| | | | | |
|---|---|---|---|---|
| H(25) | 0.2703 | 0.1799 | 0.7117 | 6.4176 |
| H(26) | 1.0016 | 0.3638 | 1.0221 | 7.2640 |
| H(27) | 0.8811 | 0.4138 | 1.0156 | 7.2640 |
| H(28) | 0.8664 | 0.3319 | 1.0349 | 7.2640 |
| H(29) | 0.9342 | 0.1985 | 0.9748 | 6.8286 |
| H(30) | 1.0083 | 0.1778 | 0.9101 | 6.8286 |
| H(31) | 1.0701 | 0.2307 | 0.9646 | 6.8286 |
| H(32) | 0.9915 | 0.1888 | 0.8013 | 6.4812 |
| H(33) | 0.8977 | 0.2222 | 0.7456 | 6.4812 |
| H(34) | 1.0354 | 0.2540 | 0.7569 | 6.4812 |
| H(35) | 0.9300 | 0.3886 | 0.7241 | 6.4753 |
| H(36) | 0.7894 | 0.3599 | 0.7202 | 6.4753 |
| H(37) | 0.8193 | 0.4376 | 0.7490 | 6.4753 |
| H(38) | 0.9017 | 0.5020 | 0.8663 | 6.0133 |
| H(39) | 0.7545 | 0.4879 | 0.8614 | 6.0133 |
| H(40) | 0.8275 | 0.4893 | 0.9326 | 6.0133 |

Estimated standard deviations in the least significant figure are given in parentheses.

**Table S21. Anisotropic Displacement Parameters for $[(CpTiCl_2)(CpTi)(Cp^*Ru)_2(\mu_3\text{-}S)_4]\cdot CH_2Cl_2$ ($6\cdot CH_2Cl_2$)**

| atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| Ru(1) | 0.0275(4) | 0.0252(5) | 0.0260(4) | -0.0028(4) | 0.0058(3) | -0.0036(4) |
| Ru(2) | 0.0201(4) | 0.0290(5) | 0.0242(4) | -0.0014(4) | 0.0046(3) | -0.0003(4) |
| Ti(1) | 0.0223(8) | 0.028(1) | 0.044(1) | 0.0005(8) | 0.0061(7) | -0.0018(8) |
| Ti(2) | 0.0300(9) | 0.040(1) | 0.0246(9) | -0.0034(8) | 0.0098(7) | -0.0010(8) |
| Cl(1) | 0.043(2) | 0.062(2) | 0.053(2) | -0.001(1) | -0.010(1) | -0.001(1) |
| Cl(2) | 0.045(2) | 0.036(2) | 0.069(2) | -0.006(1) | 0.012(1) | 0.014(1) |
| Cl(3) | 0.096(3) | 0.172(5) | 0.118(3) | 0.027(3) | -0.025(2) | -0.059(3) |
| Cl(4) | 0.121(4) | 0.281(7) | 0.131(4) | 0.069(4) | -0.018(3) | -0.089(4) |
| S(1) | 0.024(1) | 0.033(1) | 0.036(1) | -0.005(1) | 0.006(1) | -0.006(1) |
| S(2) | 0.024(1) | 0.033(1) | 0.034(1) | -0.003(1) | 0.0071(10) | -0.010(1) |
| S(3) | 0.026(1) | 0.031(1) | 0.027(1) | -0.001(1) | 0.0040(9) | 0.000(1) |
| S(4) | 0.031(1) | 0.034(1) | 0.033(1) | 0.001(1) | 0.0083(10) | 0.007(1) |
| C(1) | 0.071(9) | 0.07(1) | 0.075(10) | 0.050(8) | 0.023(8) | 0.029(8) |
| C(2) | 0.020(6) | 0.08(1) | 0.11(1) | 0.006(6) | 0.015(7) | -0.026(9) |
| C(3) | 0.045(8) | 0.061(9) | 0.11(1) | 0.022(7) | 0.045(8) | 0.003(9) |
| C(4) | 0.057(9) | 0.08(1) | 0.09(1) | 0.017(8) | 0.039(8) | -0.013(9) |
| C(5) | 0.053(8) | 0.045(9) | 0.14(1) | -0.012(7) | 0.052(9) | -0.042(9) |
| C(6) | 0.10(1) | 0.14(2) | 0.041(8) | 0.06(1) | 0.040(8) | 0.06(1) |
| C(7) | 0.055(9) | 0.16(2) | 0.029(6) | -0.03(1) | 0.007(6) | 0.013(9) |
| C(8) | 0.11(1) | 0.063(10) | 0.030(6) | -0.016(9) | 0.040(7) | -0.015(6) |
| C(9) | 0.040(7) | 0.12(1) | 0.041(7) | -0.005(8) | 0.021(5) | 0.016(8) |
| C(10) | 0.13(1) | 0.063(10) | 0.055(8) | -0.03(1) | 0.055(9) | 0.005(8) |
| C(11) | 0.039(6) | 0.023(6) | 0.047(6) | -0.008(5) | 0.006(5) | -0.007(5) |
| C(12) | 0.064(7) | 0.028(6) | 0.034(6) | -0.002(5) | 0.009(5) | -0.003(5) |
| C(13) | 0.038(6) | 0.029(6) | 0.054(7) | -0.002(5) | 0.009(5) | -0.017(5) |
| C(14) | 0.052(6) | 0.030(6) | 0.038(6) | -0.012(5) | 0.017(5) | -0.011(5) |
| C(15) | 0.060(7) | 0.033(6) | 0.031(6) | 0.001(5) | 0.003(5) | -0.002(5) |
| C(16) | 0.055(7) | 0.060(8) | 0.085(9) | -0.035(6) | 0.020(6) | -0.021(7) |
| C(17) | 0.092(10) | 0.033(7) | 0.079(9) | -0.003(6) | 0.000(7) | 0.015(6) |
| C(18) | 0.067(8) | 0.053(8) | 0.11(1) | 0.018(7) | -0.004(7) | -0.028(8) |
| C(19) | 0.096(9) | 0.065(9) | 0.059(8) | -0.031(7) | 0.039(7) | -0.036(6) |
| C(20) | 0.093(9) | 0.055(9) | 0.052(7) | -0.015(7) | -0.019(6) | -0.013(6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(21) | 0.023(5) | 0.060(8) | 0.029(5) | -0.001(5) | 0.006(4) | -0.003(5) |
| C(22) | 0.016(4) | 0.043(7) | 0.042(6) | 0.000(4) | 0.005(4) | 0.012(5) |
| C(23) | 0.014(4) | 0.052(8) | 0.041(6) | -0.005(4) | 0.009(4) | -0.006(5) |
| C(24) | 0.013(4) | 0.045(6) | 0.037(6) | -0.005(4) | 0.001(4) | 0.006(5) |
| C(25) | 0.022(5) | 0.043(7) | 0.050(6) | -0.009(5) | 0.007(4) | -0.006(5) |
| C(26) | 0.044(7) | 0.14(1) | 0.046(7) | -0.022(8) | 0.005(5) | -0.021(8) |
| C(27) | 0.031(6) | 0.08(1) | 0.105(10) | 0.002(6) | 0.005(6) | 0.041(8) |
| C(28) | 0.047(7) | 0.073(9) | 0.088(9) | -0.013(6) | 0.035(6) | -0.040(7) |
| C(29) | 0.052(7) | 0.10(1) | 0.057(7) | -0.013(7) | 0.000(6) | 0.034(7) |
| C(30) | 0.036(6) | 0.049(8) | 0.11(1) | -0.014(6) | 0.017(6) | -0.015(7) |
| C(31) | 0.061(9) | 0.24(2) | 0.11(1) | -0.03(1) | 0.011(8) | -0.10(1) |

Estimated standard deviations in the least significant figure are given in parentheses.

**Table S22. Bond Lengths (Å) Involving the Nonhydrogen Atoms in $[(CpTiCl_2)(CpTi)(Cp^*Ru)_2(\mu_3\text{-}S)_4]\cdot CH_2Cl_2$ ($6\cdot CH_2Cl_2$)**

| atom | atom | distance | atom | atom | distance |
|---|---|---|---|---|---|
| Ru(1) | Ru(2) | 2.810(1) | Ti(2) | C(6) | 2.38(1) |
| Ru(1) | Ti(2) | 2.904(2) | Ti(2) | C(7) | 2.34(1) |
| Ru(1) | S(1) | 2.382(2) | Ti(2) | C(8) | 2.359(9) |
| Ru(1) | S(3) | 2.315(3) | Ti(2) | C(9) | 2.361(9) |
| Ru(1) | S(4) | 2.311(2) | Ti(2) | C(10) | 2.37(1) |
| Ru(1) | C(11) | 2.224(9) | Cl(3) | C(31) | 1.73(1) |
| Ru(1) | C(12) | 2.251(9) | Cl(4) | C(31) | 1.62(1) |
| Ru(1) | C(13) | 2.227(9) | C(1) | C(2) | 1.38(2) |
| Ru(1) | C(14) | 2.230(9) | C(1) | C(5) | 1.39(2) |
| Ru(1) | C(15) | 2.185(9) | C(2) | C(3) | 1.33(2) |
| Ru(2) | Ti(2) | 2.963(2) | C(3) | C(4) | 1.28(2) |
| Ru(2) | S(2) | 2.382(2) | C(4) | C(5) | 1.34(2) |
| Ru(2) | S(3) | 2.316(2) | C(6) | C(7) | 1.36(2) |
| Ru(2) | S(4) | 2.313(3) | C(6) | C(10) | 1.37(2) |
| Ru(2) | C(21) | 2.176(9) | C(7) | C(8) | 1.34(2) |
| Ru(2) | C(22) | 2.264(8) | C(8) | C(9) | 1.37(1) |
| Ru(2) | C(23) | 2.315(7) | C(9) | C(10) | 1.39(2) |
| Ru(2) | C(24) | 2.265(8) | C(11) | C(12) | 1.38(1) |
| Ru(2) | C(25) | 2.207(9) | C(11) | C(15) | 1.39(1) |
| Ti(1) | Cl(1) | 2.407(3) | C(11) | C(16) | 1.52(1) |
| Ti(1) | Cl(2) | 2.413(3) | C(12) | C(13) | 1.44(1) |
| Ti(1) | S(1) | 2.539(3) | C(12) | C(17) | 1.50(1) |
| Ti(1) | S(2) | 2.534(3) | C(13) | C(14) | 1.42(1) |
| Ti(1) | S(3) | 2.570(3) | C(13) | C(18) | 1.49(1) |
| Ti(1) | C(1) | 2.38(1) | C(14) | C(15) | 1.43(1) |
| Ti(1) | C(2) | 2.39(1) | C(14) | C(19) | 1.51(1) |
| Ti(1) | C(3) | 2.37(1) | C(15) | C(20) | 1.51(1) |
| Ti(1) | C(4) | 2.41(1) | C(21) | C(22) | 1.40(1) |
| Ti(1) | C(5) | 2.40(1) | C(21) | C(25) | 1.41(1) |
| Ti(2) | S(1) | 2.299(3) | C(21) | C(26) | 1.52(1) |
| Ti(2) | S(2) | 2.297(3) | C(22) | C(23) | 1.43(1) |
| Ti(2) | S(4) | 2.277(3) | C(22) | C(27) | 1.49(1) |

