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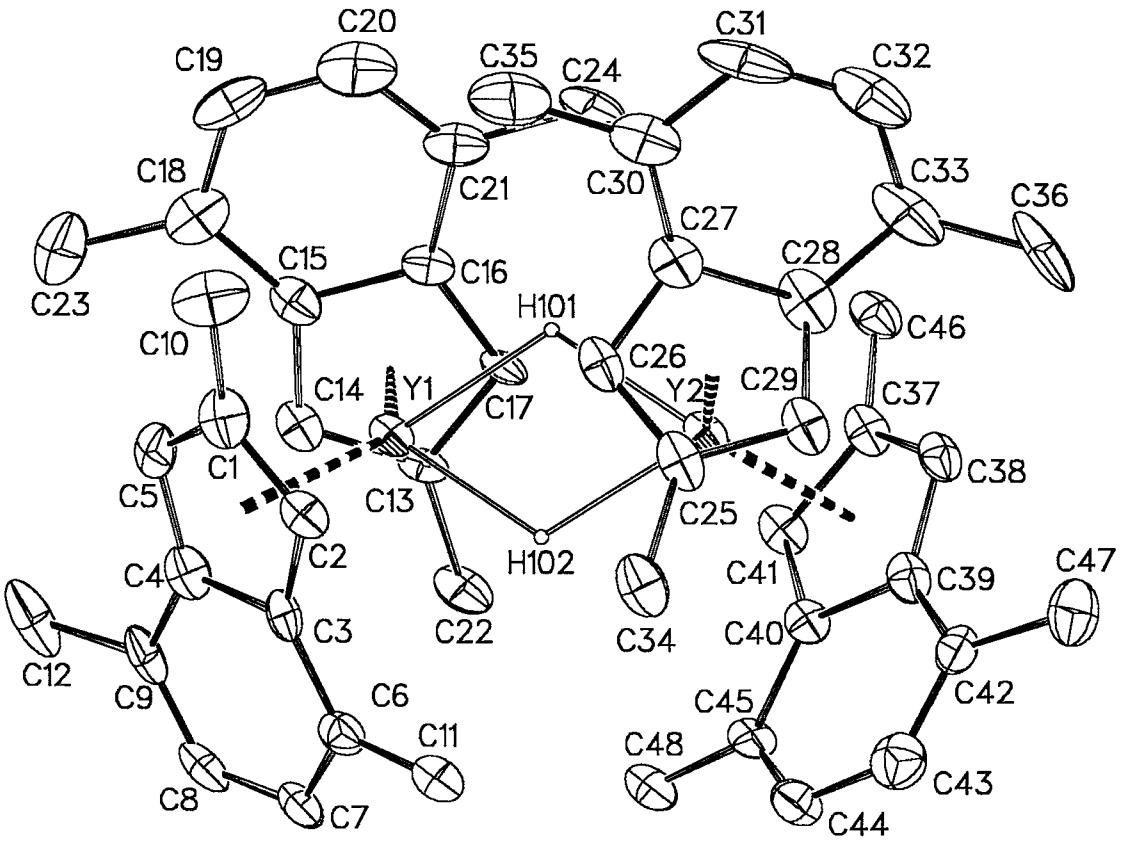
Supplementary material

Regioselective Homo- and Co-dimerization of α-Olefins Catalyzed by Bis(2,4,7-trimethylindenyl)yttrium Hydride

Winfried P. Kretschmer,[a]* Sergei Troyanov,[b] Auke Meetsma,[a] Bart Hessen,[a] and Jan H. Teuben[a]

[a]*Groningen Centre for Catalytic Olefin Polymerization, Department of Chemistry, University of Groningen, Nijenborgh 4, NL-9747 AG Groningen, The Netherlands.*
[b]*Chemistry Department, Moscow State University, 119899 Moscow, Vorobyevy Gory, Russia.*



Abstract. Bis(2,4,7-trimethylindenyl)yttrium hydride, $C_{48}H_{54}Y_2.[C_6H_6]_{0.5}$, M = 847.83, monoclinic, $P2_1/n$, a = 12.387(1), b = 21.854(1), c = 16.322(1) Å, b = 106.998(5)°, V = 4225.4(5) Å, Z = 4, D_x = 1.333 g cm^{-1}, l(MoK$\bar{\alpha}$) = 0.71073 Å, μ = 27.7 cm^{-1}, F(000) = 1764, T = 130 K, $wR(F^2)$ = 0.1871 for 6430 reflections with $F_o^2 \geq 0$ and 498 parameters and $R(F)$ = 0.0763 for 4412 reflections obeying $F_o \geq 4.0\ \sigma(F_o)$ criterion of observability.

Experimental

X-ray diffraction: Crystal and Molecular Structure.

Suitable colorless plate-shaped crystals were obtained by recrystallisation from benzene. The crystal, a parallelepiped of approximate size 0.10 x 0.20 x 0.40 mm., used for characterization and data collection was mounted on top of a glass fiber by using inert-atmosphere handling techniques and was transferred into the cold nitrogen cold stream of the low temperature unit[1] mounted on an Enraf-Nonius *CAD-4F*[2] diffractometer (Mo tube, 50 kV, 40 mA, monochromated Mo-K$\bar{\alpha}$ radiation, Dw = 0.80 + 0.34 tg q), interfaced to a *MSDOS* computer. The crystals exhibited a high background, probably caused by fluorescence of the the Y atoms, as always observed in Y containing crystals.

Unit cell parameters and orientation matrix were determined from a least-squares treatment of the *SET4*[3] setting angles of 23 reflections in the range 12.52° < q < 15.46°. The unit cell was identified as monoclinic, space group $P2_1/n$. Reduced cell calculations did not indicate any higher metric lattice symmetry[4] and examination of the final atomic coordinates of the structure did not yield extra metric symmetry elements.[5,6]

The intensities of two standard reflections, monitored every three hours of X-ray exposure time, showed no greater fluctuations during data collection than those expected from Poisson statistics. Intensity data were corrected for Lorentz and polarization effects, scale variation, but not for absorption and reduced to F_o^2.[9]

The structure was solved by Patterson methods and extension of the model was accomplished by direct methods applied to difference structure factors using the program *DIRDIF*.[8] The positional and anisotropic thermal displacement parameters for the non-hydrogen atoms were

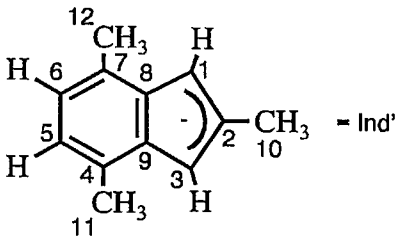
refined. A subsequent difference Fourier synthesis resulted in the location of the two hydride positions and most of the other hydrogen atoms. The two bridging hydrogen atom positions were refined with bond restraints and isotropic thermal displacement parameters. The other hydrogen atoms were included in the final refinement riding on their carrier atoms with $U = c$ x U_{equiv} of their parent atom, where $c = 1.2$ for the aromatic / non-methyl hydrogen atoms and $c = 1.5$ for the methyl hydrogen atoms and where values U_{equiv} are related to the atoms to which the H atoms are bonded. The methyl-groups were refined as rigid groups, which were allowed to rotate free.

Final refinement on F^2 carried out by full-matrix least-squares techniques converged at $wR(F^2) = 0.1871$ for 6430 reflections with $F_o^2 \geq 0$ and $R(F) = 0.0763$ for 4412 reflections with $F_o \geq 4.0\ \sigma(F_o)$ and 498 parameters. The final difference Fourier map was essentially featureless with a few peaks of max. 1.17(14) within 1.0 Å from Y; but were neglected/rejected, being artefacts. No other significant peaks having chemical meaning above the general background were observed in the final difference Fourier syntheses.

