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Table 1 ^{1}H NMR spectral data for **3a**, **3b**, **3c**, **4b**, **4c**, **5**, **6**, **7**, **8** and **9** (300 MHz, rt)

Compond	η^5-$C_5(CH_3)_5$	μ-H	μ-N=CHR	N≡CCH_3, μ-η^2:η^2-arene
3a[*1]	1.65 (s, 15H) 1.71 (s, 15H)	−13.82 (s, 1H)	2.03 (d, J_{HH} = 5.0 Hz, 3H, N=CHCH_3) 7.46 (q, J_{HH} = 5.0 Hz, 1H, N=CHCH$_3$)	0.71 (s, 6H, N≡CCH_3)
3b[*2]	1.66 (s, 15H) 1.70 (s, 15H)	−13.81 (s, 1H)	2.04 (d, J_{HH} = 5.1 Hz, 3H, N=CHCH_3) 7.48 (q, J_{HH} = 5.1 Hz, 1H, N=CHCH$_3$)	1.59 (s, 3H, μ-η^2:η^2-$C_6H_5CH_3$) 2.52 (d, J_{HH} = 7.0 Hz, 1H, μ-η^2:η^2-$C_6H_5CH_3$) 2.75–2.83 (m, 2H, μ-η^2:η^2-$C_6H_5CH_3$) 2.98 (dd, J_{HH} = 5.7 and 7.0 Hz, 1H, μ-η^2:η^2-$C_6H_5CH_3$) 5.19 (d, J_{HH} = 5.7 Hz, 1H, μ-η^2:η^2-$C_6H_5CH_3$)
3c[*1]	1.60 (s, 15H) 1.68 (s, 15H)	−13.94 (s, 1H)	1.35 (d, J_{HH} = 5.1 Hz, 3H, N=CHCH_3) 6.53 (q, J_{HH} = 5.1 Hz, 1H, N=CHCH$_3$)	3.05 (ddd, J_{HH} = 1.4, 5.7 and 6.9 Hz, 1H, μ-η^2:η^2-$C_{10}H_8$) 3.16 (ddd, J_{HH} = 1.3, 5.7 and 7.1 Hz, 1H, μ-η^2:η^2-$C_{10}H_8$) 3.32 (dd, J_{HH} = 1.4 and 7.1 Hz, 1H, μ-η^2:η^2-$C_{10}H_8$) 3.46 (dd, J_{HH} = 1.3 and 6.9 Hz, 1H, μ-η^2:η^2-$C_{10}H_8$) 7.08 (td, J_{HH} = 1.5 and 7.3 Hz, 1H, μ-η^2:η^2-$C_{10}H_8$) 7.16 (td, J_{HH} = 1.3 and 7.3 Hz, 1H, μ-η^2:η^2-$C_{10}H_8$) 7.23 (dd, J_{HH} = 1.5 and 7.3 Hz, 1H, μ-η^2:η^2-$C_{10}H_8$) 7.29 (dd, J_{HH} = 1.3 and 7.3 Hz, 1H, μ-η^2:η^2-$C_{10}H_8$)
4b[*2]	1.69 (s, 15H) 1.74 (s, 15H)	−14.14 (s, 1H)	0.92 (t, J_{HH} = 7.6 Hz, 3H, N=CHCHH'CH_3) 2.03–2.15 (m, 1H, N=CHCHH'CH$_3$) 2.18–2.29 (m, 1H, N=CHCHH'CH$_3$) 6.72 (dd, J_{HH} = 4.4 and 5.4 Hz, 1H, N=CHCHH'CH$_3$)	1.61 (s, 3H, μ-η^2:η^2-$C_6H_5CH_3$) 2.55 (d, J_{HH} = 7.2 Hz, 1H, μ-η^2:η^2-$C_6H_5CH_3$) 2.79 (dd, J_{HH} = 5.5 and 7.2 Hz, 1H, μ-η^2:η^2-$C_6H_5CH_3$) 2.84 (dd, J_{HH} = 5.5 and 7.1 Hz, 1H, μ-η^2:η^2-$C_6H_5CH_3$) 2.95 (dd, J_{HH} = 5.7 and 7.1 Hz, 1H, μ-η^2:η^2-$C_6H_5CH_3$) 5.23 (d, J_{HH} = 5.7 Hz, 1H, μ-η^2:η^2-$C_6H_5CH_3$)
4c[*1]	1.64 (s, 15H) 1.71 (s, 15H)	−13.96 (s, 1H)	0.62 (t, J_{HH} = 7.6 Hz, 3H, N=CHCHH'CH_3) 1.54 (dqd, J_{HH} = 4.4, 7.6 and 15.1 Hz, 1H, N=CHCHH'CH$_3$) 1.81 (dqd, J_{HH} = 5.7, 7.6 and 15.1 Hz, 1H, N=CHCHH'CH$_3$) 6.46 (dd, J_{HH} = 4.4 and 5.7 Hz, 1H, N=CHCHH'CH$_3$)	3.02 (ddd, J_{HH} = 1.3, 5.7 and 6.9 Hz, 1H, μ-η^2:η^2-$C_{10}H_8$) 3.14 (ddd, J_{HH} = 1.2, 5.7 and 6.9 Hz, 1H, μ-η^2:η^2-$C_{10}H_8$) 3.33 (dd, J_{HH} = 1.3 and 6.9 Hz, 1H, μ-η^2:η^2-$C_{10}H_8$) 3.46 (dd, J_{HH} = 1.2 and 6.9 Hz, 1H, μ-η^2:η^2-$C_{10}H_8$) 7.03 (td, J_{HH} = 1.5 and 7.4 Hz, 1H, μ-η^2:η^2-$C_{10}H_8$) 7.12 (td, J_{HH} = 1.4 and 7.4 Hz, 1H, μ-η^2:η^2-$C_{10}H_8$) 7.24 (dd, J_{HH} = 1.5 and 7.4 Hz, 1H, μ-η^2:η^2-$C_{10}H_8$) 7.27 (dd, J_{HH} = 1.4 and 7.4 Hz, 1H, μ-η^2:η^2-$C_{10}H_8$)

[*1] All spectra were recorded in C_6D_6. Chemical shifts are in ppm relative to $Si(CH_3)_4$ taken as 0 ppm. [*2] Recorded in THF-d_8.
[*3] Determined on the basis of ^{1}H-^{1}H COSY and ^{13}C-^{1}H HSC spectra.

Table 1 ^{1}H NMR spectral data for **3a**, **3b**, **3c**, **4b**, **4c**, **5**, **6**, **7**, **8** and **9** (300 MHz, rt) (continued)

