***Supplementary Information***

# Functional vinyl-1,8-naphthyridine copper(I) complex as efficient synergistic catalyst with KI for N-arylation coupling reactions

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## 1. General information

All the reagents were purchased from commercial suppliers and used without further purification. Column chromatography was carried out with silica gel (200-300 mesh). Thin layer chromatography was carried out using Merck silica gel $GF_{254}$ plates. $^{1}H$ NMR and $^{13}C$ NMR (500/400 MHz and 125/100 MHz, respectively) spectra were recorded on a Bruker MR-500/400 spectrometer. Chemical shifts are reported in ppm from TMS with the solvent resonance as an internal standard ($CDCl_3$: $\delta$ 7.26 ppm, DMSO-$d_6$: $\delta$ 2.54 ppm). Data are reported as follows: chemical shift, integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet) and coupling constants (Hz).

**X-ray Diffraction.** Single crystals of **C1** suitable for X-ray diffraction analysis were grown by slow diffusion of diethyl ether vapors into a dichloromethane solution. The diffraction data were collected on a Rigaku R-AXIS RAPID IP X-Ray diffractometer using a graphite monochromator with MoK$\alpha$ radiation ($\lambda$ = 0.071073 nm) at 293 K. The structures were solved by direct methods and refined by full-matrix least-squares methods on all $F2$ data (SHELX-97). Non-hydrogen atoms were refined anisotropically. The positions of hydrogen atoms were calculated and refined isotropically.

## Figure and Table captions

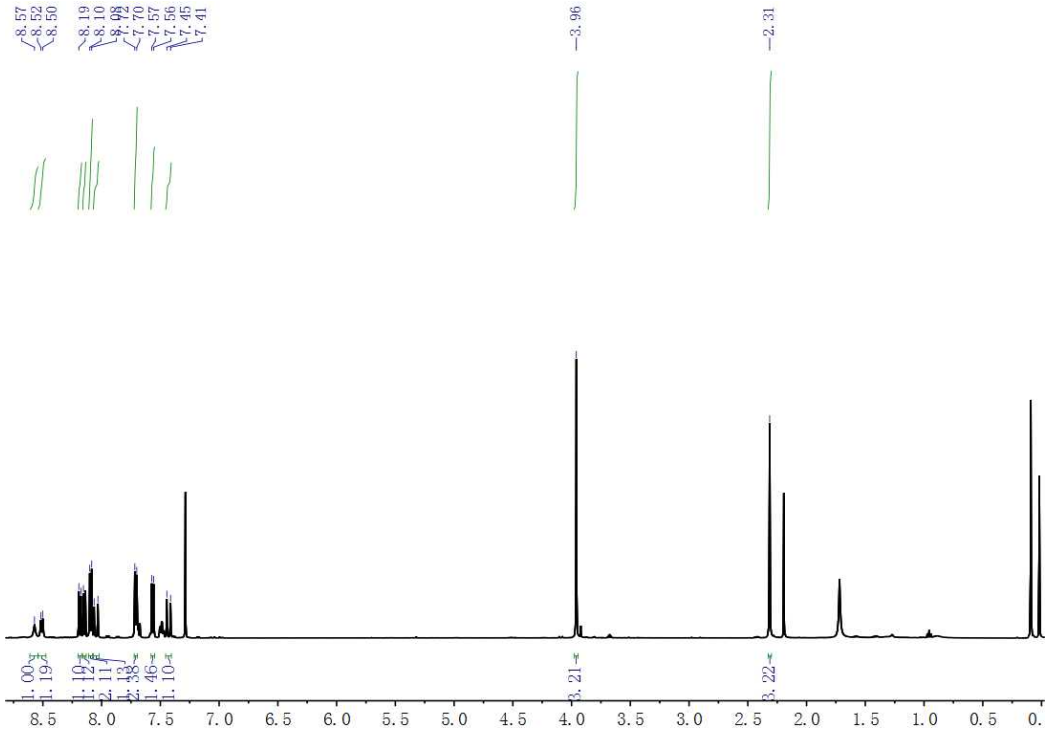


Figure S1 $^{1}H$ NMR spectra of **L1** in $CDCl_3$.

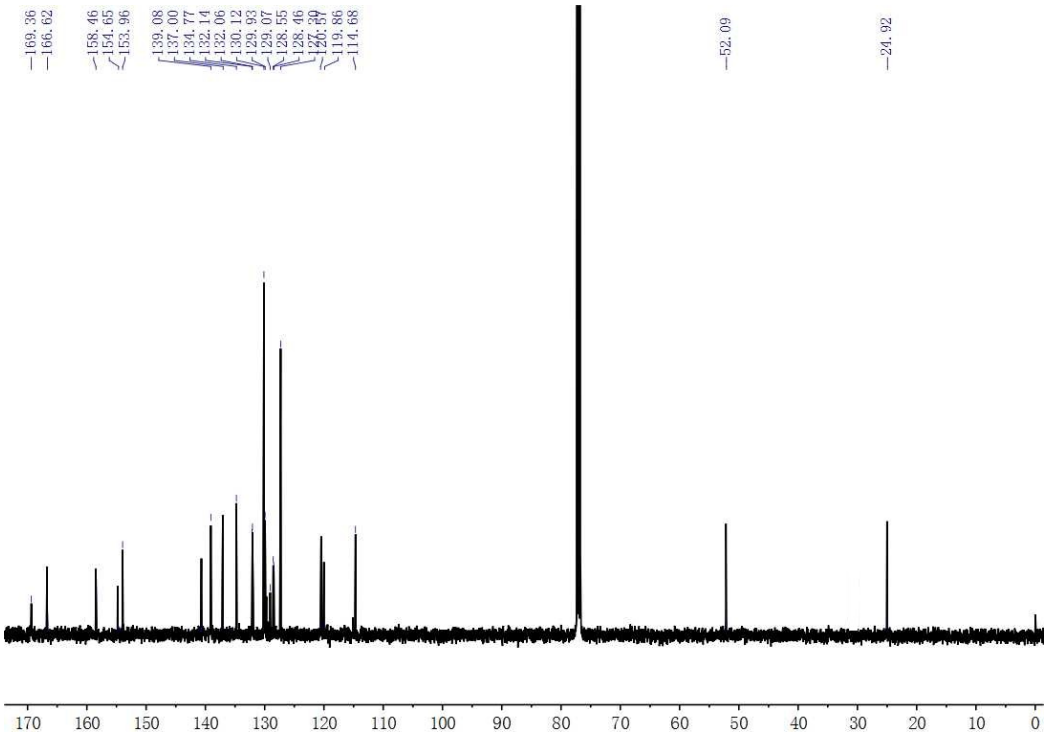


Figure S2 $^{13}C$ NMR spectra of **L1** in $CDCl_3$.

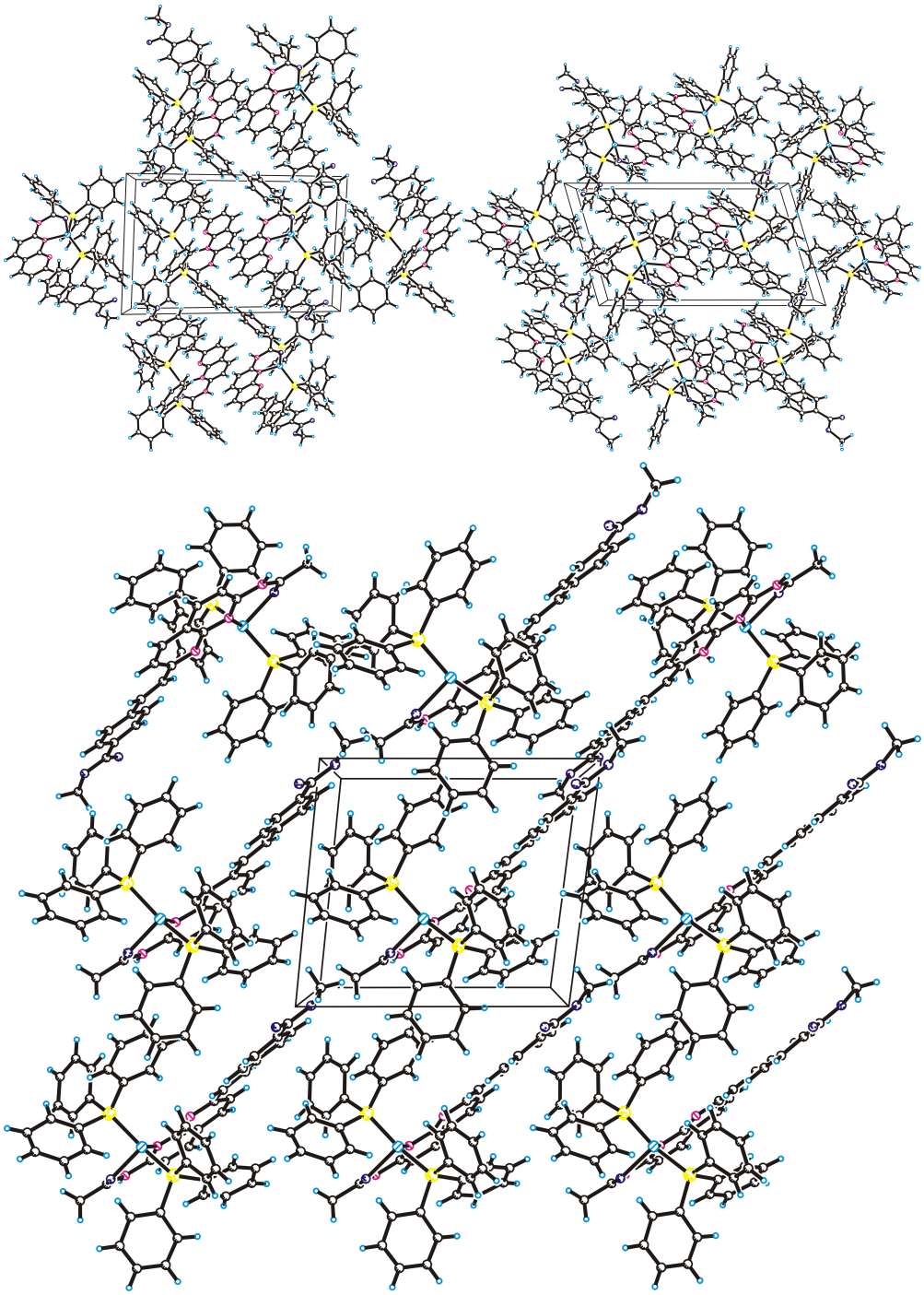

Figure S3. Perspective views and crystal packing diagram of **C1** (X, Y, Z axis).