The positional and anisotropic thermal displacement parameters for the non-hydrogen atoms and isotropic thermal displacement parameters for hydrogen atoms were refined on F^2 with full-matrix least-squares procedures minimizing the function $Q = \sum_h [w(|F_o^2 - kF_c^2|)^2]$, where $w = 1/[s^2(F_o^2) + (aP)^2 + bP]$, $P = [\max(F_o^2,0) + 2F_c^2] / 3$, F_0 and F_c are the observed and calculated structure factor amplitudes, respectively; a and b were refined. Reflections were stated observed if satisfying $F^2 > 0$ criterion of observability.

Crystal data and numerical details on data collection and refinement are given in Table 1. Final fractional atomic coordinates equivalent displacement for the non-hydrogen atoms are given in Table 2. Molecular geometry data are collected in Table 3. Tables of hydrogen atom positions, thermal displacement parameters, comprehensive distances and angles and tables of (F_o), (F_c) and $\sigma(F_o)$ are given as supplementary material for this paper. Neutral atom scattering factors and anomalous dispersion corrections were taken from *International Tables of Crystallography*.[9] All calculations performed on the HP9000/735 computer at the University of Groningen with the program packages *SHELXL*[10] (least-square refinements), *PLATON*[11] (calculation of geometric data) and a locally modified version of the program *PLUTO*[12].

Synthesis of the compounds: General considerations. All manipulations of air or moisture sensitive compounds were carried out under N_2 using glove-box, standard Schlenk or vacuum line techniques. Solvents and reagents were purified by distillation from $LiAlH_4$, potassium, Na/K alloy or sodium ketyl of benzophenone under nitrogen immediately before use. NMR spectra were recorded on a Varian Gemini 200 (^1H: 200 MHz, ^{13}C: 50.3 MHz) or Varian VXR-300 (^1H: 300 MHz, ^{13}C: 75.4 MHz) spectrometer. The ^1H and ^{13}C NMR spectra, measured at 20 °C, were referenced internally using the residual solvent resonance's, and reported in ppm. IR spectra were recorded as Nujol mulls between KBr discs on a Mattson Galaxy 4020 spectrophotometer. $(Cp^*_2YH)_2$[13] and $(Cp^*_2LaH)_2$[14] was synthesized according to published procedure.



Numbering scheme of 2,4,7-trimethylindenyl ligand.

Synthesis of 2,4,7-trimethylindanone. To a suspension of 28 g (0.2 mol) of $AlCl_3$ in 100 mL of CH_2Cl_2, kept at 0 °C by an ice bath, were added first 22 g (0.094 mol) of 2-bromoisobutyric acid bromide and then a solution of 10 g (0.094 mol) p-xylene in 50 mL CH_2Cl_2. The mixture was stirred for 2 h at 0 °C and 2 h at room temperature and then poured on ice. The dark organic layer was separated, washed with water-$NaHCO_3$ and dried over Na_2CO_3. After removal of the solvent and distillation under reduced pressure (b.p. 145 °C/ 1 mm) a pale yellow oil was obtained, which are slowly crystalllized (m.p. 35 °C). Yield: 13.2 g (0.075 mol, 81 %). ^1H NMR (toluene-d_8): δ 1.23 (d, 3H, CH_3), 2.21 (s, 3H, CH_3), 2.44 (dd, 1H, CH_2), 2.53 (s, 3H, CH_3), 2.57 (m, 1H, CH), 3.14 (dd, 1H, CH_2), 6.92 (d, 1H, CH), 7.15 (d, 1H, CH).

Synthesis of 2,4,7-trimethylindene. To a solution of 13.2 g (0.075 mol) of 2,4,7-trimethylindanone in 150 mL of tetrahydrofuran/methanol (2:1) was added under cooling with ice 3.0 g (0.082 mol) of $NaBH_4$ over a period of 90 min. After stirring for another 12 h at room temperature, the reaction mixture was poured on ice-HCl. The ether extract was washed with water-$NaHCO_3$ and dried over Na_2CO_3. Removal of the solvent gave a white solid, which contained the 2,4,7-trimethylindanol and was used without further purification. The solution of the crude indanol in 150 mL of toluene was stirred at 90 °C for 3 h after addition of 10 g (0.058 mol) of p-toluenesulphonic acid. The reaction mixture was washed with water-$NaHCO_3$, dried over Na_2CO_3 and evaporated to dryness. Distillation under reduced pressure (b.p. 140 °C/ 1 mm) yield in 8.8 g (0.056 mol, 75 %) of white needles of 2,4,7-trimethylindene (m.p. 42 °C). ^1H NMR ($CDCl_3$): δ 2.12 (s, 3H, CH_3), 2.23 (s, 3H, CH_3), 2.31 (s, 3H, CH_3), 3.11 (s, 2H, CH_2), 6.53 (q, 1H, CH), 6.77 (d, 1H, CH), 6.90 (d, 1H, CH). ^{13}C NMR ($CDCl_3$): 16.82 (10); 18.18, 18.29 (11, 12); 41.87 (3); 124.84, 125.66, 127.58 (1, 5, 6); 129.01, 129.66, 141.65, 144.19, 144.96 (2, 4, 7, 8, 9).

Preparation of 2,4,7-trimethylindenyllithium. To 37,00 g (0.234 mol) of trimethylindene dissolved in 300 mL of n-hexane, 156 mL of 1.5 M n-butyl lithium solution in hexane were added through a dropping funnel at room temperature. A white voluminous solid precipitated. Stirring was continued for 6 h. After heating the suspension for 4 h to boiling the solid was collected on a glass filter and washed with 50 ml of pentane. After drying, 37.09 g (96 %) of a white powder was obtained.

Synthesis of $(2,4,7\text{-}Me_3C_9H_4)_2Y(\mu\text{-}Cl)_2Li(THF)_2$ (1). 2.24 g (5.00 mmol) of $YCl_3(THF)_{3.5}$ was suspended in 100 mL of THF and 1.67 g (10.00 mmol) of 2,4,7-trimethylindenyl lithium was added at -80 °C. The mixture was continuously stirred and allowed to warm to room temperature over 2 h. Stirring was continued for 2 h to form a clear solution. After removal of the solvent under vacuum, the residue was treated with 80 mL of toluene/THF (10:1), stirred, allowed to settle and the solution was decanted off. Concentration to 35 mL and cooling to -30 °C gave the product in a crystalline form; yield 2.40 g (76 %) of pale yellow crystals. ^1H NMR

(benzene-d_6): δ 1.31 (m, 8H, THF), 2.35 (s, 6H, CH_3), 2.63 (s, 12H, CH_3), 3.50 (m, 8H, THF), 6.28 (s, 4H, CH), 6.89 (s, 4H, CH). ^{13}C NMR (benzene-d_6): δ 16.11 (10); 19.88 (11, 12); 25.25 (THF); 68.21 (THF); 100.27 (1, 3); 121.52 (5, 6); 128.29, 128.79, 131.09 (2, 4, 7, 8, 9). IR (cm^{-1}): 3074 (sh), 2726 (w), 1636 (w), 1359 (s), 1328 (s), 1313 (m), 1285 (m), 1254 (m), 1041 (vs), 912 (m), 890 (s), 816 (vs), 809 (vs), 797 (vs), 789 (vs), 763 (m), 736 (m), 723 (w), 660 (w), 630 (w), 503 (w). Anal. Calcd for $C_{32}H_{42}Cl_2LiO_2Y$: H, 6.77; C, 61.45; Y, 14.22. Found: H, 6.82; C, 61.50; Y, 14.15.

