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# Dichlorido-1$\kappa Cl$,3$\kappa Cl$-hexakis-[1,1,2,2,3,3($\eta^5$)-methylcyclopentadienyl]di-$\mu_2$-oxido-1:2$\kappa^2 O$:$O$;2:3$\kappa^2 O$:$O$-trihafnium(IV)

**Aleksandra Wisniewska, Katarzyna Baranowska* and Jerzy Pikies**

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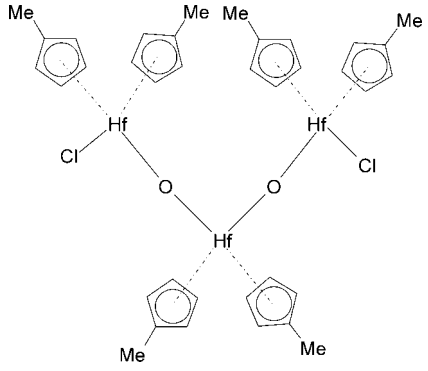
Key indicators: single-crystal X-ray study; $T$ = 120 K; mean $\sigma$(C–C) = 0.034 Å; disorder in main residue; $R$ factor = 0.061; $wR$ factor = 0.185; data-to-parameter ratio = 20.4.

The title compound, $[Hf_3(C_6H_7)_6Cl_2O_2]$, is a trinuclear molecule having two $(MeCp)_2HfCl$ units (MeCp is methylcyclopentadienyl) each connected to an $(MeCp)_2Hf$ unit by an oxide bridge. The two Hf—O—Hf bridges are nearly linear. The geometry of the three Hf atoms is tetrahedral (assuming the MeCp group occupies one coordination site); the O—Hf—O angle is 99.8 (5)°. One of the Cl atoms is disordered, with site occupancies of 0.61 (7) and 0.39 (7).

## Related literature

For another dichloridobis($\eta^5$-methylcyclopentadienyl)-hafnium(IV) compound, see: Wisniewska *et al.* (2007). For tris($\mu_2$-oxo)-tris(hafnocene) toluene solvate, see: Rogers *et al.* (1982). For ($\mu_2$-oxo)-bis(methylhafnocene), see: Fronczek *et al.* (1976). For ($\mu_2$-oxo)-bis(chlorohafnocene), see: Parkanyi *et al.* (1993).




## Experimental

### Crystal data

$[Hf_3(C_6H_7)_6Cl_2O_2]$
$M_r$ = 1113.07
Monoclinic, $P2_1/c$
$a$ = 18.9598 (10) Å
$b$ = 12.9710 (5) Å
$c$ = 14.6178 (6) Å
$\beta$ = 108.466 (4)°
$V$ = 3409.8 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 9.30 mm$^{-1}$
$T$ = 120 (2) K
0.1 × 0.08 × 0.04 mm

### Data collection

Oxford Diffraction KM4 CCD diffractometer
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2006)
$T_{min}$ = 0.283, $T_{max}$ = 0.434
11353 measured reflections
5801 independent reflections
4052 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.057

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.185
$S$ = 1.06
5801 reflections
284 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.41 e Å$^{-3}$
$\Delta\rho_{min}$ = −2.70 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Hf1—O1 | 1.925 (12) | Hf2—O2 | 2.019 (11) |
| Hf1—Cl1 | 2.446 (4) | Hf3—O2 | 1.859 (11) |
| Hf2—O1 | 1.953 (12) | Hf3—Cl2 | 2.479 (13) |
| | | | |
| O1—Hf1—Cl1 | 96.7 (4) | Hf1—O1—Hf2 | 173.3 (7) |
| O1—Hf2—O2 | 99.8 (5) | Hf3—O2—Hf2 | 178.7 (8) |
| O2—Hf3—Cl2 | 103.5 (10) | | |

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors thank Dr Jarosław Chojnacki for helpful comments.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2389).

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Wisniewska, A., Baranowska, K. & Pikies, J. (2007). *Acta Cryst.* E**63**, m2174.

  

# supporting information

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# Dichlorido-1$\kappa Cl$,3$\kappa Cl$-hexakis[1,1,2,2,3,3($\eta^5$)-methylcyclopentadienyl]di-$\mu_2$-oxido-1:2$\kappa^2 O$:$O$;2:3$\kappa^2 O$:$O$-trihafnium(IV)

**Aleksandra Wisniewska, Katarzyna Baranowska and Jerzy Pikies**

## S1. Comment

The molecular structure of (**1**) is shown in Fig.1. The crystal structure of (**1**) is build up of discrete molecules. The geometry of the central Hf atom in (**1**) is distorted pseudotetrahedral (O1—Hf2—O2 angle is 99.99 °) similar to the geometry of Cl—Hf—Cl in [($\eta^5$-$C_5H_4Me)_2HfCl_2$] (Wisniewska *et al.*, 2007). The Hf—Cl distances are in the typical range for hafnocene dichlorides. The Hf1—O1—Hf2 and Hf3—O2—Hf2 angles are large (172.91 and 178.82°.). It is typical for Hf—O—Hf moieties (Fronczek *et al.*, 1976; Parkanyi *et al.*, 1993). The related angles in cyclic tris($\mu_2$-Oxo)-tris-(hafnocene) are smaller (142.61°.) (Rogers *et al.*, 1982). The Hf—O distances 1.852Å - 2.024 Å are in typical range for hafnocene - oxygen moieties.

## S2. Experimental

The title compound [($\eta^5$-$CH_3C_5H_4)_2HfCl$-O-($\eta^5$-$CH_3C_5H_4)_2Hf$—O-($\eta^5$-$CH_3C_5H_4)_2HfCl$] (**1**) has been isolated as a colourless crystals in a reaction of $(CpMe)_2HfCl_2$ with $(iPr_2N)_2P$—$P(SiMe_3)Li$ 2,5 THF in Toluene. After standing for 1 day at room temperature, the mixture was dried under vacuum at 1 mTorr (1 Torr = 133.322 Pa) for 1 h, and the residue dissolved in pentane (4 ml) and filtered. After 2 days at 243 K, the solution yielded small colorless crystals of (**1**).

Explanation. [($\eta^5$-$CH_3C_5H_4)_2HfCl$-O-($\eta^5$-$CH_3C_5H_4)_2Hf$—O-($\eta^5$-$CH_3C_5H_4)_2HfCl$] (**1**) is a byproduct in the reaction of $(CH_3C_5H_4)Li$ with $HfCl_4$ in mol ratio 2:1. The commercially available hafnium tetrachloride contains probably $Cl_3Hf$—O-$HfCl_2$—O-$HfCl_3$, which reacts with $(CH_3C_5H_4)Li$ yielding small amounts of (**1**).

