(12) | 0.9300 |
| C(13)-C(14) | 1.380(9) |
| C(13)-C(18) | 1.402(9) |
| C(14)-C(15) | 1.386(9) |
| C(14)-H(14) | 0.9300 |
| C(15)-C(16) | 1.391(10) |
| C(15)-H(15) | 0.9300 |
| C(16)-C(17) | 1.380(10) |
| C(16)-H(16) | 0.9300 |
| C(17)-C(18) | 1.393(9) |
| C(17)-H(17) | 0.9300 |
| C(18)-H(18) | 0.9300 |
| C(19)-C(20) | 1.377(9) |
| C(19)-C(24) | 1.402(8) |
| C(20)-C(21) | 1.383(9) |
| C(20)-H(20) | 0.9300 |
| C(21)-C(22) | 1.383(9) |
| C(21)-H(21) | 0.9300 |
| C(22)-C(23) | 1.386(10) |
| C(22)-H(22) | 0.9300 |
| C(23)-C(24) | 1.401(9) |
| C(23)-H(23) | 0.9300 |
| C(25)-C(30) | 1.380(9) |
| C(25)-C(26) | 1.381(9) |
| C(26)-C(27) | 1.396(9) |
| C(26)-H(26) | 0.9300 |
| C(27)-C(28) | 1.377(10) |
| C(27)-H(27) | 0.9300 |
| C(28)-C(29) | 1.384(10) |
| C(28)-H(28) | 0.9300 |
| C(29)-C(30) | 1.401(9) |
| C(29)-H(29) | 0.9300 |
| C(30)-H(30) | 0.9300 |
| C(31)-C(36) | 1.377(9) |
| C(31)-C(32) | 1.414(9) |
| C(32)-C(33) | 1.374(9) |
| C(32)-H(32) | 0.9300 |
| C(33)-C(34) | 1.386(9) |
| C(33)-H(33) | 0.9300 |
| C(34)-C(35) | 1.391(10) |
| C(34)-H(34) | 0.9300 |
| C(35)-C(36) | 1.388(10) |
| C(35)-H(35) | 0.9300 |
| C(36)-H(36) | 0.9300 |
| C(37)-C(42) | 1.401(9) |
| C(37)-C(38) | 1.414(10) |
| C(38)-C(39) | 1.384(9) |
| C(38)-H(38) | 0.9300 |
| C(39)-C(40) | 1.385(11) |
| C(39)-H(39) | 0.9300 |
| C(40)-C(41) | 1.371(10) |
| C(40)-H(40) | 0.9300 |
| C(41)-C(42) | 1.402(9) |
| C(41)-H(41) | 0.9300 |
| C(43)-C(44) | 1.394(10) |
| C(43)-C(48) | 1.397(9) |
| C(44)-C(45) | 1.382(10) |
| C(44)-H(44) | 0.9300 |
| C(45)-C(46) | 1.387(10) |
| C(45)-H(45) | 0.9300 |
| C(46)-C(47) | 1.389(10) |
| C(46)-H(46) | 0.9300 |
| C(47)-C(48) | 1.380(9) |
| C(47)-H(47) | 0.9300 |
| C(48)-H(48) | 0.9300 |
| C(49)-C(54) | 1.384(9) |
| C(49)-C(50) | 1.386(9) |
| C(50)-C(51) | 1.374(9) |
| C(50)-H(50) | 0.9300 |
| C(51)-C(52) | 1.393(9) |
| C(51)-H(51) | 0.9300 |
| C(52)-C(53) | 1.383(10) |
| C(52)-H(52) | 0.9300 |
| C(53)-C(54) | 1.383(9) |
| C(53)-H(53) | 0.9300 |
| C(54)-H(54) | 0.9300 |
| C(55)-C(56) | 1.408(9) |
| C(55)-C(60) | 1.410(8) |
| C(56)-C(57) | 1.375(10) |
| C(56)-H(56) | 0.9300 |
| C(57)-C(58) | 1.369(10) |
| C(57)-H(57) | 0.9300 |
| C(58)-C(59) | 1.395(10) |
| C(58)-H(58) | 0.9300 |
| C(59)-C(60) | 1.396(9) |
| C(59)-H(59) | 0.9300 |
| C(61)-C(66) | 1.379(9) |
| C(61)-C(62) | 1.401(9) |
| C(62)-C(63) | 1.376(9) |
| C(62)-H(62) | 0.9300 |
| C(63)-C(64) | 1.382(9) |
| C(63)-H(63) | 0.9300 |
| C(64)-C(65) | 1.390(9) |
| C(64)-H(64) | 0.9300 |
| C(65)-C(66) | 1.389(9) |
| C(65)-H(65) | 0.9300 |
| C(66)-H(66) | 0.9300 |
| C(67)-C(72) | 1.397(8) |
| C(67)-C(68) | 1.398(9) |
| C(68)-C(69) | 1.379(9) |
| C(68)-H(68) | 0.9300 |
| C(69)-C(70) | 1.385(10) |
| C(69)-H(69) | 0.9300 |
| C(70)-C(71) | 1.393(10) |
| C(70)-H(70) | 0.9300 |
| C(71)-C(72) | 1.383(9) |
| C(71)-H(71) | 0.9300 |
| C(72)-H(72) | 0.9300 |
| C(73)-C(74) | 1.398(9) |
| C(73)-C(78) | 1.402(8) |
| C(74)-C(75) | 1.390(10) |
| C(74)-H(74) | 0.9300 |
| C(75)-C(76) | 1.383(10) |
| C(75)-H(75) | 0.9300 |
| C(76)-C(77) | 1.384(11) |
| C(76)-H(76) | 0.9300 |
| C(77)-C(78) | 1.419(9) |
| C(77)-H(77) | 0.9300 |
| C(79)-C(84) | 1.392(9) |
| C(79)-C(80) | 1.406(9) |
| C(80)-C(81) | 1.372(9) |
| C(80)-H(80) | 0.9300 |
| C(81)-C(82) | 1.392(10) |
| C(81)-H(81) | 0.9300 |
| C(82)-C(83) | 1.383(10) |
| C(82)-H(82) | 0.9300 |
| C(83)-C(84) | 1.387(9) |
| C(83)-H(83) | 0.9300 |
| C(84)-H(84) | 0.9300 |
| C(85)-C(90) | 1.394(9) |
| C(85)-C(86) | 1.394(9) |
| C(86)-C(87) | 1.382(9) |
| C(86)-H(86) | 0.9300 |
| C(87)-C(88) | 1.393(10) |
| C(87)-H(87) | 0.9300 |
| C(88)-C(89) | 1.383(11) |
| C(88)-H(88) | 0.9300 |
| C(89)-C(90) | 1.402(10) |
| C(89)-H(89) | 0.9300 |
| C(90)-H(90) | 0.9300 |
| C(91)-C(96) | 1.412(9) |
| C(91)-C(92) | 1.416(9) |
| C(92)-C(93) | 1.370(9) |
| C(92)-H(92) | 0.9300 |
| C(93)-C(94) | 1.384(10) |

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| C(93)-H(93) | 0.9300 |
| C(94)-C(95) | 1.390(10) |
| C(94)-H(94) | 0.9300 |
| C(95)-C(96) | 1.395(8) |
| C(95)-H(95) | 0.9300 |
| C(97)-C(98) | 1.396(9) |
| C(97)-C(102) | 1.395(9) |
| C(98)-C(99) | 1.380(10) |
| C(98)-H(98) | 0.9300 |
| C(99)-C(100) | 1.394(10) |
| C(99)-H(99) | 0.9300 |
| C(100)-C(101) | 1.386(10) |
| C(100)-H(100) | 0.9300 |
| C(101)-C(102) | 1.388(9) |
| C(101)-H(101) | 0.9300 |
| C(102)-H(102) | 0.9300 |
| C(103)-C(104) | 1.401(9) |
| C(103)-C(108) | 1.401(9) |
| C(104)-C(105) | 1.394(9) |
| C(104)-H(104) | 0.9300 |
| C(105)-C(106) | 1.372(10) |
| C(105)-H(105) | 0.9300 |
| C(106)-C(107) | 1.401(9) |
| C(106)-H(106) | 0.9300 |
| C(107)-C(108) | 1.377(9) |
| C(107)-H(107) | 0.9300 |
| C(108)-H(108) | 0.9300 |
| C(109)-H(109) | 0.9800 |
| C(110)-H(110) | 0.9800 |
| C(111)-C(112) | 0.89(2) |
| C(111)-Cl(11) | 0.982(16) |
| C(111)-Cl(7) | 1.723(10) |
| C(111)-Cl(8) | 1.740(11) |
| C(111)-Cl(9) | 1.743(11) |
| C(111)-Cl(10) | 1.94(2) |
| C(111)-H(111) | 0.9800 |
| Cl(7)-C(112) | 1.54(3) |
| Cl(7)-Cl(11) | 2.094(15) |
| Cl(8)-Cl(11) | 1.604(15) |
| Cl(8)-Cl(12) | 1.827(10) |
| Cl(8)-C(112) | 1.88(2) |
| Cl(9)-C(112) | 1.68(3) |
| C(112)-Cl(12) | 1.737(14) |
| C(112)-Cl(10) | 1.739(14) |
| C(112)-Cl(11) | 1.742(14) |
| C(112)-H(112) | 0.9800 |
| **Angles** | |
| C(37)-Sb(1)-C(19) | 95.1(2) |
| C(37)-Sb(1)-C(1) | 95.7(2) |
| C(19)-Sb(1)-C(1) | 93.5(2) |
| C(91)-Sb(2)-C(55) | 95.8(2) |
| C(91)-Sb(2)-C(73) | 93.4(2) |
| C(55)-Sb(2)-C(73) | 95.5(2) |
| C(13)-P(1)-C(7) | 102.6(3) |
| C(13)-P(1)-C(6) | 100.2(3) |
| C(7)-P(1)-C(6) | 101.8(3) |
| C(25)-P(2)-C(31) | 102.9(3) |
| C(25)-P(2)-C(24) | 103.9(3) |
| C(31)-P(2)-C(24) | 101.4(3) |
| C(43)-P(3)-C(49) | 103.4(3) |
| C(43)-P(3)-C(42) | 103.1(3) |
| C(49)-P(3)-C(42) | 101.1(3) |
| C(61)-P(4)-C(60) | 102.8(3) |
| C(61)-P(4)-C(67) | 103.0(3) |
| C(60)-P(4)-C(67) | 99.8(3) |
| C(85)-P(5)-C(79) | 102.3(3) |
| C(85)-P(5)-C(78) | 102.4(3) |
| C(79)-P(5)-C(78) | 102.9(3) |
| C(97)-P(6)-C(103) | 102.7(3) |
| C(97)-P(6)-C(96) | 103.4(3) |
| C(103)-P(6)-C(96) | 100.7(3) |
| C(2)-C(1)-C(6) | 119.1(6) |
| C(2)-C(1)-Sb(1) | 121.5(5) |
| C(6)-C(1)-Sb(1) | 119.5(4) |
| C(1)-C(2)-C(3) | 122.0(7) |
| C(1)-C(2)-H(2) | 119.0 |
| C(3)-C(2)-H(2) | 119.0 |
| C(4)-C(3)-C(2) | 118.8(7) |
| C(4)-C(3)-H(3) | 120.6 |
| C(2)-C(3)-H(3) | 120.6 |
| C(5)-C(4)-C(3) | 120.1(6) |
| C(5)-C(4)-H(4) | 119.9 |
| C(3)-C(4)-H(4) | 119.9 |
| C(4)-C(5)-C(6) | 121.8(7) |
| C(4)-C(5)-H(5) | 119.1 |
| C(6)-C(5)-H(5) | 119.1 |
| C(5)-C(6)-C(1) | 118.2(6) |
| C(5)-C(6)-P(1) | 124.4(5) |
| C(1)-C(6)-P(1) | 117.4(4) |
| C(8)-C(7)-C(12) | 118.8(6) |
| C(8)-C(7)-P(1) | 118.8(5) |
| C(12)-C(7)-P(1) | 122.3(5) |
| C(9)-C(8)-C(7) | 121.2(7) |
| C(9)-C(8)-H(8) | 119.4 |
| C(7)-C(8)-H(8) | 119.4 |
| C(8)-C(9)-C(10) | 120.1(7) |
| C(8)-C(9)-H(9) | 120.0 |
| C(10)-C(9)-H(9) | 120.0 |
| C(11)-C(10)-C(9) | 119.3(7) |
| C(11)-C(10)-H(10) | 120.3 |
| C(9)-C(10)-H(10) | 120.3 |
| C(10)-C(11)-C(12) | 121.2(7) |
| C(10)-C(11)-H(11) | 119.4 |
| C(12)-C(11)-H(11) | 119.4 |
| C(11)-C(12)-C(7) | 119.3(6) |
| C(11)-C(12)-H(12) | 120.3 |
| C(7)-C(12)-H(12) | 120.3 |
| C(14)-C(13)-C(18) | 119.0(6) |
| C(14)-C(13)-P(1) | 123.3(5) |
| C(18)-C(13)-P(1) | 117.7(5) |
| C(13)-C(14)-C(15) | 121.2(6) |
| C(13)-C(14)-H(14) | 119.4 |
| C(15)-C(14)-H(14) | 119.4 |
| C(14)-C(15)-C(16) | 119.4(6) |
| C(14)-C(15)-H(15) | 120.3 |
| C(16)-C(15)-H(15) | 120.3 |
| C(17)-C(16)-C(15) | 120.4(6) |
| C(17)-C(16)-H(16) | 119.8 |
| C(15)-C(16)-H(16) | 119.8 |
| C(16)-C(17)-C(18) | 119.8(6) |
| C(16)-C(17)-H(17) | 120.1 |
| C(18)-C(17)-H(17) | 120.1 |
| C(17)-C(18)-C(13) | 120.1(6) |
| C(17)-C(18)-H(18) | 119.9 |
| C(13)-C(18)-H(18) | 119.9 |
| C(20)-C(19)-C(24) | 119.1(6) |
| C(20)-C(19)-Sb(1) | 120.8(5) |
| C(24)-C(19)-Sb(1) | 120.0(4) |
| C(19)-C(20)-C(21) | 121.4(6) |
| C(19)-C(20)-H(20) | 119.3 |
| C(21)-C(20)-H(20) | 119.3 |
| C(22)-C(21)-C(20) | 120.2(6) |
| C(22)-C(21)-H(21) | 119.9 |
| C(20)-C(21)-H(21) | 119.9 |
| C(21)-C(22)-C(23) | 119.2(6) |
| C(21)-C(22)-H(22) | 120.4 |
| C(23)-C(22)-H(22) | 120.4 |
| C(22)-C(23)-C(24) | 121.0(6) |
| C(22)-C(23)-H(23) | 119.5 |
| C(24)-C(23)-H(23) | 119.5 |
| C(23)-C(24)-C(19) | 119.1(6) |
| C(23)-C(24)-P(2) | 123.5(5) |
| C(19)-C(24)-P(2) | 117.3(5) |
| C(30)-C(25)-C(26) | 118.1(6) |
| C(30)-C(25)-P(2) | 121.6(5) |
| C(26)-C(25)-P(2) | 120.0(5) |
| C(25)-C(26)-C(27) | 122.1(6) |
| C(25)-C(26)-H(26) | 119.0 |
| C(27)-C(26)-H(26) | 119.0 |
| C(28)-C(27)-C(26) | 119.3(6) |
| C(28)-C(27)-H(27) | 120.4 |
| C(26)-C(27)-H(27) | 120.4 |
| C(27)-C(28)-C(29) | 119.6(6) |
| C(27)-C(28)-H(28) | 120.2 |
| C(29)-C(28)-H(28) | 120.2 |
| C(28)-C(29)-C(30) | 120.4(6) |
| C(28)-C(29)-H(29) | 119.8 |
| C(30)-C(29)-H(29) | 119.8 |
| C(25)-C(30)-C(29) | 120.6(6) |
| C(25)-C(30)-H(30) | 119.7 |
| C(29)-C(30)-H(30) | 119.7 |
| C(36)-C(31)-C(32) | 118.6(6) |
| C(36)-C(31)-P(2) | 117.2(5) |
| C(32)-C(31)-P(2) | 124.1(5) |
| C(33)-C(32)-C(31) | 120.8(6) |
| C(33)-C(32)-H(32) | 119.6 |
| C(31)-C(32)-H(32) | 119.6 |
| C(32)-C(33)-C(34) | 119.9(6) |
| C(32)-C(33)-H(33) | 120.1 |
| C(34)-C(33)-H(33) | 120.1 |
| C(33)-C(34)-C(35) | 119.8(6) |
| C(33)-C(34)-H(34) | 120.1 |
| C(35)-C(34)-H(34) | 120.1 |
| C(36)-C(35)-C(34) | 120.1(6) |
| C(36)-C(35)-H(35) | 119.9 |
| C(34)-C(35)-H(35) | 119.9 |
| C(31)-C(36)-C(35) | 120.7(6) |
| C(31)-C(36)-H(36) | 119.6 |
| C(35)-C(36)-H(36) | 119.6 |
| C(42)-C(37)-C(38) | 119.3(6) |
| C(42)-C(37)-Sb(1) | 119.3(5) |
| C(38)-C(37)-Sb(1) | 121.4(5) |
| C(39)-C(38)-C(37) | 120.8(6) |
| C(39)-C(38)-H(38) | 119.6 |
| C(37)-C(38)-H(38) | 119.6 |
| C(40)-C(39)-C(38) | 119.0(7) |
| C(40)-C(39)-H(39) | 120.5 |
| C(38)-C(39)-H(39) | 120.5 |
| C(41)-C(40)-C(39) | 121.4(6) |
| C(41)-C(40)-H(40) | 119.3 |
| C(39)-C(40)-H(40) | 119.3 |
| C(40)-C(41)-C(42) | 120.7(6) |
| C(40)-C(41)-H(41) | 119.7 |
| C(42)-C(41)-H(41) | 119.7 |
| C(37)-C(42)-C(41) | 118.9(7) |
| C(37)-C(42)-P(3) | 118.2(5) |
| C(41)-C(42)-P(3) | 122.9(5) |
| C(44)-C(43)-C(48) | 117.5(6) |