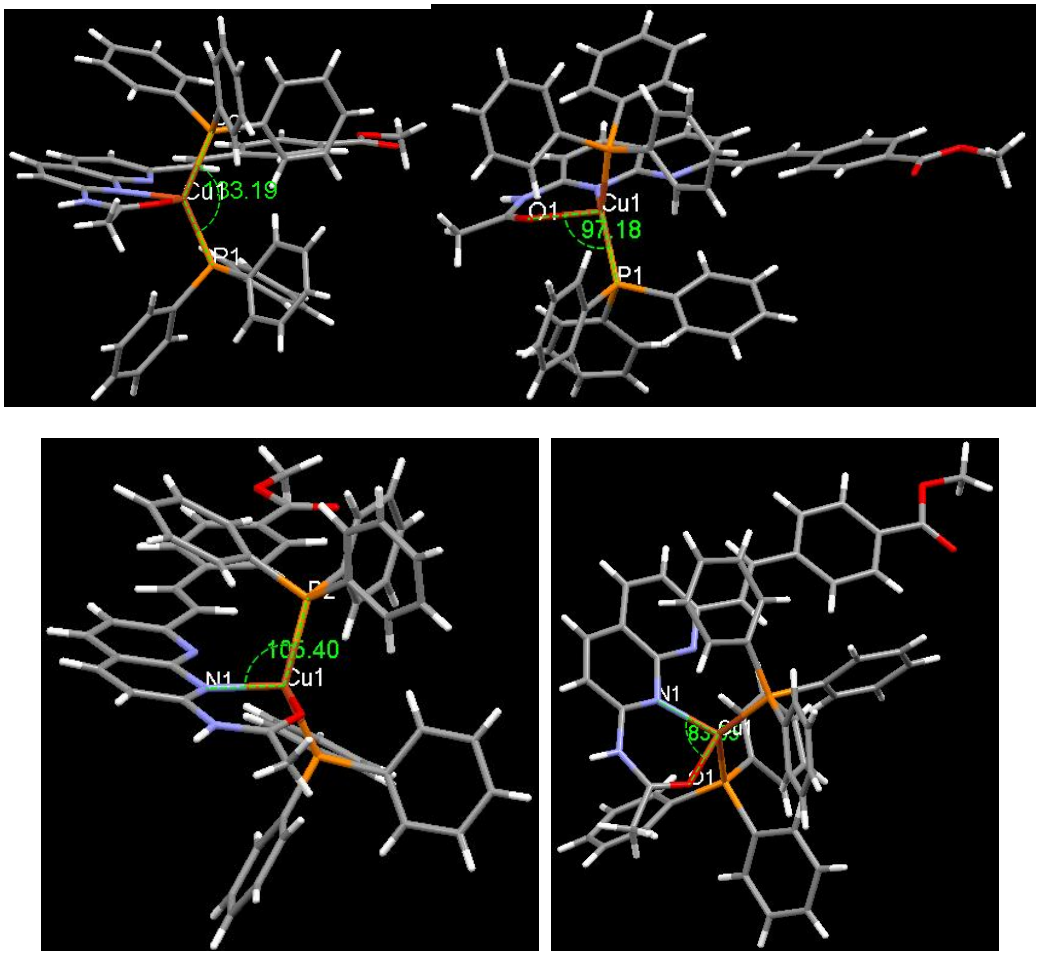


Figure S4. Selected bond angles [deg] around the Cu(Ⅰ) atom of compound **C1**.

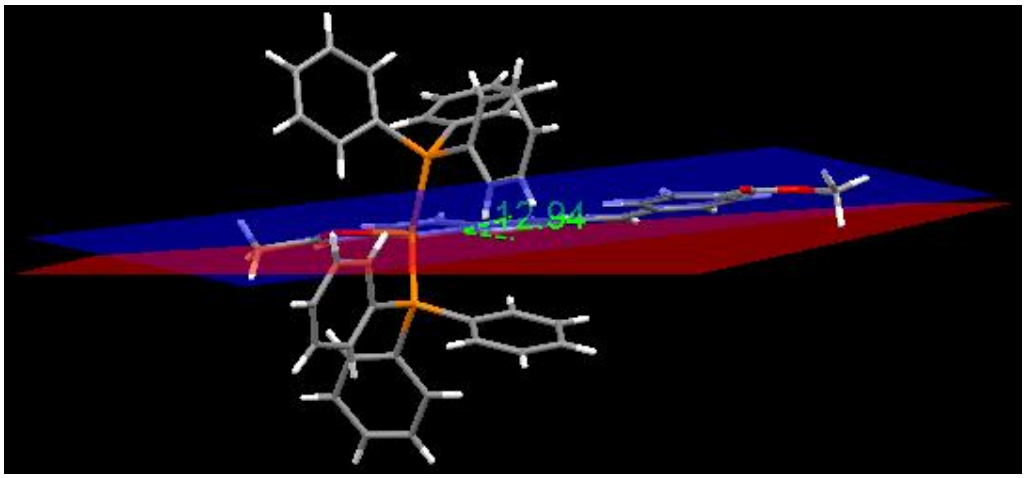


Figure S5. The plane angle [deg] of naphthyridine and benzene ring of compound **C1**.

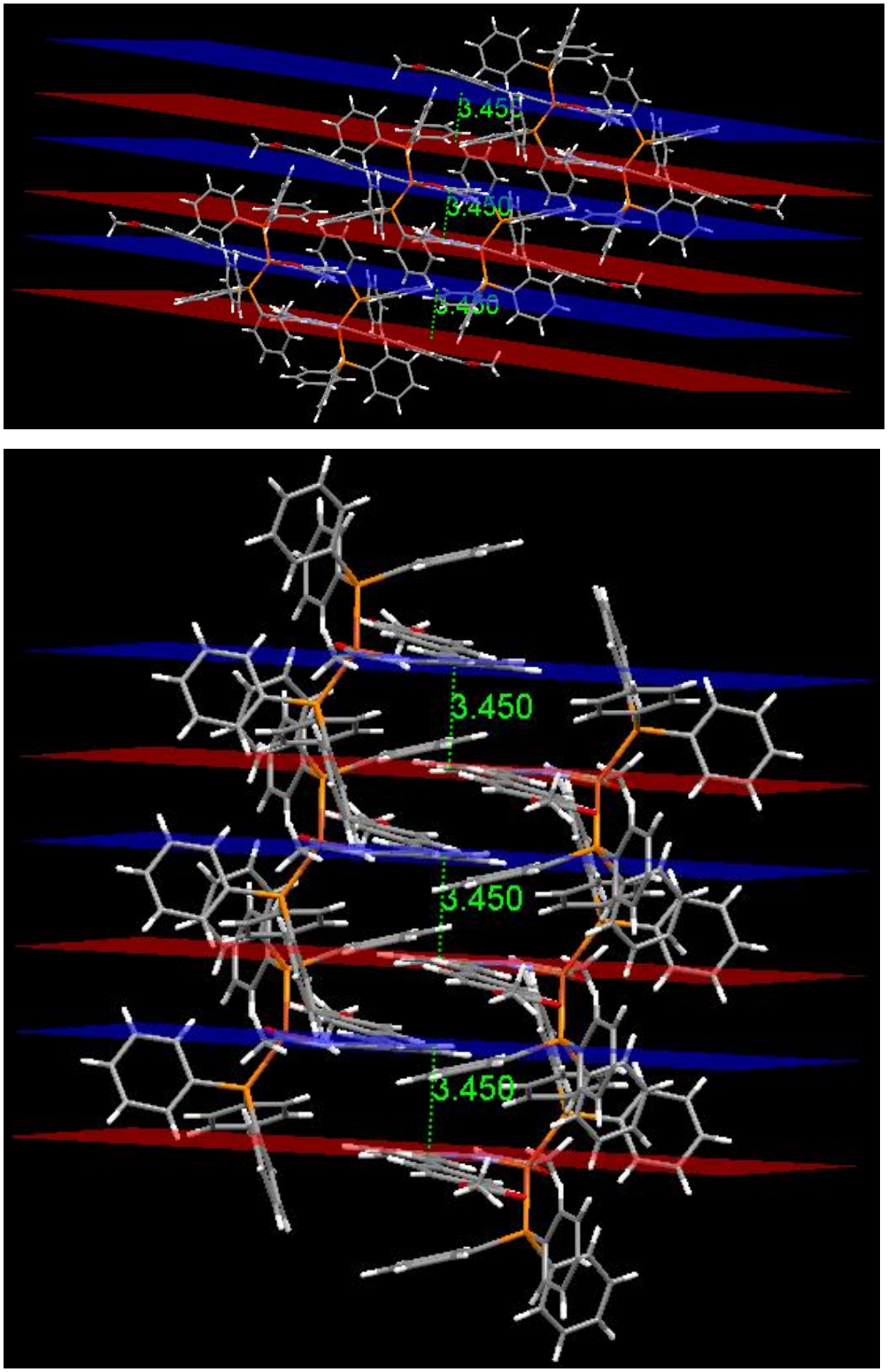


Figure S6. Crystal packing diagram and π-π stacking of **C1**.

