ORGANOMETALLICS
Organometallics, 1998, 17(11), 2297-2306, DOI:10.1021/om980132p

## Table to be deposited

**Table 1.** Atomic coordinates ($\times 10^4$, $\times 10^5$ for Ru and P atoms) and equivalent isotropic displacement coefficients ($Å^2 \times 10^3$; $Å^2 \times 10^4$ for Ru and P atoms) for the compound Ru($\eta^5$-$C_5H_5$)(9-phenyl-3,3a,4,4a-tetrahydronaphtho[2,3-c]-1-furanyl)(CO)($P^iPr_3$)(**4**).

| *Atom* | *X/a* | *Y/b* | *Z/c* | $U_{eq}$[a] |
|---|---|---|---|---|
| Ru(1) | 4820(2) | 7038(2) | 22385(2) | 269(1) |
| P | 19424(7) | 17522(7) | 24217(5) | 299(2) |
| O(1) | 2680(2) | 80(2) | 842(2) | 40(1) |
| O(2) | 1359(2) | -1395(2) | 4356(2) | 47(1) |
| C(1) | -1142(3) | 928(3) | 1111(3) | 53(1) |
| C(2) | -1611(3) | 549(4) | 2102(3) | 50(1) |
| C(3) | -1804(3) | 1590(4) | 2462(3) | 53(1) |
| C(4) | -1446(3) | 2568(4) | 1703(3) | 53(1) |
| C(5) | -1027(4) | 2170(3) | 856(3) | 56(1) |
| C(6) | 3857(3) | 840(3) | 2555(3) | 47(1) |
| C(7) | 4295(3) | -588(3) | 3293(3) | 54(1) |
| C(8) | 4761(4) | 1473(5) | 2843(5) | 95(2) |
| C(9) | 1618(3) | 2323(3) | 3522(2) | 36(1) |
| C(10) | 1950(4) | 1203(3) | 4581(2) | 52(1) |
| C(11) | 128(3) | 3273(3) | 3436(3) | 49(1) |
| C(12) | 1638(4) | 3343(3) | 1293(2) | 51(1) |
| C(13) | 2088(5) | 4379(4) | 1449(3) | 79(1) |
| C(14) | 2187(6) | 3109(4) | 326(3) | 85(2) |
| C(15) | 1081(3) | -586(3) | 3539(2) | 32(1) |
| C(16) | 1966(3) | -526(3) | 1645(2) | 28(1) |
| C(17) | 2418(2) | -1827(3) | 1838(2) | 26(1) |
| C(18) | 2105(3) | -2913(3) | 2627(2) | 27(1) |
| C(19) | 644(3) | -2857(3) | 2742(2) | 28(1) |
| C(20) | -263(3) | -2391(3) | 1861(2) | 36(1) |
| C(21) | -1600(3) | -2403(3) | 1948(3) | 45(1) |
| C(22) | -2073(3) | -2863(3) | 2902(3) | 47(1) |
| C(23) | -1202(3) | -3302(3) | 3776(3) | 44(1) |
| C(24) | 140(3) | -3292(3) | 3706(2) | 35(1) |
| C(25) | 3221(3) | -4017(3) | 3140(2) | 30(1) |
| C(26) | 3146(3) | -5266(3) | 3821(2) | 36(1) |
| C(27) | 4285(3) | -6308(3) | 4314(3) | 48(1) |

**Table to be deposited**

**Table 1 (cont.).** Atomic coordinates ($\times 10^4$, $\times 10^5$ for Ru and P atoms) and equivalent isotropic displacement coefficients ($Å^2 \times 10^3$; $Å^2 \times 10^4$ for Ru and P atoms) for the compound Ru($\eta^5$-$C_5H_5$)(9-phenyl-3,3a,4,4a-tetrahydronaphtho[2,3-c]-1-furanyl)(CO)($P^iPr_3$)(**4**).

| *Atom* | *X/a* | *Y/b* | *Z/c* | $U_{eq}$[a] |
|---|---|---|---|---|
| C(28) | 5661(4) | -6253(3) | 4164(3) | 54(1) |
| C(29) | 5838(3) | -5167(3) | 3528(3) | 48(1) |
| C(30) | 4652(3) | -3926(3) | 2926(2) | 34(1) |
| C(31) | 4803(3) | -3471(3) | 1754(2) | 38(1) |
| C(32) | 3556(3) | -2210(3) | 1150(2) | 31(1) |
| C(33) | 3867(3) | -948(3) | 692(3) | 45(1) |

[a] Equivalent isotropic *U* defined as one third of the trace of the orthogonalized *Uij* tensor.