Synthesis of $(2,4,7\text{-}Me_3C_9H_4)_2YCH(SiMe_3)_2$ (2). A 1.90 g (3.04 mmol) amount of **1** was dissolved in 50 mL of toluene and 0.50 g (3.01 mmol) of bis(trimethylsilyl)methyllithium was added at -80 °C. The mixture was continuously stirred and allowed to warm to room temperature over 2 h. After removal of the solvent under vacuum, the residue was treated with 80 mL of n-hexane, stirred, allowed to settle and the solution was decanted off. Concentration to 35 mL and cooling to -30 °C gave the product in a crystalline form; yield 1.10 g (65 %) of colourless crystals. ^1H NMR (benzene-d_6): δ -0.09 (s, 18 H, $Si(CH_3)_3$), 0.16 (d, 1H, J_{YH} = 2.7 Hz, CHSi), 2.14 (s, 3H, CH_3), 2.22 (s, 3H, CH_3), 2.27 (s, 6H, CH_3), 2.37 (s, 6H, CH_3), 6.28 (s, 2H, CH), 6.43 (s, 2H, CH), 6.53 (s, 2H, CH), 6.63 (s, 2H, CH). ^{13}C NMR (benzene-d_6): δ 2.99 ($Si(CH_3)_3$); 15.00 (10); 15.61 (10'); 18.89 (11, 12); 19.11 (11', 12'); 26.03 (d, J_{YC} = 33.5 Hz, CHSi); 99.67 (1, 3); 100.05 (1', 3'); 121.06 (5, 6); 121.50 (5', 6'); 128.34, 128.68, 128.99, 130.01, 132.63 (2, 4, 7, 8, 9, 2', 4', 7', 8', 9'). IR (cm-1): 3070 (sh), 1498 (m), 1365 (m), 1328 (w), 1312 (w), 1285 (w), 1255 (w), 1216 (s), 1163 (m), 1127 (m), 1058 (w), 1027 (w), 965 (w), 893 (s), 807 (vs), 785 (vs), 776 (s), 760 (s), 745 (w), 735 (w), 718 (m), 608 (s). Anal. Calcd for $C_{31}H_{45}Si_2Y$: H, 8.06; C, 66.16; Y, 15.80. Found: H, 8.03; C, 66.20; Y, 15.70.

Synthesis of $[(2,4,7\text{-}Me_3C_9H_4)_2Y(\mu\text{-}H)]_2 \cdot (C_6H_{12})_{0.5}$ (3). A solution of 0.40 g (0.71 mmol) of [bis(trimethylsilyl)methyl]bis(2,4,7-trimethylindenyl)yttrium (**2**) in 10 mL of cyclohexane was stirred at room temperature under an atmosphere of H_2 (1 at) for 48 h. Removal of the volatiles in vacuo gave a pale yellow solid, which was washed with neat cyclohexane and dried in vacuo; yield 0.285 g (95 %). ^1H NMR (toluene-d_8, 20 °C): δ 1.41 (s, 6 H, C_6H_{12}), 1.82 (s,

6 H, CH_3), 2.02 (s, br, 6 H, CH_3), 2.69 (t, 2 H, YH-Y, $^1J_{YH}$ = 32.7 Hz), 2.78 (s, br, 6 H, CH_3), 6.36 (s, br, 2 H, CH), 6.46 (d, 2 H, CH), 6.67 (s, br, 2 H, CH), 6.77 (s, br, 2 H). ^{1}H NMR (toluene-d_8, -20 °C): δ 1.43 (s, 10 H, C_6H_{12}), 1.82 (s, 6 H, CH_3), 2.06 (s, 6 H, CH_3), 2.68 (t, 2 H, YH-Y, J_{YH} = 29.6 Hz), 2.78 (s, 6 H, CH_3), 6.29 (d, 2 H, CH, J_{HH} = 1.1 Hz), 6.54 (d, 2 H, CH, J_{HH} = 1.1 Hz), 6.68 (d, 2 H, CH, $^1J_{HH}$ = 6.9 Hz), 6.83 (d, 2 H, CH, $^1J_{HH}$ = 6.9 Hz). ^{13}C NMR (benzene-d_6): δ 14.32 (10); 20.57 (br, 11, 12); 27.19 (C_6H_{12}); 98.70 (1, 3); 122.16 (5, 6); 128.29, 128.50, 129.20, 129.36 (2, 4, 7, 8, 9). IR (cm^{-1}): 3137 (w), 3085 (m), 3011 (s), 1818 (w), 1808 (w), 1621 (w), 1615 (w), 1598 (w), 1495 (m), 1327 (m), 1311 (m), 1286 (m), 1255 (m), 1217 (s), 1163 (m), 1126 (m), 1082 (m), 1058 (m), 965 (w), 894 (s), 825 (w), 808 (vs), 786 (vs), 775 (vs), 760 (s), 745 (m), 729 (s), 717 (m), 693 (w), 609 (s), 563 (w), 530 (w). Anal. Calcd for $C_{51}H_{60}Y_2$: H, 7.11; C, 71.99; Y, 20.90. Found: H, 7.05; C, 71.60; Y, 20.70.

$[(2,4,7\text{-}Me_3C_9H_4)_2Y(\mu\text{-}H)]_2 \cdot (C_6H_{12})_{0.5}$ (3) catalyzed dimerisation of α-olefins. The reactions were studied in sealed NMR tubes with 3 - 9 μmol (5 mg, 5.9 μmol) of **3** and 20-50 fold molar excess of α-olefin or α-olefin and styrene in a ratio 2/3 in 0.5 mL of benzene-d_6. The resulting solutions were heated to 80-100 °C, cooled to room temperature and measured. The reactions were monitored by ^{1}H NMR spectroscopy, after 10 min, 2, 6, 12 and 24 hours. After full conversion time the reaction mixture was quenched with methanol and passed over a glass filter. The ratio of the different products are based on integration of the olefinic and aliphatic proton-resonances, and the GC-MS data.

Homo-dimerisation of 1-hexene:

80% $CH_3(CH_2)_3C(=CH_2)(CH_2)_5CH_3$: ^{1}H NMR (benzene-$d_6$): δ 0.88 (t, 3H, CH_3), 0.89 (t, 3H, CH_3), 1.22 - 1.42 (m, 12 H, CH_2), 2.00 (t, 4H, $CH_2C(=CH_2)CH_2$), 4.85 (s, 2H, $=CH_2$), ^{13}C NMR (benzene-d_6): δ 14.18, 14.29 (CH_3); 22.84, 23.04, 28.21, 29.52, 30.22, 30.41, 32.17, 36.17, 36.47 (CH_2); 109.04 ($=CH_2$); 150.00 ($C=CH_2$).

17% $CH_3(CH_2)_3C(=CH_2)CH_2CH(n\text{-}C_4H_9)(CH_2)_5CH_3$: ^{1}H NMR (benzene-$d_6$): δ 0.85 - 0.94 (m, 9H, CH_3), 1.20 - 1.46 (m, 18 H, CH_2), 1.59 (m, 1H, CH), 1.90 - 2.03 (m, 4H,

$CH_2C(=CH_2)CH_2$), 4.87 (d, 1H, $=CH_2$), 4.91 (d, 1H, $=CH_2$). ^{13}C NMR (benzene-d_6): δ 13.80, 14.20, 14.30 (CH_3); 18.05, 23.05, 23.54, 27.00, 29.25, 30.22, 30.95, 32.33, 33.64, 33.96, 35.74, 35.86 (CH_2); 41.73 (CH); 110.71 ($=CH_2$); 148.91 ($C=CH_2$).

Homo-dimerisation of 3-methyl-1-butene:

90% $CH_3CH(CH_3)C(=CH_2)(CH_2)_2CH(CH_3)_2$: ^1H NMR (benzene-d_6): δ 0.87 (d, 6H, CH_3, J_{HH} = 6.59 Hz), 1.02 (d, 6H, CH_3, J_{HH} = 6.59 Hz), 1.32 (m, 2H, CH_2), 1.46 (m, 1H, CH), 2.01 (t, 2H, CH_2CH_2, J_{HH} = 8.32 Hz), 2.20 (m, 1H, CH), 4.81 (d, 1H, $=CH_2$, J_{HH} = 1.1), 4.86 (d, 1H, $=CH_2$, J_{HH} = 1.1 Hz).

9% $CH_3CH(CH_3)C(=CH_2)CH_2CH(i\text{-}C_3H_7)CH_2CH_2CH(CH_3)_2$: GC-MS (EI, 70 eV): *m/z* 210 (M^+, 1), 140 (32), 139 (67), 127 (90), 43 (100).

