ORGANOMETALLICS
Organometallics, 1998, 17(26), 5746-5757, DOI:10.1021/om980576l

**Bis($\eta^5$-cyclopentadienyl)($\eta^1$-cyclopentadienyl)($\eta^2$-butadiene)tantalum (9).**
GCOSY NMR (THF-$d_8$, 599.8 MHz, 298 K): (resonances of the butadiene ligand) δ = 6.06 / 4.54, 4.21, 2.31 (3-H / 4-H', 4-H, 2-H), 4.54 / 6.06, 4.21, 2.31 (4-H' / 3-H, 4-H, 2-H), 2.31 / 6.06, 4.54, 4.21, 1.51, 1.11 (2-H, 3-H, 4-H', 4-H, 1-H', 1-H), 1.51 / 2.31, 1.11 (1-H' / 2-H, 1-H), 1.11 / 2.31, 1.51 (1-H / 2-H, 1-H').
GHSQC NMR (THF-$d_8$, 150.8 / 599.8 MHz, 298 K): δ = 149.0 / 6.06 (C3 / 3-H), 145.5 / 6.89, 145.4 / 6.67 (C6 / 6-H, C9 / 9-H), 121.1 / 6.21, 120.8 / 6.13 (C7 / 7-H, C8 / 8-H), 104.9 / 4.54 (C4 / 4-H'), 104.9 / 4.21 (C4 / 4-H), 102.2 / 4.51, 101.6 / 5.30 (each C-Cp / Cp-H) 43.3 / 3.74 (C5 / 5-H), 24.0 / 1.51 (C1 / 1-H'), 24.0 / 1.11 (C1 / 1-H).

**2,2-Bis($\eta^5$-cyclopentadienyl)-7,7-dimethyl-2,3,6,7-tetrahydro-2-tantala-oxepine methyltris(pentafluorophenyl)borate (13a).**
GCOSY NMR (dichloromethane-$d_2$, 599.8 MHz, 198 K): δ = 6.38 / 5.31, 2.45 (4-H / 5-H, 3-H), 5.31 / 6.38, 2.03, 1.31 (5-H / 4-H, 6-H', 6-H), 2.45 / 6.38 (3-H / 4-H), 2.03 / 5.31, 1.31 (6-H' / 5-H, 6-H), 1.33 / 0.92 (both $CH_3$), 1.31 / 5.31, 2.03 (6-H / 5-H, 6-H'), 0.92 / 1.33 (both $CH_3$).
GHSQC NMR (dichloromethane-$d_2$, 150.8 / 599.8 MHz, 198K): δ = 136.0 / 6.38 (C4 / 4-H), 124.5 / 5.31 (C5 / 5-H), 111.9 / 6.26, 109.0 / 6.19 (C-Cp / Cp-H), 38.8 / 2.45 (C3 / 3-H), 38.4 / 2.03 (C6 / 6-H'), 38.4 / 1.31 /C6 / 6-H), 28.3 / 1.33 ($\underline{C}H_3/C\underline{H}_3$), 24.4 / 0.92 ($\underline{C}H_3/C\underline{H}_3$), 9.19 / 0.39 ($\underline{Me}$-$B(C_6F_5)_3$).

**2,2-Bis($\eta^5$-cyclopentadienyl)-7,7-tetramethylene-2,3,6,7-tetrahydro-2-tantala-oxepine methyltris(pentafluorophenyl)borate (13b).**
GCOSY NMR (dichloromethane-$d_2$, 599.8 MHz, 198 K): δ = 6.36 / 5.34, 2.49 (4-H / 5-H, 3-H), 5.34 / 6.36, 2.01, 1.55 (5-H / 4-H, 6-H', 6-H), 2.49 / 6.36 (3-H / 4-H), 2.01 / 5.34, 1.55 (6-H' / 5-H, 6-H), 1.55 / 5.34 / 2.01 (6-H / 5-H, 6-H').
The cross signals of the cyclopentyl fragment were not assignable.

GHSQC NMR (dichloromethane-$d_2$, 150.8 / 599.8 MHz, 198K): δ = 135.6 / 6.36 (C4 / 4-H), 124.7 / 5.34 (C5 / 5-H), 112.0 / 6.27, 109.1 / 6.18 (C-Cp / Cp-H), 39.3 / 2.49 ( C3 / 3-H), 36.1 / 2.01 (C6 / 6-H'), 36.1 / 1.55 (C6 / 6-H), 9.35 / 0.40 (Me-$B(C_6F_5)_3$). The cross signals of the cyclopentyl fragment were not assignable.

**2,2-Bis($\eta^5$-cyclopentadienyl)-7,7-pentamethylene-2,3,6,7-tetrahydro-2-tantala-oxepine methyltris(pentafluorophenyl)borate (13c).**

GCOSY NMR (dichloromethane-$d_2$, 599.8 MHz, 198 K): δ = 6.38 / 5.30, 2.48 (4-H / 5-H, 3-H), 5.30 / 6.38, 1.98, 1.24 (5-H / 4-H, 6-H', 6-H), 2.48 / 6.38 (3-H / 4-H), 1.98 / 5.30, 1.24 (6-H' / 5-H, 6-H), 1.24 / 5.30 / 1.98 (6-H / 5-H, 6-H'). The cross signals of the cyclohexyl fragment were not assignable.

GHSQC NMR (dichloromethane-$d_2$, 150.8 / 599.8 MHz, 198K): δ = 135.8 / 6.38 (C4 / 4-H), 124.3 / 5.30 (C5 / 5-H), 112.2 / 6.26, 109.6 / 6.20 (C-Cp / Cp-H), 39.5 / 2.48 (C3 / 3-H), 39.3 / 1.98 (C6 / 6-H'), 39.3 / 1.24 (C6 / 6-H), 9.36 / 0.41 (Me-$B(C_6F_5)_3$). The cross signals of the cyclohexyl fragment were not asignable.

**2,2-Bis($\eta^5$-cyclopentadienyl)-7,7-diphenyl-2,3,6,7-tetrahydro-2-tantala-oxepine methyltris(pentafluorophenyl)borate (13d).**

GCOSY NMR (dichloromethane-$d_2$, 599.8 MHz, 198 K): δ = 6.47 / 5.18, 2.76, 2.49 (4-H / 5-H, 3-H', 3-H), 5.18 / 6.47, 3.11, 2.07 (5-H / 4-H, 6-H', 6-H), 3.11 / 5.18, 2.07 (6-H' / 5-H, 6-H), 2.76 / 6.47, 2.49 (3-H' / 4-H, 3-H), 2.49 / 6.47, 2.76 (3-H / 4-H, 3-H'); 2.07 / 5.18, 3.11 (6-H / 5-H, 6-H'). The cross signals of the phenyl substituents were not assignable.

GHSQC NMR (dichloromethane-$d_2$, 150.8 / 599.8 MHz, 213K): 136.9 / 6.47 (C4 / 4-H), 124.4 / 5.18 (C5 / 5-H), 112.0 / 6.20, 109.9 / 6.13 (C-Cp / Cp-H), 40.9 / 2.76 (C3 / 3-H'), 40.9 / 2.49 (C3 / 3-H), 37.4 / 3.11 (C6 / 6-H'), 37.4 / 2.07 (C6 / 6-H), 9.27 / 0.43 (Me-$B(C_6F_5)_3$); The cross signals of the phenyl substituents were not assignable.

**2,2-Bis($\eta^5$-cyclopentadienyl)-7-methyl-7-phenyl-2,3,6,7-tetrahydro-2-tantala-oxepine methyltris(pentafluorophenyl)borate (13e).**

GCOSY NMR (dichloromethane-$d_2$, 599.8 MHz, 213 K): isomer **A**: δ = 6.26 / 5.29, 2.64, 2.45 (4-H / 5-H , 3-H', 3-H), 5.29 / 6.26, 2.93, 1.55 (5-H / 4-H, 6-H', 6-H), 2.93 / 5.29, 1.55 (6-H' / 5-H, 6-H), 2.64 / 6.26, 2.45 (3-H' / 4-H, 3-H), 2.45 / 6.26, 2.64 (3-H / 4-H, 3-H'), 1.55 / 5.29, 2.93 (6-H / 5-H, 6-H'); isomer **B**: δ = 6.54 / 5.47, 2.52 (4-H / 5-H , 3-H), 5.47 / 6.54, 2.59, 1.75 (5-H / 4-H, 6-H', 6-H), 2.59 / 5.47, 1.75 (6-H' / 5-H, 6-H), 2.52 / 6.54 (3-H / 4-H), 1.75 / 5.47, 2.50 (6-H / 5-H, 6-H'); The cross signals of the phenyl substituents were not assignable.

GHSQC NMR (dichloromethane-$d_2$, 150.8 / 599.8 MHz, 213 K): isomer **A**: δ = 135.9 / 6.26 (C4 / 4-H), 124.6 / 5.29 (C5 / 5-H), 112.2 / 6.14, 109.5 / 6.04 (C-Cp / Cp-H), 39.8 / 2.64 (C3 / 3-H'), 39.8 / 2.45 (C3 / 3-H) 36.1 / 2.93 (C6 / 6-H'), 36.1 / 1.55 (C6 / 6-H), 31.2 / 1.60 (C14 / 14-H), 9.36 / 0.41 (Me-$B(C_6F_5)_3$); isomer **B**: δ = 136.8 / 6.54 (C4 / 4-H), 124.3 / 5.47 (C5 / 5-H), 111.9 / 6.38, 109.2 / 6.28 (C-Cp / Cp-H), 39.4 / 2.52 (C3 / 3-H), 34.6 / 2.59 (C6 / 6-H'), 34.6 / 1.75 (C6 / 6-H), 25.8 / 1.25 (C14 / 14-H), isomers **A** und **B**: 9.25 / 0.41 (Me-$B(C_6F_5)_3$); The cross signals of the phenyl substituents were not assignable.

**2,2-Bis($\eta^5$-cyclopentadienyl)-2,3-dihydro-7-methyl-2-tantala-6*H*-azepine methyltris(pentafluorophenyl)borate (14a):**

GCOSY NMR (dichloromethane-$d_2$, 599.8 MHz, 198 K): δ = 6.20 / 4.80, 2.04, 1.38 (4-H / 5-H, 3-H', 3-H), 4.80 / 6.20, 3.11, 2.09 (5-H / 4-H, 6-H', 6-H), 3.11 / 4.80, 2.09 (6-H' / 5-H, 6-H), 2.09 / 4.80, 3.11 (6-H / 5-H, 6-H'), 2.04 / 6.20, 1.38 (3-H' / 4-H, 3-H), 1.38 / 6.20, 2.04 (3-H / 4-H, 3-H').

GHSQC NMR (dichloromethane-$d_2$, 150.8 / 599.8 MHz, 198 K): δ = 138.0 / 6.20 (C4 / 4-H), 112.7 / 4.80 (C5 / 5-H), 107.3 / 5.99, 104.7 / 5.92 (each C-Cp /

Cp-H), 35.2 / 3.11 (C6 / 6-H'), 35.2 / 2.09 (C6 / 6-H), 29.6 / 2.04 (C3 / 3-H'), 29.6 / 1.38 (C3 / 3-H), 26.3 / 2.11 (C8 / 8-H), 9.23 / 0.37 (Me-$B(C_6F_5)_3$ ).

**2,2-Bis($\eta^5$-cyclopentadienyl)-2,3-dihydro-7-ethyl-2-tantala-6*H*-azepine methyltris(pentafluorophenyl)borate (14b)**:

GCOSY NMR (dichloromethane-$d_2$, 599.8 MHz, 213 K): δ = 6.18 / 4.79, 2.05, 1.38 (4-H / 5-H, 3-H', 3-H), 4.79 / 6.18, 3.05, 2.07 (5-H / 4-H, 6-H', 6-H), 3.05 / 4.79, 2.07 (6-H' / 5-H, 6-H), 2.47 / 2.26, 1.00 (8-H' / 8-H, 9-H), 2.28 / 2.47, 1.00 (8-H / 8-H', 9-H), 2.07 / 4.74, 3.05 (6-H' / 5-H, 6-H), 2.05 / 6.18, 1.38 (3-H' / 4-H, 3-H), 1.38 / 6.18, 2.05 (3-H / 4-H, 3-H'), 1.00 / 2.47, 2.26 (9-H / 8-H', 8-H).

GHSQC-NMR (dichloromethane-$d_2$, 150.8 / 599.8 MHz, 213 K): δ = 138.1 / 6.18 (C4 / 4-H), 112.55 / 4.79 (C5 / 5-H), 107.4 / 5.96, 104.8 / 5.88 (C-Cp / Cp-H), 35.0 / 3.05 (C6 / 6-H'), 35.0 / 2.07 (C6 / 6-H), 33.0 / 2.47 (C8 / 8-H'), 33.0 / 2.26 (C8 / 8-H), 29.7 / 2.05 (C3 / 3-H'), 29.7 / 1.38 (C3 / 3-H), 9.4 / 0.40 (Me-$B(C_6F_5)_3$, 9.1 / 1.00 (C9 / 9-H).

**2,2-Bis($\eta^5$-cyclopentadienyl)-2,3-dihydro-7-phenyl-2-tantala-6*H*-azepine methyltris(pentafluorophenyl)borate (14c)**:

GCOSY NMR (dichloromethane-$d_2$, 599.8 MHz, 213 K): δ = 7.78 / 7.48 (9-H / 10-H), 7.57 / 7.48 (11-H / 10-H), 7.48 / 7.78, 7.57 (10-H / 9-H, 11-H), 6.34 / 4.93, 2.15, 1.62 (4-H / 5-H, 3-H', 3-H), 4.93 / 6.34, 3.99, 2.15 (5-H / 4-H, 6-H', 6-H), 3.99 / 4.93, 2.22 (6-H' / 5-H, 6-H), 2.22 / 4.93, 3.99 (6-H / 5-H, 6-H'), 2.15 / 6.34, 1.62 (3-H' / 4-H, 3-H), 1.62 / 6.34, 2.15 (3-H / 4-H, 3-H').

GHSQC NMR (dichloromethane-$d_2$, 150.8 / 599.8 MHz, 213 K): δ = 138.9 / 6.34 (C4 / 4-H), 130.7 / 5.57 (C11 / 11-H), 129.0 / 7.78 (C9 / 9-H), 128.5 / 7.48 (C10 / 10-H), 113.4 / 9.93 (C5 / 5-H), 107.4 / 6.08, 104.9 / 6.01 (C-Cp / Cp-H), 30.2 / 3.99 (C6 / 6-H'), 30.2 / 2.22 (C6 / 6-H), 24.1 / 2.15 (C3 / 3-H'), 29.1 / 1.62 (C3 / 3-H), 0.41 / 9.2 (Me-$B(C_6F_5)_3$).

**2,2-Bis($\eta^5$-cyclopentadienyl)-2,3-dihydro-7-(p-tolylmethyl)-2-tantala-6*H*-azepine methyltris(pentafluorophenyl)borate (14d)**:

GCOSY NMR (dichloromethane-$d_2$, 599.8 MHz, 198 K): δ = 7.15 / 6.96 (10-H / 11-H), 6.96 / 7.15 (11-H / 10-H), 6.19 / 4.77, 1.98, 1.38 (4-H / 5-H, 3-H', 3-H), 4.77 / 6.19, 3.18, 2.20 (5-H / 4-H, 6-H', 6-H), 3.72 / 3.56 (8-H' / 8-H), 3.18 / 4.77, 2.20 (6-H' / 5-H, 6-H), 2.20 / 4.77, 3.18 (6-H / 5-H, 6-H'), 1.98 / 6.19, 1.38 (3-H' / 4-H, 3-H), 1.38 / 6.19, 1.98 (3-H / 4-H, 3-H').

GHSQC NMR (dichloromethane-$d_2$, 150.8 / 599.8 MHz, 198K): δ = 138.3 / 6.19 (C4 / 4-H), 128.9 / 7.15 (C11 / 11-H), 128.5 / 6.96 (C10 / 10-H), 112.6 / 4.77 (C5 / 5-H), 107.2 / 5.77, 104.7 / 5.75 (C-Cp / Cp-H), 45.1 / 3.72 (C8 / 8-H'), 45.1 / 3.56 (C8 / 8-H), 34.2 / 3.18 (C6 / 6-H'), 34.2 / 2.20 (C6 / 6-H), 29.7 / 1.48 (C3 / 3-H'), 29.7 / 1.38 (C3 / 3-H), 20.6 / 229 (C13 / 13-H), 9.35 / 0.41 (Me-$B(C_6F_5)_3$).