compond	η^5-$C_5(CH_3)_5$	μ-H	μ-N=CHR	η^2-CH_2CH_2, μ-η^2:η^2-$CH_2CHCHCH_2$, μ-$CH=CH_2$
5[*1]	1.48 (s, 15H) 1.53 (s, 15H)	−16.18 (s, 1H)	2.44 (d, J_{HH} = 5.0 Hz, 3H, N=CHCH_3) 8.02 (q, J_{HH} = 5.0 Hz, 1H, N=CHCH$_3$)	0.19 (dd, J_{HH} = 8.0 and 10.6 Hz, η^2-CH_2CH_2) 0.45 (dd, J_{HH} = 8.5 and 11.5 Hz, η^2-CH_2CH_2) 1.5 (obscured by $C_5(CH_3)_5$ signal, η^2-CH_2CH_2)[*3] 1.64 (dd, J_{HH} = 8.0 and 11.5 Hz, η^2-CH_2CH_2) 1.91 (dd, J_{HH} = 7.0 and 11.0 Hz, η^2-CH_2CH_2) 1.93 (dd, J_{HH} = 8.9 and 11.5 Hz, η^2-CH_2CH_2) 2.05 (dd, J_{HH} = 8.5 and 11.0 Hz, η^2-CH_2CH_2) 2.71 (dd, J_{HH} = 8.9 and 10.6 Hz, η^2-CH_2CH_2)
6[*1]	1.48 (s, 15H) 1.53 (s, 15H)	−16.24 (s, 1H)	1.16 (t, J_{HH} = 7.6 Hz, 3H, N=CHCHH'CH_3) 2.76 (dqd, J_{HH} = 6.4, 7.6 and 14.2 Hz, 1H, N=CHCHH'CH$_3$) 2.86 (dqd, J_{HH} = 4.2, 7.6 and 14.2 Hz, 1H, N=CH)CHH'CH$_3$) 7.88 (dd, J_{HH} = 4.2 and 6.4 Hz, 1H, N=CHCHH'CH$_3$)	0.18 (dd, J_{HH} = 8.3 and 11.7 Hz, η^2-CH_2CH_2) 0.43 (dd, J_{HH} = 8.4 and 11.0 Hz, η^2-CH_2CH_2) 1.5 (obscured by $C_5(CH_3)_5$ signal, η^2-CH_2CH_2)[*3] 1.61 (dd, J_{HH} = 8.7 and 11.7 Hz, η^2-CH_2CH_2) 1.86 (dd, J_{HH} = 8.8 and 11.2 Hz, η^2-CH_2CH_2) 1.91 (dd, J_{HH} = 8.7 and 10.7 Hz, η^2-CH_2CH_2) 2.02 (dd, J_{HH} = 8.8 and 11.0 Hz, η^2-CH_2CH_2) 2.66 (dd, J_{HH} = 8.3 and 10.7 Hz, η^2-CH_2CH_2)
7[*1]	1.72 (s, 15H) 1.75 (s, 15H)	−13.12 (s, 1H)	1.99 (d, J_{HH} = 5.0 Hz, 3H, N=CHCH_3) 7.61 (q, J_{HH} = 5.0 Hz, 1H, N=CHCH$_3$)	0.40 (d, J_{HH} = 11.0 Hz, 1H, CHH'=CHCH=CH$_2$) 0.57 (d, J_{HH} = 11.4 Hz, 1H, CH$_2$=CHCH=CHH') 1.65 (d, J_{HH} = 7.8 Hz, 1H, CH$_2$=CHCH=CHH') 1.66 (d, J_{HH} = 7.5 Hz, 1H, CHH'=CHCH=CH$_2$) 2.78 (ddd, J_{HH} = 6.5, 7.5 and 11.0 Hz, 1H, CH$_2$=CHCH=CH$_2$) 2.93 (ddd, J_{HH} = 6.5, 7.8 and 11.4 Hz, 1H, CH$_2$=CHCH=CH$_2$)
8[*1]	1.72 (s, 15H) 1.75 (s, 15H)	−13.18 (s, 1H)	0.99 (t, J_{HH} = 7.7 Hz, 3H, N=CHCHH'CH_3) 2.29 (dqd, J_{HH} = 5.9, 7.7 and 14.3 Hz, 1H, N=CHCHH'CH$_3$) 2.38 (dqd, J_{HH} = 4.3, 7.7 and 14.3 Hz, 1H, N=CH)CHH'CH$_3$) 7.50 (dd, J_{HH} = 4.3 and 5.9 Hz, 1H, N=CHCHH'CH$_3$)	0.46 (d, J_{HH} = 11.0 Hz, 1H, CHH'=CHCH=CH$_2$) 0.57 (d, J_{HH} = 11.3 Hz, 1H, CH$_2$=CHCH=CHH') 1.65 (d, J_{HH} = 8.1 Hz, 1H, CH$_2$=CHCH=CHH') 1.71 (d, J_{HH} = 8.1 Hz, 1H, CHH'=CHCH=CH$_2$) 2.76 (ddd, J_{HH} = 6.3, 8.1 and 11.0 Hz, 1H, CH$_2$=CHCH=CH$_2$) 2.92 (ddd, J_{HH} = 6.3, 8.1 and 11.3 Hz, 1H, CH$_2$=CHCH=CH$_2$)

[*1] All spectra were recorded in C_6D_6. Chemical shifts are in ppm relative to $Si(CH_3)_4$ taken as 0 ppm. [*2] Recorded in THF-d_8.
[*3] Determined on the basis of ^{1}H-^{1}H COSY and ^{13}C-^{1}H HSC spectra.

Table 1 ^{1}H NMR spectral data for **3a**, **3b**, **3c**, **4b**, **4c**, **5**, **6**, **7**, **8** and **9** (300 MHz, rt) (continued)

compond	η^5-$C_5(CH_3)_5$	μ-N=CHR	η^2-CH_2CH_2, μ-η^2:η^2-$CH_2CHCHCH_2$, μ-CH=CH_2
9[*1]	1.33 (s, 15H)	2.59 (d, J_{HH} = 5.0 Hz, 3H, N=CHC*H*$_3$)	1.16 (dd, J_{HH} = 7.6 and 11.0 Hz, 1H, η^2-CH_2CH_2)
	1.68 (s, 15H)	7.30 (q, J_{HH} = 5.0 Hz, 1H, N=C*H*CH$_3$)	1.28 (dd, J_{HH} = 8.3 and 11.0 Hz, 1H, η^2-CH_2CH_2)
			1.45 (dd, J_{HH} = 1.5 and 8.9 Hz, 1H, μ-CH=C*H*H')
			1.73 (dd, J_{HH} = 8.3 and 10.4 Hz, 1H, η^2-CH_2CH_2)
			2.79 (dd, J_{HH} = 7.6 and 10.4 Hz, 1H, η^2-CH_2CH_2)
			3.36 (dd, J_{HH} = 1.5 and 5.8 Hz, 1H, μ-CH=CH*H'*)
			10.58 (dd, J_{HH} = 5.8 and 8.9 Hz, 1H, μ-C*H*=CHH')

[*1] All spectra were recorded in C_6D_6. Chemical shifts are in ppm relative to $Si(CH_3)_4$ taken as 0 ppm. [*2] Recorded in THF-d_8.
[*3] Determined on the basis of ^{1}H-^{1}H COSY and ^{13}C-^{1}H HSC spectra.

Table 2 ^{13}C NMR spectroscopic data for **3a**, **3b**, **3c**, **4b**, **4c**, **5**, **6**, **7**, **8** and **9** (75 MHz, rt)

Compond	η^5-$C_5(CH_3)_5$	μ-N=CHR	N≡CCH_3, μ-η^2:η^2-arene
3a[*1]	10.4 (q, J_{CH} = 126 Hz, $C_5(CH_3)_5$) 11.2 (q, J_{CH} = 126 Hz, $C_5(CH_3)_5$) 90.2 (s, $C_5(CH_3)_5$) 90.6 (s, $C_5(CH_3)_5$)	31.3 (dq, $^2J_{CH}$ = 14 Hz, $^1J_{CH}$ = 126 Hz, N=CHCH_3) 155.2 (qd, $^2J_{CH}$ = 7 Hz, $^1J_{CH}$ = 167 Hz, N=$CHCH_3$)	0.17 (q, J_{CH} = 136 Hz, N≡CCH_3) 116.2 (s, N≡CCH_3)
3b[*2]	10.7 (q, J_{CH} = 126 Hz, $C_5(CH_3)_5$) 11.3 (q, J_{CH} = 126 Hz, $C_5(CH_3)_5$) 90.5 (s, $C_5(CH_3)_5$) 90.6 (s, $C_5(CH_3)_5$)	32.1 (dq, $^2J_{CH}$ = 14 Hz, $^1J_{CH}$ = 126 Hz, N=CHCH_3) 157.0 (qd, $^2J_{CH}$ = 7 Hz, $^1J_{CH}$ = 167 Hz, N=$CHCH_3$)	22.4 (q, J_{CH} = 126 Hz, μ-η^2:η^2-$C_6H_5CH_3$) 51.8 (d, J_{CH} = 161 Hz, μ-η^2:η^2-$C_6H_5CH_3$) 53.7 (d, J_{CH} = 159 Hz, μ-η^2:η^2-$C_6H_5CH_3$) 55.2 (d, J_{CH} = 155 Hz, μ-η^2:η^2-$C_6H_5CH_3$) 58.9 (d, J_{CH} = 153 Hz, μ-η^2:η^2-$C_6H_5CH_3$) 118.7 (d, J_{CH} = 159 Hz, μ-η^2:η^2-$C_6H_5CH_3$) 131.1 (s, μ-η^2:η^2-$C_6H_5CH_3$)
3c[*1]	10.3 (q, J_{CH} = 126 Hz, $C_5(CH_3)_5$) 11.0 (q, J_{CH} = 126 Hz, $C_5(CH_3)_5$) 90.9 (s, $C_5(CH_3)_5$) 91.1 (s, $C_5(CH_3)_5$)	26.6 (dq, $^2J_{CH}$ = 13 Hz, $^1J_{CH}$ = 126 Hz, N=CHCH_3) 158.4 (qd, $^2J_{CH}$ = 7 Hz, $^1J_{CH}$ = 166 Hz, N=$CHCH_3$)	49.3 (d, J_{CH} = 161 Hz, μ-η^2:η^2-$C_{10}H_8$) 49.5 (d, J_{CH} = 159 Hz, μ-η^2:η^2-$C_{10}H_8$) 51.6 (d, J_{CH} = 153 Hz, μ-η^2:η^2-$C_{10}H_8$) 53.4 (d, J_{CH} = 155 Hz, μ-η^2:η^2-$C_{10}H_8$) 123.3 (d, J_{CH} = 157 Hz, μ-η^2:η^2-$C_{10}H_8$) 123.4 (d, J_{CH} = 157 Hz, μ-η^2:η^2-$C_{10}H_8$) 124.5 (d, J_{CH} = 153 Hz, μ-η^2:η^2-$C_{10}H_8$) 125.7 (d, J_{CH} = 154 Hz, μ-η^2:η^2-$C_{10}H_8$) 138.2 (s, μ-η^2:η^2-$C_{10}H_8$) 139.3 (s, μ-η^2:η^2-$C_{10}H_8$)
4b[*2]	10.6 (q, J_{CH} = 125 Hz, $C_5(CH_3)_5$) 11.3 (q, J_{CH} = 125 Hz, $C_5(CH_3)_5$) 90.6 (s, $C_5(CH_3)_5$) 90.7 (s, $C_5(CH_3)_5$)	11.5 (q, J_{CH} = 126 Hz, N=CHCH$_2CH_3$) 37.9 (t, J_{CH} = 126 Hz, N=CHCH_2CH_3) 164.6 (d, J_{CH} = 163 Hz, N=$CHCH_2CH_3$)	22.8 (q, J_{CH} = 126 Hz, μ-η^2:η^2-$C_6H_5CH_3$) 51.7 (d, J_{CH} = 160 Hz, μ-η^2:η^2-$C_6H_5CH_3$) 53.4 (d, J_{CH} = 158 Hz, μ-η^2:η^2-$C_6H_5CH_3$) 55.0 (d, J_{CH} = 154 Hz, μ-η^2:η^2-$C_6H_5CH_3$) 59.0 (d, J_{CH} = 152 Hz, μ-η^2:η^2-$C_6H_5CH_3$) 118.3 (d, J_{CH} = 154 Hz, μ-η^2:η^2-$C_6H_5CH_3$) 130.8 (s, μ-η^2:η^2-$C_6H_5CH_3$)

