labeled drawing of the dimer; crystal packing is shown in Fig. 2.

Discussion. The dimer is joined across an inversion center by an (η^5,η^1)-Cp* group which bridges the two symmetry-related Sc atoms. The η^1-methylene (C6) has been formed as the result of C—H activation of a Cp* methyl group. A somewhat surprising result is that, in all other regards, the bonding is very similar to that determined for $Cp^*_2ScCH_3$ (Thompson *et al.*, 1987). The (η^5,η^1)-ring remains planar with a maximum deviation of only 0.22 Å from the least-squares plane calculated for C1 through C10. The geometry about C6 is essentially tetrahedral; the angles C1—C6—Sc′, C1—C6—H6*A*, C1—C6—H6*B* and H6*A*—C6—H6*B* are 118.9, 107.3, 104.8 and 98.1°, respectively, giving an average value of 107.3 (8.6)°. The H6*A*—C6—H6*B* angle is slightly compressed (98.1°) while the C1—C6—Sc′ angle is somewhat opened (118.9°). The Sc′···H6*A* and Sc′···H6*B* distances are 2.76 (3) and 2.79 (3) Å indicating that there is no agostic interaction for the α-H atoms with the Sc center. The Cp*—Sc—Cp* angle (141.8°) is approximately the same as for $Cp^*_2ScCH_3$ (144.7°) suggesting that formal replacement of a methyl ligand with a bulkier (η^5,η^1)-Cp* group as the alkyl does not significantly perturb the Sc—Cp* bonding.

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A Silicon-Bridged Bis(substituted Cp) Yttrium Complex

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Abstract. *rac*-Bis(tetrahydrofuran)lithium [bis(2-trimethylsilyl-4-*tert*-butyl-η^5-cyclopentadienyl)dimethylsilane]dichloroyttrate, $[Li(C_4H_8O)_2][Y(C_{26}H_{48}Si_3)Cl_2]$, $M_r = 755.87$, triclinic, $P\bar{1}$, $a = 13.110\,(8)$, $b = 17.163\,(15)$, $c = 20.623\,(14)$ Å, $\alpha = 104.02\,(7)$, $\beta = 99.38\,(5)$, $\gamma = 100.24\,(6)$°, $V = 4326\,(6)$ Å^3, $Z = 4$, $D_x = 1.16$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71073 Å, $\mu = 15.86$ cm^{-1}, $F(000) = 1608$, room temperature, $R = 0.056$ for 6136 reflections with $F_o^2 > 3\sigma(F_o^2)$. There are two virtually identical molecules in the asymmetric unit. In each, the Y atom is tetrahedrally coordinated to a substituted Si-bridged bis(cyclopentadienyl) ligand and to two Cl ions in the cleft. The Li atom is 2.35 Å from each Cl ion, and two molecules of tetrahydrofuran are connected to the Li, completing its tetrahedral coordination.

Introduction. The Ziegler–Natta polymerization of olefins has occupied the attention of chemists for nearly four decades. Recently, the development of homogeneous transition-metal catalyst systems has afforded the possibility of mechanistic investigations into various key steps of polymer initiation, propagation and chain termination. Brintzinger and coworkers have developed a series of *ansa*-zirconocene catalysts which possess a C_2 symmetric ligand arrangement about the metal center (Roll, Brintzinger, Rieger & Zolk, 1990; Wiesenfeldt, Reinmuth, Barsties, Evertz & Brintzinger, 1989). Moreover, activation of these *ansa*-zirconocene catalysts with methylalumoxane results in production of highly isospecific polymers. Work in this laboratory has centered on the study of well defined single-component Ziegler–Natta-type catalyst systems (Piers, Shapiro, Bunel & Bercaw, 1990). We report

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Table 1. *Final heavy-atom coordinates* ($\times 10^4$) *and equivalent isotropic displacement parameters* ($Å^2 \times 10^4$)