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| C(44)-C(43)-P(3) | 117.4(5) |
| C(48)-C(43)-P(3) | 124.6(5) |
| C(45)-C(44)-C(43) | 121.1(6) |
| C(45)-C(44)-H(44) | 119.4 |
| C(43)-C(44)-H(44) | 119.4 |
| C(44)-C(45)-C(46) | 120.7(7) |
| C(44)-C(45)-H(45) | 119.6 |
| C(46)-C(45)-H(45) | 119.6 |
| C(45)-C(46)-C(47) | 118.7(6) |
| C(45)-C(46)-H(46) | 120.6 |
| C(47)-C(46)-H(46) | 120.6 |
| C(48)-C(47)-C(46) | 120.4(6) |
| C(48)-C(47)-H(47) | 119.8 |
| C(46)-C(47)-H(47) | 119.8 |
| C(47)-C(48)-C(43) | 121.4(6) |
| C(47)-C(48)-H(48) | 119.3 |
| C(43)-C(48)-H(48) | 119.3 |
| C(54)-C(49)-C(50) | 119.0(6) |
| C(54)-C(49)-P(3) | 117.5(5) |
| C(50)-C(49)-P(3) | 123.4(5) |
| C(51)-C(50)-C(49) | 120.9(6) |
| C(51)-C(50)-H(50) | 119.6 |
| C(49)-C(50)-H(50) | 119.6 |
| C(50)-C(51)-C(52) | 119.8(7) |
| C(50)-C(51)-H(51) | 120.1 |
| C(52)-C(51)-H(51) | 120.1 |
| C(53)-C(52)-C(51) | 119.8(6) |
| C(53)-C(52)-H(52) | 120.1 |
| C(51)-C(52)-H(52) | 120.1 |
| C(52)-C(53)-C(54) | 119.8(6) |
| C(52)-C(53)-H(53) | 120.1 |
| C(54)-C(53)-H(53) | 120.1 |
| C(53)-C(54)-C(49) | 120.7(6) |
| C(53)-C(54)-H(54) | 119.6 |
| C(49)-C(54)-H(54) | 119.6 |
| C(56)-C(55)-C(60) | 118.8(5) |
| C(56)-C(55)-Sb(2) | 121.5(5) |
| C(60)-C(55)-Sb(2) | 119.7(4) |
| C(57)-C(56)-C(55) | 120.3(6) |
| C(57)-C(56)-H(56) | 119.8 |
| C(55)-C(56)-H(56) | 119.8 |
| C(58)-C(57)-C(56) | 121.5(6) |
| C(58)-C(57)-H(57) | 119.3 |
| C(56)-C(57)-H(57) | 119.3 |
| C(57)-C(58)-C(59) | 119.3(6) |
| C(57)-C(58)-H(58) | 120.4 |
| C(59)-C(58)-H(58) | 120.4 |
| C(58)-C(59)-C(60) | 120.9(6) |
| C(58)-C(59)-H(59) | 119.5 |
| C(60)-C(59)-H(59) | 119.5 |
| C(59)-C(60)-C(55) | 119.2(6) |
| C(59)-C(60)-P(4) | 123.1(5) |
| C(55)-C(60)-P(4) | 117.6(4) |
| C(66)-C(61)-C(62) | 118.5(6) |
| C(66)-C(61)-P(4) | 124.1(5) |
| C(62)-C(61)-P(4) | 117.2(5) |
| C(63)-C(62)-C(61) | 120.9(6) |
| C(63)-C(62)-H(62) | 119.6 |
| C(61)-C(62)-H(62) | 119.6 |
| C(62)-C(63)-C(64) | 120.6(6) |
| C(62)-C(63)-H(63) | 119.7 |
| C(64)-C(63)-H(63) | 119.7 |
| C(63)-C(64)-C(65) | 118.7(6) |
| C(63)-C(64)-H(64) | 120.6 |
| C(65)-C(64)-H(64) | 120.6 |
| C(66)-C(65)-C(64) | 120.8(6) |
| C(66)-C(65)-H(65) | 119.6 |
| C(64)-C(65)-H(65) | 119.6 |
| C(61)-C(66)-C(65) | 120.4(6) |
| C(61)-C(66)-H(66) | 119.8 |
| C(65)-C(66)-H(66) | 119.8 |
| C(72)-C(67)-C(68) | 119.2(6) |
| C(72)-C(67)-P(4) | 117.1(5) |
| C(68)-C(67)-P(4) | 123.7(5) |
| C(69)-C(68)-C(67) | 120.8(6) |
| C(69)-C(68)-H(68) | 119.6 |
| C(67)-C(68)-H(68) | 119.6 |
| C(68)-C(69)-C(70) | 119.6(6) |
| C(68)-C(69)-H(69) | 120.2 |
| C(70)-C(69)-H(69) | 120.2 |
| C(69)-C(70)-C(71) | 120.4(6) |
| C(69)-C(70)-H(70) | 119.8 |
| C(71)-C(70)-H(70) | 119.8 |
| C(72)-C(71)-C(70) | 119.9(6) |
| C(72)-C(71)-H(71) | 120.0 |
| C(70)-C(71)-H(71) | 120.0 |
| C(71)-C(72)-C(67) | 120.1(6) |
| C(71)-C(72)-H(72) | 120.0 |
| C(67)-C(72)-H(72) | 120.0 |
| C(74)-C(73)-C(78) | 119.3(6) |
| C(74)-C(73)-Sb(2) | 121.3(5) |
| C(78)-C(73)-Sb(2) | 119.4(5) |
| C(75)-C(74)-C(73) | 121.4(6) |
| C(75)-C(74)-H(74) | 119.3 |
| C(73)-C(74)-H(74) | 119.3 |
| C(76)-C(75)-C(74) | 120.1(7) |
| C(76)-C(75)-H(75) | 120.0 |
| C(74)-C(75)-H(75) | 120.0 |
| C(77)-C(76)-C(75) | 119.3(6) |
| C(77)-C(76)-H(76) | 120.3 |
| C(75)-C(76)-H(76) | 120.3 |
| C(76)-C(77)-C(78) | 121.8(6) |
| C(76)-C(77)-H(77) | 119.1 |
| C(78)-C(77)-H(77) | 119.1 |
| C(73)-C(78)-C(77) | 118.2(6) |
| C(73)-C(78)-P(5) | 117.6(5) |
| C(77)-C(78)-P(5) | 124.1(5) |
| C(84)-C(79)-C(80) | 118.5(6) |
| C(84)-C(79)-P(5) | 122.1(5) |
| C(80)-C(79)-P(5) | 119.0(5) |
| C(81)-C(80)-C(79) | 120.7(6) |
| C(81)-C(80)-H(80) | 119.7 |
| C(79)-C(80)-H(80) | 119.7 |
| C(80)-C(81)-C(82) | 120.1(7) |
| C(80)-C(81)-H(81) | 120.0 |
| C(82)-C(81)-H(81) | 120.0 |
| C(83)-C(82)-C(81) | 120.1(7) |
| C(83)-C(82)-H(82) | 120.0 |
| C(81)-C(82)-H(82) | 120.0 |
| C(82)-C(83)-C(84) | 119.8(7) |
| C(82)-C(83)-H(83) | 120.1 |
| C(84)-C(83)-H(83) | 120.1 |
| C(83)-C(84)-C(79) | 120.8(6) |
| C(83)-C(84)-H(84) | 119.6 |
| C(79)-C(84)-H(84) | 119.6 |
| C(90)-C(85)-C(86) | 119.6(6) |
| C(90)-C(85)-P(5) | 117.4(5) |
| C(86)-C(85)-P(5) | 123.0(5) |
| C(87)-C(86)-C(85) | 120.3(6) |
| C(87)-C(86)-H(86) | 119.9 |
| C(85)-C(86)-H(86) | 119.9 |
| C(86)-C(87)-C(88) | 120.2(7) |
| C(86)-C(87)-H(87) | 119.9 |
| C(88)-C(87)-H(87) | 119.9 |
| C(89)-C(88)-C(87) | 120.3(6) |
| C(89)-C(88)-H(88) | 119.9 |
| C(87)-C(88)-H(88) | 119.9 |
| C(88)-C(89)-C(90) | 119.6(6) |
| C(88)-C(89)-H(89) | 120.2 |
| C(90)-C(89)-H(89) | 120.2 |
| C(85)-C(90)-C(89) | 120.1(6) |
| C(85)-C(90)-H(90) | 120.0 |
| C(89)-C(90)-H(90) | 120.0 |
| C(96)-C(91)-C(92) | 118.8(6) |
| C(96)-C(91)-Sb(2) | 120.0(5) |
| C(92)-C(91)-Sb(2) | 121.2(4) |
| C(93)-C(92)-C(91) | 121.4(6) |
| C(93)-C(92)-H(92) | 119.3 |
| C(91)-C(92)-H(92) | 119.3 |
| C(92)-C(93)-C(94) | 119.7(6) |
| C(92)-C(93)-H(93) | 120.1 |
| C(94)-C(93)-H(93) | 120.1 |
| C(93)-C(94)-C(95) | 120.2(6) |
| C(93)-C(94)-H(94) | 119.9 |
| C(95)-C(94)-H(94) | 119.9 |
| C(94)-C(95)-C(96) | 121.3(6) |
| C(94)-C(95)-H(95) | 119.4 |
| C(96)-C(95)-H(95) | 119.4 |
| C(95)-C(96)-C(91) | 118.7(6) |
| C(95)-C(96)-P(6) | 123.6(5) |
| C(91)-C(96)-P(6) | 117.7(5) |
| C(98)-C(97)-C(102) | 117.8(6) |
| C(98)-C(97)-P(6) | 118.7(5) |
| C(102)-C(97)-P(6) | 123.2(5) |
| C(99)-C(98)-C(97) | 121.3(6) |
| C(99)-C(98)-H(98) | 119.4 |
| C(97)-C(98)-H(98) | 119.4 |
| C(98)-C(99)-C(100) | 120.0(6) |
| C(98)-C(99)-H(99) | 120.0 |
| C(100)-C(99)-H(99) | 120.0 |
| C(101)-C(100)-C(99) | 119.7(6) |
| C(101)-C(100)-H(100) | 120.1 |
| C(99)-C(100)-H(100) | 120.1 |
| C(100)-C(101)-C(102) | 119.7(6) |
| C(100)-C(101)-H(101) | 120.2 |
| C(102)-C(101)-H(101) | 120.2 |
| C(101)-C(102)-C(97) | 121.4(6) |
| C(101)-C(102)-H(102) | 119.3 |
| C(97)-C(102)-H(102) | 119.3 |
| C(104)-C(103)-C(108) | 118.9(6) |
| C(104)-C(103)-P(6) | 118.3(5) |
| C(108)-C(103)-P(6) | 122.8(5) |
| C(105)-C(104)-C(103) | 120.0(6) |
| C(105)-C(104)-H(104) | 120.0 |
| C(103)-C(104)-H(104) | 120.0 |
| C(106)-C(105)-C(104) | 120.4(6) |
| C(106)-C(105)-H(105) | 119.8 |
| C(104)-C(105)-H(105) | 119.8 |
| C(105)-C(106)-C(107) | 120.2(6) |
| C(105)-C(106)-H(106) | 119.9 |
| C(107)-C(106)-H(106) | 119.9 |
| C(108)-C(107)-C(106) | 119.8(6) |
| C(108)-C(107)-H(107) | 120.1 |
| C(106)-C(107)-H(107) | 120.1 |
| C(107)-C(108)-C(103) | 120.8(6) |
| C(107)-C(108)-H(108) | 119.6 |
| C(103)-C(108)-H(108) | 119.6 |
| Cl(2)-C(109)-Cl(3) | 109.8(4) |

| | |
|---|---|
| Cl(2)-C(109)-Cl(1) | 109.7(4) |
| Cl(3)-C(109)-Cl(1) | 109.4(4) |
| Cl(2)-C(109)-H(109) | 109.3 |
| Cl(3)-C(109)-H(109) | 109.3 |
| Cl(1)-C(109)-H(109) | 109.3 |
| Cl(4)-C(110)-Cl(6) | 110.5(4) |
| Cl(4)-C(110)-Cl(5) | 110.8(4) |
| Cl(6)-C(110)-Cl(5) | 110.9(4) |
| Cl(4)-C(110)-H(110) | 108.2 |
| Cl(6)-C(110)-H(110) | 108.2 |
| Cl(5)-C(110)-H(110) | 108.2 |
| C(112)-C(111)-Cl(11) | 136(2) |
| C(112)-C(111)-Cl(7) | 63(2) |
| Cl(11)-C(111)-Cl(7) | 97.7(11) |
| C(112)-C(111)-Cl(8) | 84.7(17) |
| Cl(11)-C(111)-Cl(8) | 65.5(11) |
| Cl(7)-C(111)-Cl(8) | 111.6(6) |
| C(112)-C(111)-Cl(9) | 71.3(18) |
| Cl(11)-C(111)-Cl(9) | 147.9(13) |
| Cl(7)-C(111)-Cl(9) | 111.9(7) |
| Cl(8)-C(111)-Cl(9) | 111.6(7) |
| C(112)-C(111)-Cl(10) | 63.9(15) |
| Cl(11)-C(111)-Cl(10) | 156.6(16) |
| Cl(7)-C(111)-Cl(10) | 103.7(14) |
| Cl(8)-C(111)-Cl(10) | 113.8(12) |
| Cl(9)-C(111)-Cl(10) | 8.7(14) |
| C(112)-C(111)-H(111) | 167.4 |
| Cl(11)-C(111)-H(111) | 49.9 |
| Cl(7)-C(111)-H(111) | 107.1 |
| Cl(8)-C(111)-H(111) | 107.1 |
| Cl(9)-C(111)-H(111) | 107.1 |
| Cl(10)-C(111)-H(111) | 113.3 |
| C(112)-Cl(7)-C(111) | 31.1(8) |
| C(112)-Cl(7)-Cl(11) | 54.7(7) |
| C(111)-Cl(7)-Cl(11) | 27.7(5) |
| Cl(11)-Cl(8)-C(111) | 33.8(6) |
| Cl(11)-Cl(8)-Cl(12) | 113.3(6) |
| C(111)-Cl(8)-Cl(12) | 84.0(6) |
| Cl(11)-Cl(8)-C(112) | 59.3(5) |
| C(111)-Cl(8)-C(112) | 28.2(6) |
| Cl(12)-Cl(8)-C(112) | 55.8(4) |
| C(112)-Cl(9)-C(111) | 30.2(6) |
| C(111)-C(112)-Cl(7) | 85.5(19) |
| C(111)-C(112)-Cl(9) | 78.6(19) |
| Cl(7)-C(112)-Cl(9) | 125.6(12) |
| C(111)-C(112)-Cl(12) | 127(2) |
| Cl(7)-C(112)-Cl(12) | 117.5(16) |
| Cl(9)-C(112)-Cl(12) | 113.3(16) |
| C(111)-C(112)-Cl(10) | 89(2) |
| Cl(7)-C(112)-Cl(10) | 122.6(18) |
| Cl(9)-C(112)-Cl(10) | 11.2(14) |
| Cl(12)-C(112)-Cl(10) | 111.0(14) |
| C(111)-C(112)-Cl(11) | 22.9(11) |
| Cl(7)-C(112)-Cl(11) | 78.9(10) |
| Cl(9)-C(112)-Cl(11) | 100.2(14) |
| Cl(12)-C(112)-Cl(11) | 111.1(12) |
| Cl(10)-C(112)-Cl(11) | 110.7(14) |
| C(111)-C(112)-Cl(8) | 67.1(16) |
| Cl(7)-C(112)-Cl(8) | 113.1(11) |
| Cl(9)-C(112)-Cl(8) | 107.6(19) |
| Cl(12)-C(112)-Cl(8) | 60.5(8) |
| Cl(10)-C(112)-Cl(8) | 117(2) |
| Cl(11)-C(112)-Cl(8) | 52.4(8) |
| C(111)-C(112)-H(112) | 111.2 |
| Cl(7)-C(112)-H(112) | 29.2 |
| Cl(9)-C(112)-H(112) | 116.0 |
| Cl(12)-C(112)-H(112) | 108.0 |
| Cl(10)-C(112)-H(112) | 108.0 |
| Cl(11)-C(112)-H(112) | 108.0 |
| Cl(8)-C(112)-H(112) | 135.2 |
| C(112)-Cl(10)-C(111) | 27.5(7) |
| C(111)-Cl(11)-Cl(8) | 80.7(11) |
| C(111)-Cl(11)-C(112) | 20.7(11) |
| Cl(8)-Cl(11)-C(112) | 68.3(9) |
| C(111)-Cl(11)-Cl(7) | 54.6(9) |
| Cl(8)-Cl(11)-Cl(7) | 100.7(6) |
| C(112)-Cl(11)-Cl(7) | 46.4(12) |
| C(112)-Cl(12)-Cl(8) | 63.7(9) |

