Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

# Crystal structure of the $[(THF)Cs(\mu\text{-}\eta^5\text{:}\eta^5\text{-}Cp')_3Yb]_n$ oligomer

**Daniel N. Huh, Joseph W. Ziller and William J. Evans***

Department of Chemistry, University of California, Irvine, California, 92697, USA. *Correspondence e-mail: wevans@uci.edu

Received 29 May 2020
Accepted 16 June 2020

Edited by M. Zeller, Purdue University, USA

**Keywords:** lanthanide; caesium; cyclopentadienide; oligomer; crystal structure.

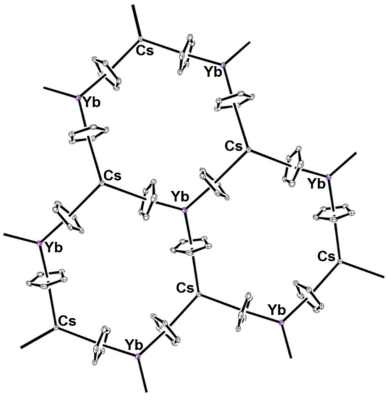
**CCDC reference**: 2010185

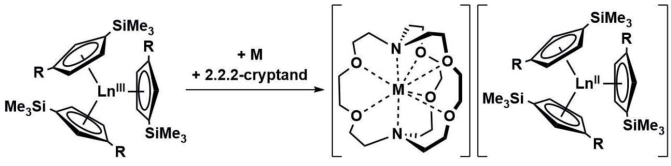
**Supporting information**: this article has supporting information at journals.iucr.org/e

The green compound poly[(tetrahydrofuran)tris[$\mu$-$\eta^5$:$\eta^5$-1-(trimethylsilyl)cyclopentadienyl]caesium(I)ytterbium(II)], $[CsYb(C_8H_{13}Si)_3(C_4H_8O)]_n$ or $[(THF)Cs(\mu\text{-}\eta^5\text{:}\eta^5\text{-}Cp')_3Yb^{II}]_n$ was synthesized by reduction of a red THF solution of $(C_5H_4SiMe_3)_3Yb^{III}$ with excess Cs metal and identified by X-ray diffraction. The compound crystallizes as a two-dimensional array of hexagons with alternating $Cs^I$ and $Yb^{II}$ ions at the vertices and cyclopentadienyl groups bridging each edge. This, based off the six-electron cyclopentadienyl rings occupying three coordination positions, gives a formally nine-coordinate tris(cyclopentadienyl) coordination environment to Yb and the Cs is ten-coordinate due to the three cyclopentadienyl rings and a coordinated molecule of THF. The complex comprises layers of $Cs_3Yb_3$ hexagons with THF ligands and $Me_3Si$ groups in between the layers. The Yb—C metrical parameters are consistent with a $4f^{14}$ $Yb^{II}$ electron configuration.

## 1. Chemical context

The new +2 oxidation states for the rare-earth metals Y, La, Ce, Pr, Gd, Tb, Ho, Er, and Lu were recently discovered by reduction of $Cp^x_3Ln$ ($Cp^x$ = $C_5H_4SiMe_3$, $C_5H_3(SiMe_3)_2$; *Ln* = rare-earth metal) using alkali metal reductants Li, Na, K, and $KC_8$ (Fig. 1) (Hitchcock *et al.*, 2008; MacDonald *et al.*, 2013; Fieser *et al.*, 2015; Evans, 2016; Palumbo *et al.*, 2018). In each of these cases, 2.2.2-cryptand was added in these reactions to encapsulate the alkali metal. It was thought that chelating agents were necessary to sequester the alkali metal to prevent interactions with cyclopentadienide ligands and subsequent ligand dissociation leading to product decomposition. This idea was challenged by examining reduction reactions of $Cp''_3M$ ($Cp''$ = $C_5H_3(SiMe_3)_2$; *M* = La, Ce, U) with Li and Cs in the absence of chelating agents (Huh *et al.*, 2018). The reaction resulted in the isolation of the first chelate-free synthesis of $La^{II}$, $Ce^{II}$, and $U^{II}$ complexes. The $[Li(THF)_4]^{1+}$ cation of the

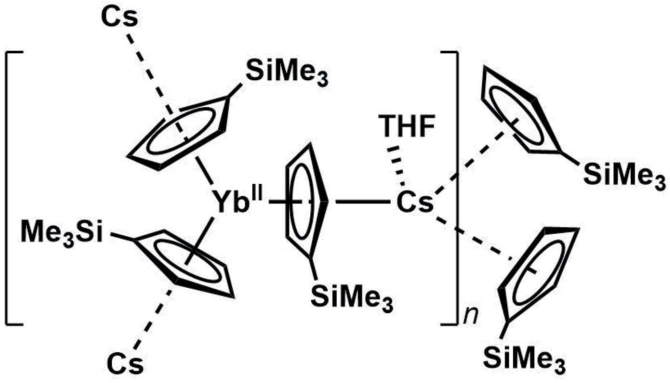



R = H, Ln = Y, La, Ce, Pr, Nd, Gd, Tb, Dy, Ho, Er, and Lu
R = $SiMe_3$, Ln = La, Ce, Pr, and Nd
M = Li, Na, K, $KC_8$

**Figure 1**
Synthesis of $(Cp^x_3Ln^{II})^{1-}$ complexes by alkali metal reduction of $Cp^x_3Ln^{III}$ precursors; $Cp^x$ = $C_5H_4SiMe_3$, $C_5H_3(SiMe_3)_2$.

Li salts in these chelate-free $M^{II}$ complexes were well-separated from the $(Cp''_3M)^{1-}$ anion. However, the Cs reductions yielded polymeric complexes of general formula $[Cp''M(\mu\text{-}Cp'')_2Cs(THF)_2]_n$ where the Cs cation has coordinated THF and cyclopentadienide ligands. Attempts to extend this chemistry to smaller rare-earth metals by reduction of $Cp'_3Ln$ ($Cp'$ = $C_5H_4SiMe_3$; $Ln$ = Y, Tb, Dy) showed evidence of $Ln^{II}$ in solution; however, the reduction products were highly unstable and decomposed even at 238 K.




In this study, we were interested in examining the reduction of $Cp'_3Yb^{III}$ with Cs metal. Unlike $Y^{II}$, $Tb^{II}$, and $Dy^{II}$ ions, $Yb^{II}$ complexes are more easily obtainable, as reflected by their less negative reduction potentials (Morss, 1976). A crystal containing the oligomeric compound; $[(THF)Cs(\mu\text{-}\eta^5\text{:}\eta^5\text{-}Cp')_3Yb]_n$, **1** ($Cp'$ = $C_5H_4SiMe_3$) was isolated by reduction of the $Cp'_3Yb^{III}$ complex (Fieser *et al.*, 2015) in THF using Cs metal (Figs. 2 and 3).

## 2. Structural commentary

All three $Cp'$ rings remain coordinated to the Yb metal center after reduction and are coordinated in a trigonal–planar fashion. The Yb atom is within 0.107 Å of the plane of the three ring centroids. Each ring bridges Yb to Cs, which also is surrounded by three cyclopentadienyl ligands as well as a coordinated molecule of THF. The three ring centroids and the oxygen of THF are arranged in a pseudo-tetrahedral geometry around Cs with a calculated four-coordinate Cs $\tau'_4$ value of 0.76 ($\tau'_4$ = 1 for tetrahedral; $\tau'_4$ = 0 for square planar; Rosiak *et al.*, 2018). The Cs metal center has a pseudo-tetrahedral geometry with Cp′(centroid)···Cs···Cp′(centroid) angles of 109.0, 114.3, and 121.4° and Cp′(centroid)···Cs···O(THF) angles of 88.8, 94.1, and 127.8°.

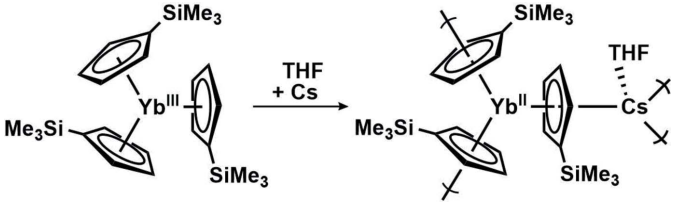



**Figure 2**
Synthesis of $[(THF)Cs(\mu\text{-}\eta^5\text{:}\eta^5\text{-}Cp')_3Yb^{II}]_n$, **1**, by caesium metal reduction of the $Cp'_3Yb^{III}$ precursor.

