Application of the Redox-Transmetalation Procedure to Access Divalent Lanthanide and Alkaline-Earth NHC Complexes**

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I. Synthesis and characterisation

I.1. General considerations

All air- and moisture-sensitive manipulations were performed under dry N₂ or Ar atmosphere using standard Schlenk techniques or in an argon-filled MBraun glovebox, unless otherwise stated. Prior to use, CH₂Cl₂ was dried by refluxing over P₂O₅ and distilled under a nitrogen atmosphere. Other solvents (THF, Et₂O and n-pentane) were dried using an MBraun solvent purification system (SPS-800) and degassed. THF was additionally distilled under nitrogen from potassium benzophenone ketyl before storage over LiAlH₄ in vacuo. THF-d₈ and C₆D₆ were stored over Na/K alloy, CDCl₃ was dried over 4 Å molecular sieves and all were degassed by freeze-pump-thaw cycles. The imidazolium salt IMe·HI was synthesised by alkylation of N-methylimidazole with MeI,[1] while IMes·HCl was prepared using the procedure of Ritter and co-workers for IPr·HCl.[2] The iodide salt IMes·HI was obtained by halogen exchange with KI in acetone using a slightly modified literature procedure.[3] The synthesis of the NHC silver complexes is described below. All other chemicals were obtained from commercial sources and used without further purification.

Elemental analyses were carried out with an Elementar vario MICRO cube. Infrared (IR) spectra were recorded in the region 4000–400 cm⁻¹ on a Bruker Tensor 37 FTIR spectrometer equipped with a room temperature DLαTGS detector, a diamond attenuated total reflection (ATR) unit and nitrogen-flushed chamber. In terms of their intensity, the signals were classified into different categories (vs = very strong, s = strong, m = medium, w = weak, and sh = shoulder).

NMR spectra were recorded on Bruker spectrometers (Avance III 300 MHz, Avance 400 MHz or Avance III 400 MHz). Chemical shifts are referenced internally using signals of the residual protio solvent (¹H) or the solvent (¹³C{¹H}) and are reported relative to tetramethylsilane. All NMR spectra were measured at 298 K, unless otherwise specified. The multiplicity of the signals is indicated as s = singlet, m = multiplet and br = broad. Assignments were determined on the basis of unambiguous chemical shifts, coupling patterns and ¹³C-DEPT experiments or 2D correlations (¹H−¹H COSY, ¹H−¹³C HSQC, ¹H−¹³C HMBC).

I.2. Synthesis of the silver complexes

The air-stable but slightly light-sensitive silver complexes 1 and 2 were prepared by reaction of the corresponding imidazolium iodides with Ag₂O in dichloromethane, according to slightly modified literature procedures.[4]
I.2.1. Synthesis of 1

To a solution of IMe·HI (2.00 g, 8.93 mmol) in CH₂Cl₂ (40 mL) was added Ag₂O (1.14 g, 4.91 mmol) and the reaction mixture was stirred overnight at room temperature under protection against light. The resulting grey suspension was evaporated to dryness under reduced pressure, extracted with hot DMF and filtered while hot over Celite. After letting the filtrate cool down to room temperature, the addition of Et₂O (200 mL) led to the precipitation of a microcrystalline white solid which was further washed with Et₂O and dried under vacuum. Yield: 2.41 g (7.28 mmol), 82%. The silver complex 1 was found insoluble in common organic solvents (THF, CH₂Cl₂, CHCl₃), which supports the formation of an ion pair. Elemental analysis data were more consistent with the general formula [Ag(IMe)₂]₂(AgI₂) formulation obtained after recrystallisation from hot DMSO.[4a]

¹H NMR (400.30 MHz, DMSO-d₆): δ [ppm]: 7.42 (s, 2H, CH₃imid.), 3.82 (s, 6H, CH₃). The ¹H NMR data are consistent with those reported in the literature.[4a] Anal. Calcd for [Ag(IMe)₂]₂(AgI₂) i.e. C₁₀H₁₆Ag₂I₂N₄ (661.81): C, 18.15; H, 2.44; N, 8.47. Found: C, 17.54%; H, 2.31%; N, 8.20.

In the following, the dimeric formula corresponding to [Ag(IMe)₂]₂(AgI₂) is considered for 1.

I.2.2. Synthesis of 2

In air, to a solution of IMes·HI (1.50 g, 3.47 mmol) in CH₂Cl₂ (40 mL) was added Ag₂O (442 mg, 1.91 mmol) and the reaction mixture was stirred overnight at room temperature under protection against light. The resulting solution was filtered over Celite and the solvent was removed under reduced pressure. The resulting off-white solid was washed with Et₂O and dried under vacuum.

Yield: 1.65 g (3.06 mmol), 88%.

The ¹H NMR spectrum of 2 in CDCl₃ revealed the presence of two compounds with similar chemical shifts, in a ratio of ca. 1:0.57, assigned to the neutral monocarbene complex [Ag(IMes)] (A) and the biscarbene ion pair [Ag(IMes)₂]⁺[AgI₂]⁻ (B), respectively.

¹H NMR (400.30 MHz, CDCl₃): δ [ppm]: 7.13 (s, 2H, CH₃imid.⁴), 7.12 (s, 1H, CH₃imid.⁸), 6.99 (s, 4H, CH₃arom.⁴⁺), 6.91 (s, 2H, CH₃arom.⁸), 2.43 (s, 3H, p-CH₃⁴), 2.34 (s, 6H, p-CH₃⁸), 2.08 (s, 12H, o-CH₃⁴⁺), 1.72 (s, 6.8H, o-CH₃⁸). The ¹H NMR data of compound B are consistent with those reported for the biscarbene complex [Ag(IMes)₂]⁺[AgI₂].[4b]

In the following, the monomeric formula corresponding to “Ag(IMes)” is considered for 2.
I.3. Synthesis of 3-8 by redox-transmetallation and characterisation

Synthesis of [EuI$_2$(IMe)$_4$] (3)

In a glovebox, a Schlenk flask was charged with 1 (200 mg, 0.302 mmol, 1.00 eq.) and freshly filed europium metal (50.5 mg, 0.332 mmol, 1.10 eq.). Outside of the glovebox, THF (10 mL) was added and the resulting suspension was stirred at room temperature for 36 hours. Decantation and careful filtration of the suspension led to an orange-red solution. Slow evaporation of the solvent in a double ampoule afforded [EuI$_2$(IMe)$_4$] (3) as highly air-sensitive dark red-purple crystals suitable for X-ray diffraction studies. The crystals were carefully washed with a small amount of THF until the washing solution remained colourless and dried under vacuum. Yield of the crystals: 55 mg (0.070 mmol), 46% (based on the IMe ligand). Anal. Calcd for C$_{20}$H$_{32}$EuI$_2$N$_8$ (790.30): C, 30.40; H, 4.08; N, 14.18. Found: C, 30.95; H, 4.36; N, 13.95. Due to the paramagnetism of 3 and its very low solubility in common organic solvents including THF-$d_8$, no NMR spectrum could be obtained.

IR (ATR): $\tilde{\nu}$ (cm$^{-1}$) = 3265 (w), 3146 (w), 3068 (vs), 2943 (s), 2849 (m), 2792 (m), 1664 (m), 1575 (vs), 1534 (w), 1447 (s), 1395 (m), 1355 (m), 1311 (m), 1247 (m), 1208 (m), 1171 (vs), 1127 (m), 1090 (m), 1068 (w), 997 (m), 937 (w), 923 (w), 809 (m), 736 (w), 713 (s), 614 (vs), 568 (w), 441 (m).

Synthesis of [SmI$_2$(IMe)$_4$] (4)

In a glovebox, a Schlenk flask was charged with 1 (210 mg, 0.317 mmol, 1.00 eq.) and freshly filed samarium metal (52.5 mg, 0.349 mmol, 1.10 eq.). Outside of the glovebox, THF (10 mL) was added and the suspension was stirred at room temperature for 36 hours. Decantation and careful filtration of the suspension led to a dark green solution. Slow evaporation of the solvent in a double ampoule afforded [SmI$_2$(IMe)$_4$] (4) as highly air-sensitive dark red-purple crystals suitable for X-ray diffraction studies. The crystals were carefully washed with a small amount of THF until the washing solution remained colourless and dried under vacuum. Yield of the crystals: 52 mg (0.066 mmol), 42% (based on the IMe ligand). Anal. Calcd for C$_{20}$H$_{32}$I$_2$N$_8$Sm (788.70): C, 30.46; H, 4.09; N, 14.21. Found: C, 32.27; H, 4.23; N, 14.78. No better elemental analysis data could be obtained despite repeated attempts. Due to the paramagnetism of 4 and its very low solubility in common organic solvents including THF-$d_8$, no NMR spectra could be obtained.

IR (ATR): $\tilde{\nu}$ (cm$^{-1}$) = 3239 (w), 3146 (w), 3105 (m), 3077 (vs), 2989 (w), 2946 (s), 2851 (w), 2797 (w), 1651 (vs), 1617 (w), 1574 (vs), 1536 (w), 1515 (s), 1444 (s), 1395 (w), 1354 (m), 1327 (s), 1287 (w), 1250 (s), 1221 (m), 1171 (vs), 1138 (m), 1105 (w), 1087 (w), 1004 (m), 912 (w), 882 (w), 825 (w), 797 (m), 768 (w), 746 (w), 713 (w), 653 (w), 614 (s), 586 (w), 505 (w).
Synthesis of [Ybl₂(IMe)₃(THF)₂] (5)

In a glovebox, a Schlenk flask was charged with 1 (210 mg, 0.317 mmol, 1.00 eq.) and freshly filed ytterbium metal (60.4 mg, 0.349 mmol, 1.10 eq.). Outside of the glovebox, THF (10 mL) was added and the suspension was stirred at room temperature for 4 days. Decantation and careful filtration of the suspension led to a dark red solution. Slow evaporation of the solvent in a double ampoule afforded [Ybl₂(IMe)₃(THF)₂] (5) as highly air-sensitive red crystals suitable for X-ray diffraction studies. The crystals were carefully washed with a small amount of THF and dried under vacuum. Yield of the crystals: 110 mg (0.144 mmol), 45% (based on the IMe ligand).

Anal. Calcd for C₁₉H₂₁₂N₄Yb·(1.7 C₄H₈O) (741.71): C, 27.21; H, 4.02; N, 7.55. Found: C, 27.15; H, 4.14; N, 7.36. These values correspond to the partial decoordination of 0.3 molecule of THF from 5.

¹H NMR (400 MHz, THF-d₆, 25 °C) δ (ppm): 6.96 (br s, Δν1/2≈ 45 Hz, 4H, CH₃imidazol), 3.90 (s, 12H, CH₃), 3.66 – 3.59 (m, ca. 8H, OCH₂THF), 1.82 – 1.74 (m, ca. 8H, CH₂THF).

¹³C{¹H} NMR (101 MHz, THF-d₆, 25 °C) δ (ppm): C₉N₇ not detected, 121.8 (CH₃imidazol), 68.0 (OCH₂THF), 38.6 (NCH₃), 26.2 (CH₂THF).

IR (ATR): ʋ (cm⁻¹) = 3145 (w), 3067 (vs), 2975 (w), 2942 (w), 2920 (w), 2851 (w), 2790 (w), 1732 (w), 1652 (w), 1616 (w), 1573 (s), 1454 (m), 1430 (w), 1372 (w), 1337 (w), 1310 (w), 1284 (w), 1237 (w), 1170 (s), 1086 (w), 1022 (m), 983 (w), 917 (w), 874 (w), 808 (m), 746 (m), 711 (w), 613 (m).

Synthesis of [Ca₁₂(IMe)₁₂(THF)₆] (6)

In a glovebox, a Schlenk flask was charged with 1 (200 mg, 0.302 mmol, 1.00 eq.) and freshly filed calcium metal (24.2 mg, 0.604 mmol, 2.00 eq.). Outside of the glovebox, THF (10 mL) was added and the suspension was stirred at room temperature for 4 days. Decantation and careful filtration of the suspension led to a clear colourless solution. Slow evaporation of the solvent in a double ampoule afforded [Ca₁₂(IMe)₁₂(THF)₆] (6) as air-sensitive colourless crystals suitable for X-ray diffraction studies. The crystals were carefully washed with a small amount of THF and dried under vacuum. Yield of the crystals: 135 mg (0.214 mmol), 71% (based on the IMe ligand).