**Table 4.** Crystal data, data collections, and structure refinements for [**4**][Cl], [**5**][Cl] and [**6**][$BPh_4$]

| | [**4**][Cl]•2$CHCl_3$ | [**5**][Cl]•5$CHCl_3$ | [**6**][$BPh_4$]•1.5$CH_2Cl_2$ |
|---|---|---|---|
| Formula | $C_{56}H_{44}Cl_8NiP_4$ | $C_{59}H_{47}AsCl_{17}NiP_3$ | $C_{159}H_{130}B_2Cl_8Ni_2P_6Sb_2$ |
| Formula Weight | 1183.10 | 1585.14 | 2892.59 |
| Crystal Size (mm) | 0.87 x 0.33 0.09 | 0.20 x 0.17 x 0.05 | 0.16 x 0.12 x 0.09 |
| Crystal System | Monoclinic | Triclinic | Monoclinic |
| Space Group | *P*2(1)/c | *P*-1 | *C*2/c |
| *a* (Å) | 16.6557(13) | 13.651(5) | 49.945(4) Å |
| *b* (Å) | 21.8350(18) | 15.423(5) | 9.6700(9) Å |
| *c* (Å) | 33.334(3) | 16.459(6) | 34.967(3) Å |
| $\alpha$ (°) | 90 | 76.245(4) | 90 |
| $\beta$ (°) | 95.711(4) | 81.548(4) | 129.231(4)°. |
| $\gamma$ (°) | 90 | 87.124(4) | 90 |
| V (Å$^3$) | 12062.5(16) | 3329(2) | 13081(2) |
| Z | 8 | 2 | 4 |
| $\rho_{calc}$ (g/cm$^3$) | 1.303 | 1.581 | 1.469 |
| $\mu$ (mm$^{-1}$) | 0.816 | 1.577 | 0.984 |
| F(000) | 4832 | 1592 | 5912 |
| T (K) | 110(2) | 110(2) | 173(2) |
| *hkl* Range | -20 → 21 | -17 → 17 | -60 → 60 |
| | -27 → 23 | -19 → 19 | -11 → 11 |
| | -42 → 42 | -21 → 21 | -42 → 42 |
| Reflns. collected | 178117 | 38868 | 62666 |
| Unique reflns. [Rint] | 25685 [0.0548] | 15051 [0.0307] | 12176 [0.0744] |
| Reflns. used for refinement | 25685 | 15051 | 12176 |
| Refined parameters | 1243 | 730 | 808 |
| GooF | 1.076 | 1.046 | 1.158 |
| R1[a], *w*R2[b] (all data) | 0.0743, 0.1414 | 0.0638, 0.1378 | 0.0848, 0.1353 |
| $\rho_{fin}$ (max., min.) (eA$^{-3}$) | 2.141, -1.558 | 2.700, -1.720 | 1.688. -1.890 |

[a]R1 = $\sum||F_o| - |F_c||/\sum|F_o|$. [b] *w*R2 $([w(F_o^2 - F_c^2)^2]/[\sum w(F_o^2)^2])^{1/2}$; $w = 1/[\sigma^2(F_o^2) + (ap)^2 + bp]$; $p = (F_o^2 + 2F_c^2)/3$ with $a = 0.0694$ for [**4**][Cl], 0.0621 for [**5**][Cl], 0.0147 for [**6**][$BPh_4$]; and $b =$ 22.8733 for [**4**][Cl], 10.4687 for [**5**][Cl], 200.2 for [**6**][$BPh_4$].

| Table 5. Bond lengths [Å] and angles [°] for [4][Cl]•2CHCl$_3$ | |
|---|---|
| **Bond lengths** | |
| Ni(1)-P(1) | 2.1116(10) |
| Ni(1)-P(3) | 2.2592(10) |
| Ni(1)-P(4) | 2.2070(10) |
| Ni(1)-Cl(1) | 2.2248(10) |
| Ni(1)-P(2) | 2.2534(10) |
| P(1)-C(1) | 1.827(4) |
| P(1)-C(19) | 1.829(4) |
| P(1)-C(37) | 1.817(3) |
| P(3)-C(31) | 1.827(4) |
| P(3)-C(25) | 1.819(4) |
| P(3)-C(20) | 1.830(4) |
| P(4)-C(38) | 1.814(3) |
| P(4)-C(49) | 1.824(4) |
| P(4)-C(43) | 1.820(4) |
| P(2)-C(7) | 1.826(4) |
| P(2)-C(2) | 1.823(4) |
| P(2)-C(13) | 1.814(4) |
| C(21)-H(21) | 0.9500 |
| C(21)-C(22) | 1.385(5) |
| C(21)-C(20) | 1.399(5) |
| C(6)-H(6) | 0.9500 |
| C(6)-C(1) | 1.393(5) |
| C(6)-C(5) | 1.384(5) |
| C(1)-C(2) | 1.390(5) |
| C(38)-C(37) | 1.394(5) |
| C(38)-C(39) | 1.392(5) |
| C(7)-C(12) | 1.387(6) |
| C(7)-C(8) | 1.393(5) |
| C(41)-H(41) | 0.9500 |
| C(41)-C(42) | 1.379(5) |
| C(41)-C(40) | 1.382(5) |
| C(19)-C(24) | 1.399(5) |
| C(19)-C(20) | 1.397(5) |
| C(37)-C(42) | 1.395(5) |
| C(49)-C(50) | 1.388(5) |
| C(49)-C(54) | 1.392(5) |
| C(2)-C(3) | 1.396(5) |
| C(13)-C(18) | 1.396(5) |
| C(13)-C(14) | 1.391(5) |
| C(39)-H(39) | 0.9500 |
| C(39)-C(40) | 1.378(5) |
| C(42)-H(42) | 0.9500 |
| C(43)-C(44) | 1.389(6) |
| C(43)-C(48) | 1.381(6) |
| C(36)-H(36) | 0.9500 |
| C(36)-C(31) | 1.392(5) |
| C(36)-C(35) | 1.396(5) |
| C(24)-H(24) | 0.9500 |
| C(24)-C(23) | 1.378(5) |
| C(31)-C(32) | 1.394(5) |
| C(5)-H(5) | 0.9500 |
| C(5)-C(4) | 1.405(5) |
| C(12)-H(12) | 0.9500 |
| C(12)-C(11) | 1.381(6) |
| C(22)-H(22) | 0.9500 |
| C(22)-C(23) | 1.382(5) |
| C(34)-H(34) | 0.9500 |
| C(34)-C(35) | 1.373(6) |
| C(34)-C(33) | 1.385(6) |
| C(16)-H(16) | 0.9500 |
| C(16)-C(17) | 1.386(6) |
| C(16)-C(15) | 1.370(7) |
| C(8)-H(8) | 0.9500 |
| C(8)-C(9) | 1.392(6) |
| C(3)-H(3) | 0.9500 |
| C(3)-C(4) | 1.374(5) |
| C(25)-C(30) | 1.388(6) |
| C(25)-C(26) | 1.381(5) |
| C(23)-H(23) | 0.9500 |
| C(50)-H(50) | 0.9500 |
| C(50)-C(51) | 1.384(6) |
| C(32)-H(32) | 0.9500 |
| C(32)-C(33) | 1.391(5) |
| C(35)-H(35) | 0.9500 |
| C(18)-H(18) | 0.9500 |
| C(18)-C(17) | 1.378(5) |
| C(14)-H(14) | 0.9500 |
| C(14)-C(15) | 1.395(6) |
| C(17)-H(17) | 0.9500 |
| C(11)-H(11) | 0.9500 |
| C(11)-C(10) | 1.374(6) |
| C(30)-H(30) | 0.9500 |
| C(30)-C(29) | 1.390(6) |
| C(4)-H(4) | 0.9500 |
| C(40)-H(40) | 0.9500 |
| C(33)-H(33) | 0.9500 |
| C(10)-H(10) | 0.9500 |
| C(10)-C(9) | 1.383(7) |
| C(52)-H(52) | 0.9500 |
| C(52)-C(53) | 1.373(6) |
| C(52)-C(51) | 1.383(7) |
| C(29)-H(29) | 0.9500 |
| C(29)-C(28) | 1.384(7) |
| C(45)-H(45) | 0.9500 |
| C(45)-C(44) | 1.377(6) |
| C(45)-C(46) | 1.376(7) |
| C(44)-H(44) | 0.9500 |
| C(46)-H(46) | 0.9500 |
| C(46)-C(47) | 1.361(7) |
| C(26)-H(26) | 0.9500 |
| C(26)-C(27) | 1.378(6) |
| C(54)-H(54) | 0.9500 |
| C(54)-C(53) | 1.382(6) |
| C(48)-H(48) | 0.9500 |
| C(48)-C(47) | 1.393(6) |
| C(28)-H(28) | 0.9500 |
| C(28)-C(27) | 1.371(7) |
| C(27)-H(27) | 0.9500 |
| C(53)-H(53) | 0.9500 |
| C(51)-H(51) | 0.9500 |
| C(15)-H(15) | 0.9500 |
| C(47)-H(47) | 0.9500 |
| C(9)-H(9) | 0.9500 |
| Ni(2)-P(5) | 2.1101(10) |
| Ni(2)-P(8) | 2.2078(10) |
| Ni(2)-P(6) | 2.2571(10) |
| Ni(2)-Cl(3) | 2.2179(10) |
| Ni(2)-P(7) | 2.2511(10) |
| P(5)-C(91) | 1.824(3) |
| P(5)-C(55) | 1.823(4) |
| P(5)-C(73) | 1.824(3) |
| P(8)-C(92) | 1.805(4) |
| P(8)-C(97) | 1.826(4) |
| P(8)-C(103) | 1.817(4) |
| P(6)-C(61) | 1.826(4) |
| P(6)-C(56) | 1.827(4) |
| P(6)-C(67) | 1.821(4) |
| P(7)-C(85) | 1.828(4) |
| P(7)-C(74) | 1.826(4) |
| P(7)-C(79) | 1.817(4) |
| Cl(14)-C(112) | 1.766(5) |
| Cl(16)-C(112) | 1.768(5) |
| Cl(13)-C(111) | 1.740(5) |
| Cl(11)-C(111) | 1.752(5) |
| Cl(12)-C(111) | 1.738(5) |
| Cl(15)-C(112) | 1.733(5) |
| C(57)-H(57) | 0.9500 |
| C(57)-C(56) | 1.397(5) |
| C(57)-C(58) | 1.390(5) |
| C(91)-C(92) | 1.391(5) |
| C(91)-C(96) | 1.395(5) |
| C(85)-C(90) | 1.376(5) |
| C(85)-C(86) | 1.390(6) |
| C(74)-C(75) | 1.383(5) |
| C(74)-C(73) | 1.398(5) |
| C(95)-H(95) | 0.9500 |
| C(95)-C(96) | 1.382(5) |
| C(95)-C(94) | 1.387(5) |
| C(92)-C(93) | 1.396(5) |
| C(61)-C(66) | 1.391(5) |
| C(61)-C(62) | 1.395(5) |
| C(79)-C(80) | 1.393(5) |
| C(79)-C(84) | 1.394(5) |
| C(75)-H(75) | 0.9500 |
| C(75)-C(76) | 1.378(5) |
| C(60)-H(60) | 0.9500 |
| C(60)-C(55) | 1.399(5) |
| C(60)-C(59) | 1.378(5) |
| C(55)-C(56) | 1.400(5) |
| C(66)-H(66) | 0.9500 |
| C(66)-C(65) | 1.392(5) |
| C(73)-C(78) | 1.398(5) |
| C(97)-C(102) | 1.389(5) |
| C(97)-C(98) | 1.388(5) |
| C(93)-H(93) | 0.9500 |
| C(93)-C(94) | 1.374(5) |
| C(78)-H(78) | 0.9500 |
| C(78)-C(77) | 1.377(5) |
| C(58)-H(58) | 0.9500 |
| C(58)-C(59) | 1.389(5) |
| C(96)-H(96) | 0.9500 |
| C(63)-H(63) | 0.9500 |
| C(63)-C(62) | 1.385(5) |
| C(63)-C(64) | 1.397(6) |
| C(102)-H(102) | 0.9500 |
| C(102)-C(101) | 1.390(6) |
| C(77)-H(77) | 0.9500 |
| C(77)-C(76) | 1.401(5) |
| C(72)-H(72) | 0.9500 |
| C(72)-C(67) | 1.394(5) |
| C(72)-C(71) | 1.383(6) |
| C(67)-C(68) | 1.378(6) |
| C(59)-H(59) | 0.9500 |
| C(62)-H(62) | 0.9500 |
| C(94)-H(94) | 0.9500 |
| C(65)-H(65) | 0.9500 |
| C(65)-C(64) | 1.374(6) |
| C(80)-H(80) | 0.9500 |
| C(80)-C(81) | 1.385(6) |
| C(103)-C(108) | 1.387(6) |
| C(103)-C(104) | 1.380(6) |
| C(68)-H(68) | 0.9500 |
| C(68)-C(69) | 1.381(6) |
| C(90)-H(90) | 0.9500 |
| C(90)-C(89) | 1.401(6) |