**Table 1**
Selected bond distances and angles for $[(THF)Cs(\mu\text{-}\eta^5\text{:}\eta^5\text{-}Cp')_3Yb]_n$, **1**.

Centroid1, centroid2, and centroid3 are the centroids of the Cp rings connected to Si1, Si2, and Si3, respectively.

| | |
|---|---|
| Yb1···centroid1 | 2.510 (1) |
| Yb1···centroid2 | 2.513 (2) |
| Yb1···centroid3 | 2.504 (1) |
| Cs1···centroid1 | 3.197 (1) |
| Cs1···centroid2 | 3.268 (2) |
| Cs1···centroid3 | 3.159 (1) |
| Cs1—O1 | 3.095 (3) |
| | |
| centroid1—Yb1···centroid2 | 120.1 |
| centroid1—Yb1···centroid3 | 116.6 |
| centroid2—Yb1···centroid3 | 122.8 |
| centroid1—Cs1···centroid2 | 121.4 |
| centroid1—Cs1···centroid3 | 109.0 |
| centroid2—Cs1···centroid3 | 114.3 |
| Yb1···centroid1···Cs1 | 175.3 |
| Yb1···centroid2···Cs1 | 172.3 |
| Yb1···centroid3···Cs1 | 176.7 |
| centroid1···Cs1···O1 | 88.8 |
| centroid2···Cs1···O1 | 94.1 |
| centroid3···Cs1···O1 | 127.8 |

**Table 2**
Bond distance (Å) ranges for Yb···Cp′(centroid) and bond angle (°) ranges for Cp′(centroid)···Yb···Cp′(centroid) in $Cp'_3Yb$ (Fieser *et al.*, 2015), [K(crypt)][$Cp'_3Yb$] (Fieser *et al.*, 2015), and $[(THF)Cs(\mu\text{-}\eta^5\text{:}\eta^5\text{-}Cp')_3Yb]_n$.

| | $Cp'_3Yb$ | [K(crypt)][$Cp'_3Yb$] | **1** |
|---|---|---|---|
| Yb···Cp′(centroid) | 2.363–2.368 | 2.503–2.513 | 2.504 (1)–2.513 (2) |
| Cs···Cp′(centroid) | | | 3.159 (1)–3.268 (2) |
| Cp′···Yb···Cp′ | 118.85–120.55 | 118.10–122.93 | 116.64–122.76 |
| Cp′···Cs···Cp′ | | | 109.0–121.4 |

The bond distances and angles in **1** are summarized in Table 1. The range of 2.504 (1)–2.513 (2) Å Cp′(centroid)···Yb bond distances in **1** is the same as that in the complex [K(crypt)][$Cp'_3Yb^{II}$] (crypt = 2.2.2-cryptand), which was

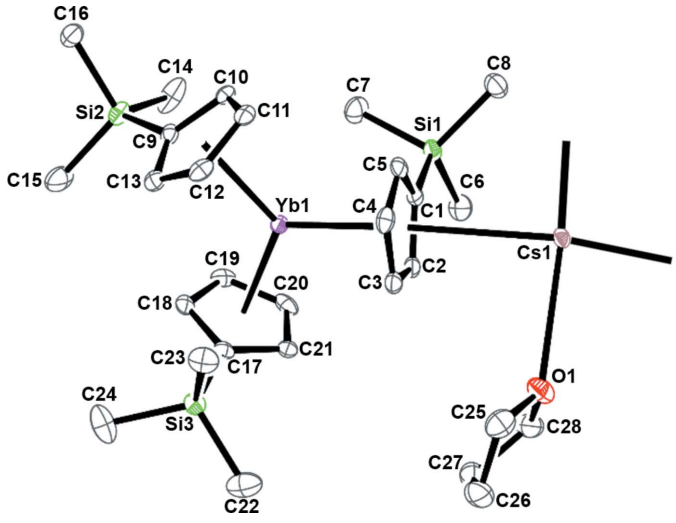



**Figure 3**
*ORTEP* representation of an asymmetric unit of $[(THF)Cs(\mu\text{-}\eta^5\text{:}\eta^5\text{-}Cp')_3Yb]_n$, **1**, with probability ellipsoids drawn at the 50% probability level. Hydrogen atoms were omitted for clarity.

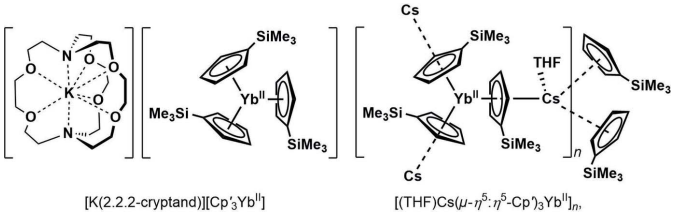



**Figure 4**
*CHEMDRAW* (Mills, 2006) representation of [K(2.2.2-cryptand)][$Cp'_3Yb^{II}$] (left) and [(THF)Cs($\mu$-$\eta^5$:$\eta^5$-Cp′)$_3Yb^{II}]_n$, **1**, (right).

fully characterized as a $4f^{14}$ $Yb^{II}$ complex, Table 2 and Fig. 4. In $Cp_3Ln$ reduction chemistry, the difference in $Ln\cdots$Cp(centroid) distances between the $Ln^{III}$ and $Ln^{II}$ complexes provides important information on the electronic configuration of the lanthanide ion (Evans, 2016). Differences in $Ln\cdots$Cp(centroid) distances for reduction of $4f^n$ $Ln^{III}$ ions to $4f^{n+1}$ $Ln^{II}$ ions range from 0.1 to 0.2 Å (Fieser *et al.*, 2015). In this study, the difference of 0.14 Å in the $Ln\cdots$Cp(centroid) distance is characteristic of a $4f^{13}$ $Yb^{III}$ reduction to a $4f^{14}$ $Yb^{II}$ ion. In contrast, $Ln^{II}$ ions with $4f^n5d^1$ configurations where the additional electron populates a *d*-orbital instead of the an *f*-orbital have differences of only 0.02–0.05 Å (Evans, 2016).

## 3. Supramolecular features

In **1**, all of the cyclopentadienyl ligands are bridging. The threefold symmetry of three bridging Cp′ ligands on each metal generates a hexagonal pattern as shown in Fig. 5. The Yb···Cp′(centroid)···Cs angles are 172.5–176.7° such that each side of the hexagon is nearly linear. The 112.4–117.3° Yb···Cs···Yb angles are smaller than the 120.8–125.6° Cs···Yb···Cs angles, which makes the hexagon slightly irregular. This could be of interest to quantum scientists trying to make thin-film layers of magnetic materials since the hexagonal pattern could lead to spin frustration with a paramagnetic lanthanide.

The side view of these layers in Fig. 6 shows how the space in between them is filled with THF and $Me_3Si$ substituent groups. The 116.6–122.8° Cp′(centroid)···Yb···Cp′(centroid) and 109.0–121.4° Cp′(centroid)···Cs···Cp′(centroid) angles generate the undulation of the hexagons shown in Fig. 6.

## 4. Database survey

The 3.159 (1), 3.197 (1), and 3.268 (2) Å Cs···Cp′(centroid) distances in **1** are shorter than the 3.278 and 3.435 Å Cs···Cp″(centroid) distances in [(THF)$_2$Cs][($\mu$-$\eta^5$:$\eta^5$-Cp″)$_2U^{II}$($\eta^5$-Cp″)]$_n$, (Huh *et al.*, 2018), the 3.396 Å Cs···$C_5H_5$(centroid) distances in {[$(Me_3Si)_2NCs]_2$·[$(C_5H_5)_2Fe$)] 0.5·($C_6H_5Me$)}$_n$, (Morris *et al.*, 2007) and the 3.337 Å Cs···$C_5Me_5$(centroid) distances in [(THF)$_2$Cs($\mu_3$-O)$_3${[Ti($C_5Me_5$)]$_3$-($\mu_3$-$CCH_2$)}] (González-del Moral *et al.*, 2005). The 3.095 (3) Å Cs—O(THF) bond distance is consistent with the Cs—O(THF) distances of 3.081 (7) to 3.119 (8) Å in [(THF)$_2$Cs][($\mu$-$\eta^5$:$\eta^5$-Cp″)$_2U^{II}$($\eta^5$-Cp″)]$_n$ (Huh *et al.*, 2018) and 3.034 (9)–3.06 (1) Å in [(THF)$_2$Cs($\mu_3$-O)$_3${[Ti($C_5Me_5$)]$_3$($\mu_3$-$CCH_2$)}] (González-del Moral *et al.*, 2005).

The extended structure of **1** differs from that of the [(THF)$_2$Cs][($\mu$-$\eta^5$:$\eta^5$-Cp″)$_2M^{II}$($\eta^5$-Cp″)]$_n$, complexes (*M* = La, U), which comprise zigzag chains of –*M*–($\mu$-Cp″)–Cs–($\mu$-Cp″)– repeat units with a terminal Cp″ attached to *M* and two terminal THF ligands attached to Cs (Huh *et al.*, 2018). These were obtained by reduction of $Cp''_3M^{III}$ compounds with Cs in THF. In those structures, La and U have a trigonal–planar tris(cyclopentadienyl) coordination like Yb in **1**, but the Cs is

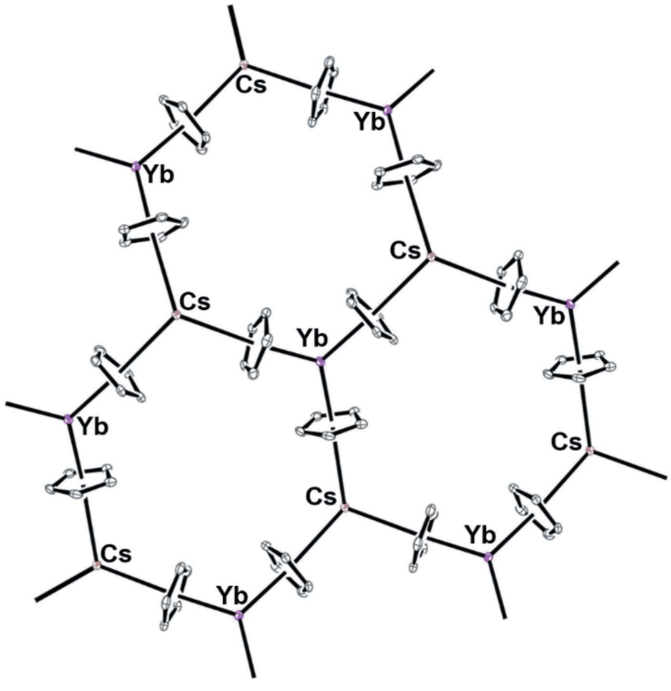



**Figure 5**
Top view of the extended structure of [(THF)Cs($\mu$-$\eta^5$:$\eta^5$-Cp′)$_3$Yb]$_n$, **1**, with the $SiMe_3$ substituent of the $C_5H_4SiMe_3$ group and the THF attached to Cs removed for clarity.