## S3. Refinement

All H atoms were refined as riding on C atoms with aromatic C—H = 0.95 Å, methyl C—H = 0.98 Å, and $U_{iso}$(H) = 1.2$U_{eq}$(C) for CH groups, 1.5$U_{eq}$(C) for $CH_3$ groups. Atom Cl2 is disordered (0.61 (7)/0.39 (7)). Two methylcyclopentadienyl molecules (C13–C18 and C19–C24) were constrained to be flat.

The largest peak/deepest hole in the final difference Fourier map was in the vicinity of the hafnium atoms.

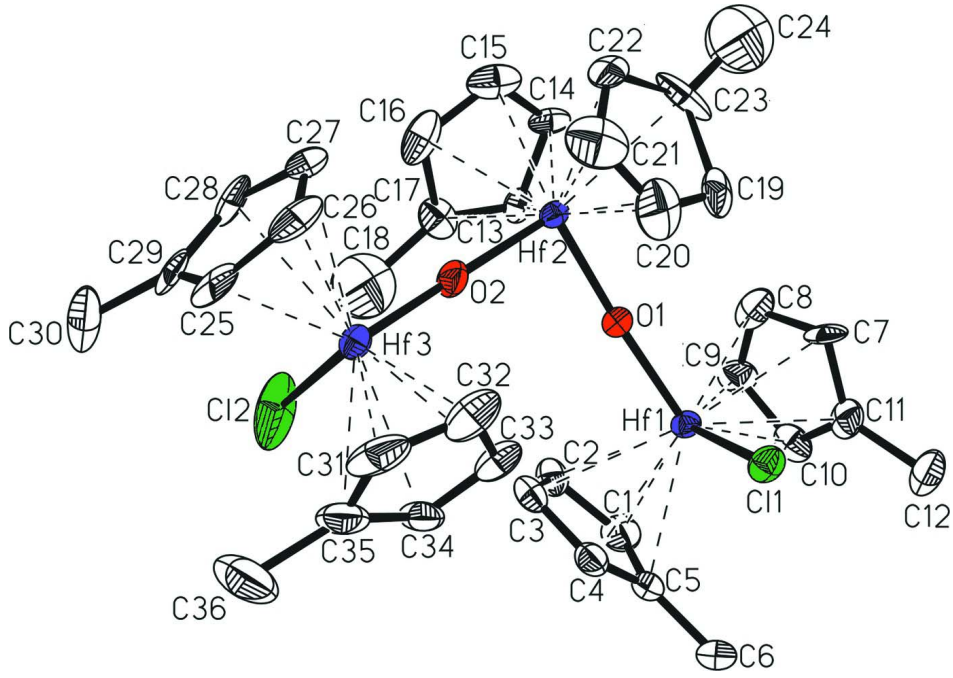


**Figure 1**

The molecular structure of (**1**), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

**Dichlorido-1$\kappa Cl$,3$\kappa Cl$-hexakis[1,1,2,2,3,3($\eta^5$)-methylcyclopentadienyl]di-$\mu_2$-oxido-1:2$\kappa^2O$:$O$;2:3$\kappa^2O$:$O$-trihafnium(IV)**

*Crystal data*

$[Hf_3(C_6H_7)_6Cl_2O_2]$
$M_r$ = 1113.07
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 18.9598 (10) Å
$b$ = 12.9710 (5) Å
$c$ = 14.6178 (6) Å
$\beta$ = 108.466 (4)°
$V$ = 3409.8 (3) Å$^3$
$Z$ = 4
$F(000)$ = 2096
$D_x$ = 2.168 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 6065 reflections
$\theta$ = 1.9–32.4°
$\mu$ = 9.30 mm$^{-1}$
$T$ = 120 K
Prism, colourless
0.1 × 0.08 × 0.04 mm

*Data collection*

Oxford Diffraction KM4 CCD diffractometer
Graphite monochromator
Detector resolution: 8.1883 pixels mm$^{-1}$
$\omega$ scans, 0.75 deg width
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2006)
$T_{min}$ = 0.283, $T_{max}$ = 0.434
11353 measured reflections
5801 independent reflections
4052 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.057
$\theta_{max}$ = 25.1°, $\theta_{min}$ = 1.9°
$h$ = −21→22
$k$ = −7→15
$l$ = −16→17

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.185$
$S = 1.06$
5801 reflections
284 parameters
6 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1162P)^2 + 4.6904P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 2.41$ e Å$^{-3}$
$\Delta\rho_{min} = -2.70$ e Å$^{-3}$

*Special details*

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

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Hf1 | 0.11659 (4) | 0.32908 (5) | 0.39912 (5) | 0.0309 (2) | |
| Hf2 | 0.31749 (4) | 0.38207 (5) | 0.56434 (5) | 0.0279 (2) | |
| Hf3 | 0.30910 (4) | 0.67984 (5) | 0.58248 (5) | 0.0331 (2) | |
| O1 | 0.2183 (6) | 0.3553 (8) | 0.4746 (9) | 0.037 (3) | |
| O2 | 0.3134 (7) | 0.5372 (8) | 0.5725 (10) | 0.049 (4) | |
| Cl1 | 0.0620 (3) | 0.3676 (3) | 0.5261 (4) | 0.0450 (11) | |
| Cl2 | 0.2938 (12) | 0.741 (3) | 0.4165 (7) | 0.056 (7) | 0.61 (7) |
| Cl2A | 0.319 (2) | 0.693 (3) | 0.4198 (12) | 0.051 (8) | 0.39 (7) |
| C1 | 0.0637 (13) | 0.3899 (16) | 0.2276 (16) | 0.059 (6) | |
| H1 | 0.0484 | 0.3399 | 0.1776 | 0.07* | |
| C2 | 0.1362 (13) | 0.4306 (14) | 0.2644 (15) | 0.052 (5) | |
| H2 | 0.1777 | 0.411 | 0.2452 | 0.062* | |
| C3 | 0.1366 (13) | 0.5039 (13) | 0.3334 (15) | 0.049 (5) | |
| H3 | 0.1774 | 0.5461 | 0.3676 | 0.059* | |
| C4 | 0.0661 (11) | 0.5041 (13) | 0.3434 (15) | 0.046 (5) | |
| H4 | 0.0514 | 0.5446 | 0.3884 | 0.056* | |
| C5 | 0.0181 (11) | 0.4330 (14) | 0.2745 (16) | 0.050 (5) | |
| C6 | −0.0606 (12) | 0.4165 (17) | 0.261 (2) | 0.070 (7) | |
| H6A | −0.0777 | 0.3549 | 0.2211 | 0.105* | |
| H6B | −0.0891 | 0.4765 | 0.2285 | 0.105* | |
| H6C | −0.0679 | 0.4069 | 0.3237 | 0.105* | |
| C7 | 0.1181 (10) | 0.1447 (13) | 0.4586 (17) | 0.051 (5) | |
| H7 | 0.1331 | 0.1332 | 0.5262 | 0.061* | |
| C8 | 0.1654 (14) | 0.1518 (14) | 0.398 (3) | 0.075 (9) | |
| H8 | 0.2179 | 0.1437 | 0.4181 | 0.09* | |