Homo-dimerisation of trimethyl(vinyl)silane:

48% *trans*-$(CH_3)_3SiCHCHCH_2CH_2Si(CH_3)_3$: ^1H NMR (benzene-d_6): δ -0.02 (s, 9H, $CH_2Si(CH_3)_3$), 0.14 (s, 9H, $CHSi(CH_3)_3$), 0.58 (m, 2H, CH_2Si, J_{HH} = 8.42 Hz), 2.11 (dt, 2H, CH_2, J_{HH} = 8.42 Hz, J_{HH} = 5.86 Hz), 5.72 (dt, 1H, CH, J_{HH} = 18.68 Hz, J_{HH} = 1.46 Hz), 6.15 (dt, 1H, CH, J_{HH} = 18.68 Hz, J_{HH} = 5.86 Hz). ^{13}C NMR (benzene-d_6): δ -1.51, -0.98 (CH_3); 15.60 (CH_2Si); 31.19 ($CHCH_2$); 127.90 ($CHCH_2$); 150.10 (*C*HSi).

24% *cis*-$(CH_3)_3SiCHCHCH_2CH_2Si(CH_3)_3$: ^1H NMR (benzene-d_6): δ -0.01 (s, 9H, $CH_2Si(CH_3)_3$), 0.18 (s, 9H, $CHSi(CH_3)_3$), 0.50 (m, 2H, CH_2Si), 2.09 (m, 2H, CH_2), 5.55 (dt, 1H, CH, J_{HH} = 13.91 Hz, J_{HH} = 1.10 Hz), 6.41 (dt, 1H, CH, J_{HH} = 13.91 Hz, J_{HH} = 7.32 Hz). ^{13}C NMR (benzene-d_6): δ -1.61, 0.45 (CH_3); 17.41 (CH_2Si); 28.32 ($CHCH_2$); 127.13 ($CHCH_2$); 152.28 (*C*HSi).

26% *trans*-$(CH_3)_3SiCH_2CHCHCH_2Si(CH_3)_3$: ^1H NMR (benzene-d_6): δ 0.02 (s, 9H, CH_3), 1.43 (dd, 4H, CH_2, J_{HH} = 4.40 Hz, J_{HH} = 2.20 Hz) 5.29 (m, 2H, CH), 6.15 (dt, 1H, CH, J_{HH} = 18.68 Hz, J_{HH} = 5.86 Hz). ^{13}C NMR (benzene-d_6): δ -1.87 (CH_3), 23.00 (CH_2), 124.67 (*C*H).

Homo-dimerisation of styrene:

87% *trans*-$C_6H_5CHCHCH_2CH_2C_6H_5$: ^{1}H NMR (benzene-d_6): δ 2.32 (ddt, 2H, CH_2, J_{HH} = 7.33 Hz, J_{HH} = 6.94 Hz, J_{HH} = 0.73 Hz), 2.57 (t, 2H, CH_2-Ph, J_{HH} = 7.33 Hz), 6.08 (dt, 1H, -CH=, J_{HH} = 15.47 Hz, J_{HH} = 6.94 Hz), 6.29 (d, 1H, =CH-Ph, J_{HH} = 15.47 Hz), 7.0-7.3 (m, 10H, C_6H_5). ^{13}C NMR (benzene-d_6): δ 35.08 (CH-CH_2-), 36.01 (-CH_2-Ph), 126.19 (o-C_6H_5), 126.38 (o-C_6H_5), 127.18 (p-C_6H_5), 128.64 (p-C_6H_5), 128.74 (m-C_6H_5), 129.89 (-CH=), 130.90 (=CH-Ph), 138.16 (C_6H_5), 141.97 (C_6H_5). GC-MS (EI, 70 eV, retention time 16:44 min): *m/z* 208 (M^+, 15), 117 (100), 115 (29), 91 (48), 65 (16).

5% *cis*-$C_6H_5CHCHCH_2CH_2C_6H_5$: GC-MS (EI, 70 eV, retention time 15:59 min): *m/z* 208 (M^+, 8), 117 (100), 115 (15), 91 (50), 65 (22).

6% *trans*-$C_6H_5CHCHCH(C_6H_5)CH_3$: ^{1}H NMR (benzene-d_6): δ 1.30 (d, 3H, CH_3, J_{HH} = 7.08 Hz), 3.41 (dq, 1H, C*H*C(Ph)CH_3, J_{HH} = 7.08 Hz, J_{HH} = 5.13 Hz), 6.05 (dd, 1H, -CH=, J_{HH} = 15.63 Hz, J_{HH} = 5.13 Hz), 6.29 (d, 1H, =CH-Ph, J_{HH} = 15.63 Hz), 7.0 - 7.3 (m, 10H, C_6H_5). ^{13}C NMR (benzene-d_6): δ 21.19 (CH_3), 42.77 (CH), 126.45 (o-C_6H_5), 126.58 (o-C_6H_5), 127.25 (p-C_6H_5), 127.60 (p-C_6H_5), 128.74 (m-C_6H_5), 129.02 (-CH=), 135.36 (=CH-Ph), 138.16 (C_6H_5), 141.97 (C_6H_5). GC-MS (EI, 70 eV, retention time 16:16 min): *m/z* 208 (M^+, 16), 194 (11), 193 (15), 178 (5), 127 (9), 115 (100), 91 (60), 65 (19).

Co-dimerization of styrene with 1-hexene:

100% conversion: 88% *trans*-$C_6H_5CHCH(CH_2)_5CH_3$: ^{1}H NMR (benzene-d_6): δ 0.89 (t, 3H, CH_3, J_{HH} = 6.84 Hz), 1.20 - 1.38 (m, 8H, CH_2), 2.09 (dt, 2H, CHC*H*$_2$, J_{HH} = 6.84 Hz, J_{HH} = 6.59 Hz), 6.13 (dt, 1H, -CH=, J_{HH} = 15.62 Hz, J_{HH} = 6.84 Hz), 6.36 (d, 1H, =CH-Ph, J_{HH} = 15.62 Hz), 7.0-7.3 (m, 5H, C_6H_5). ^{13}C NMR (benzene-d_6): δ 14.31 (CH_3); 23.00, 29.28, 29.72, 32.11, 33.41 (CH_2); 126.37 (o-C_6H_5); 127.08 (p-C_6H_5); 128.75 (m-C_6H_5); 130.46 (-CH=); 131.01 (=CH-Ph); 138.39 (C_6H_5). GC-MS (EI, 70 eV, retention time 14:11 min): *m/z* 188 (M^+, 41), 117 (100), 115 (33), 104 (94), 91 (72), 77 (10).

6% $CH_3(CH_2)_3C(=CH_2)(CH_2)_5CH_3$: GC-MS (EI, 70 eV, retention time 10:09 min): *m/z* 168 (M^+, 1), 84 (42), 83 (90), 70 (100).

3% *trans*-$C_6H_5CHCHCH_2CH_2(n\text{-}C_4H_9)(CH_2)_5CH_3$: GC-MS (EI, 70 eV, retention time 18:26 min): *m/z* 272 (M^+, 1), 129 (2), 118 (32), 117 (38), 115 (19), 104 (80), 91 (27), 85 (32), 71 (48), 57 (100).

Co-dimerization of styrene with 3-methyl-1-butene:

98% conversion: 96% *trans*-$C_6H_5CHCHCH_2CH_2CH(CH_3)_2$: ^{1}H NMR (benzene-$d_6$): δ 0.86 (d, 6H, CH_3, J_{HH} = 6.59 Hz), 1.24 (dt, 2H, CH_2CH, J_{HH} = 7.70 Hz, J_{HH} = 6.95 Hz), 1.49 (m, 1H, $CH(CH_3)_2$), 2.06 (ddt, 2H, $CHCH_2$, J_{HH} = 7.70 Hz, J_{HH} = 6.96 Hz, J_{HH} = 1.1 Hz), 6.10 (dt, 1H, -CH=, J_{HH} = 15.74 Hz, J_{HH} = 6.96 Hz), 6.35 (d, 1H, =CH-Ph, J_{HH} = 15.74 Hz), 7.0-7.3 (m, 5H, C_6H_5). ^{13}C NMR (benzene-d_6): δ 22.61 (CH_3), 27.79 (CH); 31.20, 38.78 (CH_2); 126.33 (o-C_6H_5); 127.05 (p-C_6H_5); 128.75 (m-C_6H_5); 130.28 (-CH=); 131.11 (=CH-Ph); 138.41 (C_6H_5).