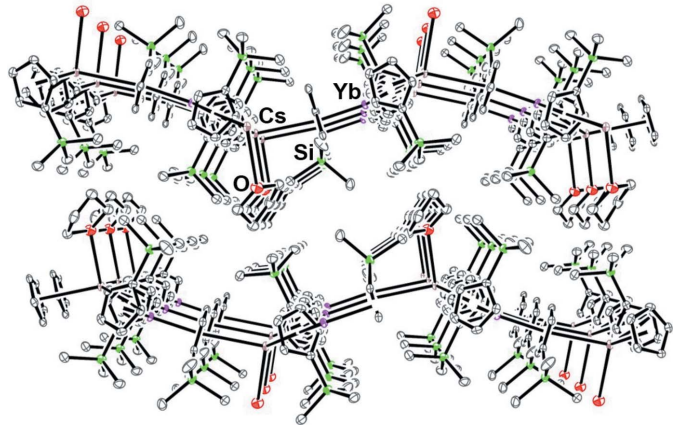



**Figure 6**
Side view of the extended structure of [(THF)Cs($\mu$-$\eta^5$:$\eta^5$-Cp′)$_3$Yb]$_n$, **1**. Magenta, Yb; brown, Cs; green, Si; red, O.

coordinated by only two cyclopentadienyl ligands to give a bent metallocene $Cp''_2Cs(THF)_2$ sub-structure with these larger rings.

A survey of the Cambridge Structural Database (CSD, version 5.41, March 2020; Groom *et al.*, 2016) also revealed four oligomeric complexes containing Yb–$Cp^x$ moieties with various types of cyclopentadienyl rings ($Cp^x$): $[Na(\mu\text{-}\eta^5{:}\eta^5\text{-}C_5H_5)_3Yb^{II}]_n$ (Apostolidis *et al.*, 1997), $[Na(\mu\text{-}\eta^5{:}\eta^5\text{-}Cp'')_2Yb^{II}{}_2(\mu\text{-}\eta^5{:}\eta^5\text{-}Cp'')_2]_n$ (Voskoboynikov *et al.*, 1997), $[(C_5Me_5)Yb(\mu\text{-}I)(\mu\text{-}\eta^5{:}\eta^5\text{-}C_5Me_5)Yb(C_5Me_5)]_n$ (Evans *et al.*, 2006) and $[Yb(\mu\text{-}\eta^5{:}\eta^5\text{-}C_5H_5)(Ph_2Pz)(THF)]_n$ ($Ph_2Pz$ = 3,5–diphenylpyrazolate) (Ali *et al.*, 2018). The $[Na(\mu\text{-}\eta^5{:}\eta^5\text{-}C_5H_5)_3Yb^{II}]_n$ (Apostolidis *et al.*, 1997) complex adopts a hexagonal net extended structure similar to that in **1** except the alkali metal does not have a coordinated solvent. The structure of $[Na(\mu\text{-}\eta^5{:}\eta^5\text{-}Cp'^{Bu})_3Sm^{II}]$ is similar (Bel'sky *et al.*, 1990). Three oligomeric complexes containing Cs–cyclopentadienyl moieties have previously been reported: $[(THF)_2Cs][(\mu\text{-}\eta^5{:}\eta^5\text{-}Cp'')_2U^{II}(\eta^5\text{-}Cp'')]_n$ (Huh *et al.*, 2018), $\{[(Me_3Si)_2NCs]_2[(C_5H_5)_2Fe)]\cdot 0.5(C_6H_5Me)\}_n$ (Morris *et al.*, 2007) and $[(THF)_2Cs(\mu_3\text{-}O)_3\{[Ti(C_5Me_5)]_3(\mu_3\text{-}CCH_2)\}]$ (González-del Moral *et al.*, 2005). An oligomeric, base-free Li–Cp′ compound was also previously reported in the literature, $[(\mu\text{-}\eta^5{:}\eta^5\text{-}Cp')Li]_n$ (Evans *et al.*, 1992).

## 5. Synthesis and crystallization

In an argon-filled glovebox, addition of a red solution of $Cp'_3Yb$ (50 mg, 0.085 mmol) in THF (2 mL) to excess Cs as a smear produced a green solution. This was stirred for 15 min at room temperature and then layered at the bottom of a vial below an $Et_2O$ (10 mL) layer for crystallization at −35°C. After 1 d, X-ray quality dark-green crystals of $[(THF)Cs(\mu\text{-}\eta^5{:}\eta^5\text{-}Cp')_3Yb^{II}]_n$ were isolated. A small number of crystals were obtained and used for crystallographic analysis. Too little sample was available for other characterization.

## 6. Refinement

Crystal data and structure refinement for $[(THF)Cs(\mu\text{-}\eta^5{:}\eta^5\text{-}Cp')_3Yb^{II}]_n$, **1** are summarized in Table 3. Hydrogen atoms were included using a riding model with $U_{iso}(H)$ values of $1.2U_{eq}(C)$ for $CH_2$ and aromatic hydrogens and $1.5U_{eq}(C)$ for $CH_3$ hydrogens with C—H distances of 0.99 ($CH_2$), 0.95 (aromatic), and 0.98 Å ($CH_3$).

## Acknowledgements

WJE would like to acknowledge the National Science Foundation for continued support.

## Funding information

Funding for this research was provided by: National Science Foundation, Directorate for Mathematical and Physical Sciences (grant No. CHE-1855328 to William J. Evans).

**Table 3**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $[CsYb(C_8H_{13}Si)_3(C_4H_8O)]$ |
| $M_r$ | 789.87 |
| Crystal system, space group | Monoclinic, $P2_1/n$ |
| Temperature (K) | 88 |
| $a, b, c$ (Å) | 9.4401 (4), 16.8718 (8), 21.0246 (10) |
| $\beta$ (°) | 92.0668 (6) |
| $V$ (Å$^3$) | 3346.4 (3) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 3.99 |
| Crystal size (mm) | 0.15 × 0.09 × 0.08 |
| | |
| Data collection | |
| Diffractometer | Bruker SMART APEXII CCD |
| Absorption correction | Multi-scan (*SADABS*; Bruker, 2014) |
| $T_{min}$, $T_{max}$ | 0.374, 0.432 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 40586, 8223, 6580 |
| $R_{int}$ | 0.055 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.667 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.032, 0.056, 1.02 |
| No. of reflections | 8223 |
| No. of parameters | 316 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 1.14, −0.62 |

Computer programs: *APEX2* (Bruker, 2014), *SAINT* (Bruker, 2013), *SHELXT2014/4* (Sheldrick, 2015*a*), *SHELXL2014/7* (Sheldrick, 2015*b*) and *SHELXTL* (Sheldrick, 2008).

## References

Ali, S. H., Deacon, G. B., Junk, P. C., Hamidi, S., Wiecko, M. & Wang, J. (2018). *Chem. Eur. J.* **24**, 230–242.
Apostolidis, C. B., Deacon, G., Dornberger, E. T., Edelmann, F., Kanellakopulos, B., MacKinnon, P. & Stalke, D. (1997). *Chem. Commun.* pp. 1047–1048.
Bel'sky, V. K., Gunko, Y. K., Bulychev, B. M., Sizov, A. I. & Soloveichik, G. L. (1990). *J. Organomet. Chem.* **390**, 35–44.
Bruker (2013). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2014). *APEX2* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Evans, W. J. (2016). *Organometallics*, **35**, 3088–3100.
Evans, W. J., Boyle, T. J. & Ziller, J. W. (1992). *Organometallics*, **11**, 3903–3907.
Evans, W. J., Champagne, T. M., Davis, B. L., Allen, N. T., Nyce, G. W., Johnston, M. A., Lin, Y.-C., Khvostov, A. & Ziller, J. W. (2006). *J. Coord. Chem.* **59**, 1069–1087.
Fieser, M. E., MacDonald, M. R., Krull, B. T., Bates, J. E., Ziller, J. W., Furche, F. & Evans, W. J. (2015). *J. Am. Chem. Soc.* **137**, 369–382.
González-del Moral, O., Martín, A., Mena, M., Morales-Varela, M. del C. & Santamaría, C. (2005). *Chem. Commun.* pp. 3682–3684.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Hitchcock, P. B., Lappert, M. F., Maron, L. & Protchenko, A. V. (2008). *Angew. Chem. Int. Ed.* **47**, 1488–1491.
Huh, D. N., Ziller, J. W. & Evans, W. J. (2018). *Inorg. Chem.* **57**, 11809–11814.
MacDonald, M. R., Bates, J. E., Ziller, J. W., Furche, F. & Evans, W. J. (2013). *J. Am. Chem. Soc.* **135**, 9857–9868.
Mills, N. (2006). *J. Am. Chem. Soc.* **128**, 13649–13650.

Morris, J. J., Noll, B. C., Honeyman, G. W., O'Hara, C. T., Kennedy, A. R., Mulvey, R. E. & Henderson, K. W. (2007). *Chem. Eur. J.* **13**, 4418–4432.
Morss, L. R. (1976). *Chem. Rev.* **76**, 827–841.
Palumbo, C. T., Darago, L. E., Windorff, C. J., Ziller, J. W. & Evans, W. J. (2018). *Organometallics*, **37**, 900–905.
Rosiak, D., Okuniewski, A. & Chojnacki, J. (2018). *Polyhedron*, **146**, 35–41.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Voskoboynikov, A. Z., Argarkov, A. Y., Shestakova, A. K., Beletskaya, I. P., Kuz'mina, L. O. & Howard, J. A. K. (1997). *J. Organomet. Chem.* **544**, 65–68.