| | | | | | |
|---|---|---|---|---|---|
| C(23) | C(24) | 1.42(1) | C(24) | C(29) | 1.50(1) |
| C(23) | C(28) | 1.51(1) | C(25) | C(30) | 1.49(1) |
| C(24) | C(25) | 1.43(1) | | | |

Estimated standard deviations in the least significant figure are given in parentheses.

**Table S23. Bond Lengths (Å) Involving the Hydrogen Atoms in $[(CpTiCl_2)(CpTi)(Cp^*Ru)_2(\mu_3\text{-}S)_4]\cdot CH_2Cl_2$ ($6\cdot CH_2Cl_2$)**

| atom | atom | distance | atom | atom | distance |
|---|---|---|---|---|---|
| C(1) | H(1) | 0.950 | C(19) | H(22) | 0.950 |
| C(2) | H(2) | 0.950 | C(20) | H(23) | 0.951 |
| C(3) | H(3) | 0.950 | C(20) | H(24) | 0.951 |
| C(4) | H(4) | 0.949 | C(20) | H(25) | 0.951 |
| C(5) | H(5) | 0.950 | C(26) | H(26) | 0.951 |
| C(6) | H(6) | 0.950 | C(26) | H(27) | 0.950 |
| C(7) | H(7) | 0.950 | C(26) | H(28) | 0.951 |
| C(8) | H(8) | 0.950 | C(27) | H(29) | 0.950 |
| C(9) | H(9) | 0.950 | C(27) | H(30) | 0.950 |
| C(10) | H(10) | 0.950 | C(27) | H(31) | 0.950 |
| C(16) | H(11) | 0.951 | C(28) | H(32) | 0.950 |
| C(16) | H(12) | 0.951 | C(28) | H(33) | 0.950 |
| C(16) | H(13) | 0.950 | C(28) | H(34) | 0.950 |
| C(17) | H(14) | 0.951 | C(29) | H(35) | 0.950 |
| C(17) | H(15) | 0.950 | C(29) | H(36) | 0.949 |
| C(17) | H(16) | 0.951 | C(29) | H(37) | 0.951 |
| C(18) | H(17) | 0.950 | C(30) | H(38) | 0.951 |
| C(18) | H(18) | 0.951 | C(30) | H(39) | 0.951 |
| C(18) | H(19) | 0.951 | C(30) | H(40) | 0.949 |
| C(19) | H(20) | 0.949 | C(31) | H(41) | 0.950 |
| C(19) | H(21) | 0.951 | C(31) | H(42) | 0.950 |

Estimated standard deviations in the least significant figure are given in parentheses.

**Table S24. Bond Angles (deg) Involving the Nonhydrogen Atoms in $[(CpTiCl_2)(CpTi)(Cp^*Ru)_2(\mu_3\text{-}S)_4]\cdot CH_2Cl_2$ ($6\cdot CH_2Cl_2$)**