Table S1. Crystal Data of **C1**.

| | |
|---|---|
| **CCDC Number** | **1587967** |
| Empirical formula | $C_{56}H_{47}BCuF_4N_3O_3P_2$ |
| Formula weight | 1022.26 |
| Temperature | 293(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | triclinic, *P-1* |
| Unit cell dimensions | *a* = 11.126(3) Å α= 90.69(3)° |
| | *b* = 11.871(3) Å β = 106.33(3)° |
| | *c* = 19.599(4) Å γ= 96.094(15)° |
| Volume | 2467.7(10) $Å^3$ |
| Z, Calculated density | 2, 1.376 $mg/m^3$ |
| Absorption coefficient | 0.571 $mm^{-1}$ |
| F(000) | 1056 |
| Crystal size | 0.20 x 0.18 x 0.12 mm |
| Theta range for data collection | 3.07 to 25.03 deg. |
| Limiting indices | $-12 \le h \le 13$, $-14 \le k \le 14$, $-23 \le l \le 23$ |
| Reflections collected / unique | 19138 / 8581 [R(int) = 0.1410] |
| Completeness to theta = 27.86 | 98.3 % |
| Absorption correction | Semi-empirical from equivalents |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 8581 / 190 / 630 |
| Goodness-of-fit on $F^2$ | 1.016 |
| Final R indices [I>2sigma(I)] | $R_1$ = 0.1411, $wR_2$ = 0.3237 |
| R indices (all data) | $R_1$ = 0.2394, $wR_2$ = 0.3700 |
| Largest diff. peak and hole | 1.445 and -0.681 e.$Å^{-3}$ |

[a] $R = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. [b] $Rw = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$.

Table S2. Bond lengths Å and angles [deg] for **C1**.

| Bond Length | Å | Angle | deg |
|---|---|---|---|
| Cu(1)-N(1) | 2.057(11) | N(1)-Cu(1)-O(1) | 83.6(4) |
| Cu(1)-O(1) | 2.217(10) | N(1)-Cu(1)-P(1) | 118.7(4) |
| Cu(1)-P(1) | 2.239(4) | O(1)-Cu(1)-P(1) | 97.2(3) |
| Cu(1)-P(2) | 2.260(4) | N(1)-Cu(1)-P(2) | 105.4(4) |
| P(1)-C(21) | 1.809(8) | O(1)-Cu(1)-P(2) | 102.9(3) |
| P(1)-C(33) | 1.812(15) | P(1)-Cu(1)-P(2) | 133.21(16) |
| P(1)-C(27) | 1.834(16) | C(21)-P(1)-C(33) | 103.9(6) |
| P(2)-C(39) | 1.797(15) | C(21)-P(1)-C(27) | 104.8(6) |
| P(2)-C(45) | 1.809(14) | C(33)-P(1)-C(27) | 101.9(7) |
| P(2)-C(51) | 1.815(9) | C(21)-P(1)-Cu(1) | 116.3(4) |
| O(1)-C(19) | 1.198(16) | C(33)-P(1)-Cu(1) | 114.3(5) |
| O(2)-C(17) | 1.169(19) | C(27)-P(1)-Cu(1) | 114.1(5) |
| O(3)-C(17) | 1.32(2) | C(39)-P(2)-C(45) | 103.4(7) |
| O(3)-C(18) | 1.478(19) | C(39)-P(2)-C(51) | 104.5(6) |
| N(1)-C(1) | 1.312(17) | C(45)-P(2)-C(51) | 104.3(6) |
| N(1)-C(5) | 1.372(17) | C(39)-P(2)-Cu(1) | 117.8(6) |
| N(2)-C(8) | 1.312(17) | C(45)-P(2)-Cu(1) | 114.8(5) |
| N(2)-C(5) | 1.343(16) | C(51)-P(2)-Cu(1) | 110.7(4) |
| N(3)-C(1) | 1.381(18) | C(19)-O(1)-Cu(1) | 127.2(10) |
| N(3)-C(19) | 1.381(19) | C(17)-O(3)-C(18) | 116.1(16) |
| N(3)-H(3A) | 0.8600 | C(1)-N(1)-C(5) | 114.1(12) |
| C(1)-C(2) | 1.38(2) | C(1)-N(1)-Cu(1) | 132.6(10) |
| C(2)-C(3) | 1.33(2) | C(5)-N(1)-Cu(1) | 112.3(9) |
| C(2)-H(2B) | 0.9300 | C(8)-N(2)-C(5) | 119.9(13) |
| C(3)-C(4) | 1.42(2) | C(1)-N(3)-C(19) | 132.1(13) |
| C(3)-H(3B) | 0.9300 | C(1)-N(3)-H(3A) | 113.9 |
| C(4)-C(5) | 1.394(19) | C(19)-N(3)-H(3A) | 113.9 |
| C(4)-C(6) | 1.40(2) | N(1)-C(1)-N(3) | 117.9(14) |
| C(6)-C(7) | 1.32(2) | N(1)-C(1)-C(2) | 127.4(14) |
| C(6)-H(6A) | 0.9300 | N(3)-C(1)-C(2) | 114.7(15) |
| C(7)-C(8) | 1.386(19) | C(3)-C(2)-C(1) | 117.7(15) |
| C(7)-H(7A) | 0.9300 | C(3)-C(2)-H(2B) | 121.2 |
| C(8)-C(9) | 1.467(19) | C(1)-C(2)-H(2B) | 121.2 |
| C(9)-C(10) | 1.348(19) | C(2)-C(3)-C(4) | 120.0(14) |
| C(9)-H(9A) | 0.9300 | C(2)-C(3)-H(3B) | 120.0 |
| C(10)-C(11) | 1.463(19) | C(4)-C(3)-H(3B) | 120.0 |
| C(10)-H(10A) | 0.9300 | C(5)-C(4)-C(6) | 117.2(14) |
| C(11)-C(16) | 1.348(19) | C(5)-C(4)-C(3) | 116.3(14) |
| C(11)-C(12) | 1.40(2) | C(6)-C(4)-C(3) | 126.4(14) |
| C(12)-C(13) | 1.40(2) | N(2)-C(5)-N(1) | 114.5(13) |
| C(12)-H(12A) | 0.9300 | N(2)-C(5)-C(4) | 121.2(14) |
| C(13)-C(14) | 1.35(2) | N(1)-C(5)-C(4) | 124.2(13) |

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|---|---|---|---|
| C(13)-H(13A) | 0.9300 | C(7)-C(6)-C(4) | 119.9(14) |
| C(14)-C(15) | 1.38(2) | C(7)-C(6)-H(6A) | 120.1 |
| C(14)-C(17) | 1.46(2) | C(4)-C(6)-H(6A) | 120.1 |
| C(15)-C(16) | 1.37(2) | C(6)-C(7)-C(8) | 120.5(14) |
| C(15)-H(15A) | 0.9300 | C(6)-C(7)-H(7A) | 119.7 |
| C(16)-H(16A) | 0.9300 | C(8)-C(7)-H(7A) | 119.7 |
| C(18)-H(18A) | 0.9600 | N(2)-C(8)-C(7) | 121.2(14) |
| C(18)-H(18B) | 0.9600 | N(2)-C(8)-C(9) | 114.0(13) |
| C(18)-H(18C) | 0.9600 | C(7)-C(8)-C(9) | 124.5(14) |
| C(19)-C(20) | 1.53(2) | C(10)-C(9)-C(8) | 124.7(14) |
| C(20)-H(20A) | 0.9600 | C(10)-C(9)-H(9A) | 117.7 |
| C(20)-H(20B) | 0.9600 | C(8)-C(9)-H(9A) | 117.7 |
| C(20)-H(20C) | 0.9600 | C(9)-C(10)-C(11) | 126.4(15) |
| C(21)-C(22) | 1.3900 | C(9)-C(10)-H(10A) | 116.8 |
| C(21)-C(26) | 1.3900 | C(11)-C(10)-H(10A) | 116.8 |
| C(22)-C(23) | 1.3900 | C(16)-C(11)-C(12) | 119.5(15) |
| C(22)-H(22A) | 0.9300 | C(16)-C(11)-C(10) | 118.6(15) |
| C(23)-C(24) | 1.3900 | C(12)-C(11)-C(10) | 121.8(14) |
| C(23)-H(23A) | 0.9300 | C(11)-C(12)-C(13) | 118.5(15) |
| C(24)-C(25) | 1.3900 | C(11)-C(12)-H(12A) | 120.8 |
| C(24)-H(24A) | 0.9300 | C(13)-C(12)-H(12A) | 120.8 |
| C(25)-C(26) | 1.3900 | C(14)-C(13)-C(12) | 122.1(16) |
| C(25)-H(25A) | 0.9300 | C(14)-C(13)-H(13A) | 119.0 |
| C(26)-H(26A) | 0.9300 | C(12)-C(13)-H(13A) | 119.0 |
| C(27)-C(32) | 1.35(2) | C(13)-C(14)-C(15) | 117.3(16) |
| C(27)-C(28) | 1.43(2) | C(13)-C(14)-C(17) | 118.8(16) |
| C(28)-C(29) | 1.38(2) | C(15)-C(14)-C(17) | 123.9(16) |
| C(28)-H(28A) | 0.9300 | C(16)-C(15)-C(14) | 121.9(16) |
| C(29)-C(30) | 1.37(2) | C(16)-C(15)-H(15A) | 119.1 |
| C(29)-H(29A) | 0.9300 | C(14)-C(15)-H(15A) | 119.1 |
| C(30)-C(31) | 1.33(2) | C(11)-C(16)-C(15) | 120.4(16) |
| C(30)-H(30A) | 0.9300 | C(11)-C(16)-H(16A) | 119.8 |
| C(31)-C(32) | 1.45(2) | C(15)-C(16)-H(16A) | 119.8 |
| C(31)-H(31A) | 0.9300 | O(2)-C(17)-O(3) | 122.6(18) |
| C(32)-H(32A) | 0.9300 | O(2)-C(17)-C(14) | 124.4(18) |
| C(33)-C(34) | 1.345(19) | O(3)-C(17)-C(14) | 112.9(16) |
| C(33)-C(38) | 1.43(2) | O(3)-C(18)-H(18A) | 109.5 |
| C(34)-C(35) | 1.38(2) | O(3)-C(18)-H(18B) | 109.5 |
| C(34)-H(34A) | 0.9300 | H(18A)-C(18)-H(18B) | 109.5 |
| C(35)-C(36) | 1.39(2) | O(3)-C(18)-H(18C) | 109.5 |
| C(35)-H(35A) | 0.9300 | H(18A)-C(18)-H(18C) | 109.5 |
| C(36)-C(37) | 1.33(2) | H(18B)-C(18)-H(18C) | 109.5 |
| C(36)-H(36A) | 0.9300 | O(1)-C(19)-N(3) | 123.6(14) |
| C(37)-C(38) | 1.41(2) | O(1)-C(19)-C(20) | 121.3(15) |