# supporting information

*Acta Cryst.* (2020). E**76**, 1131-1135 [https://doi.org/10.1107/S2056989020008051]

## Crystal structure of the [(THF)Cs($\mu$-$\eta^5$:$\eta^5$-Cp′)$_3$Yb]$_n$ oligomer

**Daniel N. Huh, Joseph W. Ziller and William J. Evans**

### Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013); program(s) used to solve structure: *SHELXT2014/4* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014/7* (Sheldrick, 2015b); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

**Poly[(tetrahydrofuran)tris[$\mu$-$\eta^5$:$\eta^5$-1-(trimethylsilyl)cyclopentadienyl]caesium(I)ytterbium(II)]**

*Crystal data*

$[CsYb(C_8H_{13}Si)_3(C_4H_8O)]$
$M_r$ = 789.87
Monoclinic, $P2_1/n$
$a$ = 9.4401 (4) Å
$b$ = 16.8718 (8) Å
$c$ = 21.0246 (10) Å
$\beta$ = 92.0668 (6)°
$V$ = 3346.4 (3) Å$^3$
$Z$ = 4
$F(000)$ = 1560
$D_x$ = 1.568 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 9869 reflections
$\theta$ = 2.3–28.5°
$\mu$ = 3.99 mm$^{-1}$
$T$ = 88 K
Prism, green
0.15 × 0.09 × 0.08 mm

*Data collection*

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
$T_{min}$ = 0.374, $T_{max}$ = 0.432
40586 measured reflections
8223 independent reflections
6580 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.055
$\theta_{max}$ = 28.3°, $\theta_{min}$ = 1.6°
$h$ = −12→12
$k$ = −22→22
$l$ = −27→27

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.056
$S$ = 1.02
8223 reflections
316 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0229P)^2 + 0.1327P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.14 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.62 e Å$^{-3}$

*Special details*

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

**Refinement**. A green crystal of approximate dimensions 0.079 x 0.086 x 0.148 mm was mounted in a cryoloop and transferred to a Bruker SMART APEX II diffractometer. The APEX2 program package was used to determine the unit-cell parameters and for data collection (90 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT and SADABS to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL program. The diffraction symmetry was 2/m and the systematic absences were consistent with the monoclinic space group P21/n that was later determined to be correct.
The structure was solved by dual space methods and refined on F2 by full-matrix least-squares techniques. The analytical scattering factors for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. The structure is polymeric.
Least-squares analysis yielded wR2 = 0.0562 and Goof = 1.017 for 316 variables refined against 8223 data (0.75 Å), R1 = 0.0315 for those 6580 data with I > 2.0sigma(I).

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Yb1 | 0.48657 (2) | 0.44122 (2) | 0.25290 (2) | 0.01341 (4) |
| Cs1 | 0.99437 (2) | 0.27157 (2) | 0.31696 (2) | 0.01493 (5) |
| Si1 | 0.69834 (10) | 0.29048 (6) | 0.15029 (5) | 0.0184 (2) |
| Si2 | 0.23952 (11) | 0.57037 (6) | 0.11663 (5) | 0.0204 (2) |
| Si3 | 0.25791 (10) | 0.45182 (6) | 0.40988 (5) | 0.0187 (2) |
| O1 | 0.8795 (3) | 0.24593 (16) | 0.45145 (12) | 0.0285 (6) |
| C1 | 0.7108 (3) | 0.33895 (19) | 0.22942 (16) | 0.0161 (7) |
| C2 | 0.6551 (3) | 0.3115 (2) | 0.28743 (17) | 0.0174 (8) |
| H2A | 0.6070 | 0.2626 | 0.2929 | 0.021* |
| C3 | 0.6826 (3) | 0.3680 (2) | 0.33517 (17) | 0.0196 (8) |
| H3A | 0.6554 | 0.3643 | 0.3781 | 0.024* |
| C4 | 0.7575 (4) | 0.4310 (2) | 0.30831 (17) | 0.0194 (8) |
| H4A | 0.7902 | 0.4774 | 0.3298 | 0.023* |
| C5 | 0.7751 (3) | 0.4129 (2) | 0.24430 (17) | 0.0184 (8) |
| H5A | 0.8231 | 0.4453 | 0.2150 | 0.022* |
| C6 | 0.6270 (4) | 0.1878 (2) | 0.15741 (18) | 0.0257 (9) |
| H6A | 0.6848 | 0.1582 | 0.1890 | 0.039* |
| H6B | 0.6299 | 0.1611 | 0.1161 | 0.039* |
| H6C | 0.5288 | 0.1902 | 0.1709 | 0.039* |
| C7 | 0.5764 (4) | 0.3487 (2) | 0.09635 (17) | 0.0276 (9) |
| H7A | 0.6159 | 0.4017 | 0.0900 | 0.041* |
| H7B | 0.4836 | 0.3533 | 0.1155 | 0.041* |
| H7C | 0.5656 | 0.3216 | 0.0552 | 0.041* |
| C8 | 0.8767 (4) | 0.2878 (2) | 0.11484 (18) | 0.0263 (9) |
| H8A | 0.9435 | 0.2601 | 0.1438 | 0.039* |
| H8B | 0.9099 | 0.3421 | 0.1081 | 0.039* |
| H8C | 0.8702 | 0.2599 | 0.0740 | 0.039* |
| C9 | 0.3846 (3) | 0.57009 (19) | 0.17806 (16) | 0.0162 (7) |
| C10 | 0.5320 (4) | 0.56244 (19) | 0.16482 (17) | 0.0173 (7) |

| | | | | |
|---|---|---|---|---|
| H10A | 0.5679 | 0.5462 | 0.1253 | 0.021* |
| C11 | 0.6148 (4) | 0.58254 (19) | 0.21886 (17) | 0.0171 (8) |
| H11A | 0.7154 | 0.5833 | 0.2220 | 0.021* |
| C12 | 0.5224 (4) | 0.60152 (19) | 0.26788 (17) | 0.0190 (8) |
| H12A | 0.5497 | 0.6163 | 0.3102 | 0.023* |
| C13 | 0.3823 (4) | 0.59465 (19) | 0.24280 (16) | 0.0180 (8) |
| H13A | 0.2992 | 0.6048 | 0.2656 | 0.022* |
| C14 | 0.2553 (5) | 0.4858 (2) | 0.0598 (2) | 0.0380 (11) |
| H14A | 0.2394 | 0.4358 | 0.0822 | 0.057* |
| H14B | 0.3503 | 0.4856 | 0.0425 | 0.057* |
| H14C | 0.1843 | 0.4916 | 0.0249 | 0.057* |
| C15 | 0.0612 (4) | 0.5700 (3) | 0.1518 (2) | 0.0379 (11) |
| H15A | 0.0433 | 0.5178 | 0.1705 | 0.057* |
| H15B | −0.0113 | 0.5811 | 0.1185 | 0.057* |
| H15C | 0.0577 | 0.6107 | 0.1849 | 0.057* |
| C16 | 0.2543 (4) | 0.6620 (2) | 0.06760 (17) | 0.0230 (8) |
| H16A | 0.3509 | 0.6665 | 0.0524 | 0.034* |
| H16B | 0.2329 | 0.7085 | 0.0936 | 0.034* |
| H16C | 0.1869 | 0.6593 | 0.0311 | 0.034* |
| C17 | 0.2651 (3) | 0.4025 (2) | 0.33118 (16) | 0.0151 (7) |
| C18 | 0.1959 (3) | 0.42821 (19) | 0.27347 (17) | 0.0169 (7) |
| H18A | 0.1408 | 0.4751 | 0.2686 | 0.020* |
| C19 | 0.2216 (3) | 0.3741 (2) | 0.22535 (17) | 0.0187 (8) |
| H19A | 0.1879 | 0.3780 | 0.1823 | 0.022* |
| C20 | 0.3061 (4) | 0.3127 (2) | 0.25131 (17) | 0.0206 (8) |
| H20A | 0.3395 | 0.2678 | 0.2291 | 0.025* |
| C21 | 0.3320 (3) | 0.3300 (2) | 0.31617 (17) | 0.0173 (8) |
| H21A | 0.3858 | 0.2981 | 0.3453 | 0.021* |
| C22 | 0.2748 (5) | 0.3775 (2) | 0.47533 (18) | 0.0346 (10) |
| H22A | 0.1956 | 0.3400 | 0.4718 | 0.052* |
| H22B | 0.2732 | 0.4047 | 0.5165 | 0.052* |
| H22C | 0.3644 | 0.3487 | 0.4721 | 0.052* |
| C23 | 0.4026 (4) | 0.5264 (2) | 0.42253 (18) | 0.0280 (9) |
| H23A | 0.3884 | 0.5702 | 0.3923 | 0.042* |
| H23B | 0.4944 | 0.5012 | 0.4158 | 0.042* |
| H23C | 0.4008 | 0.5469 | 0.4661 | 0.042* |
| C24 | 0.0843 (4) | 0.5039 (3) | 0.4147 (2) | 0.0399 (11) |
| H24A | 0.0071 | 0.4652 | 0.4106 | 0.060* |
| H24B | 0.0748 | 0.5429 | 0.3803 | 0.060* |
| H24C | 0.0798 | 0.5309 | 0.4559 | 0.060* |
| C25 | 0.8427 (4) | 0.3003 (2) | 0.50059 (19) | 0.0306 (9) |
| H25A | 0.8093 | 0.3512 | 0.4820 | 0.037* |
| H25B | 0.9255 | 0.3108 | 0.5296 | 0.037* |
| C26 | 0.7248 (4) | 0.2603 (2) | 0.53629 (19) | 0.0338 (10) |
| H26A | 0.7634 | 0.2246 | 0.5700 | 0.041* |
| H26B | 0.6615 | 0.2998 | 0.5555 | 0.041* |
| C27 | 0.6489 (4) | 0.2145 (2) | 0.4835 (2) | 0.0315 (10) |
| H27A | 0.5959 | 0.1690 | 0.5005 | 0.038* |

