Supporting Information

for

Synthesis and structural characterisation of Group 11 metal complexes with a phosphinoferrocene oxazoline

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Additional structural diagrams

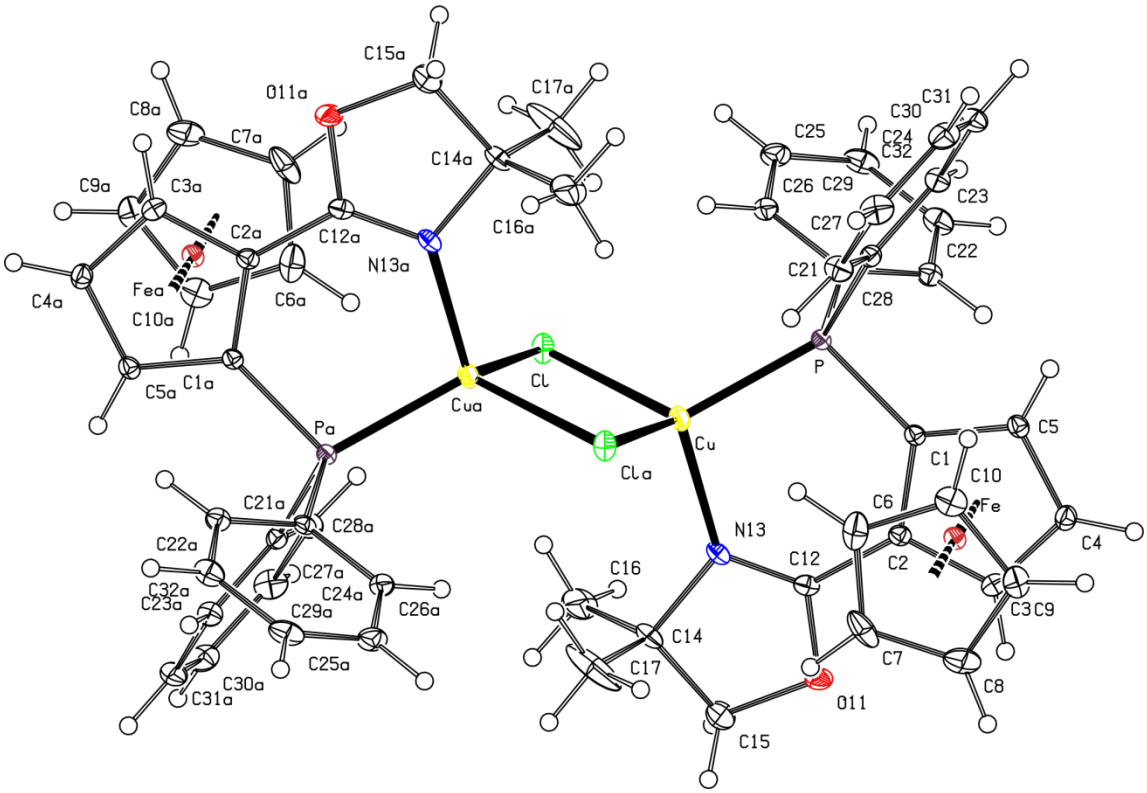

Figure S1. Displacement ellipsoid plot of the structure of **2a** (30% probability level).