Anal. Calcd for C₁₉H₂₁₂Ca₁₂N₁₂O₁₂ (630.37): C, 34.30; H, 5.12; N, 8.89. Found: C, 33.09; H, 4.69; N, 8.75. No better elemental analysis data could be obtained despite repeated attempts. The purity of 6 can be assessed from its NMR spectra (see Fig. S3-S4).

¹H NMR (400 MHz, THF-d₆, 25 °C) δ (ppm): 6.93 (s, 4H, CH₃imidazol), 3.83 (s, 12H, CH₃), 3.65 – 3.59 (m, 8H, OCH₂THF), 1.80 – 1.74 (m, 8H, CH₂THF).

¹³C{¹H} NMR (101 MHz, THF-d₆, 25 °C) δ (ppm): C₉N₇ not detected, 121.5 (CH₃imidazol), 68.0 (OCH₂THF), 38.7 (NCH₃), 26.2 (CH₂THF).
\(\text{IR (ATR): } \tilde{\nu} (\text{cm}^{-1}) = 3647 \text{ (w)}, 3572 \text{ (w)}, 3145 \text{ (m)}, 3067 \text{ (vs)}, 2979 \text{ (w)}, 2943 \text{ (w)}, 2888 \text{ (w)}, 2853 \text{ (w)}, 1730 \text{ (w)}, 1618 \text{ (w)}, 1574 \text{ (vs)}, 1450 \text{ (m)}, 1431 \text{ (w)}, 1401 \text{ (w)}, 1337 \text{ (w)}, 1284 \text{ (w)}, 1226 \text{ (w)}, 1170 \text{ (vs)}, 1085 \text{ (w)}, 1031 \text{ (s)}, 918 \text{ (w)}, 874 \text{ (m)}, 809 \text{ (s)}, 746 \text{ (s)}, 711 \text{ (w)}, 671 \text{ (w)}, 613 \text{ (s)}.\)

**Synthesis of \([\text{SrI}_2(\text{IMe})_2(\text{THF})_2]\) (7)**

In a glovebox, a Schlenk flask was charged with 1 (310 mg, 0.468 mmol, 1.00 eq.) and freshly filed strontium metal (45.1 mg, 0.515 mmol, 1.10 eq.). Outside of the glovebox, THF (10 mL) was added and the suspension was stirred at room temperature for 4 days. Decantation and careful filtration of the suspension led to a clear colourless solution. Slow evaporation of the solvent in a double ampoule afforded \([\text{SrI}_2(\text{IMe})_2(\text{THF})_2]\) (7) as air-sensitive colourless crystals suitable for X-ray diffraction studies. The crystals were carefully washed with a small amount of THF and dried under vacuum. Yield of the crystals: 151 mg (0.223 mmol), 48% (based on the IMe ligand).

Anal. Calcd for \(\text{C}_{18}\text{H}_{32}\text{I}_2\text{N}_4\text{O}_2\text{Sr} (677.91): \) C, 31.89; H, 4.76; N, 8.26. Found: C, 29.48; H, 4.24; N, 7.72.

No better elemental analysis data could be obtained despite repeated attempts. The purity of 7 can be assessed from its NMR spectra (see Fig. S5-S6).

\(^1\text{H NMR}\) (400 MHz, THF-\(d_8\), 25 °C) \(\delta\) (ppm): 6.91 (s, 4H, C\text{imidazole}), 3.78 (s, 12H, CH\(_3\)), 3.64 – 3.59 (m, ca. 2H, OCH\(_2\) residual coordinated THF), 1.80 – 1.75 (m, ca. 2H, CH\(_2\) residual coordinated THF).

\(^{13}\text{C}(^1\text{H})\text{ NMR}\) (101 MHz, THF-\(d_8\), 25 °C) \(\delta\) (ppm): \(\text{C}_{\text{NCN}}\) not detected, 121.1 (CH\(_{\text{imidazole}}\)), 68.0 (OCH\(_2\) THF), 38.4 (NCH\(_3\)), 26.2 (CH\(_2\) THF).

**IR (ATR): \(\tilde{\nu} (\text{cm}^{-1}) = 3145 \text{ (w)}, 3068 \text{ (vs)}, 2978 \text{ (w)}, 2942 \text{ (m)}, 2892 \text{ (w)}, 2853 \text{ (w)}, 1650 \text{ (w)}, 1618 \text{ (w)}, 1572 \text{ (vs)}, 1454 \text{ (m)}, 1397 \text{ (s)}, 1339 \text{ (w)}, 1306 \text{ (w)}, 1284 \text{ (w)}, 1220 \text{ (s)}, 1170 \text{ (vs)}, 1098 \text{ (w)}, 1085 \text{ (w)}, 1031 \text{ (m)}, 915 \text{ (w)}, 873 \text{ (m)}, 809 \text{ (m)}, 727 \text{ (s)}, 615 \text{ (s)}, 445 \text{ (m)}.\)**

**Synthesis of \([\text{SrI}_2(\text{IMes})(\text{THF})_3]\) (8)**

In a glovebox, a Schlenk flask was charged with 2 (342 mg, 0.633 mmol, 1.00 eq.) and freshly filed strontium metal (55.5 mg, 0.633 mmol, 1.00 eq.). Outside of the glovebox, THF (10 mL) was added and the suspension was stirred at room temperature for 2 days. Decantation and careful filtration of the suspension led to a clear colourless solution. Slow evaporation of the solvent in a double ampoule afforded \([\text{SrI}_2(\text{IMes})(\text{THF})_3]\) (8-THF) as air-sensitive colourless crystals suitable for X-ray diffraction studies. The crystals were carefully washed with a small amount of THF and dried under vacuum. Yield of the crystals: 136 mg (0.146 mmol), 23% (based on the IMes ligand).

Anal. Calcd for \(\text{C}_{33}\text{H}_{66}\text{I}_2\text{N}_4\text{O}_2\text{Sr} (934.29): \) C, 47.57; H, 6.04; N, 3.00. Found: C, 48.05; H, 5.41; N, 3.46.
NMR in C$_6$D$_6$ solution:

$^1$H NMR (400 MHz, C$_6$D$_6$, 25 °C) δ (ppm): 6.80 (s, 4H, CH$_{Ar}$), 6.50 (br s, $\Delta v_{1/2} = 25$ Hz, 2H, CH$_\text{imidazo}$), 3.68 – 3.52 (m, ca. 10H, THF), 2.18 (s, 12H, O-CH$_3$), 2.16 (s, 6H, p-C 1.48 – 1.34 (m, ca. 10H, THF).

$^{13}$C($^1$H) NMR (101 MHz, C$_6$D$_6$, 25 °C) δ (ppm): C$_\text{NCN}$ not detected, 139.0 (C$_{Ar}$), 137.4 (C$_{Ar}$), 135.5 (C$_{Ar}$), 129.2 (CH$_{Ar}$), 120.8 (CH$_\text{imidazo}$), 68.1 (OCH$_2$ THF), 25.8 (CH$_2$ THF), 21.1 (p-CH$_3$), 18.2 (o-CH$_3$).

NMR in THF-$d_8$ solution:

$^1$H NMR (400 MHz, THF-$d_8$, 25 °C) δ (ppm): 7.10 (s, 2H, CH$_\text{imidazo}$), 6.96 (s, 4H, CH$_{Ar}$), 3.65 – 3.60 (m, ca. 7H, OCH$_2$ THF), 2.31 (s, 6H, p-CH$_3$), 2.10 (s, 12H, o-CH$_3$), 1.80 – 1.74 (m, ca. 7H, CH$_2$ THF).

$^{13}$C($^1$H) NMR (101 MHz, THF-$d_8$, 25 °C) δ (ppm): C$_\text{NCN}$ not detected, 139.0 (C$_{Ar}$), 137.8 (C$_{Ar}$), 135.8 (C$_{Ar}$), 129.2 (CH$_{Ar}$), 121.5 (CH$_\text{imidazo}$), 68.0 (OCH$_2$ THF), 26.2 (CH$_2$ THF), 20.9 (p-CH$_3$), 18.1 (o-CH$_3$).

IR (ATR): $\tilde{\nu}$ (cm$^{-1}$) = 3145 (m), 3119 (w), 3065 (w), 2969 (w), 2933 (vs), 2877 (w), 2770 (w), 1636 (w), 1607 (m), 1537 (vs), 1483 (s), 1456 (w), 1380 (s), 1320 (w), 1294 (w), 1256 (w), 1228 (vs), 1163 (w), 1035 (vs), 965 (w), 929 (w), 903 (w), 859 (s), 767 (s), 736 (m), 680 (m), 570 (m).
II. NMR spectra

II.1. Complex 5

Figure S1. $^1$H NMR spectrum of 5 in THF-$d_8$ (residual protio solvent at $\delta$3.58 and 1.72 (*)).

Figure S2. $^{13}$C($^1$H) NMR spectrum of 5 in THF-$d_8$ (solvent signals at $\delta$67.21 and 25.31). Traces of C$_6$D$_6$ can be seen at $\delta$128.3 (*).
II.2. Complex 6

Figure S3. $^1$H NMR spectrum of 6 in THF-$d_8$ (residual protio solvent at $\delta$ 3.58 and 1.73 (*)).

Figure S4. $^{13}$C($^1$H) NMR spectrum of 6 in THF-$d_8$ (solvent signals at $\delta$ 67.21 and 25.31).
II.3. Complex 7

Figure S5. $^1$H NMR spectrum of 7 in THF-$d_8$ (residual protio solvent at $\delta$3.58 and 1.73 (*)).

Figure S6. $^{13}$C($^1$H) NMR spectrum of 7 in THF-$d_8$ (solvent signals at $\delta$67.21 and 25.31).
II.4. Complex 8

Figure S7. $^1$H NMR spectrum of 8 in C$_6$D$_6$ (residual protio solvent at $\delta$7.16 (*)).

Figure S8. $^{13}$C($^1$H) NMR spectrum of 8 in C$_6$D$_6$ (solvent signal at $\delta$128.06).
Figure S9. $^1$H NMR spectrum of 8 in THF-$d_8$ (residual protio solvent at $\delta$ 3.58 and 1.72 (*)).

Figure S10. $^{13}$C($^1$H) NMR spectrum of 8 in THF-$d_8$ (solvent signal at $\delta$ 67.21 and 25.31).
III. IR spectra

III.1. Complex 3

Figure S11. IR spectrum of complex 3.

III.2. Complex 4

Figure S12. IR spectrum of complex 4.
III.3. Complex 5

Figure S13. IR spectrum of complex 5.

III.4. Complex 6

Figure S14. IR spectrum of complex 6.
III.5. Complex 7

Figure S15. IR spectrum of complex 7.

III.6. Complex 8

Figure S16. IR spectrum of complex 8.
IV. X-ray crystallography

IV.1. General methods

Suitable crystals for the X-ray analysis of all compounds were obtained as described above. A suitable crystal was covered in mineral oil (Aldrich) and mounted on a glass fibre. The crystal was transferred directly to the cold stream of a STOE IPDS II (150 K) or a STOE StadiVari (100 or 150 K) diffractometer. All structures were solved by using the program SHELXS/\cite{5} and Olex2.\cite{6} The remaining non-hydrogen atoms were located from successive difference Fourier map calculations. The refinements were carried out by using full-matrix least-squares techniques on $F^2$ by using the program SHELXL.\cite{5} The H-atoms were introduced into the geometrically calculated positions (SHELXL procedures) unless otherwise stated and refined riding on the corresponding parent atoms. In each case, the locations of the largest peaks in the final difference Fourier map calculations, as well as the magnitude of the residual electron densities, were of no chemical significance. Specific comments for each data set are given below. Summary of the crystal data, data collection and refinement for compounds are given in Table S1.

Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication no. CCDC 2086921-2086926. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: +(44)1223-336-033; email: deposit@ccdc.cam.ac.uk).

The following special comments apply to the models of the structures:

- In the structure of 3, the asymmetric unit contains three independent molecules of the complex. It was a refined as a two-component inversion twin (TWIN -1.0, 0.0, 0.0, 0.0, -1.0, 0.0, 0.0, 0.0, -1.0) with a BASF value of 0.109(12).