| | | | | |
|---|---|---|---|---|
| C9 | 0.1227 (14) | 0.1712 (15) | 0.3092 (19) | 0.059 (6) |
| H9 | 0.14 | 0.1812 | 0.2555 | 0.07* |
| C10 | 0.0499 (14) | 0.1749 (12) | 0.3057 (16) | 0.051 (5) |
| H10 | 0.0084 | 0.1868 | 0.2498 | 0.062* |
| C11 | 0.0472 (13) | 0.1584 (14) | 0.3974 (19) | 0.057 (6) |
| C12 | −0.0240 (13) | 0.1464 (17) | 0.426 (2) | 0.068 (7) |
| H12A | −0.038 | 0.0735 | 0.4228 | 0.102* |
| H12B | −0.0643 | 0.186 | 0.3809 | 0.102* |
| H12C | −0.0149 | 0.1722 | 0.4915 | 0.102* |
| C13 | 0.3497 (13) | 0.3140 (18) | 0.4161 (18) | 0.066 (3) |
| H13 | 0.311 | 0.2875 | 0.3627 | 0.079* |
| C14 | 0.3922 (12) | 0.2589 (19) | 0.4995 (17) | 0.066 (3) |
| H14 | 0.3862 | 0.1879 | 0.5112 | 0.079* |
| C15 | 0.4404 (13) | 0.3201 (17) | 0.5573 (19) | 0.066 (3) |
| H15 | 0.4749 | 0.3 | 0.6174 | 0.079* |
| C16 | 0.4349 (13) | 0.4140 (19) | 0.5209 (17) | 0.066 (3) |
| H16 | 0.4644 | 0.4717 | 0.5502 | 0.079* |
| C17 | 0.3762 (12) | 0.4144 (18) | 0.4285 (17) | 0.066 (3) |
| C18 | 0.3580 (13) | 0.5119 (17) | 0.3697 (18) | 0.066 (3) |
| H18A | 0.3902 | 0.5173 | 0.329 | 0.08* |
| H18B | 0.3662 | 0.5715 | 0.413 | 0.08* |
| H18C | 0.3059 | 0.5103 | 0.3289 | 0.08* |
| C19 | 0.2593 (18) | 0.283 (2) | 0.6744 (16) | 0.081 (3) |
| H19 | 0.2137 | 0.2478 | 0.6448 | 0.097* |
| C20 | 0.2703 (18) | 0.381 (2) | 0.7065 (15) | 0.081 (3) |
| H20 | 0.2309 | 0.4285 | 0.702 | 0.097* |
| C21 | 0.3378 (18) | 0.404 (2) | 0.7429 (15) | 0.081 (3) |
| H21 | 0.3542 | 0.4707 | 0.7685 | 0.097* |
| C22 | 0.3828 (19) | 0.330 (2) | 0.7422 (16) | 0.081 (3) |
| H22 | 0.4355 | 0.3331 | 0.7667 | 0.097* |
| C23 | 0.3394 (17) | 0.242 (2) | 0.6982 (13) | 0.081 (3) |
| C24 | 0.3580 (17) | 0.1362 (19) | 0.6783 (17) | 0.081 (3) |
| H24A | 0.3199 | 0.1103 | 0.6205 | 0.08* |
| H24B | 0.36 | 0.092 | 0.7334 | 0.08* |
| H24C | 0.4065 | 0.1358 | 0.6676 | 0.08* |
| C25 | 0.3903 (12) | 0.8149 (18) | 0.6894 (18) | 0.064 (3) |
| H25 | 0.366 | 0.8746 | 0.7023 | 0.076* |
| C26 | 0.3995 (12) | 0.7254 (17) | 0.7377 (18) | 0.064 (3) |
| H26 | 0.3831 | 0.7127 | 0.7918 | 0.076* |
| C27 | 0.4380 (12) | 0.6501 (18) | 0.6960 (18) | 0.064 (3) |
| H27 | 0.4519 | 0.5816 | 0.7172 | 0.076* |
| C28 | 0.4500 (12) | 0.7013 (17) | 0.6182 (18) | 0.064 (3) |
| H28 | 0.4721 | 0.6717 | 0.5745 | 0.076* |
| C29 | 0.4241 (12) | 0.8036 (18) | 0.6143 (18) | 0.064 (3) |
| C30 | 0.4338 (12) | 0.8816 (17) | 0.5436 (17) | 0.064 (3) |
| H30A | 0.3889 | 0.924 | 0.5204 | 0.08* |
| H30B | 0.4424 | 0.8461 | 0.4889 | 0.08* |
| H30C | 0.4765 | 0.9258 | 0.5752 | 0.08* |