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|---|---|---|---|
| C(37)-H(37A) | 0.9300 | N(3)-C(19)-C(20) | 115.1(14) |
| C(38)-H(38A) | 0.9300 | C(19)-C(20)-H(20A) | 109.5 |
| C(39)-C(44) | 1.39(2) | C(19)-C(20)-H(20B) | 109.5 |
| C(39)-C(40) | 1.39(2) | H(20A)-C(20)-H(20B) | 109.5 |
| C(40)-C(41) | 1.35(2) | C(19)-C(20)-H(20C) | 109.5 |
| C(40)-H(40A) | 0.9300 | H(20A)-C(20)-H(20C) | 109.5 |
| C(41)-C(42) | 1.37(3) | H(20B)-C(20)-H(20C) | 109.5 |
| C(41)-H(41A) | 0.9300 | C(22)-C(21)-C(26) | 120.0 |
| C(42)-C(43) | 1.37(3) | C(22)-C(21)-P(1) | 118.4(6) |
| C(42)-H(42A) | 0.9300 | C(26)-C(21)-P(1) | 121.6(6) |
| C(43)-C(44) | 1.41(2) | C(23)-C(22)-C(21) | 120.0 |
| C(43)-H(43A) | 0.9300 | C(23)-C(22)-H(22A) | 120.0 |
| C(44)-H(44A) | 0.9300 | C(21)-C(22)-H(22A) | 120.0 |
| C(45)-C(46) | 1.39(2) | C(24)-C(23)-C(22) | 120.0 |
| C(45)-C(50) | 1.41(2) | C(24)-C(23)-H(23A) | 120.0 |
| C(46)-C(47) | 1.40(2) | C(22)-C(23)-H(23A) | 120.0 |
| C(46)-H(46A) | 0.9300 | C(23)-C(24)-C(25) | 120.0 |
| C(47)-C(48) | 1.29(2) | C(23)-C(24)-H(24A) | 120.0 |
| C(47)-H(47A) | 0.9300 | C(25)-C(24)-H(24A) | 120.0 |
| C(48)-C(49) | 1.33(2) | C(26)-C(25)-C(24) | 120.0 |
| C(48)-H(48A) | 0.9300 | C(26)-C(25)-H(25A) | 120.0 |
| C(49)-C(50) | 1.34(2) | C(24)-C(25)-H(25A) | 120.0 |
| C(49)-H(49A) | 0.9300 | C(25)-C(26)-C(21) | 120.0 |
| C(50)-H(50A) | 0.9300 | C(25)-C(26)-H(26A) | 120.0 |
| C(51)-C(52) | 1.3900 | C(21)-C(26)-H(26A) | 120.0 |
| C(51)-C(56) | 1.3900 | C(32)-C(27)-C(28) | 120.3(16) |
| C(52)-C(53) | 1.3900 | C(32)-C(27)-P(1) | 123.5(14) |
| C(52)-H(52A) | 0.9300 | C(28)-C(27)-P(1) | 116.2(12) |
| C(53)-C(54) | 1.3900 | C(29)-C(28)-C(27) | 118.4(16) |
| C(53)-H(53A) | 0.9300 | C(29)-C(28)-H(28A) | 120.8 |
| C(54)-C(55) | 1.3900 | C(27)-C(28)-H(28A) | 120.8 |
| C(54)-H(54A) | 0.9300 | C(30)-C(29)-C(28) | 120.2(17) |
| C(55)-C(56) | 1.3900 | C(30)-C(29)-H(29A) | 119.9 |
| C(55)-H(55A) | 0.9300 | C(28)-C(29)-H(29A) | 119.9 |
| C(56)-H(56A) | 0.9300 | C(31)-C(30)-C(29) | 122.7(18) |
| F(1)-B(1B) | 1.354(10) | C(31)-C(30)-H(30A) | 118.7 |
| F(1)-B(1) | 1.356(10) | C(29)-C(30)-H(30A) | 118.7 |
| F(2)-B(1) | 1.353(10) | C(30)-C(31)-C(32) | 118.5(19) |
| F(2)-B(1B) | 1.354(10) | C(30)-C(31)-H(31A) | 120.7 |
| F(3)-B(1) | 1.353(10) | C(32)-C(31)-H(31A) | 120.7 |
| F(3)-B(1B) | 1.354(10) | C(27)-C(32)-C(31) | 119.4(19) |
| B(1)-F(4) | 1.355(10) | C(27)-C(32)-H(32A) | 120.3 |
| B(1B)-F(4B) | 1.355(10) | C(31)-C(32)-H(32A) | 120.3 |
| | | C(34)-C(33)-C(38) | 119.0(14) |

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|---|---|---|
| | C(34)-C(33)-P(1) | 119.2(12) |
| | C(38)-C(33)-P(1) | 121.7(11) |
| | C(33)-C(34)-C(35) | 120.9(15) |
| | C(33)-C(34)-H(34A) | 119.5 |
| | C(35)-C(34)-H(34A) | 119.5 |
| | C(34)-C(35)-C(36) | 119.7(16) |
| | C(34)-C(35)-H(35A) | 120.2 |
| | C(36)-C(35)-H(35A) | 120.2 |
| | C(37)-C(36)-C(35) | 121.6(16) |
| | C(37)-C(36)-H(36A) | 119.2 |
| | C(35)-C(36)-H(36A) | 119.2 |
| | C(36)-C(37)-C(38) | 119.5(16) |
| | C(36)-C(37)-H(37A) | 120.3 |
| | C(38)-C(37)-H(37A) | 120.3 |
| | C(37)-C(38)-C(33) | 119.2(14) |
| | C(37)-C(38)-H(38A) | 120.4 |
| | C(33)-C(38)-H(38A) | 120.4 |
| | C(44)-C(39)-C(40) | 116.2(15) |
| | C(44)-C(39)-P(2) | 122.1(13) |
| | C(40)-C(39)-P(2) | 121.7(13) |
| | C(41)-C(40)-C(39) | 121.4(19) |
| | C(41)-C(40)-H(40A) | 119.3 |
| | C(39)-C(40)-H(40A) | 119.3 |
| | C(40)-C(41)-C(42) | 123(2) |
| | C(40)-C(41)-H(41A) | 118.6 |
| | C(42)-C(41)-H(41A) | 118.6 |
| | C(43)-C(42)-C(41) | 118(2) |
| | C(43)-C(42)-H(42A) | 121.0 |
| | C(41)-C(42)-H(42A) | 121.0 |
| | C(42)-C(43)-C(44) | 120(2) |
| | C(42)-C(43)-H(43A) | 120.0 |
| | C(44)-C(43)-H(43A) | 120.0 |
| | C(39)-C(44)-C(43) | 121.3(19) |
| | C(39)-C(44)-H(44A) | 119.3 |
| | C(43)-C(44)-H(44A) | 119.3 |
| | C(46)-C(45)-C(50) | 115.5(13) |
| | C(46)-C(45)-P(2) | 118.4(11) |
| | C(50)-C(45)-P(2) | 126.0(12) |
| | C(45)-C(46)-C(47) | 119.6(15) |
| | C(45)-C(46)-H(46A) | 120.2 |
| | C(47)-C(46)-H(46A) | 120.2 |
| | C(48)-C(47)-C(46) | 121.1(17) |
| | C(48)-C(47)-H(47A) | 119.4 |
| | C(46)-C(47)-H(47A) | 119.4 |

| | | |
|---|---|---|
| | C(47)-C(48)-C(49) | 121.0(17) |
| | C(47)-C(48)-H(48A) | 119.5 |
| | C(49)-C(48)-H(48A) | 119.5 |
| | C(48)-C(49)-C(50) | 121.5(17) |
| | C(48)-C(49)-H(49A) | 119.3 |
| | C(50)-C(49)-H(49A) | 119.3 |
| | C(49)-C(50)-C(45) | 121.3(16) |
| | C(49)-C(50)-H(50A) | 119.4 |
| | C(45)-C(50)-H(50A) | 119.4 |
| | C(52)-C(51)-C(56) | 120.0 |
| | C(52)-C(51)-P(2) | 116.6(7) |
| | C(56)-C(51)-P(2) | 122.9(7) |
| | C(51)-C(52)-C(53) | 120.0 |
| | C(51)-C(52)-H(52A) | 120.0 |
| | C(53)-C(52)-H(52A) | 120.0 |
| | C(54)-C(53)-C(52) | 120.0 |
| | C(54)-C(53)-H(53A) | 120.0 |
| | C(52)-C(53)-H(53A) | 120.0 |
| | C(55)-C(54)-C(53) | 120.0 |
| | C(55)-C(54)-H(54A) | 120.0 |
| | C(53)-C(54)-H(54A) | 120.0 |
| | C(54)-C(55)-C(56) | 120.0 |
| | C(54)-C(55)-H(55A) | 120.0 |
| | C(56)-C(55)-H(55A) | 120.0 |
| | C(55)-C(56)-C(51) | 120.0 |
| | C(55)-C(56)-H(56A) | 120.0 |
| | C(51)-C(56)-H(56A) | 120.0 |
| | B(1B)-F(1)-B(1) | 39.1(5) |
| | B(1)-F(2)-B(1B) | 39.2(5) |
| | B(1)-F(3)-B(1B) | 39.2(5) |
| | F(2)-B(1)-F(3) | 110.1(6) |
| | F(2)-B(1)-F(4) | 108.8(6) |
| | F(3)-B(1)-F(4) | 109.8(6) |
| | F(2)-B(1)-F(1) | 109.4(6) |
| | F(3)-B(1)-F(1) | 108.5(6) |
| | F(4)-B(1)-F(1) | 110.1(6) |
| | F(2)-B(1B)-F(1) | 109.5(6) |
| | F(2)-B(1B)-F(3) | 110.0(6) |
| | F(1)-B(1B)-F(3) | 108.6(6) |
| | F(2)-B(1B)-F(4B) | 109.3(6) |
| | F(1)-B(1B)-F(4B) | 109.8(7) |
| | F(3)-B(1B)-F(4B) | 109.6(7) |