[*1] All spectra were recorded in C_6D_6. Chemical shifts are in ppm relative to $Si(CH_3)_4$ taken as 0 ppm.
[*2] Recorded in THF-d_8.

Table 2 ^{13}C NMR spectroscopic data for **3a**, **3b**, **3c**, **4b**, **4c**, **5**, **6**, **7**, **8** and **9** (75 MHz, rt) (continued)

Compond	η^5-$C_5(CH_3)_5$	μ-N=CHR	μ-η^2:η^2-$C_{10}H_8$, η^2-CH_2CH_2
4c[*1]	10.3 (q, J_{CH} = 126 Hz, $C_5(CH_3)_5$) 11.1 (q, J_{CH} = 126 Hz, $C_5(CH_3)_5$) 91.0 (s, $C_5(CH_3)_5$) 91.3 (s, $C_5(CH_3)_5$)	12.0 (q, J_{CH} = 126 Hz, N=CHCH$_2$CH$_3$) 33.1 (t, J_{CH} = 126 Hz, N=CHCH$_2$CH$_3$) 166.1 (d, J_{CH} = 164 Hz, N=CHCH$_2$CH$_3$)	49.1 (d, J_{CH} = 162 Hz, μ-η^2:η^2-$C_{10}H_8$) 49.9 (d, J_{CH} = 159 Hz, μ-η^2:η^2-$C_{10}H_8$) 51.9 (d, J_{CH} = 153 Hz, μ-η^2:η^2-$C_{10}H_8$) 53.2 (d, J_{CH} = 154 Hz, μ-η^2:η^2-$C_{10}H_8$) 123.5 (d, J_{CH} = 156 Hz, μ-η^2:η^2-$C_{10}H_8$) 124.8 (d, J_{CH} = 154 Hz, μ-η^2:η^2-$C_{10}H_8$) 125.7 (d, J_{CH} = 154 Hz, μ-η^2:η^2-$C_{10}H_8$) 125.7 (d, J_{CH} = 154 Hz, μ-η^2:η^2-$C_{10}H_8$) 138.5 (s, μ-η^2:η^2-$C_{10}H_8$) 139.5 (s, μ-η^2:η^2-$C_{10}H_8$)
5[*1]	9.5 (q, J_{CH} = 127 Hz, $C_5(CH_3)_5$) 10.5 (q, J_{CH} = 127 Hz, $C_5(CH_3)_5$) 91.5 (s, $C_5(CH_3)_5$) 91.3 (s, $C_5(CH_3)_5$)	27.7 (dq, $^2J_{CH}$ = 13 Hz, $^1J_{CH}$ = 126 Hz, N=CHCH$_3$) 161.6 (qd, $^2J_{CH}$ = 7 Hz, $^1J_{CH}$ = 167 Hz, N=CHCH$_3$)	32.2 (dd, J_{CH} = 152 and 159 Hz, η^2-CH_2CH_2) 32.6 (dd, J_{CH} = 150 and 158 Hz, η^2-CH_2CH_2) 40.2 (t, J_{CH} = 155 Hz, η^2-CH_2CH_2) 44.2 (t, J_{CH} = 150 Hz, η^2-CH_2CH_2)
6[*1]	9.4 (q, J_{CH} = 126 Hz, $C_5(CH_3)_5$) 10.4 (q, J_{CH} = 126 Hz, $C_5(CH_3)_5$) 91.1 (s, $C_5(CH_3)_5$)	12.8 (q, J_{CH} = 126 Hz, N=CHCH$_2$CH$_3$) 34.4 (t, J_{CH} = 127 Hz, N=CHCH$_2$CH$_3$) 168.5 (d, J_{CH} = 164 Hz, N=CHCH$_2$CH$_3$)	31.9 (dd, J_{CH} = 152 and 158 Hz, η^2-CH_2CH_2) 32.5 (dd, J_{CH} = 149 and 157 Hz, η^2-CH_2CH_2) 39.7 (t, J_{CH} = 154 Hz, η^2-CH_2CH_2) 44.2 (t, J_{CH} = 153 Hz, η^2-CH_2CH_2)
7[*1]	10.7 (q, J_{CH} = 126 Hz, $C_5(CH_3)_5$) 11.2 (q, J_{CH} = 126 Hz, $C_5(CH_3)_5$) 90.1 (s, $C_5(CH_3)_5$) 90.4 (s, $C_5(CH_3)_5$)	27.5 (dq, $^2J_{CH}$ = 15 Hz, $^1J_{CH}$ = 126 Hz, N=CHCH$_3$) 159.5 (qd, $^2J_{CH}$ = 7 Hz, $^1J_{CH}$ = 166 Hz, N=CHCH$_3$)	37.4 (dd, J_{CH} = 155 and 162 Hz, μ-η^2:η^2-CH$_2$=CHCH=CH$_2$) 42.6 (dd, J_{CH} = 153 and 159 Hz, μ-η^2:η^2-CH$_2$=CHCH=CH$_2$) 51.5 (d, J_{CH} = 158 Hz, μ-η^2:η^2-CH$_2$=CHCH=CH$_2$) 52.2 (d, J_{CH} = 154 Hz, μ-η^2:η^2-CH$_2$=CHCH=CH$_2$)
8[*1]	10.7 (q, J_{CH} = 126 Hz, $C_5(CH_3)_5$) 11.2 (q, J_{CH} = 126 Hz, $C_5(CH_3)_5$) 89.9 (s, $C_5(CH_3)_5$) 90.2 (s, $C_5(CH_3)_5$)	12.0 (q, J_{CH} = 126 Hz, N=CHCH$_2$CH$_3$) 34.7 (t, J_{CH} = 127 Hz, N=CHCH$_2$CH$_3$) 166.4 (d, J_{CH} = 164 Hz, N=CHCH$_2$CH$_3$)	37.3 (t, J_{CH} = 154 Hz, μ-η^2:η^2-CH$_2$=CHCH=CH$_2$) 43.1 (t, J_{CH} = 153 Hz, μ-η^2:η^2-CH$_2$=CHCH=CH$_2$) 51.4 (d, J_{CH} = 156 Hz, μ-η^2:η^2-CH$_2$=CHCH=CH$_2$) 52.0 (d, J_{CH} = 157 Hz, μ-η^2:η^2-CH$_2$=CHCH=CH$_2$)
9[*1]	8.6 (q, J_{CH} = 127 Hz, $C_5(CH_3)_5$) 10.9 (q, J_{CH} = 126 Hz, $C_5(CH_3)_5$) 87.8 (s, $C_5(CH_3)_5$) 94.8 (s, $C_5(CH_3)_5$)	28.4 (dq, $^2J_{CH}$ = 14 Hz, $^1J_{CH}$ = 126 Hz, N=CHCH$_3$) 159.3 (qd, $^2J_{CH}$ = 7 Hz, $^1J_{CH}$ = 166 Hz, N=CHCH$_3$)	36.0 (dd, J_{CH} = 150 and 159 Hz, η^2-CH_2CH_2) 45.0 (dd, J_{CH} = 150 and 158 Hz, η^2-CH_2CH_2) 59.3 (dd, J_{CH} = 146 and 156 Hz, μ-CH=CH$_2$) 180.2 (d, J_{CH} = 156 Hz, μ-CH=CH$_2$)