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| C(100)-H(100) | 0.9500 |
| C(100)-C(101) | 1.375(6) |
| C(100)-C(99) | 1.385(6) |
| C(88)-H(88) | 0.9500 |
| C(88)-C(87) | 1.381(6) |
| C(88)-C(89) | 1.374(6) |
| C(87)-H(87) | 0.9500 |
| C(87)-C(86) | 1.374(6) |
| C(83)-H(83) | 0.9500 |
| C(83)-C(84) | 1.379(5) |
| C(83)-C(82) | 1.387(7) |
| C(76)-H(76) | 0.9500 |
| C(81)-H(81) | 0.9500 |
| C(81)-C(82) | 1.379(7) |
| C(64)-H(64) | 0.9500 |
| C(98)-H(98) | 0.9500 |
| C(98)-C(99) | 1.387(6) |
| C(70)-H(70) | 0.9500 |
| C(70)-C(71) | 1.368(7) |
| C(70)-C(69) | 1.388(7) |
| C(111)-H(111) | 1.0000 |
| C(84)-H(84) | 0.9500 |
| C(101)-H(101) | 0.9500 |
| C(71)-H(71) | 0.9500 |
| C(108)-H(108) | 0.9500 |
| C(108)-C(107) | 1.377(6) |
| C(69)-H(69) | 0.9500 |
| C(86)-H(86) | 0.9500 |
| C(89)-H(89) | 0.9500 |
| C(82)-H(82) | 0.9500 |
| C(105)-H(105) | 0.9500 |
| C(105)-C(104) | 1.399(7) |
| C(105)-C(106) | 1.364(9) |
| C(107)-H(107) | 0.9500 |
| C(107)-C(106) | 1.370(8) |
| C(104)-H(104) | 0.9500 |
| C(106)-H(106) | 0.9500 |
| C(99)-H(99) | 0.9500 |
| C(112)-H(112) | 1.0000 |
| Cl(7)-C(109) | 1.759(5) |
| Cl(5)-C(109) | 1.764(4) |
| Cl(6)-C(109) | 1.745(5) |
| C(109)-H(109) | 1.0000 |
| Cl(9)-C(110) | 1.753(4) |
| Cl(8)-C(110) | 1.732(4) |
| Cl(10)-C(110) | 1.760(5) |
| C(110)-H(110) | 1.0000 |
| **Angles** | |
| P(1)-Ni(1)-P(3) | 88.24(4) |
| P(1)-Ni(1)-P(4) | 87.11(4) |
| P(1)-Ni(1)-Cl(1) | 174.49(4) |
| P(1)-Ni(1)-P(2) | 86.96(4) |
| P(4)-Ni(1)-P(3) | 119.59(4) |
| P(4)-Ni(1)-Cl(1) | 87.39(4) |
| P(4)-Ni(1)-P(2) | 124.59(4) |
| Cl(1)-Ni(1)-P(3) | 94.70(4) |
| Cl(1)-Ni(1)-P(2) | 95.98(4) |
| P(2)-Ni(1)-P(3) | 115.22(4) |
| C(1)-P(1)-Ni(1) | 112.61(12) |
| C(1)-P(1)-C(19) | 105.77(15) |
| C(19)-P(1)-Ni(1) | 111.13(11) |
| C(37)-P(1)-Ni(1) | 112.04(12) |
| C(37)-P(1)-C(1) | 106.20(16) |
| C(37)-P(1)-C(19) | 108.76(16) |
| C(31)-P(3)-Ni(1) | 117.42(13) |
| C(31)-P(3)-C(20) | 109.30(16) |
| C(25)-P(3)-Ni(1) | 117.50(12) |
| C(25)-P(3)-C(31) | 102.81(17) |
| C(25)-P(3)-C(20) | 101.51(16) |
| C(20)-P(3)-Ni(1) | 107.05(12) |
| C(38)-P(4)-Ni(1) | 108.70(11) |
| C(38)-P(4)-C(49) | 104.41(16) |
| C(38)-P(4)-C(43) | 102.54(16) |
| C(49)-P(4)-Ni(1) | 117.54(12) |
| C(43)-P(4)-Ni(1) | 115.64(12) |
| C(43)-P(4)-C(49) | 106.42(17) |
| C(7)-P(2)-Ni(1) | 116.46(13) |
| C(2)-P(2)-Ni(1) | 107.90(12) |
| C(2)-P(2)-C(7) | 107.00(17) |
| C(13)-P(2)-Ni(1) | 117.89(12) |
| C(13)-P(2)-C(7) | 106.14(17) |
| C(13)-P(2)-C(2) | 99.71(16) |
| C(22)-C(21)-H(21) | 119.9 |
| C(22)-C(21)-C(20) | 120.2(3) |
| C(20)-C(21)-H(21) | 119.9 |
| C(1)-C(6)-H(6) | 120.1 |
| C(5)-C(6)-H(6) | 120.1 |
| C(5)-C(6)-C(1) | 119.8(3) |
| C(6)-C(1)-P(1) | 124.3(3) |
| C(2)-C(1)-P(1) | 115.3(3) |
| C(2)-C(1)-C(6) | 120.3(3) |
| C(37)-C(38)-P(4) | 116.5(2) |
| C(39)-C(38)-P(4) | 123.3(3) |
| C(39)-C(38)-C(37) | 120.2(3) |
| C(12)-C(7)-P(2) | 118.2(3) |
| C(12)-C(7)-C(8) | 119.3(4) |
| C(8)-C(7)-P(2) | 122.3(3) |
| C(42)-C(41)-H(41) | 119.5 |
| C(42)-C(41)-C(40) | 121.0(3) |
| C(40)-C(41)-H(41) | 119.5 |
| C(24)-C(19)-P(1) | 122.9(3) |
| C(20)-C(19)-P(1) | 116.7(3) |
| C(20)-C(19)-C(24) | 120.4(3) |
| C(38)-C(37)-P(1) | 115.1(3) |
| C(38)-C(37)-C(42) | 119.8(3) |
| C(42)-C(37)-P(1) | 125.0(3) |
| C(50)-C(49)-P(4) | 119.9(3) |
| C(50)-C(49)-C(54) | 118.7(3) |
| C(54)-C(49)-P(4) | 121.4(3) |
| C(1)-C(2)-P(2) | 117.2(3) |
| C(1)-C(2)-C(3) | 119.3(3) |
| C(3)-C(2)-P(2) | 123.2(3) |
| C(18)-C(13)-P(2) | 116.9(3) |
| C(14)-C(13)-P(2) | 123.9(3) |
| C(14)-C(13)-C(18) | 119.1(3) |
| C(38)-C(39)-H(39) | 120.3 |
| C(40)-C(39)-C(38) | 119.5(3) |
| C(40)-C(39)-H(39) | 120.3 |
| C(41)-C(42)-C(37) | 119.2(3) |
| C(41)-C(42)-H(42) | 120.4 |
| C(37)-C(42)-H(42) | 120.4 |
| C(44)-C(43)-P(4) | 117.6(3) |
| C(48)-C(43)-P(4) | 123.7(3) |
| C(48)-C(43)-C(44) | 118.7(4) |
| C(31)-C(36)-H(36) | 119.9 |
| C(31)-C(36)-C(35) | 120.2(4) |
| C(35)-C(36)-H(36) | 119.9 |
| C(19)-C(24)-H(24) | 120.4 |
| C(23)-C(24)-C(19) | 119.2(3) |
| C(23)-C(24)-H(24) | 120.4 |
| C(36)-C(31)-P(3) | 124.3(3) |
| C(36)-C(31)-C(32) | 118.7(3) |
| C(32)-C(31)-P(3) | 116.9(3) |
| C(6)-C(5)-H(5) | 119.9 |
| C(6)-C(5)-C(4) | 120.1(3) |
| C(4)-C(5)-H(5) | 119.9 |
| C(7)-C(12)-H(12) | 119.9 |
| C(11)-C(12)-C(7) | 120.1(4) |
| C(11)-C(12)-H(12) | 119.9 |
| C(21)-C(22)-H(22) | 120.0 |
| C(23)-C(22)-C(21) | 119.9(3) |
| C(23)-C(22)-H(22) | 120.0 |
| C(35)-C(34)-H(34) | 119.8 |
| C(35)-C(34)-C(33) | 120.5(4) |
| C(33)-C(34)-H(34) | 119.8 |
| C(17)-C(16)-H(16) | 119.7 |
| C(15)-C(16)-H(16) | 119.7 |
| C(15)-C(16)-C(17) | 120.6(4) |
| C(7)-C(8)-H(8) | 120.0 |
| C(9)-C(8)-C(7) | 120.0(4) |
| C(9)-C(8)-H(8) | 120.0 |
| C(2)-C(3)-H(3) | 119.6 |
| C(4)-C(3)-C(2) | 120.8(4) |
| C(4)-C(3)-H(3) | 119.6 |
| C(30)-C(25)-P(3) | 119.5(3) |
| C(26)-C(25)-P(3) | 121.3(3) |
| C(26)-C(25)-C(30) | 119.1(4) |
| C(24)-C(23)-C(22) | 121.1(3) |
| C(24)-C(23)-H(23) | 119.5 |
| C(22)-C(23)-H(23) | 119.5 |
| C(21)-C(20)-P(3) | 124.0(3) |
| C(19)-C(20)-P(3) | 116.8(3) |
| C(19)-C(20)-C(21) | 119.1(3) |
| C(49)-C(50)-H(50) | 119.8 |
| C(51)-C(50)-C(49) | 120.4(4) |
| C(51)-C(50)-H(50) | 119.8 |
| C(31)-C(32)-H(32) | 119.5 |
| C(33)-C(32)-C(31) | 120.9(4) |
| C(33)-C(32)-H(32) | 119.5 |
| C(36)-C(35)-H(35) | 119.9 |
| C(34)-C(35)-C(36) | 120.2(4) |
| C(34)-C(35)-H(35) | 119.9 |
| C(13)-C(18)-H(18) | 119.6 |
| C(17)-C(18)-C(13) | 120.9(4) |
| C(17)-C(18)-H(18) | 119.6 |
| C(13)-C(14)-H(14) | 120.2 |
| C(13)-C(14)-C(15) | 119.6(4) |
| C(15)-C(14)-H(14) | 120.2 |
| C(16)-C(17)-H(17) | 120.3 |
| C(18)-C(17)-C(16) | 119.4(4) |
| C(18)-C(17)-H(17) | 120.3 |
| C(12)-C(11)-H(11) | 119.6 |
| C(10)-C(11)-C(12) | 120.7(4) |
| C(10)-C(11)-H(11) | 119.6 |
| C(25)-C(30)-H(30) | 119.9 |
| C(25)-C(30)-C(29) | 120.2(4) |
| C(29)-C(30)-H(30) | 119.9 |
| C(5)-C(4)-H(4) | 120.2 |
| C(3)-C(4)-C(5) | 119.6(3) |
| C(3)-C(4)-H(4) | 120.2 |
| C(41)-C(40)-H(40) | 119.9 |
| C(39)-C(40)-C(41) | 120.3(3) |
| C(39)-C(40)-H(40) | 119.9 |
| C(34)-C(33)-C(32) | 119.4(4) |
| C(34)-C(33)-H(33) | 120.3 |
| C(32)-C(33)-H(33) | 120.3 |
| C(11)-C(10)-H(10) | 120.1 |
| C(11)-C(10)-C(9) | 119.9(4) |

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| C(9)-C(10)-H(10) | 120.1 |
| C(53)-C(52)-H(52) | 120.1 |
| C(53)-C(52)-C(51) | 119.9(4) |
| C(51)-C(52)-H(52) | 120.1 |
| C(30)-C(29)-H(29) | 120.3 |
| C(28)-C(29)-C(30) | 119.5(5) |
| C(28)-C(29)-H(29) | 120.3 |
| C(44)-C(45)-H(45) | 120.0 |
| C(46)-C(45)-H(45) | 120.0 |
| C(46)-C(45)-C(44) | 120.0(4) |
| C(43)-C(44)-H(44) | 119.6 |
| C(45)-C(44)-C(43) | 120.9(4) |
| C(45)-C(44)-H(44) | 119.6 |
| C(45)-C(46)-H(46) | 120.1 |
| C(47)-C(46)-C(45) | 119.8(4) |
| C(47)-C(46)-H(46) | 120.1 |
| C(25)-C(26)-H(26) | 119.6 |
| C(27)-C(26)-C(25) | 120.9(4) |
| C(27)-C(26)-H(26) | 119.6 |
| C(49)-C(54)-H(54) | 119.7 |
| C(53)-C(54)-C(49) | 120.7(4) |
| C(53)-C(54)-H(54) | 119.7 |
| C(43)-C(48)-H(48) | 120.1 |
| C(43)-C(48)-C(47) | 119.8(4) |
| C(47)-C(48)-H(48) | 120.1 |
| C(29)-C(28)-H(28) | 119.7 |
| C(27)-C(28)-C(29) | 120.5(4) |
| C(27)-C(28)-H(28) | 119.7 |
| C(26)-C(27)-H(27) | 120.1 |
| C(28)-C(27)-C(26) | 119.8(4) |
| C(28)-C(27)-H(27) | 120.1 |
| C(52)-C(53)-C(54) | 120.2(4) |
| C(52)-C(53)-H(53) | 119.9 |
| C(54)-C(53)-H(53) | 119.9 |
| C(50)-C(51)-H(51) | 119.9 |
| C(52)-C(51)-C(50) | 120.2(4) |
| C(52)-C(51)-H(51) | 119.9 |
| C(16)-C(15)-C(14) | 120.3(4) |
| C(16)-C(15)-H(15) | 119.8 |
| C(14)-C(15)-H(15) | 119.8 |
| C(46)-C(47)-C(48) | 120.8(5) |
| C(46)-C(47)-H(47) | 119.6 |
| C(48)-C(47)-H(47) | 119.6 |
| C(8)-C(9)-H(9) | 120.0 |
| C(10)-C(9)-C(8) | 120.0(4) |
| C(10)-C(9)-H(9) | 120.0 |
| P(5)-Ni(2)-P(8) | 87.13(4) |
| P(5)-Ni(2)-P(6) | 88.18(4) |
| P(5)-Ni(2)-Cl(3) | 174.53(4) |
| P(5)-Ni(2)-P(7) | 87.39(4) |
| P(8)-Ni(2)-P(6) | 119.53(4) |
| P(8)-Ni(2)-Cl(3) | 87.48(4) |
| P(8)-Ni(2)-P(7) | 125.14(4) |
| Cl(3)-Ni(2)-P(6) | 95.21(4) |
| Cl(3)-Ni(2)-P(7) | 95.04(4) |
| P(7)-Ni(2)-P(6) | 114.79(4) |
| C(91)-P(5)-Ni(2) | 112.00(12) |
| C(55)-P(5)-Ni(2) | 111.36(12) |
| C(55)-P(5)-C(91) | 108.40(16) |
| C(55)-P(5)-C(73) | 105.63(16) |
| C(73)-P(5)-Ni(2) | 112.13(11) |
| C(73)-P(5)-C(91) | 107.00(15) |
| C(92)-P(8)-Ni(2) | 108.73(12) |
| C(92)-P(8)-C(97) | 104.97(17) |
| C(92)-P(8)-C(103) | 102.35(17) |
| C(97)-P(8)-Ni(2) | 117.53(12) |
| C(103)-P(8)-Ni(2) | 114.70(13) |
| C(103)-P(8)-C(97) | 107.07(18) |
| C(61)-P(6)-Ni(2) | 117.25(13) |
| C(61)-P(6)-C(56) | 109.44(16) |
| C(56)-P(6)-Ni(2) | 107.01(12) |
| C(67)-P(6)-Ni(2) | 116.84(12) |
| C(67)-P(6)-C(61) | 103.89(17) |
| C(67)-P(6)-C(56) | 101.16(16) |
| C(85)-P(7)-Ni(2) | 116.57(13) |
| C(74)-P(7)-Ni(2) | 107.82(12) |
| C(74)-P(7)-C(85) | 106.37(17) |
| C(79)-P(7)-Ni(2) | 118.59(12) |
| C(79)-P(7)-C(85) | 105.46(17) |
| C(79)-P(7)-C(74) | 100.24(17) |
| C(56)-C(57)-H(57) | 119.7 |
| C(58)-C(57)-H(57) | 119.7 |
| C(58)-C(57)-C(56) | 120.7(3) |
| C(92)-C(91)-P(5) | 114.7(3) |
| C(92)-C(91)-C(96) | 120.9(3) |
| C(96)-C(91)-P(5) | 124.3(3) |
| C(90)-C(85)-P(7) | 122.7(3) |
| C(90)-C(85)-C(86) | 118.8(4) |
| C(86)-C(85)-P(7) | 118.4(3) |
| C(75)-C(74)-P(7) | 123.5(3) |
| C(75)-C(74)-C(73) | 119.6(3) |
| C(73)-C(74)-P(7) | 116.7(3) |
| C(96)-C(95)-H(95) | 119.5 |
| C(96)-C(95)-C(94) | 121.0(3) |
| C(94)-C(95)-H(95) | 119.5 |
| C(91)-C(92)-P(8) | 117.0(3) |
| C(91)-C(92)-C(93) | 118.9(3) |
| C(93)-C(92)-P(8) | 124.1(3) |
| C(66)-C(61)-P(6) | 124.5(3) |
| C(66)-C(61)-C(62) | 118.5(3) |
| C(62)-C(61)-P(6) | 117.0(3) |
| C(80)-C(79)-P(7) | 123.5(3) |
| C(80)-C(79)-C(84) | 119.1(3) |
| C(84)-C(79)-P(7) | 117.4(3) |
| C(74)-C(75)-H(75) | 119.7 |
| C(76)-C(75)-C(74) | 120.6(4) |
| C(76)-C(75)-H(75) | 119.7 |
| C(55)-C(60)-H(60) | 120.1 |
| C(59)-C(60)-H(60) | 120.1 |
| C(59)-C(60)-C(55) | 119.8(3) |
| C(60)-C(55)-P(5) | 123.5(3) |
| C(60)-C(55)-C(56) | 120.1(3) |
| C(56)-C(55)-P(5) | 116.4(3) |
| C(61)-C(66)-H(66) | 119.7 |
| C(61)-C(66)-C(65) | 120.6(4) |
| C(65)-C(66)-H(66) | 119.7 |
| C(74)-C(73)-P(5) | 115.8(3) |
| C(74)-C(73)-C(78) | 120.0(3) |
| C(78)-C(73)-P(5) | 124.0(3) |
| C(102)-C(97)-P(8) | 121.4(3) |
| C(98)-C(97)-P(8) | 119.7(3) |
| C(98)-C(97)-C(102) | 118.9(4) |
| C(92)-C(93)-H(93) | 119.8 |
| C(94)-C(93)-C(92) | 120.5(3) |
| C(94)-C(93)-H(93) | 119.8 |
| C(57)-C(56)-P(6) | 123.8(3) |
| C(57)-C(56)-C(55) | 119.0(3) |
| C(55)-C(56)-P(6) | 117.0(3) |
| C(73)-C(78)-H(78) | 120.2 |
| C(77)-C(78)-C(73) | 119.6(3) |
| C(77)-C(78)-H(78) | 120.2 |
| C(57)-C(58)-H(58) | 120.3 |
| C(59)-C(58)-C(57) | 119.5(3) |
| C(59)-C(58)-H(58) | 120.3 |
| C(91)-C(96)-H(96) | 120.7 |
| C(95)-C(96)-C(91) | 118.7(3) |
| C(95)-C(96)-H(96) | 120.7 |
| C(62)-C(63)-H(63) | 120.2 |
| C(62)-C(63)-C(64) | 119.6(4) |
| C(64)-C(63)-H(63) | 120.2 |
| C(97)-C(102)-H(102) | 119.7 |
| C(97)-C(102)-C(101) | 120.6(4) |
| C(101)-C(102)-H(102) | 119.7 |
| C(78)-C(77)-H(77) | 119.8 |
| C(78)-C(77)-C(76) | 120.3(3) |
| C(76)-C(77)-H(77) | 119.8 |
| C(67)-C(72)-H(72) | 119.9 |
| C(71)-C(72)-H(72) | 119.9 |
| C(71)-C(72)-C(67) | 120.1(4) |
| C(72)-C(67)-P(6) | 121.0(3) |
| C(68)-C(67)-P(6) | 120.2(3) |
| C(68)-C(67)-C(72) | 118.8(4) |
| C(60)-C(59)-C(58) | 120.9(3) |
| C(60)-C(59)-H(59) | 119.6 |
| C(58)-C(59)-H(59) | 119.6 |
| C(61)-C(62)-H(62) | 119.5 |
| C(63)-C(62)-C(61) | 121.1(4) |
| C(63)-C(62)-H(62) | 119.5 |
| C(95)-C(94)-H(94) | 120.0 |
| C(93)-C(94)-C(95) | 119.9(3) |
| C(93)-C(94)-H(94) | 120.0 |
| C(66)-C(65)-H(65) | 119.8 |
| C(64)-C(65)-C(66) | 120.4(4) |
| C(64)-C(65)-H(65) | 119.8 |
| C(79)-C(80)-H(80) | 120.0 |
| C(81)-C(80)-C(79) | 120.0(4) |
| C(81)-C(80)-H(80) | 120.0 |
| C(108)-C(103)-P(8) | 117.3(3) |
| C(104)-C(103)-P(8) | 123.5(3) |
| C(104)-C(103)-C(108) | 119.2(4) |
| C(67)-C(68)-H(68) | 119.5 |
| C(67)-C(68)-C(69) | 121.0(4) |
| C(69)-C(68)-H(68) | 119.5 |
| C(85)-C(90)-H(90) | 119.7 |
| C(85)-C(90)-C(89) | 120.5(4) |
| C(89)-C(90)-H(90) | 119.7 |
| C(101)-C(100)-H(100) | 120.0 |
| C(101)-C(100)-C(99) | 120.1(4) |
| C(99)-C(100)-H(100) | 120.0 |
| C(87)-C(88)-H(88) | 120.1 |
| C(89)-C(88)-H(88) | 120.1 |
| C(89)-C(88)-C(87) | 119.7(4) |
| C(88)-C(87)-H(87) | 119.8 |
| C(86)-C(87)-C(88) | 120.3(4) |
| C(86)-C(87)-H(87) | 119.8 |
| C(84)-C(83)-H(83) | 120.4 |
| C(84)-C(83)-C(82) | 119.2(4) |
| C(82)-C(83)-H(83) | 120.4 |
| C(75)-C(76)-C(77) | 119.7(3) |
| C(75)-C(76)-H(76) | 120.1 |
| C(77)-C(76)-H(76) | 120.1 |
| C(80)-C(81)-H(81) | 120.0 |
| C(82)-C(81)-C(80) | 120.1(4) |
| C(82)-C(81)-H(81) | 120.0 |
| C(63)-C(64)-H(64) | 120.1 |
| C(65)-C(64)-C(63) | 119.8(4) |
| C(65)-C(64)-H(64) | 120.1 |
| C(97)-C(98)-H(98) | 119.8 |