| | | | | |
|---|---|---|---|---|
| C31 | 0.2248 (13) | 0.7771 (18) | 0.658 (2) | 0.071 (3) |
| H31 | 0.244 | 0.8231 | 0.7109 | 0.086* |
| C32 | 0.2150 (13) | 0.6754 (18) | 0.665 (2) | 0.071 (3) |
| H32 | 0.2312 | 0.6363 | 0.7229 | 0.086* |
| C33 | 0.1776 (13) | 0.6357 (19) | 0.574 (2) | 0.071 (3) |
| H33 | 0.1589 | 0.5675 | 0.5608 | 0.086* |
| C34 | 0.1724 (13) | 0.7119 (17) | 0.508 (2) | 0.071 (3) |
| H34 | 0.1526 | 0.7046 | 0.4403 | 0.086* |
| C35 | 0.2015 (14) | 0.8040 (18) | 0.559 (2) | 0.071 (3) |
| C36 | 0.2008 (13) | 0.9084 (16) | 0.520 (2) | 0.071 (3) |
| H36A | 0.1504 | 0.9368 | 0.5024 | 0.08* |
| H36B | 0.2166 | 0.9057 | 0.462 | 0.08* |
| H36C | 0.2349 | 0.9525 | 0.5683 | 0.08* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Hf1 | 0.0263 (4) | 0.0324 (4) | 0.0300 (4) | −0.0008 (3) | 0.0031 (3) | −0.0028 (3) |
| Hf2 | 0.0227 (4) | 0.0375 (4) | 0.0232 (4) | −0.0005 (3) | 0.0069 (3) | 0.0003 (3) |
| Hf3 | 0.0318 (4) | 0.0381 (4) | 0.0296 (4) | −0.0057 (3) | 0.0101 (3) | −0.0056 (3) |
| O1 | 0.032 (7) | 0.036 (6) | 0.041 (7) | 0.001 (5) | 0.009 (6) | 0.003 (5) |
| O2 | 0.039 (8) | 0.031 (6) | 0.078 (11) | −0.008 (5) | 0.019 (8) | −0.003 (6) |
| Cl1 | 0.039 (3) | 0.046 (2) | 0.054 (3) | 0.0013 (19) | 0.021 (2) | −0.009 (2) |
| Cl2 | 0.068 (9) | 0.058 (15) | 0.042 (5) | −0.007 (9) | 0.019 (5) | 0.010 (5) |
| Cl2A | 0.086 (15) | 0.028 (13) | 0.043 (8) | 0.005 (12) | 0.026 (8) | 0.011 (6) |
| C1 | 0.058 (15) | 0.058 (12) | 0.044 (13) | −0.004 (11) | −0.005 (11) | −0.001 (10) |
| C2 | 0.068 (15) | 0.048 (10) | 0.042 (12) | 0.000 (10) | 0.021 (12) | 0.012 (9) |
| C3 | 0.066 (15) | 0.030 (8) | 0.050 (13) | 0.003 (9) | 0.018 (11) | 0.004 (9) |
| C4 | 0.045 (12) | 0.035 (8) | 0.050 (13) | −0.001 (8) | 0.003 (10) | 0.002 (9) |
| C5 | 0.043 (12) | 0.043 (10) | 0.059 (14) | 0.004 (9) | 0.009 (11) | 0.020 (10) |
| C6 | 0.043 (13) | 0.060 (12) | 0.10 (2) | 0.016 (10) | 0.013 (14) | 0.026 (13) |
| C7 | 0.021 (10) | 0.041 (9) | 0.067 (15) | 0.001 (7) | −0.018 (10) | −0.013 (10) |
| C8 | 0.047 (14) | 0.032 (10) | 0.15 (3) | −0.003 (9) | 0.035 (18) | −0.024 (14) |
| C9 | 0.061 (16) | 0.057 (12) | 0.066 (16) | 0.023 (11) | 0.031 (14) | 0.002 (11) |
| C10 | 0.076 (16) | 0.030 (9) | 0.043 (13) | −0.004 (9) | 0.010 (12) | −0.007 (8) |
| C11 | 0.056 (14) | 0.038 (10) | 0.080 (17) | −0.018 (9) | 0.024 (13) | −0.009 (10) |
| C12 | 0.051 (15) | 0.064 (13) | 0.10 (2) | −0.008 (11) | 0.035 (14) | −0.006 (13) |
| C13 | 0.070 (7) | 0.081 (6) | 0.059 (6) | 0.005 (5) | 0.035 (6) | −0.003 (5) |
| C14 | 0.070 (7) | 0.081 (6) | 0.059 (6) | 0.005 (5) | 0.035 (6) | −0.003 (5) |
| C15 | 0.070 (7) | 0.081 (6) | 0.059 (6) | 0.005 (5) | 0.035 (6) | −0.003 (5) |
| C16 | 0.070 (7) | 0.081 (6) | 0.059 (6) | 0.005 (5) | 0.035 (6) | −0.003 (5) |
| C17 | 0.070 (7) | 0.081 (6) | 0.059 (6) | 0.005 (5) | 0.035 (6) | −0.003 (5) |
| C18 | 0.070 (7) | 0.081 (6) | 0.059 (6) | 0.005 (5) | 0.035 (6) | −0.003 (5) |
| C19 | 0.106 (10) | 0.087 (7) | 0.057 (7) | 0.004 (7) | 0.038 (7) | 0.015 (6) |
| C20 | 0.106 (10) | 0.087 (7) | 0.057 (7) | 0.004 (7) | 0.038 (7) | 0.015 (6) |
| C21 | 0.106 (10) | 0.087 (7) | 0.057 (7) | 0.004 (7) | 0.038 (7) | 0.015 (6) |
| C22 | 0.106 (10) | 0.087 (7) | 0.057 (7) | 0.004 (7) | 0.038 (7) | 0.015 (6) |
| C23 | 0.106 (10) | 0.087 (7) | 0.057 (7) | 0.004 (7) | 0.038 (7) | 0.015 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C24 | 0.106 (10) | 0.087 (7) | 0.057 (7) | 0.004 (7) | 0.038 (7) | 0.015 (6) |
| C25 | 0.038 (5) | 0.078 (6) | 0.069 (7) | −0.027 (5) | 0.007 (5) | −0.018 (5) |
| C26 | 0.038 (5) | 0.078 (6) | 0.069 (7) | −0.027 (5) | 0.007 (5) | −0.018 (5) |
| C27 | 0.038 (5) | 0.078 (6) | 0.069 (7) | −0.027 (5) | 0.007 (5) | −0.018 (5) |
| C28 | 0.038 (5) | 0.078 (6) | 0.069 (7) | −0.027 (5) | 0.007 (5) | −0.018 (5) |
| C29 | 0.038 (5) | 0.078 (6) | 0.069 (7) | −0.027 (5) | 0.007 (5) | −0.018 (5) |
| C30 | 0.038 (5) | 0.078 (6) | 0.069 (7) | −0.027 (5) | 0.007 (5) | −0.018 (5) |
| C31 | 0.047 (6) | 0.066 (5) | 0.091 (8) | 0.010 (5) | 0.009 (6) | −0.015 (6) |
| C32 | 0.047 (6) | 0.066 (5) | 0.091 (8) | 0.010 (5) | 0.009 (6) | −0.015 (6) |
| C33 | 0.047 (6) | 0.066 (5) | 0.091 (8) | 0.010 (5) | 0.009 (6) | −0.015 (6) |
| C34 | 0.047 (6) | 0.066 (5) | 0.091 (8) | 0.010 (5) | 0.009 (6) | −0.015 (6) |
| C35 | 0.047 (6) | 0.066 (5) | 0.091 (8) | 0.010 (5) | 0.009 (6) | −0.015 (6) |
| C36 | 0.047 (6) | 0.066 (5) | 0.091 (8) | 0.010 (5) | 0.009 (6) | −0.015 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Hf1—O1 | 1.925 (12) | C10—H10 | 0.95 |
| Hf1—Cl1 | 2.446 (4) | C11—C12 | 1.54 (3) |
| Hf1—C9 | 2.46 (2) | C12—H12A | 0.98 |
| Hf1—C8 | 2.482 (19) | C12—H12B | 0.98 |
| Hf1—C2 | 2.493 (18) | C12—H12C | 0.98 |
| Hf1—C4 | 2.498 (18) | C13—C17 | 1.39 (3) |
| Hf1—C1 | 2.51 (2) | C13—C14 | 1.42 (3) |
| Hf1—C10 | 2.524 (18) | C13—H13 | 0.95 |
| Hf1—C3 | 2.538 (18) | C14—C15 | 1.30 (3) |
| Hf1—C7 | 2.541 (19) | C14—H14 | 0.95 |
| Hf1—C5 | 2.543 (19) | C15—C16 | 1.32 (3) |
| Hf1—C11 | 2.571 (18) | C15—H15 | 0.95 |
| Hf2—O1 | 1.953 (12) | C16—C17 | 1.45 (4) |
| Hf2—O2 | 2.019 (11) | C16—H16 | 0.95 |
| Hf2—C15 | 2.498 (18) | C17—C18 | 1.51 (3) |
| Hf2—C20 | 2.510 (19) | C18—H18A | 0.98 |
| Hf2—C14 | 2.511 (17) | C18—H18B | 0.98 |
| Hf2—C21 | 2.53 (2) | C18—H18C | 0.98 |
| Hf2—C16 | 2.536 (18) | C19—C20 | 1.36 (4) |
| Hf2—C19 | 2.57 (2) | C19—C23 | 1.54 (4) |
| Hf2—C13 | 2.586 (19) | C19—H19 | 0.95 |
| Hf2—C22 | 2.59 (2) | C20—C21 | 1.26 (4) |
| Hf2—C17 | 2.599 (15) | C20—H20 | 0.95 |
| Hf2—C23 | 2.606 (17) | C21—C22 | 1.29 (4) |
| Hf3—O2 | 1.859 (11) | C21—H21 | 0.95 |
| Hf3—C26 | 2.44 (2) | C22—C23 | 1.44 (4) |
| Hf3—Cl2A | 2.447 (17) | C22—H22 | 0.95 |
| Hf3—C32 | 2.45 (3) | C23—C24 | 1.47 (3) |
| Hf3—Cl2 | 2.479 (13) | C24—H24A | 0.98 |
| Hf3—C34 | 2.51 (2) | C24—H24B | 0.98 |
| Hf3—C27 | 2.51 (2) | C24—H24C | 0.98 |
| Hf3—C25 | 2.52 (2) | C25—C26 | 1.34 (3) |