## Table to be deposited

**Table 2.** Anisotropic displacement coefficients $U_{ij}$* (Å$^2\times10^3$; Å$^2\times10^4$ for Ru and P atoms) for the non-hydrogen atoms for the complex Ru($\eta^5$-$C_5H_5$)(9-phenyl-3,3a,4,4a-tetrahydronaphtho[2,3-c]-1-furanyl)(CO)($P^iPr_3$)(**4**).

| *Atom* | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| Ru(1) | 247(2) | 262(2) | 267(2) | -84(1) | 0(1) | -72(1) |
| P | 327(4) | 238(4) | 329(4) | -93(3) | 58(3) | -118(3) |
| O(1) | 47(1) | 30(1) | 39(1) | -8(1) | 18(1) | -18(1) |
| O(2) | 65(2) | 42(1) | 30(1) | -1(1) | -2(1) | -27(1) |
| C(1) | 39(2) | 54(2) | 59(2) | -30(2) | -24(2) | 4(2) |
| C(2) | 25(2) | 56(2) | 77(2) | -38(2) | -2(2) | -9(1) |
| C(3) | 29(2) | 67(2) | 72(2) | -41(2) | 5(2) | -11(2) |
| C(4) | 36(2) | 45(2) | 67(2) | -26(2) | -16(2) | 5(1) |
| C(5) | 53(2) | 50(2) | 45(2) | -15(2) | -18(2) | 3(2) |
| C(6) | 35(2) | 43(2) | 72(2) | -31(2) | 16(2) | -17(1) |
| C(7) | 31(2) | 46(2) | 83(3) | -29(2) | -11(2) | -4(1) |
| C(8) | 40(2) | 82(3) | 196(6) | -79(4) | 24(3) | -35(2) |
| C(9) | 39(2) | 34(2) | 40(2) | -17(1) | 3(1) | -15(1) |
| C(10) | 74(2) | 46(2) | 38(2) | -20(2) | 0(2) | -20(2) |
| C(11) | 51(2) | 53(2) | 47(2) | -30(2) | 5(2) | -11(2) |
| C(12) | 83(3) | 26(2) | 40(2) | -7(1) | 13(2) | -24(2) |
| C(13) | 138(4) | 42(2) | 66(3) | -13(2) | 22(3) | -52(3) |
| C(14) | 166(5) | 48(2) | 44(2) | -12(2) | 36(3) | -52(3) |
| C(15) | 31(1) | 34(2) | 35(2) | -15(1) | 4(1) | -15(1) |
| C(16) | 26(1) | 30(2) | 24(1) | -6(1) | 1(1) | -12(1) |
| C(17) | 23(1) | 28(1) | 28(1) | -10(1) | 3(1) | -10(1) |
| C(18) | 31(1) | 27(1) | 26(1) | -10(1) | 4(1) | -14(1) |
| C(19) | 31(1) | 26(1) | 33(1) | -13(1) | 6(1) | -15(1) |
| C(20) | 32(2) | 43(2) | 36(2) | -20(1) | 3(1) | -13(1) |
| C(21) | 35(2) | 55(2) | 58(2) | -34(2) | -1(1) | -16(2) |
| C(22) | 33(2) | 49(2) | 75(2) | -36(2) | 13(2) | -23(2) |
| C(23) | 51(2) | 43(2) | 55(2) | -25(2) | 27(2) | -30(2) |
| C(24) | 43(2) | 31(2) | 37(2) | -16(1) | 11(1) | -20(1) |
| C(25) | 32(1) | 29(2) | 32(1) | -13(1) | 0(1) | -14(1) |
| C(26) | 46(2) | 28(2) | 34(2) | -7(1) | -1(1) | -17(1) |
| C(27) | 56(2) | 29(2) | 48(2) | -3(1) | -8(2) | -14(2) |
| C(28) | 51(2) | 32(2) | 60(2) | -7(2) | -21(2) | -2(2) |
| C(29) | 32(2) | 43(2) | 64(2) | -19(2) | -10(2) | -7(1) |
| C(30) | 30(1) | 28(2) | 44(2) | -13(1) | -3(1) | -11(1) |
| C(31) | 29(2) | 37(2) | 47(2) | -19(1) | 8(1) | -11(1) |
| C(32) | 31(1) | 29(2) | 33(1) | -12(1) | 7(1) | -12(1) |
| C(33) | 50(2) | 41(2) | 48(2) | -17(2) | 26(2) | -23(2) |

* The anisotropic displacement exponent takes the form: $-2\pi^2(h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12})$.