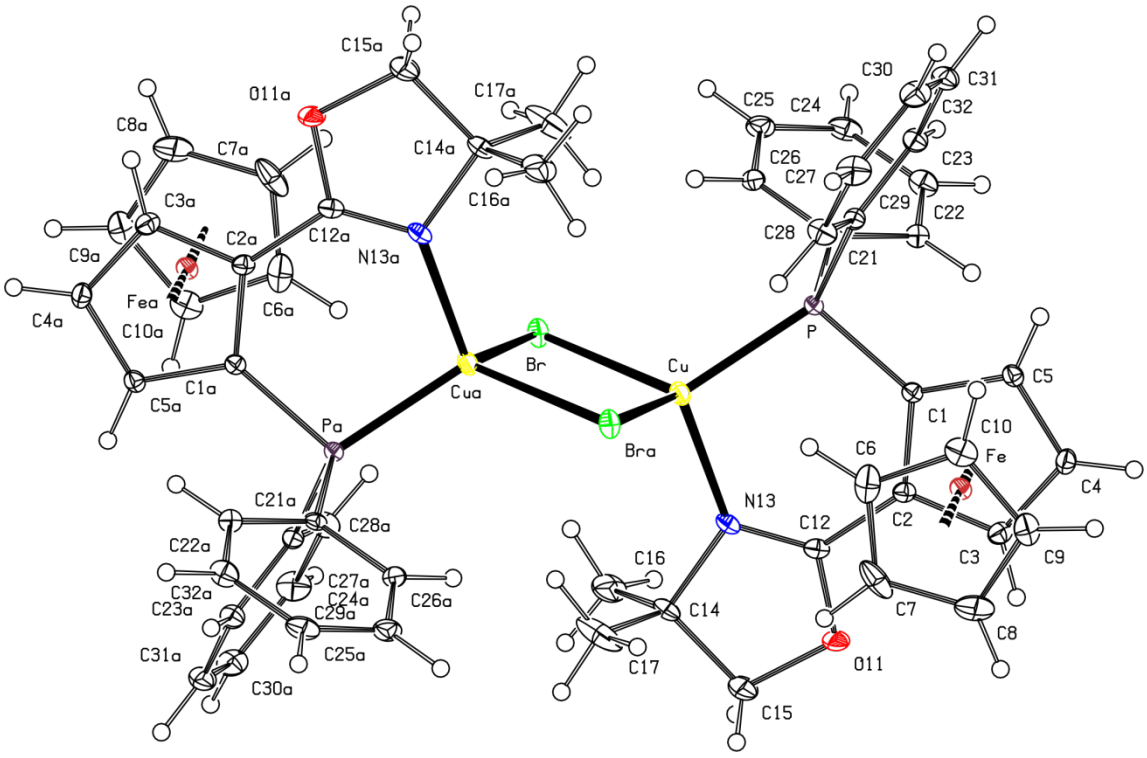

Figure S2. Displacement ellipsoid plot of the structure of **2b** (30% probability level).

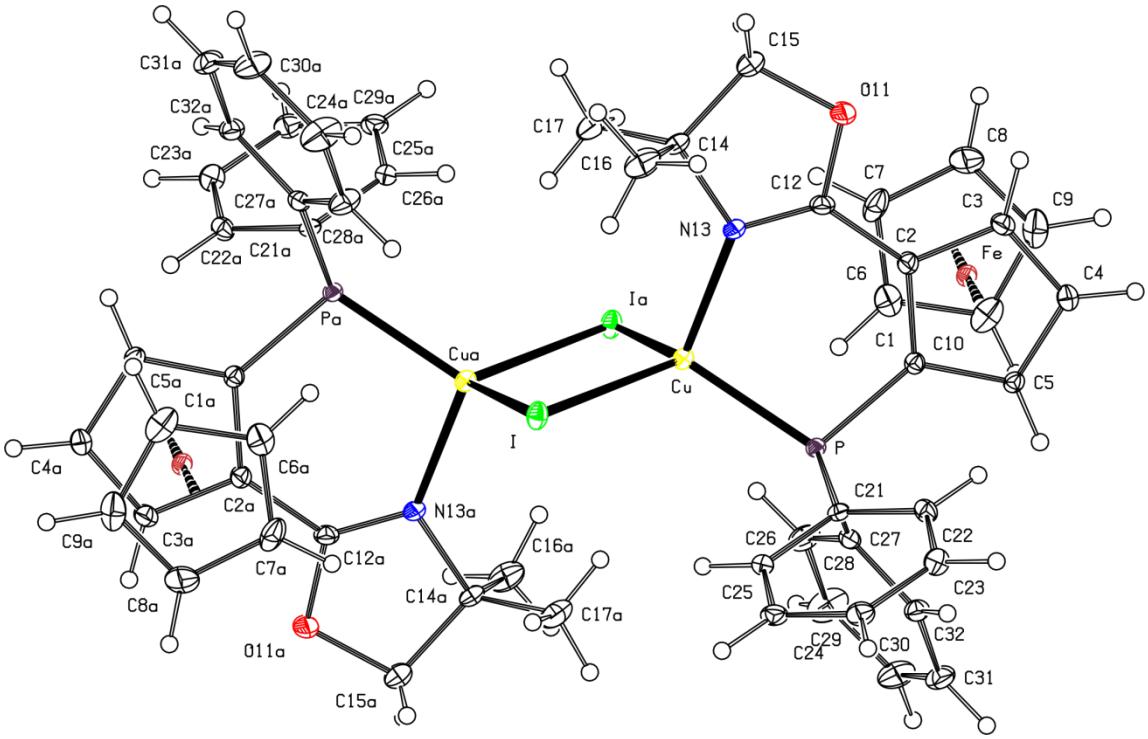

Figure S3. Displacement ellipsoid plot of the structure of **2c** (30% probability level).