| | | | | |
|---|---|---|---|---|
| H27B | 0.5827 | 0.2489 | 0.4585 | 0.038* |
| C28 | 0.7700 (4) | 0.1873 (2) | 0.44422 (18) | 0.0278 (9) |
| H28A | 0.8052 | 0.1351 | 0.4593 | 0.033* |
| H28B | 0.7388 | 0.1823 | 0.3989 | 0.033* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Yb1 | 0.01020 (7) | 0.01233 (7) | 0.01766 (8) | −0.00136 (6) | −0.00014 (6) | 0.00251 (6) |
| Cs1 | 0.01034 (10) | 0.01249 (10) | 0.02208 (12) | −0.00018 (8) | 0.00232 (8) | 0.00028 (9) |
| Si1 | 0.0150 (5) | 0.0213 (5) | 0.0190 (5) | 0.0031 (4) | 0.0009 (4) | −0.0011 (4) |
| Si2 | 0.0214 (5) | 0.0157 (5) | 0.0236 (6) | −0.0009 (4) | −0.0052 (4) | 0.0028 (4) |
| Si3 | 0.0177 (5) | 0.0192 (5) | 0.0191 (5) | −0.0009 (4) | 0.0012 (4) | −0.0017 (4) |
| O1 | 0.0207 (14) | 0.0355 (16) | 0.0295 (16) | −0.0014 (12) | 0.0062 (12) | −0.0009 (13) |
| C1 | 0.0112 (16) | 0.0161 (17) | 0.0209 (19) | 0.0018 (14) | 0.0018 (14) | 0.0027 (15) |
| C2 | 0.0130 (17) | 0.0140 (17) | 0.025 (2) | 0.0030 (14) | 0.0021 (15) | 0.0029 (15) |
| C3 | 0.0184 (18) | 0.024 (2) | 0.0162 (19) | 0.0082 (15) | 0.0003 (15) | 0.0016 (15) |
| C4 | 0.0151 (17) | 0.0177 (19) | 0.025 (2) | 0.0022 (14) | −0.0071 (15) | −0.0016 (16) |
| C5 | 0.0083 (16) | 0.0175 (18) | 0.030 (2) | −0.0002 (13) | 0.0033 (15) | 0.0049 (16) |
| C6 | 0.027 (2) | 0.023 (2) | 0.027 (2) | 0.0011 (16) | −0.0006 (17) | −0.0044 (17) |
| C7 | 0.029 (2) | 0.033 (2) | 0.021 (2) | 0.0055 (18) | −0.0059 (17) | 0.0013 (17) |
| C8 | 0.023 (2) | 0.031 (2) | 0.024 (2) | 0.0038 (17) | 0.0045 (17) | −0.0018 (17) |
| C9 | 0.0162 (17) | 0.0111 (17) | 0.0212 (19) | 0.0006 (13) | 0.0003 (14) | 0.0012 (14) |
| C10 | 0.0208 (18) | 0.0103 (16) | 0.0210 (19) | 0.0006 (14) | 0.0037 (15) | 0.0040 (15) |
| C11 | 0.0133 (17) | 0.0139 (17) | 0.024 (2) | −0.0047 (13) | −0.0014 (15) | 0.0047 (15) |
| C12 | 0.0241 (19) | 0.0118 (17) | 0.021 (2) | −0.0067 (15) | −0.0054 (15) | 0.0020 (15) |
| C13 | 0.0208 (18) | 0.0118 (17) | 0.022 (2) | −0.0011 (14) | 0.0012 (15) | 0.0009 (15) |
| C14 | 0.056 (3) | 0.020 (2) | 0.037 (3) | 0.004 (2) | −0.023 (2) | −0.0014 (19) |
| C15 | 0.022 (2) | 0.049 (3) | 0.043 (3) | 0.0003 (19) | −0.0048 (19) | 0.024 (2) |
| C16 | 0.028 (2) | 0.0204 (19) | 0.021 (2) | 0.0025 (16) | −0.0007 (16) | 0.0022 (16) |
| C17 | 0.0097 (16) | 0.0196 (18) | 0.0162 (19) | −0.0037 (14) | 0.0024 (14) | 0.0003 (15) |
| C18 | 0.0099 (16) | 0.0156 (18) | 0.025 (2) | −0.0029 (13) | 0.0026 (14) | 0.0024 (15) |
| C19 | 0.0129 (17) | 0.028 (2) | 0.0149 (19) | −0.0086 (15) | −0.0025 (14) | 0.0029 (15) |
| C20 | 0.0165 (18) | 0.0192 (19) | 0.027 (2) | −0.0062 (15) | 0.0096 (16) | −0.0061 (16) |
| C21 | 0.0124 (17) | 0.0176 (18) | 0.022 (2) | −0.0025 (14) | 0.0044 (14) | 0.0051 (15) |
| C22 | 0.056 (3) | 0.026 (2) | 0.023 (2) | −0.009 (2) | 0.006 (2) | −0.0032 (18) |
| C23 | 0.031 (2) | 0.029 (2) | 0.024 (2) | −0.0056 (18) | 0.0015 (18) | −0.0038 (17) |
| C24 | 0.028 (2) | 0.044 (3) | 0.048 (3) | 0.008 (2) | 0.002 (2) | −0.020 (2) |
| C25 | 0.034 (2) | 0.030 (2) | 0.028 (2) | −0.0032 (18) | −0.0060 (19) | 0.0018 (18) |
| C26 | 0.042 (3) | 0.032 (2) | 0.028 (2) | 0.006 (2) | 0.012 (2) | −0.0031 (19) |
| C27 | 0.024 (2) | 0.026 (2) | 0.044 (3) | 0.0008 (17) | 0.0085 (19) | 0.0089 (19) |
| C28 | 0.033 (2) | 0.025 (2) | 0.026 (2) | −0.0010 (17) | 0.0071 (18) | 0.0006 (17) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Yb1—Cnt1 | 2.510 | C7—H7B | 0.9800 |
| Yb1—Cnt2 | 2.513 | C7—H7C | 0.9800 |
| Yb1—Cnt3 | 2.504 | C8—H8A | 0.9800 |

| | | | |
|---|---|---|---|
| Cs1—Cnt1 | 3.197 | C8—H8B | 0.9800 |
| Cs1—Cnt2 | 3.268 | C8—H8C | 0.9800 |
| Cs1—Cnt3 | 3.159 | C9—C13 | 1.424 (5) |
| Yb1—C12 | 2.742 (3) | C9—C10 | 1.434 (5) |
| Yb1—C21 | 2.750 (3) | C9—Cs1$^{iii}$ | 3.587 (3) |
| Yb1—C20 | 2.757 (3) | C10—C11 | 1.398 (5) |
| Yb1—C13 | 2.775 (3) | C10—Cs1$^{iii}$ | 3.559 (3) |
| Yb1—C3 | 2.777 (3) | C10—H10A | 0.9500 |
| Yb1—C4 | 2.778 (3) | C11—C12 | 1.410 (5) |
| Yb1—C5 | 2.778 (3) | C11—Cs1$^{iii}$ | 3.427 (3) |
| Yb1—C11 | 2.779 (3) | C11—H11A | 0.9500 |
| Yb1—C17 | 2.785 (3) | C12—C13 | 1.411 (5) |
| Yb1—C2 | 2.787 (3) | C12—Cs1$^{iii}$ | 3.379 (3) |
| Yb1—C19 | 2.787 (3) | C12—H12A | 0.9500 |
| Yb1—C1 | 2.788 (3) | C13—Cs1$^{iii}$ | 3.457 (3) |
| Yb1—C18 | 2.802 (3) | C13—H13A | 0.9500 |
| Yb1—C10 | 2.802 (3) | C14—H14A | 0.9800 |
| Yb1—C9 | 2.832 (3) | C14—H14B | 0.9800 |
| Cs1—O1 | 3.095 (3) | C14—H14C | 0.9800 |
| Cs1—C2 | 3.309 (3) | C15—H15A | 0.9800 |
| Cs1—C21$^{i}$ | 3.337 (3) | C15—H15B | 0.9800 |
| Cs1—C20$^{i}$ | 3.367 (3) | C15—H15C | 0.9800 |
| Cs1—C12$^{ii}$ | 3.379 (3) | C16—Cs1$^{iii}$ | 3.810 (4) |
| Cs1—C17$^{i}$ | 3.383 (3) | C16—H16A | 0.9800 |
| Cs1—C1 | 3.390 (3) | C16—H16B | 0.9800 |
| Cs1—C3 | 3.396 (3) | C16—H16C | 0.9800 |
| Cs1—C18$^{i}$ | 3.401 (3) | C17—C21 | 1.417 (5) |
| Cs1—C19$^{i}$ | 3.407 (3) | C17—C18 | 1.425 (5) |
| Cs1—C11$^{ii}$ | 3.427 (3) | C17—Cs1$^{iv}$ | 3.383 (3) |
| Cs1—C13$^{ii}$ | 3.457 (3) | C18—C19 | 1.390 (5) |
| Cs1—C5 | 3.475 (3) | C18—Cs1$^{iv}$ | 3.401 (3) |
| Cs1—C4 | 3.499 (3) | C18—H18A | 0.9500 |
| Cs1—C10$^{ii}$ | 3.559 (3) | C19—C20 | 1.406 (5) |
| Cs1—C9$^{ii}$ | 3.587 (3) | C19—Cs1$^{iv}$ | 3.407 (3) |
| Si1—C1 | 1.854 (4) | C19—H19A | 0.9500 |
| Si1—C8 | 1.866 (4) | C20—C21 | 1.407 (5) |
| Si1—C7 | 1.866 (4) | C20—Cs1$^{iv}$ | 3.367 (3) |
| Si1—C6 | 1.867 (4) | C20—H20A | 0.9500 |
| Si2—C9 | 1.848 (4) | C21—Cs1$^{iv}$ | 3.337 (3) |
| Si2—C15 | 1.863 (4) | C21—H21A | 0.9500 |
| Si2—C16 | 1.867 (3) | C22—H22A | 0.9800 |
| Si2—C14 | 1.871 (4) | C22—H22B | 0.9800 |
| Si3—C17 | 1.856 (3) | C22—H22C | 0.9800 |
| Si3—C22 | 1.864 (4) | C23—H23A | 0.9800 |
| Si3—C24 | 1.865 (4) | C23—H23B | 0.9800 |
| Si3—C23 | 1.869 (4) | C23—H23C | 0.9800 |
| O1—C25 | 1.434 (5) | C24—H24A | 0.9800 |
| O1—C28 | 1.435 (4) | C24—H24B | 0.9800 |