**Table to be deposited**

**Table 3.** Hydrogen atom coordinates* ($\times 10^4$) and isotropic displacement coefficient ($A^2 \times 10^3$) for the compound Ru($\eta^5$-$C_5H_5$)(9-phenyl-3,3a,4,4a-tetrahydronaphtho[2,3-c]-1-furanyl)(CO)($P^iPr_3$)(**4**).

| *Atom* | *X/a* | *Y/b* | *Z/c* | *U* |
|---|---|---|---|---|
| H(1) | -965(3) | 400(3) | 650(3) | 65(2) |
| H(2) | -1780(3) | -376(4) | 2522(3) | 65(2) |
| H(3) | -2127(3) | 1616(4) | 3115(3) | 65(2) |
| H(4) | -1495(3) | 3409(4) | 1727(3) | 65(2) |
| H(5) | -614(4) | 2596(3) | 291(3) | 65(2) |
| H(6) | 4007(3) | 1006(3) | 1813(3) | 65(2) |
| H(7A) | 3752(3) | -1010(3) | 3102(3) | 65(2) |
| H(7B) | 4136(3) | -625(3) | 3993(3) | 65(2) |
| H(7C) | 5277(3) | -1044(3) | 3256(3) | 65(2) |
| H(8A) | 4516(4) | 2393(5) | 2388(5) | 65(2) |
| H(8B) | 5738(4) | 995(5) | 2811(5) | 65(2) |
| H(8C) | 4597(4) | 1414(5) | 3548(5) | 65(2) |
| H(9) | 2325(3) | 2814(3) | 3415(2) | 65(2) |
| H(10A) | 2901(4) | 597(3) | 4636(2) | 65(2) |
| H(10B) | 1314(4) | 737(3) | 4664(2) | 65(2) |
| H(10C) | 1848(4) | 1562(3) | 5117(2) | 65(2) |
| H(11A) | 66(3) | 3627(3) | 3881(3) | 65(2) |
| H(11B) | -127(3) | 4010(3) | 2725(3) | 65(2) |
| H(11C) | -503(3) | 2815(3) | 3592(3) | 65(2) |
| H(12) | 529(4) | 3795(3) | 1208(2) | 65(2) |
| H(13A) | 1730(5) | 4520(4) | 2069(3) | 65(2) |
| H(13B) | 1741(5) | 5205(4) | 856(3) | 65(2) |
| H(13C) | 3099(5) | 4057(4) | 1521(3) | 65(2) |
| H(14A) | 3219(6) | 2803(4) | 427(3) | 65(2) |
| H(14B) | 1842(6) | 3803(4) | -185(3) | 65(2) |
| H(14C) | 1923(6) | 2603(4) | 206(3) | 65(2) |
| H(20) | 36(3) | -2004(3) | 1168(2) | 65(2) |
| H(21) | -2192(3) | -2095(3) | 1347(3) | 65(2) |
| H(22) | -3083(3) | -2765(3) | 2950(3) | 65(2) |
| H(23) | -1548(3) | -3573(3) | 4497(3) | 65(2) |
| H(24) | 760(3) | -3576(3) | 4369(2) | 65(2) |
| H(26) | 2181(3) | -5370(3) | 3917(2) | 65(2) |
| H(27) | 4238(3) | -7165(3) | 4763(3) | 65(2) |
| H(28) | 6424(4) | -6958(3) | 4591(3) | 65(2) |
| H(29) | 6751(3) | -5171(3) | 3450(3) | 65(2) |
| H(30) | 4632(3) | -3179(3) | 3128(2) | 65(2) |
| H(31A) | 4892(3) | -4184(3) | 1554(2) | 65(2) |
| H(31B) | 5711(3) | -3384(3) | 1585(2) | 65(2) |
| H(32) | 3194(3) | -2390(3) | 612(2) | 65(2) |
| H(33A) | 4768(3) | -996(3) | 1062(3) | 65(2) |
| H(33B) | 3990(3) | -799(3) | 16(3) | 65(2) |

* Hydrogen atoms were located or included in calculated positions and refined riding on their respective carbon atoms with a fixed common thermal parameter.

**Table to be deposited**

**Table 4**. Full experimental details for the X-Ray analysis of the compound Ru($\eta^5$-$C_5H_5$)(9-phenyl-3,3a,4,4a-tetrahydronaphtho[2,3-c]-1-furanyl)(CO)($P^iPr_3$)(**4**).