**(1-3;6-η)-5,6-Dimethylhexa-2,5-dien-1,6-ylene-bis($\eta^5$-cyclopentadienyl)tantalum methyltris(pentafluorophenyl)borate (15a)**:

GCOSY NMR (bromobenzene-$d_5$, 599.8 MHz, 298 K): δ = 4.87 / 2.91, 2.42 (3-H / 4-H', 4-H), 4.75 / 2.11, 1.03 (2-H / 1-H', 1-H), 2.91 / 4.87, 2.42 (4-H' / 3-H, 4-H), 2.42 / 4.87, 2.91 (4-H / 3-H, 4-H'), 2.11 / 4.75, 1.03 (1-H' / 2-H, 1-H), 1.44 / 2.42 (8-H / 4-H), 1.03 / 4.75, 2.11 (1-H / 2-H, 1-H').

GHSQC NMR (dichloromethane-$d_2$, 150.8 / 599.8 MHz, 198K): δ = 112.4 / 4.75 (C2 / 2-H), 105.2 / 4.87 (C3 / 3-H), 102.8 / 5.00, 101.8 / 4.88 (C-Cp / Cp-H), 43.3 / 2.91 (C4 / 4-H'), 43.3 / 2.42 (C4 / 4-H), 36.3 / 2.11 (C1 / 1-H'), 36.3 / 1.03 (C1 / 1-H), 28.3 / 1.44 (C7 / 7-H), 20.8 / 1.37 (C8 / 8-H), 11.2 / 1.10 (Me-$B(C_6F_5)_3$).

**(1-3;6-η)-5-Propylhexa-2,5-dien-1,6-ylene-bis(η$^5$-cyclopentadienyl)tantalum methyltris(pentafluorophenyl)borate (15b) and (1-3;6-η)-6-propylhexa-2,5-dien-1,6-ylene-bis(cyclopentadienyl)tantalum methyltris(pentafluorophenyl)borate (15c):**

GCOSY NMR (dichloromethane-$d_2$, 599.8 MHz, 198 K: **15b**: δ = 5.10 / 2.84, 2.27 (3-H / 4-H', 4-H), 4.82 / 2.09, 1.03 (2-H / 1-H', 1-H), 2.84 / 5.10, 2.27 (4-H' / 3-H, 4-H), 2.27 / 5.18, 2.84 (4-H / 3-H, 4-H'), 2.09 / 4.82, 1.03 (1-H' / 2-H, 1-H), 1.03 / 4.82, 2.09 (1-H / 2-H, 1-H'); **15c**: δ = 5.00 / 2.79, 2.33 (3-H / 4-H', 4-H), 4.57 / 2.06, 0.99 (2-H / 1-H', 1-H), 2.79 / 5.00, 2.33 (4-H' / 3-H, 4-H), 2.33 / 5.00 2.79 (4-H / 3-H, 4-H'), 2.06 / 4.57, 0.99 (1-H' / 2-H, 1-H), 0.99 / 4.57, 2.06 (1-H / 2-H, 1-H'). The cross signals of the propyl substituents were not assignable.

GHSQC NMR (bromobenzene-$d_5$, 150.8 / 599.8 MHz, 198K): **15b**: δ = 154.8 / 6.62 (C6 / 6-H), 112.9 / 5.10 (C3 / 3-H), 111.5 / 4.82 (C2 / 2-H), 102.5 / 5.03, 101.8 / 4.89 (C-Cp / Cp-H), 47.2 / 1.70 (C7 / 7-H'), 47.2 / 1.56 (C7 / 7-H), 37.9 / 2.09 (C1 / 1-H'), 37.9 / 1.03 (C1 / 1-H), 35.0 / 2.84 (C4 / 4-H'), 35.0 / 2.27 (C4 / 4-H), 23.7 / 1.25 (C8 / 8-H'), 23.7 / 1.16 (C8 / 8-H), 14.2 / 0.87 (C9 / 9-H), **15c**: δ = 140.1 / 5.81 (C5 / 5-H), 114.2 / 5.00 (C3 / 3-H), 109.3 / 47.5 (C2 / 2-H), 103.0 / 5.00, 102.9 / 4.87 (C-Cp / Cp-H), 43.6 / 1.80 (C7 / 7-H'), 43.6 / 1.70 (C7 / 7-H), 39.1 / 2.79 (C4 / 4-H'), 39.1 / 2.33 (C4 / 4-H), 33.6 / 2.04 (C1 / 1-H'), 33.6 / 1.03 (C1 / 1-H), 21.3 / 1.25 (C8 / 8-H) 13.9 (C9 / 9-H); the cross resonance of the methyltris(pentafluorophenyl)borate anions is identical for both isomers: δ = 11.2 / 1.11 (Me-B($C_6F_5$)$_3$).

**Table 1.** Crystal data and structure refinement for **10**.

| | |
|---|---|
| Identification code | ERK_689 |
| Empirical formula | $C_{34}\ H_{21}\ B\ Cl_2\ F_{15}\ Ta$ |
| Formula weight | 977.17 |
| Temperature | 173(2) K |
| Wavelength | 0.71073 Å |
| Crystal system | orthorhombic |
| Space group | $P2_12_12_1$ No.19 |
| Unit cell dimensions | a = 12.714(3) Å<br>b = 14.821(3) Å<br>c = 17.367(3) Å |
| Volume | 3272.5(12) $Å^3$ |
| Z | 4 |
| Density (calculated) | 1.983 $Mg/m^3$ |
| Absorption coefficient | 3.635 $mm^{-1}$ |
| F(000) | 1888 |
| Crystal size | 0.20 x 0.15 x 0.10 mm |
| Theta range for data collection | 2.72 to 26.26°. |
| Index ranges | 0<=h<=15, 0<=k<=18, 0<=l<=21 |
| Reflections collected | 3693 |
| Independent reflections | 3693 [R(int) = 0.0000] |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 3692 / 2 / 461 |
| Goodness-of-fit on $F^2$ | 1.059 |
| Final R indices [$I>2\sigma(I)$] | R1 = 0.0384, $wR^2$ = 0.0918 |
| R indices (all data) | R1 = 0.0622, $wR^2$ = 0.1021 |
| Absolute structure parameter | -0.01(2) |
| Largest diff. peak and hole | 1.069 and -0.963 $eÅ^{-3}$ |

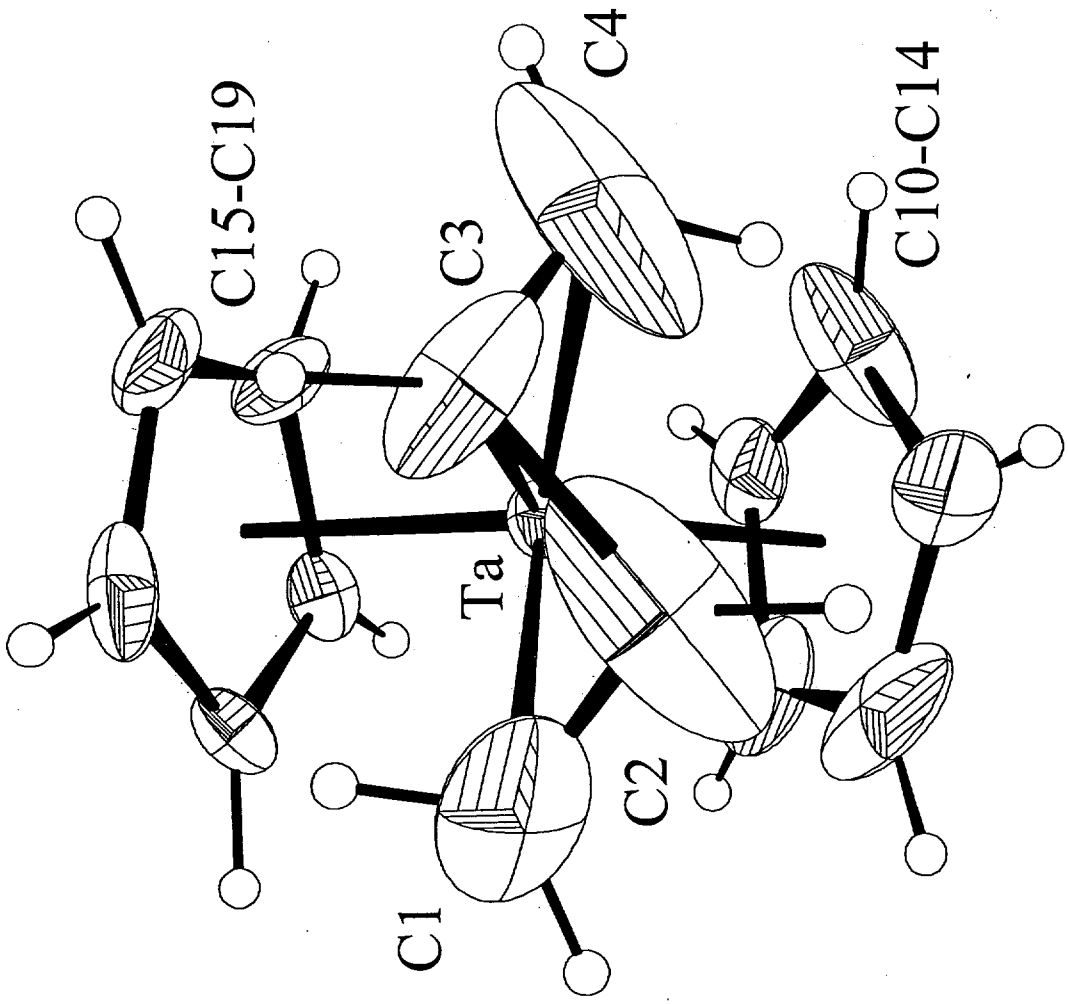
C15-C19
C3
C4
C10-C14
Ta
C2
C1

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

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Ta | 438(1) | 2287(1) | 8283(1) | 31(1) |
| C(1) | -689(21) | 2252(16) | 9403(11) | 127(9) |
| C(2) | 238(29) | 1894(22) | 9559(11) | 213(23) |
| C(3) | 970(19) | 2714(14) | 9503(8) | 97(8) |
| C(4) | 1804(24) | 2363(21) | 9145(19) | 265(28) |
| C(10) | 1538(8) | 1125(10) | 7805(8) | 116(9) |
| C(11) | 943(11) | 757(9) | 8422(7) | 212(20) |
| C(12) | -134(10) | 769(8) | 8206(9) | 140(12) |
| C(13) | -205(9) | 1145(8) | 7455(8) | 90(7) |
| C(14) | 829(11) | 1365(8) | 7208(6) | 65(5) |
| C(15) | 814(6) | 3426(7) | 7326(5) | 54(4) |
| C(16) | -209(7) | 3080(6) | 7182(4) | 41(3) |
| C(17) | -860(5) | 3314(6) | 7816(5) | 43(3) |
| C(18) | -239(8) | 3804(6) | 8352(4) | 64(4) |
| C(19) | 795(7) | 3873(6) | 8049(6) | 70(5) |
| B | 8417(10) | 6423(9) | 10625(7) | 32(3) |
| C(21) | 9644(9) | 6034(6) | 10682(6) | 29(2) |
| C(22) | 10183(9) | 6138(8) | 11385(6) | 37(3) |
| F(22) | 9698(6) | 6567(5) | 11984(3) | 45(2) |
| C(23) | 11196(9) | 5863(8) | 11515(8) | 39(3) |
| F(23) | 11654(6) | 6033(6) | 12194(4) | 64(2) |
| C(24) | 11741(9) | 5461(8) | 10939(9) | 46(3) |
| F(24) | 12753(5) | 5194(5) | 11039(5) | 62(2) |
| C(25) | 11271(8) | 5344(7) | 10255(7) | 37(3) |
| F(25) | 11798(5) | 4917(5) | 9663(5) | 57(2) |
| C(26) | 10240(8) | 5638(7) | 10130(6) | 30(2) |
| F(26) | 9873(5) | 5510(5) | 9407(4) | 42(2) |
| C(31) | 7806(7) | 6077(7) | 9819(6) | 28(2) |
| C(32) | 7710(8) | 5179(8) | 9636(7) | 35(3) |
| F(32) | 8241(5) | 4550(4) | 10051(4) | 45(2) |
| C(33) | 7097(10) | 4836(8) | 9044(7) | 37(3) |
| F(33) | 7049(6) | 3932(5) | 8921(5) | 56(2) |
| C(34) | 6520(9) | 5404(9) | 8597(7) | 39(3) |
| F(34) | 5926(6) | 5088(6) | 8024(4) | 59(2) |
| C(35) | 6569(9) | 6312(8) | 8748(6) | 35(3) |
| F(35) | 6011(6) | 6896(5) | 8308(5) | 54(2) |
| C(36) | 7208(9) | 6633(7) | 9342(6) | 37(3) |
| F(36) | 7179(6) | 7528(4) | 9442(4) | 47(2) |
| C(41) | 8567(8) | 7520(6) | 10652(5) | 26(2) |
| C(42) | 8132(9) | 8103(8) | 11203(6) | 38(3) |
| F(42) | 7438(6) | 7794(5) | 11718(4) | 55(2) |
| C(43) | 8333(10) | 9012(7) | 11222(6) | 39(3) |
| F(43) | 7871(7) | 9537(5) | 11768(5) | 63(2) |
| C(44) | 8996(10) | 9390(8) | 10700(8) | 45(3) |
| F(44) | 9189(7) | 10297(5) | 10712(5) | 60(2) |
| C(45) | 9423(9) | 8865(7) | 10137(7) | 37(3) |
| F(45) | 10066(6) | 9231(5) | 9605(5) | 58(2) |
| C(46) | 9213(9) | 7950(7) | 10129(6) | 36(3) |
| F(46) | 9648(6) | 7477(4) | 9541(4) | 47(2) |
| C(51) | 7697(10) | 6001(8) | 11320(8) | 45(3) |
| C(60) | 9478(15) | 7935(14) | 3279(12) | 109(8) |
| Cl(61) | 10394(4) | 8643(3) | 3712(2) | 78(1) |
| Cl(62) | 8191(4) | 8213(3) | 3553(3) | 81(1) |

 



**Table 3.** Bond lengths [Å] and angles [°] for **10**.

| | |
|---|---|
| Ta-C(13) | 2.365(10) |
| Ta-C(14) | 2.366(10) |
| Ta-C(12) | 2.367(11) |
| Ta-C(10) | 2.368(13) |
| Ta-C(11) | 2.369(12) |
| Ta-C(17) | 2.387(8) |
| Ta-C(16) | 2.390(8) |
| Ta-C(18) | 2.411(8) |
| Ta-C(15) | 2.416(8) |
| Ta-C(19) | 2.430(9) |
| C(1)-C(2) | 1.32(3) |
| C(2)-C(3) | 1.53(4) |
| C(3)-C(4) | 1.33(3) |
| C(10)-C(14) | 1.42 |
| C(10)-C(11) | 1.42 |
| C(11)-C(12) | 1.42 |
| C(12)-C(13) | 1.42 |
| C(13)-C(14) | 1.42 |
| C(15)-C(16) | 1.42 |
| C(15)-C(19) | 1.42 |
| C(16)-C(17) | 1.42 |
| C(17)-C(18) | 1.42 |
| C(18)-C(19) | 1.42 |
| B-C(41) | 1.64(2) |
| B-C(51) | 1.64(2) |
| B-C(21) | 1.67(2) |
| B-C(31) | 1.68(2) |
| C(21)-C(26) | 1.356(14) |
| C(21)-C(22) | 1.41(2) |
| C(22)-F(22) | 1.366(13) |
| C(22)-C(23) | 1.37(2) |
| C(23)-F(23) | 1.339(14) |
| C(23)-C(24) | 1.35(2) |
| C(24)-C(25) | 1.34(2) |
| C(24)-F(24) | 1.357(13) |
| C(25)-F(25) | 1.381(13) |
| C(25)-C(26) | 1.398(14) |
| C(26)-F(26) | 1.352(12) |
| C(31)-C(32) | 1.37(2) |
| C(31)-C(36) | 1.39(2) |
| C(32)-F(32) | 1.357(13) |
| C(32)-C(33) | 1.39(2) |
| C(33)-F(33) | 1.358(13) |
| C(33)-C(34) | 1.36(2) |
| C(34)-F(34) | 1.335(13) |
| C(34)-C(35) | 1.37(2) |
| C(35)-F(35) | 1.355(12) |
| C(35)-C(36) | 1.40(2) |
| C(36)-F(36) | 1.339(13) |
| C(41)-C(46) | 1.38(2) |
| C(41)-C(42) | 1.403(14) |
| C(42)-F(42) | 1.336(13) |
| C(42)-C(43) | 1.37(2) |
| C(43)-C(44) | 1.36(2) |
| C(43)-F(43) | 1.359(13) |
| C(44)-C(45) | 1.36(2) |
| C(44)-F(44) | 1.367(13) |
| C(45)-F(45) | 1.349(13) |
| C(45)-C(46) | 1.38(2) |
| C(46)-F(46) | 1.357(12) |
| C(60)-Cl(61) | 1.74(2) |
| C(60)-Cl(62) | 1.75(2) |