| | | | |
|---|---|---|---|
| Hf3—C33 | 2.52 (2) | C25—C29 | 1.44 (3) |
| Hf3—C35 | 2.54 (2) | C25—H25 | 0.95 |
| Hf3—C31 | 2.55 (2) | C26—C27 | 1.46 (3) |
| Hf3—C28 | 2.57 (2) | C26—H26 | 0.95 |
| C1—C5 | 1.38 (3) | C27—C28 | 1.40 (3) |
| C1—C2 | 1.41 (3) | C27—H27 | 0.95 |
| C1—H1 | 0.95 | C28—C29 | 1.41 (3) |
| C2—C3 | 1.39 (3) | C28—H28 | 0.95 |
| C2—H2 | 0.95 | C29—C30 | 1.50 (3) |
| C3—C4 | 1.39 (3) | C30—H30A | 0.98 |
| C3—H3 | 0.95 | C30—H30B | 0.98 |
| C4—C5 | 1.45 (3) | C30—H30C | 0.98 |
| C4—H4 | 0.95 | C31—C32 | 1.34 (3) |
| C5—C6 | 1.46 (3) | C31—C35 | 1.43 (4) |
| C6—H6A | 0.98 | C31—H31 | 0.95 |
| C6—H6B | 0.98 | C32—C33 | 1.39 (4) |
| C6—H6C | 0.98 | C32—H32 | 0.95 |
| C7—C11 | 1.37 (3) | C33—C34 | 1.36 (4) |
| C7—C8 | 1.45 (3) | C33—H33 | 0.95 |
| C7—H7 | 0.95 | C34—C35 | 1.42 (3) |
| C8—C9 | 1.31 (4) | C34—H34 | 0.95 |
| C8—H8 | 0.95 | C35—C36 | 1.47 (3) |
| C9—C10 | 1.37 (3) | C36—H36A | 0.98 |
| C9—H9 | 0.95 | C36—H36B | 0.98 |
| C10—C11 | 1.37 (3) | C36—H36C | 0.98 |

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|---|---|---|---|
| O1—Hf1—Cl1 | 96.7 (4) | C1—C2—Hf1 | 74.5 (12) |
| O1—Hf1—C9 | 104.2 (7) | C3—C2—H2 | 125.8 |
| Cl1—Hf1—C9 | 132.8 (6) | C1—C2—H2 | 125.8 |
| O1—Hf1—C8 | 81.9 (7) | Hf1—C2—H2 | 116 |
| Cl1—Hf1—C8 | 116.4 (7) | C2—C3—C4 | 107.1 (19) |
| C9—Hf1—C8 | 30.9 (8) | C2—C3—Hf1 | 72.2 (10) |
| O1—Hf1—C2 | 89.2 (6) | C4—C3—Hf1 | 72.4 (10) |
| Cl1—Hf1—C2 | 134.2 (5) | C2—C3—H3 | 126.5 |
| C9—Hf1—C2 | 88.5 (7) | C4—C3—H3 | 126.5 |
| C8—Hf1—C2 | 109.5 (9) | Hf1—C3—H3 | 120.7 |
| O1—Hf1—C4 | 103.7 (5) | C3—C4—C5 | 109.8 (19) |
| Cl1—Hf1—C4 | 81.5 (5) | C3—C4—Hf1 | 75.6 (11) |
| C9—Hf1—C4 | 131.4 (8) | C5—C4—Hf1 | 75.0 (10) |
| C8—Hf1—C4 | 160.9 (9) | C3—C4—H4 | 125.1 |
| C2—Hf1—C4 | 53.1 (7) | C5—C4—H4 | 125.1 |
| O1—Hf1—C1 | 121.8 (6) | Hf1—C4—H4 | 116.2 |
| Cl1—Hf1—C1 | 124.2 (6) | C1—C5—C4 | 104.4 (19) |
| C9—Hf1—C1 | 78.4 (8) | C1—C5—C6 | 130 (2) |
| C8—Hf1—C1 | 108.3 (10) | C4—C5—C6 | 125 (2) |
| C2—Hf1—C1 | 32.7 (7) | C1—C5—Hf1 | 73.0 (12) |
| C4—Hf1—C1 | 53.1 (7) | C4—C5—Hf1 | 71.6 (11) |
| O1—Hf1—C10 | 133.6 (6) | C6—C5—Hf1 | 120.5 (13) |