[*1] All spectra were recorded in C_6D_6. Chemical shifts are in ppm relative to $Si(CH_3)_4$ taken as 0 ppm.
[*2] Recorded in THF-d_8.

L2424-5

Compound 4c

X-ray Structure Report

Data Collection

An orange prismatic crystal of $C_{33}H_{45}NRu_2$ having approximate dimensions of $0.30 \times 0.50 \times 1.00$ mm was mounted on glass fiber. All measurements were made on a Rigaku AFC5R diffractometer with graphite monochromated Mo-Kα radiation and a 12kW rotating anode generator.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 19 carefully centered reflections in the range $19.4 < 2\theta < 23.5°$ corresponded to a primitive triclinic cell with dimensions:

a = 11.144(2) Å	α = 96.17(2)°
b = 16.361(3) Å	β = 105.24(2)°
c = 8.644(2) Å	γ = 82.48(2)°
V = 1503.2(5) Å^3	

For Z = 2 and F.W.= 657.87, the calculated density is 1.45g/cm^3. Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

$P\bar{1}$ (#2)

The data were collected at a temperature of 23 ± 1°C using the ω scan technique to a maximum 2θ value of 50.0°. Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.40° with a take-off angle of 6.0°. Scans of (1.15 + 0.14 tan θ)° were made at a speed of 16.0° /min (in omega). The weak reflections ($I < 3.0\sigma(I)$) were rescanned (maximum of 3 scans) and the counts were accumulated to ensure good counting statistics. Stationary background counts were recorded on each side of the reflection. The ratio of peak counting time to background counting time was 2:1. The diameter of the incident beam collimator was 1.0 mm, the crystal to detector distance was 285 mm, and the detector aperture was 6.0×6.0 mm (horizontal × vertical).

Data Reduction

Of the 5584 reflections which were colected, 5288 were unique (R_{int} = 0.011). Overthe course of data collection, the standards decreased by -1.7 %. A linear correction factors was applied to the data to account for this phenomenon.

The linear absorption coefficient, μ, for Mo-Kα radiation is 10.3 cm^{-1}. An empirical absorption correction based on azimuthal scans of several reflections was applied which resulted in transmission factors ranging from 0.92 to 1.00. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Some hydrogen atoms were refined isotropically, the rest were included in fixed positions. The final cycle of full-matrix least-squares refinement[3] was based on 4136 observed reflections ($I > 3.0\sigma(I)$) and 329 variable parameters and converged (largest parameter was 0.32 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma\left||Fo| - |Fc|\right| / \Sigma|Fo| = 0.037$$

$$R\omega = \sqrt{(\Sigma\omega(|Fo| - |Fc|)^2 / \Sigma\omega Fo^2)} = 0.036$$

The standard deviation of an observation of unit weight[4] was 2.49. The weighting scheme was based on counting statistics and included a factor (p = 0.007) to downweight the intense reflections. Plots of $\Sigma\omega(|Fo| - |Fc|)^2$ versus $|Fo|$, reflection order in data collection, sin θ/λ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.90 and -0.72 e$^-$/Å^3, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in F_{calc}[6]; the values for Δf' and Δf" were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[8]. All calculations were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation.

References

(1) MITHRIL90: Gilmore, C. J.; MITHRIL - an integrated direct methods computer program. Univ. of Glasgow, Scotland (1990).

(2) DIRDIF92: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., Garcia-Granda, S., Gould, R.O., Smits, J.M.M. and Smykalla, C. (1992). The DIRDIF program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least-Squares:

Function minimized: $\Sigma\omega(|Fo|-|Fc|)^2$

where $w = \dfrac{1}{\sigma^2(Fo)} = \dfrac{4Fo^2}{\sigma^2(Fo^2)}$

$$\sigma^2(Fo^2) = \frac{S^2(C+R^2B)+(pFo^2)^2}{Lp^2}$$

S = Scan rate
C = Total Integrated Peak Count
R = Ratio of Scan Time to background counting time
B = Total Background Count
Lp = Lorentz-polarization factor
p = p-factor

(4) Standard deviation on an observation of unit weight:

$$\sqrt{\Sigma\omega(|Fo|-|Fc|)^2 / (No-Nv)}$$

where: No = number of observations
Nv = number of variables

(5) Cromer, D.T. & Waber, J.T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2A (1974).

(6) Ibers, J.A. & Hamilton, W.C.; Acta Crystallogr., 17, 781 (1964).

(7) Creaph, D.C. & McAuley, W.J.; "International Tables for X-ray Crystallography", Vol C.(A.J.C.Wilson,ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8)Creaph, D.C. & Hubbell, J.H.; "International Tables for X-ray Crystallography", Vol C.(A.J.C.Wilson,ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1992).

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EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{33}H_{45}NRu_2$
Formula Weight	657.87
Crystal Color, Habit	orange, prismatic
Crystal Dimensions	0.30 × 0.50 × 1.00 mm
Crystal System	triclinic
Lattice Type	Primitive
No. of reflections Used for Unit Cell Determination (2θ range)	19(19.4-23.5°)
Omega Scan Peak Width at Half-Height	0.40°
Lattice Parameters	a = 11.144(2) Å b = 16.361(3) Å c = 8.644(2) Å α = 96.17(2) β = 105.24(2) γ = 82.48(2) V = 1503.2(5) Å^3
Space Group	$P\bar{1}$ (#2)
Z value	2
D *calc*	1.453g/cm^3
F000	676.00
μ(MoKα)	10.26 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC5R
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Attenuator	Zr foil (factors = 1.00,3.60,11.82,43.09)
Take-off Angle	6.0°
Detector Aperture	6.0 mm horizontal 6.0 mm vertical
Crystal to Detector Distance	285 mm
Temperature	23.0°C
Scan Type	ω
Scan Rate	16.0°/min (in ω) - up to 3 scans
Scan Width	(1.15+0.14 tan θ)°
$2\theta_{max}$	50.0°
No. of Reflections Measured	Total: 5584 Unique: 5288 (R_{int} = 0.011)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.9201-0.9997)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (MITHRIL 90)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma\omega(\lvert Fo\rvert - \lvert Fc\rvert)^2$
Least Squares Weights	$\frac{1}{\sigma^2(Fo)} = \frac{4Fo^2}{\sigma^2(Fo^2)}$

p-factor	0.01
Anomalous Dispersion	All non-hydrogen atoms
No. Observations ($I > 3.00\sigma(I)$)	4136
No. Variables	329
Reflection/Parameter Ratio	12.57
Residuals: R; Rw	0.037; 0.036
Goodness of Fit Indicator	2.49
Max Shift/Error in Final Cycle	0.32
Maximum peak in Final Diff. Map	0.90 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.72 $e^-/Å^3$

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Compound 8

X-ray Structure Report

Data Collection

An yellow-orange prismatic crystal of $C_{27}H_{43}NRu_2$ having approximate dimensions of $0.20 \times 0.40 \times 0.20$ mm was mounted on glass fiber. All measurements were made on a Rigaku AFC5R diffractometer with graphite monochromated Mo-Kα radiation and a 12kW rotating anode generator.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 20 carefully centered reflections in the range $19.6 < 2\theta < 20.7°$ corresponded to a primitive orthorhombic cell with dimensions:

a = 15.166(7) Å
b = 25.605(5) Å
c = 13.590(6) Å
V = 5277(3) Å^3

For Z = 8 and F.W.= 583.78, the calculated density is 1.47g/cm^3. Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

P_{bca} (#61)

The data were collected at a temperature of 23 ± 1°C using the ω scan technique to a maximum 2θ value of 50.0°. Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.47° with a take-off angle of 6.0°. Scans of (0.97 + 0.14 tan θ)° were made at a speed of 16.0° /min (in omega). The weak reflections ($I < 3.0\sigma(I)$) were rescanned (maximum of 3 scans) and the counts were accumulated to ensure good counting statistics. Stationary background counts were recorded on each side of the reflection. The ratio of peak counting time to background counting time was 2:1. The diameter of the incident beam collimator was 1.0 mm, the crystal to detector distance was 285 mm, and the detector aperture was 6.0×6.0 mm (horizontal × vertical).