| atom | atom | atom | angle | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|
| Ru(2) | Ru(1) | Ti(2) | 62.44(4) | S(4) | Ru(1) | C(13) | 89.7(3) |
| Ru(2) | Ru(1) | S(1) | 96.82(6) | S(4) | Ru(1) | C(14) | 121.4(3) |
| Ru(2) | Ru(1) | S(3) | 52.66(6) | S(4) | Ru(1) | C(15) | 151.2(3) |
| Ru(2) | Ru(1) | S(4) | 52.61(7) | C(11) | Ru(1) | C(12) | 36.0(3) |
| Ru(2) | Ru(1) | C(11) | 172.4(2) | C(11) | Ru(1) | C(13) | 61.6(3) |
| Ru(2) | Ru(1) | C(12) | 137.5(3) | C(11) | Ru(1) | C(14) | 61.8(3) |
| Ru(2) | Ru(1) | C(13) | 110.8(2) | C(11) | Ru(1) | C(15) | 36.8(3) |
| Ru(2) | Ru(1) | C(14) | 112.9(2) | C(12) | Ru(1) | C(13) | 37.6(3) |
| Ru(2) | Ru(1) | C(15) | 141.9(3) | C(12) | Ru(1) | C(14) | 62.0(3) |
| Ti(2) | Ru(1) | S(1) | 50.38(7) | C(12) | Ru(1) | C(15) | 61.6(3) |
| Ti(2) | Ru(1) | S(3) | 87.74(7) | C(13) | Ru(1) | C(14) | 37.2(3) |
| Ti(2) | Ru(1) | S(4) | 50.21(7) | C(13) | Ru(1) | C(15) | 62.6(4) |
| Ti(2) | Ru(1) | C(11) | 122.1(2) | C(14) | Ru(1) | C(15) | 37.8(3) |
| Ti(2) | Ru(1) | C(12) | 116.0(2) | Ru(1) | Ru(2) | Ti(2) | 60.34(4) |
| Ti(2) | Ru(1) | C(13) | 136.0(3) | Ru(1) | Ru(2) | S(2) | 95.73(6) |
| Ti(2) | Ru(1) | C(14) | 171.5(3) | Ru(1) | Ru(2) | S(3) | 52.64(6) |
| Ti(2) | Ru(1) | C(15) | 149.8(3) | Ru(1) | Ru(2) | S(4) | 52.56(6) |
| S(1) | Ru(1) | S(3) | 80.02(8) | Ru(1) | Ru(2) | C(21) | 157.6(3) |
| S(1) | Ru(1) | S(4) | 100.04(8) | Ru(1) | Ru(2) | C(22) | 125.4(2) |
| S(1) | Ru(1) | C(11) | 90.6(2) | Ru(1) | Ru(2) | C(23) | 113.6(2) |
| S(1) | Ru(1) | C(12) | 114.0(3) | Ru(1) | Ru(2) | C(24) | 128.7(2) |
| S(1) | Ru(1) | C(13) | 150.8(2) | Ru(1) | Ru(2) | C(25) | 162.5(3) |
| S(1) | Ru(1) | C(14) | 138.0(3) | Ti(2) | Ru(2) | S(2) | 49.45(7) |
| S(1) | Ru(1) | C(15) | 101.3(3) | Ti(2) | Ru(2) | S(3) | 86.33(6) |
| S(3) | Ru(1) | S(4) | 104.63(9) | Ti(2) | Ru(2) | S(4) | 49.27(7) |
| S(3) | Ru(1) | C(11) | 131.1(3) | Ti(2) | Ru(2) | C(21) | 115.1(2) |
| S(3) | Ru(1) | C(12) | 156.3(2) | Ti(2) | Ru(2) | C(22) | 126.0(2) |
| S(3) | Ru(1) | C(13) | 124.3(3) | Ti(2) | Ru(2) | C(23) | 156.8(2) |
| S(3) | Ru(1) | C(14) | 94.6(3) | Ti(2) | Ru(2) | C(24) | 165.7(2) |
| S(3) | Ru(1) | C(15) | 97.9(3) | Ti(2) | Ru(2) | C(25) | 131.1(2) |
| S(4) | Ru(1) | C(11) | 124.3(3) | S(2) | Ru(2) | S(3) | 80.95(8) |
| S(4) | Ru(1) | C(12) | 92.1(3) | S(2) | Ru(2) | S(4) | 97.73(8) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| S(2) | Ru(2) | C(21) | 95.7(2) | Cl(2) | Ti(1) | S(1) | 150.9(1) |
| S(2) | Ru(2) | C(22) | 130.7(3) | Cl(2) | Ti(1) | S(2) | 86.8(1) |
| S(2) | Ru(2) | C(23) | 148.8(2) | Cl(2) | Ti(1) | S(3) | 78.60(9) |
| S(2) | Ru(2) | C(24) | 116.3(3) | Cl(2) | Ti(1) | C(1) | 85.7(4) |
| S(2) | Ru(2) | C(25) | 87.3(2) | Cl(2) | Ti(1) | C(2) | 118.9(4) |
| S(3) | Ru(2) | S(4) | 104.56(9) | Cl(2) | Ti(1) | C(3) | 130.4(3) |
| S(3) | Ru(2) | C(21) | 148.7(3) | Cl(2) | Ti(1) | C(4) | 104.4(4) |
| S(3) | Ru(2) | C(22) | 144.0(2) | Cl(2) | Ti(1) | C(5) | 77.6(3) |
| S(3) | Ru(2) | C(23) | 108.0(2) | S(1) | Ti(1) | S(2) | 82.10(9) |
| S(3) | Ru(2) | C(24) | 92.1(2) | S(1) | Ti(1) | S(3) | 72.47(8) |
| S(3) | Ru(2) | C(25) | 111.3(3) | S(1) | Ti(1) | C(1) | 122.6(4) |
| S(4) | Ru(2) | C(21) | 106.8(3) | S(1) | Ti(1) | C(2) | 89.1(4) |
| S(4) | Ru(2) | C(22) | 89.3(2) | S(1) | Ti(1) | C(3) | 77.5(3) |
| S(4) | Ru(2) | C(23) | 108.2(3) | S(1) | Ti(1) | C(4) | 98.5(4) |
| S(4) | Ru(2) | C(24) | 144.2(2) | S(1) | Ti(1) | C(5) | 129.2(4) |
| S(4) | Ru(2) | C(25) | 144.1(3) | S(2) | Ti(1) | S(3) | 73.37(8) |
| C(21) | Ru(2) | C(22) | 36.7(3) | S(2) | Ti(1) | C(1) | 124.5(4) |
| C(21) | Ru(2) | C(23) | 60.9(3) | S(2) | Ti(1) | C(2) | 126.4(4) |
| C(21) | Ru(2) | C(24) | 61.3(3) | S(2) | Ti(1) | C(3) | 94.5(4) |
| C(21) | Ru(2) | C(25) | 37.4(3) | S(2) | Ti(1) | C(4) | 75.0(3) |
| C(22) | Ru(2) | C(23) | 36.2(3) | S(2) | Ti(1) | C(5) | 91.1(4) |
| C(22) | Ru(2) | C(24) | 60.6(3) | S(3) | Ti(1) | C(1) | 155.7(3) |
| C(22) | Ru(2) | C(25) | 61.9(3) | S(3) | Ti(1) | C(2) | 151.6(3) |
| C(23) | Ru(2) | C(24) | 36.0(3) | S(3) | Ti(1) | C(3) | 148.8(3) |
| C(23) | Ru(2) | C(25) | 61.5(3) | S(3) | Ti(1) | C(4) | 148.0(3) |
| C(24) | Ru(2) | C(25) | 37.2(3) | S(3) | Ti(1) | C(5) | 152.2(3) |
| Cl(1) | Ti(1) | Cl(2) | 91.2(1) | C(1) | Ti(1) | C(2) | 33.6(4) |
| Cl(1) | Ti(1) | S(1) | 86.5(1) | C(1) | Ti(1) | C(3) | 53.3(4) |
| Cl(1) | Ti(1) | S(2) | 152.3(1) | C(1) | Ti(1) | C(4) | 54.2(4) |
| Cl(1) | Ti(1) | S(3) | 79.16(9) | C(1) | Ti(1) | C(5) | 33.7(4) |
| Cl(1) | Ti(1) | C(1) | 82.8(4) | C(2) | Ti(1) | C(3) | 32.4(4) |
| Cl(1) | Ti(1) | C(2) | 78.3(3) | C(2) | Ti(1) | C(4) | 54.2(4) |
| Cl(1) | Ti(1) | C(3) | 107.5(4) | C(2) | Ti(1) | C(5) | 55.6(4) |
| Cl(1) | Ti(1) | C(4) | 131.9(3) | C(3) | Ti(1) | C(4) | 31.1(4) |
| Cl(1) | Ti(1) | C(5) | 115.5(5) | C(3) | Ti(1) | C(5) | 52.8(4) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C(4) | Ti(1) | C(5) | 32.3(4) | S(4) | Ti(2) | C(10) | 99.9(4) |
| Ru(1) | Ti(2) | Ru(2) | 57.22(3) | C(6) | Ti(2) | C(7) | 33.4(5) |
| Ru(1) | Ti(2) | S(1) | 52.94(7) | C(6) | Ti(2) | C(8) | 55.6(4) |
| Ru(1) | Ti(2) | S(2) | 95.13(7) | C(6) | Ti(2) | C(9) | 55.9(4) |
| Ru(1) | Ti(2) | S(4) | 51.26(7) | C(6) | Ti(2) | C(10) | 33.5(4) |
| Ru(1) | Ti(2) | C(6) | 124.2(5) | C(7) | Ti(2) | C(8) | 33.1(4) |
| Ru(1) | Ti(2) | C(7) | 154.7(5) | C(7) | Ti(2) | C(9) | 55.4(4) |
| Ru(1) | Ti(2) | C(8) | 164.3(4) | C(7) | Ti(2) | C(10) | 55.6(5) |
| Ru(1) | Ti(2) | C(9) | 131.0(4) | C(8) | Ti(2) | C(9) | 33.8(4) |
| Ru(1) | Ti(2) | C(10) | 113.8(3) | C(8) | Ti(2) | C(10) | 56.2(4) |
| Ru(2) | Ti(2) | S(1) | 94.60(8) | C(9) | Ti(2) | C(10) | 34.2(4) |
| Ru(2) | Ti(2) | S(2) | 51.99(6) | Ru(1) | S(1) | Ti(1) | 102.93(9) |
| Ru(2) | Ti(2) | S(4) | 50.33(7) | Ru(1) | S(1) | Ti(2) | 76.68(8) |
| Ru(2) | Ti(2) | C(6) | 122.5(4) | Ti(1) | S(1) | Ti(2) | 91.8(1) |
| Ru(2) | Ti(2) | C(7) | 118.1(3) | Ru(2) | S(2) | Ti(1) | 102.36(9) |
| Ru(2) | Ti(2) | C(8) | 137.9(4) | Ru(2) | S(2) | Ti(2) | 78.56(8) |
| Ru(2) | Ti(2) | C(9) | 171.7(4) | Ti(1) | S(2) | Ti(2) | 91.98(9) |
| Ru(2) | Ti(2) | C(10) | 149.1(5) | Ru(1) | S(3) | Ru(2) | 74.70(7) |
| S(1) | Ti(2) | S(2) | 92.9(1) | Ru(1) | S(3) | Ti(1) | 103.89(8) |
| S(1) | Ti(2) | S(4) | 103.6(1) | Ru(2) | S(3) | Ti(1) | 103.14(9) |
| S(1) | Ti(2) | C(6) | 134.4(5) | Ru(1) | S(4) | Ru(2) | 74.83(8) |
| S(1) | Ti(2) | C(7) | 145.7(3) | Ru(1) | S(4) | Ti(2) | 78.53(9) |
| S(1) | Ti(2) | C(8) | 114.4(4) | Ru(2) | S(4) | Ti(2) | 80.4(1) |
| S(1) | Ti(2) | C(9) | 90.9(3) | Ti(1) | C(1) | C(2) | 73.5(6) |
| S(1) | Ti(2) | C(10) | 101.4(4) | Ti(1) | C(1) | C(5) | 73.9(7) |
| S(2) | Ti(2) | S(4) | 101.3(1) | C(2) | C(1) | C(5) | 108(1) |
| S(2) | Ti(2) | C(6) | 129.9(6) | Ti(1) | C(2) | C(1) | 72.9(6) |
| S(2) | Ti(2) | C(7) | 99.2(4) | Ti(1) | C(2) | C(3) | 73.2(6) |
| S(2) | Ti(2) | C(8) | 94.8(3) | C(1) | C(2) | C(3) | 104(1) |
| S(2) | Ti(2) | C(9) | 121.6(4) | Ti(1) | C(3) | C(2) | 74.4(7) |
| S(2) | Ti(2) | C(10) | 150.8(3) | Ti(1) | C(3) | C(4) | 75.9(7) |
| S(4) | Ti(2) | C(6) | 84.8(3) | C(2) | C(3) | C(4) | 114(1) |
| S(4) | Ti(2) | C(7) | 105.2(5) | Ti(1) | C(4) | C(3) | 73.0(8) |
| S(4) | Ti(2) | C(8) | 137.7(4) | Ti(1) | C(4) | C(5) | 73.5(7) |
| S(4) | Ti(2) | C(9) | 134.0(4) | C(3) | C(4) | C(5) | 108(1) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Ti(1) | C(5) | C(1) | 72.4(7) | C(14) | C(13) | C(18) | 126.5(9) |
| Ti(1) | C(5) | C(4) | 74.2(8) | Ru(1) | C(14) | C(13) | 71.3(5) |
| C(1) | C(5) | C(4) | 107(1) | Ru(1) | C(14) | C(15) | 69.4(5) |
| Ti(2) | C(6) | C(7) | 71.8(8) | Ru(1) | C(14) | C(19) | 126.9(6) |
| Ti(2) | C(6) | C(10) | 72.9(7) | C(13) | C(14) | C(15) | 107.0(8) |
| C(7) | C(6) | C(10) | 107(1) | C(13) | C(14) | C(19) | 128(1) |
| Ti(2) | C(7) | C(6) | 74.8(8) | C(15) | C(14) | C(19) | 125(1) |
| Ti(2) | C(7) | C(8) | 74.3(7) | Ru(1) | C(15) | C(11) | 73.1(5) |
| C(6) | C(7) | C(8) | 110(1) | Ru(1) | C(15) | C(14) | 72.8(5) |
| Ti(2) | C(8) | C(7) | 72.7(7) | Ru(1) | C(15) | C(20) | 127.5(7) |
| Ti(2) | C(8) | C(9) | 73.2(6) | C(11) | C(15) | C(14) | 108.1(9) |
| C(7) | C(8) | C(9) | 108(1) | C(11) | C(15) | C(20) | 127(1) |
| Ti(2) | C(9) | C(8) | 73.0(6) | C(14) | C(15) | C(20) | 124.3(9) |
| Ti(2) | C(9) | C(10) | 73.2(6) | Ru(2) | C(21) | C(22) | 75.1(5) |
| C(8) | C(9) | C(10) | 108(1) | Ru(2) | C(21) | C(25) | 72.5(5) |
| Ti(2) | C(10) | C(6) | 73.6(7) | Ru(2) | C(21) | C(26) | 125.7(6) |
| Ti(2) | C(10) | C(9) | 72.6(7) | C(22) | C(21) | C(25) | 110.2(8) |
| C(6) | C(10) | C(9) | 107(1) | C(22) | C(21) | C(26) | 125(1) |
| Ru(1) | C(11) | C(12) | 73.1(5) | C(25) | C(21) | C(26) | 125(1) |
| Ru(1) | C(11) | C(15) | 70.1(6) | Ru(2) | C(22) | C(21) | 68.2(5) |
| Ru(1) | C(11) | C(16) | 126.6(6) | Ru(2) | C(22) | C(23) | 73.8(5) |
| C(12) | C(11) | C(15) | 109.9(9) | Ru(2) | C(22) | C(27) | 128.0(6) |
| C(12) | C(11) | C(16) | 124.0(9) | C(21) | C(22) | C(23) | 107.5(8) |
| C(15) | C(11) | C(16) | 126(1) | C(21) | C(22) | C(27) | 126.6(9) |
| Ru(1) | C(12) | C(11) | 70.9(5) | C(23) | C(22) | C(27) | 125.5(9) |
| Ru(1) | C(12) | C(13) | 70.3(5) | Ru(2) | C(23) | C(22) | 69.9(4) |
| Ru(1) | C(12) | C(17) | 127.9(7) | Ru(2) | C(23) | C(24) | 70.1(5) |
| C(11) | C(12) | C(13) | 107.6(9) | Ru(2) | C(23) | C(28) | 134.6(6) |
| C(11) | C(12) | C(17) | 126.9(9) | C(22) | C(23) | C(24) | 107.1(8) |
| C(13) | C(12) | C(17) | 125(1) | C(22) | C(23) | C(28) | 126.1(9) |
| Ru(1) | C(13) | C(12) | 72.1(5) | C(24) | C(23) | C(28) | 125.6(9) |
| Ru(1) | C(13) | C(14) | 71.5(5) | Ru(2) | C(24) | C(23) | 73.9(5) |
| Ru(1) | C(13) | C(18) | 127.9(7) | Ru(2) | C(24) | C(25) | 69.2(5) |
| C(12) | C(13) | C(14) | 107.5(8) | Ru(2) | C(24) | C(29) | 128.1(6) |
| C(12) | C(13) | C(18) | 126(1) | C(23) | C(24) | C(25) | 109.0(8) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C(23) | C(24) | C(29) | 124.1(9) | C(21) | C(25) | C(24) | 106.1(9) |
| C(25) | C(24) | C(29) | 127(1) | C(21) | C(25) | C(30) | 129(1) |
| Ru(2) | C(25) | C(21) | 70.1(5) | C(24) | C(25) | C(30) | 124(1) |
| Ru(2) | C(25) | C(24) | 73.6(5) | Cl(3) | C(31) | Cl(4) | 116.8(8) |
| Ru(2) | C(25) | C(30) | 130.0(6) | | | | |