$U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
Y*a*	1810 (.4)	7217 (.3)	4009 (.3)	432 (2)
Cl1*a*	3262 (1)	6960 (1)	3292 (1)	719 (5)
Cl2*a*	2931 (1)	8756 (1)	4442 (1)	708 (5)
Si1*a*	−400 (1)	6062 (1)	4245 (1)	611 (5)
Si2*a*	1161 (2)	8070 (1)	5831 (1)	813 (6)
Si3*a*	372 (1)	5333 (1)	2407 (1)	632 (5)
C1*a*	−1428 (5)	6446 (4)	4683 (3)	976 (23)
C2*a*	−793 (5)	4914 (4)	3970 (3)	903 (21)
C3*a*	978 (4)	6434 (4)	4793 (3)	531 (16)
C4*a*	1549 (4)	7246 (3)	5231 (3)	525 (17)
C5*a*	2638 (5)	7228 (4)	5301 (3)	587 (18)
C6*a*	2789 (5)	6479 (4)	4926 (3)	563 (17)
C7*a*	1748 (5)	5989 (3)	4610 (3)	571 (18)
C8*a*	567 (6)	7615 (5)	6447 (3)	1259 (29)
C9*a*	245 (6)	8639 (4)	5464 (4)	1368 (30)
C10*a*	2392 (6)	8882 (4)	6303 (3)	1038 (26)
C11*a*	3807 (5)	6180 (4)	4988 (4)	696 (21)
C12*a*	4745 (5)	6882 (4)	5048 (4)	1049 (26)
C13*a*	3780 (5)	5484 (5)	4385 (4)	1252 (29)
C14*a*	3948 (5)	5889 (4)	5634 (4)	1177 (26)
C15*a*	−204 (4)	6555 (3)	3552 (3)	475 (17)
C16*a*	280 (4)	6335 (3)	2977 (3)	450 (15)
C17*a*	585 (4)	7071 (4)	2782 (3)	508 (16)
C18*a*	295 (4)	7738 (3)	3200 (3)	523 (18)
C19*a*	−156 (4)	7421 (4)	3682 (3)	529 (17)
C20*a*	1199 (5)	4727 (3)	2801 (3)	954 (23)
C21*a*	−985 (5)	4682 (4)	2047 (4)	1240 (29)
C22*a*	965 (5)	5552 (3)	1698 (3)	902 (23)
C23*a*	317 (5)	8576 (4)	3081 (3)	679 (20)
C24*a*	1242 (6)	8841 (4)	2763 (3)	960 (23)
C25*a*	372 (6)	9235 (4)	3732 (4)	1043 (26)
C26*a*	−726 (6)	8500 (4)	2585 (4)	1278 (27)
Y*b*	3053 (.4)	2441 (.3)	867 (.3)	450 (2)
Cl1*b*	2749 (1)	3843 (1)	1553 (1)	642 (4)
Cl2*b*	4415 (1)	3364 (1)	406 (1)	751 (5)
Si1*b*	1996 (1)	449 (1)	726 (1)	536 (5)
Si2*b*	2974 (1)	900 (1)	−942 (1)	725 (6)
Si3*b*	2180 (1)	2113 (1)	2530 (1)	632 (5)
C1*b*	2456 (5)	−477 (3)	297 (3)	765 (19)
C2*b*	829 (4)	83 (3)	1066 (3)	627 (18)
C3*b*	1682 (4)	1105 (3)	156 (3)	441 (16)
C4*b*	2233 (4)	1382 (3)	−330 (3)	535 (18)
C5*b*	1854 (4)	2088 (4)	−425 (3)	578 (18)
C6*b*	1106 (4)	2267 (3)	−28 (3)	496 (17)
C7*b*	1026 (4)	1661 (3)	330 (3)	463 (16)
C8*b*	4245 (5)	652 (4)	−590 (3)	997 (22)
C9*b*	3356 (5)	1625 (4)	−1452 (3)	1007 (23)
C10*b*	2094 (5)	−67 (4)	−1534 (3)	1039 (25)
C11*b*	402 (4)	2873 (3)	−76 (3)	518 (17)
C12*b*	1022 (5)	3688 (4)	−149 (3)	797 (20)
C13*b*	−476 (5)	2469 (4)	−728 (3)	795 (20)
C14*b*	−114 (5)	3050 (4)	525 (3)	769 (19)
C15*b*	3123 (4)	1210 (3)	1392 (3)	465 (16)
C16*b*	3090 (4)	1899 (3)	1949 (3)	464 (17)
C17*b*	4127 (5)	2438 (3)	2100 (3)	548 (18)
C18*b*	4772 (5)	2123 (4)	1669 (3)	534 (18)
C19*b*	4131 (5)	1370 (3)	1230 (3)	555 (18)
C20*b*	872 (4)	2259 (3)	2133 (3)	699 (18)
C21*b*	2823 (5)	3081 (4)	3217 (3)	892 (22)
C22*b*	1952 (6)	1256 (4)	2931 (3)	1061 (23)
C23*b*	5959 (5)	2444 (4)	1766 (4)	767 (25)
C24*b*	6521 (5)	2046 (4)	2261 (4)	1257 (32)
C25*b*	6284 (4)	3375 (4)	2056 (4)	1076 (30)
C26*b*	6324 (5)	2187 (4)	1100 (4)	1068 (29)
Li*a*	4084 (8)	8380 (6)	3729 (5)	776 (34)
O1*a*	4148 (4)	8946 (4)	3036 (3)	1111 (18)
C27*a*	4386 (7)	9815 (7)	3176 (6)	1758 (44)
C28*a*	4541 (11)	9997 (11)	2520 (11)	2677 (77)
C29*a*	3822 (11)	9301 (14)	2042 (8)	2627 (79)
C30*a*	3910 (8)	8591 (7)	2320 (6)	1723 (44)
O2*a*	5548 (4)	8631 (3)	4200 (3)	1040 (19)
C31*a*	6340 (10)	8477 (9)	3881 (7)	2243 (63)
C32*a*	7242 (17)	8569 (16)	4334 (10)	3091 (105)
C33*a*	7130 (14)	8873 (11)	4969 (9)	2576 (83)
C34*a*	6003 (9)	8994 (5)	4901 (6)	1534 (43)
Li*b*	4128 (8)	4571 (6)	1161 (6)	792 (33)
O1*b*	5229 (4)	5223 (3)	1958 (3)	1035 (19)
C27*b*	6245 (8)	5647 (6)	1925 (5)	1492 (40)