4% $CH_3CH(CH_3)C(=CH_2)(CH_2)_2CH(CH_3)_2$: see above.

Co-dimerization of styrene with 3,3-dimethyl-1-butene:

14% conversion: 93% *trans*-$C_6H_5CHCHCH_2CH_2C(CH_3)_3$: ^{1}H NMR (benzene-$d_6$): δ 0.86 (s, 9H, CH_3), 1.06 (t, 2H, CH_2C, J_{HH} = 7.70 Hz), 2.05 (ddt, 2H, $CHCH_2$, J_{HH} = 7.70 Hz, J_{HH} = 6.96 Hz, J_{HH} = 1.1 Hz), 6.10 (dt, 1H, -CH=, J_{HH} = 15.80 Hz, J_{HH} = 6.96 Hz), 6.40 (d, 1H, =CH-Ph, J_{HH} = 15.80 Hz), 7.0-7.3 (m, 5H, C_6H_5).

Co-dimerization of styrene with trimethyl(vinyl)silane:

100% conversion: 92% *trans*-$C_6H_5CHCHCH_2CH_2Si(CH_3)_3$: ^{1}H NMR (benzene-$d_6$): δ -0.01 (s, 9H, CH_3), 0.60 (m, 2H, CH_2Si, J_{HH} = 8.03 Hz), 2.11 (dt, 2H, CH_2, J_{HH} = 8.03 Hz, J_{HH} = 6.59 Hz), 6.18 (dt, 1H, -CH=, J_{HH} = 15.75 Hz, J_{HH} = 6.59 Hz), 6.29 (d, 1H, =CH-Ph, J_{HH} = 15.75 Hz), 7.0-7.3 (m, 5H, C_6H_5). ^{13}C NMR (benzene-d_6): δ -1.54 (CH_3), 16.43 (CH_2Si), 27.71 ($CHCH_2$), 126.35 (o-C_6H_5), 127.03 (p-C_6H_5), 128.75 (-CH=), 128.80 (m-C_6H_5), 133.58 (=CH-Ph), 138.47 (C_6H_5). GC-MS (EI, 70 eV, retention time 13:25 min): *m/z* 204 (M^+, 9), 130 (6), 115 (5), 91 (6), 73 (100).

6% isomers of *$(CH_3)_3SiC_4H_8Si(CH_3)_3$*: GC-MS (EI, 70 eV, retention time 8:04 min): *m/z* 200 (M^+, 5), 112 (2), 97 (8), 73 (100).

Co-dimerization of styrene with 3-phenyl-1-propene:

98% conversion: 90% *trans-$C_6H_5CHCH(CH_2)_3C_6H_5$*: ^{1}H NMR (benzene-d_6): δ 1.62 (tt, 2H, $CH_2CH_2CH_2$, J_{HH} = 7.96 Hz, J_{HH} = 6.94 Hz), 2.03 (ddt, 2H, $CHCH_2$, J_{HH} = 6.94 Hz, J_{HH} = 6.94 Hz, J_{HH} = 0.70 Hz), 2.48 (t, 2H, CH_2-Ph, J_{HH} = 7.96 Hz), 6.06 (dt, 1H, -CH=, J_{HH} = 15.75 Hz, J_{HH} = 6.94 Hz), 6.30 (d, 1H, =CH-Ph, J_{HH} = 15.75 Hz), 7.0-7.3 (m, 10H, C_6H_5). ^{13}C NMR (benzene-d_6): δ 31.29 ($CH_2CH_2CH_2$), 32.40 (CH-CH_2-), 35.12 (-CH_2-Ph), 126.06 (o-C_6H_5), 126.36 (o-C_6H_5), 127.13 (p-C_6H_5), 128.60 (p-C_6H_5), 128.75 (m-C_6H_5), 130.46 (-CH=), 130.78 (=CH-Ph), 138.26 (C_6H_5), 142.49 (C_6H_5).

4% *$C_6H_5CH_2C(=CH_2)(CH_2)_3C_6H_5$*: ^{1}H NMR (benzene-$d_6$): δ 1.64 (tt, 2H, $CH_2CH_2CH_2$), 2.10 - 2.40 (m, 4 H, $CH_2CH_2CH_2$), 2.35 (s, 2H, $C_6H_5CH_2C$), 4.60 (d, 1H, $=CH_2$), 4.63 (d, 1H, $=CH_2$), 7.00 - 7.03 (m, 10H, C_6H_5).

Co-dimerization of styrene with 3-(tert-butylthio)-1-propene:

68% conversion: 94% *trans-$C_6H_5CHCH(CH_2)_3SC(CH_3)_3$*: ^{1}H NMR (benzene-$d_6$): δ 1.22 (s, 9H, CH_3), 1.62 (tt, 2H, $CH_2CH_2CH_2$), 2.17 (dt, 2H, $CHCH_2$), 2.40 (t, 2H, CH_2S), 6.02 (dt, 1H, -CH=, J_{HH} = 15.75 Hz, J_{HH} = 6.95 Hz), 6.28 (d, 1H, =CH-Ph, J_{HH} = 15.75 Hz), 7.0-7.3 (m, 5H, C_6H_5).

Co-dimerization of styrene with 2-(3'-butenyl)-2-methyl-1,3-dithiane:

92% conversion: 98% *trans-$C_6H_5CHCH(CH_2)_3C(CH_3)S(CH_2)_3S$*: ^{1}H NMR (benzene-$d_6$): δ 1.49 (m, 2H, SCH_2CH_2), 1.56 (s, 3H, CH_3), 1.68 (tt, 2H, $CH_2CH_2CH_2$), 1.94 (t, 2H, CH_2CCH_3), 2.33 (dt, 2H, $CHCH_2$), 2.40 (m, 4H, SCH_2), 6.09 (dt, 1H, -CH=, J_{HH} = 15.38 Hz, J_{HH} = 6.98 Hz), 6.34 (d, 1H, =CH-Ph, J_{HH} = 15.38 Hz), 7.0-7.3 (m, 5H, C_6H_5).

Co-dimerization of styrene with 2-methyl-2-(5'-hexenyl)-1,3-dithiane:

98% conversion: 99% *trans*-$C_6H_5CHCH(CH_2)_5C(CH_3)S(CH_2)_3S$: ^{1}H NMR (benzene-$d_6$): δ 1.25 (m, 4H, $CHCH_2CH_2CH_2$), 1.49 (m, 4H, CH_2CH_2C, SCH_2CH_2), 1.58 (s, 3H, CH_3), 1.90 (t, 2H, CH_2CCH_3), 2.30 (dt, 2H, $CHCH_2$), 2.49 (m, 4H, SCH_2), 6.06 (dt, 1H, -CH=, J_{HH} = 15.97 Hz, J_{HH} = 6.59 Hz), 6.34 (d, 1H, =CH-Ph, J_{HH} = 15.97 Hz), 7.0-7.3 (m, 5H, C_6H_5). ^{13}C NMR (benzene-d_6): δ 24.66, 25.48, 29.39, 29.56, 33.20, 42.09 (CH_2); 26.38 (SCH_2); 28.00 (CH_3); 49.43 (CCH_3); 126.38 (o-C_6H_5); 127.10 (p-C_6H_5); 128.45 (m-C_6H_5); 130.53 (-CH=); 130.90 (=CH-Ph); 138.35 (C_6H_5).