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|---|---|---|---|
| Cl1—Hf1—C10 | 108.2 (5) | C5—C6—H6A | 109.5 |
| C9—Hf1—C10 | 31.8 (7) | C5—C6—H6B | 109.5 |
| C8—Hf1—C10 | 52.1 (8) | H6A—C6—H6B | 109.5 |
| C2—Hf1—C10 | 99.5 (7) | C5—C6—H6C | 109.5 |
| C4—Hf1—C10 | 118.0 (7) | H6A—C6—H6C | 109.5 |
| C1—Hf1—C10 | 74.7 (7) | H6B—C6—H6C | 109.5 |
| O1—Hf1—C3 | 79.4 (6) | C11—C7—C8 | 105 (2) |
| Cl1—Hf1—C3 | 104.7 (5) | C11—C7—Hf1 | 75.7 (11) |
| C9—Hf1—C3 | 120.3 (7) | C8—C7—Hf1 | 71.0 (12) |
| C8—Hf1—C3 | 136.4 (8) | C11—C7—H7 | 127.5 |
| C2—Hf1—C3 | 32.0 (6) | C8—C7—H7 | 127.5 |
| C4—Hf1—C3 | 32.0 (6) | Hf1—C7—H7 | 118.1 |
| C1—Hf1—C3 | 53.3 (7) | C9—C8—C7 | 108 (2) |
| C10—Hf1—C3 | 127.8 (7) | C9—C8—Hf1 | 73.5 (13) |
| O1—Hf1—C7 | 94.0 (5) | C7—C8—Hf1 | 75.4 (11) |
| Cl1—Hf1—C7 | 83.9 (5) | C9—C8—H8 | 126.1 |
| C9—Hf1—C7 | 53.2 (8) | C7—C8—H8 | 126.1 |
| C8—Hf1—C7 | 33.6 (8) | Hf1—C8—H8 | 117.1 |
| C2—Hf1—C7 | 141.2 (7) | C8—C9—C10 | 110 (2) |
| C4—Hf1—C7 | 158.2 (6) | C8—C9—Hf1 | 75.7 (14) |
| C1—Hf1—C7 | 126.4 (7) | C10—C9—Hf1 | 76.8 (11) |
| C10—Hf1—C7 | 52.3 (7) | C8—C9—H9 | 124.9 |
| C3—Hf1—C7 | 169.6 (7) | C10—C9—H9 | 124.9 |
| O1—Hf1—C5 | 133.8 (5) | Hf1—C9—H9 | 114.5 |
| Cl1—Hf1—C5 | 92.6 (5) | C9—C10—C11 | 108 (2) |
| C9—Hf1—C5 | 102.0 (8) | C9—C10—Hf1 | 71.4 (12) |
| C8—Hf1—C5 | 132.6 (9) | C11—C10—Hf1 | 76.3 (11) |
| C2—Hf1—C5 | 54.1 (7) | C9—C10—H10 | 126.1 |
| C4—Hf1—C5 | 33.5 (6) | C11—C10—H10 | 126.1 |
| C1—Hf1—C5 | 31.7 (7) | Hf1—C10—H10 | 118.2 |
| C10—Hf1—C5 | 84.5 (7) | C7—C11—C10 | 109 (2) |
| C3—Hf1—C5 | 54.5 (7) | C7—C11—C12 | 125 (2) |
| C7—Hf1—C5 | 132.1 (6) | C10—C11—C12 | 126 (2) |
| O1—Hf1—C11 | 125.0 (6) | C7—C11—Hf1 | 73.3 (11) |
| Cl1—Hf1—C11 | 81.1 (5) | C10—C11—Hf1 | 72.5 (11) |
| C9—Hf1—C11 | 52.2 (7) | C12—C11—Hf1 | 125.0 (14) |
| C8—Hf1—C11 | 52.6 (7) | C11—C12—H12A | 109.5 |
| C2—Hf1—C11 | 130.6 (7) | C11—C12—H12B | 109.5 |
| C4—Hf1—C11 | 129.6 (7) | H12A—C12—H12B | 109.5 |
| C1—Hf1—C11 | 102.7 (8) | C11—C12—H12C | 109.5 |
| C10—Hf1—C11 | 31.3 (7) | H12A—C12—H12C | 109.5 |
| C3—Hf1—C11 | 154.6 (8) | H12B—C12—H12C | 109.5 |
| C7—Hf1—C11 | 31.1 (7) | C17—C13—C14 | 106 (2) |
| C5—Hf1—C11 | 101.1 (7) | C17—C13—Hf2 | 75.0 (10) |
| O1—Hf2—O2 | 99.8 (5) | C14—C13—Hf2 | 70.9 (9) |
| O1—Hf2—C15 | 128.9 (7) | C17—C13—H13 | 127 |
| O2—Hf2—C15 | 112.2 (6) | C14—C13—H13 | 127 |
| O1—Hf2—C20 | 92.0 (8) | Hf2—C13—H13 | 119.1 |