| | |
|---|---|
| C(99)-C(98)-C(97) | 120.4(4) |
| C(99)-C(98)-H(98) | 119.8 |
| C(71)-C(70)-H(70) | 120.0 |
| C(71)-C(70)-C(69) | 119.9(4) |
| C(69)-C(70)-H(70) | 120.0 |
| Cl(13)-C(111)-Cl(11) | 111.8(3) |
| Cl(13)-C(111)-H(111) | 107.9 |
| Cl(11)-C(111)-H(111) | 107.9 |
| Cl(12)-C(111)-Cl(13) | 111.1(3) |
| Cl(12)-C(111)-Cl(11) | 110.0(3) |
| Cl(12)-C(111)-H(111) | 107.9 |
| C(79)-C(84)-H(84) | 119.5 |
| C(83)-C(84)-C(79) | 121.0(4) |
| C(83)-C(84)-H(84) | 119.5 |
| C(102)-C(101)-H(101) | 120.0 |
| C(100)-C(101)-C(102) | 119.9(4) |
| C(100)-C(101)-H(101) | 120.0 |
| C(72)-C(71)-H(71) | 119.8 |
| C(70)-C(71)-C(72) | 120.5(4) |
| C(70)-C(71)-H(71) | 119.8 |
| C(103)-C(108)-H(108) | 119.5 |
| C(107)-C(108)-C(103) | 120.9(4) |
| C(107)-C(108)-H(108) | 119.5 |
| C(68)-C(69)-C(70) | 119.6(5) |
| C(68)-C(69)-H(69) | 120.2 |
| C(70)-C(69)-H(69) | 120.2 |
| C(85)-C(86)-H(86) | 119.6 |
| C(87)-C(86)-C(85) | 120.8(4) |
| C(87)-C(86)-H(86) | 119.6 |
| C(90)-C(89)-H(89) | 120.1 |
| C(88)-C(89)-C(90) | 119.8(4) |
| C(88)-C(89)-H(89) | 120.1 |
| C(83)-C(82)-H(82) | 119.7 |
| C(81)-C(82)-C(83) | 120.7(4) |
| C(81)-C(82)-H(82) | 119.7 |
| C(104)-C(105)-H(105) | 119.7 |
| C(106)-C(105)-H(105) | 119.7 |
| C(106)-C(105)-C(104) | 120.6(5) |
| C(108)-C(107)-H(107) | 120.1 |
| C(106)-C(107)-C(108) | 119.7(5) |
| C(106)-C(107)-H(107) | 120.1 |
| C(103)-C(104)-C(105) | 119.3(5) |
| C(103)-C(104)-H(104) | 120.4 |
| C(105)-C(104)-H(104) | 120.4 |
| C(105)-C(106)-C(107) | 120.3(5) |
| C(105)-C(106)-H(106) | 119.9 |
| C(107)-C(106)-H(106) | 119.9 |
| C(100)-C(99)-C(98) | 120.1(4) |
| C(100)-C(99)-H(99) | 120.0 |
| C(98)-C(99)-H(99) | 120.0 |
| Cl(14)-C(112)-Cl(16) | 109.0(3) |
| Cl(14)-C(112)-H(112) | 108.6 |
| Cl(16)-C(112)-H(112) | 108.6 |
| Cl(15)-C(112)-Cl(14) | 111.8(2) |
| Cl(15)-C(112)-Cl(16) | 110.0(3) |
| Cl(15)-C(112)-H(112) | 108.6 |
| Cl(7)-C(109)-Cl(5) | 110.0(2) |
| Cl(7)-C(109)-H(109) | 108.4 |
| Cl(5)-C(109)-H(109) | 108.4 |
| Cl(6)-C(109)-Cl(7) | 111.1(2) |
| Cl(6)-C(109)-Cl(5) | 110.5(3) |
| Cl(6)-C(109)-H(109) | 108.4 |
| Cl(9)-C(110)-Cl(10) | 109.9(2) |
| Cl(9)-C(110)-H(110) | 108.4 |
| Cl(8)-C(110)-Cl(9) | 111.8(2) |
| Cl(8)-C(110)-Cl(10) | 109.9(2) |
| Cl(8)-C(110)-H(110) | 108.4 |
| Cl(10)-C(110)-H(110) | 108.4 |

| Table 6. Bond lengths [Å] and angles [°] for [5][Cl]•5CHCl$_3$ | |
|---|---|
| **Bond lengths** | |
| As(1)-Ni(1) | 2.1981(7) |
| As(1)-C(1) | 1.924(3) |
| As(1)-C(37) | 1.926(3) |
| As(1)-C(19) | 1.920(3) |
| Ni(1)-Cl(1) | 2.2186(10) |
| Ni(1)-P(2) | 2.2608(12) |
| Ni(1)-P(3) | 2.2586(10) |
| Ni(1)-P(1) | 2.2835(10) |
| P(2)-C(20) | 1.826(3) |
| P(2)-C(25) | 1.824(4) |
| P(2)-C(31) | 1.830(4) |
| P(3)-C(49) | 1.828(3) |
| P(3)-C(43) | 1.827(3) |
| P(3)-C(38) | 1.826(3) |
| P(1)-C(13) | 1.822(4) |
| P(1)-C(2) | 1.824(4) |
| P(1)-C(7) | 1.823(4) |
| Cl(6)-C(56) | 1.760(4) |
| Cl(8)-C(56) | 1.754(4) |
| Cl(7)-C(56) | 1.753(4) |
| Cl(5)-C(55) | 1.746(4) |
| Cl(3)-C(55) | 1.738(4) |
| Cl(4)-C(55) | 1.730(4) |
| C(1)-C(2) | 1.394(5) |
| C(1)-C(6) | 1.392(5) |
| C(13)-C(14) | 1.396(5) |
| C(13)-C(18) | 1.388(5) |
| C(20)-C(19) | 1.384(5) |
| C(20)-C(21) | 1.396(5) |
| C(37)-C(38) | 1.398(4) |
| C(37)-C(42) | 1.388(5) |
| C(19)-C(24) | 1.390(4) |
| C(49)-C(54) | 1.390(5) |
| C(49)-C(50) | 1.396(5) |
| C(43)-C(44) | 1.385(5) |
| C(43)-C(48) | 1.380(5) |
| C(44)-H(44) | 0.9500 |
| C(44)-C(45) | 1.384(5) |
| C(38)-C(39) | 1.395(5) |
| C(25)-C(30) | 1.390(5) |
| C(25)-C(26) | 1.394(5) |
| C(3)-H(3) | 0.9500 |
| C(3)-C(2) | 1.405(5) |
| C(3)-C(4) | 1.382(6) |
| C(24)-H(24) | 0.9500 |
| C(24)-C(23) | 1.385(5) |
| C(53)-H(53) | 0.9500 |
| C(53)-C(54) | 1.385(5) |
| C(53)-C(52) | 1.379(6) |
| C(54)-H(54) | 0.9500 |
| C(36)-H(36) | 0.9500 |
| C(36)-C(31) | 1.393(5) |
| C(36)-C(35) | 1.394(6) |
| C(40)-H(40) | 0.9500 |
| C(40)-C(39) | 1.379(5) |
| C(40)-C(41) | 1.387(5) |
| C(39)-H(39) | 0.9500 |
| C(31)-C(32) | 1.398(5) |
| C(4)-H(4) | 0.9500 |
| C(4)-C(5) | 1.379(6) |
| C(6)-H(6) | 0.9500 |
| C(6)-C(5) | 1.392(5) |
| C(21)-H(21) | 0.9500 |
| C(21)-C(22) | 1.384(5) |
| C(5)-H(5) | 0.9500 |
| C(42)-H(42) | 0.9500 |
| C(42)-C(41) | 1.386(5) |
| C(30)-H(30) | 0.9500 |
| C(30)-C(29) | 1.388(6) |
| C(46)-H(46) | 0.9500 |
| C(46)-C(45) | 1.380(6) |
| C(46)-C(47) | 1.375(7) |
| C(45)-H(45) | 0.9500 |
| C(10)-H(10) | 0.9500 |
| C(10)-C(9) | 1.362(10) |
| C(10)-C(11) | 1.375(9) |
| C(23)-H(23) | 0.9500 |
| C(23)-C(22) | 1.385(5) |
| C(7)-C(8) | 1.396(6) |
| C(7)-C(12) | 1.395(6) |
| C(26)-H(26) | 0.9500 |
| C(26)-C(27) | 1.382(5) |
| C(15)-H(15) | 0.9500 |
| C(15)-C(16) | 1.369(6) |
| C(15)-C(14) | 1.391(5) |
| C(50)-H(50) | 0.9500 |
| C(50)-C(51) | 1.383(5) |
| C(56)-H(56) | 1.0000 |
| C(55)-H(55) | 1.0000 |
| C(33)-H(33) | 0.9500 |
| C(33)-C(32) | 1.386(6) |
| C(33)-C(34) | 1.392(7) |
| C(16)-H(16) | 0.9500 |
| C(16)-C(17) | 1.372(7) |
| C(48)-H(48) | 0.9500 |
| C(48)-C(47) | 1.399(6) |
| C(41)-H(41) | 0.9500 |
| C(22)-H(22) | 0.9500 |
| C(14)-H(14) | 0.9500 |
| C(32)-H(32) | 0.9500 |
| C(27)-H(27) | 0.9500 |
| C(27)-C(28) | 1.380(6) |
| C(35)-H(35) | 0.9500 |
| C(35)-C(34) | 1.375(7) |
| C(8)-H(8) | 0.9500 |
| C(8)-C(9) | 1.394(7) |
| C(51)-H(51) | 0.9500 |
| C(51)-C(52) | 1.391(6) |
| C(18)-H(18) | 0.9500 |
| C(18)-C(17) | 1.382(6) |
| C(17)-H(17) | 0.9500 |
| C(34)-H(34) | 0.9500 |
| C(28)-H(28) | 0.9500 |
| C(28)-C(29) | 1.377(7) |
| C(9)-H(9) | 0.9500 |
| C(52)-H(52) | 0.9500 |
| C(29)-H(29) | 0.9500 |
| C(47)-H(47) | 0.9500 |
| C(12)-H(12) | 0.9500 |
| C(12)-C(11) | 1.392(6) |
| C(11)-H(11) | 0.9500 |
| Cl(9)-C(57) | 1.756(4) |
| Cl(10)-C(57) | 1.760(4) |
| Cl(11)-C(57) | 1.763(4) |
| C(57)-H(57) | 1.0000 |
| Cl(14)-C(58) | 1.740(5) |
| Cl(13)-C(58) | 1.756(5) |
| Cl(12)-C(58) | 1.732(5) |
| C(58)-H(58) | 1.0000 |
| Cl(15)-C(59) | 1.720(7) |
| Cl(17)-C(59) | 1.724(6) |
| Cl(16)-C(59) | 1.750(6) |
| C(59)-H(59) | 1.0000 |
| **Angles** | |
| C(1)-As(1)-Ni(1) | 110.87(10) |
| C(1)-As(1)-C(37) | 107.88(14) |
| C(37)-As(1)-Ni(1) | 110.59(10) |
| C(19)-As(1)-Ni(1) | 110.78(10) |
| C(19)-As(1)-C(1) | 107.44(13) |
| C(19)-As(1)-C(37) | 109.18(13) |
| As(1)-Ni(1)-Cl(1) | 178.02(3) |
| As(1)-Ni(1)-P(2) | 85.88(3) |
| As(1)-Ni(1)-P(3) | 86.22(4) |
| As(1)-Ni(1)-P(1) | 85.98(4) |
| Cl(1)-Ni(1)-P(2) | 92.96(3) |
| Cl(1)-Ni(1)-P(3) | 93.03(4) |
| Cl(1)-Ni(1)-P(1) | 95.99(4) |
| P(2)-Ni(1)-P(1) | 119.31(4) |
| P(3)-Ni(1)-P(2) | 121.38(4) |
| P(3)-Ni(1)-P(1) | 117.88(4) |
| C(20)-P(2)-Ni(1) | 110.55(11) |
| C(20)-P(2)-C(31) | 104.52(16) |
| C(25)-P(2)-Ni(1) | 119.14(11) |
| C(25)-P(2)-C(20) | 101.11(16) |
| C(25)-P(2)-C(31) | 104.67(16) |
| C(31)-P(2)-Ni(1) | 115.07(12) |
| C(49)-P(3)-Ni(1) | 116.24(11) |
| C(43)-P(3)-Ni(1) | 116.77(11) |
| C(43)-P(3)-C(49) | 104.76(15) |
| C(38)-P(3)-Ni(1) | 110.80(11) |
| C(38)-P(3)-C(49) | 105.79(15) |
| C(38)-P(3)-C(43) | 100.87(15) |
| C(13)-P(1)-Ni(1) | 118.92(12) |
| C(13)-P(1)-C(2) | 101.92(16) |
| C(13)-P(1)-C(7) | 104.56(16) |
| C(2)-P(1)-Ni(1) | 110.35(12) |
| C(7)-P(1)-Ni(1) | 114.24(14) |
| C(7)-P(1)-C(2) | 105.39(18) |
| C(2)-C(1)-As(1) | 114.7(2) |
| C(6)-C(1)-As(1) | 123.5(3) |
| C(6)-C(1)-C(2) | 121.7(3) |
| C(14)-C(13)-P(1) | 118.0(3) |
| C(18)-C(13)-P(1) | 123.3(3) |
| C(18)-C(13)-C(14) | 118.7(3) |
| C(19)-C(20)-P(2) | 117.8(2) |
| C(19)-C(20)-C(21) | 118.9(3) |
| C(21)-C(20)-P(2) | 123.4(3) |
| C(38)-C(37)-As(1) | 114.5(2) |
| C(42)-C(37)-As(1) | 123.7(2) |
| C(42)-C(37)-C(38) | 121.5(3) |
| C(20)-C(19)-As(1) | 114.4(2) |
| C(20)-C(19)-C(24) | 121.6(3) |
| C(24)-C(19)-As(1) | 123.8(2) |
| C(54)-C(49)-P(3) | 123.0(3) |
| C(54)-C(49)-C(50) | 119.0(3) |
| C(50)-C(49)-P(3) | 118.0(3) |
| C(44)-C(43)-P(3) | 117.2(3) |
| C(48)-C(43)-P(3) | 123.8(3) |
| C(48)-C(43)-C(44) | 119.0(3) |
| C(43)-C(44)-H(44) | 119.6 |
| C(45)-C(44)-C(43) | 120.9(3) |
| C(45)-C(44)-H(44) | 119.6 |
| C(37)-C(38)-P(3) | 117.6(2) |
| C(39)-C(38)-P(3) | 123.9(3) |
| C(39)-C(38)-C(37) | 118.4(3) |