Data Reduction

A total of 5171 reflections which were collected. Overthe course of data collection, the standards decreased by -1.1 %. A linear correction factors was applied to the data to account for this phenomenon.

The linear absorption coefficient, μ, for Mo-Kα radiation is 11.6 cm^{-1}. An empirical absorption correction based on azimuthal scans of several reflections was applied which resulted in transmission factors ranging from 0.92 to 0.99. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Some hydrogen atoms were refined isotropically, the rest were included in fixed positions. The final cycle of full-matrix least-squares refinement[3] was based on 3415 observed reflections ($I > 3.0\sigma(I)$) and 275 variable parameters and converged (largest parameter was 0.08 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma \| Fo| - |Fc| \| / \Sigma |Fo| = 0.035$$

$$R\omega = \sqrt{(\Sigma \omega (|Fo| - |Fc|)^2 / \Sigma \omega Fo^2)} = 0.028$$

The standard deviation of an observation of unit weight[4] was 2.26. The weighting scheme was based on counting statistics and included a factor (p = 0.001) to downweight the intense reflections. Plots of $\Sigma\omega(|Fo| - |Fc|)^2$ versus $|Fo|$, reflection order in data collection, sin θ/λ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.47 and -0.38 e$^-$/Å^3, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in F_{calc}[6]; the values for Δf' and Δf" were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[8]. All calculations were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation.

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References

(1) MITHRIL90: Gilmore, C. J.; MITHRIL - an integrated direct methods computer program. Univ. of Glasgow, Scotland (1990).

(2) DIRDIF92: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., Garcia-Granda, S., Gould, R.O., Smits, J.M.M. and Smykalla, C. (1992). The DIRDIF program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least-Squares:

Function minimized: $\Sigma\omega(|Fo|-|Fc|)^2$

where $w = \dfrac{1}{\sigma^2(Fo)} = \dfrac{4Fo^2}{\sigma^2(Fo^2)}$

$$\sigma^2(Fo^2) = \frac{S^2(C+R^2B)+(pFo^2)^2}{Lp^2}$$

S = Scan rate
C = Total Integrated Peak Count
R = Ratio of Scan Time to background counting time
B = Total Background Count
Lp = Lorentz-polarization factor
p = p-factor

(4) Standard deviation on an observation of unit weight:

$$\sqrt{\Sigma\omega(|Fo|-|Fc|)^2 / (No-Nv)}$$

where: No = number of observations
Nv = number of variables

(5) Cromer, D.T. & Waber, J.T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2A (1974).

(6) Ibers, J.A. & Hamilton, W.C.; Acta Crystallogr., 17, 781 (1964).

(7) Creaph, D.C. & McAuley, W.J.; "International Tables for X-ray Crystallography", Vol C,(A.J.C.Wilson,ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8)Creaph, D.C. & Hubbell, J.H.; "International Tables for X-ray Crystallography", Vol C,(A.J.C.Wilson,ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1992).

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EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{27}H_{43}NRu_2$
Formula Weight	583.78
Crystal Color, Habit	yellow-orange, prismatic
Crystal Dimensions	0.20 × 0.40 × 0.20 mm
Crystal System	orthorhombic
Lattice Type	Primitive
No. of reflections Used for Unit Cell Determination (2θ range)	20(19.6-20.7°)
Omega Scan Peak Width at Half-Height	0.47°
Lattice Parameters	a = 15.166(7) Å b = 25.605(5) Å c = 13.590(6) Å V = 5277(3) Å^3
Space Group	P_{bca} (#61)
Z value	8
D *calc*	1.469g/cm^3
F000	2400.00
μ(MoKα)	11.58 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC5R
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Attenuator	Zr foil (factors = 1.00,3.60,11.82,43.09)
Take-off Angle	6.0°
Detector Aperture	6.0 mm horizontal 6.0 mm vertical
Crystal to Detector Distance	285 mm
Temperature	23.0℃
Scan Type	ω
Scan Rate	16.0°/min (in ω) - up to 3 scans
Scan Width	(0.97+0.14 tan θ)°
2θ*max*	50.0°
No. of Reflections Measured	Total: 5171
Corrections	Lorentz-polarization Absorption (trans. factors: 0.9210-0.9939)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (MITHRIL 90)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma\omega(\lvert Fo\rvert - \lvert Fc\rvert)^2$
Least Squares Weights	$\frac{1}{\sigma^2(Fo)} = \frac{4Fo^2}{\sigma^2(Fo^2)}$
p-factor	0.001
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I > 3.00σ(I))	3415

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No. Variables	275
Reflection/Parameter Ratio	12.42
Residuals: R; Rw	0.035; 0.028
Goodness of Fit Indicator	2.26
Max Shift/Error in Final Cycle	0.08
Maximum peak in Final Diff. Map	0.47 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.38 $e^-/Å^3$

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Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Ru(1)	0.42520(4)	0.22902(3)	0.36691(5)	3.45(1)
Ru(2)	0.17386(4)	0.19623(3)	0.27143(5)	3.66(1)
N(1)	0.2593(4)	0.2994(3)	0.2902(4)	3.7(1)
C(1)	0.2133(7)	0.3738(4)	0.2669(7)	6.9(2)
C(2)	0.2723(10)	0.4431(5)	0.2880(9)	10.6(3)
C(3)	0.219(1)	0.4996(5)	0.1462(10)	13.3(3)
C(4)	0.3794(5)	0.1871(3)	0.5726(6)	4.2(1)
C(5)	0.4062(5)	0.2698(4)	0.6114(6)	4.5(1)
C(6)	0.2477(5)	0.1696(3)	0.5224(6)	4.4(1)
C(7)	0.1534(5)	0.2377(4)	0.5162(6)	4.7(2)
C(8)	0.3090(6)	0.3357(4)	0.6343(6)	4.8(2)
C(9)	0.3372(7)	0.4137(4)	0.7044(7)	6.2(2)
C(10)	0.2450(10)	0.4759(5)	0.7281(9)	7.9(2)
C(11)	0.1227(9)	0.4591(5)	0.6801(9)	8.0(3)
C(12)	0.0888(7)	0.3839(5)	0.6091(8)	6.9(2)
C(13)	0.1835(6)	0.3193(4)	0.5860(6)	5.0(2)
C(14)	0.5455(5)	0.2678(4)	0.2196(7)	4.7(2)
C(15)	0.5999(5)	0.2834(4)	0.3870(7)	4.7(2)
C(16)	0.6277(5)	0.2050(4)	0.4558(7)	4.9(2)
C(17)	0.5862(5)	0.1423(4)	0.3328(8)	4.9(2)
C(18)	0.5361(5)	0.1825(4)	0.1857(7)	4.8(2)
C(19)	0.4997(6)	0.1399(5)	0.0221(8)	8.2(2)
C(20)	0.5103(6)	0.3298(5)	0.0962(8)	7.8(2)
C(21)	0.6394(6)	0.3637(4)	0.4722(9)	7.6(2)