- In the structure of 4, the asymmetric unit contains three independent molecules of the complex. It was a refined as a two-component inversion twin (TWIN -1.0, 0.0, 0.0, 0.0, -1.0, 0.0, 0.0, 0.0, -1.0) with a BASF value of 0.33(4). A DFIX restrain was added on one N-CH$_3$ bond distance (C60-N24) to avoid the occurrence of an A alert in the checkCIF report. Rigid body (RIGU) restraints with standard uncertainties were added to six different NHC rings. One B alert (PLAT342 - Low Bond Precision on C-C Bonds) appears in the checkCIF report and is due to weak diffraction of the crystal at high angles.
- In the structure of 5, rigid body (RIGU) restraints with standard uncertainties have been added on both NHC rings. One B alert (PLAT342 - Low Bond Precision on C-C Bonds) appears in the checkCIF report and is due to weak diffraction of the crystal at high angles.

- In the structure of 7, one coordinated THF ligand (O2, C15, C16, C17, C18) is disordered over two positions with an occupancy ratio freely refined to 0.58/0.42. Similarity restraints on the respective bond distances (SADI) and displacement parameters (SIMU 0.01 0.02) were used. Additionally, one similarity restraint on displacement parameters (SIMU 0.01 0.02) has been added to the second coordinated THF ligand (O1, C11, C12, C13, C14). One B alert (PLAT342 - Low Bond Precision on C-C Bonds) appears in the checkCIF report and is due to weak diffraction of the crystal at high angles.

- In the structure of 8, the non-coordinating THF molecule (O4, C34, C35, C36, C37) is disordered over two positions with an occupancy ratio freely refined to 0.62/0.38. Similarity restraints on the respective bond distances (SADI) and displacement parameters (SIMU, RIGU) were used. Additionally, one rigid body (RIGU 0.002 0.002) restrain has been added to one coordinated THF ligand (O3, C30, C31, C32, C33).
## IV.1. Summary of crystal data

**Table S1.** Crystal data, data collection and refinement for complexes 3-8.

| Compounds | 3 | 4 | 5 | 6 | 7 | 8·THF |
|-----------|---|---|---|---|---|------|
| Chemical formula | C_{20}H_{2}EuI_{2}N_{8} | C_{20}H_{32}I_{2}Sm | C_{18}H_{32}I_{2}O_{2}Yb | C_{18}H_{32}CaI_{2}N_{8}O_{2} | C_{18}H_{32}I_{2}O_{2}Sr | C_{18}H_{32}I_{2}O_{2}Sr |
| CCDC Number | 2086921 | 2086922 | 2086923 | 2086924 | 2086925 | 2086926 |
| Formula Mass | 790.29 | 788.68 | 763.31 | 630.35 | 677.89 | 934.25 |
| Crystal system | Orthorhombic | Orthorhombic | Monoclinic | Monoclinic | Monoclinic | Orthorhombic |
| a/Å | 23.828(5) | 23.7920(7) | 9.5164(15) | 9.547(2) | 9.735(3) | 18.6377(6) |
| b/Å | 45.506(9) | 45.429(2) | 16.087(2) | 16.185(4) | 16.330(3) | 19.3653(5) |
| c/Å | 15.611(3) | 15.5221(5) | 16.455(2) | 16.553(5) | 16.577(5) | 22.6375(10) |
| α° | 94.340(12) | 94.67(2) | 93.77(2) | | | |
| β° | 94.340(12) | 94.67(2) | 93.77(2) | | | |
| γ° | 94.340(12) | 94.67(2) | 93.77(2) | | | |
| Unit cell volume/Å³ | 16927(6) | 16777.1(11) | 2511.8(6) | 2549.4(11) | 2629.5(11) | 8170.4(5) |
| Temperature/K | 100 | 100 | 100 | 150 | 150 | 150 |
| Space group | Iba2 | Iba2 | P2₁/n | P2₁/n | P2₁/n | Pbca |
| No. of formula units per unit cell, Z | 24 | 24 | 4 | 4 | 4 | 8 |
| Absorption coefficient, μ/mm⁻¹ | 4.433 | 4.330 | 6.200 | 2.686 | 4.416 | 2.868 |
| No. of reflections measured | 127473 | 126545 | 11477 | 14285 | 10716 | 31788 |
| No. of independent reflections | 21654 | 18507 | 5456 | 6117 | 4955 | 11284 |
| R_{int} | 0.0386 | 0.0791 | 0.0713 | 0.0606 | 0.0903 | 0.0520 |
| Final R₁ values (I > 2σ(I)) | 0.0353 | 0.0738 | 0.0682 | 0.0670 | 0.0726 | 0.0429 |
| Final wR(F²) values (I > 2σ(I)) | 0.0833 | 0.1766 | 0.1341 | 0.1477 | 0.1339 | 0.0913 |
| Final R₁ values (all data) | 0.0433 | 0.1131 | 0.1384 | 0.1174 | 0.1885 | 0.0776 |
| Final wR(F²) values (all data) | 0.0883 | 0.2159 | 0.1673 | 0.1816 | 0.1722 | 0.1089 |
| Goodness of fit on F² | 1.028 | 1.053 | 1.012 | 1.105 | 1.014 | 1.028 |
| Flack parameter | 0.109(12) | 0.33(4) | - | - | - | - |

S18
IV.2. Crystal structures

IV.2.1. The molecular structure of 3 in the solid state

**Figure S17.** Molecular structure of 3 in the solid state with thermal ellipsoids at the 40% probability level. H atoms have been omitted for clarity. Selected bond distances (Å) and angles [°]: Eu1-I1 3.3228(8), Eu1-I2 3.3072(8), Eu1-C1 2.811(8), Eu1-C6 2.799(9), Eu1-C11 2.815(8), Eu1-C16 2.811(8); I1-Eu1-I2 174.91(2), C1-Eu1-I1 89.6(2), C1-Eu1-I2 92.5(2), C1-Eu1-C6 85.4(3), C1-Eu1-C11 170.6(3), C1-Eu1-C16 85.7(2), C6-Eu1-I1 88.2(2), C6-Eu1-I2 87.3(2). The asymmetric unit of 3 contains three independent molecules with very similar metrical data, only one molecule is displayed here.

IV.2.2. The molecular structure of 4 in the solid state

**Figure S18.** Molecular structure of 4 in the solid state with thermal ellipsoids at the 40% probability level. H atoms have been omitted for clarity. Selected bond distances (Å) and angles [°]: Sm1-I1 3.236(2), Sm1-I2 3.254(2), Sm1-C1 2.74(3), Sm1-C6 2.85(2), Sm1-C11 2.79(3), Sm1-C16 2.83(3); I1-Sm1-I2 177.69(7), C1-Sm1-I1 98.6(7), C1-Sm1-I2 81.5(7), C1-Sm1-C6 94.6(8), C1-Sm1-C11 168.2(9), C1-Sm1-C16 86.8(9), C6-Sm1-I1 97.3(5), C6-Sm1-I2 84.9(5). The asymmetric unit of 4 contains three independent molecules with very similar metrical data, only one molecule is displayed here.
IV.2.3. The molecular structure of 5 in the solid state

![Molecular structure of 5](image)

**Figure S19.** Molecular structure of 5 in the solid state with thermal ellipsoids at the 40% probability level. H atoms have been omitted for clarity. Selected bond distances (Å) and angles [°]: Yb-I1 3.1358(13), Yb-I2 3.1380(13), Yb-O1 2.442(10), Yb-O2 2.430(10), Yb-C1 2.626(14), Yb-C6 2.603(14); I1-Yb-I2 176.67(4), O1-Yb-I1 86.6(3), O1-Yb-I2 90.0(3), O1-Yb-C1 88.8(4), O1-Yb-C6 163.1(4), O2-Yb-I1 89.0(3), O2-Yb-I2 90.4(3), O2-Yb-O1 78.3(4), O2-Yb-C1 167.1(4), O2-Yb-C6 84.8(4), C1-Yb-I1 90.6(3), C1-Yb-I2 89.2(3), C6-Yb-I1 93.5(3), C6-Yb-I2 89.7(3), C1-Yb-C6 108.1(4).

IV.2.4. The molecular structure of 6 in the solid state

![Molecular structure of 6](image)

**Figure S20.** Molecular structure of 6 in the solid state with thermal ellipsoids at the 40% probability level. H atoms have been omitted for clarity. Selected bond distances (Å) and angles [°]: I1-Ca 3.157(2), I2-Ca 3.161(2), Ca-O1 2.382(6), Ca-O2 2.403(6), Ca-C1 2.597(8), Ca-C6 2.632(8); I1-Ca-I2 176.98(6), O1-Ca-I1 90.0(2), O1-Ca-I2 90.0(2), O1-Ca-O2 80.0(2), O1-Ca-C1 169.4(2), O1-Ca-C6 85.2(3), O2-Ca-I1 89.5(2), O2-Ca-I2 87.5(2), O2-Ca-C1 89.4(2), O2-Ca-C6 165.2(3), C1-Ca-I1 90.3(2), C1-Ca-I2 89.1(2), C1-Ca-C6 105.4(3), C6-Ca-I1 89.7(2), C6-Ca-I2 93.3(2).
**IV.2.5. The molecular structure of 7 in the solid state**

*Figure S21.* Molecular structure of 7 in the solid state with thermal ellipsoids at the 40% probability level. Only one disordered position for one of the coordinated THF ligands is depicted and H atoms have been omitted for clarity. Selected bond distances (Å) and angles [°]: I1-Sr 3.270(2), I2-Sr 3.262(2), Sr-O1 2.528(10), Sr-C1 2.762(13), Sr-C6 2.745(12), Sr-O2A 2.49(4); I1-Sr-I2 177.60(5), O1-Sr-I1 90.7(3), O1-Sr-I2 90.1(3), O1-Sr-C1 167.7(3), O1-Sr-C6 85.4(4), C1-Sr-I1 88.9(3), C1-Sr-I2 89.9(3), C6-Sr-I1 92.4(3), C6-Sr-I2 90.0(3), C6-Sr-C1 106.9(4), O2A-Sr-I1 87(2), O2A-Sr-I2 91(2), O2A-Sr-O1 79(3), O2A-Sr-C1 89(3), O2A-Sr-C6 164(3).

**IV.2.6. The molecular structure of 8 in the solid state**

*Figure S22.* Molecular structure of 8-THF in the solid state with thermal ellipsoids at the 40% probability level. H atoms and non-coordinating solvent molecules have been omitted for clarity. Selected bond distances (Å) and angles [°]: Sr-I1 3.2284(5), Sr-I2 3.2458(4), Sr-O1 2.549(3), Sr-O2 2.541(3), Sr-O3 2.564(3), Sr-C1 2.779(4); I1-Sr-I2 177.258(15), O1-Sr-I2 91.97(7), O1-Sr-I1 85.90(7), O1-Sr-O3 76.05(11), O1-Sr-C1 103.79(10), O3-Sr-I2 88.09(7), O3-Sr-I1 89.73(7), O3-Sr-C1 177.12(11), O2-Sr-I2 94.46(7), O2-Sr-I1 86.76(7), O2-Sr-C1 101.01(11), C1-Sr-I2 89.04(8), C1-Sr-I1 93.14(8).
V. DFT calculations

V.1. Reaction energies

To investigate the bonding properties in the [MI₂(IMe)₄] and [MI₂(IMe)₂THF₂] molecules, quantum chemical RI-DFT calculations were performed using the BP-86 functional (see Table S2). The basis sets were of def2-SV(P) quality for all atoms as given in the program package TURBOMOLE. For iodine, samarium and strontium effective core potentials (ecp) of 46, 52 and 28 core electrons were used. Under the given symmetry constraints (D₄ or C₂ for the tetra- and the bis-NHC adducts, resp.) small values of imaginary frequencies remain. As they are in no way related to the metal atom – ligand vibrations under discussion, we ignored them.