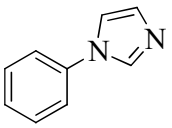
Table S3. Torsion angles for compound **C1**[deg].

| Torsion angles/deg | | Torsion angles/deg | |
|---|---|---|---|
| N(1)-Cu(1)-P(1)-C(21) | 98.0(6) | C(24)-C(25)-C(26)-C(21) | 0.0 |
| O(1)-Cu(1)-P(1)-C(21) | -175.3(5) | C(22)-C(21)-C(26)-C(25) | 0.0 |
| P(2)-Cu(1)-P(1)-C(21) | -60.0(5) | P(1)-C(21)-C(26)-C(25) | -178.0(8) |
| N(1)-Cu(1)-P(1)-C(33) | -23.1(7) | C(21)-P(1)-C(27)-C(32) | -88.1(15) |
| O(1)-Cu(1)-P(1)-C(33) | 63.6(6) | C(33)-P(1)-C(27)-C(32) | 19.9(16) |
| P(2)-Cu(1)-P(1)-C(33) | 178.8(5) | Cu(1)-P(1)-C(27)-C(32) | 143.6(14) |
| N(1)-Cu(1)-P(1)-C(27) | -139.8(6) | C(21)-P(1)-C(27)-C(28) | 89.8(11) |
| O(1)-Cu(1)-P(1)-C(27) | -53.1(6) | C(33)-P(1)-C(27)-C(28) | -162.2(11) |
| P(2)-Cu(1)-P(1)-C(27) | 62.1(5) | Cu(1)-P(1)-C(27)-C(28) | -38.5(12) |
| N(1)-Cu(1)-P(2)-C(39) | -134.6(6) | C(32)-C(27)-C(28)-C(29) | -2(2) |
| O(1)-Cu(1)-P(2)-C(39) | 138.6(6) | P(1)-C(27)-C(28)-C(29) | -179.6(13) |
| P(1)-Cu(1)-P(2)-C(39) | 25.6(6) | C(27)-C(28)-C(29)-C(30) | 1(3) |
| N(1)-Cu(1)-P(2)-C(45) | 103.3(6) | C(28)-C(29)-C(30)-C(31) | -4(3) |
| O(1)-Cu(1)-P(2)-C(45) | 16.4(6) | C(29)-C(30)-C(31)-C(32) | 8(3) |
| P(1)-Cu(1)-P(2)-C(45) | -96.6(6) | C(28)-C(27)-C(32)-C(31) | 5(3) |
| N(1)-Cu(1)-P(2)-C(51) | -14.4(5) | P(1)-C(27)-C(32)-C(31) | -177.0(16) |
| O(1)-Cu(1)-P(2)-C(51) | -101.3(5) | C(30)-C(31)-C(32)-C(27) | -8(3) |
| P(1)-Cu(1)-P(2)-C(51) | 145.7(4) | C(21)-P(1)-C(33)-C(34) | 169.3(12) |
| N(1)-Cu(1)-O(1)-C(19) | 12.0(13) | C(27)-P(1)-C(33)-C(34) | 60.6(14) |
| P(1)-Cu(1)-O(1)-C(19) | -106.1(13) | Cu(1)-P(1)-C(33)-C(34) | -62.9(13) |
| P(2)-Cu(1)-O(1)-C(19) | 116.4(13) | C(21)-P(1)-C(33)-C(38) | -8.7(13) |
| O(1)-Cu(1)-N(1)-C(1) | 3.4(14) | C(27)-P(1)-C(33)-C(38) | -117.4(12) |
| P(1)-Cu(1)-N(1)-C(1) | 98.1(14) | Cu(1)-P(1)-C(33)-C(38) | 119.1(11) |
| P(2)-Cu(1)-N(1)-C(1) | -98.3(14) | C(38)-C(33)-C(34)-C(35) | -2(2) |
| O(1)-Cu(1)-N(1)-C(5) | 170.8(10) | P(1)-C(33)-C(34)-C(35) | 179.9(13) |
| P(1)-Cu(1)-N(1)-C(5) | -94.5(9) | C(33)-C(34)-C(35)-C(36) | 1(3) |
| P(2)-Cu(1)-N(1)-C(5) | 69.1(10) | C(34)-C(35)-C(36)-C(37) | 0(3) |
| C(5)-N(1)-C(1)-N(3) | 178.4(13) | C(35)-C(36)-C(37)-C(38) | 0(3) |
| Cu(1)-N(1)-C(1)-N(3) | -14(2) | C(36)-C(37)-C(38)-C(33) | -1(2) |
| C(5)-N(1)-C(1)-C(2) | 1(2) | C(34)-C(33)-C(38)-C(37) | 2(2) |
| Cu(1)-N(1)-C(1)-C(2) | 168.2(13) | P(1)-C(33)-C(38)-C(37) | 179.8(12) |
| C(19)-N(3)-C(1)-N(1) | 15(3) | C(45)-P(2)-C(39)-C(44) | -53.8(14) |
| C(19)-N(3)-C(1)-C(2) | -167.2(17) | C(51)-P(2)-C(39)-C(44) | 55.1(14) |
| N(1)-C(1)-C(2)-C(3) | -1(3) | Cu(1)-P(2)-C(39)-C(44) | 178.4(11) |
| N(3)-C(1)-C(2)-C(3) | -178.4(15) | C(45)-P(2)-C(39)-C(40) | 127.5(13) |
| C(1)-C(2)-C(3)-C(4) | 4(2) | C(51)-P(2)-C(39)-C(40) | -123.5(13) |
| C(2)-C(3)-C(4)-C(5) | -7(2) | Cu(1)-P(2)-C(39)-C(40) | -0.2(15) |
| C(2)-C(3)-C(4)-C(6) | 177.3(16) | C(44)-C(39)-C(40)-C(41) | 4(2) |
| C(8)-N(2)-C(5)-N(1) | -180.0(12) | P(2)-C(39)-C(40)-C(41) | -177.1(14) |
| C(8)-N(2)-C(5)-C(4) | 3(2) | C(39)-C(40)-C(41)-C(42) | -3(3) |
| C(1)-N(1)-C(5)-N(2) | 179.0(12) | C(40)-C(41)-C(42)-C(43) | 3(4) |
| Cu(1)-N(1)-C(5)-N(2) | 9.1(15) | C(41)-C(42)-C(43)-C(44) | -4(3) |