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Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(22)	0.7009(6)	0.1897(5)	0.6237(8)	7.9(2)
C(23)	0.6068(6)	0.0513(4)	0.3506(9)	7.7(2)
C(24)	0.1142(6)	0.0853(4)	0.1229(9)	6.0(2)
C(25)	0.0302(10)	0.1117(7)	0.2148(9)	8.8(3)
C(26)	-0.0263(7)	0.1892(9)	0.165(1)	10.9(4)
C(27)	0.0229(8)	0.2093(5)	0.045(1)	8.3(2)
C(28)	0.1087(6)	0.1467(5)	0.0204(7)	5.6(2)
C(29)	0.1864(10)	0.0019(5)	0.125(1)	17.0(4)
C(30)	-0.010(1)	0.067(1)	0.330(1)	25.6(7)
C(31)	-0.1347(8)	0.242(1)	0.221(2)	28.8(7)
C(32)	-0.014(1)	0.2850(6)	-0.049(2)	23.5(5)
C(33)	0.1723(8)	0.1403(8)	-0.1155(9)	15.5(4)
H(1)	0.340(5)	0.154(4)	0.271(7)	9(1)
H(2)	0.1181	0.3837	0.2261	19.1500
H(3)	0.3565	0.4232	0.2920	18.8551
H(4)	0.2649	0.4714	0.3858	10.9991
H(5)	0.2231	0.4691	0.0482	13.4258
H(6)	0.1331	0.5182	0.1432	18.8551
H(7)	0.2654	0.5449	0.1644	13.4258
H(8)	0.4534	0.1318	0.6321	6.2483
H(9)	0.4996	0.2801	0.6986	6.2483
H(10)	0.2181	0.1081	0.5411	6.2483
H(11)	0.0721	0.2166	0.5122	6.2483
H(12)	0.4485	0.4255	0.7679	6.2483

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Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(13)	0.2819	0.5421	0.7916	6.2483
H(14)	0.0484	0.5187	0.7021	6.2483
H(15)	-0.0161	0.3680	0.5605	15.9832
H(16)	0.4197	0.1619	-0.0325	9.9276
H(17)	0.5596	0.1470	-0.0351	9.9276
H(18)	0.5005	0.0822	0.0316	9.9276
H(19)	0.5246	0.3833	0.1475	9.4254
H(20)	0.5595	0.3164	0.0207	9.4254
H(21)	0.4242	0.3296	0.0419	9.4254
H(22)	0.6727	0.3568	0.5843	8.9965
H(23)	0.7011	0.3813	0.4301	8.9965
H(24)	0.5688	0.4045	0.4590	8.9965
H(25)	0.6537	0.1620	0.6750	9.6622
H(26)	0.7776	0.1571	0.6228	9.6622
H(27)	0.7174	0.2416	0.6819	9.6622
H(28)	0.5711	0.0393	0.4322	9.4987
H(29)	0.5700	0.0230	0.2518	9.4987
H(30)	0.6946	0.0350	0.3795	9.4987
H(31)	0.1298	-0.0389	0.0950	20.7522
H(32)	0.2373	-0.0021	0.0520	20.7522
H(33)	0.2373	-0.0054	0.2307	20.7522
H(34)	-0.0001	0.0982	0.4296	27.7777
H(35)	-0.0938	0.0560	0.2875	27.7777
H(36)	0.0415	0.0142	0.3471	27.7777

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(37)	-0.1098	0.2959	0.2539	36.7781
H(38)	-0.2047	0.2458	0.1278	36.7781
H(39)	-0.1547	0.2186	0.3017	36.7781
H(40)	0.0571	0.3126	-0.0378	27.3238
H(41)	-0.0459	0.2673	-0.1608	27.3238
H(42)	-0.0765	0.3188	-0.0119	27.3238
H(43)	0.2303	0.0899	-0.1083	19.1500
H(44)	0.1121	0.1364	-0.2144	19.1500
H(45)	0.2172	0.1856	-0.1059	19.1500

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

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Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ru(1)	0.0436(3)	0.0467(3)	0.0415(3)	-0.0048(2)	0.0126(2)	0.0016(2)
Ru(2)	0.0407(3)	0.0547(3)	0.0464(3)	-0.0007(2)	0.0169(2)	0.0059(2)
N(1)	0.058(3)	0.043(3)	0.041(2)	0.004(2)	0.022(2)	0.007(2)
C(1)	0.166(8)	0.054(4)	0.056(4)	-0.025(5)	0.048(4)	-0.003(3)
C(2)	0.25(1)	0.088(6)	0.074(5)	-0.023(7)	0.056(6)	0.000(5)
C(3)	0.33(1)	0.078(6)	0.091(6)	-0.002(7)	0.033(8)	0.043(5)
C(4)	0.066(4)	0.056(4)	0.037(3)	0.001(3)	0.014(3)	0.010(3)
C(5)	0.068(4)	0.061(4)	0.037(3)	0.000(3)	0.010(3)	0.002(3)
C(6)	0.077(4)	0.050(3)	0.050(3)	-0.004(3)	0.034(3)	0.014(3)
C(7)	0.062(4)	0.075(4)	0.053(4)	-0.009(3)	0.028(3)	0.008(3)
C(8)	0.092(5)	0.060(4)	0.037(3)	-0.005(4)	0.026(3)	0.002(3)
C(9)	0.117(6)	0.071(5)	0.049(4)	-0.010(4)	0.028(4)	-0.006(3)
C(10)	0.174(9)	0.067(5)	0.070(5)	-0.007(6)	0.058(6)	-0.010(4)
C(11)	0.164(8)	0.068(5)	0.085(6)	0.029(6)	0.077(6)	0.002(4)
C(12)	0.113(6)	0.088(5)	0.066(4)	0.024(5)	0.048(4)	0.008(4)
C(13)	0.089(5)	0.062(4)	0.046(3)	0.008(4)	0.038(3)	0.005(3)
C(14)	0.043(3)	0.076(4)	0.065(4)	-0.007(3)	0.021(3)	0.015(3)
C(15)	0.047(3)	0.060(4)	0.075(4)	-0.015(3)	0.015(3)	0.000(3)
C(16)	0.038(3)	0.083(5)	0.063(4)	-0.006(3)	0.008(3)	0.009(3)
C(17)	0.045(3)	0.056(4)	0.085(5)	0.002(3)	0.025(3)	-0.003(3)
C(18)	0.044(3)	0.085(5)	0.059(4)	-0.010(3)	0.026(3)	-0.010(3)
C(19)	0.077(5)	0.153(7)	0.083(5)	-0.019(5)	0.041(4)	-0.044(5)
C(20)	0.080(5)	0.127(7)	0.105(6)	0.008(4)	0.046(4)	0.049(5)
C(21)	0.072(5)	0.088(5)	0.129(6)	-0.031(4)	0.024(4)	-0.009(5)

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Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(22)	0.063(5)	0.135(7)	0.088(5)	0.005(4)	-0.003(4)	0.024(5)
C(23)	0.084(5)	0.071(5)	0.146(7)	0.007(4)	0.052(5)	0.006(5)
C(24)	0.071(5)	0.060(4)	0.079(5)	-0.010(4)	-0.013(4)	0.000(4)
C(25)	0.110(8)	0.182(10)	0.064(5)	-0.099(7)	0.018(5)	0.009(6)
C(26)	0.031(4)	0.21(1)	0.16(1)	-0.031(6)	0.026(5)	-0.096(9)
C(27)	0.069(6)	0.074(5)	0.132(8)	-0.009(4)	-0.049(5)	0.018(5)
C(28)	0.052(4)	0.117(6)	0.046(4)	-0.033(4)	0.005(3)	0.003(4)
C(29)	0.19(1)	0.075(6)	0.26(1)	0.024(6)	-0.123(9)	-0.047(7)
C(30)	0.41(2)	0.55(3)	0.098(8)	-0.43(2)	0.032(10)	0.02(1)
C(31)	0.041(5)	0.57(3)	0.39(2)	-0.005(10)	0.045(9)	-0.33(2)
C(32)	0.34(2)	0.107(8)	0.29(2)	-0.071(10)	-0.24(1)	0.087(9)
C(33)	0.133(8)	0.43(2)	0.054(5)	-0.154(10)	0.034(5)	-0.044(7)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