Table S2. Results of the quantum chemical DFT calculations: energies, bond distances and vibrational frequencies of interest, Ahlrichs-Heinzmann population analyses (6 modified atomic orbitals were chosen for Sm and Sr, resp.).

| Cmpd. | 4 (Sm) | 4* (Sr) | 7 (Sr) | 7* (Sm) |
|-------|--------|---------|--------|---------|
| General formula | [MI₂(IMe)₄] | [MI₂(IMe)₂THF₂] |        |         |
| Eₜₒᵣ/a.u.* | −1270.539575 | −1272.402178 | −1127.768752 | −1125.906671 |
| r(M–C)/Å | 2.840 | 2.784 | 2.741 | 2.786 |
| r(M–I)/Å | 3.331 | 3.290 | 3.238 | 3.281 |
| r(M–O)/Å | - | - | 2.582 | 2.654 |
| v (Sm–C)/cm⁻¹ | 320/317/317 | 322/319/319 | 320/320 | 318/320 |
| Q(M) | 0.81 | 0.63 | 0.90 | 0.98 |
| Q(I) | −0.89 | −0.88 | −0.73 | −0.73 |
| Q(IMe) | 0.24 | 0.28 | −0.10 | −0.10 |
| Q(C) | −0.32 | −0.31 | −0.49 | −0.51 |
| Q(THF) | - | - | 0.37 | 0.34 |
| Q(O) | - | - | −0.24 | −0.24 |
| SEN(M–C) | 0.35 | 0.36 | 0.05 | 0.05 |
| SEN(M–O) | - | - | 0.12 | 0.11 |
| SEN(Sm–I)** | 0.00 | 0.02 | 0.36 | 0.35 |

* Eₜₒᵣ: THF: −232.2792442, IMe: −304.5852812, SrI₂: −53.83509089, SmI₂: −51.97452612 a.u.
** SEN: SmI₂: 0.60, SrI₂: 0.61; Q: Sm: 0.93, Sr:0.88.
V.2. Cartesian coordinates

Complex 4' [SmI₂(IME₂)₂(THF)₂]

| Cartesian Coordinates (a.u.) |
|-----------------------------|
|                            |
| -2.18713383976614          | -4.91615871490102   | 8.91731280630249     | h   |
| -1.33849793727846          | -3.51784201134637   | 7.60346232517625     | c   |
| 1.43189012840919           | -4.20854842573277   | 6.90387323121852      | c   |
| -1.45009900583378           | -1.64279875584704   | 8.53622937778231      | h   |
| -2.73748811771067           | -3.52287425129562   | 5.02763202681708      | c   |
| 1.20796377676969           | -5.14714225583571   | 4.17128856038685      | c   |
| 2.27573578238536           | -5.64004657109418   | 8.18336962952157      | h   |
| 2.66269658360677           | -2.50722084862028   | 6.9359458983370      | h   |
| -0.7769543720896           | -3.60138335400230   | 3.1288655893306      | o   |
| -3.95620054845673           | -5.23042645719265   | 4.81265798691340      | h   |
| -3.90735758036934           | -1.82996613089064   | 4.63200116410015      | h   |
| 0.62833649860056           | -7.17792270700616   | 4.08208031827120      | h   |
| 2.92462846081125           | -4.84632089101017   | 3.00354096241096      | h   |
| -0.00000000000000          | 0.00000000000000   | -0.2728854794486      | sm  |
| -0.53707329901954           | -3.67688187800399   | -4.00359568472528      | c   |
| 1.03783245807107           | -1.3920150420624   | -6.00456918554126      | n   |
| -2.06284185440047           | -5.76840040433359   | -3.94286904506172      | n   |
| 0.53533062634135           | -6.45200144679788   | -7.14232490314543      | c   |
| 3.08739593605271           | -2.4412449287187   | -6.73434574146673      | c   |
| -1.44579080627099           | -7.4932420113751   | -5.8261027361980      | h   |
| -4.01282125132836           | -6.1542359110286   | -2.02767939897004      | h   |
| 1.593402031191988          | -7.15260701579870  | -8.77981236469985      | h   |
| 4.88454817009081           | -3.01624528394260  | -5.81352954625213      | h   |
| 3.30212956834594           | -2.44453797672732  | -8.82189229897447      | h   |
| 2.61805926966703           | -0.50685126981948  | -6.07273780816814      | h   |
| -2.4621906060065           | -9.27898157515340  | -6.09112106747085     | c   |
| -5.59231351868228          | -7.26811136338887  | -2.84100346092499      | h   |
| -3.21995458030292          | -7.16143193332936  | -0.36442853432533      | c   |
| -4.73782150581967          | -4.2836707734671   | -1.40615065131457      | c   |
| 2.18713383976614           | 4.91615871490102   | 8.91731280630249      | h   |
| 1.33849793727846           | 3.51784201134637   | 7.60346232517625      | c   |
| -1.43189012840919          | 4.20854842573277   | 6.90387323121852      | c   |
| 1.45009900583378           | 1.64279875584704   | 8.53622937778231      | h   |
| 2.73748811771067           | 3.52287425129562   | 5.02763202681708      | c   |
| -1.20796377676969          | 5.14714225583571   | 4.17128856038685      | c   |
| -2.27573578238536          | 5.64004657109418   | 8.18336962952157      | h   |
| -2.66269658360677          | 2.50722084862028   | 6.9359458983370      | c   |
| 0.77869543720896           | 3.60138335400230   | 3.1288655893306      | o   |
| 3.95620054845673           | 5.23042647519265   | 4.81265798691340      | c   |
| 3.90973578036934           | 1.82996613089064   | 4.63200116410015      | h   |
| -0.62833649860056          | 7.17792270700616   | 4.08208031827120      | h   |
| -2.92462846081125          | 4.84632089101017   | 3.00354096241096      | h   |
| 0.5370329901954           | 3.67688187800399   | -4.00359568472528      | c   |
| -1.03783245807107          | 4.13920150420624   | -6.00456918554126      | c   |
| 2.06284185440047           | 5.76840040433359   | -3.94286904506172      | h   |
| -0.53533062643135         | 6.45200144677988   | -7.14232490314543      | c   |
| #  | symmetry | wave number | IR intensity | selection rules |
|----|----------|-------------|--------------|-----------------|
| 1  | b        | -18.21      | 0.00000      | YES  YES        |
| 2  | b        | -2.44       | 0.00000      | YES  YES        |
| 3  | -        | 0.00        | 0.00000      | -    -          |
| 4  | -        | 0.00        | 0.00000      | -    -          |
| 5  | -        | 0.00        | 0.00000      | -    -          |
| 6  | -        | 0.00        | 0.00000      | -    -          |
| 7  | -        | 0.00        | 0.00000      | -    -          |
| 8  | -        | 0.00        | 0.00000      | -    -          |
| 9  | a        | 19.74       | 2.79043      | YES  YES        |
| 10 | b        | 23.33       | 2.89340      | YES  YES        |
| 11 | a        | 25.43       | 0.02659      | YES  YES        |
| 12 | b        | 28.70       | 1.35120      | YES  YES        |
| 13 | a        | 32.56       | 0.00293      | YES  YES        |
| 14 | a        | 40.12       | 0.15608      | YES  YES        |
| 15 | b        | 46.02       | 2.61411      | YES  YES        |
| 16 | a        | 48.10       | 2.38852      | YES  YES        |
| 17 | a        | 57.86       | 0.83938      | YES  YES        |
| 18 | b        | 61.27       | 1.30621      | YES  YES        |
| 19 | a        | 63.33       | 5.97882      | YES  YES        |
| 20 | b        | 64.26       | 6.03905      | YES  YES        |
| 21 | a        | 74.59       | 0.36959      | YES  YES        |
| 22 | b        | 77.94       | 0.66730      | YES  YES        |
| 23 | a        | 79.36       | 0.01383      | YES  YES        |
| 24 | a        | 92.32       | 0.27261      | YES  YES        |
| 25 | b        | 92.99       | 5.85614      | YES  YES        |
| 26 | a        | 100.54      | 0.89980      | YES  YES        |
| 27 | a        | 108.61      | 0.03550      | YES  YES        |
| 28 | b        | 109.94      | 5.78003      | YES  YES        |
| 29 | b        | 112.26      | 0.26901      | YES  YES        |
| 30 | a        | 119.33      | 0.86169      | YES  YES        |
| 31 | b        | 119.42      | 0.44309      | YES  YES        |
| 32 | b        | 130.12      | 11.68374     | YES  YES        |
| 33 | a        | 130.89      | 0.71826      | YES  YES        |
|   |   |   |   |   |
|---|---|---|---|---|
| 34 | a | 137.18 | 0.77970 | YES | YES |
| 35 | b | 140.38 | 8.25372 | YES | YES |