| | | | |
|---|---|---|---|
| C(1)-N(1)-C(5)-C(4) | -4(2) | C(40)-C(39)-C(44)-C(43) | -5(2) |
| Cu(1)-N(1)-C(5)-C(4) | -174.2(11) | P(2)-C(39)-C(44)-C(43) | 175.9(13) |
| C(6)-C(4)-C(5)-N(2) | 0(2) | C(42)-C(43)-C(44)-C(39) | 6(3) |
| C(3)-C(4)-C(5)-N(2) | -176.4(13) | C(39)-P(2)-C(45)-C(46) | -92.1(13) |
| C(6)-C(4)-C(5)-N(1) | -176.5(13) | C(51)-P(2)-C(45)-C(46) | 158.8(12) |
| C(3)-C(4)-C(5)-N(1) | 7(2) | Cu(1)-P(2)-C(45)-C(46) | 37.5(13) |
| C(5)-C(4)-C(6)-C(7) | -3(2) | C(39)-P(2)-C(45)-C(50) | 85.2(15) |
| C(3)-C(4)-C(6)-C(7) | 173.5(15) | C(51)-P(2)-C(45)-C(50) | -23.9(15) |
| C(4)-C(6)-C(7)-C(8) | 2(2) | Cu(1)-P(2)-C(45)-C(50) | -145.1(12) |
| C(5)-N(2)-C(8)-C(7) | -4(2) | C(50)-C(45)-C(46)-C(47) | 0(2) |
| C(5)-N(2)-C(8)-C(9) | 170.1(12) | P(2)-C(45)-C(46)-C(47) | 177.5(12) |
| C(6)-C(7)-C(8)-N(2) | 1(2) | C(45)-C(46)-C(47)-C(48) | 1(2) |
| C(6)-C(7)-C(8)-C(9) | -172.0(14) | C(46)-C(47)-C(48)-C(49) | -2(3) |
| N(2)-C(8)-C(9)-C(10) | 174.3(14) | C(47)-C(48)-C(49)-C(50) | 2(3) |
| C(7)-C(8)-C(9)-C(10) | -12(2) | C(48)-C(49)-C(50)-C(45) | -1(3) |
| C(8)-C(9)-C(10)-C(11) | 177.3(14) | C(46)-C(45)-C(50)-C(49) | 0(2) |
| C(9)-C(10)-C(11)-C(16) | -177.9(15) | P(2)-C(45)-C(50)-C(49) | -177.6(14) |
| C(9)-C(10)-C(11)-C(12) | 1(2) | C(39)-P(2)-C(51)-C(52) | -167.9(7) |
| C(16)-C(11)-C(12)-C(13) | -2(3) | C(45)-P(2)-C(51)-C(52) | -59.6(7) |
| C(10)-C(11)-C(12)-C(13) | 179.3(15) | Cu(1)-P(2)-C(51)-C(52) | 64.3(6) |
| C(11)-C(12)-C(13)-C(14) | -1(3) | C(39)-P(2)-C(51)-C(56) | 20.7(8) |
| C(12)-C(13)-C(14)-C(15) | 6(3) | C(45)-P(2)-C(51)-C(56) | 129.0(7) |
| C(12)-C(13)-C(14)-C(17) | -176.8(16) | Cu(1)-P(2)-C(51)-C(56) | -107.1(6) |
| C(13)-C(14)-C(15)-C(16) | -7(2) | C(56)-C(51)-C(52)-C(53) | 0.0 |
| C(17)-C(14)-C(15)-C(16) | 175.5(15) | P(2)-C(51)-C(52)-C(53) | -171.6(7) |
| C(12)-C(11)-C(16)-C(15) | 1(2) | C(51)-C(52)-C(53)-C(54) | 0.0 |
| C(10)-C(11)-C(16)-C(15) | 179.4(14) | C(52)-C(53)-C(54)-C(55) | 0.0 |
| C(14)-C(15)-C(16)-C(11) | 4(3) | C(53)-C(54)-C(55)-C(56) | 0.0 |
| C(18)-O(3)-C(17)-O(2) | 5(3) | C(54)-C(55)-C(56)-C(51) | 0.0 |
| C(18)-O(3)-C(17)-C(14) | -172.4(15) | C(52)-C(51)-C(56)-C(55) | 0.0 |
| C(13)-C(14)-C(17)-O(2) | 4(3) | P(2)-C(51)-C(56)-C(55) | 171.1(8) |
| C(15)-C(14)-C(17)-O(2) | -179(2) | B(1B)-F(2)-B(1)-F(3) | -59.5(7) |
| C(13)-C(14)-C(17)-O(3) | -178.9(15) | B(1B)-F(2)-B(1)-F(4) | -179.9(9) |
| C(15)-C(14)-C(17)-O(3) | -2(2) | B(1B)-F(2)-B(1)-F(1) | 59.7(7) |
| Cu(1)-O(1)-C(19)-N(3) | -15(2) | B(1B)-F(3)-B(1)-F(2) | 59.5(7) |
| Cu(1)-O(1)-C(19)-C(20) | 164.4(12) | B(1B)-F(3)-B(1)-F(4) | 179.3(9) |
| C(1)-N(3)-C(19)-O(1) | 1(3) | B(1B)-F(3)-B(1)-F(1) | -60.3(7) |
| C(1)-N(3)-C(19)-C(20) | -179.2(17) | B(1B)-F(1)-B(1)-F(2) | -59.8(7) |
| C(33)-P(1)-C(21)-C(22) | 86.8(7) | B(1B)-F(1)-B(1)-F(3) | 60.4(7) |
| C(27)-P(1)-C(21)-C(22) | -166.7(7) | B(1B)-F(1)-B(1)-F(4) | -179.4(9) |
| Cu(1)-P(1)-C(21)-C(22) | -39.7(7) | B(1)-F(2)-B(1B)-F(1) | -59.9(7) |
| C(33)-P(1)-C(21)-C(26) | -95.2(8) | B(1)-F(2)-B(1B)-F(3) | 59.3(7) |
| C(27)-P(1)-C(21)-C(26) | 11.4(8) | B(1)-F(2)-B(1B)-F(4B) | 179.8(10) |
| Cu(1)-P(1)-C(21)-C(26) | 138.3(5) | B(1)-F(1)-B(1B)-F(2) | 59.8(7) |

| | | | |
|---|---|---|---|
| C(26)-C(21)-C(22)-C(23) | 0.0 | B(1)-F(1)-B(1B)-F(3) | -60.3(7) |
| P(1)-C(21)-C(22)-C(23) | 178.1(8) | B(1)-F(1)-B(1B)-F(4B) | 179.8(9) |
| C(21)-C(22)-C(23)-C(24) | 0.0 | B(1)-F(3)-B(1B)-F(2) | -59.3(7) |
| C(22)-C(23)-C(24)-C(25) | 0.0 | B(1)-F(3)-B(1B)-F(1) | 60.5(7) |
| C(23)-C(24)-C(25)-C(26) | 0.0 | B(1)-F(3)-B(1B)-F(4B) | -179.6(9) |

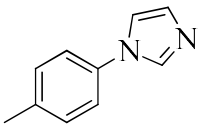
**2. Experimental data for products**



1-phenyl-1H-imidazole (**1**)[1]

$^1$H NMR ($CDCl_3$, 400 MHz) δ: 7.81 (s, 1H), 7.48～7.51 (m, 3H), 7.32～7.36 (m, 4H), 7.28 (d, J＝11.5 Hz, 1H), 7.21 (s, 1H);

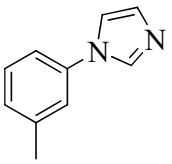
$^{13}$C NMR ($CDCl_3$, 100 MHz) δ: 144.3, 139.0, 137.4, 135.2, 129.8, 128.4, 123.1, 122.4, 116.4.



1-(*p*-tolyl)-1H-imidazole (**2**)[2]

$^1$H NMR ($CDCl_3$, 400 MHz) δ: 7.71 (s, 1H), 7.14 (s, 5H), 7.09 (s, 1H), 2.28 (s, 3H);

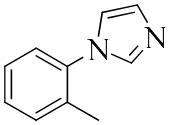
$^{13}$C NMR ($CDCl_3$, 100 MHz) δ: 137.25, 135.36, 134.89, 130.13, 130.01, 121.24, 118.14, 20.69.



1-*m*-tolyl-1H-imidazole (**3**)[3]:

$^1$H NMR ($CDCl_3$, 400 MHz) δ: 8.232 (s, 1H), 7.713 (s, 1H), 7.475 (s, 1H), 7.395 (d, J＝10.8 Hz, 1H), 7.353 (d, J＝8.0 Hz, 1H), 7.148 (d, J＝7.6 Hz, 1H), 7.093 (s, 1H), 2.353 (s, 3H).

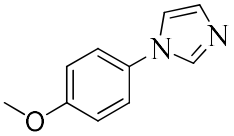
$^{13}$C NMR (100 MHz, $CDCl_3$) δ: 139.8, 137.4, 134.7, 130.2, 129.7, 129, 121.5, 116.5, 20.9.



1-*o*-tolyl-1H-imidazole (**4**) [4]:

$^1$H NMR (400 MHz, $CDCl_3$) δ: 7.60 (br s, 1H), 7.37～7.28 (m, 3H), 7.24～7.20 (m, 2H), 7.05 (br s, 1H), 2.19 (s, 3H);

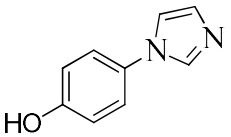
$^{13}$C NMR (100 MHz, $CDCl_3$) δ: 148.3, 138.3, 135.6, 130.8, 130.1, 118.4, 114.1, 111.1, 11.7.



1-(4-methoxyphenyl)-1H-imidazole (**5**)[2]

$^1$H NMR ($CDCl_3$, 400 MHz) δ: 7.75 (s, 1H), 7.28 (d, J＝8.9 Hz, 2H), 7.18 (d, J＝7.3 Hz, 2H), 6.95 (d, J＝8.9 Hz, 2H), 3.83 (s, 3H);

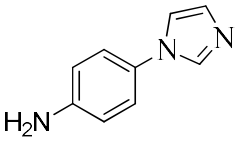
$^{13}$C NMR ($CDCl_3$, 100 MHz) δ: 158.88, 135.46, 160.67, 129.98, 123.25, 118.42, 114.86, 55.60



4-imidazol-1-yl-phenol (**6**) [5]

$^1$H NMR (400 MHz, DMSO): δ 9.75 (s, 1H), 8.06 (s, 1H), 7.57 (d, 1H), 7.38-7.42 (m, 2H), 7.06 (s, 1H), 6.85-6.89 (m, 2H).

$^{13}$C NMR (100 MHz, DMSO): δ 156.91, 135.96, 129.78, 129.43, 122.74, 118.90, 116.53.

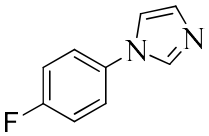


1-imidazol-1-yl-phenylamine (**7**) [6]

$^1$H NMR (400 MHz, $CDCl_3$): δ 7.70 (s, 1H), 7.11-7.15 (m, 4H), 6.70-6.72 (m, 2H), 2.16 (s, 2H).

$^{13}$C NMR (100 MHz, $CDCl_3$): δ 146.32, 135.83, 129.64, 128.58, 123.24, 118.88,

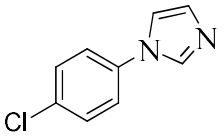
115.48.



1-(4-fluorophenyl)-1H-imidazole (**8**)[7]:

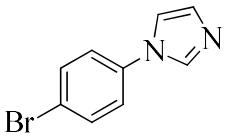
$^1$H NMR ($CDCl_3$, 400 MHz) δ : 7.80 (s, 1H), 7.36～7.32 (m, 2H), 7.22～7.12 (m, 4H);

$^{13}$C NMR ($CDCl_3$, 100MHz) δ: 163.40, 163.01, 133.56, 130.22, 123.58, 123.40, 118.72, 116.98, 116.60



1-(4-chlorophenyl)-1H-imidazole (**9**)[8]:

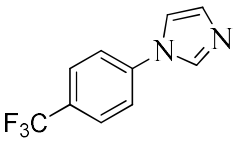
$^1$H NMR (DMSO-d6, 400 MHz) δ: 8.290 (s, 1H), 7.773 (s, 1H), 7.721～7.571 (dd, J ＝8.8, 51.2 Hz, 4H), 7.124 (s, 1H).