*Crystal data:*

| | |
|---|---|
| Formula | $C_{33}H_{41}O_2PRu$ |
| Molecular weight | 601.70 |
| Color and habit | Yellow, prismatic block |
| Size (mm) | 0.5 x 0.5 x 0.8 |
| Symmetry | Triclinic, *P*-1(no. 2) |
| Unit cell determination | Least-squares fit to 62 reflections. |
| | ($20 \leq 2\theta \leq 35\infty$) |
| Unit cell dimensions | 10.415(3), 11.819(4), 14.114(5) Å |
| | 68.15(2), 86.69(2), 69.110(10)° |
| Packing: $V$ (Å$^3$), $Z$ | 1500.9(9), 2 |
| $D_{calc}$(g cm$^{-3}$), $F$ (000) | 1.331, 628 |

*Experimental data:*

| | |
|---|---|
| Diffractometer | Four-circle Siemens-P4. |
| Radiation and technique | Mo-$K_\alpha$ ($\lambda$ = 0.71073 Å) |
| | Bisecting geometry |
| Monochromator | Graphite oriented |
| Collection mode/range | $\theta / 2\theta$ scan ($3 \leq 2\theta \leq 50\infty$) |
| Number of reflections: | |
| measured | 7179 (*h*: -11, 12; *k*: -12, 12; *l*: -16, 16) |
| unique | 5120 (merging R factor 0.0495) |
| Standard reflections | 3 standards; measured every 100 reflections. |
| | No decay observed. |
| Absorption correction | Semiempirical method ($\psi$-scan)* |
| Max. and min. trans. fact. | 0.799, 0.753 |
| $\mu$ (mm$^{-1}$) and $\mu$·R | 0.60, 0.18 |
| Temperature (K) | 200.0(2) |

**Table to be deposited**

**Table 4 (cont.).** Full experimental details for the X-Ray analysis of the compound Ru($\eta^5$-$C_5H_5$)(9-phenyl-3,3a,4,4a-tetrahydronaphtho[2,3-c]-1-furanyl)(CO)($P^iPr_3$)(**4**).

| | |
|---|---|
| *Solution and refinement:* | SHELXTL PLUS and SHELX93, Systems ALPHA AXP |
| Solution mode | Patterson |
| Refinement | Full-matrix least-squares on $F^2$'s. All reflections. |
| Hydrogen atoms | From observed or calculated positions. Refined riding on C atoms with a common thermal parameter. |
| No. parameters | 335 |
| Weighting scheme | $w^{-1} = \sigma^2(F_o^2) + (0.0393P)^2 + 0.60\ P$ where $P=[\text{Max}\ (F_o^2, 0) + 2F_c^2]/3$ |
| $\Delta F$ final (Max.) | 0.60 e/Å$^3$ [close to Ru atom (0.99 Å)] |
| $\Delta F$ final (Min.) | -0.89 e/Å$^3$ |
| Max. thermal values (Å$^2$) | $U_{33}$ (C8) = 0.20(1) |
| Max. shift/esd | 0.023 |
| $R_1$[a] [$F^2 > 2\sigma(F^2)$] | 0.0297 |
| $wR_2$[b] [all data] | 0.0755 |
| $S$[c] [all data] | 1.059 |
| Data-to-Parameter Ratio | 15.3:1 |

Atomic scattering factors from the International Tables for X-Ray Crystallography; Vol. C (1992). Anomalous dispersion applied for Ru and P atoms.

[a] $R_1(F) = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$. [b] $wR_2(F^2) = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$. [c] Goof = S = $\{\Sigma[w(F_o^2 - F_c^2)^2]/(n-p)\}^{1/2}$, where n is the number of reflections, and p is the number of refined parameters.

---

* North, A. C. T.; Phillips, D. C.; Mathews, F. S. *Acta Crystallogr., Sect. A* **1968**, *24*, 351.

## Table to be deposited

**Table 5**. Bond lengths [Å] and angles [deg] for Ru($\eta^5$-$C_5H_5$)(9-phenyl-3,3a,4,4a-tetrahydronaphtho[2,3-c]-1-furanyl)(CO)($P^iPr_3$)(**4**).