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Table 3. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Ru(1)	Ru(2)	2.8103(8)	Ru(1)	N(1)	2.037(4)
Ru(1)	C(4)	2.173(5)	Ru(1)	C(5)	2.202(5)
Ru(1)	C(14)	2.261(5)	Ru(1)	C(15)	2.204(5)
Ru(1)	C(16)	2.181(5)	Ru(1)	C(17)	2.200(5)
Ru(1)	C(18)	2.253(5)	Ru(1)	H(1)	1.67(6)
Ru(2)	N(1)	2.016(4)	Ru(2)	C(6)	2.178(5)
Ru(2)	C(7)	2.212(5)	Ru(2)	C(24)	2.179(6)
Ru(2)	C(25)	2.177(7)	Ru(2)	C(26)	2.191(7)
Ru(2)	C(27)	2.227(7)	Ru(2)	C(28)	2.201(6)
N(1)	C(1)	1.272(7)	C(1)	C(2)	1.356(9)
C(1)	H(2)	1.02	C(2)	C(3)	1.559(10)
C(2)	H(3)	0.94	C(2)	H(4)	0.94
C(3)	H(5)	0.95	C(3)	H(6)	0.96
C(3)	H(7)	0.94	C(4)	C(5)	1.409(7)
C(4)	C(6)	1.475(7)	C(4)	H(8)	1.20
C(5)	C(8)	1.462(7)	C(5)	H(9)	1.13
C(6)	C(7)	1.424(7)	C(6)	H(10)	1.14
C(7)	C(13)	1.447(8)	C(7)	H(11)	1.00
C(8)	C(9)	1.389(8)	C(8)	C(13)	1.404(8)
C(9)	C(10)	1.388(9)	C(9)	H(12)	1.25
C(10)	C(11)	1.37(1)	C(10)	H(13)	1.23
C(11)	C(12)	1.368(10)	C(11)	H(14)	1.23
C(12)	C(13)	1.430(8)	C(12)	H(15)	1.19
C(14)	C(15)	1.424(7)	C(14)	C(18)	1.406(7)

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Table 3. Bond Lengths(Å) (continued)

atom	atom	distance	atom	atom	distance
C(14)	C(20)	1.493(8)	C(15)	C(16)	1.434(8)
C(15)	C(21)	1.496(8)	C(16)	C(17)	1.423(7)
C(16)	C(22)	1.496(8)	C(17)	C(18)	1.439(8)
C(17)	C(23)	1.496(8)	C(18)	C(19)	1.487(8)
C(19)	H(16)	0.94	C(19)	H(17)	0.95
C(19)	H(18)	0.96	C(20)	H(19)	0.95
C(20)	H(20)	0.95	C(20)	H(21)	0.95
C(21)	H(22)	0.96	C(21)	H(23)	0.95
C(21)	H(24)	0.95	C(22)	H(25)	0.95
C(22)	H(26)	0.95	C(22)	H(27)	0.95
C(23)	H(28)	0.94	C(23)	H(29)	0.95
C(23)	H(30)	0.95	C(24)	C(25)	1.38(1)
C(24)	C(28)	1.395(8)	C(24)	C(29)	1.490(10)
C(25)	C(26)	1.40(1)	C(25)	C(30)	1.49(1)
C(26)	C(27)	1.37(1)	C(26)	C(31)	1.55(1)
C(27)	C(28)	1.347(10)	C(27)	C(32)	1.51(1)
C(28)	C(33)	1.512(9)	C(29)	H(31)	0.95
C(29)	H(32)	0.94	C(29)	H(33)	0.95
C(30)	H(34)	0.94	C(30)	H(35)	0.94
C(30)	H(36)	0.97	C(31)	H(37)	0.95
C(31)	H(38)	0.96	C(31)	H(39)	0.92
C(32)	H(40)	0.94	C(32)	H(41)	0.96
C(32)	H(42)	0.93	C(33)	H(43)	0.98
C(33)	H(44)	0.94	C(33)	H(45)	0.93

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Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
Ru(2)	Ru(1)	N(1)	45.8(1)	Ru(2)	Ru(1)	C(4)	72.3(1)
Ru(2)	Ru(1)	C(5)	90.5(1)	Ru(2)	Ru(1)	C(14)	129.4(1)
Ru(2)	Ru(1)	C(15)	162.3(2)	Ru(2)	Ru(1)	C(16)	158.2(2)
Ru(2)	Ru(1)	C(17)	125.6(2)	Ru(2)	Ru(1)	C(18)	114.4(1)
Ru(2)	Ru(1)	H(1)	40(1)	N(1)	Ru(1)	C(4)	95.6(2)
N(1)	Ru(1)	C(5)	85.6(2)	N(1)	Ru(1)	C(14)	103.0(2)
N(1)	Ru(1)	C(15)	118.6(2)	N(1)	Ru(1)	C(16)	155.9(2)
N(1)	Ru(1)	C(17)	154.3(2)	N(1)	Ru(1)	C(18)	118.1(2)
N(1)	Ru(1)	H(1)	81(1)	C(4)	Ru(1)	C(5)	37.6(2)
C(4)	Ru(1)	C(14)	158.0(2)	C(4)	Ru(1)	C(15)	122.5(2)
C(4)	Ru(1)	C(16)	96.2(2)	C(4)	Ru(1)	C(17)	104.1(2)
C(4)	Ru(1)	C(18)	139.3(2)	C(4)	Ru(1)	H(1)	81(1)
C(5)	Ru(1)	C(14)	131.8(2)	C(5)	Ru(1)	C(15)	97.0(2)
C(5)	Ru(1)	C(16)	91.0(2)	C(5)	Ru(1)	C(17)	120.0(2)
C(5)	Ru(1)	C(18)	153.4(2)	C(5)	Ru(1)	H(1)	115(1)
C(14)	Ru(1)	C(15)	37.2(2)	C(14)	Ru(1)	C(16)	62.3(2)
C(14)	Ru(1)	C(17)	62.3(2)	C(14)	Ru(1)	C(18)	36.3(2)
C(14)	Ru(1)	H(1)	112(1)	C(15)	Ru(1)	C(16)	38.2(2)
C(15)	Ru(1)	C(17)	63.6(2)	C(15)	Ru(1)	C(18)	62.2(2)
C(15)	Ru(1)	H(1)	143(1)	C(16)	Ru(1)	C(17)	37.9(2)
C(16)	Ru(1)	C(18)	62.5(2)	C(16)	Ru(1)	H(1)	120(2)
C(17)	Ru(1)	C(18)	37.7(2)	C(17)	Ru(1)	H(1)	84(1)
C(18)	Ru(1)	H(1)	81(1)	Ru(1)	Ru(2)	N(1)	46.4(1)
Ru(1)	Ru(2)	C(6)	71.9(1)	Ru(1)	Ru(2)	C(7)	89.9(1)

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Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
Ru(1)	Ru(2)	C(24)	122.4(2)	Ru(1)	Ru(2)	C(25)	151.8(4)
Ru(1)	Ru(2)	C(26)	168.9(4)	Ru(1)	Ru(2)	C(27)	134.1(3)
Ru(1)	Ru(2)	C(28)	115.4(2)	N(1)	Ru(2)	C(6)	95.7(2)
N(1)	Ru(2)	C(7)	85.0(2)	N(1)	Ru(2)	C(24)	146.5(2)
N(1)	Ru(2)	C(25)	161.5(4)	N(1)	Ru(2)	C(26)	124.1(4)
N(1)	Ru(2)	C(27)	102.8(2)	N(1)	Ru(2)	C(28)	112.4(2)
C(6)	Ru(2)	C(7)	37.8(2)	C(6)	Ru(2)	C(24)	110.7(2)
C(6)	Ru(2)	C(25)	96.2(3)	C(6)	Ru(2)	C(26)	117.7(4)
C(6)	Ru(2)	C(27)	153.9(3)	C(6)	Ru(2)	C(28)	147.2(3)
C(7)	Ru(2)	C(24)	128.5(3)	C(7)	Ru(2)	C(25)	95.9(3)
C(7)	Ru(2)	C(26)	95.2(3)	C(7)	Ru(2)	C(27)	125.3(3)
C(7)	Ru(2)	C(28)	154.7(2)	C(24)	Ru(2)	C(25)	36.9(3)
C(24)	Ru(2)	C(26)	61.1(3)	C(24)	Ru(2)	C(27)	60.9(3)
C(24)	Ru(2)	C(28)	37.1(2)	C(25)	Ru(2)	C(26)	37.4(3)
C(25)	Ru(2)	C(27)	61.7(3)	C(25)	Ru(2)	C(28)	61.6(3)
C(26)	Ru(2)	C(27)	36.2(3)	C(26)	Ru(2)	C(28)	60.0(3)
C(27)	Ru(2)	C(28)	35.4(3)	Ru(1)	N(1)	Ru(2)	87.8(2)
Ru(1)	N(1)	C(1)	141.8(5)	Ru(2)	N(1)	C(1)	130.3(5)
N(1)	C(1)	C(2)	129.4(8)	N(1)	C(1)	H(2)	116.5
C(2)	C(1)	H(2)	114.2	C(1)	C(2)	C(3)	112.1(8)
C(1)	C(2)	H(3)	104.4	C(1)	C(2)	H(4)	108.3
C(3)	C(2)	H(3)	110.0	C(3)	C(2)	H(4)	110.9
H(3)	C(2)	H(4)	111.0	C(2)	C(3)	H(5)	109.5
C(2)	C(3)	H(6)	108.6	C(2)	C(3)	H(7)	108.4