1-(4-bromo-phenyl)-1H-imidazole (**10**) [9]

$^1$H NMR (400 MHz, $CDCl_3$): δ 7.82 (s, 1H), 7.57-7.79 (m, 2H), 7.14-7.28 (m, 3H), 7.12 (s, 1H).

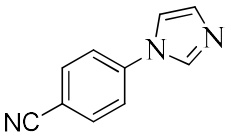
$^{13}$C NMR (100 MHz, $CDCl_3$): δ 136.36, 135.48, 133.02, 130.73, 122.99, 120.96, 118.12.



1-(4-(trifluoromethyl)phenyl)-1H-imidazole (**11**)[2]

$^1$H NMR ($CDCl_3$, 400 MHz) δ: 7.90 (brs, 1H), 7.71 (m, 2H), 7.46～7.34 (m, 4H);

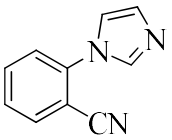
$^{13}$C NMR ($CDCl_3$, 100 MHz) δ: 129.61, 129.25, 127.65, 127.22, 124.79, 122.22, 121.24.



4-imidazol-1-yl-benzonitrile (**12**)[6]

$^1$H NMR (400 MHz, $CDCl_3$): δ 7.96 (s, 1H), 7.77-7.84 (m, 2H), 7.53-7.58 (m, 2H), 7.31-7.36 (d, 1H), 7.23 (s, 1H).

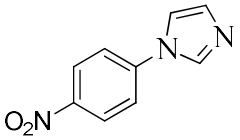
$^{13}$C NMR (100 MHz, $CDCl_3$): δ 140.47, 135.32, 134.12, 131.45, 121.15, 117.90, 117.59, 110.93.



2-(1H-imidazol-1-yl)benzonitrile (**13**)[10]:

$^1$H NMR ($CDCl_3$, 400 MHz) δ: 7.90 (s, 1H) , 7.71 (s, 1H), 7.65～7.60 (m, 3H), 7.30 (s, 1H), 7.22 (s, 1H);

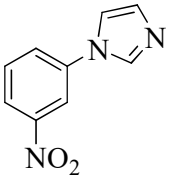
$^{13}$C NMR ($CDCl_3$, 100 MHz) δ: 138.16, 135.49, 131.26, 131.17, 130.91, 125.58, 124,36, 117.96, 117,67, 114.25.



1-(4-nitrophenyl)-1H-imidazole (**14**)[2]

$^1$H NMR ($CDCl_3$, 400 MHz) δ: 8.4 (d, J＝8.8 Hz, 2H), 7.99 (s, 1H), 7.59 (d, J＝9.2 Hz, 2H), 7.39 (s, 1H), 7.29 (s, 1H);

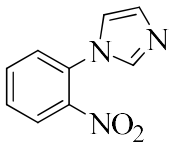
$^{13}$C NMR ($CDCl_3$, 100 MHz) δ: 142.0, 135.4, 131.7, 125.8, 121.0, 117.6, 109.8.



1-(3-nitrophenyl)-1H-imidazole (**15**)[10]:

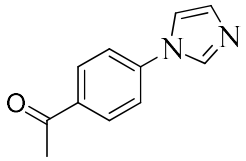
$^1$H NMR ($CDCl_3$, 400 MHz) δ: 8.19 (s, 1H), 8.15 (d, J＝8.4 Hz, 1H), 7.90 (s, 1H), 7.72～7.63 (m, 2H), 7.34 (s, 1H), 7.21 (s, 1H);

$^{13}$C NMR ($CDCl_3$, 100 MHz) δ: 149.11, 138.28, 135.45, 131.41, 131.08, 126.68, 122.12, 118.11, 116.32.



1-(2-nitrophenyl)-1H-imidazole (**16**)[11]:

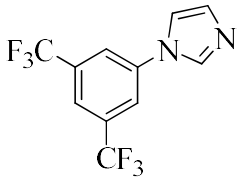
$^1$H NMR (DMSO-$d_6$, 400 MHz) δ: 8.155～8.178 (dd, J＝0.8, 8 Hz, 1H), 7.855～7.916 (m, 2H), 7.690～7.753 (m, 2H), 7.426 (s, 1H), 7.088 (s, 1H).



1-(4-imidazol-1-yl-phenyl)-ethanone (**17**) [6]

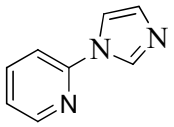
$^1$H NMR (400 MHz, $CDCl_3$): δ 8.11-8.14 (m, 2H), 8.01 (s, 1H), 7.52-7.56 (m, 2H), 7.40 (s, 1H), 7.28 (s, 1H), 2.67 (s, 3H).

$^{13}$C NMR (100 MHz, $CDCl_3$): δ 196.52, 140.68, 135.74, 135.35, 131.08, 130.30, 120.67, 117.70, 26.58.



1-(3,5-bis(trifluoromethyl)phenyl)-1H-imidazole (**18**)[12]:

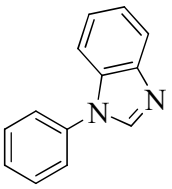
$^1$H NMR (DMSO-$d_6$, 400 MHz) δ: 8.597 (s, 1H), 8.452 (s, 2H), 8.087～8.099 (m, 2H), 7.176 (t, J＝1.2 Hz, 1H).



1-(pyridine)-1H-imidazole (**19**) [1]

$^1$H NMR (400 MHz, $CDCl_3$): δ 8.40-8.43 (m, 1H), 8.32-8.34 (m, 1H), 7.75-7.78 (m, 1H), 7.60-7.63 (m, 1H), 7.29-7.34 (m, 1H), 7.14-7.20 (m, 2H).

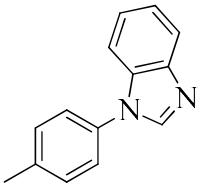
$^{13}$C NMR (100 MHz, $CDCl_3$): δ 148.80, 148.73, 138.88, 134.76, 130.34, 121.85, 116.00, 112.10.



1-phenyl-1H-benzo[*d*]imidazole (**20**)[13]:

$^1$H NMR ($CDCl_3$, 400 MHz) δ: 8.10 s, 1H), 7.88～7.76 (m, 1H), 7.61～7.46 (m, 6H), 7.34 (t, J＝4.2 Hz, 2H);

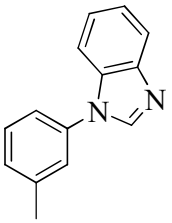
$^{13}$C NMR ($CDCl_3$, 100 MHz) δ: 143.87, 141.83, 136.12, 133.27, 129.90, 128.01, 123.89, 123.15, 122.22, 120.14, 110.11.



1-(*p*-tolyl)-1H-benzo[d]imidazole (**21**)[2]

$^1$H NMR ($CDCl_3$, 400 MHz) δ: 7.66～7.69 (m, 1H), 7.53～7.50 (m, 1H), 7.39～7.35 (m, 2H), 7.28～7.32 (m, 3H), 7.22～7.12 (m, 2 H), 6.63 (dd, J＝3.2, 1.0 Hz, 1H), 2.41 (s, 3H);

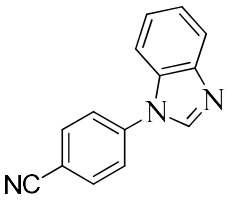
$^{13}$C NMR ($CDCl_3$, 100 MHz) δ: 137.32, 136.17, 135.85, 129.95, 127.90, 124.11, 120.85, 120.01, 110.31, 103.02, 20.86.



1-*m*-tolyl-1H-benzo[*d*]imidazole (**22**) [14]:

$^1$H NMR (400 MHz, $CDCl_3$) δ: 8.05 (br s, 1H), 7.78～7.84 (m, 1H), 7.39～7.45 (m, 1H), 7.21～7.33 (m, 6H), 2.40 (s, 3H);

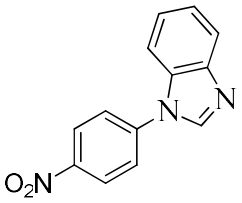
$^{13}$C NMR (100 MHz, $CDCl_3$) δ: 149, 145.6, 142, 138, 132, 130.5, 124, 123.6, 122.9, 122.7, 120.3, 110.1, 109.8, 20.5.



4-(1H-benzo[*d*]imidazol-1-yl)benzonitrile (**23**)[15]

$^1$H NMR (400 MHz, $CDCl_3$): δ 8.19 (s, 1H), 7.89-7.92 (m, 3H), 7.68-7.72 (m, 2H), 7.57-7.60 (m, 1H), 7.38-7.42 (m, 2H).

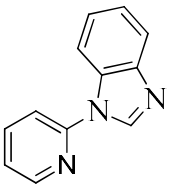
$^{13}$C NMR (100 MHz, $CDCl_3$): δ 144.22, 141.63, 140.07, 134.24, 132.78, 131.80, 129.08, 124.50, 123.94, 123.64, 121.01, 117.89, 111.52, 110.31.



1-(4-nitrophenyl)-1H-benzo[d]imidazole (**24**)[15]

$^1$H NMR ($CDCl_3$, 400 MHz) δ: 8.50 (dt, J＝8.4, 2.4 Hz, 2H), 8.21 (s, 1H), 7.93～7.90 (m, 1H), 7.76 (dt, J＝8.4, 2.4 Hz, 2H), 7.60～7.64 (m, 1H), 7.44～7.40 (m, 2H);

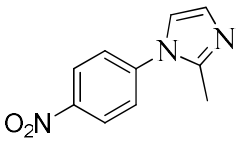
$^{13}$C NMR ($CDCl_3$, 100 MHz) δ: 147.56, 143.5, 143.22, 138.32, 136.45, 123.89, 123.03, 122.67, 115.23.