| 36 | a | 146.51 | 0.53989 | YES | YES |
| 37 | b | 146.82 | 1.84351 | YES | YES |
| 38 | b | 153.57 | 10.51475 | YES | YES |
| 39 | a | 159.53 | 12.59832 | YES | YES |
| 40 | a | 201.50 | 12.50426 | YES | YES |
| 41 | b | 205.23 | 23.28662 | YES | YES |
| 42 | a | 274.19 | 0.13100 | YES | YES |
| 43 | b | 275.32 | 0.19216 | YES | YES |
| 44 | a | 317.81 | 4.05065 | YES | YES |
| 45 | b | 318.62 | 7.88654 | YES | YES |
| 46 | b | 320.42 | 24.73885 | YES | YES |
| 47 | a | 321.99 | 4.26064 | YES | YES |
| 48 | a | 451.44 | 2.84321 | YES | YES |
| 49 | b | 451.62 | 6.55551 | YES | YES |
| 50 | b | 606.18 | 2.42772 | YES | YES |
| 51 | a | 606.61 | 8.43751 | YES | YES |
| 52 | a | 609.91 | 3.21292 | YES | YES |
| 53 | b | 610.62 | 1.57756 | YES | YES |
| 54 | a | 612.78 | 0.22671 | YES | YES |
| 55 | b | 612.89 | 0.60999 | YES | YES |
| 56 | b | 637.59 | 0.16535 | YES | YES |
| 57 | a | 638.49 | 0.00585 | YES | YES |
| 58 | b | 664.26 | 13.09402 | YES | YES |
| 59 | a | 689.37 | 51.12863 | YES | YES |
| 60 | b | 689.55 | 29.88388 | YES | YES |
| 61 | a | 736.71 | 6.58253 | YES | YES |
| 62 | a | 737.27 | 14.20018 | YES | YES |
| 63 | b | 777.63 | 0.12190 | YES | YES |
| 64 | b | 777.68 | 0.04964 | YES | YES |
| 65 | a | 786.44 | 0.20891 | YES | YES |
| 66 | b | 790.56 | 15.21701 | YES | YES |
| 67 | a | 857.09 | 2.03505 | YES | YES |
| 68 | a | 857.81 | 12.22338 | YES | YES |
| 69 | b | 898.08 | 4.03762 | YES | YES |
| 70 | b | 898.89 | 0.88049 | YES | YES |
| 71 | a | 903.63 | 42.25867 | YES | YES |
| 72 | b | 908.70 | 140.18668 | YES | YES |
| 73 | a | 927.64 | 6.85747 | YES | YES |
| 74 | b | 929.05 | 0.61023 | YES | YES |
| 75 | a | 951.68 | 3.48008 | YES | YES |
| 76 | b | 953.04 | 1.73533 | YES | YES |
| 77 | a | 996.69 | 0.16622 | YES | YES |
| 78 | b | 996.97 | 1.76145 | YES | YES |
| 79 | a | 1009.97 | 0.15303 | YES | YES |
| 80 | b | 1010.08 | 0.09181 | YES | YES |
| 81 | a | 1031.62 | 18.13955 | YES | YES |
| 82 | b | 1032.42 | 10.08054 | YES | YES |
| 83 | a | 1039.22 | 0.04152 | YES | YES |
| 84 | a | 1039.22 | 0.04152 | YES | YES |
|   |   |                   |                   |   |   |
|---|---|-------------------|-------------------|---|---|
| 85 | b | 1041.51           | 109.59416         | YES | YES |
| 86 | b | 1056.29           | 6.29870           | YES | YES |
| 87 | a | 1056.35           | 6.30051           | YES | YES |
| 88 | b | 1072.38           | 2.88974           | YES | YES |
| 89 | a | 1073.21           | 0.01171           | YES | YES |
| 90 | b | 1087.83           | 9.59143           | YES | YES |
| 91 | a | 1088.02           | 6.90894           | YES | YES |
| 92 | b | 1114.58           | 8.13148           | YES | YES |
| 93 | a | 1114.69           | 3.47535           | YES | YES |
| 94 | b | 1114.82           | 3.50120           | YES | YES |
| 95 | a | 1114.99           | 0.30107           | YES | YES |
| 96 | b | 1120.09           | 4.77668           | YES | YES |
| 97 | a | 1120.23           | 0.56270           | YES | YES |
| 98 | b | 1181.75           | 5.31588           | YES | YES |
| 99 | a | 1182.56           | 1.23142           | YES | YES |
|100 | b | 1198.56           | 25.99160          | YES | YES |
|101 | a | 1198.66           | 12.40946          | YES | YES |
|102 | b | 1202.25           | 3.17979           | YES | YES |
|103 | a | 1202.53           | 5.80571           | YES | YES |
|104 | a | 1214.06           | 1.95113           | YES | YES |
|105 | b | 1214.97           | 2.83496           | YES | YES |
|106 | b | 1253.47           | 2.70919           | YES | YES |
|107 | a | 1254.14           | 0.45185           | YES | YES |
|108 | b | 1271.85           | 3.38522           | YES | YES |
|109 | a | 1275.06           | 1.46110           | YES | YES |
|110 | b | 1288.27           | 2.57925           | YES | YES |
|111 | a | 1288.64           | 0.17685           | YES | YES |
|112 | a | 1323.09           | 0.11698           | YES | YES |
|113 | b | 1323.10           | 3.50076           | YES | YES |
|114 | b | 1329.54           | 2.11209           | YES | YES |
|115 | a | 1331.43           | 2.51937           | YES | YES |
|116 | a | 1344.01           | 4.92826           | YES | YES |
|117 | b | 1344.26           | 6.85320           | YES | YES |
|118 | a | 1356.98           | 0.99944           | YES | YES |
|119 | b | 1357.06           | 1.09749           | YES | YES |
|120 | b | 1357.90           | 0.14579           | YES | YES |
|121 | a | 1359.37           | 11.69482          | YES | YES |
|122 | b | 1392.91           | 27.30830          | YES | YES |
|123 | a | 1393.70           | 8.69105           | YES | YES |
|124 | b | 1416.76           | 3.55828           | YES | YES |
|125 | a | 1417.09           | 4.35988           | YES | YES |
|126 | a | 1421.30           | 0.54789           | YES | YES |
|127 | b | 1424.15           | 6.22433           | YES | YES |
|128 | b | 1431.06           | 10.91232          | YES | YES |
|129 | a | 1435.21           | 0.23417           | YES | YES |
|130 | b | 1435.42           | 9.80883           | YES | YES |
|131 | a | 1435.71           | 1.19189           | YES | YES |
|132 | b | 1438.44           | 0.69681           | YES | YES |
|133 | b | 1440.09           | 6.43222           | YES | YES |
|134 | a | 1443.76           | 31.83585          | YES | YES |
|135 | b | 1447.14           | 4.32918           | YES | YES |
|   |    |  |  |  |  |  |  |  |  |
|---|---|---|---|---|---|---|---|---|---|
| 136 | a | 1447.82 | 46.20022 | YES | YES |
| 137 | a | 1448.01 | 0.63062 | YES | YES |
| 138 | b | 1449.41 | 35.19710 | YES | YES |
| 139 | a | 1449.66 | 2.31857 | YES | YES |
| 140 | b | 1450.20 | 5.21907 | YES | YES |
| 141 | a | 1450.50 | 3.41199 | YES | YES |
| 142 | b | 1450.66 | 0.63062 | YES | YES |
| 143 | a | 1451.20 | 35.19710 | YES | YES |
| 144 | b | 1451.41 | 2.31857 | YES | YES |
| 145 | a | 1451.66 | 5.21907 | YES | YES |
| 146 | b | 1452.20 | 35.19710 | YES | YES |
| 147 | a | 1452.41 | 2.31857 | YES | YES |
| 148 | b | 1452.66 | 5.21907 | YES | YES |
| 149 | a | 1453.26 | 32.54501 | YES | YES |
| 150 | a | 1454.01 | 0.63062 | YES | YES |
| 151 | b | 1454.20 | 35.19710 | YES | YES |
| 152 | b | 1454.41 | 2.31857 | YES | YES |
| 153 | a | 1454.66 | 5.21907 | YES | YES |
| 154 | a | 1455.20 | 32.54501 | YES | YES |
| 155 | b | 1455.41 | 2.31857 | YES | YES |
| 156 | a | 1456.01 | 5.21907 | YES | YES |
| 157 | b | 1456.20 | 32.54501 | YES | YES |
| 158 | a | 1456.41 | 2.31857 | YES | YES |
| 159 | b | 1456.66 | 5.21907 | YES | YES |
| 160 | b | 1457.20 | 32.54501 | YES | YES |
| 161 | a | 1457.41 | 2.31857 | YES | YES |
| 162 | a | 1458.01 | 5.21907 | YES | YES |
| 163 | b | 1458.20 | 32.54501 | YES | YES |
| 164 | a | 1459.20 | 2.31857 | YES | YES |
| 165 | b | 1459.41 | 5.21907 | YES | YES |
| 166 | b | 1459.66 | 32.54501 | YES | YES |
| 167 | a | 1460.20 | 2.31857 | YES | YES |
| 168 | b | 1460.41 | 5.21907 | YES | YES |
| 169 | a | 1460.66 | 32.54501 | YES | YES |
| 170 | a | 1461.20 | 2.31857 | YES | YES |
| 171 | b | 1461.41 | 5.21907 | YES | YES |
| 172 | a | 1461.66 | 32.54501 | YES | YES |
| 173 | b | 1462.20 | 2.31857 | YES | YES |
| 174 | b | 1462.41 | 5.21907 | YES | YES |
| 175 | a | 1462.66 | 32.54501 | YES | YES |
| 176 | b | 1463.20 | 2.31857 | YES | YES |
| 177 | a | 1463.41 | 5.21907 | YES | YES |
| 178 | a | 1463.66 | 32.54501 | YES | YES |
| 179 | b | 1464.20 | 2.31857 | YES | YES |
| 180 | a | 1464.41 | 5.21907 | YES | YES |
| 181 | b | 1464.66 | 32.54501 | YES | YES |