 



| | |
|---|---|
| C(13)-Ta-C(14) | 34.93(13) |
| C(13)-Ta-C(12) | 34.93(14) |
| C(14)-Ta-C(12) | 58.1(2) |
| C(13)-Ta-C(10) | 58.1(2) |
| C(14)-Ta-C(10) | 34.9(2) |
| C(12)-Ta-C(10) | 58.1(2) |
| C(13)-Ta-C(11) | 58.1(2) |
| C(14)-Ta-C(11) | 58.1(2) |
| C(12)-Ta-C(11) | 34.9(2) |
| C(10)-Ta-C(11) | 34.9(2) |
| C(13)-Ta-C(17) | 90.7(4) |
| C(14)-Ta-C(17) | 104.2(4) |
| C(12)-Ta-C(17) | 112.0(4) |
| C(10)-Ta-C(17) | 138.9(4) |
| C(11)-Ta-C(17) | 146.4(4) |
| C(13)-Ta-C(16) | 75.4(4) |
| C(14)-Ta-C(16) | 74.1(3) |
| C(12)-Ta-C(16) | 108.5(5) |
| C(10)-Ta-C(16) | 106.3(4) |
| C(11)-Ta-C(16) | 130.2(4) |
| C(17)-Ta-C(16) | 34.59(10) |
| C(13)-Ta-C(18) | 125.1(4) |
| C(14)-Ta-C(18) | 130.8(3) |
| C(12)-Ta-C(18) | 141.2(4) |
| C(10)-Ta-C(18) | 155.0(4) |
| C(11)-Ta-C(18) | 169.9(4) |
| C(17)-Ta-C(18) | 34.42(10) |
| C(16)-Ta-C(18) | 57.18(13) |
| C(13)-Ta-C(15) | 98.7(5) |
| C(14)-Ta-C(15) | 79.6(4) |
| C(12)-Ta-C(15) | 133.3(5) |
| C(10)-Ta-C(15) | 98.6(4) |
| C(11)-Ta-C(15) | 133.3(4) |
| C(17)-Ta-C(15) | 57.15(12) |
| C(16)-Ta-C(15) | 34.36(10) |
| C(18)-Ta-C(15) | 56.84(13) |
| C(13)-Ta-C(19) | 131.0(4) |
| C(14)-Ta-C(19) | 112.8(4) |
| C(12)-Ta-C(19) | 165.4(5) |
| C(10)-Ta-C(19) | 122.3(4) |
| C(11)-Ta-C(19) | 153.2(4) |
| C(17)-Ta-C(19) | 56.98(13) |
| C(16)-Ta-C(19) | 56.94(13) |
| C(18)-Ta-C(19) | 34.11(11) |
| C(15)-Ta-C(19) | 34.08(11) |
| C(1)-C(2)-C(3) | 102(2) |
| C(4)-C(3)-C(2) | 102(2) |
| C(14)-C(10)-C(11) | 108.0 |
| C(14)-C(10)-Ta | 72.5(4) |
| C(11)-C(10)-Ta | 72.6(4) |
| C(12)-C(11)-C(10) | 108.0 |
| C(12)-C(11)-Ta | 72.5(4) |
| C(10)-C(11)-Ta | 72.5(4) |
| C(13)-C(12)-C(11) | 108.0 |
| C(13)-C(12)-Ta | 72.5(4) |
| C(11)-C(12)-Ta | 72.6(5) |
| C(12)-C(13)-C(14) | 108.0 |
| C(12)-C(13)-Ta | 72.6(4) |
| C(14)-C(13)-Ta | 72.6(4) |
| C(10)-C(14)-C(13) | 108.0 |
| C(10)-C(14)-Ta | 72.6(5) |
| C(13)-C(14)-Ta | 72.5(4) |
| C(16)-C(15)-C(19) | 108.0 |
| C(16)-C(15)-Ta | 71.8(3) |
| C(19)-C(15)-Ta | 73.5(3) |

| | |
|---|---|
| C(17)-C(16)-C(15) | 108.0 |
| C(17)-C(16)-Ta | 72.6(3) |
| C(15)-C(16)-Ta | 73.8(3) |
| C(16)-C(17)-C(18) | 108.0 |
| C(16)-C(17)-Ta | 72.8(3) |
| C(18)-C(17)-Ta | 73.7(3) |
| C(19)-C(18)-C(17) | 108.0 |
| C(19)-C(18)-Ta | 73.6(3) |
| C(17)-C(18)-Ta | 71.8(3) |
| C(18)-C(19)-C(15) | 108.0 |
| C(18)-C(19)-Ta | 72.2(3) |
| C(15)-C(19)-Ta | 72.5(3) |
| C(41)-B-C(51) | 115.0(9) |
| C(41)-B-C(21) | 103.5(9) |
| C(51)-B-C(21) | 110.3(9) |
| C(41)-B-C(31) | 112.3(9) |
| C(51)-B-C(31) | 103.9(9) |
| C(21)-B-C(31) | 112.1(9) |
| C(26)-C(21)-C(22) | 112.9(10) |
| C(26)-C(21)-B | 129.1(10) |
| C(22)-C(21)-B | 118.0(9) |
| F(22)-C(22)-C(23) | 115.9(10) |
| F(22)-C(22)-C(21) | 119.4(9) |
| C(23)-C(22)-C(21) | 124.7(12) |
| F(23)-C(23)-C(24) | 120.8(11) |
| F(23)-C(23)-C(22) | 119.9(12) |
| C(24)-C(23)-C(22) | 119.3(12) |
| C(25)-C(24)-C(23) | 118.9(10) |
| C(25)-C(24)-F(24) | 119.9(13) |
| C(23)-C(24)-F(24) | 121.2(12) |
| C(24)-C(25)-F(25) | 120.1(10) |
| C(24)-C(25)-C(26) | 121.0(11) |
| F(25)-C(25)-C(26) | 118.8(11) |
| F(26)-C(26)-C(21) | 121.7(9) |
| F(26)-C(26)-C(25) | 115.1(10) |
| C(21)-C(26)-C(25) | 123.2(11) |
| C(32)-C(31)-C(36) | 112.7(10) |
| C(32)-C(31)-B | 121.9(9) |
| C(36)-C(31)-B | 124.5(10) |
| F(32)-C(32)-C(31) | 119.9(10) |
| F(32)-C(32)-C(33) | 115.0(9) |
| C(31)-C(32)-C(33) | 125.1(10) |
| F(33)-C(33)-C(34) | 119.8(11) |
| F(33)-C(33)-C(32) | 120.2(10) |
| C(34)-C(33)-C(32) | 120.0(10) |
| F(34)-C(34)-C(33) | 120.9(12) |
| F(34)-C(34)-C(35) | 120.8(12) |
| C(33)-C(34)-C(35) | 118.3(11) |
| F(35)-C(35)-C(34) | 119.7(10) |
| F(35)-C(35)-C(36) | 120.2(10) |
| C(34)-C(35)-C(36) | 120.0(10) |
| F(36)-C(36)-C(31) | 121.6(10) |
| F(36)-C(36)-C(35) | 114.7(10) |
| C(31)-C(36)-C(35) | 123.7(10) |
| C(46)-C(41)-C(42) | 113.6(9) |
| C(46)-C(41)-B | 120.6(9) |
| C(42)-C(41)-B | 125.8(9) |
| F(42)-C(42)-C(43) | 116.4(10) |
| F(42)-C(42)-C(41) | 120.3(10) |
| C(43)-C(42)-C(41) | 123.2(11) |
| C(44)-C(43)-F(43) | 119.9(10) |
| C(44)-C(43)-C(42) | 120.2(11) |
| F(43)-C(43)-C(42) | 119.9(11) |
| C(43)-C(44)-C(45) | 119.4(11) |
| C(43)-C(44)-F(44) | 120.4(12) |
| C(45)-C(44)-F(44) | 120.1(12) |

| | |
|---|---|
| F(45)-C(45)-C(44) | 120.2(10) |
| F(45)-C(45)-C(46) | 120.3(11) |
| C(44)-C(45)-C(46) | 119.4(11) |
| F(46)-C(46)-C(41) | 120.0(9) |
| F(46)-C(46)-C(45) | 115.8(10) |
| C(41)-C(46)-C(45) | 124.1(10) |
| Cl(61)-C(60)-Cl(62) | 111.5(9) |

 



**Table 4.** Anisotropic displacement parameters ($Å^2 \times 10^3$) for **10**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [ h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12} ]$

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Ta | 35(1) | 29(1) | 29(1) | 2(1) | -4(1) | 3(1) |
| C(1) | 196(26) | 109(16) | 76(13) | 25(14) | 73(16) | -12(21) |
| C(2) | 263(42) | 337(51) | 40(10) | 92(19) | 64(18) | 191(41) |
| C(3) | 186(24) | 85(11) | 20(6) | -3(8) | -22(9) | -67(17) |
| C(4) | 269(40) | 264(42) | 264(38) | -198(35) | -238(35) | 190(36) |
| C(10) | 137(19) | 152(21) | 59(10) | 31(12) | 42(12) | 91(17) |
| C(11) | 84(14) | 75(14) | 476(58) | 61(24) | 179(25) | 26(11) |
| C(12) | 164(24) | 49(10) | 207(27) | -70(16) | 111(22) | -50(13) |
| C(13) | 149(21) | 47(9) | 74(11) | -27(8) | -14(13) | -23(12) |
| C(14) | 85(11) | 41(8) | 69(10) | -13(7) | 36(9) | 12(8) |
| C(15) | 65(9) | 52(8) | 43(7) | 19(6) | -11(6) | -26(7) |
| C(16) | 54(8) | 40(6) | 30(5) | 12(5) | -6(5) | 11(6) |
| C(17) | 40(6) | 52(8) | 37(6) | 3(6) | -1(5) | 18(6) |
| C(18) | 99(12) | 31(6) | 60(8) | -6(6) | -37(10) | 21(7) |
| C(19) | 75(10) | 32(7) | 104(14) | 23(8) | -21(9) | -17(7) |
| B | 32(6) | 31(6) | 33(6) | -1(5) | 2(5) | 3(5) |
| C(21) | 30(5) | 22(4) | 36(5) | 4(4) | 3(5) | -3(5) |
| C(22) | 47(7) | 34(6) | 30(5) | 10(5) | -8(5) | 1(5) |
| F(22) | 59(4) | 50(4) | 27(3) | -1(3) | -1(3) | 3(4) |
| C(23) | 28(6) | 34(6) | 54(8) | 8(6) | -10(6) | -5(5) |
| F(23) | 61(5) | 74(5) | 57(5) | 14(4) | -32(4) | -11(4) |
| C(24) | 26(6) | 30(6) | 83(10) | 0(6) | -24(6) | 4(5) |
| F(24) | 28(4) | 61(5) | 95(6) | 12(5) | -8(4) | 7(4) |
| C(25) | 28(5) | 26(5) | 57(7) | -1(5) | 6(5) | 3(5) |
| F(25) | 37(4) | 46(4) | 87(6) | -18(4) | 14(4) | 1(3) |
| C(26) | 28(6) | 26(5) | 38(5) | 2(4) | -4(5) | 3(4) |
| F(26) | 38(4) | 52(4) | 35(3) | -16(3) | 2(3) | -1(3) |
| C(31) | 14(4) | 33(5) | 36(5) | 8(5) | 0(4) | -1(4) |
| C(32) | 28(6) | 35(6) | 43(7) | 3(5) | 6(5) | 4(5) |
| F(32) | 46(4) | 28(3) | 63(5) | 7(3) | -7(4) | 2(3) |
| C(33) | 45(7) | 31(6) | 36(6) | -9(5) | 1(6) | 5(5) |
| F(33) | 58(5) | 35(4) | 76(5) | -10(4) | 1(4) | -5(4) |
| C(34) | 31(6) | 56(8) | 30(6) | -15(6) | -2(5) | -5(6) |
| F(34) | 56(4) | 62(5) | 58(5) | -20(4) | -16(4) | 0(4) |
| C(35) | 35(6) | 36(6) | 35(6) | 3(5) | -2(5) | 10(5) |
| F(35) | 62(4) | 49(4) | 51(4) | -4(4) | -28(4) | 12(3) |
| C(36) | 42(6) | 33(6) | 37(6) | -8(5) | 2(5) | 1(5) |
| F(36) | 59(4) | 31(4) | 52(4) | -1(3) | -19(3) | 9(3) |
| C(41) | 36(5) | 19(6) | 24(5) | -5(4) | -4(4) | 0(4) |
| C(42) | 44(6) | 42(6) | 27(5) | 1(5) | 4(5) | 6(5) |
| F(42) | 64(4) | 46(4) | 55(4) | -4(4) | 29(4) | 3(4) |
| C(43) | 56(7) | 28(5) | 33(6) | -17(5) | -4(5) | 3(6) |
| F(43) | 92(6) | 39(4) | 58(5) | -21(4) | 14(5) | 8(4) |
| C(44) | 47(7) | 30(6) | 58(8) | 3(6) | -22(6) | -6(5) |
| F(44) | 76(5) | 34(4) | 71(5) | -1(4) | -9(4) | -6(4) |
| C(45) | 36(6) | 32(5) | 42(6) | 7(5) | -11(5) | 4(5) |
| F(45) | 62(5) | 49(4) | 63(5) | 25(4) | 11(4) | -5(4) |
| C(46) | 41(6) | 36(6) | 32(5) | 0(5) | -4(5) | 6(4) |
| F(46) | 60(4) | 42(4) | 38(3) | 6(3) | 22(3) | 6(4) |
| C(51) | 53(8) | 28(6) | 56(8) | 19(6) | 14(7) | 0(6) |
| C(60) | 92(12) | 123(17) | 113(14) | -85(14) | 18(14) | -37(12) |
| Cl(61) | 66(2) | 82(3) | 86(3) | -25(2) | 14(2) | -19(3) |
| Cl(62) | 81(3) | 57(2) | 103(3) | -2(2) | -30(2) | -10(2) |

**Table 5.** Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$ x $10^3$) for **10**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1A) | -746(21) | 2879(16) | 9296(11) | 153 |
| H(1B) | -1300(21) | 1883(16) | 9399(11) | 153 |
| H(2) | 408(29) | 1285(22) | 9676(11) | 256 |
| H(3) | 858(19) | 3314(14) | 9677(8) | 117 |
| H(4A) | 1807(24) | 1744(21) | 9003(19) | 319 |
| H(4B) | 2395(24) | 2732(21) | 9033(19) | 319 |
| H(10) | 2280(8) | 1198(10) | 7794(8) | 139 |
| H(11) | 1218(16) | 540(14) | 8896(8) | 254 |
| H(12) | -706(13) | 562(12) | 8510(12) | 168 |
| H(13) | -833(11) | 1234(14) | 7169(11) | 108 |
| H(14) | 1013(16) | 1626(12) | 6727(7) | 78 |
| H(15) | 1407(6) | 3368(7) | 6997(5) | 64 |
| H(16) | -420(10) | 2750(9) | 6739(5) | 49 |
| H(17) | -1583(6) | 3168(10) | 7872(7) | 52 |
| H(18) | -475(11) | 4044(9) | 8829(5) | 76 |
| H(19) | 1373(9) | 4167(9) | 8288(8) | 84 |
| H(51A) | 7984(42) | 6190(49) | 11819(8) | 68 |
| H(51B) | 7703(58) | 5341(8) | 11287(32) | 68 |
| H(51C) | 6973(19) | 6221(49) | 11271(31) | 68 |
| H(60A) | 9627(15) | 7303(14) | 3427(12) | 131 |
| H(60B) | 9543(15) | 7982(14) | 2713(12) | 131 |