Table 1 (*cont.*)

	x	y	z	U_{eq}
C28*b*	6714 (13)	6188 (10)	2621 (10)	2485 (81)
C29*b*	6127 (15)	5857 (11)	3055 (8)	2715 (90)
C30*b*	5115 (7)	5376 (6)	2646 (5)	1452 (39)
O2*b*	3806 (4)	5367 (3)	713 (3)	1018 (17)
C31*b*	3480 (7)	5239 (5)	−5 (5)	1193 (31)
C32*b*	2784 (9)	5833 (8)	−63 (7)	1821 (51)
C33*b*	3178 (10)	6511 (7)	561 (8)	1849 (51)
C34*b*	3759 (8)	6177 (7)	1041 (5)	1634 (42)

Table 2. *Selected bond distances* (Å) *and angles* (°)

Y*a*—Cp1*a*	2.383	Y*b*—Cp1*b*	2.396
Y*a*—Cp2*a*	2.385	Y*b*—Cp2*b*	2.389
Y*a*—Cl1*a*	2.628 (2)	Y*b*—Cl1*b*	2.614 (1)
Y*a*—Cl2*a*	2.642 (2)	Y*b*—Cl2*b*	2.623 (2)
Li*a*—Cl1*a*	2.366 (11)	Li*b*—Cl1*b*	2.377 (11)
Li*a*—Cl2*a*	2.340 (11)	Li*b*—Cl2*b*	2.401 (11)
Li*a*—O1*a*	1.917 (12)	Li*b*—O1*b*	1.950 (12)
Li*a*—O2*a*	1.925 (12)	Li*b*—O2*b*	1.893 (12)
Si1*a*—C1*a*	1.869 (7)	Si1*b*—C1*b*	1.872 (6)
Si1*a*—C2*a*	1.863 (6)	Si1*b*—C2*b*	1.858 (6)
Si1*a*—C3*a*	1.878 (6)	Si1*b*—C3*b*	1.862 (5)
Si1*a*—C15*a*	1.858 (6)	Si1*b*—C15*b*	1.887 (6)
Si2*a*—C4*a*	1.845 (6)	Si2*b*—C4*b*	1.843 (6)
Si2*a*—C8*a*	1.850 (8)	Si2*b*—C8*b*	1.869 (7)
Si2*a*—C9*a*	1.856 (8)	Si2*b*—C9*b*	1.868 (7)
Si2*a*—C10*a*	1.878 (7)	Si2*b*—C10*b*	1.859 (7)
Cp1*a*—Y*a*—Cp2*a*	122.1	Cp1*b*—Y*b*—Cp2*b*	122.5
Cp1*a*—Y*a*—Cl1*a*	114.2	Cp1*b*—Y*b*—Cl1*b*	112.4
Cp1*a*—Y*a*—Cl2*a*	107.0	Cp1*b*—Y*b*—Cl2*b*	108.6
Cp2*a*—Y*a*—Cl1*a*	108.6	Cp2*b*—Y*b*—Cl1*b*	108.1
Cp2*a*—Y*a*—Cl2*a*	114.2	Cp2*b*—Y*b*—Cl2*b*	114.3
Cl1*a*—Y*a*—Cl2*a*	84.6 (0)	Cl1*b*—Y*b*—Cl2*b*	84.6 (0)
Cl1*a*—Li*a*—Cl2*a*	97.8 (4)	Cl1*b*—Li*b*—Cl2*b*	95.1 (4)
Cl1*a*—Li*a*—O1*a*	113.7 (5)	Cl1*b*—Li*b*—O1*b*	107.9 (5)
Cl1*a*—Li*a*—O2*a*	115.5 (5)	Cl1*b*—Li*b*—O2*b*	117.9 (5)
Cl2*a*—Li*a*—O1*a*	114.3 (5)	Cl2*b*—Li*b*—O1*b*	120.3 (5)
Cl2*a*—Li*a*—O2*a*	113.9 (5)	Cl2*b*—Li*b*—O2*b*	113.3 (5)
O1*a*—Li*a*—O2*a*	102.4 (6)	O1*b*—Li*b*—O2*b*	103.0 (6)
Cl5*a*—Si1*a*—C3*a*	99.1 (3)	Cl5*b*—Si1*b*—C3*b*	99.5 (2)

herein the crystal structure of the C_2 symmetric complex *rac*-$(CH_3)_2Si[2\text{-}Si(CH_3)_3\text{-}4\text{-}C(CH_3)_3C_5H_2]_2\text{-}YCl_2Li(\overline{OCH_2CH_2CH_2CH_2})_2$.