| | | | |
|---|---|---|---|
| C1—C5 | 1.418 (5) | C24—H24C | 0.9800 |
| C1—C2 | 1.423 (5) | C25—C26 | 1.522 (5) |
| C2—C3 | 1.402 (5) | C25—H25A | 0.9900 |
| C2—H2A | 0.9500 | C25—H25B | 0.9900 |
| C3—C4 | 1.407 (5) | C26—C27 | 1.511 (6) |
| C3—H3A | 0.9500 | C26—H26A | 0.9900 |
| C4—C5 | 1.396 (5) | C26—H26B | 0.9900 |
| C4—H4A | 0.9500 | C27—C28 | 1.507 (5) |
| C5—H5A | 0.9500 | C27—H27A | 0.9900 |
| C6—H6A | 0.9800 | C27—H27B | 0.9900 |
| C6—H6B | 0.9800 | C28—H28A | 0.9900 |
| C6—H6C | 0.9800 | C28—H28B | 0.9900 |
| C7—H7A | 0.9800 | | |

| | | | |
|---|---|---|---|
| Cnt1—Yb1—Cnt2 | 120.1 | C15—Si2—C14 | 110.1 (2) |
| Cnt1—Yb1—Cnt3 | 116.6 | C16—Si2—C14 | 105.67 (18) |
| Cnt2—Yb1—Cnt3 | 122.8 | C17—Si3—C22 | 110.60 (16) |
| Cnt1—Cs1—O1 | 88.8 | C17—Si3—C24 | 108.68 (17) |
| Cnt2—Cs1—O1 | 94.1 | C22—Si3—C24 | 109.2 (2) |
| Cnt3—Cs1—O1 | 127.8 | C17—Si3—C23 | 112.26 (16) |
| Cnt1—Cs1—Cnt3 | 109.0 | C22—Si3—C23 | 107.77 (19) |
| Cnt1—Cs1—Cnt2 | 121.4 | C24—Si3—C23 | 108.32 (19) |
| Cnt2—Cs1—Cnt3 | 114.3 | C25—O1—C28 | 109.0 (3) |
| Yb1—Cnt1—Cs1 | 175.3 | C25—O1—Cs1 | 132.2 (2) |
| Yb1—Cnt2—Cs1 | 172.5 | C28—O1—Cs1 | 105.9 (2) |
| Yb1—Cnt3—Cs1 | 176.7 | C5—C1—C2 | 105.4 (3) |
| C12—Yb1—C21 | 133.07 (10) | C5—C1—Si1 | 126.8 (3) |
| C12—Yb1—C20 | 148.28 (10) | C2—C1—Si1 | 127.7 (3) |
| C21—Yb1—C20 | 29.62 (10) | C5—C1—Yb1 | 74.82 (18) |
| C12—Yb1—C13 | 29.63 (10) | C2—C1—Yb1 | 75.16 (18) |
| C21—Yb1—C13 | 118.73 (10) | Si1—C1—Yb1 | 114.08 (15) |
| C20—Yb1—C13 | 121.02 (10) | C5—C1—Cs1 | 81.47 (19) |
| C12—Yb1—C3 | 106.89 (10) | C2—C1—Cs1 | 74.58 (18) |
| C21—Yb1—C3 | 75.43 (10) | Si1—C1—Cs1 | 111.25 (13) |
| C20—Yb1—C3 | 93.17 (11) | Yb1—C1—Cs1 | 134.51 (12) |
| C13—Yb1—C3 | 133.57 (10) | C3—C2—C1 | 109.1 (3) |
| C12—Yb1—C4 | 84.54 (10) | C3—C2—Yb1 | 75.02 (19) |
| C21—Yb1—C4 | 104.58 (10) | C1—C2—Yb1 | 75.27 (19) |
| C20—Yb1—C4 | 121.05 (10) | C3—C2—Cs1 | 81.44 (19) |
| C13—Yb1—C4 | 114.11 (10) | C1—C2—Cs1 | 80.94 (19) |
| C3—Yb1—C4 | 29.34 (10) | Yb1—C2—Cs1 | 138.44 (12) |
| C12—Yb1—C5 | 93.42 (10) | C3—C2—H2A | 125.4 |
| C21—Yb1—C5 | 116.94 (10) | C1—C2—H2A | 125.4 |
| C20—Yb1—C5 | 118.11 (10) | Yb1—C2—H2A | 116.2 |
| C13—Yb1—C5 | 120.08 (10) | Cs1—C2—H2A | 105.3 |
| C3—Yb1—C5 | 48.02 (10) | C2—C3—C4 | 108.0 (3) |
| C4—Yb1—C5 | 29.10 (10) | C2—C3—Yb1 | 75.79 (19) |
| C12—Yb1—C11 | 29.58 (10) | C4—C3—Yb1 | 75.34 (19) |

| | | | |
|---|---|---|---|
| C21—Yb1—C11 | 162.49 (10) | C2—C3—Cs1 | 74.48 (18) |
| C20—Yb1—C11 | 161.12 (11) | C4—C3—Cs1 | 82.34 (19) |
| C13—Yb1—C11 | 48.43 (10) | Yb1—C3—Cs1 | 134.71 (12) |
| C3—Yb1—C11 | 104.80 (10) | C2—C3—H3A | 126.0 |
| C4—Yb1—C11 | 76.00 (10) | C4—C3—H3A | 126.0 |
| C5—Yb1—C11 | 72.15 (10) | Yb1—C3—H3A | 115.1 |
| C12—Yb1—C17 | 104.81 (10) | Cs1—C3—H3A | 110.0 |
| C21—Yb1—C17 | 29.67 (9) | C5—C4—C3 | 107.5 (3) |
| C20—Yb1—C17 | 49.15 (10) | C5—C4—Yb1 | 75.45 (19) |
| C13—Yb1—C17 | 89.55 (10) | C3—C4—Yb1 | 75.31 (19) |
| C3—Yb1—C17 | 91.45 (10) | C5—C4—Cs1 | 77.52 (19) |
| C4—Yb1—C17 | 115.93 (10) | C3—C4—Cs1 | 74.17 (18) |
| C5—Yb1—C17 | 139.21 (10) | Yb1—C4—Cs1 | 130.28 (12) |
| C11—Yb1—C17 | 134.15 (10) | C5—C4—H4A | 126.3 |
| C12—Yb1—C2 | 132.66 (10) | C3—C4—H4A | 126.3 |
| C21—Yb1—C2 | 69.27 (10) | Yb1—C4—H4A | 115.3 |
| C20—Yb1—C2 | 74.47 (10) | Cs1—C4—H4A | 114.4 |
| C13—Yb1—C2 | 161.85 (10) | C4—C5—C1 | 109.9 (3) |
| C3—Yb1—C2 | 29.18 (10) | C4—C5—Yb1 | 75.44 (19) |
| C4—Yb1—C2 | 48.21 (10) | C1—C5—Yb1 | 75.66 (18) |
| C5—Yb1—C2 | 47.93 (10) | C4—C5—Cs1 | 79.4 (2) |
| C11—Yb1—C2 | 119.41 (10) | C1—C5—Cs1 | 74.73 (19) |
| C17—Yb1—C2 | 95.49 (10) | Yb1—C5—Cs1 | 131.24 (12) |
| C12—Yb1—C19 | 122.04 (10) | C4—C5—H5A | 125.0 |
| C21—Yb1—C19 | 48.35 (10) | C1—C5—H5A | 125.0 |
| C20—Yb1—C19 | 29.37 (10) | Yb1—C5—H5A | 115.8 |
| C13—Yb1—C19 | 92.85 (10) | Cs1—C5—H5A | 112.9 |
| C3—Yb1—C19 | 121.44 (10) | Si1—C6—H6A | 109.5 |
| C4—Yb1—C19 | 150.23 (10) | Si1—C6—H6B | 109.5 |
| C5—Yb1—C19 | 142.33 (10) | H6A—C6—H6B | 109.5 |
| C11—Yb1—C19 | 133.69 (10) | Si1—C6—H6C | 109.5 |
| C17—Yb1—C19 | 48.72 (10) | H6A—C6—H6C | 109.5 |
| C2—Yb1—C19 | 103.58 (10) | H6B—C6—H6C | 109.5 |
| C12—Yb1—C1 | 122.63 (10) | Si1—C7—H7A | 109.5 |
| C21—Yb1—C1 | 94.75 (10) | Si1—C7—H7B | 109.5 |
| C20—Yb1—C1 | 89.08 (10) | H7A—C7—H7B | 109.5 |
| C13—Yb1—C1 | 146.41 (10) | Si1—C7—H7C | 109.5 |
| C3—Yb1—C1 | 48.85 (10) | H7A—C7—H7C | 109.5 |
| C4—Yb1—C1 | 48.90 (10) | H7B—C7—H7C | 109.5 |
| C5—Yb1—C1 | 29.52 (9) | Si1—C8—H8A | 109.5 |
| C11—Yb1—C1 | 98.33 (10) | Si1—C8—H8B | 109.5 |
| C17—Yb1—C1 | 123.39 (10) | H8A—C8—H8B | 109.5 |
| C2—Yb1—C1 | 29.57 (9) | Si1—C8—H8C | 109.5 |
| C19—Yb1—C1 | 113.15 (10) | H8A—C8—H8C | 109.5 |
| C12—Yb1—C18 | 100.20 (10) | H8B—C8—H8C | 109.5 |
| C21—Yb1—C18 | 48.09 (10) | C13—C9—C10 | 105.1 (3) |
| C20—Yb1—C18 | 48.09 (10) | C13—C9—Si2 | 129.1 (3) |
| C13—Yb1—C18 | 74.83 (10) | C10—C9—Si2 | 124.3 (3) |