| | | | |
|---|---|---|---|
| O2—Hf2—C20 | 85.6 (7) | C15—C14—C13 | 110 (2) |
| C15—Hf2—C20 | 128.0 (9) | C15—C14—Hf2 | 74.4 (10) |
| O1—Hf2—C14 | 99.8 (7) | C13—C14—Hf2 | 76.7 (9) |
| O2—Hf2—C14 | 133.9 (7) | C15—C14—H14 | 125 |
| C15—Hf2—C14 | 30.1 (7) | C13—C14—H14 | 125 |
| C20—Hf2—C14 | 134.6 (8) | Hf2—C14—H14 | 115.8 |
| O1—Hf2—C21 | 120.8 (8) | C14—C15—C16 | 111 (3) |
| O2—Hf2—C21 | 79.7 (7) | C14—C15—Hf2 | 75.5 (10) |
| C15—Hf2—C21 | 103.9 (9) | C16—C15—Hf2 | 76.3 (9) |
| C20—Hf2—C21 | 28.9 (8) | C14—C15—H15 | 124.7 |
| C14—Hf2—C21 | 122.9 (9) | C16—C15—H15 | 124.7 |
| O1—Hf2—C16 | 126.6 (7) | Hf2—C15—H15 | 115.3 |
| O2—Hf2—C16 | 84.6 (6) | C15—C16—C17 | 108 (2) |
| C15—Hf2—C16 | 30.4 (7) | C15—C16—Hf2 | 73.2 (9) |
| C20—Hf2—C16 | 141.2 (9) | C17—C16—Hf2 | 76.0 (10) |
| C14—Hf2—C16 | 50.6 (8) | C15—C16—H16 | 125.8 |
| C21—Hf2—C16 | 112.4 (9) | C17—C16—H16 | 125.8 |
| O1—Hf2—C19 | 79.5 (8) | Hf2—C16—H16 | 117 |
| O2—Hf2—C19 | 115.5 (7) | C13—C17—C16 | 105 (2) |
| C15—Hf2—C19 | 117.1 (8) | C13—C17—C18 | 135 (2) |
| C20—Hf2—C19 | 31.0 (8) | C16—C17—C18 | 120 (2) |
| C14—Hf2—C19 | 108.9 (8) | C13—C17—Hf2 | 74.0 (9) |
| C21—Hf2—C19 | 50.7 (9) | C16—C17—Hf2 | 71.2 (9) |
| C16—Hf2—C19 | 145.6 (9) | C18—C17—Hf2 | 119.7 (7) |
| O1—Hf2—C13 | 79.0 (6) | C17—C18—H18A | 109.5 |
| O2—Hf2—C13 | 114.4 (6) | C17—C18—H18B | 109.5 |
| C15—Hf2—C13 | 52.0 (8) | H18A—C18—H18B | 109.5 |
| C20—Hf2—C13 | 159.0 (8) | C17—C18—H18C | 109.5 |
| C14—Hf2—C13 | 32.4 (7) | H18A—C18—H18C | 109.5 |
| C21—Hf2—C13 | 154.7 (9) | H18B—C18—H18C | 109.5 |
| C16—Hf2—C13 | 52.2 (8) | C20—C19—C23 | 102 (3) |
| C19—Hf2—C13 | 128.1 (8) | C20—C19—Hf2 | 72.2 (10) |
| O1—Hf2—C22 | 132.9 (7) | C23—C19—Hf2 | 74.1 (10) |
| O2—Hf2—C22 | 102.4 (7) | C20—C19—H19 | 128.8 |
| C15—Hf2—C22 | 78.6 (9) | C23—C19—H19 | 128.8 |
| C20—Hf2—C22 | 49.5 (10) | Hf2—C19—H19 | 117.6 |
| C14—Hf2—C22 | 93.8 (8) | C21—C20—C19 | 113 (3) |
| C21—Hf2—C22 | 29.1 (8) | C21—C20—Hf2 | 76.5 (12) |
| C16—Hf2—C22 | 96.6 (9) | C19—C20—Hf2 | 76.8 (10) |
| C19—Hf2—C22 | 53.4 (9) | C21—C20—H20 | 123.4 |
| C13—Hf2—C22 | 126.0 (8) | C19—C20—H20 | 123.4 |
| O1—Hf2—C17 | 94.0 (7) | Hf2—C20—H20 | 114.8 |
| O2—Hf2—C17 | 85.3 (6) | C20—C21—C22 | 114 (3) |
| C15—Hf2—C17 | 52.4 (8) | C20—C21—Hf2 | 74.6 (12) |
| C20—Hf2—C17 | 169.8 (8) | C22—C21—Hf2 | 78.0 (11) |
| C14—Hf2—C17 | 52.1 (7) | C20—C21—H21 | 123 |
| C21—Hf2—C17 | 143.8 (9) | C22—C21—H21 | 123 |
| C16—Hf2—C17 | 32.9 (8) | Hf2—C21—H21 | 115.7 |

| | | | |
|---|---|---|---|
| C19—Hf2—C17 | 158.9 (8) | C21—C22—C23 | 108 (3) |
| C13—Hf2—C17 | 31.0 (7) | C21—C22—Hf2 | 72.9 (12) |
| C22—Hf2—C17 | 128.7 (9) | C23—C22—Hf2 | 74.5 (11) |
| O1—Hf2—C23 | 105.7 (8) | C21—C22—H22 | 125.9 |
| O2—Hf2—C23 | 130.6 (7) | C23—C22—H22 | 125.9 |
| C15—Hf2—C23 | 83.0 (8) | Hf2—C22—H22 | 118.6 |
| C20—Hf2—C23 | 52.4 (8) | C22—C23—C24 | 134 (3) |
| C14—Hf2—C23 | 82.2 (8) | C22—C23—C19 | 102 (2) |
| C21—Hf2—C23 | 50.9 (8) | C24—C23—C19 | 124 (3) |
| C16—Hf2—C23 | 111.0 (9) | C22—C23—Hf2 | 73.3 (11) |
| C19—Hf2—C23 | 34.7 (8) | C24—C23—Hf2 | 119.6 (8) |
| C13—Hf2—C23 | 111.5 (8) | C19—C23—Hf2 | 71.3 (10) |
| C22—Hf2—C23 | 32.1 (8) | C23—C24—H24A | 109.5 |
| C17—Hf2—C23 | 132.9 (8) | C23—C24—H24B | 109.5 |
| O2—Hf3—C26 | 106.2 (7) | H24A—C24—H24B | 109.5 |
| O2—Hf3—Cl2A | 88.4 (10) | C23—C24—H24C | 109.5 |
| C26—Hf3—Cl2A | 129.8 (8) | H24A—C24—H24C | 109.5 |
| O2—Hf3—C32 | 94.1 (7) | H24B—C24—H24C | 109.5 |
| C26—Hf3—C32 | 87.4 (8) | C26—C25—C29 | 107 (2) |
| Cl2A—Hf3—C32 | 140.3 (12) | C26—C25—Hf3 | 71.2 (12) |
| O2—Hf3—Cl2 | 103.5 (10) | C29—C25—Hf3 | 77.8 (12) |
| C26—Hf3—Cl2 | 131.5 (6) | C26—C25—H25 | 126.3 |
| Cl2A—Hf3—Cl2 | 18.0 (4) | C29—C25—H25 | 126.3 |
| C32—Hf3—Cl2 | 127.7 (9) | Hf3—C25—H25 | 116.8 |
| O2—Hf3—C34 | 101.3 (7) | C25—C26—C27 | 111 (2) |
| C26—Hf3—C34 | 133.3 (8) | C25—C26—Hf3 | 77.6 (14) |
| Cl2A—Hf3—C34 | 87.3 (13) | C27—C26—Hf3 | 75.4 (13) |
| C32—Hf3—C34 | 53.3 (9) | C25—C26—H26 | 124.5 |
| Cl2—Hf3—C34 | 74.9 (9) | C27—C26—H26 | 124.5 |
| O2—Hf3—C27 | 80.9 (7) | Hf3—C26—H26 | 114.4 |
| C26—Hf3—C27 | 34.3 (7) | C28—C27—C26 | 105 (2) |
| Cl2A—Hf3—C27 | 107.3 (12) | C28—C27—Hf3 | 76.3 (14) |
| C32—Hf3—C27 | 112.3 (9) | C26—C27—Hf3 | 70.3 (13) |
| Cl2—Hf3—C27 | 118.9 (8) | C28—C27—H27 | 127.7 |
| C34—Hf3—C27 | 165.4 (9) | C26—C27—H27 | 127.7 |
| O2—Hf3—C25 | 135.0 (7) | Hf3—C27—H27 | 118 |
| C26—Hf3—C25 | 31.3 (7) | C27—C28—C29 | 110 (2) |
| Cl2A—Hf3—C25 | 109.7 (7) | C27—C28—Hf3 | 71.8 (13) |
| C32—Hf3—C25 | 96.2 (8) | C29—C28—Hf3 | 76.6 (13) |
| Cl2—Hf3—C25 | 104.2 (8) | C27—C28—H28 | 125.2 |
| C34—Hf3—C25 | 119.8 (8) | C29—C28—H28 | 125.2 |
| C27—Hf3—C25 | 54.7 (8) | Hf3—C28—H28 | 118.2 |
| O2—Hf3—C33 | 80.7 (6) | C28—C29—C25 | 107 (2) |
| C26—Hf3—C33 | 119.3 (8) | C28—C29—C30 | 123 (2) |
| Cl2A—Hf3—C33 | 110.2 (10) | C25—C29—C30 | 130 (2) |
| C32—Hf3—C33 | 32.4 (8) | C28—C29—Hf3 | 72.0 (11) |
| Cl2—Hf3—C33 | 102.6 (8) | C25—C29—Hf3 | 69.7 (11) |
| C34—Hf3—C33 | 31.4 (8) | C30—C29—Hf3 | 124.5 (15) |