Experimental. A crystal with a most irregular triangular prism shape, 0.63 × 0.67 × 1.18 mm, was used for data collection on a CAD-4 diffractometer, with ω scans. 25 reflections with $26 < 2\theta < 29°$ were used for the determination of the cell dimensions. An absorption correction was not applied: ψ scans of six high χ reflections suggested corrections of ±7% to I, but the corrections resulted in a poorer goodness of fit for merging the data. The crystal was somewhat obscured by grease in its capillary, so no analytical absorption correction could be made; $(\sin\theta/\lambda)_{max} = 0.59$ Å^{-1}; h from −15 to 15, k from −20 to 20, l from 0 to 24. Three standard reflections ($1\overline{2}\overline{5}$, $\overline{3}24$ and $15\overline{2}$) showed no variations greater than those predicted by counting statistics. 16 018 reflections were measured, of which 15 167 were independent. Goodness of fit for merging was 1.35, and R_{int} for 372 reflections with exactly two observations was 0.051. All reflections, F_o^2 positive and negative, were used in solution and refinement of the structure. The structure was solved from a Patterson map, which gave coordinates of Y atoms; remaining atoms were found by successive structure factor–Fourier calculations. F_o^2 values were used in full-matrix least-squares refinement, with $w = 1/\sigma^2(F_o^2)$. H atoms were positioned by calculation (C—H = 0.95 Å) assuming staggered geometries on methyl groups; H-atom parameters were not refined, but the atoms were repositioned near the conclusion of the refinement. R on $F = 0.134$ for 12 716 reflections with $F_o^2 > 0$ (wR on $F^2 = 0.010$); R on $F = 0.056$ for 6136 reflections with $F_o^2 > 3\sigma(F_o^2)$ (wR on $F^2 = 0.007$); and $S = 1.33$ for 15 167 reflections and 775 parameters. Variances $[\sigma^2(F_o^2)]$ were derived from counting statistics plus an additional term, $(0.014I)^2$; variances of the merged data by propagation of e.s.d. plus another additional term, $(0.014\bar{I})^2$. In the final cycle, maximum shift/e.s.d. was 0.09 in the Y molecule, and 1.56 for y of C32 in thf*a* [several parameters of this thf group continued to shift (with no change in the residuals) for at least five full-matrix cycles after the remainder of the structure had settled down, presumably because of disorder]. In the final difference map one peak of 1.01 e Å^{-3} was found near Y*a*; other peaks were ±0.86 e Å^{-3}. Scattering factors were taken from Cromer & Waber (1974) and dispersion corrections (f') from Cromer (1974). Programs used were those of the *CRYM* crystallographic computing system (Duchamp, 1964) and *ORTEP*II (Johnson, 1976). Final heavy-atom parameters are given in Table 1.*