| | |
|---|---|
| Ru(1)-C(15) | 1.858(3) |
| Ru(1)-C(16) | 2.088(3) |
| Ru(1)-C(1) | 2.267(3) |
| Ru(1)-C(5) | 2.275(3) |
| Ru(1)-C(2) | 2.277(3) |
| Ru(1)-C(4) | 2.289(3) |
| Ru(1)-C(3) | 2.290(3) |
| Ru(1)-P | 2.3545(9) |
| P-C(9) | 1.881(3) |
| P-C(6) | 1.880(3) |
| P-C(12) | 1.891(3) |
| O(1)-C(16) | 1.424(3) |
| O(1)-C(33) | 1.462(4) |
| O(2)-C(15) | 1.161(3) |
| C(1)-C(2) | 1.417(5) |
| C(1)-C(5) | 1.423(5) |
| C(1)-H(1) | 1.03 |
| C(2)-C(3) | 1.447(5) |
| C(2)-H(2) | 1.10 |
| C(3)-C(4) | 1.401(5) |
| C(3)-H(3) | 0.97 |
| C(4)-C(5) | 1.432(5) |
| C(4)-H(4) | 0.99 |
| C(5)-H(5) | 0.94 |
| C(6)-C(7) | 1.529(5) |
| C(6)-C(8) | 1.544(5) |
| C(6)-H(6) | 1.01 |
| C(7)-H(7A) | 0.98 |
| C(7)-H(7B) | 0.98 |
| C(7)-H(7C) | 0.98 |
| C(8)-H(8A) | 0.98 |
| C(8)-H(8B) | 0.98 |
| C(8)-H(8C) | 0.98 |
| C(9)-C(10) | 1.538(4) |
| C(9)-C(11) | 1.536(4) |
| C(9)-H(9) | 1.06 |
| C(10)-H(10A) | 0.98 |
| C(10)-H(10B) | 0.98 |
| C(10)-H(10C) | 0.98 |
| C(11)-H(11A) | 0.86 |
| C(11)-H(11B) | 1.03 |
| C(11)-H(11C) | 0.96 |
| C(12)-C(14) | 1.531(5) |
| C(12)-C(13) | 1.545(5) |
| C(12)-H(12) | 1.08 |
| C(13)-H(13A) | 0.98 |
| C(13)-H(13B) | 0.98 |
| C(13)-H(13C) | 0.98 |
| C(14)-H(14A) | 1.00 |

**Table to be deposited**

**Table 5 (cont.).** Bond lengths [Å] and angles [deg] for Ru($\eta^5$-$C_5H_5$)(9-phenyl-3,3a,4,4a-tetrahydronaphtho[2,3-c]-1-furanyl)(CO)($P^iPr_3$)(**4**).

| | |
|---|---|
| C(14)-H(14B) | 0.84 |
| C(14)-H(14C) | 0.81 |
| C(16)-C(17) | 1.359(4) |
| C(17)-C(18) | 1.479(3) |
| C(17)-C(32) | 1.537(4) |
| C(18)-C(25) | 1.374(4) |
| C(18)-C(19) | 1.500(4) |
| C(19)-C(24) | 1.408(4) |
| C(19)-C(20) | 1.413(4) |
| C(20)-C(21) | 1.396(4) |
| C(20)-H(20) | 1.00 |
| C(21)-C(22) | 1.385(5) |
| C(21)-H(21) | 0.95 |
| C(22)-C(23) | 1.389(5) |
| C(22)-H(22) | 1.02 |
| C(23)-C(24) | 1.400(4) |
| C(23)-H(23) | 1.03 |
| C(24)-H(24) | 1.04 |
| C(25)-C(26) | 1.458(4) |
| C(25)-C(30) | 1.537(4) |
| C(26)-C(27) | 1.350(4) |
| C(26)-H(26) | 1.05 |
| C(27)-C(28) | 1.458(5) |
| C(27)-H(27) | 0.99 |
| C(28)-C(29) | 1.334(5) |
| C(28)-H(28) | 0.95 |
| C(29)-C(30) | 1.517(4) |
| C(29)-H(29) | 0.95 |
| C(30)-C(31) | 1.555(4) |
| C(30)-H(30) | 1.02 |
| C(31)-C(32) | 1.561(4) |
| C(31)-H(31A) | 0.96 |
| C(31)-H(31B) | 0.99 |
| C(32)-C(33) | 1.533(4) |
| C(32)-H(32) | 0.99 |
| C(33)-H(33A) | 1.07 |
| C(33)-H(33B) | 0.91 |

| | |
|---|---|
| C(16)-Ru(1)-C(5) | 103.72(12) |
| C(1)-Ru(1)-C(5) | 36.52(13) |
| C(15)-Ru(1)-C(2) | 97.37(13) |
| C(16)-Ru(1)-C(2) | 110.50(11) |
| C(1)-Ru(1)-C(2) | 36.33(13) |
| C(5)-Ru(1)-C(2) | 61.0(2) |
| C(15)-Ru(1)-C(4) | 129.84(13) |
| C(16)-Ru(1)-C(4) | 140.09(11) |
| C(1)-Ru(1)-C(4) | 60.65(13) |
| C(5)-Ru(1)-C(4) | 36.58(12) |

## Table to be deposited

**Table 5 (cont.).** Bond lengths [Å] and angles [deg] for Ru($\eta^5$-$C_5H_5$)(9-phenyl-3,3a,4,4a-tetrahydronaphtho[2,3-c]-1-furanyl)(CO)($P^iPr_3$)(**4**).