**Table 1.** Crystal data and structure refinement for **14a**.

| | |
|---|---|
| Identification code | ERK_713 |
| Empirical formula | $C_{35}$ $H_{22}$ B $F_{15}$ N Ta |
| Formula weight | 933.30 |
| Temperature | 173(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | triclinic, P1bar (No. 2) |
| Unit cell dimensions | a = 10.020(1) Å α = 80.38(1)°.<br>b = 10.813(1) Å β = 84.55(1)°.<br>c = 15.027(1) Å γ = 81.00(1)°. |
| Volume | 1581.5(2) Å$^3$ |
| Z, Calculated density | 2, 1.960 Mg/m$^3$ |
| Absorption coefficient | 3.593 mm$^{-1}$ |
| F(000) | 904 |
| Crystal size | 0.30 x 0.30 x 0.20 mm |
| Theta range for data collection | 2.19 to 26.29°. |
| Index ranges | -12<=h<=12, -13<=k<=13, 0<=l<=18 |
| Reflections collected / unique | 6675 / 6420 [R(int) = 0.0265] |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 6420 / 0 / 480 |
| Goodness-of-fit on $F^2$ | 1.159 |
| Final R indices [I>2σ(I)] | R1 = 0.0357, w$R^2$ = 0.1034 |
| R indices (all data) | R1 = 0.0395, w$R^2$ = 0.1050 |
| Largest diff. peak and hole | 1.456 and -3.311 eÅ$^{-3}$ |

**Table 2.** Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$ x $10^3$) for **14a**.
U(eq) is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Ta(2) | 1302(1) | 3231(1) | 2786(1) | 22(1) |
| N(1) | 3168(5) | 2505(4) | 2862(3) | 30(1) |
| C(3) | 801(6) | 1465(6) | 3716(4) | 33(1) |
| C(4) | 1611(7) | 1198(6) | 4521(4) | 39(1) |
| C(5) | 2937(7) | 771(7) | 4537(4) | 40(2) |
| C(6) | 3889(7) | 511(6) | 3736(5) | 41(2) |
| C(7) | 4171(6) | 1688(5) | 3060(4) | 30(1) |
| C(71) | 5566(7) | 1771(7) | 2661(5) | 43(2) |
| C(10) | 1863(8) | 2944(8) | 1222(4) | 50(2) |
| C(11) | 896(9) | 4038(7) | 1237(5) | 50(2) |
| C(12) | -327(8) | 3653(7) | 1648(5) | 47(2) |
| C(13) | -93(8) | 2342(7) | 1913(5) | 46(2) |
| C(14) | 1249(9) | 1902(7) | 1656(5) | 54(2) |
| C(15) | 889(8) | 5433(6) | 2896(5) | 44(2) |
| C(16) | 2020(7) | 4917(5) | 3393(5) | 41(2) |
| C(17) | 1575(6) | 4081(6) | 4138(5) | 35(1) |
| C(18) | 190(7) | 4084(7) | 4090(5) | 40(2) |
| C(19) | -238(6) | 4921(7) | 3339(6) | 47(2) |
| B | 4465(6) | 13296(5) | 7747(4) | 19(1) |
| C(21) | 5322(5) | 13000(5) | 6785(3) | 21(1) |
| C(22) | 6697(5) | 12508(5) | 6672(3) | 20(1) |
| F(22) | 7453(3) | 12114(3) | 7394(2) | 31(1) |
| C(23) | 7402(5) | 12403(5) | 5853(4) | 26(1) |
| F(23) | 8727(3) | 11935(4) | 5811(2) | 37(1) |
| C(24) | 6749(6) | 12776(6) | 5067(4) | 28(1) |
| F(24) | 7409(4) | 12669(4) | 4256(2) | 42(1) |
| C(25) | 5402(6) | 13256(6) | 5121(3) | 26(1) |
| F(25) | 4727(4) | 13613(4) | 4368(2) | 39(1) |
| C(26) | 4737(5) | 13359(5) | 5969(4) | 24(1) |
| F(26) | 3401(3) | 13859(3) | 5954(2) | 30(1) |
| C(31) | 5377(5) | 12742(5) | 8629(3) | 23(1) |
| C(32) | 5929(6) | 13446(5) | 9149(4) | 27(1) |
| F(32) | 5784(4) | 14730(3) | 8954(3) | 45(1) |
| C(33) | 6695(6) | 12941(6) | 9873(4) | 34(1) |
| F(33) | 7215(4) | 13694(4) | 10338(3) | 50(1) |
| C(34) | 6961(6) | 11642(6) | 10111(4) | 34(1) |
| F(34) | 7724(4) | 11129(4) | 10807(2) | 47(1) |
| C(35) | 6448(6) | 10889(5) | 9620(4) | 29(1) |
| F(35) | 6725(4) | 9616(3) | 9830(3) | 41(1) |
| C(36) | 5682(5) | 11440(5) | 8907(4) | 24(1) |
| F(36) | 5277(4) | 10631(3) | 8423(2) | 32(1) |
| C(41) | 3066(5) | 12611(5) | 7939(3) | 20(1) |
| C(42) | 2151(6) | 12872(5) | 8674(4) | 24(1) |
| F(42) | 2415(4) | 13670(3) | 9214(2) | 34(1) |
| C(43) | 961(6) | 12356(6) | 8903(4) | 28(1) |
| F(43) | 128(4) | 12671(4) | 9609(2) | 41(1) |
| C(44) | 628(6) | 11511(5) | 8398(4) | 29(1) |
| F(44) | -508(4) | 10981(4) | 8624(3) | 41(1) |
| C(45) | 1483(6) | 11217(5) | 7670(4) | 27(1) |
| F(45) | 1175(4) | 10392(4) | 7169(3) | 43(1) |
| C(46) | 2657(5) | 11753(5) | 7468(4) | 23(1) |
| F(46) | 3440(4) | 11358(3) | 6755(2) | 34(1) |
| C(51) | 4044(6) | 14832(5) | 7621(4) | 25(1) |

**Table 3.** Bond lengths [Å] and angles [°] for **14a**.

| | |
|---|---|
| Ta(2)-N(1) | 1.918(5) |
| Ta(2)-C(3) | 2.264(6) |
| Ta(2)-C(15) | 2.383(6) |
| Ta(2)-C(11) | 2.394(6) |
| Ta(2)-C(16) | 2.401(6) |
| Ta(2)-C(13) | 2.405(7) |
| Ta(2)-C(19) | 2.407(6) |
| Ta(2)-C(18) | 2.409(6) |
| Ta(2)-C(14) | 2.410(7) |
| Ta(2)-C(12) | 2.415(7) |
| Ta(2)-C(17) | 2.420(6) |
| Ta(2)-C(10) | 2.423(6) |
| N(1)-C(7) | 1.253(7) |
| C(3)-C(4) | 1.484(9) |
| C(4)-C(5) | 1.338(10) |
| C(5)-C(6) | 1.499(9) |
| C(6)-C(7) | 1.536(9) |
| C(7)-C(71) | 1.478(8) |
| C(10)-C(14) | 1.404(12) |
| C(10)-C(11) | 1.408(11) |
| C(11)-C(12) | 1.409(12) |
| C(12)-C(13) | 1.396(11) |
| C(13)-C(14) | 1.396(12) |
| C(15)-C(19) | 1.398(11) |
| C(15)-C(16) | 1.406(10) |
| C(16)-C(17) | 1.401(10) |
| C(17)-C(18) | 1.396(9) |
| C(18)-C(19) | 1.380(11) |
| B-C(51) | 1.632(7) |
| B-C(31) | 1.655(7) |
| B-C(21) | 1.662(7) |
| B-C(41) | 1.666(7) |
| C(21)-C(26) | 1.380(7) |
| C(21)-C(22) | 1.402(7) |
| C(22)-F(22) | 1.355(6) |
| C(22)-C(23) | 1.372(8) |
| C(23)-F(23) | 1.344(6) |
| C(23)-C(24) | 1.375(8) |
| C(24)-F(24) | 1.343(6) |
| C(24)-C(25) | 1.368(8) |
| C(25)-F(25) | 1.343(6) |
| C(25)-C(26) | 1.394(7) |
| C(26)-F(26) | 1.364(6) |
| C(31)-C(32) | 1.381(8) |
| C(31)-C(36) | 1.395(7) |
| C(32)-F(32) | 1.358(7) |
| C(32)-C(33) | 1.379(8) |
| C(33)-F(33) | 1.347(7) |
| C(33)-C(34) | 1.380(9) |
| C(34)-F(34) | 1.346(6) |
| C(34)-C(35) | 1.369(9) |
| C(35)-F(35) | 1.351(7) |
| C(35)-C(36) | 1.375(8) |
| C(36)-F(36) | 1.356(6) |
| C(41)-C(46) | 1.388(7) |
| C(41)-C(42) | 1.404(7) |
| C(42)-F(42) | 1.348(6) |
| C(42)-C(43) | 1.385(8) |
| C(43)-F(43) | 1.342(7) |
| C(43)-C(44) | 1.378(9) |
| C(44)-F(44) | 1.343(6) |
| C(44)-C(45) | 1.373(8) |

| | |
|---|---|
| C(45)-F(45) | 1.347(7) |
| C(45)-C(46) | 1.377(8) |
| C(46)-F(46) | 1.354(6) |
| | |
| N(1)-Ta(2)-C(3) | 86.7(2) |
| N(1)-Ta(2)-C(15) | 113.6(2) |
| C(3)-Ta(2)-C(15) | 133.8(3) |
| N(1)-Ta(2)-C(11) | 109.1(3) |
| C(3)-Ta(2)-C(11) | 132.5(3) |
| C(15)-Ta(2)-C(11) | 81.6(3) |
| N(1)-Ta(2)-C(16) | 83.2(2) |
| C(3)-Ta(2)-C(16) | 120.2(2) |
| C(15)-Ta(2)-C(16) | 34.2(2) |
| C(11)-Ta(2)-C(16) | 106.3(3) |
| N(1)-Ta(2)-C(13) | 118.7(2) |
| C(3)-Ta(2)-C(13) | 76.5(2) |
| C(15)-Ta(2)-C(13) | 120.4(3) |
| C(11)-Ta(2)-C(13) | 56.3(3) |
| C(16)-Ta(2)-C(13) | 154.6(2) |
| N(1)-Ta(2)-C(19) | 138.2(2) |
| C(3)-Ta(2)-C(19) | 104.0(3) |
| C(15)-Ta(2)-C(19) | 33.9(3) |
| C(11)-Ta(2)-C(19) | 93.2(3) |
| C(16)-Ta(2)-C(19) | 56.4(2) |
| C(13)-Ta(2)-C(19) | 103.1(3) |
| N(1)-Ta(2)-C(18) | 116.8(2) |
| C(3)-Ta(2)-C(18) | 77.9(2) |
| C(15)-Ta(2)-C(18) | 55.9(3) |
| C(11)-Ta(2)-C(18) | 126.3(3) |
| C(16)-Ta(2)-C(18) | 56.0(2) |
| C(13)-Ta(2)-C(18) | 116.3(3) |
| C(19)-Ta(2)-C(18) | 33.3(3) |
| N(1)-Ta(2)-C(14) | 86.1(3) |
| C(3)-Ta(2)-C(14) | 81.5(3) |
| C(15)-Ta(2)-C(14) | 137.9(3) |
| C(11)-Ta(2)-C(14) | 56.4(3) |
| C(16)-Ta(2)-C(14) | 154.9(3) |
| C(13)-Ta(2)-C(14) | 33.7(3) |
| C(19)-Ta(2)-C(14) | 135.0(3) |
| C(18)-Ta(2)-C(14) | 147.8(3) |
| N(1)-Ta(2)-C(12) | 136.5(2) |
| C(3)-Ta(2)-C(12) | 105.6(3) |
| C(15)-Ta(2)-C(12) | 87.9(3) |
| C(11)-Ta(2)-C(12) | 34.1(3) |
| C(16)-Ta(2)-C(12) | 121.5(2) |
| C(13)-Ta(2)-C(12) | 33.7(3) |
| C(19)-Ta(2)-C(12) | 80.0(3) |
| C(18)-Ta(2)-C(12) | 106.6(3) |
| C(14)-Ta(2)-C(12) | 56.0(3) |
| N(1)-Ta(2)-C(17) | 85.4(2) |
| C(3)-Ta(2)-C(17) | 86.9(2) |
| C(15)-Ta(2)-C(17) | 56.2(2) |
| C(11)-Ta(2)-C(17) | 137.3(3) |
| C(16)-Ta(2)-C(17) | 33.8(2) |
| C(13)-Ta(2)-C(17) | 149.2(3) |
| C(19)-Ta(2)-C(17) | 55.8(2) |
| C(18)-Ta(2)-C(17) | 33.6(2) |
| C(14)-Ta(2)-C(17) | 165.9(2) |
| C(12)-Ta(2)-C(17) | 135.7(2) |
| N(1)-Ta(2)-C(10) | 80.6(2) |
| C(3)-Ta(2)-C(10) | 114.3(3) |
| C(15)-Ta(2)-C(10) | 110.0(3) |
| C(11)-Ta(2)-C(10) | 34.0(3) |
| C(16)-Ta(2)-C(10) | 121.7(3) |
| C(13)-Ta(2)-C(10) | 56.0(3) |
| C(19)-Ta(2)-C(10) | 127.2(3) |

| | |
|---|---|
| C(18)-Ta(2)-C(10) | 160.2(3) |
| C(14)-Ta(2)-C(10) | 33.8(3) |
| C(12)-Ta(2)-C(10) | 56.1(3) |
| C(17)-Ta(2)-C(10) | 153.7(3) |
| C(7)-N(1)-Ta(2) | 158.3(5) |
| C(4)-C(3)-Ta(2) | 111.1(4) |
| C(5)-C(4)-C(3) | 126.5(6) |
| C(4)-C(5)-C(6) | 126.2(6) |
| C(5)-C(6)-C(7) | 115.1(5) |
| N(1)-C(7)-C(71) | 124.3(6) |
| N(1)-C(7)-C(6) | 116.5(5) |
| C(71)-C(7)-C(6) | 119.2(5) |
| C(14)-C(10)-C(11) | 107.7(7) |
| C(14)-C(10)-Ta(2) | 72.6(4) |
| C(11)-C(10)-Ta(2) | 71.9(4) |
| C(10)-C(11)-C(12) | 107.8(7) |
| C(10)-C(11)-Ta(2) | 74.1(4) |
| C(12)-C(11)-Ta(2) | 73.8(4) |
| C(13)-C(12)-C(11) | 107.8(7) |
| C(13)-C(12)-Ta(2) | 72.8(4) |
| C(11)-C(12)-Ta(2) | 72.2(4) |
| C(14)-C(13)-C(12) | 108.6(7) |
| C(14)-C(13)-Ta(2) | 73.3(4) |
| C(12)-C(13)-Ta(2) | 73.6(4) |
| C(13)-C(14)-C(10) | 108.0(7) |
| C(13)-C(14)-Ta(2) | 73.0(4) |
| C(10)-C(14)-Ta(2) | 73.6(4) |
| C(19)-C(15)-C(16) | 108.1(7) |
| C(19)-C(15)-Ta(2) | 74.0(4) |
| C(16)-C(15)-Ta(2) | 73.6(3) |
| C(17)-C(16)-C(15) | 107.3(6) |
| C(17)-C(16)-Ta(2) | 73.8(3) |
| C(15)-C(16)-Ta(2) | 72.2(4) |
| C(18)-C(17)-C(16) | 107.8(6) |
| C(18)-C(17)-Ta(2) | 72.8(3) |
| C(16)-C(17)-Ta(2) | 72.4(4) |
| C(19)-C(18)-C(17) | 108.8(6) |
| C(19)-C(18)-Ta(2) | 73.3(4) |
| C(17)-C(18)-Ta(2) | 73.6(3) |
| C(18)-C(19)-C(15) | 107.9(6) |
| C(18)-C(19)-Ta(2) | 73.4(4) |
| C(15)-C(19)-Ta(2) | 72.1(4) |
| C(51)-B-C(31) | 112.6(4) |
| C(51)-B-C(21) | 105.5(4) |
| C(31)-B-C(21) | 111.5(4) |
| C(51)-B-C(41) | 109.1(4) |
| C(31)-B-C(41) | 106.3(4) |
| C(21)-B-C(41) | 111.9(4) |
| C(26)-C(21)-C(22) | 112.0(5) |
| C(26)-C(21)-B | 120.9(5) |
| C(22)-C(21)-B | 126.7(4) |
| F(22)-C(22)-C(23) | 114.2(5) |
| F(22)-C(22)-C(21) | 120.9(5) |
| C(23)-C(22)-C(21) | 124.9(5) |
| F(23)-C(23)-C(22) | 120.6(5) |
| F(23)-C(23)-C(24) | 119.6(5) |
| C(22)-C(23)-C(24) | 119.8(5) |
| F(24)-C(24)-C(25) | 120.0(5) |
| F(24)-C(24)-C(23) | 121.1(5) |
| C(25)-C(24)-C(23) | 118.8(5) |
| F(25)-C(25)-C(24) | 120.5(5) |
| F(25)-C(25)-C(26) | 120.5(5) |
| C(24)-C(25)-C(26) | 119.1(5) |
| F(26)-C(26)-C(21) | 119.8(5) |
| F(26)-C(26)-C(25) | 114.8(5) |
| C(21)-C(26)-C(25) | 125.4(5) |