Co-dimerization of styrene with 3-butenal-diethylacetal:

45% conversion: 90% *trans*-$C_6H_5CHCH(CH_2)_3CH(OCH_2CH_3)_2$: ^{1}H NMR (benzene-$d_6$): δ 1.12 (t, 6H, CH_3), 1.54 (tt, 2H, $CHCH_2CH_2$), 1.68 (dt, 2H, CH_2CH_2CH), 2.38 (dt, 2H, $CHCH_2$), 3.32 (dq, 2H, OCH_2), 3.50 (dq, 2H, OCH_2), 4.44 (t, 1H, CH_2CH), 6.10 (dt, 1H, -CH=, J_{HH} = 15.38 Hz, J_{HH} = 6.98 Hz), 6.30 (d, 1H, =CH-Ph, J_{HH} = 15.38 Hz), 7.0-7.3 (m, 5H, C_6H_5). ^{13}C NMR (benzene-d_6): δ 15.62 (CH_3); 24.94, 33.19, 33.50 (CH_2); 60.74 (OCH_2); 102.93 ($CH(OR)_2$); 126.53 (o-C_6H_5); 127.17 (p-C_6H_5); 128.71 (m-C_6H_5); 130.67 (-CH=); 130.72 (=CH-Ph); 137.92 (C_6H_5).

NMR tube reaction of 3 with 3-phenyl-1-propene. To a NMR tube charged with a benzene-*d*6 solution of 15 mg (17.6 mmol) of **3** was added 10 μL (76.2 mmol) of 3-phenyl-1-propen. After 24 hours at 50 °C all allylbenzene had been consumed to give $Ind'_2Y(\eta^3\text{-}CH_2CHCHPh)$ together with propylbenzene, β-methylstyrene and dimers. ^{1}H NMR (benzene-d_6): δ 1.40 (C_6H_{12}), 1.93 (s, 3H, CH_3), 2.21 (s, 6H, CH_3), 2.28 (s, 3H, CH_3), 2.34 (s, 6H, CH_3), 2.46 (m, 2H, CH_2), 4.47 (dd, 1H, $CHPh$, J_{HH} = 13.9 Hz, J_{YH} = 3.6 Hz), 6.20 (br, 4H, CH), 6.60 (br, 4H, CH), 6.95-7.30 (m, 5H, Ph), 7.61 (dddd, 1H, CH_2CH, J_{HH} = 13.9 Hz, J_{HH} = 9.6 Hz, J_{HH} = 9.5 Hz, J_{YH} = 3.5 Hz).

NMR tube reaction of 3 with 3-(*tert*-butylthio)-1-propene. To a NMR tube charged with a benzene-*d*6 solution of 15 mg (17.6 mmol) of **3** was added 3.1 μL (18.0 mmol) of 3-(*tert*-

butylthio)-1-propen. After 24 hours at room temperature, all 3-(*tert*-butylthio)-1-propen had been consumed to give Ind'$_2$YCH$_2$CH$_2$CH$_2$SC(CH$_3$)$_3$ as the predominant product. ^{1}H NMR (benzene-d_6): δ -1.07 (m, 2H, YCH$_2$), 0.95 (s, 9H, CMe$_3$), 1.40 (C$_6$H$_{12}$), 2.05 (s, 6H, CH$_3$), 2.12 (m, 2H, CH$_2$C*H*$_2$), 2.29 (m, 2H, CH$_2$S), 2.48 (s, 12H, CH$_3$), 6.26 (br, 4H, CH), 6.76 (s, 4H, CH). ^{13}C NMR (benzene-d_6): δ 15.40 (10); 19.96 (11, 12); 27.19 (C$_6$H$_{12}$); 30.41 (br, CH$_2$*C*H$_2$, C(*C*H$_3$)$_3$); 31.11 (*C*Me$_3$); 37.22 (CH$_2$S); 41.40 (d, YCH$_2$, J_{YC} = 46.4 Hz); 98.38 (1, 3); 121.43 (5, 6); 128.29, 128.50, 129.78, 131.51 (2, 4, 7, 8, 9).

Synthesis of Cp*$_2$YCH(Ph)CH$_3$. To a suspension of 20 mg (28 μmol) of (Cp*$_2$YH)$_2$ in 5 ml of cyclohexane was added 9 μL (0.065 mmol) of styrene. Removal of the solvent in vacuo gave a bright orange solid in quantitative yield. ^{1}H NMR (C$_6$D$_6$, 20 °C): δ 1.60 (d, 3H, CH$_3$, J_{HH} = 6.22 Hz), 1.68 (s, 15H, CH$_3$), 1.95 (s, 15H, CH$_3$), 2.76 (dq, 1 H, C*H*CH$_3$, J_{HH} = 6.22 Hz, J_{YH} = 7 Hz), 6.50 (br, 1H, C$_6$H$_5$), 6.63 (t, 1H, C$_6$H$_5$, J_{HH} = 7.68 Hz), 6.98 (t, 2H, C$_6$H$_5$, J_{HH} = 7.22), 7.21 (d, 1H, C$_6$H$_5$, J_{HH} = 4.40). ^{13}C NMR (C$_6$D$_6$, 20 °C): δ 10.40, 11.27 (Cp*, J_{CH} = 126 Hz); 12.60 (CH*C*H$_3$, J_{CH} = 123 Hz); 49.20 (*C*HCH$_3$, J_{CH} = 131 Hz, J_{YC} = 16.8 Hz); 111.6 (br, C$_6$H$_5$); 117.28, 117.44 (Cp*); 118.30 (C$_6$H$_5$, J_{CH} = 161.1 Hz); 128.50 133.40, 154.65 (C$_6$H$_5$).

Synthesis of Cp*$_2$LaCH(Ph)CH$_3$. To a suspension of 25 mg (0.030 mmol) of (Cp*$_2$LaH)$_2$ in 5 ml of cyclohexane was added 9 μL (0.065 mmol) of styrene. Removal of the solvent in vacuo gave a bright orange solid in quantitative yield. ^{1}H NMR (C$_6$D$_6$, 20 °C): δ 1.68 (s, 15H, CH$_3$), 1.71 (d, 3H, CH$_3$, J_{HH} = 5.86 Hz), 1.96 (s, 15H, CH$_3$), 2.37 (q, 1 H, C*H*CH$_3$, J_{HH} = 5.86 Hz), 5.59 (br, 1H, C$_6$H$_5$), 6.49 (t, 1H, C$_6$H$_5$, J_{HH} = 7.32 Hz), 6.60 - 7.20 (br, 3H, C$_6$H$_5$). ^{1}H NMR (toluene-d_8, -30 °C): δ 1.69 (s, 15H, CH$_3$), 1.72 (d, 3H, CH$_3$, J_{HH} = 5.86 Hz), 1.97 (s, 15H, CH$_3$), 2.40 (q, 1 H, C*H*CH$_3$, J_{HH} = 5.86 Hz), 5.53 (d, 1H, C$_6$H$_5$, J_{HH} = 7.32 Hz), 6.51 (t, 1H, C$_6$H$_5$, J_{HH} = 7.33 Hz), 6.60 (t, 1H, C$_6$H$_5$, J_{HH} = 8.33 Hz), 6.92 (d, 1H, C$_6$H$_5$, J_{HH} = 8.33 Hz), 7.22 (m, 1H, C$_6$H$_5$). ^{13}C NMR (toluene-d_8, -30 °C): δ 10.03, 10.92 (Cp*, J_{CH} = 125.1 Hz); 11.57 (CH*C*H$_3$, J_{CH} = 115.6 Hz); 64.53 (*C*HCH$_3$, J_{CH} = 136.2 Hz); 106.60 (C$_6$H$_5$, J_{CH} =

141.8 Hz), 116.00 (C_6H_5, J_{CH} = 162.3 Hz), 118.81, 119.14 (Cp*); 120.07 (C_6H_5, J_{CH} = 155.6 Hz); 131.70 (C_6H_5, J_{CH} = 156.7 Hz); 132.60 (C_6H_5, J_{CH} = 154.8 Hz); 149.67 (C_6H_5).

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Table 1.

a. Crystal data and details of the structure determination.