**Complex 4 [SmI₂(IMe)₄]**

*Cartesian coordinates (a.u.)*

3.79432198153452 -3.79432198153452 0.00000000000000 c
6.05829736860230 -7.37785698566997 -0.90152430814280 c
7.37785698566997 -6.05829736860230 0.90152430814280 c
3.90391765192269 -5.96147882292272 -1.41702205975946 n

S27
Vibrational Spectrum

| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|-----------------|
|   | cm⁻¹ | km/mol   | IR          | RAMAN        |                 |
| 1 | e    | -15.35   | 0.00000     | YES          | YES             |
| 2 | e    | -15.35   | 0.00000     | YES          | YES             |
| 3 | b1   | -12.04   | 0.00000     | NO           | YES             |
| 4 |      | -0.00    | 0.00000     |              |                 |
| 5 |      | 0.00     | 0.00000     |              |                 |
| 6 |      | 0.00     | 0.00000     |              |                 |
| 7 |      | 0.00     | 0.00000     |              |                 |
| 8 |      | 0.00     | 0.00000     |              |                 |
| 9 |      | 0.00     | 0.00000     |              |                 |
| 10| b2   | 7.86     | 3.10959     | YES          | YES             |
| 11| e    | 17.62    | 0.52654     | YES          | YES             |
| 12| e    | 17.63    | 0.52687     | YES          | YES             |
| 13| b1   | 28.74    | 0.00000     | NO           | YES             |
| 14| e    | 31.52    | 3.37426     | YES          | YES             |
| 15| e    | 31.52    | 3.37467     | YES          | YES             |
| 16| b2   | 43.49    | 0.00000     | YES          | YES             |
| 17| b1   | 63.26    | 0.00000     | NO           | YES             |
| 18| e    | 71.56    | 2.00295     | YES          | YES             |
| 19| e    | 71.56    | 2.00280     | YES          | YES             |
| 20| b2   | 72.92    | 0.05982     | YES          | YES             |
| 21| b1   | 77.07    | 0.00000     | NO           | YES             |
| 22| b2   | 80.22    | 2.41772     | YES          | YES             |
| 23| e    | 80.33    | 6.56000     | YES          | YES             |
| 24| e    | 80.33    | 6.56071     | YES          | YES             |
| 25| b1   | 81.56    | 0.00000     | NO           | YES             |
| 26| e    | 85.00    | 0.70453     | YES          | YES             |
| 27| e    | 85.00    | 0.70558     | YES          | YES             |
| 28| b2   | 86.10    | 0.00000     | YES          | YES             |
| 29| b2   | 101.63   | 15.83937    | YES          | YES             |
| 30| b1   | 102.14   | 0.00000     | NO           | YES             |
| 31| e    | 108.47   | 0.65678     | YES          | YES             |
| 32| e    | 108.48   | 0.65688     | YES          | YES             |
| 33| b2   | 110.20   | 0.00000     | YES          | YES             |
| 34| b1   | 110.82   | 0.00000     | NO           | YES             |
| 35| b1   | 113.35   | 0.00000     | NO           | YES             |
| 36| e    | 116.85   | 1.25155     | YES          | YES             |
| 37| e    | 116.85   | 1.25152     | YES          | YES             |
| 38| b2   | 121.56   | 10.86236    | YES          | YES             |
| 39| b1   | 127.75   | 0.00000     | NO           | YES             |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 40 | e | 143.71 | 12.74284 | YES | YES |
| 41 | e | 143.71 | 12.74305 | YES | YES |
| 42 | b2 | 196.77 | 44.03568 | YES | YES |
| 43 | e | 199.17 | 15.31672 | YES | YES |
| 44 | e | 199.17 | 15.31667 | YES | YES |
| 45 | b1 | 203.95 | 0.00000 | NO | YES |
| 46 | b2 | 271.28 | 0.00000 | NO | YES |
| 47 | e | 273.84 | 0.57462 | YES | YES |
| 48 | e | 273.84 | 0.57466 | YES | YES |
| 49 | a1 | 276.51 | 0.00000 | NO | YES |
| 50 | e | 317.25 | 17.43886 | YES | YES |
| 51 | e | 317.25 | 17.43903 | YES | YES |
| 52 | b2 | 317.87 | 0.00000 | NO | YES |
| 53 | a1 | 320.11 | 0.00000 | NO | YES |
| 54 | a2 | 450.92 | 4.99570 | YES | NO |
| 55 | e | 452.09 | 6.54508 | YES | YES |
| 56 | e | 452.09 | 6.54511 | YES | YES |
| 57 | b1 | 453.29 | 0.00000 | NO | YES |
| 58 | a1 | 604.37 | 0.00000 | NO | YES |
| 59 | e | 605.04 | 2.20144 | YES | YES |
| 60 | e | 605.04 | 2.20138 | YES | YES |
| 61 | b2 | 605.58 | 0.00000 | NO | YES |
| 62 | a1 | 616.99 | 0.00000 | NO | YES |
| 63 | e | 617.13 | 1.26177 | YES | YES |
| 64 | e | 617.13 | 1.26183 | YES | YES |
| 65 | b2 | 617.30 | 0.00000 | NO | YES |
| 66 | a2 | 632.18 | 0.74862 | YES | NO |
| 67 | e | 632.61 | 0.14709 | YES | YES |
| 68 | e | 632.61 | 0.14709 | YES | YES |
| 69 | b1 | 633.53 | 0.00000 | NO | YES |
| 70 | a2 | 686.33 | 67.01562 | YES | NO |
| 71 | e | 686.80 | 45.82218 | YES | YES |
| 72 | e | 686.80 | 45.82211 | YES | YES |
| 73 | b1 | 687.13 | 0.00000 | NO | YES |
| 74 | b1 | 736.31 | 0.00000 | NO | YES |
| 75 | e | 736.47 | 9.76669 | YES | YES |
| 76 | e | 736.47 | 9.76669 | YES | YES |
| 77 | a2 | 737.00 | 24.43786 | YES | NO |
| 78 | b2 | 773.31 | 0.00000 | NO | YES |
| 79 | e | 773.40 | 0.26298 | YES | YES |
| 80 | e | 773.40 | 0.26298 | YES | YES |
| 81 | a1 | 773.51 | 0.00000 | NO | YES |
| 82 | b2 | 993.07 | 4.48894 | YES | YES |
| 83 | e | 993.83 | 1.50341 | YES | YES |
| 84 | e | 993.83 | 1.50339 | YES | YES |
| 85 | b1 | 994.82 | 0.00000 | NO | YES |
| 86 | b2 | 1005.31 | 0.00000 | YES | YES |
| 87 | e | 1005.46 | 0.09931 | YES | YES |
| 88 | e | 1005.46 | 0.09929 | YES | YES |
| 89 | b1 | 1005.85 | 0.00000 | NO | YES |
| 90 | e | 1052.67 | 8.55314 | YES | YES |
|   |     |         |            |      |     |   |
|---|-----|---------|-----------|------|-----|---|
| 91|  e  | 1052.67 | 8.55314   | YES  | YES|
| 92|  b2 | 1052.69 | 0.00000   | NO   | YES|
| 93|  a1 | 1052.89 | 0.00000   | NO   | YES|
| 94|  b1 | 1065.49 | 0.00000   | NO   | YES|
| 95|  e  | 1065.93 | 1.67947   | YES  | YES|
| 96|  e  | 1065.93 | 1.67959   | YES  | YES|
| 97|  a2 | 1066.84 | 5.85042   | YES  | NO |
| 98|  a1 | 1083.04 | 0.00000   | NO   | YES|
| 99|  e  | 1083.14 | 19.91320  | YES  | YES|
|100|  e  | 1083.14 | 19.91330  | YES  | YES|
|101|  b2 | 1083.38 | 0.00000   | NO   | YES|
|102|  b2 | 1115.02 | 0.00000   | YES  | YES|
|103|  e  | 1115.15 | 1.17246   | YES  | YES|
|104|  e  | 1115.15 | 1.17395   | YES  | YES|
|105|  b1 | 1115.52 | 0.00000   | NO   | YES|
|106|  b2 | 1116.49 | 9.29360   | YES  | YES|
|107|  e  | 1116.74 | 15.31371  | YES  | YES|
|108|  e  | 1116.74 | 15.31513  | YES  | YES|
|109|  b1 | 1117.12 | 0.00000   | NO   | YES|
|110|  a2 | 1195.51 | 34.87694  | YES  | NO |
|111|  e  | 1195.74 | 18.23373  | YES  | YES|
|112|  e  | 1195.74 | 18.23377  | YES  | YES|
|113|  b1 | 1196.24 | 0.00000   | NO   | YES|
|114|  a2 | 1313.00 | 5.39320   | YES  | NO |
|115|  e  | 1313.85 | 4.40062   | YES  | YES|
|116|  e  | 1313.85 | 4.40063   | YES  | YES|
|117|  b1 | 1314.69 | 0.00000   | NO   | YES|
|118|  b2 | 1335.83 | 0.00000   | NO   | YES|
|119|  e  | 1336.29 | 2.25274   | YES  | YES|
|120|  e  | 1336.29 | 2.25275   | YES  | YES|
|121|  a1 | 1337.88 | 0.00000   | NO   | YES|
|122|  b2 | 1355.97 | 0.00000   | NO   | YES|
|123|  e  | 1356.05 | 2.25547   | YES  | YES|
|124|  e  | 1356.05 | 2.25542   | YES  | YES|
|125|  a1 | 1356.25 | 0.00000   | NO   | YES|
|126|  a2 | 1388.17 | 48.44517  | YES  | NO |
|127|  e  | 1390.21 | 24.81133  | YES  | YES|
|128|  e  | 1390.21 | 24.81131  | YES  | YES|
|129|  b1 | 1394.14 | 0.00000   | NO   | YES|
|130|  b2 | 1412.71 | 0.00000   | YES  | YES|
|131|  e  | 1416.21 | 2.47910   | YES  | YES|
|132|  e  | 1416.21 | 2.47858   | YES  | YES|
|133|  b1 | 1419.35 | 0.00000   | NO   | YES|
|134|  e  | 1431.11 | 0.19867   | YES  | YES|
|135|  e  | 1431.11 | 0.19853   | YES  | YES|
|136|  b2 | 1431.53 | 0.00000   | YES  | YES|
|137|  b2 | 1432.07 | 35.90473  | YES  | YES|
|138|  e  | 1434.90 | 18.25552  | YES  | YES|
|139|  e  | 1434.90 | 18.25608  | YES  | YES|
|140|  b1 | 1435.28 | 0.00000   | NO   | YES|
|141|  b1 | 1436.33 | 0.00000   | NO   | YES|
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 142 | b2 | 1438.91 | 4.04445 | YES | YES |
| 143 | e  | 1439.84 | 12.72150 | YES | YES |
| 144 | e  | 1439.84 | 12.71737 | YES | YES |
| 145 | b1 | 1440.65 | 0.00000 | NO  | YES |
| 146 | e  | 1443.09 | 15.88549 | YES | YES |
| 147 | e  | 1443.09 | 15.88210 | YES | YES |
| 148 | b2 | 1443.82 | 0.00000 | NO  | YES |
| 149 | b2 | 1445.01 | 29.83187 | YES | YES |
| 150 | b1 | 1445.61 | 0.00000 | NO  | YES |
| 151 | e  | 1448.54 | 16.14795 | YES | YES |
| 152 | e  | 1448.54 | 16.14834 | YES | YES |
| 153 | b1 | 1450.28 | 0.00000 | NO  | YES |
| 154 | e  | 1563.69 | 0.08263 | YES | YES |
| 155 | e  | 1563.69 | 0.08263 | YES | YES |
| 156 | a1 | 1563.74 | 0.00000 | NO  | YES |
| 157 | b2 | 1563.93 | 0.00000 | NO  | YES |
| 158 | b1 | 2943.76 | 0.00000 | NO  | YES |
| 159 | e  | 2943.91 | 98.61729 | YES | YES |
| 160 | e  | 2943.91 | 98.45692 | YES | YES |
| 161 | e  | 2944.15 | 144.17951 | YES | YES |
| 162 | e  | 2944.15 | 144.02006 | YES | YES |
| 163 | b2 | 2944.25 | 0.00000 | YES | YES |
| 164 | b2 | 2945.24 | 2.86605 | YES | YES |
| 165 | b1 | 2945.48 | 0.00000 | NO  | YES |
| 166 | b1 | 3034.34 | 0.00000 | NO  | YES |
| 167 | e  | 3034.40 | 15.11581 | YES | YES |
| 168 | e  | 3034.40 | 15.11303 | YES | YES |
| 169 | b1 | 3035.32 | 0.00000 | NO  | YES |
| 170 | e  | 3035.80 | 70.22851 | YES | YES |
| 171 | e  | 3035.80 | 70.22545 | YES | YES |
| 172 | b2 | 3035.92 | 0.00000 | YES | YES |
| 173 | b2 | 3036.34 | 0.33902 | YES | YES |
| 174 | e  | 3054.38 | 0.08302 | YES | YES |
| 175 | e  | 3054.39 | 0.08322 | YES | YES |
| 176 | b2 | 3054.58 | 0.00000 | YES | YES |
| 177 | b1 | 3054.85 | 0.00000 | NO  | YES |
| 178 | e  | 3055.36 | 26.08431 | YES | YES |
| 179 | e  | 3055.36 | 26.08512 | YES | YES |
| 180 | b2 | 3056.25 | 123.07812 | YES | YES |
| 181 | b1 | 3056.98 | 0.00000 | NO  | YES |
| 182 | a2 | 3172.87 | 0.81702 | YES | NO  |
| 183 | e  | 3172.87 | 0.57608 | YES | YES |
| 184 | e  | 3172.87 | 0.57608 | YES | YES |
| 185 | b1 | 3172.87 | 0.00000 | NO  | YES |
| 186 | b2 | 3193.11 | 0.00000 | NO  | YES |
| 187 | e  | 3193.11 | 1.46876 | YES | YES |
| 188 | e  | 3193.11 | 1.46876 | YES | YES |
| 189 | a1 | 3193.13 | 0.00000 | NO  | YES |
**Complex 7 [Srl₂(IMe)₂(THF)₂]**