| | |
|---|---|
| C(32)-C(31)-C(36) | 112.8(5) |
| C(32)-C(31)-B | 126.7(5) |
| C(36)-C(31)-B | 120.4(5) |
| F(32)-C(32)-C(33) | 114.2(5) |
| F(32)-C(32)-C(31) | 121.1(5) |
| C(33)-C(32)-C(31) | 124.7(5) |
| F(33)-C(33)-C(32) | 121.1(6) |
| F(33)-C(33)-C(34) | 119.5(5) |
| C(32)-C(33)-C(34) | 119.4(5) |
| F(34)-C(34)-C(35) | 120.8(6) |
| F(34)-C(34)-C(33) | 120.4(6) |
| C(35)-C(34)-C(33) | 118.8(5) |
| F(35)-C(35)-C(34) | 119.6(5) |
| F(35)-C(35)-C(36) | 120.8(5) |
| C(34)-C(35)-C(36) | 119.6(5) |
| F(36)-C(36)-C(35) | 116.0(5) |
| F(36)-C(36)-C(31) | 119.2(5) |
| C(35)-C(36)-C(31) | 124.7(5) |
| C(46)-C(41)-C(42) | 112.3(5) |
| C(46)-C(41)-B | 128.4(4) |
| C(42)-C(41)-B | 119.3(4) |
| F(42)-C(42)-C(43) | 115.7(5) |
| F(42)-C(42)-C(41) | 119.8(5) |
| C(43)-C(42)-C(41) | 124.5(5) |
| F(43)-C(43)-C(44) | 119.7(5) |
| F(43)-C(43)-C(42) | 120.8(5) |
| C(44)-C(43)-C(42) | 119.5(5) |
| F(44)-C(44)-C(45) | 121.1(5) |
| F(44)-C(44)-C(43) | 120.1(5) |
| C(45)-C(44)-C(43) | 118.7(5) |
| F(45)-C(45)-C(44) | 119.6(5) |
| F(45)-C(45)-C(46) | 120.7(5) |
| C(44)-C(45)-C(46) | 119.8(5) |
| F(46)-C(46)-C(45) | 114.3(5) |
| F(46)-C(46)-C(41) | 120.5(5) |
| C(45)-C(46)-C(41) | 125.2(5) |

**Table 4.** Anisotropic displacement parameters ($Å^2 \times 10^3$) for **14a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [ h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12} ]$

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Ta(2) | 24(1) | 18(1) | 25(1) | -4(1) | -6(1) | -3(1) |
| N(1) | 36(3) | 23(2) | 32(3) | -4(2) | -6(2) | -9(2) |
| C(3) | 31(3) | 39(3) | 29(3) | -5(2) | 4(2) | -9(3) |
| C(4) | 46(4) | 33(3) | 32(3) | 5(3) | 2(3) | -1(3) |
| C(5) | 43(4) | 42(4) | 30(3) | 1(3) | -6(3) | 6(3) |
| C(6) | 42(4) | 33(3) | 42(4) | -4(3) | 1(3) | 10(3) |
| C(7) | 22(3) | 25(3) | 43(3) | -16(2) | -5(2) | 5(2) |
| C(71) | 34(3) | 36(3) | 61(4) | -18(3) | 5(3) | -5(3) |
| C(10) | 49(4) | 78(6) | 18(3) | -7(3) | 3(3) | 0(4) |
| C(11) | 78(6) | 45(4) | 27(3) | 5(3) | -20(3) | -7(4) |
| C(12) | 52(4) | 50(4) | 40(4) | -7(3) | -23(3) | 0(3) |
| C(13) | 57(4) | 47(4) | 41(4) | -9(3) | -22(3) | -12(3) |
| C(14) | 79(6) | 40(4) | 48(4) | -16(3) | -32(4) | 7(4) |
| C(15) | 56(4) | 20(3) | 56(4) | -11(3) | -14(3) | 7(3) |
| C(16) | 39(3) | 15(3) | 73(5) | -16(3) | -14(3) | -5(2) |
| C(17) | 31(3) | 33(3) | 46(4) | -19(3) | -11(3) | 0(2) |
| C(18) | 32(3) | 49(4) | 44(4) | -30(3) | 18(3) | -10(3) |
| C(19) | 23(3) | 52(4) | 72(5) | -40(4) | -13(3) | 14(3) |
| B | 21(3) | 20(3) | 17(2) | -3(2) | -1(2) | -3(2) |
| C(21) | 23(2) | 19(2) | 20(2) | -2(2) | -2(2) | -5(2) |
| C(22) | 20(2) | 19(2) | 21(2) | -1(2) | -4(2) | -5(2) |
| F(22) | 25(2) | 40(2) | 27(2) | 3(1) | -8(1) | -1(1) |
| C(23) | 19(2) | 25(3) | 32(3) | -2(2) | 0(2) | -4(2) |
| F(23) | 23(2) | 48(2) | 35(2) | -4(2) | 3(1) | 2(2) |
| C(24) | 33(3) | 34(3) | 20(3) | -7(2) | 5(2) | -11(2) |
| F(24) | 39(2) | 59(2) | 26(2) | -8(2) | 3(2) | -7(2) |
| C(25) | 26(3) | 33(3) | 17(2) | -4(2) | -1(2) | -3(2) |
| F(25) | 36(2) | 59(2) | 20(2) | -3(2) | -7(1) | -3(2) |
| C(26) | 25(3) | 23(3) | 24(3) | -2(2) | -5(2) | -4(2) |
| F(26) | 19(2) | 42(2) | 25(2) | -5(1) | -3(1) | 5(1) |
| C(31) | 24(3) | 22(3) | 21(2) | -1(2) | -5(2) | -4(2) |
| C(32) | 32(3) | 28(3) | 23(3) | -5(2) | -5(2) | -3(2) |
| F(32) | 63(3) | 24(2) | 56(2) | -9(2) | -31(2) | -7(2) |
| C(33) | 36(3) | 40(3) | 30(3) | -12(3) | -12(2) | -5(3) |
| F(33) | 55(3) | 56(3) | 47(2) | -25(2) | -26(2) | -3(2) |
| C(34) | 29(3) | 48(4) | 21(3) | -3(2) | -9(2) | 3(3) |
| F(34) | 46(2) | 63(3) | 28(2) | 1(2) | -19(2) | 6(2) |
| C(35) | 30(3) | 24(3) | 29(3) | 8(2) | -3(2) | -3(2) |
| F(35) | 45(2) | 29(2) | 43(2) | 10(2) | -9(2) | 2(2) |
| C(36) | 25(3) | 23(3) | 23(3) | -2(2) | -2(2) | -2(2) |
| F(36) | 42(2) | 20(2) | 36(2) | -5(1) | -11(2) | -4(1) |
| C(41) | 20(2) | 17(2) | 20(2) | 1(2) | -4(2) | 1(2) |
| C(42) | 27(3) | 24(3) | 22(2) | -1(2) | -6(2) | -4(2) |
| F(42) | 43(2) | 39(2) | 25(2) | -12(1) | 3(1) | -15(2) |
| C(43) | 28(3) | 31(3) | 22(3) | 4(2) | -2(2) | -4(2) |
| F(43) | 36(2) | 56(2) | 31(2) | -9(2) | 11(2) | -12(2) |
| C(44) | 24(3) | 28(3) | 33(3) | 8(2) | -8(2) | -8(2) |
| F(44) | 28(2) | 49(2) | 47(2) | 0(2) | -2(2) | -19(2) |
| C(45) | 27(3) | 23(3) | 32(3) | -4(2) | -6(2) | -6(2) |
| F(45) | 44(2) | 39(2) | 53(2) | -17(2) | -4(2) | -20(2) |
| C(46) | 23(2) | 20(2) | 25(3) | -5(2) | -1(2) | -1(2) |
| F(46) | 35(2) | 30(2) | 41(2) | -19(2) | 7(2) | -9(1) |
| C(51) | 31(3) | 19(2) | 24(3) | 0(2) | -4(2) | -5(2) |

**Table 5.** Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$ x $10^3$) for **14a**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(3A) | -175 | 1578 | 3914 | 40 |
| H(3B) | 989 | 734 | 3382 | 40 |
| H(4) | 1140 | 1346 | 5082 | 47 |
| H(5) | 3310 | 618 | 5109 | 48 |
| H(6A) | 3510 | -65 | 3411 | 49 |
| H(6B) | 4761 | 59 | 3958 | 49 |
| H(71A) | 5574 | 2552 | 2225 | 64 |
| H(71B) | 5888 | 1039 | 2352 | 64 |
| H(71C) | 6161 | 1776 | 3141 | 64 |
| H(10) | 2768 | 2917 | 965 | 60 |
| H(11) | 1042 | 4884 | 1011 | 60 |
| H(12) | -1161 | 4189 | 1729 | 56 |
| H(13) | -740 | 1835 | 2219 | 56 |
| H(14) | 1673 | 1045 | 1756 | 65 |
| H(15) | 890 | 6027 | 2353 | 53 |
| H(16) | 2919 | 5101 | 3250 | 49 |
| H(17) | 2119 | 3597 | 4594 | 42 |
| H(18) | -367 | 3591 | 4506 | 48 |
| H(19) | -1138 | 5115 | 3156 | 56 |
| H(51A) | 3619 | 15078 | 8193 | 37 |
| H(51B) | 3404 | 15099 | 7148 | 37 |
| H(51C) | 4856 | 15242 | 7447 | 37 |

**Table 1.** Crystal data and structure refinement for **14d**.

| | |
|---|---|
| Identification code | ERK_741 |
| Empirical formula | $C_{42}$ $H_{28}$ B $F_{15}$ N Ta |
| Formula weight | 1023.41 |
| Temperature | 223(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | monoclinic, $P2_1/n$ (No.14) |
| Unit cell dimensions | a = 14.464(3) Å<br>b = 12.383(2) Å  β = 90.39(2)°.<br>c = 21.057(3) Å |
| Volume | 3771.4(11) Å$^3$ |
| Z, Calculated density | 4, 1.802 Mg/m$^3$ |
| Absorption coefficient | 3.023 mm$^{-1}$ |
| F(000) | 2000 |
| Crystal size | 0.30 x 0.20 x 0.20 mm |
| Theta range for data collection | 2.37 to 26.30°. |
| Index ranges | -18<=h<=18, 0<=k<=15, 0<=l<=26 |
| Reflections collected / unique | 7858 / 7648 [R(int) = 0.0383] |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 7648 / 0 / 543 |
| Goodness-of-fit on $F^2$ | 1.169 |
| Final R indices [I>2σ(I)] | R1 = 0.0387, w$R^2$ = 0.1046 |
| R indices (all data) | R1 = 0.0563, w$R^2$ = 0.1109 |
| Largest diff. peak and hole | 0.836 and -0.990 eÅ$^{-3}$ |

**Table 2.** Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$ x $10^3$) for **14b**.
U(eq) is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Ta(2) | 2529(1) | 1818(1) | 244(1) | 33(1) |
| C(3) | 2242(6) | 3416(5) | 742(4) | 56(2) |
| C(4) | 2913(6) | 3661(6) | 1220(4) | 56(2) |
| C(5) | 3040(6) | 3188(6) | 1794(4) | 57(2) |
| C(6) | 2503(6) | 2265(6) | 2032(3) | 51(2) |
| C(7) | 2663(5) | 1208(5) | 1683(3) | 43(2) |
| N(1) | 2652(4) | 1248(4) | 1080(2) | 38(1) |
| C(71) | 2811(6) | 184(6) | 2047(3) | 55(2) |
| C(72) | 2860(5) | -799(6) | 1625(3) | 49(2) |
| C(73) | 2057(5) | -1288(6) | 1428(4) | 53(2) |
| C(74) | 2097(6) | -2147(6) | 1012(4) | 59(2) |
| C(75) | 2915(6) | -2524(6) | 778(4) | 60(2) |
| C(76) | 3704(7) | -2023(7) | 979(5) | 77(3) |
| C(77) | 3691(6) | -1181(7) | 1390(4) | 66(2) |
| C(78) | 2928(10) | -3467(8) | 315(5) | 104(4) |
| C(10) | 4089(6) | 1209(8) | 142(5) | 71(2) |
| C(11) | 3696(6) | 1242(10) | -488(5) | 81(3) |
| C(12) | 3527(6) | 2322(9) | -624(4) | 69(3) |
| C(13) | 3790(6) | 2944(8) | -101(4) | 71(2) |
| C(14) | 4131(5) | 2251(8) | 358(4) | 67(2) |
| C(15) | 1351(5) | 1962(6) | -557(3) | 50(2) |
| C(16) | 1617(6) | 889(7) | -538(4) | 59(2) |
| C(17) | 1386(7) | 475(8) | 54(5) | 73(3) |
| C(18) | 954(5) | 1279(9) | 391(4) | 70(3) |
| C(19) | 927(5) | 2205(8) | 11(4) | 68(2) |
| B | 1176(5) | 2930(6) | -2825(4) | 40(2) |
| C(21) | 714(4) | 1706(5) | -2835(3) | 38(1) |
| C(22) | 634(5) | 1146(6) | -3402(3) | 47(2) |
| F(22) | 926(3) | 1617(4) | -3947(2) | 58(1) |
| C(23) | 279(5) | 115(6) | -3465(4) | 56(2) |
| F(23) | 237(4) | -346(4) | -4051(2) | 84(2) |
| C(24) | 6(5) | -442(6) | -2945(4) | 58(2) |
| F(24) | -332(4) | -1455(4) | -2997(3) | 87(2) |
| C(25) | 84(5) | 63(6) | -2368(4) | 50(2) |
| F(25) | -198(4) | -479(4) | -1848(2) | 71(1) |
| C(26) | 440(4) | 1094(5) | -2330(3) | 40(1) |
| F(26) | 463(3) | 1478(3) | -1730(2) | 55(1) |
| C(31) | 2277(5) | 2698(5) | -3001(3) | 40(1) |
| C(32) | 2817(4) | 2089(5) | -2607(3) | 42(2) |
| F(32) | 2466(3) | 1717(3) | -2048(2) | 50(1) |
| C(33) | 3739(5) | 1846(6) | -2709(4) | 53(2) |
| F(33) | 4231(3) | 1288(4) | -2284(3) | 75(1) |
| C(34) | 4146(5) | 2217(6) | -3259(4) | 57(2) |
| F(34) | 5031(3) | 1985(4) | -3378(3) | 82(2) |
| C(35) | 3620(6) | 2795(7) | -3689(4) | 61(2) |
| F(35) | 3999(4) | 3128(5) | -4222(3) | 85(2) |
| C(36) | 2696(5) | 3030(6) | -3544(3) | 48(2) |
| F(36) | 2295(3) | 3635(4) | -3993(2) | 67(1) |
| C(41) | 1090(4) | 3569(5) | -2136(3) | 37(1) |
| C(42) | 1785(5) | 4111(5) | -1822(3) | 45(2) |
| F(42) | 2653(3) | 4104(4) | -2026(2) | 57(1) |
| C(43) | 1648(6) | 4721(6) | -1269(3) | 52(2) |
| F(43) | 2396(4) | 5195(4) | -990(2) | 72(1) |
| C(44) | 795(6) | 4821(6) | -1022(3) | 57(2) |
| F(44) | 663(4) | 5418(4) | -496(2) | 84(2) |

| | | | | |
|---|---|---|---|---|
| C(45) | 72(5) | 4329(6) | -1326(4) | 53(2) |
| F(45) | -790(4) | 4440(4) | -1097(3) | 81(2) |
| C(46) | 224(5) | 3722(5) | -1860(3) | 46(2) |
| F(46) | -531(3) | 3258(4) | -2120(2) | 55(1) |
| C(51) | 631(5) | 3723(6) | -3330(3) | 52(2) |