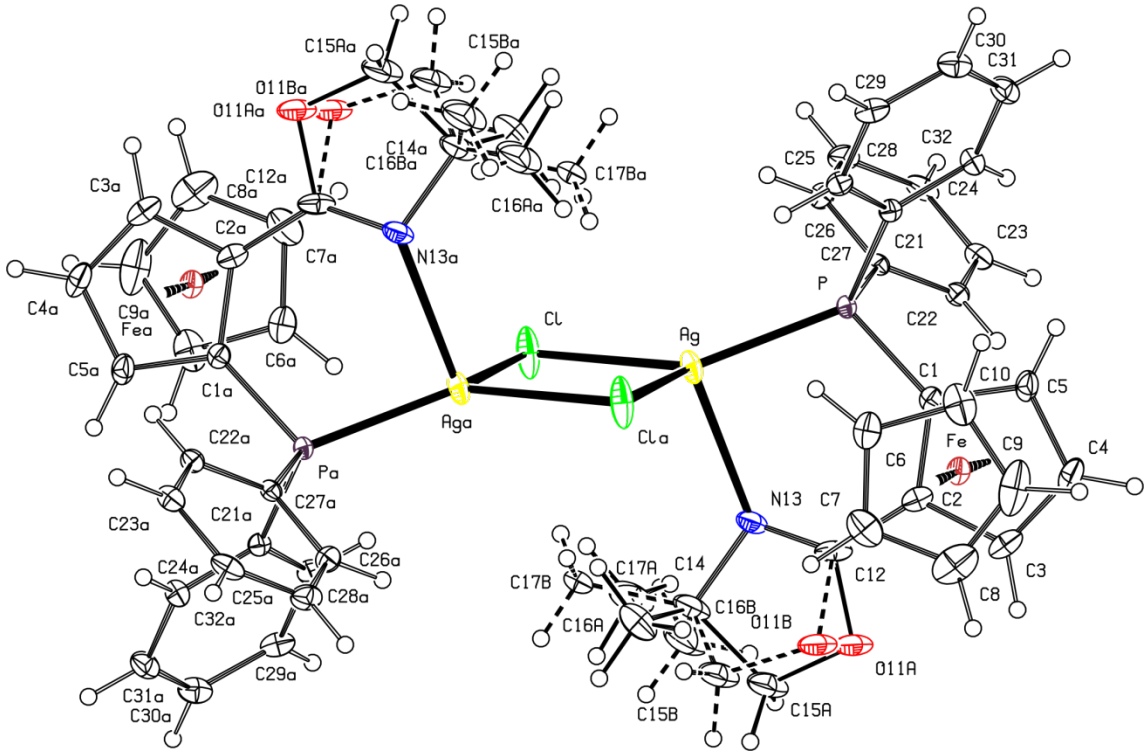

Figure S4. Displacement ellipsoid plot of the structure of **3** (30% probability level).