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| C27—Hf3—C33 | 137.4 (8) | C29—C30—H30A | 109.5 |
| C25—Hf3—C33 | 125.9 (8) | C29—C30—H30B | 109.5 |
| O2—Hf3—C35 | 132.4 (7) | H30A—C30—H30B | 109.5 |
| C26—Hf3—C35 | 105.7 (8) | C29—C30—H30C | 109.5 |
| Cl2A—Hf3—C35 | 97.3 (14) | H30A—C30—H30C | 109.5 |
| C32—Hf3—C35 | 53.3 (9) | H30B—C30—H30C | 109.5 |
| Cl2—Hf3—C35 | 79.9 (11) | C32—C31—C35 | 108 (2) |
| C34—Hf3—C35 | 32.7 (7) | C32—C31—Hf3 | 70.4 (14) |
| C27—Hf3—C35 | 139.5 (8) | C35—C31—Hf3 | 73.2 (14) |
| C25—Hf3—C35 | 87.2 (8) | C32—C31—H31 | 126 |
| C33—Hf3—C35 | 53.0 (8) | C35—C31—H31 | 126 |
| O2—Hf3—C31 | 125.1 (7) | Hf3—C31—H31 | 122 |
| C26—Hf3—C31 | 80.1 (8) | C31—C32—C33 | 110 (3) |
| Cl2A—Hf3—C31 | 129.7 (14) | C31—C32—Hf3 | 78.6 (16) |
| C32—Hf3—C31 | 31.0 (7) | C33—C32—Hf3 | 76.8 (16) |
| Cl2—Hf3—C31 | 111.9 (11) | C31—C32—H32 | 125.1 |
| C34—Hf3—C31 | 53.2 (9) | C33—C32—H32 | 125.1 |
| C27—Hf3—C31 | 113.7 (8) | Hf3—C32—H32 | 111.8 |
| C25—Hf3—C31 | 74.3 (8) | C34—C33—C32 | 108 (2) |
| C33—Hf3—C31 | 52.2 (8) | C34—C33—Hf3 | 73.6 (14) |
| C35—Hf3—C31 | 32.6 (8) | C32—C33—Hf3 | 70.9 (14) |
| O2—Hf3—C28 | 93.2 (6) | C34—C33—H33 | 126 |
| C26—Hf3—C28 | 53.6 (8) | C32—C33—H33 | 126 |
| Cl2A—Hf3—C28 | 78.4 (10) | Hf3—C33—H33 | 121.2 |
| C32—Hf3—C28 | 140.8 (9) | C33—C34—C35 | 108 (3) |
| Cl2—Hf3—C28 | 87.5 (7) | C33—C34—Hf3 | 74.9 (14) |
| C34—Hf3—C28 | 159.4 (8) | C35—C34—Hf3 | 74.7 (14) |
| C27—Hf3—C28 | 31.9 (8) | C33—C34—H34 | 125.9 |
| C25—Hf3—C28 | 53.7 (8) | C35—C34—H34 | 125.9 |
| C33—Hf3—C28 | 169.1 (8) | Hf3—C34—H34 | 116.5 |
| C35—Hf3—C28 | 134.3 (8) | C34—C35—C31 | 106 (2) |
| C31—Hf3—C28 | 127.8 (8) | C34—C35—C36 | 128 (3) |
| Hf1—O1—Hf2 | 173.3 (7) | C31—C35—C36 | 126 (2) |
| Hf3—O2—Hf2 | 178.7 (8) | C34—C35—Hf3 | 72.6 (13) |
| C5—C1—C2 | 110.2 (19) | C31—C35—Hf3 | 74.2 (13) |
| C5—C1—Hf1 | 75.3 (12) | C36—C35—Hf3 | 123.1 (17) |
| C2—C1—Hf1 | 72.8 (11) | C35—C36—H36A | 109.5 |
| C5—C1—H1 | 124.9 | C35—C36—H36B | 109.5 |
| C2—C1—H1 | 124.9 | H36A—C36—H36B | 109.5 |
| Hf1—C1—H1 | 118.7 | C35—C36—H36C | 109.5 |
| C3—C2—C1 | 108 (2) | H36A—C36—H36C | 109.5 |
| C3—C2—Hf1 | 75.8 (11) | H36B—C36—H36C | 109.5 |