| | |
|---|---|
| C(2)-Ru(1)-C(4) | 60.72(13) |
| C(15)-Ru(1)-C(3) | 99.20(13) |
| C(16)-Ru(1)-C(3) | 147.01(11) |
| C(1)-Ru(1)-C(3) | 60.68(13) |
| C(5)-Ru(1)-C(3) | 60.50(14) |
| C(2)-Ru(1)-C(3) | 36.93(12) |
| C(4)-Ru(1)-C(3) | 35.63(13) |
| C(15)-Ru(1)-P | 91.94(9) |
| C(16)-Ru(1)-P | 94.05(8) |
| C(1)-Ru(1)-P | 140.73(10) |
| C(5)-Ru(1)-P | 105.50(11) |
| C(2)-Ru(1)-P | 153.85(9) |
| C(4)-Ru(1)-P | 94.73(10) |
| C(3)-Ru(1)-P | 117.45(9) |
| C(9)-P-C(6) | 104.73(14) |
| C(9)-P-C(12) | 101.51(14) |
| C(6)-P-C(12) | 105.0(2) |
| C(9)-P-Ru(1) | 114.73(9) |
| C(6)-P-Ru(1) | 117.91(10) |
| C(12)-P-Ru(1) | 111.30(12) |
| C(16)-O(1)-C(33) | 108.1(2) |
| C(2)-C(1)-C(5) | 108.8(3) |
| C(2)-C(1)-Ru(1) | 72.2(2) |
| C(5)-C(1)-Ru(1) | 72.0(2) |
| C(2)-C(1)-H(1) | 124.6(2) |
| C(5)-C(1)-H(1) | 126.6(2) |
| Ru(1)-C(1)-H(1) | 124.11(9) |
| C(1)-C(2)-C(3) | 107.0(3) |
| C(1)-C(2)-Ru(1) | 71.5(2) |
| C(3)-C(2)-Ru(1) | 72.0(2) |
| C(1)-C(2)-H(2) | 126.2(2) |
| C(3)-C(2)-H(2) | 126.7(2) |
| Ru(1)-C(2)-H(2) | 121.01(10) |
| C(4)-C(3)-C(2) | 108.3(3) |
| C(4)-C(3)-Ru(1) | 72.1(2) |
| C(2)-C(3)-Ru(1) | 71.0(2) |
| C(4)-C(3)-H(3) | 125.4(2) |
| C(2)-C(3)-H(3) | 126.3(2) |
| Ru(1)-C(3)-H(3) | 122.79(10) |
| C(3)-C(4)-C(5) | 108.5(3) |
| C(3)-C(4)-Ru(1) | 72.2(2) |
| C(5)-C(4)-Ru(1) | 71.2(2) |
| C(3)-C(4)-H(4) | 126.5(2) |
| C(5)-C(4)-H(4) | 124.9(2) |
| Ru(1)-C(4)-H(4) | 123.80(9) |
| C(1)-C(5)-C(4) | 107.4(3) |
| C(1)-C(5)-Ru(1) | 71.5(2) |
| C(4)-C(5)-Ru(1) | 72.2(2) |

**Table to be deposited**

**Table 5 (cont.).** Bond lengths [Å] and angles [deg] for Ru($\eta^5$-$C_5H_5$)(9-phenyl-3,3a,4,4a-tetrahydronaphtho[2,3-c]-1-furanyl)(CO)($P^iPr_3$)(**4**).