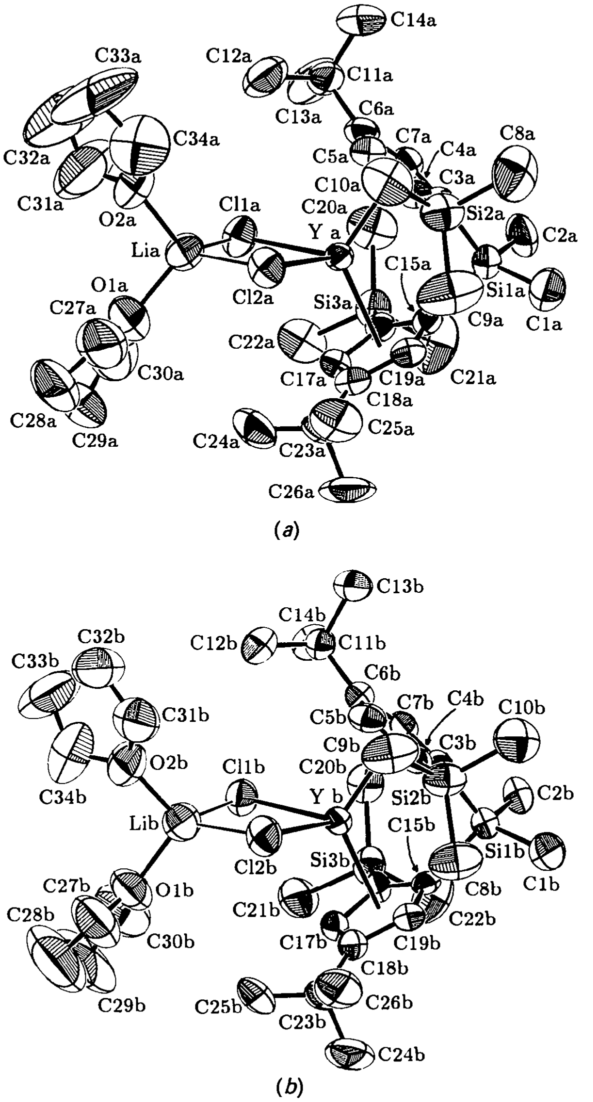

Fig. 1. An *ORTEP*II (Johnson, 1976) drawing showing the atomic numbering systems of (*a*) molecule *A* (C16*a*, between C15*a* and C17*a*, is not labeled) and (*b*) molecule *B* (C16*b* not labeled). Atoms are shown as 50% probability ellipsoids, with H atoms omitted.

Discussion. Fig. 1 shows labeled drawings of molecules *A* and *B*; selected distances and angles for these are given in Table 2. Because the two molecules are so similar, this discussion uses average distances with the scatter standard deviation given in square brackets. Fig. 2 shows the unit-cell packing. The