Estimated standard deviations in the least significant figure are given in parentheses.

**Table S25. Bond Angles (deg) Involving the Hydrogen Atoms in $[(CpTiCl_2)(CpTi)(Cp^*Ru)_2(\mu_3\text{-}S)_4]\cdot CH_2Cl_2$ ($6\cdot CH_2Cl_2$)**

| atom | atom | atom | angle | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|
| Ti(1) | C(1) | H(1) | 118.50 | C(11) | C(16) | H(13) | 109.60 |
| C(2) | C(1) | H(1) | 126.10 | H(11) | C(16) | H(12) | 109.33 |
| C(5) | C(1) | H(1) | 126.19 | H(11) | C(16) | H(13) | 109.43 |
| Ti(1) | C(2) | H(2) | 118.21 | H(12) | C(16) | H(13) | 109.42 |
| C(1) | C(2) | H(2) | 127.93 | C(12) | C(17) | H(14) | 109.55 |
| C(3) | C(2) | H(2) | 128.03 | C(12) | C(17) | H(15) | 109.63 |
| Ti(1) | C(3) | H(3) | 117.91 | C(12) | C(17) | H(16) | 109.59 |
| C(2) | C(3) | H(3) | 123.19 | H(14) | C(17) | H(15) | 109.35 |
| C(4) | C(3) | H(3) | 123.21 | H(14) | C(17) | H(16) | 109.30 |
| Ti(1) | C(4) | H(4) | 119.40 | H(15) | C(17) | H(16) | 109.41 |
| C(3) | C(4) | H(4) | 125.92 | C(13) | C(18) | H(17) | 109.63 |
| C(5) | C(4) | H(4) | 125.97 | C(13) | C(18) | H(18) | 109.57 |
| Ti(1) | C(5) | H(5) | 118.77 | C(13) | C(18) | H(19) | 109.55 |
| C(1) | C(5) | H(5) | 126.73 | H(17) | C(18) | H(18) | 109.39 |
| C(4) | C(5) | H(5) | 126.75 | H(17) | C(18) | H(19) | 109.38 |
| Ti(2) | C(6) | H(6) | 120.83 | H(18) | C(18) | H(19) | 109.30 |
| C(7) | C(6) | H(6) | 126.38 | C(14) | C(19) | H(20) | 109.56 |
| C(10) | C(6) | H(6) | 126.33 | C(14) | C(19) | H(21) | 109.45 |
| Ti(2) | C(7) | H(7) | 117.77 | C(14) | C(19) | H(22) | 109.48 |
| C(6) | C(7) | H(7) | 124.87 | H(20) | C(19) | H(21) | 109.47 |
| C(8) | C(7) | H(7) | 124.91 | H(20) | C(19) | H(22) | 109.52 |
| Ti(2) | C(8) | H(8) | 119.83 | H(21) | C(19) | H(22) | 109.35 |
| C(7) | C(8) | H(8) | 126.16 | C(15) | C(20) | H(23) | 109.60 |
| C(9) | C(8) | H(8) | 126.21 | C(15) | C(20) | H(24) | 109.57 |
| Ti(2) | C(9) | H(9) | 119.39 | C(15) | C(20) | H(25) | 109.59 |
| C(8) | C(9) | H(9) | 126.26 | H(23) | C(20) | H(24) | 109.35 |
| C(10) | C(9) | H(9) | 126.22 | H(23) | C(20) | H(25) | 109.37 |
| Ti(2) | C(10) | H(10) | 119.31 | H(24) | C(20) | H(25) | 109.35 |
| C(6) | C(10) | H(10) | 126.26 | C(21) | C(26) | H(26) | 109.53 |
| C(9) | C(10) | H(10) | 126.43 | C(21) | C(26) | H(27) | 109.59 |
| C(11) | C(16) | H(11) | 109.52 | C(21) | C(26) | H(28) | 109.52 |
| C(11) | C(16) | H(12) | 109.53 | H(26) | C(26) | H(27) | 109.44 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| H(26) | C(26) | H(28) | 109.35 | C(24) | C(29) | H(37) | 109.44 |
| H(27) | C(26) | H(28) | 109.40 | H(35) | C(29) | H(36) | 109.52 |
| C(22) | C(27) | H(29) | 109.51 | H(35) | C(29) | H(37) | 109.40 |
| C(22) | C(27) | H(30) | 109.52 | H(36) | C(29) | H(37) | 109.47 |
| C(22) | C(27) | H(31) | 109.48 | C(25) | C(30) | H(38) | 109.48 |
| H(29) | C(27) | H(30) | 109.45 | C(25) | C(30) | H(39) | 109.48 |
| H(29) | C(27) | H(31) | 109.43 | C(25) | C(30) | H(40) | 109.56 |
| H(30) | C(27) | H(31) | 109.43 | H(38) | C(30) | H(39) | 109.35 |
| C(23) | C(28) | H(32) | 109.48 | H(38) | C(30) | H(40) | 109.48 |
| C(23) | C(28) | H(33) | 109.50 | H(39) | C(30) | H(40) | 109.47 |
| C(23) | C(28) | H(34) | 109.51 | Cl(3) | C(31) | H(41) | 107.70 |
| H(32) | C(28) | H(33) | 109.42 | Cl(3) | C(31) | H(42) | 107.68 |
| H(32) | C(28) | H(34) | 109.46 | Cl(4) | C(31) | H(41) | 107.51 |
| H(33) | C(28) | H(34) | 109.46 | Cl(4) | C(31) | H(42) | 107.52 |
| C(24) | C(29) | H(35) | 109.47 | H(41) | C(31) | H(42) | 109.45 |
| C(24) | C(29) | H(36) | 109.53 | | | | |

Estimated standard deviations in the least significant figure are given in parentheses.