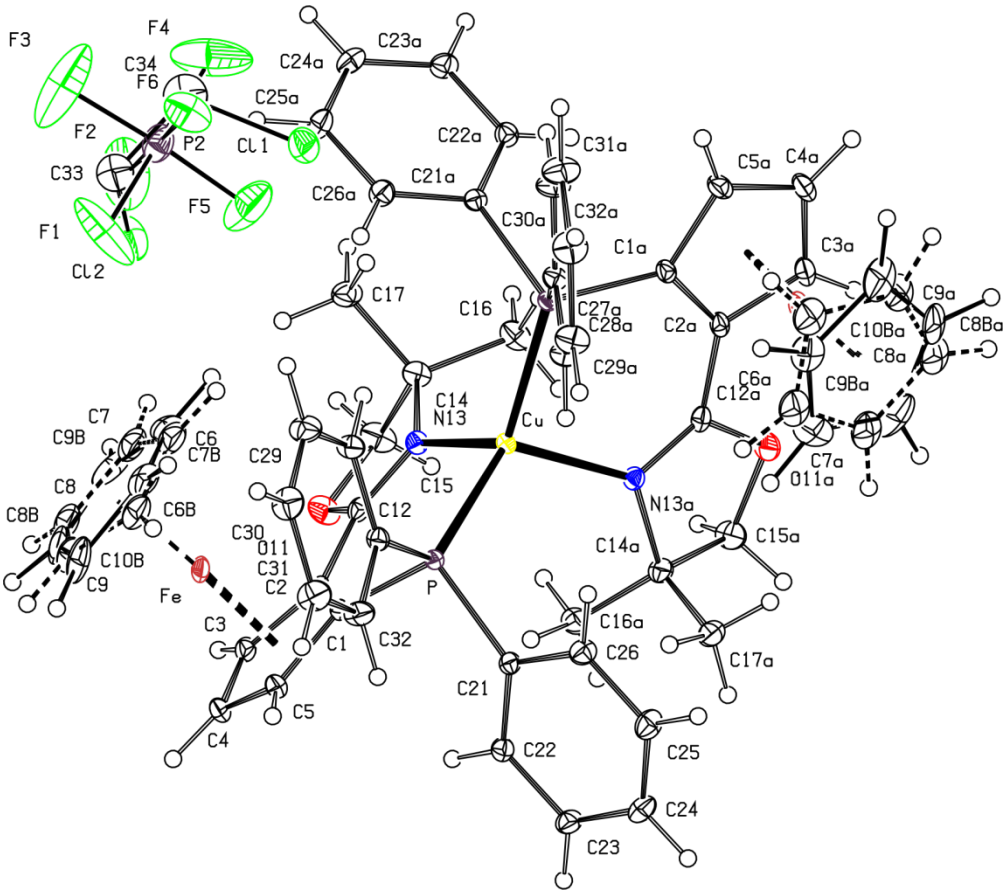

Figure S5. Displacement ellipsoid plot of of **5**·$C_2H_4Cl_2$ (30% probability level).