**Table 3.** Bond lengths [Å] and angles [°] for **14b**.

| | |
|---|---|
| Ta(2)-N(1) | 1.903(5) |
| Ta(2)-C(3) | 2.278(7) |
| Ta(2)-C(17) | 2.378(8) |
| Ta(2)-C(14) | 2.389(8) |
| Ta(2)-C(10) | 2.390(8) |
| Ta(2)-C(15) | 2.396(6) |
| Ta(2)-C(18) | 2.395(7) |
| Ta(2)-C(16) | 2.397(7) |
| Ta(2)-C(11) | 2.401(8) |
| Ta(2)-C(13) | 2.411(8) |
| Ta(2)-C(19) | 2.413(7) |
| Ta(2)-C(12) | 2.419(7) |
| C(3)-C(4) | 1.426(11) |
| C(4)-C(5) | 1.354(11) |
| C(5)-C(6) | 1.472(11) |
| C(6)-C(7) | 1.520(10) |
| C(7)-N(1) | 1.270(8) |
| C(7)-C(71) | 1.497(9) |
| C(71)-C(72) | 1.509(10) |
| C(72)-C(73) | 1.372(10) |
| C(72)-C(77) | 1.387(12) |
| C(73)-C(74) | 1.379(11) |
| C(74)-C(75) | 1.368(12) |
| C(75)-C(76) | 1.364(13) |
| C(75)-C(78) | 1.521(12) |
| C(76)-C(77) | 1.355(13) |
| C(10)-C(14) | 1.369(13) |
| C(10)-C(11) | 1.441(13) |
| C(11)-C(12) | 1.388(15) |
| C(12)-C(13) | 1.395(13) |
| C(13)-C(14) | 1.381(13) |
| C(15)-C(19) | 1.381(12) |
| C(15)-C(16) | 1.384(11) |
| C(16)-C(17) | 1.390(12) |
| C(17)-C(18) | 1.376(14) |
| C(18)-C(19) | 1.399(13) |
| B-C(51) | 1.645(10) |
| B-C(21) | 1.657(10) |
| B-C(41) | 1.658(10) |
| B-C(31) | 1.663(10) |
| C(21)-C(26) | 1.368(9) |
| C(21)-C(22) | 1.383(9) |
| C(22)-F(22) | 1.358(8) |
| C(22)-C(23) | 1.382(10) |
| C(23)-C(24) | 1.355(12) |
| C(23)-F(23) | 1.360(9) |
| C(24)-F(24) | 1.351(9) |
| C(24)-C(25) | 1.371(11) |
| C(25)-F(25) | 1.351(9) |
| C(25)-C(26) | 1.379(9) |
| C(26)-F(26) | 1.350(7) |
| C(31)-C(36) | 1.362(9) |
| C(31)-C(32) | 1.364(9) |
| C(32)-F(32) | 1.365(8) |
| C(32)-C(33) | 1.385(10) |
| C(33)-F(33) | 1.332(8) |
| C(33)-C(34) | 1.382(11) |
| C(34)-F(34) | 1.337(8) |
| C(34)-C(35) | 1.378(12) |
| C(35)-F(35) | 1.319(9) |
| C(35)-C(36) | 1.404(11) |
| C(36)-F(36) | 1.335(8) |

| | |
|---|---|
| C(41)-C(42) | 1.374(9) |
| C(41)-C(46) | 1.397(9) |
| C(42)-F(42) | 1.330(8) |
| C(42)-C(43) | 1.405(10) |
| C(43)-C(44) | 1.347(11) |
| C(43)-F(43) | 1.361(8) |
| C(44)-F(44) | 1.346(8) |
| C(44)-C(45) | 1.366(11) |
| C(45)-F(45) | 1.347(8) |
| C(45)-C(46) | 1.371(10) |
| C(46)-F(46) | 1.347(8) |

| | |
|---|---|
| N(1)-Ta(2)-C(3) | 85.0(2) |
| N(1)-Ta(2)-C(17) | 87.5(3) |
| C(3)-Ta(2)-C(17) | 123.8(4) |
| N(1)-Ta(2)-C(14) | 84.6(3) |
| C(3)-Ta(2)-C(14) | 86.5(3) |
| C(17)-Ta(2)-C(14) | 147.9(4) |
| N(1)-Ta(2)-C(10) | 83.3(3) |
| C(3)-Ta(2)-C(10) | 119.3(3) |
| C(17)-Ta(2)-C(10) | 114.8(4) |
| C(14)-Ta(2)-C(10) | 33.3(3) |
| N(1)-Ta(2)-C(15) | 137.7(2) |
| C(3)-Ta(2)-C(15) | 97.4(3) |
| C(17)-Ta(2)-C(15) | 56.1(3) |
| C(14)-Ta(2)-C(15) | 137.6(3) |
| C(10)-Ta(2)-C(15) | 128.9(3) |
| N(1)-Ta(2)-C(18) | 82.0(3) |
| C(3)-Ta(2)-C(18) | 90.4(4) |
| C(17)-Ta(2)-C(18) | 33.5(3) |
| C(14)-Ta(2)-C(18) | 166.4(3) |
| C(10)-Ta(2)-C(18) | 145.4(4) |
| C(15)-Ta(2)-C(18) | 55.9(3) |
| N(1)-Ta(2)-C(16) | 120.3(3) |
| C(3)-Ta(2)-C(16) | 129.2(3) |
| C(17)-Ta(2)-C(16) | 33.9(3) |
| C(14)-Ta(2)-C(16) | 134.9(3) |
| C(10)-Ta(2)-C(16) | 107.6(3) |
| C(15)-Ta(2)-C(16) | 33.6(3) |
| C(18)-Ta(2)-C(16) | 55.7(3) |
| N(1)-Ta(2)-C(11) | 114.9(3) |
| C(3)-Ta(2)-C(11) | 133.1(4) |
| C(17)-Ta(2)-C(11) | 100.1(4) |
| C(14)-Ta(2)-C(11) | 56.3(3) |
| C(10)-Ta(2)-C(11) | 35.0(3) |
| C(15)-Ta(2)-C(11) | 94.0(3) |
| C(18)-Ta(2)-C(11) | 132.3(4) |
| C(16)-Ta(2)-C(11) | 78.6(3) |
| N(1)-Ta(2)-C(13) | 115.3(3) |
| C(3)-Ta(2)-C(13) | 77.1(3) |
| C(17)-Ta(2)-C(13) | 151.7(3) |
| C(14)-Ta(2)-C(13) | 33.4(3) |
| C(10)-Ta(2)-C(13) | 55.9(3) |
| C(15)-Ta(2)-C(13) | 106.3(3) |
| C(18)-Ta(2)-C(13) | 157.2(4) |
| C(16)-Ta(2)-C(13) | 119.0(3) |
| C(11)-Ta(2)-C(13) | 56.1(4) |
| N(1)-Ta(2)-C(19) | 110.2(3) |
| C(3)-Ta(2)-C(19) | 75.1(3) |
| C(17)-Ta(2)-C(19) | 55.9(3) |
| C(14)-Ta(2)-C(19) | 154.8(3) |
| C(10)-Ta(2)-C(19) | 161.8(3) |
| C(15)-Ta(2)-C(19) | 33.4(3) |
| C(18)-Ta(2)-C(19) | 33.8(3) |
| C(16)-Ta(2)-C(19) | 55.4(3) |
| C(11)-Ta(2)-C(19) | 127.3(3) |

| | |
|---|---|
| C(13)-Ta(2)-C(19) | 123.4(3) |
| N(1)-Ta(2)-C(12) | 137.9(3) |
| C(3)-Ta(2)-C(12) | 103.6(3) |
| C(17)-Ta(2)-C(12) | 118.1(3) |
| C(14)-Ta(2)-C(12) | 55.6(3) |
| C(10)-Ta(2)-C(12) | 56.3(3) |
| C(15)-Ta(2)-C(12) | 82.8(3) |
| C(18)-Ta(2)-C(12) | 138.0(3) |
| C(16)-Ta(2)-C(12) | 86.2(3) |
| C(11)-Ta(2)-C(12) | 33.5(4) |
| C(13)-Ta(2)-C(12) | 33.6(3) |
| C(19)-Ta(2)-C(12) | 111.8(3) |
| C(4)-C(3)-Ta(2) | 112.6(5) |
| C(5)-C(4)-C(3) | 128.7(8) |
| C(4)-C(5)-C(6) | 124.8(7) |
| C(5)-C(6)-C(7) | 114.9(6) |
| N(1)-C(7)-C(71) | 123.1(6) |
| N(1)-C(7)-C(6) | 116.7(6) |
| C(71)-C(7)-C(6) | 120.2(6) |
| C(7)-N(1)-Ta(2) | 159.9(5) |
| C(7)-C(71)-C(72) | 112.8(5) |
| C(73)-C(72)-C(77) | 118.4(8) |
| C(73)-C(72)-C(71) | 119.5(7) |
| C(77)-C(72)-C(71) | 122.0(7) |
| C(72)-C(73)-C(74) | 119.6(8) |
| C(75)-C(74)-C(73) | 122.2(8) |
| C(76)-C(75)-C(74) | 117.2(8) |
| C(76)-C(75)-C(78) | 122.3(9) |
| C(74)-C(75)-C(78) | 120.5(9) |
| C(77)-C(76)-C(75) | 122.2(9) |
| C(76)-C(77)-C(72) | 120.5(8) |
| C(14)-C(10)-C(11) | 107.2(9) |
| C(14)-C(10)-Ta(2) | 73.3(5) |
| C(11)-C(10)-Ta(2) | 72.9(5) |
| C(12)-C(11)-C(10) | 106.6(9) |
| C(12)-C(11)-Ta(2) | 74.0(5) |
| C(10)-C(11)-Ta(2) | 72.1(5) |
| C(11)-C(12)-C(13) | 108.8(9) |
| C(11)-C(12)-Ta(2) | 72.6(5) |
| C(13)-C(12)-Ta(2) | 72.9(4) |
| C(14)-C(13)-C(12) | 107.7(9) |
| C(14)-C(13)-Ta(2) | 72.4(5) |
| C(12)-C(13)-Ta(2) | 73.5(5) |
| C(10)-C(14)-C(13) | 109.8(9) |
| C(10)-C(14)-Ta(2) | 73.4(5) |
| C(13)-C(14)-Ta(2) | 74.1(5) |
| C(19)-C(15)-C(16) | 108.0(8) |
| C(19)-C(15)-Ta(2) | 74.0(4) |
| C(16)-C(15)-Ta(2) | 73.2(4) |
| C(15)-C(16)-C(17) | 108.2(8) |
| C(15)-C(16)-Ta(2) | 73.2(4) |
| C(17)-C(16)-Ta(2) | 72.3(4) |
| C(18)-C(17)-C(16) | 108.0(8) |
| C(18)-C(17)-Ta(2) | 74.0(5) |
| C(16)-C(17)-Ta(2) | 73.8(5) |
| C(17)-C(18)-C(19) | 108.0(8) |
| C(17)-C(18)-Ta(2) | 72.5(5) |
| C(19)-C(18)-Ta(2) | 73.8(5) |
| C(15)-C(19)-C(18) | 107.8(8) |
| C(15)-C(19)-Ta(2) | 72.6(4) |
| C(18)-C(19)-Ta(2) | 72.4(4) |
| C(51)-B-C(21) | 110.2(6) |
| C(51)-B-C(41) | 104.0(5) |
| C(21)-B-C(41) | 114.6(5) |
| C(51)-B-C(31) | 114.5(6) |
| C(21)-B-C(31) | 103.1(5) |

| | |
|---|---|
| C(41)-B-C(31) | 110.8(5) |
| C(26)-C(21)-C(22) | 111.8(6) |
| C(26)-C(21)-B | 128.0(6) |
| C(22)-C(21)-B | 120.1(6) |
| F(22)-C(22)-C(23) | 115.6(6) |
| F(22)-C(22)-C(21) | 119.3(6) |
| C(23)-C(22)-C(21) | 125.1(7) |
| C(24)-C(23)-F(23) | 120.4(7) |
| C(24)-C(23)-C(22) | 120.2(7) |
| F(23)-C(23)-C(22) | 119.3(8) |
| F(24)-C(24)-C(23) | 121.0(8) |
| F(24)-C(24)-C(25) | 121.6(8) |
| C(23)-C(24)-C(25) | 117.4(7) |
| F(25)-C(25)-C(24) | 118.0(7) |
| F(25)-C(25)-C(26) | 121.8(7) |
| C(24)-C(25)-C(26) | 120.2(7) |
| F(26)-C(26)-C(21) | 121.9(6) |
| F(26)-C(26)-C(25) | 112.9(6) |
| C(21)-C(26)-C(25) | 125.2(6) |
| C(36)-C(31)-C(32) | 115.0(6) |
| C(36)-C(31)-B | 124.6(6) |
| C(32)-C(31)-B | 120.4(6) |
| F(32)-C(32)-C(31) | 119.8(6) |
| F(32)-C(32)-C(33) | 115.1(6) |
| C(31)-C(32)-C(33) | 125.1(7) |
| F(33)-C(33)-C(34) | 120.5(7) |
| F(33)-C(33)-C(32) | 121.2(7) |
| C(34)-C(33)-C(32) | 118.2(7) |
| F(34)-C(34)-C(35) | 120.9(8) |
| F(34)-C(34)-C(33) | 119.9(8) |
| C(35)-C(34)-C(33) | 119.2(7) |
| F(35)-C(35)-C(34) | 119.4(7) |
| F(35)-C(35)-C(36) | 121.5(8) |
| C(34)-C(35)-C(36) | 119.2(7) |
| F(36)-C(36)-C(31) | 124.8(7) |
| F(36)-C(36)-C(35) | 111.9(6) |
| C(31)-C(36)-C(35) | 123.3(7) |
| C(42)-C(41)-C(46) | 112.9(6) |
| C(42)-C(41)-B | 126.5(6) |
| C(46)-C(41)-B | 120.1(6) |
| F(42)-C(42)-C(41) | 122.2(6) |
| F(42)-C(42)-C(43) | 114.2(6) |
| C(41)-C(42)-C(43) | 123.7(7) |
| C(44)-C(43)-F(43) | 121.4(7) |
| C(44)-C(43)-C(42) | 120.3(7) |
| F(43)-C(43)-C(42) | 118.3(7) |
| F(44)-C(44)-C(43) | 120.2(7) |
| F(44)-C(44)-C(45) | 121.2(8) |
| C(43)-C(44)-C(45) | 118.5(7) |
| F(45)-C(45)-C(44) | 119.6(7) |
| F(45)-C(45)-C(46) | 120.2(7) |
| C(44)-C(45)-C(46) | 120.2(7) |
| F(46)-C(46)-C(45) | 115.7(6) |
| F(46)-C(46)-C(41) | 120.0(6) |
| C(45)-C(46)-C(41) | 124.3(7) |

**Table 4.** Anisotropic displacement parameters ($Å^2 \times 10^3$) for **14d**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [ h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12} ]$