**Table S26. Atomic Coordinates and B(eq) Values for $[(TiCl_3)(CpTi)(Cp^*Ru)_2(\mu_3\text{-}S)_4]\cdot CH_2Cl_2$ ($7\cdot CH_2Cl_2$)**

| atom | x | y | z | B(eq) |
|---|---|---|---|---|
| Ru(1) | 0.02148(6) | 0.15847(3) | 0.21070(3) | 2.22(1) |
| Ru(2) | 0.21705(6) | 0.12630(3) | 0.32364(3) | 2.26(1) |
| Ti(1) | -0.0796(1) | 0.16664(7) | 0.39855(7) | 3.31(3) |
| Ti(2) | -0.0117(1) | 0.03139(6) | 0.29974(7) | 2.78(3) |
| Cl(1) | -0.2347(2) | 0.2564(1) | 0.3770(1) | 4.78(6) |
| Cl(2) | 0.0286(2) | 0.2166(1) | 0.5027(1) | 4.38(5) |
| Cl(3) | -0.2463(2) | 0.1085(1) | 0.4669(1) | 5.50(6) |
| Cl(4) | 0.1575(3) | 0.4169(2) | 0.3808(2) | 10.4(1) |
| Cl(5) | -0.1111(4) | 0.4504(2) | 0.4253(2) | 12.7(1) |
| S(1) | -0.1656(2) | 0.11582(9) | 0.28047(9) | 2.70(4) |
| S(2) | 0.0722(2) | 0.07180(9) | 0.41201(10) | 2.90(4) |
| S(3) | 0.0766(2) | 0.22098(9) | 0.31781(10) | 2.73(4) |
| S(4) | 0.1527(2) | 0.06147(9) | 0.21919(9) | 2.65(4) |
| C(1) | 0.031(1) | -0.0830(5) | 0.284(2) | 9.3(4) |
| C(2) | -0.018(3) | -0.0757(7) | 0.350(1) | 11.8(7) |
| C(3) | -0.143(3) | -0.0536(9) | 0.346(1) | 11.6(7) |
| C(4) | -0.177(2) | -0.0497(6) | 0.272(1) | 9.5(5) |
| C(5) | -0.067(2) | -0.0687(6) | 0.2353(6) | 7.5(4) |
| C(6) | -0.1165(8) | 0.1724(4) | 0.1111(4) | 3.5(2) |
| C(7) | 0.0030(9) | 0.1463(4) | 0.0851(4) | 4.1(2) |
| C(8) | 0.1088(8) | 0.1902(5) | 0.1012(4) | 4.4(2) |
| C(9) | 0.0567(10) | 0.2470(4) | 0.1365(4) | 4.6(2) |
| C(10) | -0.0878(9) | 0.2365(4) | 0.1451(4) | 4.1(2) |
| C(11) | -0.2545(10) | 0.1430(6) | 0.0984(5) | 9.6(4) |
| C(12) | 0.017(1) | 0.0811(5) | 0.0399(5) | 10.8(4) |
| C(13) | 0.2495(10) | 0.1836(7) | 0.0724(5) | 10.9(4) |
| C(14) | 0.131(1) | 0.3108(5) | 0.1542(6) | 11.4(4) |
| C(15) | -0.190(1) | 0.2842(6) | 0.1742(5) | 11.5(4) |
| C(16) | 0.4048(7) | 0.0736(4) | 0.3542(5) | 3.7(2) |
| C(17) | 0.4276(7) | 0.1114(4) | 0.2895(4) | 3.0(2) |
| C(18) | 0.4151(7) | 0.1794(4) | 0.3055(4) | 3.3(2) |
| C(19) | 0.3860(7) | 0.1852(4) | 0.3824(5) | 3.8(2) |

| | | | | |
|---|---|---|---|---|
| C(20) | 0.3813(7) | 0.1192(5) | 0.4131(4) | 4.1(2) |
| C(21) | 0.4200(9) | -0.0018(5) | 0.3635(6) | 7.2(3) |
| C(22) | 0.4766(8) | 0.0805(4) | 0.2177(5) | 5.3(2) |
| C(23) | 0.4462(9) | 0.2378(4) | 0.2557(5) | 6.4(3) |
| C(24) | 0.3769(8) | 0.2495(5) | 0.4253(5) | 6.4(3) |
| C(25) | 0.3652(9) | 0.1022(6) | 0.4952(5) | 7.1(3) |
| C(26) | 0.006(1) | 0.3905(5) | 0.4091(8) | 10.7(4) |
| H(1) | 0.1209 | -0.0963 | 0.2723 | 11.1947 |
| H(2) | 0.0312 | -0.0850 | 0.3961 | 14.1107 |
| H(3) | -0.1995 | -0.0427 | 0.3872 | 13.9007 |
| H(4) | -0.2617 | -0.0361 | 0.2502 | 11.4350 |
| H(5) | -0.0615 | -0.0714 | 0.1821 | 9.0025 |
| H(6) | -0.2973 | 0.1382 | 0.1452 | 11.4684 |
| H(7) | -0.3071 | 0.1721 | 0.0666 | 11.4684 |
| H(8) | -0.2469 | 0.1000 | 0.0751 | 11.4684 |
| H(9) | -0.0687 | 0.0588 | 0.0364 | 12.9179 |
| H(10) | 0.0457 | 0.0916 | -0.0093 | 12.9179 |
| H(11) | 0.0815 | 0.0524 | 0.0643 | 12.9179 |
| H(12) | 0.2885 | 0.1424 | 0.0899 | 13.1124 |
| H(13) | 0.2459 | 0.1838 | 0.0190 | 13.1124 |
| H(14) | 0.3033 | 0.2205 | 0.0902 | 13.1124 |
| H(15) | 0.2067 | 0.3012 | 0.1866 | 13.6504 |
| H(16) | 0.1610 | 0.3305 | 0.1090 | 13.6504 |
| H(17) | 0.0719 | 0.3413 | 0.1784 | 13.6504 |
| H(18) | -0.1452 | 0.3233 | 0.1936 | 13.8392 |
| H(19) | -0.2514 | 0.2969 | 0.1345 | 13.8392 |
| H(20) | -0.2384 | 0.2630 | 0.2131 | 13.8392 |
| H(21) | 0.3390 | -0.0200 | 0.3828 | 8.6574 |
| H(22) | 0.4367 | -0.0217 | 0.3160 | 8.6574 |
| H(23) | 0.4939 | -0.0111 | 0.3975 | 8.6574 |
| H(24) | 0.4124 | 0.0482 | 0.1996 | 6.3506 |
| H(25) | 0.4868 | 0.1149 | 0.1810 | 6.3506 |
| H(26) | 0.5615 | 0.0590 | 0.2273 | 6.3506 |
| H(27) | 0.5391 | 0.2364 | 0.2430 | 7.6759 |
| H(28) | 0.3910 | 0.2354 | 0.2110 | 7.6759 |

| | | | | |
|---|---|---|---|---|
| H(29) | 0.4283 | 0.2789 | 0.2813 | 7.6759 |
| H(30) | 0.4617 | 0.2722 | 0.4247 | 7.7094 |
| H(31) | 0.3085 | 0.2773 | 0.4027 | 7.7094 |
| H(32) | 0.3547 | 0.2400 | 0.4758 | 7.7094 |
| H(33) | 0.3499 | 0.1425 | 0.5227 | 8.5775 |
| H(34) | 0.2901 | 0.0726 | 0.5002 | 8.5775 |
| H(35) | 0.4453 | 0.0807 | 0.5142 | 8.5775 |
| H(36) | -0.0311 | 0.3613 | 0.3713 | 12.8687 |
| H(37) | 0.0201 | 0.3659 | 0.4545 | 12.8687 |

Estimated standard deviations in the least significant figure are given in parentheses.

**Table S27. Anisotropic Displacement Parameters for $[(TiCl_3)(CpTi)(Cp^*Ru)_2(\mu_3\text{-}S)_4]\cdot CH_2Cl_2$ ($7\cdot CH_2Cl_2$)**

| atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|
| Ru(1) | 0.0308(3) | 0.0272(3) | 0.0261(3) | -0.0013(3) | -0.0015(2) | 0.0050(3) |
| Ru(2) | 0.0304(3) | 0.0279(3) | 0.0274(3) | 0.0007(3) | -0.0029(2) | 0.0026(2) |
| Ti(1) | 0.0464(8) | 0.0438(8) | 0.0353(8) | 0.0013(7) | -0.0035(6) | -0.0036(7) |
| Ti(2) | 0.0440(8) | 0.0279(7) | 0.0337(7) | -0.0048(6) | -0.0007(6) | 0.0040(6) |
| Cl(1) | 0.054(1) | 0.068(1) | 0.060(1) | 0.023(1) | -0.008(1) | -0.010(1) |
| Cl(2) | 0.064(1) | 0.064(1) | 0.037(1) | 0.006(1) | -0.0085(10) | -0.013(1) |
| Cl(3) | 0.058(1) | 0.098(2) | 0.054(1) | -0.009(1) | 0.022(1) | 0.009(1) |
| Cl(4) | 0.122(3) | 0.098(2) | 0.177(3) | 0.001(2) | 0.009(3) | 0.041(2) |
| Cl(5) | 0.171(4) | 0.106(3) | 0.210(4) | -0.006(3) | 0.053(3) | 0.006(3) |
| S(1) | 0.0301(9) | 0.042(1) | 0.0301(9) | -0.0031(8) | -0.0012(7) | 0.0025(8) |
| S(2) | 0.038(1) | 0.041(1) | 0.0307(10) | 0.0007(9) | -0.0012(8) | 0.0076(8) |
| S(3) | 0.039(1) | 0.0312(10) | 0.0330(10) | 0.0049(8) | 0.0007(8) | -0.0023(8) |
| S(4) | 0.037(1) | 0.0319(10) | 0.0318(9) | 0.0036(8) | 0.0003(8) | -0.0015(8) |
| C(1) | 0.069(8) | 0.023(5) | 0.26(2) | 0.003(5) | -0.01(1) | 0.00(1) |
| C(2) | 0.31(3) | 0.042(9) | 0.09(1) | -0.07(1) | -0.07(2) | 0.041(9) |
| C(3) | 0.22(2) | 0.07(1) | 0.16(2) | -0.09(1) | 0.13(2) | -0.04(1) |
| C(4) | 0.075(9) | 0.035(6) | 0.25(2) | -0.019(6) | -0.06(1) | 0.01(1) |
| C(5) | 0.17(1) | 0.037(7) | 0.079(8) | -0.048(8) | -0.01(1) | -0.011(6) |
| C(6) | 0.044(5) | 0.065(6) | 0.024(4) | -0.011(4) | -0.008(3) | 0.021(4) |
| C(7) | 0.077(6) | 0.051(5) | 0.027(4) | 0.017(5) | -0.007(4) | 0.011(4) |
| C(8) | 0.047(5) | 0.088(7) | 0.030(4) | 0.000(5) | -0.003(4) | 0.023(5) |
| C(9) | 0.086(7) | 0.047(5) | 0.039(5) | -0.028(5) | -0.029(5) | 0.025(4) |
| C(10) | 0.086(7) | 0.054(5) | 0.017(4) | 0.035(5) | -0.003(4) | 0.012(4) |
| C(11) | 0.086(8) | 0.20(1) | 0.076(7) | -0.078(8) | -0.044(6) | 0.069(8) |
| C(12) | 0.27(2) | 0.090(9) | 0.044(6) | 0.062(10) | -0.030(8) | -0.026(6) |
| C(13) | 0.062(7) | 0.30(2) | 0.058(7) | 0.030(9) | 0.025(5) | 0.075(9) |
| C(14) | 0.24(1) | 0.088(8) | 0.100(9) | -0.103(9) | -0.084(9) | 0.066(7) |
| C(15) | 0.23(1) | 0.17(1) | 0.040(6) | 0.16(1) | 0.017(7) | 0.029(7) |
| C(16) | 0.031(4) | 0.041(5) | 0.068(6) | 0.007(4) | -0.004(4) | 0.005(4) |
| C(17) | 0.031(4) | 0.042(5) | 0.039(4) | 0.004(3) | -0.005(3) | -0.005(4) |
| C(18) | 0.034(4) | 0.046(5) | 0.044(5) | -0.004(4) | -0.008(4) | 0.007(4) |
| C(19) | 0.030(4) | 0.056(5) | 0.056(5) | 0.002(4) | -0.010(4) | -0.012(4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(20) | 0.032(4) | 0.083(7) | 0.039(5) | -0.005(4) | -0.012(4) | 0.019(5) |
| C(21) | 0.067(7) | 0.064(7) | 0.14(1) | 0.021(5) | -0.009(7) | 0.027(7) |
| C(22) | 0.040(5) | 0.089(7) | 0.073(6) | -0.007(5) | 0.014(4) | -0.028(6) |
| C(23) | 0.068(6) | 0.064(6) | 0.109(8) | -0.041(5) | -0.029(6) | 0.041(6) |
| C(24) | 0.047(6) | 0.105(8) | 0.091(7) | -0.003(5) | -0.016(5) | -0.053(6) |
| C(25) | 0.058(6) | 0.17(1) | 0.042(5) | -0.006(7) | -0.016(5) | 0.021(6) |
| C(26) | 0.103(10) | 0.061(8) | 0.24(2) | -0.002(7) | -0.01(1) | 0.044(9) |

Estimated standard deviations in the least significant figure are given in parentheses.

**Table S28. Bond Lengths (Å) Involving the Nonhydrogen Atoms in $[(TiCl_3)(CpTi)(Cp^*Ru)_2(\mu_3\text{-}S)_4]\cdot CH_2Cl_2$ ($7\cdot CH_2Cl_2$)**

| atom | atom | distance | atom | atom | distance |
|---|---|---|---|---|---|
| Ru(1) | Ru(2) | 2.8141(8) | Ti(2) | C(3) | 2.30(1) |
| Ru(1) | Ti(2) | 2.995(1) | Ti(2) | C(4) | 2.33(1) |
| Ru(1) | S(1) | 2.406(2) | Ti(2) | C(5) | 2.345(9) |
| Ru(1) | S(3) | 2.321(2) | Cl(4) | C(26) | 1.68(1) |
| Ru(1) | S(4) | 2.317(2) | Cl(5) | C(26) | 1.68(1) |
| Ru(1) | C(6) | 2.217(6) | C(1) | C(2) | 1.30(2) |
| Ru(1) | C(7) | 2.247(7) | C(1) | C(5) | 1.31(2) |
| Ru(1) | C(8) | 2.242(8) | C(2) | C(3) | 1.31(2) |
| Ru(1) | C(9) | 2.227(7) | C(3) | C(4) | 1.36(2) |
| Ru(1) | C(10) | 2.198(7) | C(4) | C(5) | 1.33(2) |
| Ru(2) | Ti(2) | 2.956(1) | C(6) | C(7) | 1.38(1) |
| Ru(2) | S(2) | 2.409(2) | C(6) | C(10) | 1.43(1) |
| Ru(2) | S(3) | 2.330(2) | C(6) | C(11) | 1.49(1) |
| Ru(2) | S(4) | 2.329(2) | C(7) | C(8) | 1.38(1) |
| Ru(2) | C(16) | 2.179(7) | C(7) | C(12) | 1.53(1) |
| Ru(2) | C(17) | 2.199(7) | C(8) | C(9) | 1.39(1) |
| Ru(2) | C(18) | 2.248(7) | C(8) | C(13) | 1.50(1) |
| Ru(2) | C(19) | 2.262(7) | C(9) | C(10) | 1.45(1) |
| Ru(2) | C(20) | 2.239(7) | C(9) | C(14) | 1.49(1) |
| Ti(1) | Cl(1) | 2.367(2) | C(10) | C(15) | 1.48(1) |
| Ti(1) | Cl(2) | 2.329(2) | C(16) | C(17) | 1.397(9) |
| Ti(1) | Cl(3) | 2.371(2) | C(16) | C(20) | 1.41(1) |
| Ti(1) | S(1) | 2.455(2) | C(16) | C(21) | 1.51(1) |
| Ti(1) | S(2) | 2.408(2) | C(17) | C(18) | 1.381(9) |
| Ti(1) | S(3) | 2.391(2) | C(17) | C(22) | 1.508(9) |
| Ti(2) | S(1) | 2.276(2) | C(18) | C(19) | 1.41(1) |
| Ti(2) | S(2) | 2.282(2) | C(18) | C(23) | 1.49(1) |
| Ti(2) | S(4) | 2.274(2) | C(19) | C(20) | 1.42(1) |
| Ti(2) | C(1) | 2.32(1) | C(19) | C(24) | 1.49(1) |
| Ti(2) | C(2) | 2.30(1) | C(20) | C(25) | 1.51(1) |

Estimated standard deviations in the least significant figure are given in parentheses.

**Table S29. Bond Lengths (Å) Involving the Hydrogen Atoms in $[(TiCl_3)(CpTi)(Cp^*Ru)_2(\mu_3\text{-}S)_4]\cdot CH_2Cl_2$ ($7\cdot CH_2Cl_2$)**

| atom | atom | distance | atom | atom | distance |
|---|---|---|---|---|---|
| C(1) | H(1) | 0.950 | C(15) | H(20) | 0.950 |
| C(2) | H(2) | 0.950 | C(21) | H(21) | 0.950 |
| C(3) | H(3) | 0.950 | C(21) | H(22) | 0.950 |
| C(4) | H(4) | 0.950 | C(21) | H(23) | 0.950 |
| C(5) | H(5) | 0.950 | C(22) | H(24) | 0.950 |
| C(11) | H(6) | 0.950 | C(22) | H(25) | 0.950 |
| C(11) | H(7) | 0.950 | C(22) | H(26) | 0.950 |
| C(11) | H(8) | 0.950 | C(23) | H(27) | 0.950 |
| C(12) | H(9) | 0.950 | C(23) | H(28) | 0.950 |
| C(12) | H(10) | 0.950 | C(23) | H(29) | 0.950 |
| C(12) | H(11) | 0.950 | C(24) | H(30) | 0.950 |
| C(13) | H(12) | 0.950 | C(24) | H(31) | 0.950 |
| C(13) | H(13) | 0.950 | C(24) | H(32) | 0.950 |
| C(13) | H(14) | 0.950 | C(25) | H(33) | 0.950 |
| C(14) | H(15) | 0.950 | C(25) | H(34) | 0.950 |
| C(14) | H(16) | 0.950 | C(25) | H(35) | 0.950 |
| C(14) | H(17) | 0.950 | C(26) | H(36) | 0.950 |
| C(15) | H(18) | 0.950 | C(26) | H(37) | 0.950 |
| C(15) | H(19) | 0.950 | | | |

Estimated standard deviations in the least significant figure are given in parentheses.