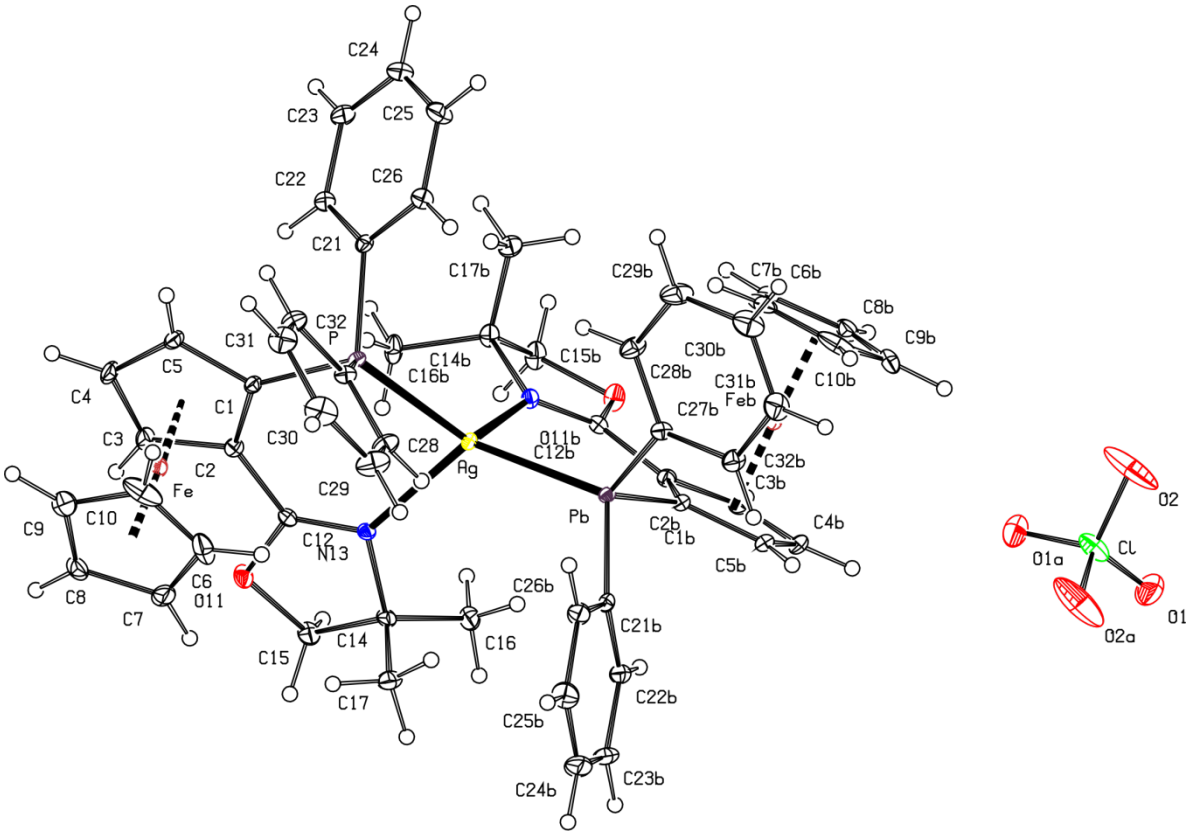

Figure S6. Displacement ellipsoid plot of the structure of **6** (30% probability level).

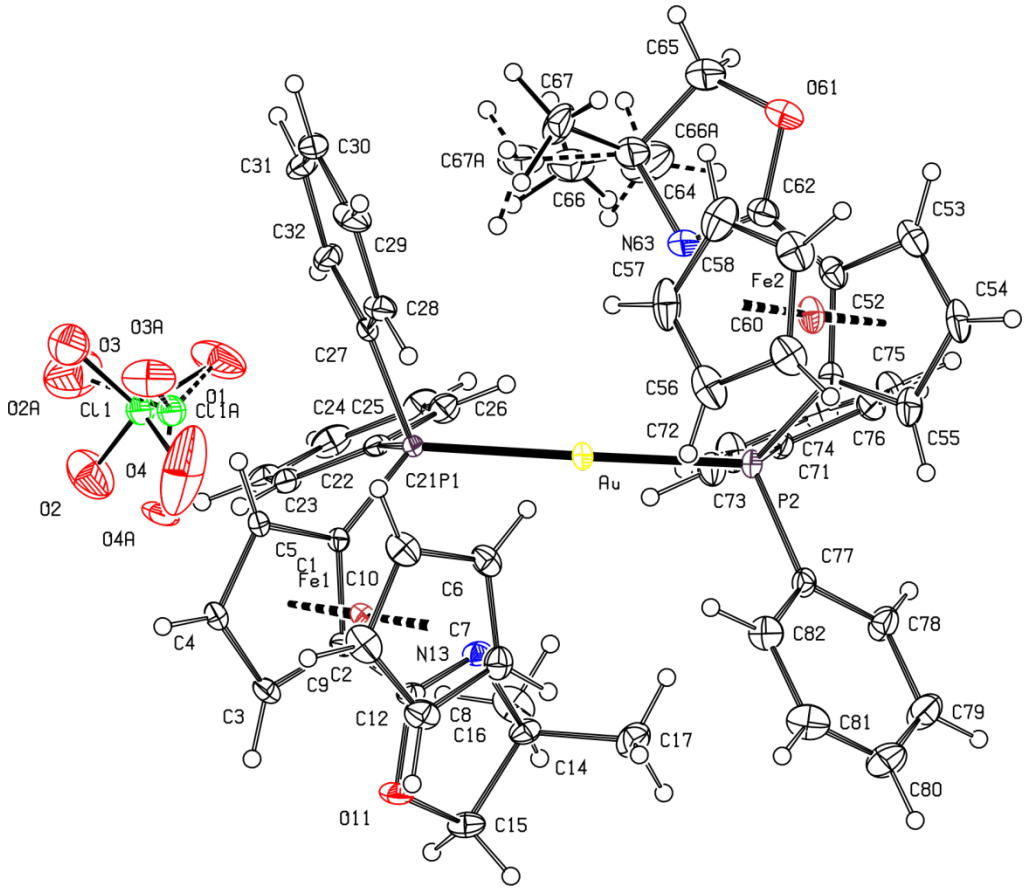

Figure S7. Displacement ellipsoid plot of the structure of **7** (30% probability level).