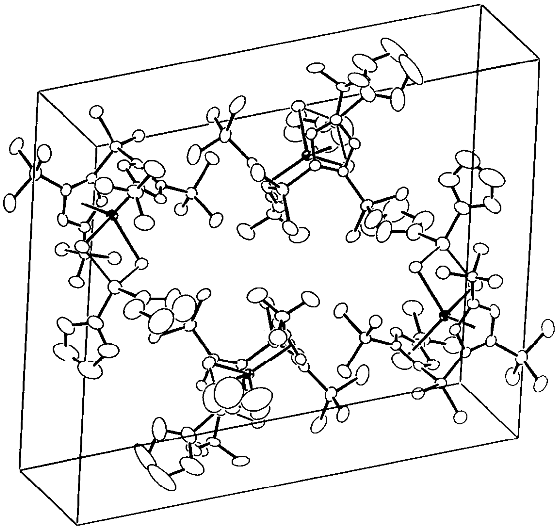

Fig. 2. An *ORTEP*II (Johnson, 1976) view of the contents of a unit cell, with one unit cell outlined. Y atoms have their principal ellipsoids outlined. Atoms are shown as 50% probability ellipsoids and H atoms are omitted. The *c* axis is horizontal and the view is perpendicular to the *bc* plane. The *A* molecules are closer to the center of the cell and the *B* molecules are in the upper-left and lower-right corners.

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* Lists of assigned H-atom parameters, anisotropic displacement parameters, complete distances and angles, and observed and calculated structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55177 (75 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HH0616]

centroids of the Cp rings are 2.388 [6] Å from the Y atoms, but the Cp planes are not perpendicular to the Y—Cp vectors. Y—C(Cp ring) distances range from 2.585 (5) to 2.817 (6) Å, with the C atoms closest to the Si bridge being closest to Y. This effect is caused by the bridging Si atom; it 'pinches' the Cp rings together and the Y atom can no longer fit between them perfectly. This effect is also seen in the angle between the two Cp planes: this is 113 (4)°, whereas the Cp1—Y—Cp2 angle is 122.3°. {The Cp(C)—Si1—Cp(C) angle is 99.3 [3]°.} Other distances in the Y molecule are normal: Y—Cl 2.627 [12], Si—C 1.863 [12], C—C (Cp rings) 1.422 [17] Å. In each molecule there is a strain evidenced by two normal C(Cp)—Si—CH_3 angles of 108.4 [4]° and a third larger angle of 117.0[10]°, to the methyl C atom near the other Cp ring. This strain appears in all four independent Cp rings and reflects a steric crowding between the —$Si(CH_3)_3$ group and the rest of the molecule: from the affected CH_3 group, C—C distances are 3.81 [4] Å to a methyl C atom on the Si bridge (C1 or C2), 4.02 [5] Å to a methyl C atom on the ^{t}Bu group of the opposite bridge and only 3.68 [3] Å to a Cp C atom in the opposite Cp ring. The 'radius' of a —CH_3 group is taken as 2.0 Å; thus the first contact is 0.09 Å short while the second is at just the van der Waals distance. The 3.68 Å contact is short enough to imply the severe strain of bending a C—Si—C bond by 8° or so.

The $Li(thf)_2^+$ group is joined to the two Cl atoms of the Y molecule, with Li—Cl distances averaging 2.371 [25] Å, almost exactly the sum of the crystal radii for Li^+ and Cl^- and shorter than the Li—C distance (2.57 Å) in LiCl (Wells, 1962). Coordination about the Li^+ atom is approximately tetrahedral (Fig. 1), with normal Li—O distances {1.92 [2] Å}. The thf molecules have large apparent thermal motions, indicating a moderate disorder.

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A Bis(pyrazolyl)(bipyridyl)platinum Complex

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Abstract. (4,4′-Dimethyl-2,2′-bipyridyl)bis(3,5-dimethylpyrazolium)platinum(II) 0.5-tetrahydrofuran solvate monohydrate, $[Pt(C_5H_7N_2)_2(C_{12}H_{12}N_2)].0.5C_4H_8O.H_2O$, $M_r = 623.65$, monoclinic, $P2_1/n$, $a = 8.625$ (2), $b = 20.593$ (8), $c = 14.451$ (4) Å, $\beta = 90.32$ (2)°, $V = 2566.7$ (14) Å^3, $Z = 4$, $D_x = 1.61$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71073 Å, $\mu = 55.50$ cm^{-1}, $F(000) = 1232$, room temperature, $R = 0.0387$ for 2874 reflections with $F_o^2 > 3\sigma(F_o^2)$. The square-planar Pt complex has normal Pt—N(bipyridyl) bonds [2.009 (8) Å] and slightly short Pt—N(pyrazolyl) bonds [1.983 (7) Å]. The ligand molecules have normal distances and angles; the planes of the pyrazolyl ligands are twisted by about

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