**Table S30. Bond Angles (deg) Involving the Nonhydrogen Atoms in $[(TiCl_3)(CpTi)(Cp^*Ru)_2(\mu_3\text{-}S)_4]\cdot CH_2Cl_2$ ($7\cdot CH_2Cl_2$)**

| atom | atom | atom | angle | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|
| Ru(2) | Ru(1) | Ti(2) | 61.08(3) | S(4) | Ru(1) | C(8) | 93.5(2) |
| Ru(2) | Ru(1) | S(1) | 94.14(5) | S(4) | Ru(1) | C(9) | 126.4(3) |
| Ru(2) | Ru(1) | S(3) | 52.92(4) | S(4) | Ru(1) | C(10) | 151.7(2) |
| Ru(2) | Ru(1) | S(4) | 52.92(4) | C(6) | Ru(1) | C(7) | 36.0(3) |
| Ru(2) | Ru(1) | C(6) | 171.3(2) | C(6) | Ru(1) | C(8) | 60.9(3) |
| Ru(2) | Ru(1) | C(7) | 135.9(2) | C(6) | Ru(1) | C(9) | 62.1(3) |
| Ru(2) | Ru(1) | C(8) | 114.2(2) | C(6) | Ru(1) | C(10) | 37.8(3) |
| Ru(2) | Ru(1) | C(9) | 119.0(2) | C(7) | Ru(1) | C(8) | 35.8(3) |
| Ru(2) | Ru(1) | C(10) | 148.4(2) | C(7) | Ru(1) | C(9) | 60.4(3) |
| Ti(2) | Ru(1) | S(1) | 48.35(5) | C(7) | Ru(1) | C(10) | 61.6(3) |
| Ti(2) | Ru(1) | S(3) | 92.34(5) | C(8) | Ru(1) | C(9) | 36.3(3) |
| Ti(2) | Ru(1) | S(4) | 48.65(5) | C(8) | Ru(1) | C(10) | 62.4(3) |
| Ti(2) | Ru(1) | C(6) | 116.9(2) | C(9) | Ru(1) | C(10) | 38.3(3) |
| Ti(2) | Ru(1) | C(7) | 115.3(2) | Ru(1) | Ru(2) | Ti(2) | 62.48(3) |
| Ti(2) | Ru(1) | C(8) | 138.2(3) | Ru(1) | Ru(2) | S(2) | 99.19(5) |
| Ti(2) | Ru(1) | C(9) | 174.5(3) | Ru(1) | Ru(2) | S(3) | 52.62(4) |
| Ti(2) | Ru(1) | C(10) | 144.2(3) | Ru(1) | Ru(2) | S(4) | 52.54(4) |
| S(1) | Ru(1) | S(3) | 85.89(6) | Ru(1) | Ru(2) | C(16) | 147.7(2) |
| S(1) | Ru(1) | S(4) | 96.36(6) | Ru(1) | Ru(2) | C(17) | 117.7(2) |
| S(1) | Ru(1) | C(6) | 89.6(2) | Ru(1) | Ru(2) | C(18) | 111.8(2) |
| S(1) | Ru(1) | C(7) | 115.7(2) | Ru(1) | Ru(2) | C(19) | 133.8(2) |
| S(1) | Ru(1) | C(8) | 150.0(2) | Ru(1) | Ru(2) | C(20) | 170.4(2) |
| S(1) | Ru(1) | C(9) | 135.8(3) | Ti(2) | Ru(2) | S(2) | 49.06(5) |
| S(1) | Ru(1) | C(10) | 98.6(2) | Ti(2) | Ru(2) | S(3) | 93.15(5) |
| S(3) | Ru(1) | S(4) | 105.76(6) | Ti(2) | Ru(2) | S(4) | 49.23(5) |
| S(3) | Ru(1) | C(6) | 135.3(2) | Ti(2) | Ru(2) | C(16) | 111.7(2) |
| S(3) | Ru(1) | C(7) | 151.9(2) | Ti(2) | Ru(2) | C(17) | 126.7(2) |
| S(3) | Ru(1) | C(8) | 118.4(3) | Ti(2) | Ru(2) | C(18) | 159.8(2) |
| S(3) | Ru(1) | C(9) | 91.7(2) | Ti(2) | Ru(2) | C(19) | 160.3(2) |
| S(3) | Ru(1) | C(10) | 99.2(2) | Ti(2) | Ru(2) | C(20) | 126.5(2) |
| S(4) | Ru(1) | C(6) | 118.9(2) | S(2) | Ru(2) | S(3) | 91.50(6) |
| S(4) | Ru(1) | C(7) | 90.3(2) | S(2) | Ru(2) | S(4) | 96.92(6) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| S(2) | Ru(2) | C(16) | 97.9(2) | Cl(3) | Ti(1) | S(1) | 90.70(8) |
| S(2) | Ru(2) | C(17) | 134.6(2) | Cl(3) | Ti(1) | S(2) | 90.51(9) |
| S(2) | Ru(2) | C(18) | 146.8(2) | Cl(3) | Ti(1) | S(3) | 173.95(9) |
| S(2) | Ru(2) | C(19) | 111.8(2) | S(1) | Ti(1) | S(2) | 87.90(7) |
| S(2) | Ru(2) | C(20) | 86.5(2) | S(1) | Ti(1) | S(3) | 83.30(7) |
| S(3) | Ru(2) | S(4) | 105.09(6) | S(2) | Ti(1) | S(3) | 90.05(8) |
| S(3) | Ru(2) | C(16) | 153.5(2) | Ru(1) | Ti(2) | Ru(2) | 56.45(3) |
| S(3) | Ru(2) | C(17) | 131.3(2) | Ru(1) | Ti(2) | S(1) | 52.18(5) |
| S(3) | Ru(2) | C(18) | 97.8(2) | Ru(1) | Ti(2) | S(2) | 97.20(6) |
| S(3) | Ru(2) | C(19) | 92.0(2) | Ru(1) | Ti(2) | S(4) | 49.92(5) |
| S(3) | Ru(2) | C(20) | 119.9(2) | Ru(1) | Ti(2) | C(1) | 136.9(6) |
| S(4) | Ru(2) | C(16) | 98.3(2) | Ru(1) | Ti(2) | C(2) | 169.6(7) |
| S(4) | Ru(2) | C(17) | 86.7(2) | Ru(1) | Ti(2) | C(3) | 151.4(8) |
| S(4) | Ru(2) | C(18) | 111.1(2) | Ru(1) | Ti(2) | C(4) | 123.6(4) |
| S(4) | Ru(2) | C(19) | 146.2(2) | Ru(1) | Ti(2) | C(5) | 118.6(3) |
| S(4) | Ru(2) | C(20) | 134.9(2) | Ru(2) | Ti(2) | S(1) | 93.28(6) |
| C(16) | Ru(2) | C(17) | 37.2(2) | Ru(2) | Ti(2) | S(2) | 52.89(5) |
| C(16) | Ru(2) | C(18) | 61.7(3) | Ru(2) | Ti(2) | S(4) | 50.88(5) |
| C(16) | Ru(2) | C(19) | 61.6(3) | Ru(2) | Ti(2) | C(1) | 119.8(3) |
| C(16) | Ru(2) | C(20) | 37.1(3) | Ru(2) | Ti(2) | C(2) | 123.8(6) |
| C(17) | Ru(2) | C(18) | 36.2(2) | Ru(2) | Ti(2) | C(3) | 148.4(8) |
| C(17) | Ru(2) | C(19) | 60.6(3) | Ru(2) | Ti(2) | C(4) | 173.7(7) |
| C(17) | Ru(2) | C(20) | 61.3(3) | Ru(2) | Ti(2) | C(5) | 140.6(6) |
| C(18) | Ru(2) | C(19) | 36.4(2) | S(1) | Ti(2) | S(2) | 95.55(8) |
| C(18) | Ru(2) | C(20) | 61.2(3) | S(1) | Ti(2) | S(4) | 101.40(8) |
| C(19) | Ru(2) | C(20) | 36.7(3) | S(1) | Ti(2) | C(1) | 145.1(4) |
| Cl(1) | Ti(1) | Cl(2) | 95.05(9) | S(1) | Ti(2) | C(2) | 135.2(8) |
| Cl(1) | Ti(1) | Cl(3) | 89.60(9) | S(1) | Ti(2) | C(3) | 102.2(7) |
| Cl(1) | Ti(1) | S(1) | 87.96(8) | S(1) | Ti(2) | C(4) | 90.9(4) |
| Cl(1) | Ti(1) | S(2) | 175.86(9) | S(1) | Ti(2) | C(5) | 113.7(6) |
| Cl(1) | Ti(1) | S(3) | 89.41(8) | S(2) | Ti(2) | S(4) | 102.27(8) |
| Cl(2) | Ti(1) | Cl(3) | 96.12(9) | S(2) | Ti(2) | C(1) | 112.7(7) |
| Cl(2) | Ti(1) | S(1) | 172.56(9) | S(2) | Ti(2) | C(2) | 89.6(4) |
| Cl(2) | Ti(1) | S(2) | 89.06(8) | S(2) | Ti(2) | C(3) | 97.8(7) |
| Cl(2) | Ti(1) | S(3) | 89.92(8) | S(2) | Ti(2) | C(4) | 131.3(7) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| S(2) | Ti(2) | C(5) | 142.8(4) | Ti(2) | C(3) | C(4) | 74.3(8) |
| S(4) | Ti(2) | C(1) | 92.4(5) | C(2) | C(3) | C(4) | 106(2) |
| S(4) | Ti(2) | C(2) | 120.9(8) | Ti(2) | C(4) | C(3) | 71.6(8) |
| S(4) | Ti(2) | C(3) | 147.2(4) | Ti(2) | C(4) | C(5) | 74.1(7) |
| S(4) | Ti(2) | C(4) | 123.6(7) | C(3) | C(4) | C(5) | 107(1) |
| S(4) | Ti(2) | C(5) | 94.2(4) | Ti(2) | C(5) | C(1) | 72.8(7) |
| C(1) | Ti(2) | C(2) | 32.7(5) | Ti(2) | C(5) | C(4) | 72.8(7) |
| C(1) | Ti(2) | C(3) | 55.7(5) | C(1) | C(5) | C(4) | 110(1) |
| C(1) | Ti(2) | C(4) | 55.3(4) | Ru(1) | C(6) | C(7) | 73.2(4) |
| C(1) | Ti(2) | C(5) | 32.6(4) | Ru(1) | C(6) | C(10) | 70.4(4) |
| C(2) | Ti(2) | C(3) | 33.2(5) | Ru(1) | C(6) | C(11) | 127.4(5) |
| C(2) | Ti(2) | C(4) | 54.7(6) | C(7) | C(6) | C(10) | 108.3(7) |
| C(2) | Ti(2) | C(5) | 53.5(5) | C(7) | C(6) | C(11) | 126.0(9) |
| C(3) | Ti(2) | C(4) | 34.1(5) | C(10) | C(6) | C(11) | 125.4(9) |
| C(3) | Ti(2) | C(5) | 55.3(5) | Ru(1) | C(7) | C(6) | 70.8(4) |
| C(4) | Ti(2) | C(5) | 33.1(4) | Ru(1) | C(7) | C(8) | 71.9(4) |
| Ru(1) | S(1) | Ti(1) | 92.66(7) | Ru(1) | C(7) | C(12) | 127.4(5) |
| Ru(1) | S(1) | Ti(2) | 79.47(6) | C(6) | C(7) | C(8) | 110.0(8) |
| Ti(1) | S(1) | Ti(2) | 87.74(7) | C(6) | C(7) | C(12) | 125.6(9) |
| Ru(2) | S(2) | Ti(1) | 87.99(7) | C(8) | C(7) | C(12) | 124.2(9) |
| Ru(2) | S(2) | Ti(2) | 78.06(6) | Ru(1) | C(8) | C(7) | 72.3(5) |
| Ti(1) | S(2) | Ti(2) | 88.76(7) | Ru(1) | C(8) | C(9) | 71.2(5) |
| Ru(1) | S(3) | Ru(2) | 74.46(5) | Ru(1) | C(8) | C(13) | 130.9(6) |
| Ru(1) | S(3) | Ti(1) | 96.51(7) | C(7) | C(8) | C(9) | 108.3(8) |
| Ru(2) | S(3) | Ti(1) | 90.23(7) | C(7) | C(8) | C(13) | 125(1) |
| Ru(1) | S(4) | Ru(2) | 74.55(5) | C(9) | C(8) | C(13) | 126(1) |
| Ru(1) | S(4) | Ti(2) | 81.42(7) | Ru(1) | C(9) | C(8) | 72.4(5) |
| Ru(2) | S(4) | Ti(2) | 79.89(6) | Ru(1) | C(9) | C(10) | 69.8(4) |
| Ti(2) | C(1) | C(2) | 72.9(8) | Ru(1) | C(9) | C(14) | 128.8(6) |
| Ti(2) | C(1) | C(5) | 74.6(7) | C(8) | C(9) | C(10) | 108.0(7) |
| C(2) | C(1) | C(5) | 107(2) | C(8) | C(9) | C(14) | 126(1) |
| Ti(2) | C(2) | C(1) | 74.5(8) | C(10) | C(9) | C(14) | 125(1) |
| Ti(2) | C(2) | C(3) | 73.1(9) | Ru(1) | C(10) | C(6) | 71.8(4) |
| C(1) | C(2) | C(3) | 111(2) | Ru(1) | C(10) | C(9) | 71.9(4) |
| Ti(2) | C(3) | C(2) | 73.8(9) | Ru(1) | C(10) | C(15) | 126.1(5) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C(6) | C(10) | C(9) | 105.4(7) | Ru(2) | C(18) | C(23) | 129.9(5) |
| C(6) | C(10) | C(15) | 126(1) | C(17) | C(18) | C(19) | 107.5(7) |
| C(9) | C(10) | C(15) | 129(1) | C(17) | C(18) | C(23) | 127.6(8) |
| Ru(2) | C(16) | C(17) | 72.2(4) | C(19) | C(18) | C(23) | 124.3(8) |
| Ru(2) | C(16) | C(20) | 73.7(4) | Ru(2) | C(19) | C(18) | 71.3(4) |
| Ru(2) | C(16) | C(21) | 125.6(6) | Ru(2) | C(19) | C(20) | 70.8(4) |
| C(17) | C(16) | C(20) | 107.6(7) | Ru(2) | C(19) | C(24) | 128.5(5) |
| C(17) | C(16) | C(21) | 127.1(8) | C(18) | C(19) | C(20) | 107.9(7) |
| C(20) | C(16) | C(21) | 124.9(8) | C(18) | C(19) | C(24) | 125.7(8) |
| Ru(2) | C(17) | C(16) | 70.6(4) | C(20) | C(19) | C(24) | 126.1(8) |
| Ru(2) | C(17) | C(18) | 73.9(4) | Ru(2) | C(20) | C(16) | 69.2(4) |
| Ru(2) | C(17) | C(22) | 128.1(5) | Ru(2) | C(20) | C(19) | 72.6(4) |
| C(16) | C(17) | C(18) | 109.6(7) | Ru(2) | C(20) | C(25) | 127.2(5) |
| C(16) | C(17) | C(22) | 122.9(7) | C(16) | C(20) | C(19) | 107.4(7) |
| C(18) | C(17) | C(22) | 127.0(7) | C(16) | C(20) | C(25) | 126.8(9) |
| Ru(2) | C(18) | C(17) | 70.0(4) | C(19) | C(20) | C(25) | 125.7(9) |
| Ru(2) | C(18) | C(19) | 72.3(4) | Cl(4) | C(26) | Cl(5) | 116.9(6) |