| | |
|---|---|
| C(30)-C(25)-P(2) | 123.1(3) |
| C(30)-C(25)-C(26) | 119.2(3) |
| C(26)-C(25)-P(2) | 117.7(3) |
| C(2)-C(3)-H(3) | 119.8 |
| C(4)-C(3)-H(3) | 119.8 |
| C(4)-C(3)-C(2) | 120.3(3) |
| C(19)-C(24)-H(24) | 120.7 |
| C(23)-C(24)-C(19) | 118.6(3) |
| C(23)-C(24)-H(24) | 120.7 |
| C(54)-C(53)-H(53) | 119.9 |
| C(52)-C(53)-H(53) | 119.9 |
| C(52)-C(53)-C(54) | 120.2(3) |
| C(49)-C(54)-H(54) | 119.8 |
| C(53)-C(54)-C(49) | 120.4(3) |
| C(53)-C(54)-H(54) | 119.8 |
| C(31)-C(36)-H(36) | 120.1 |
| C(31)-C(36)-C(35) | 119.7(4) |
| C(35)-C(36)-H(36) | 120.1 |
| C(39)-C(40)-H(40) | 119.9 |
| C(39)-C(40)-C(41) | 120.3(3) |
| C(41)-C(40)-H(40) | 119.9 |
| C(38)-C(39)-H(39) | 119.8 |
| C(40)-C(39)-C(38) | 120.5(3) |
| C(40)-C(39)-H(39) | 119.8 |
| C(1)-C(2)-P(1) | 117.9(2) |
| C(1)-C(2)-C(3) | 118.0(3) |
| C(3)-C(2)-P(1) | 124.0(3) |
| C(36)-C(31)-P(2) | 121.7(3) |
| C(36)-C(31)-C(32) | 118.9(3) |
| C(32)-C(31)-P(2) | 119.4(3) |
| C(3)-C(4)-H(4) | 119.6 |
| C(5)-C(4)-C(3) | 120.8(3) |
| C(5)-C(4)-H(4) | 119.6 |
| C(1)-C(6)-H(6) | 120.5 |
| C(5)-C(6)-C(1) | 119.0(3) |
| C(5)-C(6)-H(6) | 120.5 |
| C(20)-C(21)-H(21) | 120.0 |
| C(22)-C(21)-C(20) | 120.1(3) |
| C(22)-C(21)-H(21) | 120.0 |
| C(4)-C(5)-C(6) | 120.1(4) |
| C(4)-C(5)-H(5) | 119.9 |
| C(6)-C(5)-H(5) | 119.9 |
| C(37)-C(42)-H(42) | 120.6 |
| C(41)-C(42)-C(37) | 118.7(3) |
| C(41)-C(42)-H(42) | 120.6 |
| C(25)-C(30)-H(30) | 120.3 |
| C(29)-C(30)-C(25) | 119.5(4) |
| C(29)-C(30)-H(30) | 120.3 |
| C(45)-C(46)-H(46) | 120.3 |
| C(47)-C(46)-H(46) | 120.3 |
| C(47)-C(46)-C(45) | 119.5(4) |
| C(44)-C(45)-H(45) | 119.9 |
| C(46)-C(45)-C(44) | 120.1(4) |
| C(46)-C(45)-H(45) | 119.9 |
| C(9)-C(10)-H(10) | 119.7 |
| C(9)-C(10)-C(11) | 120.6(5) |
| C(11)-C(10)-H(10) | 119.7 |
| C(24)-C(23)-H(23) | 119.6 |
| C(22)-C(23)-C(24) | 120.8(3) |
| C(22)-C(23)-H(23) | 119.6 |
| C(8)-C(7)-P(1) | 123.1(4) |
| C(12)-C(7)-P(1) | 117.7(3) |
| C(12)-C(7)-C(8) | 119.1(4) |
| C(25)-C(26)-H(26) | 119.8 |
| C(27)-C(26)-C(25) | 120.5(4) |
| C(27)-C(26)-H(26) | 119.8 |
| C(16)-C(15)-H(15) | 119.8 |
| C(16)-C(15)-C(14) | 120.5(4) |
| C(14)-C(15)-H(15) | 119.8 |
| C(49)-C(50)-H(50) | 119.8 |
| C(51)-C(50)-C(49) | 120.4(3) |
| C(51)-C(50)-H(50) | 119.8 |
| Cl(6)-C(56)-H(56) | 108.7 |
| Cl(8)-C(56)-Cl(6) | 110.9(2) |
| Cl(8)-C(56)-H(56) | 108.7 |
| Cl(7)-C(56)-Cl(6) | 109.4(2) |
| Cl(7)-C(56)-Cl(8) | 110.3(2) |
| Cl(7)-C(56)-H(56) | 108.7 |
| Cl(5)-C(55)-H(55) | 108.8 |
| Cl(3)-C(55)-Cl(5) | 108.5(2) |
| Cl(3)-C(55)-H(55) | 108.8 |
| Cl(4)-C(55)-Cl(5) | 109.7(2) |
| Cl(4)-C(55)-Cl(3) | 112.2(2) |
| Cl(4)-C(55)-H(55) | 108.8 |
| C(32)-C(33)-H(33) | 120.0 |
| C(32)-C(33)-C(34) | 120.1(4) |
| C(34)-C(33)-H(33) | 120.0 |
| C(15)-C(16)-H(16) | 120.0 |
| C(15)-C(16)-C(17) | 120.1(4) |
| C(17)-C(16)-H(16) | 120.0 |
| C(43)-C(48)-H(48) | 120.0 |
| C(43)-C(48)-C(47) | 120.0(4) |
| C(47)-C(48)-H(48) | 120.0 |
| C(40)-C(41)-H(41) | 119.7 |
| C(42)-C(41)-C(40) | 120.6(3) |
| C(42)-C(41)-H(41) | 119.7 |
| C(21)-C(22)-C(23) | 120.1(3) |
| C(21)-C(22)-H(22) | 120.0 |
| C(23)-C(22)-H(22) | 120.0 |
| C(13)-C(14)-H(14) | 120.1 |
| C(15)-C(14)-C(13) | 119.9(3) |
| C(15)-C(14)-H(14) | 120.1 |
| C(31)-C(32)-H(32) | 119.6 |
| C(33)-C(32)-C(31) | 120.7(4) |
| C(33)-C(32)-H(32) | 119.6 |
| C(26)-C(27)-H(27) | 119.9 |
| C(28)-C(27)-C(26) | 120.3(4) |
| C(28)-C(27)-H(27) | 119.9 |
| C(36)-C(35)-H(35) | 119.4 |
| C(34)-C(35)-C(36) | 121.2(4) |
| C(34)-C(35)-H(35) | 119.4 |
| C(7)-C(8)-H(8) | 120.2 |
| C(9)-C(8)-C(7) | 119.6(5) |
| C(9)-C(8)-H(8) | 120.2 |
| C(50)-C(51)-H(51) | 120.1 |
| C(50)-C(51)-C(52) | 119.9(3) |
| C(52)-C(51)-H(51) | 120.1 |
| C(13)-C(18)-H(18) | 119.7 |
| C(17)-C(18)-C(13) | 120.6(4) |
| C(17)-C(18)-H(18) | 119.7 |
| C(16)-C(17)-C(18) | 120.3(4) |
| C(16)-C(17)-H(17) | 119.9 |
| C(18)-C(17)-H(17) | 119.9 |
| C(33)-C(34)-H(34) | 120.3 |
| C(35)-C(34)-C(33) | 119.4(4) |
| C(35)-C(34)-H(34) | 120.3 |
| C(27)-C(28)-H(28) | 120.3 |
| C(29)-C(28)-C(27) | 119.4(4) |
| C(29)-C(28)-H(28) | 120.3 |
| C(10)-C(9)-C(8) | 120.7(5) |
| C(10)-C(9)-H(9) | 119.6 |
| C(8)-C(9)-H(9) | 119.6 |
| C(53)-C(52)-C(51) | 120.0(3) |
| C(53)-C(52)-H(52) | 120.0 |
| C(51)-C(52)-H(52) | 120.0 |
| C(30)-C(29)-H(29) | 119.4 |
| C(28)-C(29)-C(30) | 121.2(4) |
| C(28)-C(29)-H(29) | 119.4 |
| C(46)-C(47)-C(48) | 120.5(4) |
| C(46)-C(47)-H(47) | 119.7 |
| C(48)-C(47)-H(47) | 119.7 |
| C(7)-C(12)-H(12) | 119.9 |
| C(11)-C(12)-C(7) | 120.2(5) |
| C(11)-C(12)-H(12) | 119.9 |
| C(10)-C(11)-C(12) | 119.9(6) |
| C(10)-C(11)-H(11) | 120.0 |
| C(12)-C(11)-H(11) | 120.0 |
| Cl(9)-C(57)-Cl(10) | 110.9(2) |
| Cl(9)-C(57)-Cl(11) | 109.4(2) |
| Cl(9)-C(57)-H(57) | 108.8 |
| Cl(10)-C(57)-Cl(11) | 110.1(2) |
| Cl(10)-C(57)-H(57) | 108.8 |
| Cl(11)-C(57)-H(57) | 108.8 |
| Cl(14)-C(58)-Cl(13) | 111.2(3) |
| Cl(14)-C(58)-H(58) | 107.1 |
| Cl(13)-C(58)-H(58) | 107.1 |
| Cl(12)-C(58)-Cl(14) | 112.6(3) |
| Cl(12)-C(58)-Cl(13) | 111.4(3) |
| Cl(12)-C(58)-H(58) | 107.1 |
| Cl(15)-C(59)-Cl(17) | 113.1(4) |
| Cl(15)-C(59)-Cl(16) | 109.8(4) |
| Cl(15)-C(59)-H(59) | 107.6 |
| Cl(17)-C(59)-Cl(16) | 110.9(4) |
| Cl(17)-C(59)-H(59) | 107.6 |
| Cl(16)-C(59)-H(59) | 107.6 |

| Table 7. Bond lengths [Å] and angles [°] for [6][$BPh_4$]•1.5$CH_2Cl_2$ | |
|---|---|
| **Bond lengths** | |
| Sb(1)-Ni(1) | 2.3548(9) |
| Sb(1)-C(1) | 2.117(6) |
| Sb(1)-C(19) | 2.103(5) |
| Sb(1)-C(37) | 2.110(6) |
| Ni(1)-Cl(1) | 2.2425(16) |
| Ni(1)-P(1) | 2.3160(16) |
| Ni(1)-P(2) | 2.3024(16) |
| Ni(1)-P(3) | 2.3013(17) |
| Cl(2)-C(79) | 1.750(10) |
| Cl(3)-C(79) | 1.763(12) |
| P(1)-C(2) | 1.831(6) |
| P(1)-C(7) | 1.836(6) |
| P(1)-C(13) | 1.835(6) |
| P(2)-C(20) | 1.842(6) |
| P(2)-C(25) | 1.828(6) |
| P(2)-C(31) | 1.825(6) |
| P(3)-C(38) | 1.836(6) |
| P(3)-C(43) | 1.826(6) |
| P(3)-C(49) | 1.817(6) |
| C(1)-C(2) | 1.403(8) |
| C(1)-C(6) | 1.392(8) |
| C(2)-C(3) | 1.412(8) |
| C(3)-H(3) | 0.9500 |
| C(3)-C(4) | 1.394(9) |
| C(4)-H(4) | 0.9500 |
| C(4)-C(5) | 1.383(9) |
| C(5)-H(5) | 0.9500 |
| C(5)-C(6) | 1.383(8) |
| C(6)-H(6) | 0.9500 |
| C(7)-C(8) | 1.386(8) |
| C(7)-C(12) | 1.401(8) |
| C(8)-H(8) | 0.9500 |
| C(8)-C(9) | 1.389(9) |
| C(9)-H(9) | 0.9500 |
| C(9)-C(10) | 1.382(9) |
| C(10)-H(10) | 0.9500 |
| C(10)-C(11) | 1.373(10) |
| C(11)-H(11) | 0.9500 |
| C(11)-C(12) | 1.394(9) |
| C(12)-H(12) | 0.9500 |
| C(13)-C(14) | 1.409(8) |
| C(13)-C(18) | 1.400(8) |
| C(14)-H(14) | 0.9500 |
| C(14)-C(15) | 1.386(9) |
| C(15)-H(15) | 0.9500 |
| C(15)-C(16) | 1.393(9) |
| C(16)-H(16) | 0.9500 |
| C(16)-C(17) | 1.366(9) |
| C(17)-H(17) | 0.9500 |
| C(17)-C(18) | 1.397(8) |
| C(18)-H(18) | 0.9500 |
| C(19)-C(20) | 1.398(8) |
| C(19)-C(24) | 1.396(8) |
| C(20)-C(21) | 1.401(8) |
| C(21)-H(21) | 0.9500 |
| C(21)-C(22) | 1.383(9) |
| C(22)-H(22) | 0.9500 |
| C(22)-C(23) | 1.396(9) |
| C(23)-H(23) | 0.9500 |
| C(23)-C(24) | 1.387(8) |
| C(24)-H(24) | 0.9500 |
| C(25)-C(26) | 1.407(8) |
| C(25)-C(30) | 1.386(8) |
| C(26)-H(26) | 0.9500 |
| C(26)-C(27) | 1.387(8) |
| C(27)-H(27) | 0.9500 |
| C(27)-C(28) | 1.388(8) |
| C(28)-H(28) | 0.9500 |
| C(28)-C(29) | 1.385(9) |
| C(29)-H(29) | 0.9500 |
| C(29)-C(30) | 1.395(8) |
| C(30)-H(30) | 0.9500 |
| C(31)-C(32) | 1.385(8) |
| C(31)-C(36) | 1.399(8) |
| C(32)-H(32) | 0.9500 |
| C(32)-C(33) | 1.385(8) |
| C(33)-H(33) | 0.9500 |
| C(33)-C(34) | 1.382(9) |
| C(34)-H(34) | 0.9500 |
| C(34)-C(35) | 1.368(9) |
| C(35)-H(35) | 0.9500 |
| C(35)-C(36) | 1.386(8) |
| C(36)-H(36) | 0.9500 |
| C(37)-C(38) | 1.403(9) |
| C(37)-C(42) | 1.396(9) |
| C(38)-C(39) | 1.398(9) |
| C(39)-H(39) | 0.9500 |
| C(39)-C(40) | 1.377(9) |
| C(40)-H(40) | 0.9500 |
| C(40)-C(41) | 1.400(10) |
| C(41)-H(41) | 0.9500 |
| C(41)-C(42) | 1.398(9) |
| C(42)-H(42) | 0.9500 |
| C(43)-C(44) | 1.406(8) |
| C(43)-C(48) | 1.393(9) |
| C(44)-H(44) | 0.9500 |
| C(44)-C(45) | 1.371(9) |
| C(45)-H(45) | 0.9500 |
| C(45)-C(46) | 1.383(11) |
| C(46)-H(46) | 0.9500 |
| C(46)-C(47) | 1.381(11) |
| C(47)-H(47) | 0.9500 |
| C(47)-C(48) | 1.388(9) |
| C(48)-H(48) | 0.9500 |
| C(49)-C(50) | 1.409(9) |
| C(49)-C(54) | 1.386(9) |
| C(50)-H(50) | 0.9500 |
| C(50)-C(51) | 1.386(9) |
| C(51)-H(51) | 0.9500 |
| C(51)-C(52) | 1.362(10) |
| C(52)-H(52) | 0.9500 |
| C(52)-C(53) | 1.371(11) |
| C(53)-H(53) | 0.9500 |
| C(53)-C(54) | 1.418(10) |
| C(54)-H(54) | 0.9500 |
| C(55)-C(56) | 1.401(9) |
| C(55)-C(60) | 1.396(9) |
| C(55)-B(1) | 1.649(9) |
| C(56)-H(56) | 0.9500 |
| C(56)-C(57) | 1.382(10) |
| C(57)-H(57) | 0.9500 |
| C(57)-C(58) | 1.380(11) |
| C(58)-H(58) | 0.9500 |
| C(58)-C(59) | 1.391(11) |
| C(59)-H(59) | 0.9500 |
| C(59)-C(60) | 1.400(9) |
| C(60)-H(60) | 0.9500 |
| C(61)-C(62) | 1.418(9) |
| C(61)-C(66) | 1.404(8) |
| C(61)-B(1) | 1.640(9) |
| C(62)-H(62) | 0.9500 |
| C(62)-C(63) | 1.393(9) |
| C(63)-H(63) | 0.9500 |
| C(63)-C(64) | 1.384(9) |
| C(64)-H(64) | 0.9500 |
| C(64)-C(65) | 1.389(10) |
| C(65)-H(65) | 0.9500 |
| C(65)-C(66) | 1.397(9) |
| C(66)-H(66) | 0.9500 |
| C(67)-C(68) | 1.415(9) |
| C(67)-C(72) | 1.389(9) |
| C(67)-B(1) | 1.657(9) |
| C(68)-H(68) | 0.9500 |
| C(68)-C(69) | 1.399(9) |
| C(69)-H(69) | 0.9500 |
| C(69)-C(70) | 1.376(11) |
| C(70)-H(70) | 0.9500 |
| C(70)-C(71) | 1.358(10) |
| C(71)-H(71) | 0.9500 |
| C(71)-C(72) | 1.396(9) |
| C(72)-H(72) | 0.9500 |
| C(73)-C(74) | 1.411(8) |
| C(73)-C(78) | 1.400(8) |
| C(73)-B(1) | 1.652(9) |
| C(74)-H(74) | 0.9500 |
| C(74)-C(75) | 1.396(8) |
| C(75)-H(75) | 0.9500 |
| C(75)-C(76) | 1.389(9) |
| C(76)-H(76) | 0.9500 |
| C(76)-C(77) | 1.387(9) |
| C(77)-H(77) | 0.9500 |
| C(77)-C(78) | 1.391(9) |
| C(78)-H(78) | 0.9500 |
| C(79)-H(79A) | 0.9900 |
| C(79)-H(79B) | 0.9900 |
| C(80)-H(80A) | 0.9900 |
| C(80)-H(80B) | 0.9900 |
| C(80)-Cl(4) | 1.799(14) |
| C(80)-Cl(5) | 1.758(15) |
| Sb(1)-Ni(1) | 2.3548(9) |
| Sb(1)-C(1) | 2.117(6) |
| Sb(1)-C(19) | 2.103(5) |
| Sb(1)-C(37) | 2.110(6) |
| Ni(1)-Cl(1) | 2.2425(16) |
| Ni(1)-P(1) | 2.3160(16) |
| Ni(1)-P(2) | 2.3024(16) |
| Ni(1)-P(3) | 2.3013(17) |
| **Angles** | |
| C(1)-Sb(1)-Ni(1) | 107.48(17) |
| C(19)-Sb(1)-Ni(1) | 107.67(17) |
| C(19)-Sb(1)-C(1) | 112.7(2) |
| C(19)-Sb(1)-C(37) | 109.1(2) |
| C(37)-Sb(1)-Ni(1) | 107.99(18) |
| C(37)-Sb(1)-C(1) | 111.7(2) |
| Cl(1)-Ni(1)-Sb(1) | 177.31(5) |
| Cl(1)-Ni(1)-P(1) | 97.31(6) |
| Cl(1)-Ni(1)-P(2) | 93.53(6) |
| Cl(1)-Ni(1)-P(3) | 95.19(6) |
| P(1)-Ni(1)-Sb(1) | 85.09(5) |
| P(2)-Ni(1)-Sb(1) | 84.40(5) |
| P(2)-Ni(1)-P(1) | 113.02(6) |
| P(3)-Ni(1)-Sb(1) | 84.62(5) |
| P(3)-Ni(1)-P(1) | 119.75(6) |