| | | | |
|---|---|---|---|
| C3—Yb1—C18 | 120.22 (10) | C13—C9—Yb1 | 73.08 (19) |
| C4—Yb1—C18 | 145.35 (10) | C10—C9—Yb1 | 74.11 (18) |
| C5—Yb1—C18 | 164.74 (10) | Si2—C9—Yb1 | 128.22 (15) |
| C11—Yb1—C18 | 123.02 (10) | C13—C9—Cs1$^{iii}$ | 73.26 (18) |
| C17—Yb1—C18 | 29.55 (9) | C10—C9—Cs1$^{iii}$ | 77.33 (18) |
| C2—Yb1—C18 | 116.83 (10) | Si2—C9—Cs1$^{iii}$ | 104.19 (12) |
| C19—Yb1—C18 | 28.80 (10) | Yb1—C9—Cs1$^{iii}$ | 127.59 (11) |
| C1—Yb1—C18 | 137.11 (10) | C11—C10—C9 | 109.8 (3) |
| C12—Yb1—C10 | 48.31 (10) | C11—C10—Yb1 | 74.58 (19) |
| C21—Yb1—C10 | 156.10 (10) | C9—C10—Yb1 | 76.40 (19) |
| C20—Yb1—C10 | 132.46 (11) | C11—C10—Cs1$^{iii}$ | 73.21 (18) |
| C13—Yb1—C10 | 48.00 (10) | C9—C10—Cs1$^{iii}$ | 79.51 (18) |
| C3—Yb1—C10 | 128.46 (10) | Yb1—C10—Cs1$^{iii}$ | 129.76 (12) |
| C4—Yb1—C10 | 99.32 (10) | C11—C10—H10A | 125.1 |
| C5—Yb1—C10 | 84.76 (10) | C9—C10—H10A | 125.1 |
| C11—Yb1—C10 | 29.00 (10) | Yb1—C10—H10A | 115.8 |
| C17—Yb1—C10 | 134.24 (10) | Cs1$^{iii}$—C10—H10A | 114.2 |
| C2—Yb1—C10 | 130.23 (10) | C10—C11—C12 | 107.9 (3) |
| C19—Yb1—C10 | 108.45 (10) | C10—C11—Yb1 | 76.42 (18) |
| C1—Yb1—C10 | 101.51 (10) | C12—C11—Yb1 | 73.76 (18) |
| C18—Yb1—C10 | 109.46 (10) | C10—C11—Cs1$^{iii}$ | 83.81 (19) |
| C12—Yb1—C9 | 49.06 (10) | C12—C11—Cs1$^{iii}$ | 76.14 (19) |
| C21—Yb1—C9 | 128.10 (10) | Yb1—C11—Cs1$^{iii}$ | 136.45 (12) |
| C20—Yb1—C9 | 113.55 (10) | C10—C11—H11A | 126.1 |
| C13—Yb1—C9 | 29.39 (9) | C12—C11—H11A | 126.1 |
| C3—Yb1—C9 | 153.27 (10) | Yb1—C11—H11A | 115.9 |
| C4—Yb1—C9 | 124.75 (10) | Cs1$^{iii}$—C11—H11A | 107.2 |
| C5—Yb1—C9 | 114.22 (10) | C11—C12—C13 | 107.7 (3) |
| C11—Yb1—C9 | 48.76 (10) | C11—C12—Yb1 | 76.66 (19) |
| C17—Yb1—C9 | 105.13 (10) | C13—C12—Yb1 | 76.46 (19) |
| C2—Yb1—C9 | 158.00 (10) | C11—C12—Cs1$^{iii}$ | 79.95 (19) |
| C19—Yb1—C9 | 84.94 (10) | C13—C12—Cs1$^{iii}$ | 81.20 (19) |
| C1—Yb1—C9 | 128.44 (10) | Yb1—C12—Cs1$^{iii}$ | 140.67 (13) |
| C18—Yb1—C9 | 80.25 (10) | C11—C12—H12A | 126.1 |
| C10—Yb1—C9 | 29.49 (9) | C13—C12—H12A | 126.1 |
| O1—Cs1—C2 | 80.28 (8) | Yb1—C12—H12A | 113.2 |
| O1—Cs1—C21$^{i}$ | 114.33 (8) | Cs1$^{iii}$—C12—H12A | 106.1 |
| C2—Cs1—C21$^{i}$ | 148.98 (8) | C12—C13—C9 | 109.6 (3) |
| O1—Cs1—C20$^{i}$ | 138.03 (8) | C12—C13—Yb1 | 73.92 (19) |
| C2—Cs1—C20$^{i}$ | 137.32 (9) | C9—C13—Yb1 | 77.53 (19) |
| C21$^{i}$—Cs1—C20$^{i}$ | 24.23 (8) | C12—C13—Cs1$^{iii}$ | 75.02 (18) |
| O1—Cs1—C12$^{ii}$ | 110.63 (8) | C9—C13—Cs1$^{iii}$ | 83.51 (19) |
| C2—Cs1—C12$^{ii}$ | 92.69 (8) | Yb1—C13—Cs1$^{iii}$ | 135.26 (12) |
| C21$^{i}$—Cs1—C12$^{ii}$ | 105.96 (8) | C12—C13—H13A | 125.2 |
| C20$^{i}$—Cs1—C12$^{ii}$ | 89.07 (8) | C9—C13—H13A | 125.2 |
| O1—Cs1—C17$^{i}$ | 107.40 (7) | Yb1—C13—H13A | 115.3 |
| C2—Cs1—C17$^{i}$ | 127.34 (8) | Cs1$^{iii}$—C13—H13A | 108.8 |
| C21$^{i}$—Cs1—C17$^{i}$ | 24.34 (8) | Si2—C14—H14A | 109.5 |

| | | | |
|---|---|---|---|
| C20$^{i}$—Cs1—C17$^{i}$ | 39.93 (8) | Si2—C14—H14B | 109.5 |
| C12$^{ii}$—Cs1—C17$^{i}$ | 128.47 (8) | H14A—C14—H14B | 109.5 |
| O1—Cs1—C1 | 104.30 (7) | Si2—C14—H14C | 109.5 |
| C2—Cs1—C1 | 24.49 (8) | H14A—C14—H14C | 109.5 |
| C21$^{i}$—Cs1—C1 | 129.35 (8) | H14B—C14—H14C | 109.5 |
| C20$^{i}$—Cs1—C1 | 113.14 (8) | Si2—C15—H15A | 109.5 |
| C12$^{ii}$—Cs1—C1 | 88.68 (8) | Si2—C15—H15B | 109.5 |
| C17$^{i}$—Cs1—C1 | 114.09 (8) | H15A—C15—H15B | 109.5 |
| O1—Cs1—C3 | 68.30 (8) | Si2—C15—H15C | 109.5 |
| C2—Cs1—C3 | 24.09 (8) | H15A—C15—H15C | 109.5 |
| C21$^{i}$—Cs1—C3 | 133.69 (8) | H15B—C15—H15C | 109.5 |
| C20$^{i}$—Cs1—C3 | 136.14 (9) | Si2—C16—Cs1$^{iii}$ | 96.16 (13) |
| C12$^{ii}$—Cs1—C3 | 116.22 (8) | Si2—C16—H16A | 109.5 |
| C17$^{i}$—Cs1—C3 | 109.40 (8) | Cs1$^{iii}$—C16—H16A | 66.8 |
| C1—Cs1—C3 | 39.65 (8) | Si2—C16—H16B | 109.5 |
| O1—Cs1—C18$^{i}$ | 124.90 (8) | Cs1$^{iii}$—C16—H16B | 52.7 |
| C2—Cs1—C18$^{i}$ | 109.78 (8) | H16A—C16—H16B | 109.5 |
| C21$^{i}$—Cs1—C18$^{i}$ | 39.23 (8) | Si2—C16—H16C | 109.5 |
| C20$^{i}$—Cs1—C18$^{i}$ | 39.10 (8) | Cs1$^{iii}$—C16—H16C | 153.3 |
| C12$^{ii}$—Cs1—C18$^{i}$ | 122.27 (8) | H16A—C16—H16C | 109.5 |
| C17$^{i}$—Cs1—C18$^{i}$ | 24.24 (8) | H16B—C16—H16C | 109.5 |
| C1—Cs1—C18$^{i}$ | 91.83 (8) | C21—C17—C18 | 105.5 (3) |
| C3—Cs1—C18$^{i}$ | 98.84 (8) | C21—C17—Si3 | 128.0 (3) |
| O1—Cs1—C19$^{i}$ | 146.73 (8) | C18—C17—Si3 | 126.4 (3) |
| C2—Cs1—C19$^{i}$ | 114.55 (8) | C21—C17—Yb1 | 73.79 (18) |
| C21$^{i}$—Cs1—C19$^{i}$ | 39.29 (8) | C18—C17—Yb1 | 75.89 (18) |
| C20$^{i}$—Cs1—C19$^{i}$ | 23.95 (8) | Si3—C17—Yb1 | 118.31 (14) |
| C12$^{ii}$—Cs1—C19$^{i}$ | 98.71 (9) | C21—C17—Cs1$^{iv}$ | 75.99 (18) |
| C17$^{i}$—Cs1—C19$^{i}$ | 39.57 (8) | C18—C17—Cs1$^{iv}$ | 78.58 (18) |
| C1—Cs1—C19$^{i}$ | 91.36 (8) | Si3—C17—Cs1$^{iv}$ | 108.65 (13) |
| C3—Cs1—C19$^{i}$ | 112.73 (8) | Yb1—C17—Cs1$^{iv}$ | 132.98 (11) |
| C18$^{i}$—Cs1—C19$^{i}$ | 23.56 (8) | C19—C18—C17 | 109.5 (3) |
| O1—Cs1—C11$^{ii}$ | 87.61 (8) | C19—C18—Yb1 | 75.02 (19) |
| C2—Cs1—C11$^{ii}$ | 82.35 (8) | C17—C18—Yb1 | 74.57 (18) |
| C21$^{i}$—Cs1—C11$^{ii}$ | 123.61 (8) | C19—C18—Cs1$^{iv}$ | 78.45 (19) |
| C20$^{i}$—Cs1—C11$^{ii}$ | 111.22 (8) | C17—C18—Cs1$^{iv}$ | 77.18 (18) |
| C12$^{ii}$—Cs1—C11$^{ii}$ | 23.90 (8) | Yb1—C18—Cs1$^{iv}$ | 131.52 (11) |
| C17$^{i}$—Cs1—C11$^{ii}$ | 147.92 (8) | C19—C18—H18A | 125.3 |
| C1—Cs1—C11$^{ii}$ | 88.14 (8) | C17—C18—H18A | 125.3 |
| C3—Cs1—C11$^{ii}$ | 102.45 (8) | Yb1—C18—H18A | 117.0 |
| C18$^{i}$—Cs1—C11$^{ii}$ | 146.18 (8) | Cs1$^{iv}$—C18—H18A | 111.4 |
| C19$^{i}$—Cs1—C11$^{ii}$ | 122.61 (8) | C18—C19—C20 | 108.2 (3) |
| O1—Cs1—C13$^{ii}$ | 110.19 (8) | C18—C19—Yb1 | 76.18 (19) |
| C2—Cs1—C13$^{ii}$ | 116.34 (8) | C20—C19—Yb1 | 74.12 (19) |
| C21$^{i}$—Cs1—C13$^{ii}$ | 85.36 (8) | C18—C19—Cs1$^{iv}$ | 77.99 (19) |
| C20$^{i}$—Cs1—C13$^{ii}$ | 73.64 (8) | C20—C19—Cs1$^{iv}$ | 76.46 (19) |
| C12$^{ii}$—Cs1—C13$^{ii}$ | 23.79 (8) | Yb1—C19—Cs1$^{iv}$ | 131.87 (12) |
| C17$^{i}$—Cs1—C13$^{ii}$ | 109.44 (8) | C18—C19—H19A | 125.9 |