**Cartesian Coordinates (a.u.)**

| X         | Y         | Z         |
|-----------|-----------|-----------|
| -2.6470530627665 | -4.92048951960288 | 8.80759345087798 h |
| -1.35083731452290 | -3.49459065349433 | 7.56915248977705 c |
| 1.39905540536908 | -4.25512811281484 | 6.86321400102224 c |
| -1.40372711183054 | -1.66240715222572 | 8.58741939202274 h |
| -2.72197301412441 | -3.32703479049768 | 4.98513578366990 c |
| 1.16904188314912 | -5.06135333176225 | 4.08934079349660 c |
| 2.17597357348423 | -5.77438069427468 | 8.08266801171073 h |
| 2.69099500192078 | -2.60403797076009 | 6.9873410852813 h |
| -0.74891289498982 | -3.39789039308871 | 3.10007564606983 c |
| -0.400498269140231 | -4.97209344399914 | 4.67911448939465 h |
| -3.82533232373409 | -1.57633544186408 | 4.65635809375690 h |
| 0.51310787705504 | -7.06249502631838 | 3.90485656875185 h |
| 2.90482565348853 | -4.77506618457968 | 2.94680554107892 h |
| 0.00000000000000 | 0.00000000000000 | -0.31932770977704 sr |
| -0.51207030037787 | -3.67346967163144 | -3.93364731037198 c |
| 1.00811204346624 | -4.11722688132853 | -5.98223715787188 n |
| -2.01683538358488 | -5.78065629390621 | -3.83881960368172 n |
| 0.49447129929345 | -6.43127699522731 | -7.1130369492075 c |
| 3.02206261140842 | -2.40495500837033 | -6.77474160276619 h |
| -1.43818424132098 | -7.49458624717076 | -5.74457113106785 h |
| -3.91595933294368 | -6.19363694994741 | -1.87908964523830 c |
| 1.51183911445461 | -7.11593779454468 | -8.78265271309844 h |
| 4.48435623926159 | -2.96278327335258 | -5.90217341877421 h |
| 3.17705407803228 | -2.41690739905490 | -8.86751081509336 h |
| 2.55964529078232 | -0.47092747338492 | -6.10900349280122 h |
| -2.44620889189593 | -9.28840662775504 | -5.98612030505304 c |
| -5.48048663658590 | -7.35809302525451 | -2.64902675180969 c |
| -3.06482147170747 | -7.16465539154018 | -0.22304014235536 c |
| -4.67895080494396 | -4.33600849594734 | -1.26505415226951 h |
| 2.26470530627665 | 4.92048951960288 | 8.80759345087798 h |
| 1.35083731452290 | 3.49459065349433 | 7.56915248977705 c |
| -1.39905540536908 | 4.25512811281484 | 6.86321400102224 c |
| 1.40372711183054 | 1.66240715222572 | 8.58741939202274 h |
| 2.72197301412414 | 3.32703479049768 | 4.98513578366990 c |
| -1.16904188314912 | 5.06135333176225 | 4.08934079349660 c |
| -2.17597357348423 | 5.77438069427468 | 8.08266801171073 h |
| -2.69099500192078 | 2.60403797076009 | 6.9873410852813 h |
| 0.74891289498982 | 3.39789039308871 | 3.10007564606983 o |
| 4.00498269140231 | 4.97209344399914 | 4.67911448939465 h |
| 3.82533232373409 | 1.57633544186408 | 4.65635809375690 h |
| -0.51310787705504 | 7.06249502631838 | 3.90485656875185 h |
| 2.90482565348853 | 4.77506618457968 | 2.94680554107892 h |
| 0.51207030037787 | 3.67346967163144 | -3.93364731037198 c |
| -1.00811204346624 | 4.11722688132853 | -5.98223715787188 n |
| 2.01683538358384 | 5.78065629390621 | -3.83881960368172 n |
| -0.49447129929345 | 6.43127699522731 | -7.1130369492075 c |
| -3.02206261140842 | 2.40495500837033 | -6.77474160276619 c |
| 1.43818424132098 | 7.49458624717076 | -5.74457113106785 c |
| #   | symmetry | wave number | IR intensity | selection rules |
|-----|----------|-------------|--------------|-----------------|
| 1   | b        | -11.72      | 0.00000      | YES             |
| 2   | b        | -0.00       | 0.00000      | -               |
| 3   | b        | -0.00       | 0.00000      | -               |
| 4   | b        | -0.00       | 0.00000      | -               |
| 5   | b        | -0.00       | 0.00000      | -               |
| 6   | b        | -0.00       | 0.00000      | -               |
| 7   | b        | -0.00       | 0.00000      | -               |
| 8   | b        | 14.84       | 1.33050      | YES             |
| 9   | a        | 22.38       | 2.89285      | YES             |
| 10  | a        | 27.89       | 0.02041      | YES             |
| 11  | b        | 27.95       | 3.00216      | YES             |
| 12  | a        | 33.79       | 0.03300      | YES             |
| 13  | b        | 40.59       | 3.16539      | YES             |
| 14  | a        | 52.84       | 0.61458      | YES             |
| 15  | a        | 57.86       | 0.04058      | YES             |
| 16  | b        | 61.33       | 0.96905      | YES             |
| 17  | a        | 64.97       | 0.79858      | YES             |
| 18  | b        | 69.34       | 0.71435      | YES             |
| 19  | a        | 70.66       | 5.82390      | YES             |
| 20  | b        | 74.50       | 5.46527      | YES             |
| 21  | a        | 76.66       | 1.97890      | YES             |
| 22  | a        | 80.14       | 0.08539      | YES             |
| 23  | b        | 84.53       | 1.36960      | YES             |
| 24  | a        | 97.05       | 0.11641      | YES             |
| 25  | b        | 103.04      | 3.53203      | YES             |
| 26  | a        | 107.77      | 0.78735      | YES             |
| 27  | b        | 116.77      | 0.04675      | YES             |
| 28  | b        | 121.36      | 2.88268      | YES             |
| 29  | a        | 125.54      | 0.11139      | YES             |
| 30  | b        | 127.30      | 2.28851      | YES             |
| 31  | a        | 134.53      | 0.32624      | YES             |
| 32  | b        | 142.56      | 0.75645      | YES             |
| 33  | a        | 144.90      | 1.45436      | YES             |
| 34  | a        | 146.95      | 1.45746      | YES             |
| 35  | b        | 147.79      | 6.86691      | YES             |
|   |   |   |   |   |
|---|---|---|---|---|
|   |   |   |   |   |
| 36 | a | 155.96 | 0.78385 | YES | YES |
| 37 | b | 162.10 | 20.36396 | YES | YES |
| 38 | b | 185.63 | 17.15857 | YES | YES |
| 39 | a | 186.89 | 13.20445 | YES | YES |
| 40 | a | 204.32 | 19.09576 | YES | YES |
| 41 | b | 207.48 | 31.52863 | YES | YES |
| 42 | a | 274.68 | 0.15130 | YES | YES |
| 43 | b | 275.05 | 0.22052 | YES | YES |
| 44 | a | 319.63 | 1.80622 | YES | YES |
| 45 | b | 319.99 | 4.64339 | YES | YES |
| 46 | b | 322.63 | 7.19623 | YES | YES |
| 47 | b | 322.71 | 8.87544 | YES | YES |
| 48 | b | 612.80 | 0.27547 | YES | YES |
| 49 | b | 612.88 | 0.56446 | YES | YES |
| 50 | b | 639.41 | 0.18111 | YES | YES |
| 51 | a | 640.27 | 0.00749 | YES | YES |
| 52 | a | 665.98 | 0.92821 | YES | YES |
| 53 | a | 667.02 | 14.42668 | YES | YES |
| 54 | b | 688.78 | 53.38155 | YES | YES |
| 55 | a | 688.94 | 27.71098 | YES | YES |
| 56 | a | 737.71 | 7.13992 | YES | YES |
| 57 | b | 738.07 | 14.12029 | YES | YES |
| 58 | b | 776.89 | 0.11101 | YES | YES |
| 59 | a | 776.95 | 0.04929 | YES | YES |
| 60 | b | 795.55 | 0.10909 | YES | YES |
| 61 | a | 798.99 | 16.70025 | YES | YES |
| 62 | a | 861.50 | 2.25483 | YES | YES |
| 63 | b | 862.39 | 12.78882 | YES | YES |
| 64 | b | 898.88 | 7.20291 | YES | YES |
| 65 | b | 899.94 | 0.03605 | YES | YES |
| 66 | b | 905.99 | 41.95356 | YES | YES |
| 67 | a | 911.40 | 136.44360 | YES | YES |
| 68 | b | 927.88 | 7.93188 | YES | YES |
| 69 | a | 928.72 | 0.63907 | YES | YES |
| 70 | a | 952.80 | 2.66150 | YES | YES |
| 71 | b | 953.33 | 2.09471 | YES | YES |
| 72 | a | 996.74 | 0.20153 | YES | YES |
| 73 | b | 996.95 | 1.81320 | YES | YES |
| 74 | a | 1011.77 | 0.18273 | YES | YES |
| 75 | b | 1011.92 | 0.13289 | YES | YES |
| 76 | a | 1032.71 | 20.76451 | YES | YES |
| 77 | b | 1032.99 | 6.45907 | YES | YES |
| 78 | a | 1039.50 | 0.03264 | YES | YES |
| 79 | b | 1041.60 | 115.33058 | YES | YES |
| 80 | b | 1056.51 | 6.96454 | YES | YES |
|   |   |   |   |   |
|---|---|---|---|---|
| 87 | a | 1056.77 | 7.01915 | YES |
| 88 | b | 1071.84 | 2.83077 | YES |
| 89 | a | 1072.90 | 0.12498 | YES |
| 90 | b | 1089.25 | 9.63899 | YES |
| 91 | a | 1089.59 | 6.72508 | YES |
| 92 | b | 1114.42 | 11.57888 | YES |
| 93 | a | 1114.73 | 4.33364 | YES |
| 94 | a | 1117.37 | 0.00606 | YES |
| 95 | b | 1117.56 | 0.81692 | YES |
| 96 | b | 1119.11 | 3.73433 | YES |
| 97 | a | 1119.35 | 0.27181 | YES |
| 98 | b | 1182.03 | 4.66843 | YES |
| 99 | a | 1182.60 | 1.68448 | YES |
|100 | b | 1199.22 | 24.57870 | YES |
|101 | a | 1199.35 | 13.05042 | YES |
|102 | b | 1201.87 | 2.49250 | YES |
|103 | a | 1202.05 | 6.37555 | YES |
|104 | a | 1214.32 | 1.51734 | YES |
|105 | b | 1216.49 | 3.28818 | YES |
|106 | b | 1254.45 | 3.06124 | YES |
|107 | a | 1255.36 | 0.24510 | YES |
|108 | b | 1272.73 | 3.77983 | YES |
|109 | a | 1274.83 | 1.34487 | YES |
|110 | b | 1288.72 | 1.87242 | YES |
|111 | a | 1289.35 | 0.18891 | YES |
|112 | a | 1321.35 | 0.13807 | YES |
|113 | b | 1321.39 | 3.80816 | YES |
|114 | b | 1330.36 | 2.44646 | YES |
|115 | a | 1331.13 | 1.84853 | YES |
|116 | a | 1344.66 | 4.50750 | YES |
|117 | b | 1344.83 | 6.13646 | YES |
|118 | b | 1357.07 | 0.65263 | YES |
|119 | a | 1357.22 | 0.64590 | YES |
|120 | b | 1357.71 | 0.48745 | YES |
|121 | a | 1358.96 | 8.53817 | YES |
|122 | b | 1392.49 | 25.82079 | YES |
|123 | a | 1393.76 | 9.69585 | YES |
|124 | b | 1416.30 | 4.99931 | YES |
|125 | a | 1417.14 | 5.33532 | YES |
|126 | b | 1430.74 | 10.40377 | YES |
|127 | b | 1431.32 | 6.92497 | YES |
|128 | a | 1431.99 | 0.52838 | YES |
|129 | a | 1435.83 | 0.10605 | YES |
|130 | b | 1435.91 | 8.44083 | YES |
|131 | a | 1436.18 | 1.05183 | YES |
|132 | b | 1439.26 | 7.73376 | YES |
|133 | a | 1444.03 | 38.29524 | YES |
|134 | b | 1444.33 | 4.76213 | YES |
|135 | a | 1447.33 | 0.25199 | YES |
|136 | b | 1447.72 | 2.75466 | YES |
|137 | a | 1448.53 | 33.88084 | YES |
|   |   |   |   |   |
|---|---|---|---|---|
| 138 | b | 1449.25 | 30.61009 | YES | YES |
| 139 | a | 1449.86 | 0.48308 | YES | YES |
| 140 | b | 1453.82 | 6.86136 | YES | YES |
| 141 | a | 1455.11 | 11.94360 | YES | YES |
| 142 | b | 1468.40 | 5.87706 | YES | YES |
| 143 | a | 1475.72 | 5.70860 | YES | YES |
| 144 | b | 1563.64 | 0.52706 | YES | YES |
| 145 | a | 1563.73 | 0.11193 | YES | YES |
| 146 | b | 2899.02 | 128.86055 | YES | YES |
| 147 | a | 2899.30 | 0.08676 | YES | YES |
| 148 | b | 2925.96 | 79.18510 | YES | YES |
| 149 | a | 2926.22 | 0.15763 | YES | YES |
| 150 | b | 2946.47 | 107.69638 | YES | YES |
| 151 | a | 2946.47 | 5.60441 | YES | YES |
| 152 | b | 2954.09 | 19.52717 | YES | YES |
| 153 | a | 2954.93 | 34.43150 | YES | YES |
| 154 | b | 2976.87 | 28.27422 | YES | YES |
| 155 | a | 2976.94 | 0.83111 | YES | YES |
| 156 | a | 2983.32 | 55.11853 | YES | YES |
| 157 | b | 2984.46 | 0.57706 | YES | YES |
| 158 | a | 3024.49 | 8.34197 | YES | YES |
| 159 | b | 3024.84 | 3.44683 | YES | YES |
| 160 | a | 3026.55 | 13.72653 | YES | YES |
| 161 | b | 3027.02 | 11.93415 | YES | YES |
| 162 | a | 3037.27 | 22.59865 | YES | YES |
| 163 | b | 3037.63 | 2.12634 | YES | YES |
| 164 | a | 3038.28 | 29.90744 | YES | YES |
| 165 | b | 3038.32 | 22.97109 | YES | YES |
| 166 | b | 3043.54 | 56.41870 | YES | YES |
| 167 | a | 3044.27 | 0.12893 | YES | YES |
| 168 | b | 3048.90 | 0.25865 | YES | YES |
| 169 | a | 3049.38 | 6.64868 | YES | YES |
| 170 | a | 3055.69 | 0.75514 | YES | YES |
| 171 | b | 3055.79 | 23.66335 | YES | YES |
| 172 | a | 3061.29 | 10.61504 | YES | YES |
| 173 | b | 3061.71 | 6.27207 | YES | YES |
| 174 | b | 3176.46 | 0.98419 | YES | YES |
| 175 | a | 3176.47 | 0.48718 | YES | YES |
| 176 | b | 3196.48 | 0.45316 | YES | YES |
| 177 | a | 3196.49 | 0.20020 | YES | YES |

Complex 7' [Sr₂IMe₄]

Cartesian Coordinates (a.u.)