Chemical formula	$C_{48}H_{54}Y_2 \cdot [C_6H_6]_{0.5}$
Formula weight, g.mol^{-1}	847.83
Crystal system	monoclinic
Space group, no.	$P2_1/n$
a, Å	12.387(1)
b, Å	21.854(1)
c, Å	16.322(1)
β, deg	106.998(5)
V, Å^3	4225.4(5)
Z	4
D_{cacl}, g·cm^{-3}	1.333
F(000), electrons	1764
μ(Mo *K*), cm^{-1}	27.66
Approx. crystal dimension, mm	0.10 x 0.20 x 0.40

b. Data collection.

Radiation	Mo *Kα*
Wavelength, Å	0.71073
Monochromator	Graphite
Temperature, K	130
range; min. max., deg	1.61, 25.0
ω/2 scan, deg	Δω = 0.80 + 0.34 tg
Data set	*h*: 0→14; k: 0→25; l: -19→18
Crystal-to-receiving-aperture distance, mm	173
Horizontal, vertical aperture, mm	3.2 + tg ; 4.0
Reference reflections,	31-5, 1.7
r.m.s. dev. in %	-1-3-5, 1.0
Drift correction	0.973 - 1.000
X-ray exposure time, h	105.0
Total data	7422
Unique data	7143
Observed data ($F_o \geq 4.0\ \sigma\ (F_o)$)	4412

$R_{sig} = \Sigma \sigma(F_o^2) / \Sigma [F_o^2]$	0.117

c. Refinement.

Number of reflections	6430
Number of refined parameters	498
Final agreement factors:	
$R(F) = \Sigma(\|\|F_o\|-\|F_c\|\|)/\Sigma F_o$	0.0763
for $F_o > 4.0\ \sigma(F_o)$	
$wR(F^2) = [\Sigma[w(F_o^2-F_c^2)^2]/\Sigma w(F_o^2)^2]^{1/2}$	0.1871
for $F_o^2 > 0$	
Weighting scheme: *a*, *b*	0.1046, 2.4527
$w = 1/[\sigma^2 (F_o)^2 + (aP)^2 + bP]$	
and $P = [\max(F_o^2,0) + 2F_c^2]/3$.	
GooF = S = $[\Sigma[w(F_o^2-F_c^2)^2]/(n-p)]^{1/2}$	1.040
n = number of reflections	
p = number of parameters refined	
Residual electron density in final difference Fourier map, e/Å^3	1.17(14)
Max. (shift/σ) final cycle	<0.001

Table 2.

Final fractional atomic coordinates and equivalent isotropic thermal displacement Parameters for non-H atoms with e.s.d.'s in parentheses. Atoms of the Asymmetric Unit.

Atom	*x*	*y*	*z*	U_{eq} (Å^2)*
Y(1)	-0.04339(6)	0.36339(4)	0.22168(5)	0.0193(3)
C(1)	0.0580(8)	0.3809(4)	0.3880(5)	0.032(3)
C(2)	0.0328(7)	0.3197(4)	0.3779(5)	0.024(3)
C(3)	-0.0879(7)	0.3114(4)	0.3543(5)	0.024(3)
C(4)	-0.1338(7)	0.3714(4)	0.3505(5)	0.025(3)
C(5)	-0.0444(8)	0.4135(4)	0.3678(5)	0.027(3)
C(6)	-0.1557(7)	0.2577(4)	0.3373(5)	0.024(3)
C(7)	-0.2716(7)	0.2677(4)	0.3135(5)	0.027(3)
C(8)	-0.3169(7)	0.3257(4)	0.3124(5)	0.029(3)
C(9)	-0.2549(8)	0.3778(4)	0.3290(6)	0.030(3)
C(10)	0.1724(8)	0.4098(5)	0.4144(6)	0.042(3)

C(11)	-0.1067(8)	0.1954(4)	0.3447(6)	0.032(3)
C(12)	-0.3047(9)	0.4399(5)	0.3348(7)	0.049(4)
C(13)	-0.2146(6)	0.3948(4)	0.0882(5)	0.018(3)
C(14)	-0.2027(7)	0.4415(4)	0.1475(5)	0.024(3)
C(15)	-0.1013(7)	0.4748(4)	0.1549(5)	0.027(3)
C(16)	-0.0459(6)	0.4430(4)	0.0997(5)	0.022(3)
C(17)	-0.1162(6)	0.3942(4)	0.0599(5)	0.019(3)
C(18)	-0.0541(8)	0.5279(4)	0.1999(6)	0.036(3)
C(19)	0.0471(8)	0.5462(5)	0.1930(7)	0.045(4)
C(20)	0.1058(8)	0.5136(5)	0.1449(7)	0.047(4)
C(21)	0.0633(7)	0.4640(4)	0.0969(6)	0.031(3)
C(22)	-0.3134(7)	0.3523(4)	0.0607(6)	0.031(3)
C(23)	-0.1197(9)	0.5649(5)	0.2471(7)	0.046(4)
C(24)	0.1222(7)	0.4313(5)	0.0409(6)	0.034(3)
H(101)	0.83(4)	0.8333(19)	0.164(4)	0.030(16)
H(102)	-0.030(5)	0.270(2)	0.203(4)	0.02(2)
Y(2)	0.09462(6)	0.24319(4)	0.14266(5)	0.0194(3)
C(25)	0.2311(7)	0.1915(4)	0.2790(5)	0.024(3)
C(26)	0.2545(7)	0.2536(4)	0.2876(5)	0.025(3)
C(27)	0.3080(6)	0.2714(4)	0.2252(5)	0.026(3)
C(28)	0.3131(7)	0.2168(5)	0.1753(5)	0.029(3)
C(29)	0.2615(7)	0.1688(4)	0.2090(5)	0.028(3)
C(30)	0.3529(7)	0.3275(5)	0.2068(6)	0.036(3)
C(31)	0.4030(8)	0.3275(6)	0.1412(7)	0.052(4)
C(32)	0.4112(8)	0.2752(6)	0.0949(7)	0.051(4)
C(33)	0.3700(7)	0.2190(6)	0.1095(6)	0.044(4)
C(34)	0.1815(8)	0.1528(4)	0.3348(6)	0.035(3)
C(35)	0.3482(8)	0.3834(5)	0.2596(8)	0.054(4)
C(36)	0.3852(8)	0.1619(6)	0.0641(6)	0.054(4)
C(37)	-0.0007(7)	0.2351(4)	-0.0272(5)	0.025(3)
C(38)	0.0657(7)	0.1826(4)	-0.0027(5)	0.025(3)
C(39)	0.0163(7)	0.1436(4)	0.0474(5)	0.025(3)
C(40)	-0.0803(6)	0.1770(4)	0.0570(5)	0.020(3)
C(41)	-0.0886(7)	0.2327(4)	0.0115(5)	0.023(3)
C(42)	0.0447(7)	0.0857(4)	0.0833(6)	0.027(3)
C(43)	-0.0186(8)	0.0626(5)	0.1330(6)	0.037(3)
C(44)	-0.1116(8)	0.0959(4)	0.1450(6)	0.030(3)
C(45)	-0.1446(6)	0.1505(4)	0.1078(5)	0.023(3)
C(46)	0.0197(7)	0.2862(4)	-0.0832(5)	0.029(3)
C(47)	0.1362(8)	0.0474(4)	0.0646(7)	0.043(4)
C(48)	-0.2477(7)	0.1831(4)	0.1159(6)	0.029(3)
C(49)	-0.5276(9)	0.4662(5)	-0.0751(7)	0.049(4)
C(50)	-0.4355(9)	0.5060(6)	-0.0531(8)	0.056(4)
C(51)	-0.5922(9)	0.4620(6)	-0.0199(9)	0.059(5)

*) $U_{eq} = 1/3_{ij} U_{ij} a_i^* a_j^* \mathbf{a_i.a_j}$

Table 3.

Selected data on the geometry. Standard deviations in the last decimal place are given in parentheses.