1-(pyridine)-1H-benzonitrile (**25**) [2]

$^1$H NMR (400 MHz, $CDCl_3$): δ 8.53-8.56 (m, 2H), 8.00-8.02 (m, 1H), 7.81-7.86 (m, 2H), 7.51-7.53 (m, 1H), 7.23-7.36 (m, 3H).

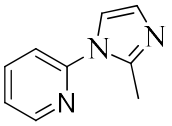
$^{13}$C NMR (100 MHz, $CDCl_3$): δ 149.90, 149.48, 144.69, 141.34, 138.96, 132.13, 124.22, 123.30, 121.86, 120.65, 114.34, 112.65.



2-methyl-1-(4-nitrophenyl)-1H-imidazole (**26**) [16]

$^{1}$H NMR (400 MHz, $CDCl_3$): δ 8.31-8.35 (m, 2H), 7.45-7.48 (m, 2H), 7.04-7.05 (d, 2H), 2.40 (s, 3H).

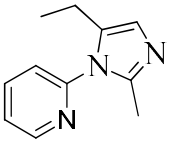
$^{13}$C NMR (100 MHz, $CDCl_3$): δ 146.91, 144.60, 143.17, 128.76, 125.79, 125.15, 120.24, 14.11.



2-(2-methyl-1H-imidazol-1-yl)pyridine (**27**)

$^{1}$H NMR (400 MHz, $CDCl_3$): δ 8.37-8.39 (d, 1H), 7.66-7.71 (m, 1H), 7.12-7.17 (m, 3H), 6.86 (s, 1H), 2.43-2.46 (m, 3H).

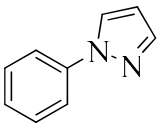
$^{13}$C NMR (100 MHz, $CDCl_3$): δ 150.45, 148.93, 144.69, 138.63, 127.66, 122.24, 118.84, 117.02, 15.20.



2-(5-ethyl-2-methyl-1H-imidazol-1-yl)pyridine (**28**) [16]

$^{1}$H NMR (400 MHz, $CDCl_3$): δ 8.45-8.47 (m, 1H), 7.72-7.77 (m, 1H), 7.18-7.22 (m, 2H), 6.87 (d, 1H), 2.82-2.88 (m, 2H), 2.09-2.18 (d, 3H), 1.18-1.22 (m, 3H).

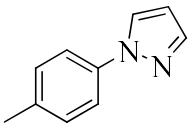
$^{13}$C NMR (100 MHz, $CDCl_3$): δ 150.71, 149.23, 149.07, 138.56, 136.72, 122.10, 117.35, 115.22, 21.78, 13.41, 12.51.



1-phenyl-1H-pyrazole (**29**) [17]:

$^{1}$H NMR (400 MHz, $CDCl_3$) δ: 7.83 (s, 1H), 7.64 (d, J＝8.3 Hz, 3H), 7.33 (t, J＝8.3 Hz, 2H), 7.21 (t, J＝7.1 Hz, 1H), 6.37 (s, 1H);

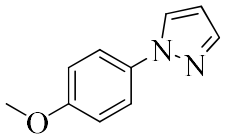
$^{13}$C NMR (100 MHz, $CDCl_3$) δ: 141.1, 140.2, 129.4, 126.8, 126.4, 119.2, 107.6.



1-*p*-tolyl-1H-pyrazole (**30**) [17]:

$^{1}$HNMR (400 MHz, $CDCl_3$) δ: 7.83 (d, J＝2.3 Hz, 1H), 7.62 (s, 1H), 7.52 (d, J＝8.3 Hz, 2H), 7.2 (d, J＝8.3 Hz, 2H), 6.37 (s, 1H), 2.33 (s, 3H);

$^{13}$C NMR (100 MHz, $CDCl_3$) δ: 140.7, 138, 136.1, 126.7, 129.9, 119.1, 107.3, 20.9.




1-(4-methoxyphenyl)-1H-pyrazole (**31**) [17]:

$^{1}$H NMR (400 MHz, $CDCl_3$) δ: 7.76 (d, J＝2.3 Hz, 1H), 7.61 (s, 1H), 7.53 (d, J＝8.3 Hz, 2H), 6.91 (d, J＝8.3 Hz, 2H), 6.37 (s, 1H), 3.70 (s, 3H);

$^{13}$C NMR (100 MHz, $CDCl_3$) δ: 157.5, 140.2, 133.4, 127.3, 119.9, 114.5, 107.2, 55.3.

**References**


[1] Suresh P, Pitchumani K, *J Org Chem*, 73 (2008) 9121.

[2] Ma H C, Jiang X Z, *J Org Chem*, 72 (2007) 8943.

[3]Zhang J, Yin H, Han S. Chin. J. Org. Chem. 2012, 32, 1429

[4] Collman J P, Zhong M. Org. Lett. 2000, 2, 1233.

[5] Altman R A, Koval E D, Buchwald S L. *J. Org. Chem.* 72 (2007) 6190.

[6] Zhu L, Guo P, Li G, et al, *J Org Chem*, 72 (2007) 8535.

[7] Kantam M L, Venkanna G T, Sridhar C, Sreedhar B, Choudary B M. J. Org. Chem. 2006, 71, 9522.

[8]Lv X, Bao W. J. Org. Chem. 2007, 72, 3863.

[9] Altman R A , Buchwald S L, *Org Lett*, 8 (2006) 2779.

[10] Yang M, Liu F. J. Org. Chem. 2007, 72, 8969.

[11] Choudary B, Sridhar C, Kantam M, Venkanna G, Sreedhar B. J. Am. Chem. Soc. 2005, 127, 9948.

[12] Cheng D, Gan F, Qian W, Bao W. Green Chem. 2008, 10, 171.

[13] Xie Y X, Pi S F, Wang J, Yin D L, Li J H. J. Org. Chem. 2006, 71, 8324

[14] Zhang Z J, Mao J C, Zhu D, Wu F, Chen H L, Wan B S. Tetrahedron 2006, 62, 4435.

[15] Yang K, Qiu Y, Li Z, et al, *J Org Chem*, 76 (2011) 3151.

[16]Wang Y, Wu Z, Wang L, et al, *Chem-Eur J*, 15 (2009) 8971.

[17] Correa A, Bolm C. Angew. Chem., Int. Ed. 2007, 46, 8862.

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) x

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

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Temperature:   293 K
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| Sum formula | C56 H47 B Cu F4 N3 O3 P2 | C56 H47 B Cu F4 N3 O3 P2 |
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The following ALERTS were generated. Each ALERT has the format
**test-name_ALERT_alert-type_alert-level**.
Click on the hyperlinks for more details of the test.

## Alert level B

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PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) ...................       0.37 Report
PLAT341_ALERT_3_B Low Bond Precision on  C-C Bonds ...............     0.0230 Ang.
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Th(Min) ...         17 Report
PLAT930_ALERT_2_B Check Twin Law ( 0 0  1)[ 1 0  2] Estimated BASF       0.27
PLAT930_ALERT_2_B Check Twin Law ( 2 0 -1)[ 1 0  0] Estimated BASF       0.28
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## Alert level C

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            identifier.
            kelly
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
RFACG01_ALERT_3_C  The value of the R factor is > 0.10
            R factor given   0.141
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
            Rint given   0.141
PLAT020_ALERT_3_C The value of Rint is greater than 0.12 .........      0.141 Report
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections too Low ....         43 %
PLAT082_ALERT_2_C High R1 Value ..................................       0.14 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.12 Report
PLAT234_ALERT_4_C Large Hirshfeld Difference N1     --  C1      ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C13    --  C14     ..       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C27    --  C28     ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C48    --  C49     ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C49    --  C50     ..       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C53    --  C54     ..       0.22 Ang.
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....         N3 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C24 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C31 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....        C55 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C17 Check
PLAT242_ALERT_2_C Low       Ueq as Compared to Neighbors for .....        C19 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....       2.8 Note
PLAT334_ALERT_2_C Small Average Benzene  C-C Dist. C11    -C16          1.37 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     14.469 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      4.307 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      2.666 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.595        128 Report
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## Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         7 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         7 Report
PLAT005_ALERT_5_G No _iucr_refine_instructions_details  in the CIF    Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............         1 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ    Please Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical         ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      45.00 Why ?
PLAT093_ALERT_1_G No su's on H-positions, refinement reported as .      mixed Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage =           40 Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  F4B    ..  C20     ..       2.78 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        202 Check
             B1B  -F1   -B1      1.555   1.555   1.555             39.10 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        203 Check
             B1   -F2   -B1B     1.555   1.555   1.555             39.20 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... #        204 Check
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             B1   -F3   -B1B     1.555   1.555   1.555            39.20 Deg.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       190 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..         ! Info
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL      2014 Note
PLAT931_ALERT_5_G Found Twin Law ( 0 0  1)[       ] Estimated BASF      0.27 Check
PLAT931_ALERT_5_G Found Twin Law ( 2 0 -1)[       ] Estimated BASF      0.28 Check
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   6 ALERT level B = A potentially serious problem, consider carefully
  26 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  20 ALERT level G = General information/check it is not something unexpected

   7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  16 ALERT type 2 Indicator that the structure model may be wrong or deficient
  13 ALERT type 3 Indicator that the structure quality may be low
  12 ALERT type 4 Improvement, methodology, query or suggestion
   4 ALERT type 5 Informative message, check
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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

**Publication of your CIF in IUCr journals**

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

**Publication of your CIF in other journals**

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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**PLATON version of 21/06/2015; check.def file version of 21/06/2015**

**Datablock x** - ellipsoid plot