| | | | |
|---|---|---|---|
| C1—Cs1—C13$^{ii}$ | 111.22 (8) | C20—C19—H19A | 125.9 |
| C3—Cs1—C13$^{ii}$ | 139.38 (8) | Yb1—C19—H19A | 115.9 |
| C18$^{i}$—Cs1—C13$^{ii}$ | 111.98 (8) | Cs1$^{iv}$—C19—H19A | 112.2 |
| C19$^{i}$—Cs1—C13$^{ii}$ | 90.34 (8) | C19—C20—C21 | 107.4 (3) |
| C11$^{ii}$—Cs1—C13$^{ii}$ | 38.65 (8) | C19—C20—Yb1 | 76.50 (19) |
| O1—Cs1—C5 | 105.94 (7) | C21—C20—Yb1 | 74.91 (19) |
| C2—Cs1—C5 | 38.83 (8) | C19—C20—Cs1$^{iv}$ | 79.59 (19) |
| C21$^{i}$—Cs1—C5 | 110.42 (8) | C21—C20—Cs1$^{iv}$ | 76.66 (18) |
| C20$^{i}$—Cs1—C5 | 101.17 (8) | Yb1—C20—Cs1$^{iv}$ | 134.91 (12) |
| C12$^{ii}$—Cs1—C5 | 109.56 (8) | C19—C20—H20A | 126.3 |
| C17$^{i}$—Cs1—C5 | 91.53 (8) | C21—C20—H20A | 126.3 |
| C1—Cs1—C5 | 23.80 (8) | Yb1—C20—H20A | 114.7 |
| C3—Cs1—C5 | 38.38 (8) | Cs1$^{iv}$—C20—H20A | 110.3 |
| C18$^{i}$—Cs1—C5 | 71.25 (8) | C20—C21—C17 | 109.3 (3) |
| C19$^{i}$—Cs1—C5 | 77.29 (8) | C20—C21—Yb1 | 75.48 (19) |
| C11$^{ii}$—Cs1—C5 | 111.87 (8) | C17—C21—Yb1 | 76.54 (18) |
| C13$^{ii}$—Cs1—C5 | 129.48 (8) | C20—C21—Cs1$^{iv}$ | 79.11 (19) |
| O1—Cs1—C4 | 84.87 (8) | C17—C21—Cs1$^{iv}$ | 79.67 (18) |
| C2—Cs1—C4 | 38.88 (8) | Yb1—C21—Cs1$^{iv}$ | 136.70 (12) |
| C21$^{i}$—Cs1—C4 | 112.41 (8) | C20—C21—H21A | 125.3 |
| C20$^{i}$—Cs1—C4 | 112.73 (8) | C17—C21—H21A | 125.3 |
| C12$^{ii}$—Cs1—C4 | 127.43 (8) | Yb1—C21—H21A | 114.7 |
| C17$^{i}$—Cs1—C4 | 88.95 (8) | Cs1$^{iv}$—C21—H21A | 108.6 |
| C1—Cs1—C4 | 39.03 (8) | Si3—C22—H22A | 109.5 |
| C3—Cs1—C4 | 23.49 (8) | Si3—C22—H22B | 109.5 |
| C18$^{i}$—Cs1—C4 | 75.59 (8) | H22A—C22—H22B | 109.5 |
| C19$^{i}$—Cs1—C4 | 89.67 (8) | Si3—C22—H22C | 109.5 |
| C11$^{ii}$—Cs1—C4 | 121.18 (8) | H22A—C22—H22C | 109.5 |
| C13$^{ii}$—Cs1—C4 | 150.24 (8) | H22B—C22—H22C | 109.5 |
| C5—Cs1—C4 | 23.09 (8) | Si3—C23—H23A | 109.5 |
| O1—Cs1—C10$^{ii}$ | 74.63 (7) | Si3—C23—H23B | 109.5 |
| C2—Cs1—C10$^{ii}$ | 98.69 (8) | H23A—C23—H23B | 109.5 |
| C21$^{i}$—Cs1—C10$^{ii}$ | 111.34 (8) | Si3—C23—H23C | 109.5 |
| C20$^{i}$—Cs1—C10$^{ii}$ | 108.30 (8) | H23A—C23—H23C | 109.5 |
| C12$^{ii}$—Cs1—C10$^{ii}$ | 38.08 (8) | H23B—C23—H23C | 109.5 |
| C17$^{i}$—Cs1—C10$^{ii}$ | 133.90 (8) | Si3—C24—H24A | 109.5 |
| C1—Cs1—C10$^{ii}$ | 109.52 (8) | Si3—C24—H24B | 109.5 |
| C3—Cs1—C10$^{ii}$ | 113.49 (8) | H24A—C24—H24B | 109.5 |
| C18$^{i}$—Cs1—C10$^{ii}$ | 147.28 (8) | Si3—C24—H24C | 109.5 |
| C19$^{i}$—Cs1—C10$^{ii}$ | 127.76 (8) | H24A—C24—H24C | 109.5 |
| C11$^{ii}$—Cs1—C10$^{ii}$ | 22.98 (8) | H24B—C24—H24C | 109.5 |
| C13$^{ii}$—Cs1—C10$^{ii}$ | 37.70 (8) | O1—C25—C26 | 105.8 (3) |
| C5—Cs1—C10$^{ii}$ | 133.23 (8) | O1—C25—H25A | 110.6 |
| C4—Cs1—C10$^{ii}$ | 136.14 (8) | C26—C25—H25A | 110.6 |
| O1—Cs1—C9$^{ii}$ | 87.86 (7) | O1—C25—H25B | 110.6 |
| C2—Cs1—C9$^{ii}$ | 120.23 (8) | C26—C25—H25B | 110.6 |
| C21$^{i}$—Cs1—C9$^{ii}$ | 88.67 (8) | H25A—C25—H25B | 108.7 |
| C20$^{i}$—Cs1—C9$^{ii}$ | 85.71 (8) | C27—C26—C25 | 101.6 (3) |

| | | | |
|---|---|---|---|
| C12$^{ii}$—Cs1—C9$^{ii}$ | 38.69 (8) | C27—C26—H26A | 111.5 |
| C17$^{i}$—Cs1—C9$^{ii}$ | 112.18 (8) | C25—C26—H26A | 111.5 |
| C1—Cs1—C9$^{ii}$ | 125.32 (8) | C27—C26—H26B | 111.5 |
| C3—Cs1—C9$^{ii}$ | 136.64 (8) | C25—C26—H26B | 111.5 |
| C18$^{i}$—Cs1—C9$^{ii}$ | 124.31 (8) | H26A—C26—H26B | 109.3 |
| C19$^{i}$—Cs1—C9$^{ii}$ | 106.95 (8) | C28—C27—C26 | 102.1 (3) |
| C11$^{ii}$—Cs1—C9$^{ii}$ | 38.49 (8) | C28—C27—H27A | 111.3 |
| C13$^{ii}$—Cs1—C9$^{ii}$ | 23.23 (8) | C26—C27—H27A | 111.3 |
| C5—Cs1—C9$^{ii}$ | 147.92 (8) | C28—C27—H27B | 111.3 |
| C4—Cs1—C9$^{ii}$ | 158.85 (8) | C26—C27—H27B | 111.3 |
| C10$^{ii}$—Cs1—C9$^{ii}$ | 23.16 (7) | H27A—C27—H27B | 109.2 |
| C1—Si1—C8 | 109.90 (16) | O1—C28—C27 | 106.8 (3) |
| C1—Si1—C7 | 109.33 (16) | O1—C28—Cs1 | 52.50 (16) |
| C8—Si1—C7 | 108.40 (17) | C27—C28—Cs1 | 137.3 (2) |
| C1—Si1—C6 | 110.42 (16) | O1—C28—H28A | 110.4 |
| C8—Si1—C6 | 110.06 (17) | C27—C28—H28A | 110.4 |
| C7—Si1—C6 | 108.70 (18) | Cs1—C28—H28A | 112.0 |
| C9—Si2—C15 | 112.34 (18) | O1—C28—H28B | 110.4 |
| C9—Si2—C16 | 108.64 (16) | C27—C28—H28B | 110.4 |
| C15—Si2—C16 | 107.99 (17) | Cs1—C28—H28B | 60.1 |
| C9—Si2—C14 | 111.75 (17) | H28A—C28—H28B | 108.6 |

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+3/2, y-1/2, -z+1/2$; (iii) $-x+3/2, y+1/2, -z+1/2$; (iv) $x-1, y, z$.