|   |   |   |   |   |
|---|---|---|---|---|
| 3.71980389154317 | -3.71980389154317 | 0.00000000000000 | c |
| 5.97984510846662 | -7.31169521301540 | -0.89184622738920 | c |
| 7.31169521301540 | -5.97984510846662 | 0.89184622738920 | c |
| 3.82125789402472 | -5.89951405469525 | -1.40201886975880 | n |
| 5.89951405469525 | -3.82125789402472 | 1.40201886975880 | n |
| 6.38502604399808 | -9.11844247563602 | -1.82158722788010 | h |
| # | mode | symmetry | wave number | IR intensity | selection rules |
|---|------|----------|-------------|--------------|-----------------|
| 1 | e    | -12.61   | 0.00000     | YES          | YES             |
| 2 | e    | -12.61   | 0.00000     | YES          | YES             |
| 3 | b1   | -11.95   | 0.00000     | NO           | YES             |
| 4 |      | -0.00    | 0.00000     |              |                 |
| 5 |      | 0.00     | 0.00000     |              |                 |
| 6 |      | 0.00     | 0.00000     |              |                 |
| 7 |      | 0.00     | 0.00000     |              |                 |
| 8 |      | 0.00     | 0.00000     |              |                 |
| 9 |      | 0.00     | 0.00000     |              |                 |
| 10| b2   | 9.25     | 3.26505     | YES          | YES             |
| 11| e    | 22.91    | 0.43719     | YES          | YES             |
| 12| e    | 22.91    | 0.43726     | YES          | YES             |
| 13| b1   | 29.62    | 0.00000     | NO           | YES             |
| 14| e    | 37.23    | 3.34067     | YES          | YES             |
| 15| e    | 37.23    | 3.34096     | YES          | YES             |
| 16| b2   | 48.44    | 0.00000     | YES          | YES             |
| 17| b1   | 64.43    | 0.00000     | NO           | YES             |
| 18| e    | 76.85    | 1.71747     | YES          | YES             |
| 19| e    | 76.85    | 1.71750     | YES          | YES             |
| 20| b2   | 79.87    | 0.35124     | YES          | YES             |
| 21| b1   | 84.88    | 0.00000     | NO           | YES             |
| 22| b1   | 86.15    | 0.00000     | NO           | YES             |
| 23| e    | 86.68    | 7.08385     | YES          | YES             |
| 24| e    | 86.68    | 7.08480     | YES          | YES             |
| 25| b2   | 88.54    | 0.42708     | YES          | YES             |
| 26| b2   | 90.82    | 0.00000     | YES          | YES             |
| 27| e    | 91.11    | 0.63951     | YES          | YES             |
| 28| e    | 91.11    | 0.64062     | YES          | YES             |
| 29| b2   | 106.18   | 9.18417     | YES          | YES             |
| 30| b2   | 109.01   | 0.00000     | YES          | YES             |
| 31| b1   | 109.97   | 0.00000     | NO           | YES             |
| 32| b1   | 111.78   | 0.00000     | NO           | YES             |
| 33| e    | 113.88   | 0.06969     | YES          | YES             |
| 34| e    | 113.88   | 0.06971     | YES          | YES             |
| 35| b1   | 121.07   | 0.00000     | NO           | YES             |
| 36| e    | 123.13   | 2.80977     | YES          | YES             |
| 37| e    | 123.13   | 2.80975     | YES          | YES             |
| 38| b1   | 132.53   | 0.00000     | NO           | YES             |
| 39| b2   | 139.32   | 22.49970    | YES          | YES             |
| 40| e    | 174.34   | 14.53356    | YES          | YES             |
| 41| e    | 174.34   | 14.53366    | YES          | YES             |
|   | Symbol | X    | Y      | Result | Decision |
|---|--------|------|--------|--------|----------|
| 42| a2     | 204.46 | 52.73457 | YES    | NO       |
| 43| e      | 206.88 | 19.74130 | YES    | YES      |
| 44| e      | 206.88 | 19.74143 | YES    | YES      |
| 45| b1     | 211.58 | 0.00000  | NO     | YES      |
| 46| b2     | 271.68 | 0.00000  | NO     | YES      |
| 47| e      | 274.78 | 0.81569  | YES    | YES      |
| 48| e      | 274.78 | 0.81575  | YES    | YES      |
| 49| a1     | 278.00 | 0.00000  | NO     | YES      |
| 50| b2     | 318.65 | 0.00000  | NO     | YES      |
| 51| e      | 318.95 | 17.54129 | YES    | YES      |
| 52| e      | 318.95 | 17.54142 | YES    | YES      |
| 53| a1     | 321.55 | 0.00000  | NO     | YES      |
| 54| a2     | 451.72 | 4.97482  | YES    | NO       |
| 55| e      | 452.89 | 6.97165  | YES    | YES      |
| 56| e      | 452.89 | 6.97171  | YES    | YES      |
| 57| b1     | 454.06 | 0.00000  | NO     | YES      |
| 58| a1     | 604.32 | 0.00000  | NO     | YES      |
| 59| e      | 605.07 | 2.23413  | YES    | YES      |
| 60| e      | 605.07 | 2.23405  | YES    | YES      |
| 61| b2     | 605.48 | 0.00000  | NO     | YES      |
| 62| a1     | 616.82 | 0.00000  | NO     | YES      |
| 63| e      | 616.98 | 1.10396  | YES    | YES      |
| 64| e      | 616.98 | 1.10403  | YES    | YES      |
| 65| b2     | 617.09 | 0.00000  | NO     | YES      |
| 66| a2     | 634.96 | 0.86984  | YES    | NO       |
| 67| e      | 635.67 | 0.10184  | YES    | YES      |
| 68| e      | 635.67 | 0.10184  | YES    | YES      |
| 69| b1     | 636.74 | 0.00000  | NO     | YES      |
| 70| a2     | 686.88 | 68.12864 | YES    | NO       |
| 71| e      | 687.37 | 44.72587 | YES    | YES      |
| 72| e      | 687.37 | 44.72582 | YES    | YES      |
| 73| b1     | 687.71 | 0.00000  | NO     | YES      |
| 74| b1     | 737.12 | 0.00000  | NO     | YES      |
| 75| e      | 737.30 | 10.51175 | YES    | YES      |
| 76| e      | 737.30 | 10.51175 | YES    | YES      |
| 77| a2     | 737.80 | 10.51175 | YES    | YES      |
| 78| b2     | 773.73 | 0.00000  | NO     | YES      |
| 79| e      | 773.83 | 0.26464  | YES    | YES      |
| 80| e      | 773.83 | 0.26465  | YES    | YES      |
| 81| a1     | 773.95 | 0.00000  | NO     | YES      |
| 82| b2     | 993.23 | 4.25758  | YES    | YES      |
| 83| e      | 994.02 | 1.30808  | YES    | YES      |
| 84| e      | 994.02 | 1.30805  | YES    | YES      |
| 85| b1     | 995.04 | 0.00000  | NO     | YES      |
| 86| b2     | 1007.21| 0.00000  | YES    | YES      |
| 87| e      | 1007.63| 0.05775  | YES    | YES      |
| 88| e      | 1007.63| 0.05773  | YES    | YES      |
| 89| b1     | 1007.94| 0.00000  | NO     | YES      |
| 90| e      | 1053.25| 9.23589  | YES    | YES      |
| 91| e      | 1053.25| 9.23589  | YES    | YES      |
| 92| b2     | 1053.26| 0.00000  | NO     | YES      |
|    |    |     |     |     |     |
|----|----|-----|-----|-----|-----|
|    |    | 1053.52 | 0.00000 | NO | YES |
| 94 | b1 | 1062.88 | 0.00000 | NO | YES |
| 95 | e  | 1063.46 | 1.38125 | YES | YES |
| 96 | e  | 1063.46 | 1.38136 | YES | YES |
| 97 | a2 | 1064.46 | 5.21212 | YES | NO  |
| 98 | a1 | 1083.85 | 0.00000 | NO | YES |
| 99 | b2 | 1084.39 | 0.00000 | NO | YES |
|100 | e  | 1084.49 | 19.02423 | YES | YES |
|101 | e  | 1084.49 | 19.02418 | YES | YES |
|102 | b2 | 1115.70 | 0.00000 | YES | YES |
|103 | e  | 1115.81 | 1.38125 | YES | YES |
|104 | e  | 1115.81 | 1.38136 | YES | YES |
|105 | b1 | 1116.40 | 0.00000 | NO  | YES |
|106 | b2 | 1117.25 | 0.00000 | NO  | YES |
|107 | e  | 1117.77 | 16.97016 | YES | YES |
|108 | e  | 1117.77 | 16.97108 | YES | YES |
|109 | b1 | 1118.19 | 0.00000 | NO  | YES |
|110 | a2 | 1195.20 | 0.00000 | NO  | YES |
|111 | e  | 1195.44 | 18.97547 | YES | YES |
|112 | e  | 1195.44 | 18.97552 | YES | YES |
|113 | b1 | 1195.98 | 0.00000 | NO  | YES |
|114 | a2 | 1235.72 | 0.00000 | NO  | YES |
|115 | e  | 1312.96 | 4.98408 | YES | YES |
|116 | e  | 1312.96 | 4.98408 | YES | YES |
|117 | b1 | 1313.72 | 0.00000 | NO  | YES |
|118 | b2 | 1335.29 | 0.00000 | NO  | YES |
|119 | e  | 1335.90 | 1.51351 | YES | YES |
|120 | e  | 1335.90 | 1.51349 | YES | YES |
|121 | a1 | 1337.46 | 0.00000 | NO  | YES |
|122 | b2 | 1355.66 | 0.00000 | NO  | YES |
|123 | e  | 1355.75 | 2.06812 | YES | YES |
|124 | e  | 1355.75 | 2.06812 | YES | YES |
|125 | a1 | 1355.91 | 0.00000 | NO  | YES |
|126 | a2 | 1387.93 | 52.11094 | YES | NO  |
|127 | e  | 1389.90 | 23.87481 | YES | YES |
|128 | e  | 1389.90 | 23.87479 | YES | YES |
|129 | b1 | 1393.96 | 0.00000 | NO  | YES |
|130 | b2 | 1412.76 | 0.00000 | YES | YES |
|131 | e  | 1416.44 | 2.13281 | YES | YES |
|132 | e  | 1416.44 | 2.13235 | YES | YES |
|133 | b1 | 1420.12 | 0.00000 | NO  | YES |
|134 | e  | 1430.83 | 0.77514 | YES | YES |
|135 | e  | 1430.83 | 0.77492 | YES | YES |
|136 | b2 | 1431.20 | 0.00000 | YES | YES |
|137 | b2 | 1432.09 | 19.90005 | YES | YES |
|138 | e  | 1433.86 | 19.90027 | YES | YES |
|139 | e  | 1433.86 | 19.90027 | YES | YES |
|140 | b1 | 1434.48 | 0.00000 | NO  | YES |
|141 | b1 | 1436.01 | 0.00000 | NO  | YES |
|142 | b2 | 1438.42 | 1.32310 | YES | YES |
|143 | e  | 1439.34 | 14.58727 | YES | YES |
|   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|
| 144 | e | 1439.34 | 14.58390 | YES | YES |
| 145 | b1 | 1439.91 | 0.00000 | NO | YES |
| 146 | e | 1443.21 | 17.02467 | YES | YES |
| 147 | e | 1443.21 | 17.02179 | YES | YES |
| 148 | b2 | 1443.53 | 0.00000 | YES | YES |
| 149 | a2 | 1444.97 | 27.94135 | YES | NO |
| 150 | b1 | 1446.97 | 0.00000 | NO | YES |
| 151 | e | 1449.94 | 18.02009 | YES | YES |
| 152 | e | 1449.94 | 18.02041 | YES | YES |
| 153 | b1 | 1451.87 | 0.00000 | NO | YES |
| 154 | a1 | 1565.21 | 0.00000 | NO | YES |
| 155 | e | 1565.21 | 0.19988 | YES | YES |
| 156 | e | 1565.21 | 0.19988 | YES | YES |
| 157 | b2 | 1565.42 | 0.00000 | NO | YES |
| 158 | b1 | 2945.56 | 0.00000 | NO | YES |
| 159 | e | 2945.63 | 132.49318 | YES | YES |
| 160 | e | 2945.63 | 132.40175 | YES | YES |
| 161 | e | 2945.96 | 114.90942 | YES | YES |
| 162 | e | 2945.96 | 114.81870 | YES | YES |
| 163 | b2 | 2946.01 | 0.00000 | YES | YES |
| 164 | b2 | 2946.97 | 3.16299 | YES | YES |
| 165 | b1 | 2947.20 | 0.00000 | NO | YES |
| 166 | b1 | 3036.45 | 0.00000 | NO | YES |
| 167 | e | 3036.46 | 17.09725 | YES | YES |
| 168 | e | 3036.46 | 17.09616 | YES | YES |
| 169 | b1 | 3037.16 | 0.00000 | NO | YES |
| 170 | e | 3038.05 | 58.80697 | YES | YES |
| 171 | e | 3038.05 | 58.80572 | YES | YES |
| 172 | b2 | 3038.17 | 0.00000 | YES | YES |
| 173 | b2 | 3038.34 | 0.50627 | YES | YES |
| 174 | e | 3055.65 | 0.00026 | YES | YES |
| 175 | e | 3055.65 | 0.00024 | YES | YES |
| 176 | b2 | 3055.87 | 0.00000 | YES | YES |
| 177 | b1 | 3056.17 | 0.00000 | NO | YES |
| 178 | e | 3056.73 | 40.20873 | YES | YES |
| 179 | e | 3056.73 | 40.20923 | YES | YES |
| 180 | b2 | 3058.01 | 127.11637 | YES | YES |
| 181 | b1 | 3058.79 | 0.00000 | NO | YES |
| 182 | a2 | 3173.17 | 0.82248 | YES | NO |
| 183 | e | 3173.17 | 0.59332 | YES | YES |
| 184 | e | 3173.17 | 0.59331 | YES | YES |
| 185 | b1 | 3173.17 | 0.00000 | NO | YES |
| 186 | b2 | 3193.50 | 0.00000 | NO | YES |
| 187 | e | 3193.50 | 1.27037 | YES | YES |
| 188 | e | 3193.50 | 1.27037 | YES | YES |
| 189 | a1 | 3193.52 | 0.00000 | NO | YES |
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[8] TURBOMOLE Version 7.4, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH since 2007.