| | |
|---|---|
| P(3)-Ni(1)-P(2) | 124.68(6) |
| C(2)-P(1)-Ni(1) | 114.70(19) |
| C(2)-P(1)-C(7) | 102.4(3) |
| C(2)-P(1)-C(13) | 103.0(3) |
| C(7)-P(1)-Ni(1) | 118.78(18) |
| C(13)-P(1)-Ni(1) | 112.9(2) |
| C(13)-P(1)-C(7) | 103.2(3) |
| C(20)-P(2)-Ni(1) | 114.49(19) |
| C(25)-P(2)-Ni(1) | 111.63(18) |
| C(25)-P(2)-C(20) | 103.5(3) |
| C(31)-P(2)-Ni(1) | 120.1(2) |
| C(31)-P(2)-C(20) | 103.2(3) |
| C(31)-P(2)-C(25) | 102.0(3) |
| C(38)-P(3)-Ni(1) | 115.4(2) |
| C(43)-P(3)-Ni(1) | 121.3(2) |
| C(43)-P(3)-C(38) | 99.1(3) |
| C(49)-P(3)-Ni(1) | 110.0(2) |
| C(49)-P(3)-C(38) | 104.1(3) |
| C(49)-P(3)-C(43) | 105.1(3) |
| C(2)-C(1)-Sb(1) | 112.9(4) |
| C(6)-C(1)-Sb(1) | 126.0(4) |
| C(6)-C(1)-C(2) | 121.1(5) |
| C(1)-C(2)-P(1) | 119.8(4) |
| C(1)-C(2)-C(3) | 118.3(5) |
| C(3)-C(2)-P(1) | 121.8(4) |
| C(2)-C(3)-H(3) | 120.1 |
| C(4)-C(3)-C(2) | 119.8(6) |
| C(4)-C(3)-H(3) | 120.1 |
| C(3)-C(4)-H(4) | 119.7 |
| C(5)-C(4)-C(3) | 120.6(5) |
| C(5)-C(4)-H(4) | 119.7 |
| C(4)-C(5)-H(5) | 119.8 |
| C(6)-C(5)-C(4) | 120.4(6) |
| C(6)-C(5)-H(5) | 119.8 |
| C(1)-C(6)-H(6) | 120.2 |
| C(5)-C(6)-C(1) | 119.6(6) |
| C(5)-C(6)-H(6) | 120.2 |
| C(8)-C(7)-P(1) | 120.1(5) |
| C(8)-C(7)-C(12) | 118.4(6) |
| C(12)-C(7)-P(1) | 121.6(5) |
| C(7)-C(8)-H(8) | 119.5 |
| C(7)-C(8)-C(9) | 121.0(6) |
| C(9)-C(8)-H(8) | 119.5 |
| C(8)-C(9)-H(9) | 120.0 |
| C(10)-C(9)-C(8) | 120.0(6) |
| C(10)-C(9)-H(9) | 120.0 |
| C(9)-C(10)-H(10) | 120.1 |
| C(11)-C(10)-C(9) | 119.9(6) |
| C(11)-C(10)-H(10) | 120.1 |
| C(10)-C(11)-H(11) | 119.8 |
| C(10)-C(11)-C(12) | 120.5(6) |
| C(12)-C(11)-H(11) | 119.8 |
| C(7)-C(12)-H(12) | 120.0 |
| C(11)-C(12)-C(7) | 120.1(6) |
| C(11)-C(12)-H(12) | 120.0 |
| C(14)-C(13)-P(1) | 118.3(5) |
| C(18)-C(13)-P(1) | 123.7(5) |
| C(18)-C(13)-C(14) | 117.9(5) |
| C(13)-C(14)-H(14) | 119.6 |
| C(15)-C(14)-C(13) | 120.7(6) |
| C(15)-C(14)-H(14) | 119.6 |
| C(14)-C(15)-H(15) | 119.9 |
| C(14)-C(15)-C(16) | 120.2(6) |
| C(16)-C(15)-H(15) | 119.9 |
| C(15)-C(16)-H(16) | 120.1 |
| C(17)-C(16)-C(15) | 119.7(6) |
| C(17)-C(16)-H(16) | 120.1 |
| C(16)-C(17)-H(17) | 119.6 |
| C(16)-C(17)-C(18) | 120.9(6) |
| C(18)-C(17)-H(17) | 119.6 |
| C(13)-C(18)-H(18) | 119.8 |
| C(17)-C(18)-C(13) | 120.4(6) |
| C(17)-C(18)-H(18) | 119.8 |
| C(20)-C(19)-Sb(1) | 112.8(4) |
| C(24)-C(19)-Sb(1) | 125.0(4) |
| C(24)-C(19)-C(20) | 121.9(5) |
| C(19)-C(20)-P(2) | 118.9(4) |
| C(19)-C(20)-C(21) | 118.0(5) |
| C(21)-C(20)-P(2) | 123.1(5) |
| C(20)-C(21)-H(21) | 119.8 |
| C(22)-C(21)-C(20) | 120.4(6) |
| C(22)-C(21)-H(21) | 119.8 |
| C(21)-C(22)-H(22) | 119.6 |
| C(21)-C(22)-C(23) | 120.9(5) |
| C(23)-C(22)-H(22) | 119.6 |
| C(22)-C(23)-H(23) | 120.1 |
| C(24)-C(23)-C(22) | 119.7(6) |
| C(24)-C(23)-H(23) | 120.1 |
| C(19)-C(24)-H(24) | 120.5 |
| C(23)-C(24)-C(19) | 119.1(6) |
| C(23)-C(24)-H(24) | 120.5 |
| C(26)-C(25)-P(2) | 117.7(4) |
| C(30)-C(25)-P(2) | 122.4(5) |
| C(30)-C(25)-C(26) | 119.8(5) |
| C(25)-C(26)-H(26) | 120.2 |
| C(27)-C(26)-C(25) | 119.6(5) |
| C(27)-C(26)-H(26) | 120.2 |
| C(26)-C(27)-H(27) | 120.1 |
| C(26)-C(27)-C(28) | 119.9(6) |
| C(28)-C(27)-H(27) | 120.1 |
| C(27)-C(28)-H(28) | 119.5 |
| C(29)-C(28)-C(27) | 120.9(6) |
| C(29)-C(28)-H(28) | 119.5 |
| C(28)-C(29)-H(29) | 120.3 |
| C(28)-C(29)-C(30) | 119.4(6) |
| C(30)-C(29)-H(29) | 120.3 |
| C(25)-C(30)-C(29) | 120.3(6) |
| C(25)-C(30)-H(30) | 119.8 |
| C(29)-C(30)-H(30) | 119.8 |
| C(32)-C(31)-P(2) | 120.1(4) |
| C(32)-C(31)-C(36) | 118.8(5) |
| C(36)-C(31)-P(2) | 120.8(5) |
| C(31)-C(32)-H(32) | 120.0 |
| C(33)-C(32)-C(31) | 120.0(6) |
| C(33)-C(32)-H(32) | 120.0 |
| C(32)-C(33)-H(33) | 119.6 |
| C(34)-C(33)-C(32) | 120.8(6) |
| C(34)-C(33)-H(33) | 119.6 |
| C(33)-C(34)-H(34) | 120.3 |
| C(35)-C(34)-C(33) | 119.5(6) |
| C(35)-C(34)-H(34) | 120.3 |
| C(34)-C(35)-H(35) | 119.7 |
| C(34)-C(35)-C(36) | 120.6(6) |
| C(36)-C(35)-H(35) | 119.7 |
| C(31)-C(36)-H(36) | 119.9 |
| C(35)-C(36)-C(31) | 120.2(6) |
| C(35)-C(36)-H(36) | 119.9 |
| C(38)-C(37)-Sb(1) | 112.6(4) |
| C(42)-C(37)-Sb(1) | 126.4(5) |
| C(42)-C(37)-C(38) | 121.0(6) |
| C(37)-C(38)-P(3) | 119.4(5) |
| C(39)-C(38)-P(3) | 122.0(5) |
| C(39)-C(38)-C(37) | 118.5(6) |
| C(38)-C(39)-H(39) | 119.5 |
| C(40)-C(39)-C(38) | 121.0(6) |
| C(40)-C(39)-H(39) | 119.5 |
| C(39)-C(40)-H(40) | 119.8 |
| C(39)-C(40)-C(41) | 120.3(6) |
| C(41)-C(40)-H(40) | 119.8 |
| C(40)-C(41)-H(41) | 120.1 |
| C(42)-C(41)-C(40) | 119.8(6) |
| C(42)-C(41)-H(41) | 120.1 |
| C(37)-C(42)-C(41) | 119.3(6) |
| C(37)-C(42)-H(42) | 120.4 |
| C(41)-C(42)-H(42) | 120.4 |
| C(44)-C(43)-P(3) | 117.1(5) |
| C(48)-C(43)-P(3) | 123.4(5) |
| C(48)-C(43)-C(44) | 118.8(6) |
| C(43)-C(44)-H(44) | 119.5 |
| C(45)-C(44)-C(43) | 120.9(7) |
| C(45)-C(44)-H(44) | 119.5 |
| C(44)-C(45)-H(45) | 120.2 |
| C(44)-C(45)-C(46) | 119.5(7) |
| C(46)-C(45)-H(45) | 120.2 |
| C(45)-C(46)-H(46) | 119.7 |
| C(47)-C(46)-C(45) | 120.6(7) |
| C(47)-C(46)-H(46) | 119.7 |
| C(46)-C(47)-H(47) | 119.9 |
| C(46)-C(47)-C(48) | 120.1(7) |
| C(48)-C(47)-H(47) | 119.9 |
| C(43)-C(48)-H(48) | 120.1 |
| C(47)-C(48)-C(43) | 119.9(6) |
| C(47)-C(48)-H(48) | 120.1 |
| C(50)-C(49)-P(3) | 118.6(5) |
| C(54)-C(49)-P(3) | 122.3(5) |
| C(54)-C(49)-C(50) | 118.7(6) |
| C(49)-C(50)-H(50) | 119.8 |
| C(51)-C(50)-C(49) | 120.4(7) |
| C(51)-C(50)-H(50) | 119.8 |
| C(50)-C(51)-H(51) | 119.7 |
| C(52)-C(51)-C(50) | 120.7(7) |
| C(52)-C(51)-H(51) | 119.7 |
| C(51)-C(52)-H(52) | 119.8 |
| C(51)-C(52)-C(53) | 120.3(7) |
| C(53)-C(52)-H(52) | 119.8 |
| C(52)-C(53)-H(53) | 119.8 |
| C(52)-C(53)-C(54) | 120.4(7) |
| C(54)-C(53)-H(53) | 119.8 |
| C(49)-C(54)-C(53) | 119.6(7) |
| C(49)-C(54)-H(54) | 120.2 |
| C(53)-C(54)-H(54) | 120.2 |
| C(56)-C(55)-B(1) | 122.7(6) |
| C(60)-C(55)-C(56) | 114.7(6) |
| C(60)-C(55)-B(1) | 122.5(5) |
| C(55)-C(56)-H(56) | 118.1 |
| C(57)-C(56)-C(55) | 123.9(7) |
| C(57)-C(56)-H(56) | 118.1 |
| C(56)-C(57)-H(57) | 120.2 |
| C(58)-C(57)-C(56) | 119.5(7) |
| C(58)-C(57)-H(57) | 120.2 |
| C(57)-C(58)-H(58) | 120.2 |
| C(57)-C(58)-C(59) | 119.6(7) |
| C(59)-C(58)-H(58) | 120.2 |
| C(58)-C(59)-H(59) | 120.4 |
| C(58)-C(59)-C(60) | 119.2(7) |
| C(60)-C(59)-H(59) | 120.4 |
| C(55)-C(60)-C(59) | 123.1(7) |
| C(55)-C(60)-H(60) | 118.4 |

| | |
|---|---|
| C(59)-C(60)-H(60) | 118.4 |
| C(62)-C(61)-B(1) | 121.5(5) |
| C(66)-C(61)-C(62) | 114.7(6) |
| C(66)-C(61)-B(1) | 123.8(6) |
| C(61)-C(62)-H(62) | 118.6 |
| C(63)-C(62)-C(61) | 122.9(6) |
| C(63)-C(62)-H(62) | 118.6 |
| C(62)-C(63)-H(63) | 119.9 |
| C(64)-C(63)-C(62) | 120.2(6) |
| C(64)-C(63)-H(63) | 119.9 |
| C(63)-C(64)-H(64) | 120.5 |
| C(63)-C(64)-C(65) | 118.9(6) |
| C(65)-C(64)-H(64) | 120.5 |
| C(64)-C(65)-H(65) | 119.8 |
| C(64)-C(65)-C(66) | 120.3(6) |
| C(66)-C(65)-H(65) | 119.8 |
| C(61)-C(66)-H(66) | 118.6 |
| C(65)-C(66)-C(61) | 122.8(6) |
| C(65)-C(66)-H(66) | 118.6 |
| C(68)-C(67)-B(1) | 120.5(6) |
| C(72)-C(67)-C(68) | 114.4(6) |
| C(72)-C(67)-B(1) | 125.1(6) |
| C(67)-C(68)-H(68) | 118.5 |
| C(69)-C(68)-C(67) | 122.9(7) |
| C(69)-C(68)-H(68) | 118.5 |
| C(68)-C(69)-H(69) | 120.4 |
| C(70)-C(69)-C(68) | 119.1(7) |
| C(70)-C(69)-H(69) | 120.4 |
| C(69)-C(70)-H(70) | 119.9 |
| C(71)-C(70)-C(69) | 120.3(7) |
| C(71)-C(70)-H(70) | 119.9 |
| C(70)-C(71)-H(71) | 120.0 |
| C(70)-C(71)-C(72) | 120.0(7) |
| C(72)-C(71)-H(71) | 120.0 |
| C(67)-C(72)-C(71) | 123.3(7) |
| C(67)-C(72)-H(72) | 118.4 |
| C(71)-C(72)-H(72) | 118.4 |
| C(74)-C(73)-B(1) | 122.5(5) |
| C(78)-C(73)-C(74) | 113.8(5) |
| C(78)-C(73)-B(1) | 123.5(5) |
| C(73)-C(74)-H(74) | 118.3 |
| C(75)-C(74)-C(73) | 123.3(6) |
| C(75)-C(74)-H(74) | 118.3 |
| C(74)-C(75)-H(75) | 119.9 |
| C(76)-C(75)-C(74) | 120.2(6) |
| C(76)-C(75)-H(75) | 119.9 |
| C(75)-C(76)-H(76) | 120.8 |
| C(77)-C(76)-C(75) | 118.4(6) |
| C(77)-C(76)-H(76) | 120.8 |
| C(76)-C(77)-H(77) | 120.0 |
| C(76)-C(77)-C(78) | 120.1(6) |
| C(78)-C(77)-H(77) | 120.0 |
| C(73)-C(78)-H(78) | 118.0 |
| C(77)-C(78)-C(73) | 124.1(6) |
| C(77)-C(78)-H(78) | 118.0 |
| Cl(2)-C(79)-Cl(3) | 108.6(7) |
| Cl(2)-C(79)-H(79A) | 110.0 |
| Cl(2)-C(79)-H(79B) | 110.0 |
| Cl(3)-C(79)-H(79A) | 110.0 |
| Cl(3)-C(79)-H(79B) | 110.0 |
| H(79A)-C(79)-H(79B) | 108.3 |
| H(80A)-C(80)-H(80B) | 108.4 |
| Cl(4)-C(80)-H(80A) | 110.0 |
| Cl(4)-C(80)-H(80B) | 110.0 |
| Cl(5)-C(80)-H(80A) | 110.0 |
| Cl(5)-C(80)-H(80B) | 110.0 |
| Cl(5)-C(80)-Cl(4) | 108.4(9) |
| C(55)-B(1)-C(67) | 110.8(5) |
| C(55)-B(1)-C(73) | 107.5(5) |
| C(61)-B(1)-C(55) | 107.9(5) |
| C(61)-B(1)-C(67) | 111.9(5) |
| C(61)-B(1)-C(73) | 109.8(5) |
| C(73)-B(1)-C(67) | 108.8(5) |
| C(1)-Sb(1)-Ni(1) | 107.48(17) |
| C(19)-Sb(1)-Ni(1) | 107.67(17) |
| C(19)-Sb(1)-C(1) | 112.7(2) |
| C(19)-Sb(1)-C(37) | 109.1(2) |
| C(37)-Sb(1)-Ni(1) | 107.99(18) |
| C(37)-Sb(1)-C(1) | 111.7(2) |
| Cl(1)-Ni(1)-Sb(1) | 177.31(5) |
| Cl(1)-Ni(1)-P(1) | 97.31(6) |
| Cl(1)-Ni(1)-P(2) | 93.53(6) |
| Cl(1)-Ni(1)-P(3) | 95.19(6) |
| P(1)-Ni(1)-Sb(1) | 85.09(5) |
| P(2)-Ni(1)-Sb(1) | 84.40(5) |
| P(2)-Ni(1)-P(1) | 113.02(6) |
| P(3)-Ni(1)-Sb(1) | 84.62(5) |
| P(3)-Ni(1)-P(1) | 119.75(6) |
| P(3)-Ni(1)-P(2) | 124.68(6) |
| C(2)-P(1)-Ni(1) | 114.70(19) |
| C(2)-P(1)-C(7) | 102.4(3) |
| C(2)-P(1)-C(13) | 103.0(3) |
| C(7)-P(1)-Ni(1) | 118.78(18) |
| C(13)-P(1)-Ni(1) | 112.9(2) |
| C(13)-P(1)-C(7) | 103.2(3) |
| C(20)-P(2)-Ni(1) | 114.49(19) |
| C(25)-P(2)-Ni(1) | 111.63(18) |