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Ta(2) | 37(1) | 36(1) | 26(1) | 2(1) | -1(1) | 1(1) |
| C(3) | 83(6) | 32(4) | 53(4) | 3(3) | 0(4) | 4(3) |
| C(4) | 68(5) | 41(4) | 60(5) | 1(3) | -2(4) | -10(4) |
| C(5) | 69(5) | 46(4) | 55(4) | -16(4) | -6(4) | 0(4) |
| C(6) | 69(5) | 50(4) | 33(3) | -5(3) | 8(3) | -2(4) |
| C(7) | 57(4) | 42(4) | 31(3) | 1(3) | -4(3) | -12(3) |
| N(1) | 42(3) | 34(3) | 38(3) | -3(2) | -3(2) | 5(2) |
| C(71) | 81(5) | 48(4) | 37(4) | 7(3) | -12(3) | -14(4) |
| C(72) | 56(4) | 46(4) | 43(4) | 19(3) | -11(3) | -5(3) |
| C(73) | 52(4) | 48(4) | 60(5) | 10(4) | 3(3) | -8(3) |
| C(74) | 72(5) | 47(4) | 56(5) | 7(4) | 0(4) | -16(4) |
| C(75) | 79(6) | 46(4) | 57(5) | 15(4) | 10(4) | -2(4) |
| C(76) | 76(6) | 51(5) | 104(8) | 10(5) | 7(5) | 16(5) |
| C(77) | 54(5) | 57(5) | 87(6) | 11(4) | -20(4) | -1(4) |
| C(78) | 171(13) | 51(5) | 91(8) | -14(5) | 25(8) | 0(7) |
| C(10) | 50(5) | 83(7) | 79(6) | 5(5) | 9(4) | 23(5) |
| C(11) | 63(6) | 102(8) | 79(7) | -37(6) | 32(5) | 4(5) |
| C(12) | 48(4) | 123(8) | 38(4) | 11(5) | 12(3) | -11(5) |
| C(13) | 65(5) | 76(6) | 72(6) | 3(5) | 13(4) | -24(5) |
| C(14) | 42(4) | 91(7) | 67(5) | 4(5) | 0(4) | -5(4) |
| C(15) | 50(4) | 59(5) | 42(4) | 2(3) | -15(3) | -1(3) |
| C(16) | 59(5) | 61(5) | 57(5) | -10(4) | -13(4) | -9(4) |
| C(17) | 80(6) | 57(5) | 81(6) | 22(5) | -32(5) | -29(5) |
| C(18) | 36(4) | 117(8) | 57(5) | 20(5) | 0(3) | -15(5) |
| C(19) | 36(4) | 82(6) | 84(6) | -5(5) | -19(4) | 13(4) |
| B | 37(4) | 44(4) | 38(4) | 1(3) | 3(3) | 0(3) |
| C(21) | 35(3) | 39(3) | 40(3) | -4(3) | -4(2) | 7(3) |
| C(22) | 43(4) | 48(4) | 50(4) | -6(3) | -6(3) | 8(3) |
| F(22) | 63(3) | 68(3) | 42(2) | -7(2) | 5(2) | 5(2) |
| C(23) | 54(4) | 49(4) | 64(5) | -21(4) | -2(4) | -1(3) |
| F(23) | 104(4) | 73(3) | 76(3) | -42(3) | -6(3) | 1(3) |
| C(24) | 54(4) | 39(4) | 82(6) | -5(4) | -4(4) | 2(3) |
| F(24) | 106(4) | 44(3) | 112(5) | -19(3) | -9(4) | -11(3) |
| C(25) | 48(4) | 39(4) | 62(5) | 0(3) | -3(3) | 4(3) |
| F(25) | 87(3) | 50(3) | 74(3) | 16(2) | 8(3) | -6(2) |
| C(26) | 41(3) | 37(3) | 41(3) | -2(3) | -1(3) | 5(3) |
| F(26) | 70(3) | 52(2) | 42(2) | 2(2) | -10(2) | -9(2) |
| C(31) | 44(4) | 34(3) | 40(3) | -3(3) | -2(3) | -2(3) |
| C(32) | 38(3) | 39(4) | 48(4) | -2(3) | 1(3) | -5(3) |
| F(32) | 50(2) | 59(3) | 41(2) | 14(2) | -3(2) | 5(2) |
| C(33) | 48(4) | 38(4) | 74(5) | 3(4) | -14(4) | 1(3) |
| F(33) | 54(3) | 63(3) | 106(4) | 18(3) | -17(3) | 9(2) |
| C(34) | 34(4) | 50(4) | 87(6) | -9(4) | 12(4) | -5(3) |
| F(34) | 45(3) | 71(3) | 129(5) | -1(3) | 13(3) | 8(2) |
| C(35) | 52(4) | 62(5) | 69(5) | -3(4) | 20(4) | -8(4) |
| F(35) | 73(3) | 94(4) | 87(4) | 18(3) | 35(3) | -7(3) |
| C(36) | 56(4) | 43(4) | 46(4) | 1(3) | 6(3) | -6(3) |
| F(36) | 64(3) | 81(3) | 55(3) | 25(2) | 6(2) | -2(2) |
| C(41) | 41(3) | 33(3) | 36(3) | 2(3) | -3(3) | 3(3) |
| C(42) | 48(4) | 37(3) | 50(4) | 5(3) | -1(3) | -4(3) |
| F(42) | 51(2) | 58(3) | 63(3) | -15(2) | 6(2) | -12(2) |
| C(43) | 68(5) | 43(4) | 45(4) | -4(3) | -8(3) | -15(4) |
| F(43) | 90(3) | 71(3) | 55(3) | -19(2) | -12(2) | -26(3) |
| C(44) | 87(6) | 41(4) | 42(4) | -7(3) | 8(4) | -8(4) |
| F(44) | 118(4) | 68(3) | 66(3) | -28(3) | 29(3) | -22(3) |
| C(45) | 58(4) | 38(4) | 64(5) | 2(3) | 21(4) | 2(3) |

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| | | | | | | |
|---|---|---|---|---|---|---|
| F(45) | 76(3) | 66(3) | 101(4) | -16(3) | 41(3) | 2(3) |
| C(46) | 49(4) | 35(3) | 53(4) | 3(3) | 1(3) | 0(3) |
| F(46) | 43(2) | 61(3) | 61(3) | -2(2) | 2(2) | -2(2) |
| C(51) | 61(5) | 53(4) | 41(4) | 5(3) | -8(3) | 10(4) |

**Table 5.** Hydrogen coordinates ( x $10^4$) and isotropic displacement parameters ($Å^2$ x $10^3$) for **14d**.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(3A) | 2235 | 3997 | 426 | 67 |
| H(3B) | 1629 | 3385 | 936 | 67 |
| H(4) | 3323 | 4226 | 1123 | 68 |
| H(5) | 3505 | 3471 | 2060 | 68 |
| H(6A) | 1844 | 2445 | 2004 | 61 |
| H(6B) | 2655 | 2159 | 2482 | 61 |
| H(71A) | 2304 | 92 | 2349 | 66 |
| H(71B) | 3387 | 242 | 2292 | 66 |
| H(73) | 1483 | -1040 | 1576 | 64 |
| H(74) | 1543 | -2484 | 886 | 70 |
| H(76) | 4276 | -2271 | 828 | 93 |
| H(77) | 4249 | -853 | 1516 | 79 |
| H(78A) | 2928 | -4140 | 551 | 157 |
| H(78B) | 3480 | -3427 | 57 | 157 |
| H(78C) | 2385 | -3435 | 43 | 157 |
| H(10) | 4281 | 589 | 364 | 85 |
| H(11) | 3576 | 649 | -754 | 97 |
| H(12) | 3277 | 2589 | -1006 | 83 |
| H(13) | 3742 | 3699 | -67 | 85 |
| H(14) | 4359 | 2463 | 758 | 80 |
| H(15) | 1443 | 2441 | -897 | 60 |
| H(16) | 1905 | 506 | -868 | 71 |
| H(17) | 1503 | -231 | 198 | 87 |
| H(18) | 719 | 1218 | 805 | 84 |
| H(19) | 667 | 2874 | 122 | 81 |
| H(51A) | -19 | 3755 | -3221 | 78 |
| H(51B) | 695 | 3439 | -3757 | 78 |
| H(51C) | 894 | 4442 | -3310 | 78 |

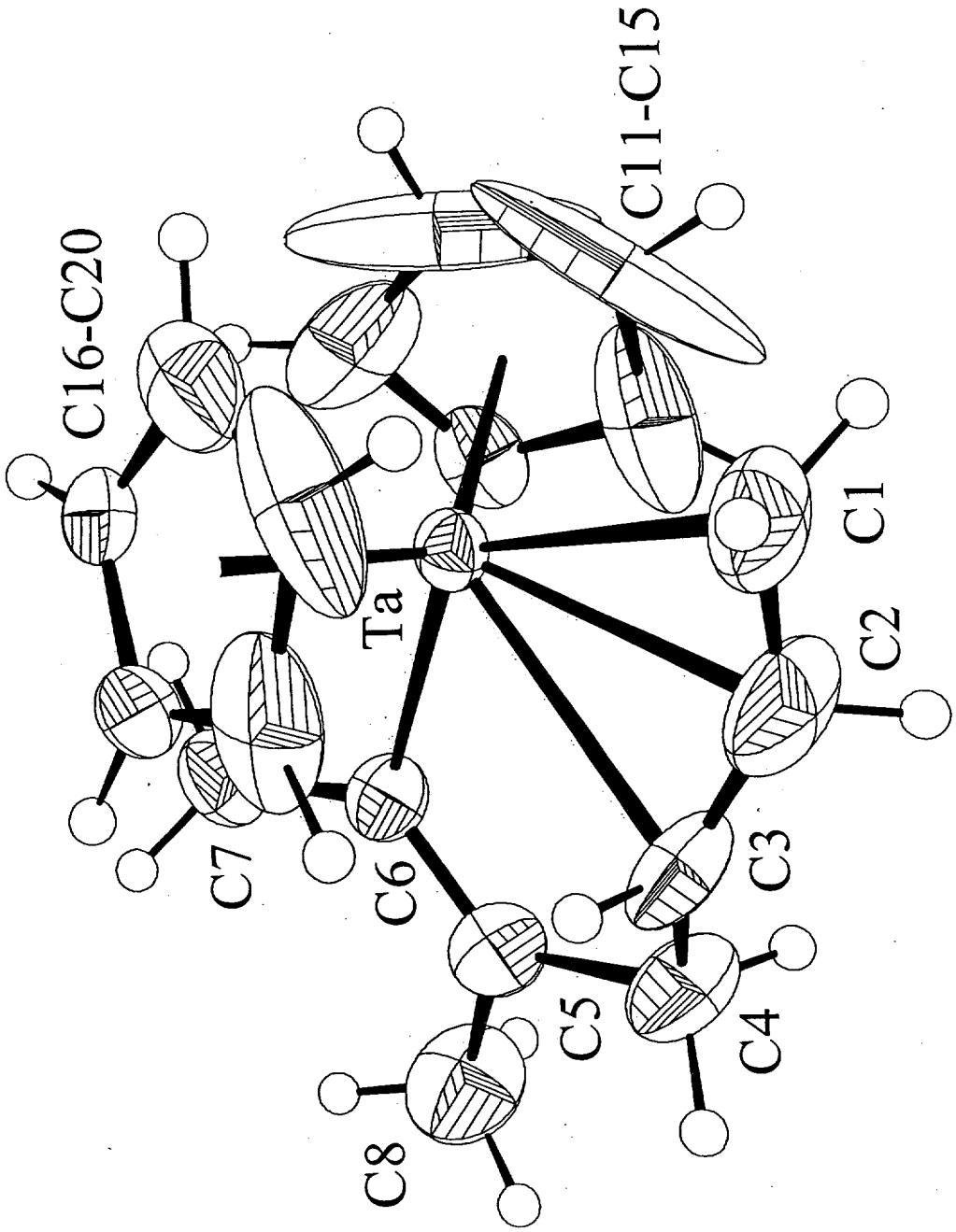

**Table 1.** Crystal data and structure refinement for **15a**.

| | |
|---|---|
| Identification code | ERK_764 |
| Empirical formula | $C_{37}$ $H_{25}$ B $F_{15}$ Ta |
| Formula weight | 946.33 |
| Temperature | 223(2) K |
| Wavelength | 0.71073 Å |
| Crystal system, space group | monoclinic, $P2_1/n$ (No. 14) |
| Unit cell dimensions | a = 12.722(1) Å<br>b = 14.150(1) Å  β = 107.50(1)°.<br>c = 19.317(1) Å |
| Volume | 3316.4(4) Å$^3$ |
| Z, Calculated density | 4, 1.895 Mg/m$^3$ |
| Absorption coefficient | 3.428 mm$^{-1}$ |
| F(000) | 1840 |
| Crystal size | 0.50 x 0.50 x 0.25 mm |
| Theta range for data collection | 2.21 to 26.32°. |
| Index ranges | -15<=h<=15, 0<=k<=17, 0<=l<=24 |
| Reflections collected / unique | 6941 / 6739 [R(int) = 0.0320] |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 6739 / 0 / 500 |
| Goodness-of-fit on $F^2$ | 1.008 |
| Final R indices [I>2σ(I)] | R1 = 0.0322, $wR^2$ = 0.0888 |
| R indices (all data) | R1 = 0.0468, $wR^2$ = 0.0934 |
| Largest diff. peak and hole | 1.334 and -1.778 eÅ$^{-3}$ |

**Table 2.** Atomic coordinates ( x $10^4$) and equivalent isotropic displacement parameters ($Å^2$ x $10^3$) for **15a**.
U(eq) is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Ta | 1771(1) | 2262(1) | 38(1) | 30(1) |
| C(6) | 3582(4) | 1955(3) | 628(2) | 38(1) |
| C(5) | 4175(4) | 2405(4) | 1237(3) | 45(1) |
| C(4A) | 3627(4) | 3125(4) | 1572(3) | 58(1) |
| C(3A) | 2445(8) | 2990(10) | 1308(7) | 48(4) |
| C(2A) | 1619(5) | 3462(5) | 897(4) | 76(2) |
| C(4B) | 3627(4) | 3125(4) | 1572(3) | 58(1) |
| C(3B) | 2645(11) | 3433(9) | 1000(8) | 52(4) |
| C(2B) | 1619(5) | 3462(5) | 897(4) | 76(2) |
| C(1) | 639(5) | 3359(5) | 405(4) | 75(2) |
| C(7) | 4190(4) | 1219(4) | 306(3) | 51(1) |
| C(8) | 5395(5) | 2265(5) | 1609(4) | 75(2) |
| C(11) | 1168(10) | 3334(13) | -937(9) | 212(12) |
| C(12) | 1094(9) | 2539(15) | -1220(6) | 205(12) |
| C(13) | 2115(8) | 2149(6) | -1106(3) | 88(3) |
| C(14) | 2883(5) | 2806(3) | -716(3) | 49(1) |
| C(15) | 2277(8) | 3559(5) | -599(5) | 102(3) |
| C(16) | 253(6) | 1379(5) | 207(7) | 102(3) |
| C(17) | 1192(8) | 1137(4) | 794(4) | 88(3) |
| C(18) | 1905(4) | 656(3) | 506(2) | 45(1) |
| C(19) | 1448(4) | 620(3) | -225(3) | 49(1) |
| C(20) | 426(5) | 1055(4) | -396(5) | 80(2) |
| B | 3046(4) | 7194(3) | 11069(2) | 29(1) |
| C(21) | 2736(3) | 7296(3) | 10172(2) | 29(1) |
| C(22) | 2761(3) | 8112(3) | 9779(2) | 32(1) |
| F(22) | 3183(2) | 8930(2) | 10119(1) | 42(1) |
| C(23) | 2377(4) | 8180(3) | 9033(2) | 37(1) |
| F(23) | 2456(3) | 9005(2) | 8702(1) | 53(1) |
| C(24) | 1929(4) | 7404(4) | 8627(2) | 43(1) |
| F(24) | 1562(3) | 7457(2) | 7903(2) | 64(1) |
| C(25) | 1895(4) | 6573(3) | 8984(2) | 42(1) |
| F(25) | 1469(3) | 5792(2) | 8599(2) | 63(1) |
| C(26) | 2296(3) | 6540(3) | 9728(2) | 36(1) |
| F(26) | 2244(2) | 5677(2) | 10024(1) | 49(1) |
| C(31) | 4042(3) | 6422(3) | 11414(2) | 28(1) |
| C(32) | 4300(3) | 6186(3) | 12141(2) | 34(1) |
| F(32) | 3788(2) | 6637(2) | 12572(1) | 49(1) |
| C(33) | 5082(4) | 5528(3) | 12485(2) | 41(1) |
| F(33) | 5245(2) | 5329(3) | 13196(1) | 60(1) |
| C(34) | 5685(4) | 5081(3) | 12114(3) | 41(1) |
| F(34) | 6447(2) | 4434(2) | 12439(2) | 61(1) |
| C(35) | 5497(3) | 5294(3) | 11393(2) | 38(1) |
| F(35) | 6087(2) | 4870(2) | 11009(2) | 58(1) |
| C(36) | 4693(3) | 5947(3) | 11064(2) | 31(1) |
| F(36) | 4596(2) | 6138(2) | 10361(1) | 45(1) |
| C(41) | 3486(3) | 8203(3) | 11492(2) | 32(1) |
| C(42) | 2914(4) | 8763(3) | 11837(2) | 42(1) |
| F(42) | 1851(3) | 8579(2) | 11804(2) | 62(1) |
| C(43) | 3346(5) | 9561(4) | 12237(3) | 53(1) |
| F(43) | 2725(4) | 10057(3) | 12565(2) | 88(1) |
| C(44) | 4386(5) | 9846(3) | 12286(3) | 58(2) |
| F(44) | 4824(4) | 10619(2) | 12675(2) | 91(1) |
| C(45) | 5001(4) | 9332(3) | 11936(3) | 50(1) |
| F(45) | 6018(3) | 9602(2) | 11965(2) | 72(1) |
| C(46) | 4542(4) | 8532(3) | 11563(2) | 36(1) |
| F(46) | 5169(2) | 8064(2) | 11221(2) | 47(1) |
| C(51) | 1918(4) | 6810(4) | 11218(3) | 42(1) |