Table S1. Selected crystallographic data and structure refinement parameters.[a]

Compound	**2a**	**2b**	**2c**
Formula	$C_{54}H_{52}Cl_2Cu_2Fe_2N_2O_2P_2$	$C_{54}H_{52}Br_2Cu_2Fe_2N_2O_2P_2$	$C_{54}H_{52}I_2Cu_2Fe_2N_2O_2P_2$
M	1132.59	1221.51	1315.49
Crystal system	triclinic	triclinic	triclinic
Space group	P–1 (no. 2)	P–1 (no. 2)	P–1 (no. 2)
T/K	150(2)	150(2)	150(2)
a/Å	8.6022(1)	8.7044(2)	9.8304(3)
b/Å	10.3705(2)	10.3913(3)	10.1402(3)
c/Å	14.6183(2)	14.6913(4)	14.1354(3)
α/°	72.2224(6)	71.9240(8)	93.457(1)
β/°	77.6107(6)	76.678(1)	104.929(1)
γ/°	77.8137(6)	76.9869(9)	111.613(1)
V/Å^3	1197.94(3)	1212.17(6)	1246.73(6)
Z	1	1	1
μ(Mo Kα)/mm^{-1}	1.692	3.211	2.757
Diffrns collected	17883	17963	12916
Independent diffrns	5508	5575	5719
Observed[a] diffrns	5010	5015	4980
R_{int}[b]/%	1.71	1.95	2.19
No. of parameters	300	300	300
R[b] obsd diffrns/%	2.29	2.13	2.48
R, wR[b] all data/%	2.63, 6.13	2.57, 5.26	3.16, 5.60
Δρ/e Å^{-3}	0.39, –0.28	0.43, –0.33	0.63, –0.42
CCDC entry	1838560	1838561	1838562

[a] Diffractions with $I > 2\sigma(I)$. [b] Definitions: $R_{int} = \Sigma\,|F_o^2 - F_o^2(\text{mean})|/\Sigma F_o^2$, where F_o^2(mean) is the average intensity of symmetry-equivalent diffractions. $R = \Sigma\,||F_o| - |F_c||/\Sigma\,|F_o|$, $wR = [\Sigma\{w(F_o^2 - F_c^2)^2\}/\Sigma w(F_o^2)^2]^{1/2}$.

Table S1 continued

Compound	**3**	**5**·$C_2H_4Cl_2$	**6**
Formula	$C_{54}H_{52}Cl_2Ag_2Fe_2N_2O_2P_2$	$C_{56}H_{52}Cl_2CuF_6Fe_2N_2O_2P_3$	$C_{54}H_{52}AgClFe_2N_2O_6P_2$
M	1221.25	1238.04	1141.93
Crystal system	monoclinic	monoclinic	orthorhombic
Space group	$P2_1/c$ (no. 14)	$C2/c$ (no. 15)	$P2_12_12$ (no. 18)
T/K	150(2)	150(2)	120(2)
a/Å	11.4719(3)	24.3010(4)	11.2448(7)
b/Å	12.1037(3)	11.9534(3)	19.970(1)
c/Å	17.9417(4)	19.8877(3)	11.2323(8)
α/°	90	90	90
β/°	100.1631(9)	111.2931(6)	90
γ/°	90	90	90
V/Å^3	2452.2(1)	5382.6(2)	2522.4(3)
Z	2	4	2
μ(Mo Kα)/mm^{-1}	1.585	1.177	1.120
Diffrns collected	19272	20596	28692
Independent diffrns	5634	6187	5822
Observed[a] diffrns	4694	5660	5796
R_{int}[b]/%	2.63	1.71	2.91
No. of parameters	321	422	311
R[b] obsd diffrns/%	2.82	3.35	1.69
R, wR[b] all data/%	3.75, 6.78	3.70, 8.43	1.71, 4.04
Δρ/e Å^{-3}	0.62, –0.42	0.88, –0.54	0.25, –0.38
CCDC entry	1838563	1838564	1838565

Table S1 continued

Compound	**7**
Formula	$C_{54}H_{52}AuClFe_2N_2O_6P_2$
M	1231.03
Crystal system	monoclinic
Space group	$P2_1/n$ (no. 14)
T/K	120(2)
a/Å	14.6573(6)
b/Å	19.9271(7)
c/Å	16.6591(7)
α/°	90
β/°	94.443(2)
γ/°	90
V/Å^3	4851.1(3)
Z	4
μ(Mo Kα)/mm^{-1}	3.782
Diffrns collected	68585
Independent diffrns	11169
Observed[a] diffrns	10035
R_{int}[b]/%	3.99
No. of parameters	670
R[b] obsd diffrns/%	3.13
R, wR[b] all data/%	3.68, 7.25
Δρ/e Å^{-3}	2.89, –1.51
CCDC entry	1838566