Interatomic Distances (Å)

Y(1)	-C(1)	2.665(8)		C(6)	-C(7)	1.391(13)	
Y(1)	-C(2)	2.626(8)		C(6)	-C(11)	1.481(13)	
Y(1)	-C(3)	2.642(8)		C(7)	-C(8)	1.384(12)	
Y(1)	-C(4)	2.661(8)		C(8)	-C(9)	1.356(13)	
Y(1)	-C(5)	2.628(8)		C(9)	-C(12)	1.505(14)	
Y(1)	-C(13)	2.648(8)		C(13)	-C(14)	1.384(12)	
Y(1)	-C(14)	2.622(9)		C(13)	-C(17)	1.424(11)	
Y(1)	-C(15)	2.678(9)		C(13)	-C(22)	1.497(12)	
Y(1)	-C(16)	2.637(8)		C(14)	-C(15)	1.426(13)	
Y(1)	-C(17)	2.617(8)		C(15)	-C(16)	1.458(12)	
C(1)	-C(2)	1.372(12)		C(15)	-C(18)	1.406(12)	
C(1)	-C(5)	1.407(14)		C(16)	-C(17)	1.410(12)	
C(1)	-C(10)	1.495(14)		C(16)	-C(21)	1.442(12)	
C(2)	-C(3)	1.442(13)		C(18)	-C(19)	1.352(15)	
C(3)	-C(4)	1.423(12)		C(18)	-C(23)	1.508(15)	
C(3)	-C(6)	1.422(12)		C(19)	-C(20)	1.409(15)	
C(4)	-C(5)	1.403(13)		C(20)	-C(21)	1.351(14)	
C(4)	-C(9)	1.444(14)		C(21)	-C(24)	1.506(13)	

Bond angles (deg.)

C(1)	-Y(1)	-C(2)	30.1(3)	C(2)	-C(1)	-C(10)	127.5(9)
C(1)	-Y(1)	-C(3)	51.4(3)	C(5)	-C(1)	-C(10)	124.5(8)
C(1)	-Y(1)	-C(4)	50.8(3)	Y(1)	-C(2)	-C(1)	76.5(5)
C(1)	-Y(1)	-C(5)	30.8(3)	Y(1)	-C(2)	-C(3)	74.7(5)
C(1)	-Y(1)	-C(13)	145.7(3)	C(1)	-C(2)	-C(3)	109.7(8)
C(1)	-Y(1)	-C(14)	116.3(3)	Y(1)	-C(3)	-C(2)	73.5(5)
C(1)	-Y(1)	-C(15)	105.9(3)	Y(1)	-C(3)	-C(4)	75.2(5)
C(1)	-Y(1)	-C(16)	124.9(3)	Y(1)	-C(3)	-C(6)	116.6(5)
C(1)	-Y(1)	-C(17)	155.8(3)	C(2)	-C(3)	-C(4)	105.4(7)
C(2)	-Y(1)	-C(3)	31.8(3)	C(2)	-C(3)	-C(6)	131.5(8)
C(2)	-Y(1)	-C(4)	51.1(3)	C(4)	-C(3)	-C(6)	123.1(8)
C(2)	-Y(1)	-C(5)	50.7(3)	Y(1)	-C(4)	-C(3)	73.7(5)
C(2)	-Y(1)	-C(13)	150.1(3)	Y(1)	-C(4)	-C(5)	73.3(5)
C(2)	-Y(1)	-C(14)	133.9(3)	Y(1)	-C(4)	-C(9)	117.5(6)
C(2)	-Y(1)	-C(15)	134.7(3)	C(3)	-C(4)	-C(5)	108.3(8)
C(2)	-Y(1)	-C(16)	153.4(3)	C(3)	-C(4)	-C(9)	118.2(8)
C(2)	-Y(1)	-C(17)	173.4(3)	C(5)	-C(4)	-C(9)	133.5(8)
C(3)	-Y(1)	-C(4)	31.1(3)	Y(1)	-C(5)	-C(1)	76.0(5)
C(3)	-Y(1)	-C(5)	51.5(3)	Y(1)	-C(5)	-C(4)	75.9(5)
C(3)	-Y(1)	-C(13)	118.5(3)	C(1)	-C(5)	-C(4)	108.6(8)

C(3)	-Y(1)	-C(14)	110.4(3)
C(3)	-Y(1)	-C(15)	129.0(3)
C(3)	-Y(1)	-C(16)	160.6(3)
C(3)	-Y(1)	-C(17)	147.6(3)
C(4)	-Y(1)	-C(5)	30.8(3)
C(4)	-Y(1)	-C(13)	102.2(3)
C(4)	-Y(1)	-C(14)	83.6(3)
C(4)	-Y(1)	-C(15)	97.9(3)
C(4)	-Y(1)	-C(16)	129.7(3)
C(4)	-Y(1)	-C(17)	132.8(3)
C(5)	-Y(1)	-C(13)	115.1(3)
C(5)	-Y(1)	-C(14)	86.9(3)
C(5)	-Y(1)	-C(15)	85.3(3)
C(5)	-Y(1)	-C(16)	114.1(3)
C(5)	-Y(1)	-C(17)	135.8(3)
C(13)	-Y(1)	-C(14)	30.5(3)
C(13)	-Y(1)	-C(15)	51.3(3)
C(13)	-Y(1)	-C(16)	51.5(2)
C(13)	-Y(1)	-C(17)	31.4(2)
C(14)	-Y(1)	-C(15)	31.2(3)
C(14)	-Y(1)	-C(16)	51.7(3)
C(14)	-Y(1)	-C(17)	51.4(3)
C(15)	-Y(1)	-C(16)	31.8(3)
C(15)	-Y(1)	-C(17)	51.9(3)
C(16)	-Y(1)	-C(17)	31.1(3)
Y(1)	-C(1)	-C(2)	73.4(5)
Y(1)	-C(1)	-C(5)	73.1(5)
Y(1)	-C(1)	-C(10)	118.6(6)
C(2)	-C(1)	-C(5)	107.9(8)
Y(1)	-C(17)	-C(13)	75.5(5)
Y(1)	-C(17)	-C(16)	75.2(5)
C(13)	-C(17)	-C(16)	108.4(7)
C(15)	-C(18)	-C(19)	117.1(9)
C(15)	-C(18)	-C(23)	120.4(9)
C(19)	-C(18)	-C(23)	122.4(9)

C(3)	-C(6)	-C(7)	115.3(8)
C(3)	-C(6)	-C(11)	122.5(8)
C(7)	-C(6)	-C(11)	122.2(8)
C(6)	-C(7)	-C(8)	121.9(8)
C(7)	-C(8)	-C(9)	124.2(9)
C(4)	-C(9)	-C(8)	117.0(8)
C(4)	-C(9)	-C(12)	119.2(8)
C(8)	-C(9)	-C(12)	123.4(9)
Y(1)	-C(13)	-C(14)	73.7(5)
Y(1)	-C(13)	-C(17)	73.1(4)
Y(1)	-C(13)	-C(22)	118.3(6)
C(14)	-C(13)	-C(17)	107.9(7)
C(14)	-C(13)	-C(22)	125.3(8)
C(17)	-C(13)	-C(22)	126.8(8)
Y(1)	-C(14)	-C(13)	75.8(5)
Y(1)	-C(14)	-C(15)	76.6(5)
C(13)	-C(14)	-C(15)	110.3(7)
Y(1)	-C(15)	-C(14)	72.2(5)
Y(1)	-C(15)	-C(16)	72.5(5)
Y(1)	-C(15)	-C(18)	121.1(6)
C(14)	-C(15)	-C(16)	105.4(7)
C(14)	-C(15)	-C(18)	133.4(8)
C(16)	-C(15)	-C(18)	121.1(8)
Y(1)	-C(16)	-C(15)	75.6(5)
Y(1)	-C(16)	-C(17)	73.6(5)
Y(1)	-C(16)	-C(21)	115.5(6)
C(15)	-C(16)	-C(17)	107.8(7)
C(15)	-C(16)	-C(21)	118.9(8)
C(17)	-C(16)	-C(21)	133.2(8)
C(18)	-C(19)	-C(20)	122.6(10)
C(19)	-C(20)	-C(21)	123.5(10)
C(16)	-C(21)	-C(20)	116.6(8)
C(16)	-C(21)	-C(24)	119.6(8)
C(20)	-C(21)	-C(24)	123.8(9)