**Table 3**. Bond lengths [Å] and angles [°] for **15a**.

| | |
|---|---|
| Ta-C(6) | 2.283(4) |
| Ta-C(12) | 2.355(9) |
| Ta-C(11) | 2.360(9) |
| Ta-C(1) | 2.365(5) |
| Ta-C(13) | 2.383(6) |
| Ta-C(20) | 2.385(5) |
| Ta-C(19) | 2.388(4) |
| Ta-C(16) | 2.403(6) |
| Ta-C(15) | 2.404(5) |
| Ta-C(17) | 2.420(5) |
| Ta-C(2A) | 2.421(5) |
| Ta-C(2B) | 2.421(5) |
| Ta-C(18) | 2.433(4) |
| Ta-C(14) | 2.441(5) |
| Ta-C(3B) | 2.488(11) |
| Ta-C(3A) | 2.558(9) |
| C(6)-C(5) | 1.351(7) |
| C(6)-C(7) | 1.537(6) |
| C(5)-C(4B) | 1.489(8) |
| C(5)-C(4A) | 1.489(8) |
| C(5)-C(8) | 1.514(7) |
| C(4A)-C(3A) | 1.449(10) |
| C(3A)-C(2A) | 1.295(14) |
| C(2A)-C(1) | 1.329(9) |
| C(4B)-C(3B) | 1.464(14) |
| C(3B)-C(2B) | 1.261(15) |
| C(2B)-C(1) | 1.329(9) |
| C(11)-C(12) | 1.24(3) |
| C(11)-C(15) | 1.40(2) |
| C(12)-C(13) | 1.37(2) |
| C(13)-C(14) | 1.394(9) |
| C(14)-C(15) | 1.373(8) |
| C(16)-C(20) | 1.331(11) |
| C(16)-C(17) | 1.420(12) |
| C(17)-C(18) | 1.380(8) |
| C(18)-C(19) | 1.355(7) |
| C(19)-C(20) | 1.386(8) |
| B-C(51) | 1.638(6) |
| B-C(31) | 1.654(6) |
| B-C(41) | 1.658(6) |
| B-C(21) | 1.665(6) |
| C(21)-C(26) | 1.380(6) |
| C(21)-C(22) | 1.386(6) |
| C(22)-F(22) | 1.358(5) |
| C(22)-C(23) | 1.380(6) |
| C(23)-F(23) | 1.349(5) |
| C(23)-C(24) | 1.371(7) |
| C(24)-F(24) | 1.337(5) |
| C(24)-C(25) | 1.370(7) |
| C(25)-F(25) | 1.352(5) |
| C(25)-C(26) | 1.373(6) |
| C(26)-F(26) | 1.359(5) |
| C(31)-C(32) | 1.384(5) |
| C(31)-C(36) | 1.390(5) |
| C(32)-F(32) | 1.360(5) |
| C(32)-C(33) | 1.379(6) |
| C(33)-C(34) | 1.354(7) |
| C(33)-F(33) | 1.354(5) |
| C(34)-F(34) | 1.343(5) |
| C(34)-C(35) | 1.373(6) |
| C(35)-F(35) | 1.346(5) |
| C(35)-C(36) | 1.383(6) |

| | |
|---|---|
| C(36)-F(36) | 1.353(5) |
| C(41)-C(42) | 1.375(6) |
| C(41)-C(46) | 1.389(6) |
| C(42)-F(42) | 1.360(6) |
| C(42)-C(43) | 1.384(7) |
| C(43)-F(43) | 1.349(6) |
| C(43)-C(44) | 1.360(8) |
| C(44)-F(44) | 1.348(6) |
| C(44)-C(45) | 1.384(8) |
| C(45)-F(45) | 1.335(6) |
| C(45)-C(46) | 1.373(6) |
| C(46)-F(46) | 1.353(5) |

| | |
|---|---|
| C(6)-Ta-C(12) | 123.2(4) |
| C(6)-Ta-C(11) | 123.9(3) |
| C(12)-Ta-C(11) | 30.5(6) |
| C(6)-Ta-C(1) | 126.1(2) |
| C(12)-Ta-C(1) | 97.7(5) |
| C(11)-Ta-C(1) | 74.7(4) |
| C(6)-Ta-C(13) | 90.6(3) |
| C(12)-Ta-C(13) | 33.5(4) |
| C(11)-Ta-C(13) | 53.8(5) |
| C(1)-Ta-C(13) | 128.3(3) |
| C(6)-Ta-C(20) | 123.3(2) |
| C(12)-Ta-C(20) | 75.8(4) |
| C(11)-Ta-C(20) | 98.8(5) |
| C(1)-Ta-C(20) | 97.9(2) |
| C(13)-Ta-C(20) | 86.4(3) |
| C(6)-Ta-C(19) | 90.2(2) |
| C(12)-Ta-C(19) | 87.5(5) |
| C(11)-Ta-C(19) | 117.5(6) |
| C(1)-Ta-C(19) | 128.4(2) |
| C(13)-Ta-C(19) | 78.8(2) |
| C(20)-Ta-C(19) | 33.8(2) |
| C(6)-Ta-C(16) | 124.4(2) |
| C(12)-Ta-C(16) | 99.6(4) |
| C(11)-Ta-C(16) | 111.2(4) |
| C(1)-Ta-C(16) | 73.4(3) |
| C(13)-Ta-C(16) | 118.0(3) |
| C(20)-Ta-C(16) | 32.3(3) |
| C(19)-Ta-C(16) | 55.2(2) |
| C(6)-Ta-C(15) | 90.9(3) |
| C(12)-Ta-C(15) | 54.2(5) |
| C(11)-Ta-C(15) | 34.2(4) |
| C(1)-Ta-C(15) | 86.2(3) |
| C(13)-Ta-C(15) | 54.8(3) |
| C(20)-Ta-C(15) | 129.9(3) |
| C(19)-Ta-C(15) | 133.6(2) |
| C(16)-Ta-C(15) | 144.7(3) |
| C(6)-Ta-C(17) | 91.0(3) |
| C(12)-Ta-C(17) | 130.5(4) |
| C(11)-Ta-C(17) | 145.0(4) |
| C(1)-Ta-C(17) | 85.8(3) |
| C(13)-Ta-C(17) | 133.6(2) |
| C(20)-Ta-C(17) | 54.9(3) |
| C(19)-Ta-C(17) | 54.8(2) |
| C(16)-Ta-C(17) | 34.2(3) |
| C(15)-Ta-C(17) | 171.3(2) |
| C(6)-Ta-C(2A) | 93.9(2) |
| C(12)-Ta-C(2A) | 120.7(6) |
| C(11)-Ta-C(2A) | 91.3(6) |
| C(1)-Ta-C(2A) | 32.2(2) |
| C(13)-Ta-C(2A) | 139.2(3) |
| C(20)-Ta-C(2A) | 123.1(3) |
| C(19)-Ta-C(2A) | 141.6(2) |
| C(16)-Ta-C(2A) | 92.2(3) |

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| C(15)-Ta-C(2A) | 84.5(3) |
| C(17)-Ta-C(2A) | 86.9(3) |
| C(6)-Ta-C(2B) | 93.9(2) |
| C(12)-Ta-C(2B) | 120.7(6) |
| C(11)-Ta-C(2B) | 91.3(6) |
| C(1)-Ta-C(2B) | 32.2(2) |
| C(13)-Ta-C(2B) | 139.2(3) |
| C(20)-Ta-C(2B) | 123.1(3) |
| C(19)-Ta-C(2B) | 141.6(2) |
| C(16)-Ta-C(2B) | 92.2(3) |
| C(15)-Ta-C(2B) | 84.5(3) |
| C(17)-Ta-C(2B) | 86.9(3) |
| C(6)-Ta-C(18) | 71.9(2) |
| C(12)-Ta-C(18) | 120.1(5) |
| C(11)-Ta-C(18) | 150.0(6) |
| C(1)-Ta-C(18) | 118.9(2) |
| C(13)-Ta-C(18) | 105.6(2) |
| C(20)-Ta-C(18) | 54.8(2) |
| C(19)-Ta-C(18) | 32.6(2) |
| C(16)-Ta-C(18) | 55.5(2) |
| C(15)-Ta-C(18) | 154.7(2) |
| C(17)-Ta-C(18) | 33.0(2) |
| C(2A)-Ta-C(18) | 114.3(2) |
| C(2B)-Ta-C(18) | 114.3(2) |
| C(6)-Ta-C(14) | 71.3(2) |
| C(12)-Ta-C(14) | 55.2(3) |
| C(11)-Ta-C(14) | 55.1(3) |
| C(1)-Ta-C(14) | 119.1(2) |
| C(13)-Ta-C(14) | 33.6(2) |
| C(20)-Ta-C(14) | 119.9(3) |
| C(19)-Ta-C(14) | 105.9(2) |
| C(16)-Ta-C(14) | 151.5(3) |
| C(15)-Ta-C(14) | 32.9(2) |
| C(17)-Ta-C(14) | 154.7(2) |
| C(2A)-Ta-C(14) | 111.6(2) |
| C(2B)-Ta-C(14) | 111.6(2) |
| C(18)-Ta-C(14) | 121.8(2) |
| C(6)-Ta-C(3B) | 66.2(3) |
| C(12)-Ta-C(3B) | 127.1(6) |
| C(11)-Ta-C(3B) | 97.7(7) |
| C(1)-Ta-C(3B) | 61.0(3) |
| C(13)-Ta-C(3B) | 124.9(5) |
| C(20)-Ta-C(3B) | 148.4(5) |
| C(19)-Ta-C(3B) | 144.7(4) |
| C(16)-Ta-C(3B) | 116.2(5) |
| C(15)-Ta-C(3B) | 75.3(5) |
| C(17)-Ta-C(3B) | 97.8(5) |
| C(2B)-Ta-C(3B) | 29.7(3) |
| C(18)-Ta-C(3B) | 112.3(4) |
| C(14)-Ta-C(3B) | 91.5(4) |
| C(6)-Ta-C(3A) | 66.5(2) |
| C(12)-Ta-C(3A) | 146.7(6) |
| C(11)-Ta-C(3A) | 116.2(7) |
| C(1)-Ta-C(3A) | 60.5(3) |
| C(13)-Ta-C(3A) | 144.5(4) |
| C(20)-Ta-C(3A) | 128.6(4) |
| C(19)-Ta-C(3A) | 125.6(4) |
| C(16)-Ta-C(3A) | 97.5(4) |
| C(15)-Ta-C(3A) | 96.9(4) |
| C(17)-Ta-C(3A) | 76.2(4) |
| C(2A)-Ta-C(3A) | 30.0(3) |
| C(18)-Ta-C(3A) | 93.1(4) |
| C(14)-Ta-C(3A) | 111.0(3) |
| C(5)-C(6)-C(7) | 117.0(4) |
| C(5)-C(6)-Ta | 124.1(3) |
| C(7)-C(6)-Ta | 118.9(3) |

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| C(6)-C(5)-C(4B) | 119.3(4) |
| C(6)-C(5)-C(4A) | 119.3(4) |
| C(6)-C(5)-C(8) | 125.2(5) |
| C(4B)-C(5)-C(8) | 115.5(5) |
| C(4A)-C(5)-C(8) | 115.5(5) |
| C(3A)-C(4A)-C(5) | 109.2(5) |
| C(2A)-C(3A)-C(4A) | 135.5(13) |
| C(2A)-C(3A)-Ta | 69.2(5) |
| C(4A)-C(3A)-Ta | 113.8(5) |
| C(3A)-C(2A)-C(1) | 142.6(9) |
| C(3A)-C(2A)-Ta | 80.8(4) |
| C(1)-C(2A)-Ta | 71.6(3) |
| C(3B)-C(4B)-C(5) | 106.3(6) |
| C(2B)-C(3B)-C(4B) | 137.5(15) |
| C(2B)-C(3B)-Ta | 72.2(6) |
| C(4B)-C(3B)-Ta | 117.0(7) |
| C(3B)-C(2B)-C(1) | 144.4(9) |
| C(3B)-C(2B)-Ta | 78.1(6) |
| C(1)-C(2B)-Ta | 71.6(3) |
| C(2B)-C(1)-Ta | 76.2(3) |
| C(2A)-C(1)-Ta | 76.2(3) |
| C(12)-C(11)-C(15) | 110.2(11) |
| C(12)-C(11)-Ta | 74.5(7) |
| C(15)-C(11)-Ta | 74.6(5) |
| C(11)-C(12)-C(13) | 110.5(11) |
| C(11)-C(12)-Ta | 74.9(8) |
| C(13)-C(12)-Ta | 74.4(5) |
| C(12)-C(13)-C(14) | 107.3(10) |
| C(12)-C(13)-Ta | 72.1(5) |
| C(14)-C(13)-Ta | 75.5(3) |
| C(15)-C(14)-C(13) | 105.6(7) |
| C(15)-C(14)-Ta | 72.0(3) |
| C(13)-C(14)-Ta | 71.0(3) |
| C(14)-C(15)-C(11) | 106.4(10) |
| C(14)-C(15)-Ta | 75.0(3) |
| C(11)-C(15)-Ta | 71.2(4) |
| C(20)-C(16)-C(17) | 107.2(6) |
| C(20)-C(16)-Ta | 73.1(3) |
| C(17)-C(16)-Ta | 73.5(4) |
| C(18)-C(17)-C(16) | 107.1(6) |
| C(18)-C(17)-Ta | 74.0(3) |
| C(16)-C(17)-Ta | 72.2(3) |
| C(19)-C(18)-C(17) | 108.1(6) |
| C(19)-C(18)-Ta | 71.9(2) |
| C(17)-C(18)-Ta | 73.0(3) |
| C(18)-C(19)-C(20) | 108.1(6) |
| C(18)-C(19)-Ta | 75.5(3) |
| C(20)-C(19)-Ta | 73.0(3) |
| C(16)-C(20)-C(19) | 109.5(7) |
| C(16)-C(20)-Ta | 74.6(4) |
| C(19)-C(20)-Ta | 73.2(3) |
| C(51)-B-C(31) | 108.4(3) |
| C(51)-B-C(41) | 112.6(3) |
| C(31)-B-C(41) | 105.4(3) |
| C(51)-B-C(21) | 105.4(3) |
| C(31)-B-C(21) | 112.9(3) |
| C(41)-B-C(21) | 112.2(3) |
| C(26)-C(21)-C(22) | 112.2(4) |
| C(26)-C(21)-B | 120.3(3) |
| C(22)-C(21)-B | 127.2(3) |
| F(22)-C(22)-C(23) | 114.1(4) |
| F(22)-C(22)-C(21) | 121.1(3) |
| C(23)-C(22)-C(21) | 124.8(4) |
| F(23)-C(23)-C(24) | 120.0(4) |
| F(23)-C(23)-C(22) | 120.2(4) |
| C(24)-C(23)-C(22) | 119.9(4) |