| | |
|---|---|
| C(1)-C(5)-H(5) | 126.9(2) |
| C(4)-C(5)-H(5) | 125.0(2) |
| Ru(1)-C(5)-H(5) | 114.20(11) |
| C(7)-C(6)-C(8) | 108.6(3) |
| C(7)-C(6)-P | 113.4(2) |
| C(8)-C(6)-P | 115.8(3) |
| C(7)-C(6)-H(6) | 116.9(2) |
| C(8)-C(6)-H(6) | 102.6(3) |
| P-C(6)-H(6) | 99.04(12) |
| C(6)-C(7)-H(7A) | 109.4(2) |
| C(6)-C(7)-H(7B) | 109.4(2) |
| C(6)-C(7)-H(7C) | 109.6(2) |
| C(6)-C(8)-H(8A) | 111.5(3) |
| C(6)-C(8)-H(8B) | 110.1(2) |
| C(6)-C(8)-H(8C) | 106.8(3) |
| C(10)-C(9)-C(11) | 109.4(3) |
| C(10)-C(9)-P | 113.8(2) |
| C(11)-C(9)-P | 111.7(2) |
| C(10)-C(9)-H(9) | 109.9(2) |
| C(11)-C(9)-H(9) | 110.8(2) |
| P-C(9)-H(9) | 101.01(9) |
| C(9)-C(10)-H(10A) | 109.5(2) |
| C(9)-C(10)-H(10B) | 109.4(2) |
| C(9)-C(10)-H(10C) | 109.6(2) |
| C(9)-C(11)-H(11A) | 108.7(2) |
| C(9)-C(11)-H(11B) | 110.7(2) |
| C(9)-C(11)-H(11C) | 110.8(2) |
| C(14)-C(12)-C(13) | 110.8(3) |
| C(14)-C(12)-P | 111.6(2) |
| C(13)-C(12)-P | 117.7(3) |
| C(14)-C(12)-H(12) | 111.1(3) |
| C(13)-C(12)-H(12) | 102.5(2) |
| P-C(12)-H(12) | 102.32(12) |
| C(12)-C(13)-H(13A) | 110.0(2) |
| C(12)-C(13)-H(13B) | 110.0(2) |
| C(12)-C(13)-H(13C) | 108.4(2) |
| C(12)-C(14)-H(14A) | 106.3(3) |
| C(12)-C(14)-H(14B) | 109.0(2) |
| C(12)-C(14)-H(14C) | 112.8(2) |
| O(2)-C(15)-Ru(1) | 175.0(2) |
| C(17)-C(16)-O(1) | 109.5(2) |
| C(17)-C(16)-Ru(1) | 134.1(2) |
| O(1)-C(16)-Ru(1) | 116.4(2) |
| C(16)-C(17)-C(18) | 132.0(2) |
| C(16)-C(17)-C(32) | 111.5(2) |
| C(18)-C(17)-C(32) | 116.2(2) |
| C(25)-C(18)-C(17) | 116.2(2) |
| C(25)-C(18)-C(19) | 122.8(2) |

**Table to be deposited**

**Table 5 (cont.).** Bond lengths [Å] and angles [deg] for Ru($\eta^5$-$C_5H_5$)(9-phenyl-3,3a,4,4a-tetrahydronaphtho[2,3-c]-1-furanyl)(CO)($P^iPr_3$)(**4**).

| | |
|---|---|
| C(17)-C(18)-C(19) | 120.6(2) |
| C(24)-C(19)-C(20) | 117.8(2) |
| C(24)-C(19)-C(18) | 122.4(2) |
| C(20)-C(19)-C(18) | 119.8(2) |
| C(21)-C(20)-C(19) | 120.9(3) |
| C(21)-C(20)-H(20) | 119.3(2) |
| C(19)-C(20)-H(20) | 119.8(2) |
| C(22)-C(21)-C(20) | 120.7(3) |
| C(22)-C(21)-H(21) | 119.7(2) |
| C(20)-C(21)-H(21) | 119.7(2) |
| C(21)-C(22)-C(23) | 119.2(3) |
| C(21)-C(22)-H(22) | 119.3(2) |
| C(23)-C(22)-H(22) | 121.1(2) |
| C(22)-C(23)-C(24) | 121.1(3) |
| C(22)-C(23)-H(23) | 121.2(2) |
| C(24)-C(23)-H(23) | 117.5(2) |
| C(23)-C(24)-C(19) | 120.4(3) |
| C(23)-C(24)-H(24) | 120.0(2) |
| C(19)-C(24)-H(24) | 119.6(2) |
| C(18)-C(25)-C(26) | 125.1(2) |
| C(18)-C(25)-C(30) | 116.5(2) |
| C(26)-C(25)-C(30) | 118.3(2) |
| C(27)-C(26)-C(25) | 122.1(3) |
| C(27)-C(26)-H(26) | 118.7(2) |
| C(25)-C(26)-H(26) | 119.2(2) |
| C(26)-C(27)-C(28) | 121.4(3) |
| C(26)-C(27)-H(27) | 122.2(2) |
| C(28)-C(27)-H(27) | 116.3(2) |
| C(29)-C(28)-C(27) | 120.9(3) |
| C(29)-C(28)-H(28) | 119.6(2) |
| C(27)-C(28)-H(28) | 119.0(2) |
| C(28)-C(29)-C(30) | 123.2(3) |
| C(28)-C(29)-H(29) | 118.3(2) |
| C(30)-C(29)-H(29) | 118.5(2) |
| C(29)-C(30)-C(25) | 113.9(2) |
| C(29)-C(30)-C(31) | 111.9(3) |
| C(25)-C(30)-C(31) | 109.8(2) |
| C(29)-C(30)-H(30) | 110.3(2) |
| C(25)-C(30)-H(30) | 104.19(14) |
| C(31)-C(30)-H(30) | 106.1(2) |
| C(30)-C(31)-C(32) | 111.0(2) |
| C(30)-C(31)-H(31A) | 107.6(2) |
| C(32)-C(31)-H(31A) | 112.4(2) |
| C(30)-C(31)-H(31B) | 112.17(14) |
| C(32)-C(31)-H(31B) | 113.14(14) |
| C(33)-C(32)-C(17) | 100.3(2) |
| C(33)-C(32)-C(31) | 115.7(2) |
| C(17)-C(32)-C(31) | 112.8(2) |