Estimated standard deviations in the least significant figure are given in parentheses.

**Table S31. Bond Angles (deg) Involving the Hydrogen Atoms in $[(TiCl_3)(CpTi)(Cp^*Ru)_2(\mu_3\text{-}S)_4]\cdot CH_2Cl_2$ ($7\cdot CH_2Cl_2$)**

| atom | atom | atom | angle | atom | atom | atom | angle |
|---|---|---|---|---|---|---|---|
| Ti(2) | C(1) | H(1) | 117.96 | H(13) | C(13) | H(14) | 109.47 |
| C(2) | C(1) | H(1) | 126.68 | C(9) | C(14) | H(15) | 109.48 |
| C(5) | C(1) | H(1) | 126.63 | C(9) | C(14) | H(16) | 109.47 |
| Ti(2) | C(2) | H(2) | 119.66 | C(9) | C(14) | H(17) | 109.47 |
| C(1) | C(2) | H(2) | 124.37 | H(15) | C(14) | H(16) | 109.48 |
| C(3) | C(2) | H(2) | 124.43 | H(15) | C(14) | H(17) | 109.47 |
| Ti(2) | C(3) | H(3) | 117.16 | H(16) | C(14) | H(17) | 109.47 |
| C(2) | C(3) | H(3) | 127.05 | C(10) | C(15) | H(18) | 109.47 |
| C(4) | C(3) | H(3) | 127.09 | C(10) | C(15) | H(19) | 109.47 |
| Ti(2) | C(4) | H(4) | 119.50 | C(10) | C(15) | H(20) | 109.47 |
| C(3) | C(4) | H(4) | 126.69 | H(18) | C(15) | H(19) | 109.47 |
| C(5) | C(4) | H(4) | 126.75 | H(18) | C(15) | H(20) | 109.47 |
| Ti(2) | C(5) | H(5) | 120.89 | H(19) | C(15) | H(20) | 109.47 |
| C(1) | C(5) | H(5) | 125.22 | C(16) | C(21) | H(21) | 109.48 |
| C(4) | C(5) | H(5) | 125.17 | C(16) | C(21) | H(22) | 109.47 |
| C(6) | C(11) | H(6) | 109.47 | C(16) | C(21) | H(23) | 109.48 |
| C(6) | C(11) | H(7) | 109.48 | H(21) | C(21) | H(22) | 109.47 |
| C(6) | C(11) | H(8) | 109.47 | H(21) | C(21) | H(23) | 109.47 |
| H(6) | C(11) | H(7) | 109.47 | H(22) | C(21) | H(23) | 109.47 |
| H(6) | C(11) | H(8) | 109.47 | C(17) | C(22) | H(24) | 109.47 |
| H(7) | C(11) | H(8) | 109.47 | C(17) | C(22) | H(25) | 109.47 |
| C(7) | C(12) | H(9) | 109.47 | C(17) | C(22) | H(26) | 109.47 |
| C(7) | C(12) | H(10) | 109.48 | H(24) | C(22) | H(25) | 109.47 |
| C(7) | C(12) | H(11) | 109.47 | H(24) | C(22) | H(26) | 109.47 |
| H(9) | C(12) | H(10) | 109.47 | H(25) | C(22) | H(26) | 109.47 |
| H(9) | C(12) | H(11) | 109.46 | C(18) | C(23) | H(27) | 109.47 |
| H(10) | C(12) | H(11) | 109.47 | C(18) | C(23) | H(28) | 109.47 |
| C(8) | C(13) | H(12) | 109.48 | C(18) | C(23) | H(29) | 109.48 |
| C(8) | C(13) | H(13) | 109.47 | H(27) | C(23) | H(28) | 109.46 |
| C(8) | C(13) | H(14) | 109.47 | H(27) | C(23) | H(29) | 109.47 |
| H(12) | C(13) | H(13) | 109.47 | H(28) | C(23) | H(29) | 109.47 |
| H(12) | C(13) | H(14) | 109.47 | C(19) | C(24) | H(30) | 109.47 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| C(19) | C(24) | H(31) | 109.47 | H(33) | C(25) | H(34) | 109.47 |
| C(19) | C(24) | H(32) | 109.47 | H(33) | C(25) | H(35) | 109.47 |
| H(30) | C(24) | H(31) | 109.47 | H(34) | C(25) | H(35) | 109.47 |
| H(30) | C(24) | H(32) | 109.47 | Cl(4) | C(26) | H(36) | 107.58 |
| H(31) | C(24) | H(32) | 109.47 | Cl(4) | C(26) | H(37) | 107.58 |
| C(20) | C(25) | H(33) | 109.47 | Cl(5) | C(26) | H(36) | 107.58 |
| C(20) | C(25) | H(34) | 109.47 | Cl(5) | C(26) | H(37) | 107.57 |
| C(20) | C(25) | H(35) | 109.47 | H(36) | C(26) | H(37) | 109.46 |

Estimated standard deviations in the least significant figure are given in parentheses.