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

**Table 8. XYZ coordinates for the optimized structure of $[4]^+$**

| | | | |
|---|---|---|---|
| Ni | -0.292681 | 0.003853 | 0.001431 |
| Cl | -2.507231 | 0.006464 | -0.006401 |
| P | 1.833468 | 0.001447 | 0.005363 |
| P | -0.149441 | 0.365804 | 2.258321 |
| P | -0.146783 | -2.132371 | -0.813323 |
| P | -0.142578 | 1.769182 | -1.445455 |
| C | 2.518673 | -0.091085 | 1.692275 |
| C | 3.855946 | -0.392163 | 1.989083 |
| H | 4.555962 | -0.636391 | 1.199595 |
| C | 4.285282 | -0.422696 | 3.314357 |
| H | 5.317496 | -0.661272 | 3.539897 |
| C | 3.383380 | -0.167784 | 4.350840 |
| H | 3.717570 | -0.203439 | 5.380490 |
| C | 2.046940 | 0.102648 | 4.063923 |
| H | 1.338124 | 0.248841 | 4.870748 |
| C | 1.604120 | 0.148123 | 2.734160 |
| C | -0.641206 | 2.025343 | 2.835222 |
| C | 0.204824 | 2.849692 | 3.592824 |
| H | -3.683240 | 5.252481 | -1.864232 |
| C | -1.513732 | 1.003074 | -5.798521 |
| C | -0.212646 | 1.449986 | -5.565784 |
| H | 1.243416 | 2.023657 | -4.099846 |
| C | -1.013594 | 5.407061 | 0.231656 |
| C | -1.916035 | 0.937666 | -3.413576 |
| C | -2.191429 | 5.796157 | -0.409493 |
| H | 0.411254 | 4.710413 | 4.647392 |
| C | -2.166208 | -0.430270 | 4.088675 |
| H | -2.578405 | 1.872079 | 1.888815 |
| C | -2.756309 | -1.326650 | 4.981307 |
| H | -1.905175 | 5.457201 | 4.157329 |
| H | -3.390678 | 4.034218 | 2.764043 |
| H | 1.214516 | 2.534980 | 3.825100 |
| H | -2.564477 | 0.695453 | -2.578686 |
| C | -2.169631 | 3.739891 | -1.686306 |
| H | -2.662206 | -3.497929 | -5.764877 |
| H | -0.536744 | -2.209345 | -5.736021 |
| C | -1.923721 | -3.415332 | 0.890801 |
| H | 4.555896 | 1.352676 | -0.030399 |
| C | -0.986448 | -2.570098 | -2.379089 |
| C | 2.521702 | 1.508870 | -0.756160 |
| H | -3.669651 | -1.046748 | 5.492426 |
| H | 1.350465 | 4.090334 | -2.647136 |
| C | -0.620773 | 1.431842 | -3.173404 |
| H | 0.504509 | -2.323589 | 3.146632 |
| C | 3.858947 | -1.516732 | -1.323860 |
| C | 4.291527 | -2.646425 | -2.015469 |
| C | 3.390786 | -3.670095 | -2.320864 |
| H | 3.727171 | -4.541992 | -2.868405 |
| H | 1.345867 | -4.329722 | -2.231621 |
| C | -0.632884 | -3.465536 | 0.333538 |
| H | 1.217215 | -4.586556 | 0.261487 |
| H | -3.723493 | -4.167139 | -3.622068 |
| H | -2.655558 | -3.608095 | -1.479635 |
| H | 0.517354 | -1.603673 | -3.600269 |
| H | 5.324265 | 3.389660 | -1.179906 |
| H | 3.730105 | 4.754860 | -2.503514 |
| H | -2.620513 | -3.254131 | 5.931100 |
| H | -0.528395 | -3.880772 | 4.743831 |
| C | 1.610022 | 2.292155 | -1.486955 |
| H | -1.862577 | 0.852173 | -6.813193 |
| C | 0.233573 | 1.667875 | -4.261251 |
| H | -3.362506 | 0.367905 | -4.892203 |
| C | -0.983323 | 3.345912 | -1.051867 |
| C | -2.360086 | 0.740571 | -4.719901 |
| H | -2.652729 | 6.746814 | -0.170091 |
| H | -0.561174 | 6.048728 | 0.977680 |
| H | -2.619762 | 3.113519 | -2.444715 |
| H | 0.415251 | -6.389478 | 1.730483 |
| H | -3.373787 | -4.403393 | 2.125604 |
| H | -1.893870 | -6.332187 | 2.639623 |
| H | 0.489341 | 3.893227 | 0.437397 |
| C | 1.606293 | -2.432267 | -1.241672 |
| C | -2.192323 | -3.285109 | -2.402276 |
| C | -2.199321 | -3.231932 | -4.822088 |
| H | 5.325127 | -2.721411 | -2.330562 |
| C | 2.520073 | -1.411847 | -0.920154 |
| C | 4.291891 | 3.076339 | -1.276191 |
| C | -1.936491 | 2.475375 | 2.521398 |
| C | -2.374971 | -4.449586 | 1.708855 |
| C | -0.989062 | -2.917128 | 4.564578 |
| C | -0.405170 | -2.172625 | -3.595004 |
| H | -2.623428 | 0.537256 | 3.929786 |
| C | -1.549975 | 4.505650 | 3.779937 |
| C | -0.242928 | -5.562178 | 1.492043 |
| C | 2.056433 | 3.464821 | -2.113210 |
| C | -2.167306 | -2.566654 | 5.226945 |
| C | -0.404463 | -2.033084 | 3.660889 |
| H | 4.557730 | -0.711212 | -1.134760 |
| C | 2.052710 | -3.558451 | -1.948432 |
| C | 0.210405 | -4.539466 | 0.657274 |
| C | -1.539794 | -5.528018 | 2.005597 |
| C | -0.249115 | 4.084773 | 4.058367 |
| C | -2.388249 | 3.701925 | 3.005250 |
| C | -0.979864 | -0.773081 | 3.424925 |
| H | -2.562780 | -2.561091 | 0.695404 |
| C | -2.794981 | -3.608884 | -3.618767 |
| C | -1.002379 | -2.513147 | -4.806583 |
| C | 3.858996 | 1.914649 | -0.639943 |
| C | 3.393212 | 3.846643 | -2.018956 |
| C | -2.769894 | 4.957462 | -1.361691 |
| C | -0.418695 | 4.185963 | -0.077113 |
| H | 0.454152 | 1.641507 | -6.398364 |

**Table 9. XYZ coordinates for the optimized structure of [5]$^+$**

| | | | |
|---|---|---|---|
| As | 1.829345 | -0.002392 | -0.002982 |
| H | -2.652977 | -2.615300 | -6.247016 |
| C | -1.019437 | -1.771581 | -5.123106 |
| H | -0.548835 | -1.317476 | -5.986396 |
| C | -0.440643 | -1.621048 | -3.865229 |
| H | 0.475406 | -1.049428 | -3.767065 |
| C | 2.525192 | 1.651197 | -0.715160 |
| C | 3.873128 | 2.029166 | -0.687414 |
| H | 4.624691 | 1.379496 | -0.255393 |
| C | 4.252086 | 3.271633 | -1.193321 |
| H | 5.293418 | 3.568803 | -1.168923 |
| C | 3.288305 | 4.139890 | -1.713350 |
| H | -3.724646 | -3.634739 | -4.253047 |
| H | 3.583696 | 5.110316 | -2.093094 |
| H | 1.200682 | -0.394251 | 4.915050 |
| C | 1.945185 | 3.769160 | -1.731115 |
| H | 1.197977 | 4.458679 | -2.106844 |
| C | 1.549279 | 2.514533 | -1.241091 |
| C | -0.736499 | 1.874054 | -2.931489 |
| C | -2.042338 | 1.424826 | -3.201472 |
| H | -2.673805 | 1.081799 | -2.389632 |
| C | -2.520584 | 1.402857 | -4.510449 |
| H | -3.531117 | 1.063314 | -4.703079 |
| C | -1.699368 | 1.798058 | -5.567652 |
| H | -2.074816 | 1.782422 | -6.583925 |
| C | -0.389135 | 2.203198 | -5.311982 |
| H | 0.258966 | 2.498028 | -6.129036 |
| C | -1.024802 | -1.260020 | 3.289181 |
| C | -2.219351 | -1.031372 | 3.985913 |
| H | 1.109020 | 2.569383 | -3.824379 |
| C | -1.025430 | 3.479454 | -0.550284 |
| C | -2.221432 | 3.967115 | -1.094793 |
| H | -2.689784 | 3.461316 | -1.928683 |
| C | -2.805396 | 5.126733 | -0.581816 |
| H | -3.725996 | 5.497508 | -1.016386 |
| C | -2.201157 | 5.812858 | 0.471076 |
| H | -2.650251 | 6.719911 | 0.857690 |
| C | -1.012894 | 5.328989 | 1.022596 |
| H | -0.540746 | 5.852337 | 1.844860 |
| C | -0.393863 | -5.697799 | 0.753507 |
| C | -0.433236 | 4.164797 | 0.524217 |
| H | 0.485194 | 3.797539 | 0.967808 |
| H | 5.287205 | -2.807132 | -2.513258 |
| C | 3.280895 | -3.563137 | -2.729413 |
| H | 3.574327 | -4.380009 | -3.377354 |
| C | 1.938372 | -3.390086 | -2.398384 |
| H | 1.189506 | -4.060813 | -2.803674 |
| C | 1.545322 | -2.334848 | -1.560095 |
| C | -0.739434 | -3.473131 | -0.156023 |
| C | 0.087805 | -4.586179 | 0.060189 |
| H | 1.104776 | -4.595966 | -0.310674 |
| C | 0.091588 | 2.245160 | -4.002281 |
| H | 0.253494 | -6.553226 | 0.907649 |
| C | -1.703896 | -5.714839 | 1.232608 |
| H | -2.079854 | -6.585886 | 1.756006 |
| C | -2.524161 | -4.601269 | 1.044659 |
| H | -3.534230 | -4.596272 | 1.436153 |
| C | -2.045288 | -3.480687 | 0.368205 |
| H | -2.675818 | -2.605499 | 0.259168 |
| C | -1.030169 | -2.214084 | -2.735902 |
| C | -2.222932 | -2.934072 | -2.887295 |
| H | -2.689969 | -3.406210 | -2.033184 |
| C | -2.806294 | -3.069513 | -4.148269 |
| C | -2.204465 | -2.496258 | -5.267976 |
| Ni | -0.378837 | -0.000887 | -0.000557 |
| P | -0.206822 | -2.012938 | -1.116243 |
| P | -0.204355 | 1.973842 | -1.186187 |
| C | 1.549819 | -0.181832 | 2.796782 |
| Cl | -2.583882 | -0.006114 | -0.000744 |
| C | 2.525520 | -0.211442 | 1.785831 |
| P | -0.204051 | 0.041082 | 2.300855 |
| H | 0.250345 | 4.049967 | 5.240375 |
| C | 2.522969 | -1.447382 | -1.079867 |
| H | 0.482221 | -2.735521 | 2.800683 |
| C | -0.433391 | -2.533545 | 3.345034 |
| H | -0.538917 | -4.519709 | 4.149384 |
| H | -2.688746 | -0.056859 | 3.963484 |
| C | -1.011056 | -3.545937 | 4.107325 |
| H | -3.721796 | -1.862738 | 5.275536 |
| C | 0.088531 | 2.339963 | 3.950055 |
| H | -2.080723 | 4.804837 | 4.839884 |
| C | -2.197564 | -3.309165 | 4.804906 |
| H | -2.645384 | -4.096645 | 5.399195 |
| C | 3.870108 | -1.614972 | -1.422600 |
| H | -3.529926 | 3.543612 | 3.263111 |
| H | -2.667764 | 1.535827 | 2.117841 |
| C | -1.703492 | 3.918838 | 4.343145 |
| C | -0.735930 | 1.602365 | 3.086375 |
| C | -2.520839 | 3.205262 | 3.465054 |
| H | 4.623499 | -0.916311 | -1.079146 |
| C | 4.246450 | -2.677747 | -2.242407 |
| C | -2.039994 | 2.063059 | 2.827320 |
| C | -0.394774 | 3.492934 | 4.570963 |
| C | -2.801983 | -2.054444 | 4.736064 |
| H | 1.104215 | 2.021162 | 4.146322 |
| C | 3.873271 | -0.424598 | 2.099305 |
| C | 4.253183 | -0.601701 | 3.428773 |
| H | 5.294631 | -0.770845 | 3.673875 |
| C | 3.290091 | -0.579347 | 4.441199 |
| C | 1.946844 | -0.378991 | 4.128971 |
| H | 3.585956 | -0.730595 | 5.472103 |
| H | 4.624050 | -0.477316 | 1.320172 |

**Table 10. XYZ coordinates for the optimized structure of [6]$^{+}$**

| | | | |
|---|---|---|---|
| C | -1.899265 | 0.284064 | 4.555610 |
| Ni | -0.480778 | 0.094930 | 0.051940 |
| H | -0.149362 | 5.741712 | 3.106238 |
| P | -0.278292 | -2.228026 | -0.385274 |
| P | -0.194001 | 1.454353 | -1.829527 |
| H | -4.043947 | 4.025012 | 2.508386 |
| H | 3.281304 | 1.798663 | 5.619563 |
| C | -0.196424 | 3.623372 | 2.745866 |
| C | -2.968052 | 3.915576 | 2.580498 |
| H | -3.018291 | 1.809971 | 2.150765 |
| C | -2.392114 | 2.658480 | 2.399601 |
| C | -0.997743 | 2.495739 | 2.505415 |
| H | 0.880773 | 3.525928 | 2.807652 |
| H | -2.352358 | 1.259476 | 4.437177 |
| H | -3.006839 | -0.147050 | 6.345670 |
| C | -2.265691 | -0.511334 | 5.643654 |
| H | -1.950598 | -2.366585 | 6.689111 |
| C | -1.671501 | -1.757551 | 5.837162 |
| H | -0.246313 | -3.183860 | 5.073417 |
| C | -0.710903 | -2.215574 | 4.932998 |
| H | 0.389483 | -1.801365 | 3.140740 |
| C | -0.355219 | -1.433091 | 3.837526 |
| C | -0.942988 | -0.173233 | 3.637980 |
| H | 4.674342 | 0.469554 | 1.785733 |
| C | 3.852888 | 0.740375 | 2.440100 |
| H | 5.146453 | 1.210101 | 4.092503 |
| C | 4.121861 | 1.154212 | 3.744075 |
| H | 0.978016 | -0.392904 | -6.324357 |
| C | 3.070453 | 1.485432 | 4.603940 |
| C | 0.201561 | -0.246654 | -5.581962 |
| H | 0.939442 | 1.642026 | 4.847275 |
| C | 1.750017 | 1.406477 | 4.166303 |
| C | 1.461622 | 1.006876 | 2.851315 |
| C | 2.526081 | 0.669359 | 1.997407 |
| H | -1.414227 | 2.798952 | -4.185785 |
| C | -1.650226 | 3.379884 | -3.302467 |
| H | -2.702656 | 4.885281 | -4.416539 |
| C | -2.385769 | 4.557284 | -3.433272 |
| H | -3.292712 | 6.218691 | -2.405733 |
| H | -2.573569 | 5.444054 | -0.157565 |
| H | -1.357752 | -1.077073 | -6.811497 |
| C | -2.716090 | 5.306686 | -2.302962 |
| C | -2.310726 | 4.874163 | -1.040268 |
| H | -1.282152 | 3.357993 | 0.080448 |
| C | -1.577408 | 3.696278 | -0.903727 |
| C | -1.235273 | 2.940718 | -2.032685 |
| H | 1.536264 | 0.673124 | -4.171393 |
| C | 0.518478 | 0.351888 | -4.358961 |
| C | -2.164872 | 5.027481 | 2.845644 |
| H | -2.615739 | 6.002162 | 2.992817 |
| C | -0.778971 | 4.880680 | 2.913823 |
| Sb | 1.866167 | 0.069122 | 0.083237 |
| C | 1.467909 | -2.794311 | -0.591139 |
| C | 2.524750 | -1.885723 | -0.378934 |
| Cl | -2.672638 | 0.199940 | -0.033869 |
| H | -2.747160 | -2.087275 | 1.104185 |
| C | 1.834627 | 3.166288 | -2.890327 |
| C | -2.103969 | -0.452267 | -4.888363 |
| H | 0.724352 | -4.642422 | 1.139756 |
| C | -0.480222 | 0.562030 | -3.398127 |
| C | 4.188593 | 2.951292 | -2.355396 |
| H | -2.654973 | -5.582207 | 3.599591 |
| C | 2.574095 | 1.486434 | -1.316289 |
| H | -2.828508 | -4.412543 | -5.024520 |
| C | -2.347384 | -3.979434 | -4.155173 |
| C | -0.995990 | -3.637077 | -4.198404 |
| H | 4.669262 | -1.579320 | -0.371069 |
| H | -0.423269 | -3.791300 | -5.105340 |
| C | -1.793742 | 0.131141 | -3.662849 |
| C | -2.455970 | -3.224687 | -1.858923 |
| H | -4.129569 | -4.015575 | -2.944781 |
| H | -3.035253 | -3.081968 | -0.956479 |
| C | -3.077374 | -3.758885 | -2.987000 |
| C | -0.372482 | -3.088315 | -3.078393 |
| H | 0.674141 | -2.817223 | -3.139354 |
| C | -0.956573 | -3.288564 | 0.949003 |
| C | -1.089913 | -2.900213 | -1.885973 |
| C | 1.526824 | 2.102033 | -2.029026 |
| C | -2.238054 | -2.983425 | 1.443294 |
| H | 1.042077 | 3.671952 | -3.429553 |
| H | -3.120318 | -0.769135 | -5.088556 |
| H | -2.566478 | 0.266022 | -2.913231 |
| C | -2.846473 | -3.812326 | 2.384721 |
| C | 1.787496 | -4.106671 | -0.982221 |
| P | -0.280907 | 0.837357 | 2.261054 |
| C | -2.178008 | -4.936133 | 2.871720 |
| H | 3.378938 | 4.412496 | -3.712723 |
| C | -0.278023 | -4.401793 | 1.469740 |
| C | 3.899800 | 1.901720 | -1.482144 |
| H | 5.212675 | 3.282200 | -2.482315 |
| C | 3.155571 | 3.586201 | -3.048186 |
| C | -1.109765 | -0.633374 | -5.854040 |
| C | -0.886537 | -5.217031 | 2.425724 |
| H | -3.838792 | -3.569253 | 2.746757 |
| H | 4.705285 | 1.430651 | -0.929325 |
| H | -0.351603 | -6.077236 | 2.812403 |
| C | 3.116542 | -4.501001 | -1.132041 |
| H | 3.343254 | -5.517248 | -1.432281 |
| C | 4.153175 | -3.593594 | -0.903442 |
| C | 3.858898 | -2.282120 | -0.531180 |
| H | 5.184537 | -3.902822 | -1.025933 |
| H | 0.992781 | -4.815853 | -1.184757 |