## Table to be deposited

**Table 5 (cont.).** Bond lengths [Å] and angles [deg] for Ru($\eta^5$-$C_5H_5$)(9-phenyl-3,3a,4,4a-tetrahydronaphtho[2,3-c]-1-furanyl)(CO)($P^iPr_3$)(**4**).

| | |
|---|---|
| C(33)-C(32)-H(32) | 111.1(2) |
| C(17)-C(32)-H(32) | 110.55(14) |
| C(31)-C(32)-H(32) | 106.5(2) |
| O(1)-C(33)-C(32) | 106.4(2) |
| O(1)-C(33)-H(33A) | 107.9(2) |
| C(32)-C(33)-H(33A) | 113.4(2) |
| O(1)-C(33)-H(33B) | 112.7(2) |
| C(32)-C(33)-H(33B) | 107.3(2) |

Weighted least-squares planes through the starred atoms
(Nardelli, Musatti, Domiano & Andreetti Ric.Sci.(1965),15(II-A),807).
Equation of the plane: m1*X+m2*Y+m3*Z=d

Plane 1

m1 = -0.67194(0.00112)
m2 = -0.12646(0.00136)
m3 = -0.72973(0.00099)
D = -2.87471(0.00218)

| Atom | d | s | d/s | (d/s)**2 |
|---|---|---|---|---|
| C16 * | -0.0460 | 0.0027 | -16.995 | 288.824 |
| O1 * | 0.0616 | 0.0021 | 28.697 | 823.543 |
| C33 * | -0.1741 | 0.0035 | -50.162 | 2516.179 |
| C32 * | 0.0847 | 0.0029 | 29.375 | 862.900 |
| C17 * | -0.0198 | 0.0026 | -7.458 | 55.616 |
| | | | | ========== |
| | | Sum((d/s)**2) for starred atoms | | 4547.062 |

Chi-squared at 95% for 2 degrees of freedom: 5.99
The group of atoms deviates significantly from planarity

Plane 2

m1 = -0.49754(0.00119)
m2 = -0.74698(0.00093)
m3 = -0.44099(0.00116)
D = -0.89922(0.00606)

| Atom | d | s | d/s | (d/s)**2 |
|---|---|---|---|---|
| C17 * | -0.3256 | 0.0028 | -114.840 | 13188.246 |
| C32 * | 0.1773 | 0.0030 | 58.832 | 3461.250 |
| C31 * | 0.2250 | 0.0033 | 68.301 | 4665.088 |
| C30 * | -0.4136 | 0.0031 | -132.952 | 17676.236 |
| C25 * | 0.2059 | 0.0030 | 69.080 | 4771.997 |
| C18 * | 0.1620 | 0.0029 | 56.640 | 3208.049 |
| | | | | ========== |
| | | Sum((d/s)**2) for starred atoms | | 46970.867 |

Chi-squared at 95% for 3 degrees of freedom: 7.81
The group of atoms deviates significantly from planarity

Plane 3

m1 = -0.12025(0.00129)
m2 = -0.63800(0.00108)
m3 = -0.76059(0.00089)
D = -1.55951(0.00916)

| Atom | d | s | d/s | (d/s)**2 |
|---|---|---|---|---|
| C25 * | -0.0217 | 0.0028 | -7.712 | 59.474 |
| C30 * | 0.0168 | 0.0030 | 5.565 | 30.972 |
| C29 * | -0.0013 | 0.0037 | -0.355 | 0.126 |
| C28 * | -0.0121 | 0.0037 | -3.302 | 10.903 |
| C27 * | -0.0003 | 0.0035 | -0.096 | 0.009 |
| C26 * | 0.0167 | 0.0029 | 5.668 | 32.129 |
| | | | | ========== |
| | | Sum((d/s)**2) for starred atoms | | 133.613 |

Chi-squared at 95% for 3 degrees of freedom: 7.81
The group of atoms deviates significantly from planarity

Dihedral angles formed by LSQ-planes

| Plane - plane | | angle (e.s.d.) |
|---|---|---|
| 1 | 2 | 41.36( 0.10) |
| 1 | 3 | 44.23( 0.11) |
| 2 | 3 | 29.33( 0.09) |