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Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
H(5)	C(3)	H(6)	109.3	H(5)	C(3)	H(7)	110.9
H(6)	C(3)	H(7)	110.1	Ru(1)	C(4)	C(5)	72.3(3)
Ru(1)	C(4)	C(6)	107.7(3)	Ru(1)	C(4)	H(8)	112.4
C(5)	C(4)	C(6)	119.0(5)	C(5)	C(4)	H(8)	120.1
C(6)	C(4)	H(8)	115.6	Ru(1)	C(5)	C(4)	70.1(3)
Ru(1)	C(5)	C(8)	119.7(4)	Ru(1)	C(5)	H(9)	112.2
C(4)	C(5)	C(8)	121.1(5)	C(4)	C(5)	H(9)	116.6
C(8)	C(5)	H(9)	111.3	Ru(2)	C(6)	C(4)	108.0(3)
Ru(2)	C(6)	C(7)	72.3(3)	Ru(2)	C(6)	H(10)	109.4
C(4)	C(6)	C(7)	117.8(5)	C(4)	C(6)	H(10)	122.1
C(7)	C(6)	H(10)	114.8	Ru(2)	C(7)	C(6)	69.8(3)
Ru(2)	C(7)	C(13)	119.9(4)	Ru(2)	C(7)	H(11)	100.7
C(6)	C(7)	C(13)	121.4(5)	C(6)	C(7)	H(11)	109.0
C(13)	C(7)	H(11)	122.8	C(5)	C(8)	C(9)	122.1(6)
C(5)	C(8)	C(13)	118.9(5)	C(9)	C(8)	C(13)	119.1(6)
C(8)	C(9)	C(10)	122.0(7)	C(8)	C(9)	H(12)	119.4
C(10)	C(9)	H(12)	117.9	C(9)	C(10)	C(11)	118.3(7)
C(9)	C(10)	H(13)	115.8	C(11)	C(10)	H(13)	125.8
C(10)	C(11)	C(12)	122.4(7)	C(10)	C(11)	H(14)	113.3
C(12)	C(11)	H(14)	124.3	C(11)	C(12)	C(13)	119.4(7)
C(11)	C(12)	H(15)	124.4	C(13)	C(12)	H(15)	116.1
C(7)	C(13)	C(8)	119.5(5)	C(7)	C(13)	C(12)	121.8(6)
C(8)	C(13)	C(12)	118.7(6)	Ru(1)	C(14)	C(15)	69.2(3)
Ru(1)	C(14)	C(18)	71.5(3)	Ru(1)	C(14)	C(20)	128.0(4)

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Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(15)	C(14)	C(18)	108.8(5)	C(15)	C(14)	C(20)	126.5(6)
C(18)	C(14)	C(20)	124.6(6)	Ru(1)	C(15)	C(14)	73.6(3)
Ru(1)	C(15)	C(16)	70.1(3)	Ru(1)	C(15)	C(21)	128.4(4)
C(14)	C(15)	C(16)	107.1(5)	C(14)	C(15)	C(21)	126.8(6)
C(16)	C(15)	C(21)	125.5(6)	Ru(1)	C(16)	C(15)	71.8(3)
Ru(1)	C(16)	C(17)	71.8(3)	Ru(1)	C(16)	C(22)	127.7(4)
C(15)	C(16)	C(17)	108.7(5)	C(15)	C(16)	C(22)	126.0(6)
C(17)	C(16)	C(22)	125.0(6)	Ru(1)	C(17)	C(16)	70.3(3)
Ru(1)	C(17)	C(18)	73.1(3)	Ru(1)	C(17)	C(23)	127.6(4)
C(16)	C(17)	C(18)	106.9(5)	C(16)	C(17)	C(23)	125.8(6)
C(18)	C(17)	C(23)	126.8(6)	Ru(1)	C(18)	C(14)	72.2(3)
Ru(1)	C(18)	C(17)	69.2(3)	Ru(1)	C(18)	C(19)	131.7(4)
C(14)	C(18)	C(17)	108.5(5)	C(14)	C(18)	C(19)	125.4(6)
C(17)	C(18)	C(19)	125.5(6)	C(18)	C(19)	H(16)	110.0
C(18)	C(19)	H(17)	108.7	C(18)	C(19)	H(18)	109.0
H(16)	C(19)	H(17)	110.2	H(16)	C(19)	H(18)	110.1
H(17)	C(19)	H(18)	108.7	C(14)	C(20)	H(19)	109.4
C(14)	C(20)	H(20)	109.6	C(14)	C(20)	H(21)	109.7
H(19)	C(20)	H(20)	109.4	H(19)	C(20)	H(21)	109.3
H(20)	C(20)	H(21)	109.4	C(15)	C(21)	H(22)	109.3
C(15)	C(21)	H(23)	110.1	C(15)	C(21)	H(24)	109.6
H(22)	C(21)	H(23)	109.4	H(22)	C(21)	H(24)	108.8
H(23)	C(21)	H(24)	109.7	C(16)	C(22)	H(25)	109.9
C(16)	C(22)	H(26)	110.4	C(16)	C(22)	H(27)	108.6

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Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
H(25)	C(22)	H(26)	109.5	H(25)	C(22)	H(27)	109.0
H(26)	C(22)	H(27)	109.4	C(17)	C(23)	H(28)	109.5
C(17)	C(23)	H(29)	109.4	C(17)	C(23)	H(30)	108.4
H(28)	C(23)	H(29)	110.4	H(28)	C(23)	H(30)	109.6
H(29)	C(23)	H(30)	109.6	Ru(2)	C(24)	C(25)	71.4(4)
Ru(2)	C(24)	C(28)	72.3(4)	Ru(2)	C(24)	C(29)	126.6(5)
C(25)	C(24)	C(28)	107.9(7)	C(25)	C(24)	C(29)	124.5(10)
C(28)	C(24)	C(29)	127.3(9)	Ru(2)	C(25)	C(24)	71.6(4)
Ru(2)	C(25)	C(26)	71.9(5)	Ru(2)	C(25)	C(30)	127.0(6)
C(24)	C(25)	C(26)	106.1(7)	C(24)	C(25)	C(30)	129(1)
C(26)	C(25)	C(30)	123(1)	Ru(2)	C(26)	C(25)	70.8(5)
Ru(2)	C(26)	C(27)	73.3(4)	Ru(2)	C(26)	C(31)	126.1(6)
C(25)	C(26)	C(27)	109.2(8)	C(25)	C(26)	C(31)	126(1)
C(27)	C(26)	C(31)	123(1)	Ru(2)	C(27)	C(26)	70.5(5)
Ru(2)	C(27)	C(28)	71.2(4)	Ru(2)	C(27)	C(32)	126.1(5)
C(26)	C(27)	C(28)	107.7(8)	C(26)	C(27)	C(32)	127(1)
C(28)	C(27)	C(32)	124(1)	Ru(2)	C(28)	C(24)	70.6(3)
Ru(2)	C(28)	C(27)	73.4(4)	Ru(2)	C(28)	C(33)	129.3(4)
C(24)	C(28)	C(27)	109.1(7)	C(24)	C(28)	C(33)	126.4(9)
C(27)	C(28)	C(33)	123.9(9)	C(24)	C(29)	H(31)	109.1
C(24)	C(29)	H(32)	109.4	C(24)	C(29)	H(33)	108.9
H(31)	C(29)	H(32)	110.3	H(31)	C(29)	H(33)	109.4
H(32)	C(29)	H(33)	109.8	C(25)	C(30)	H(34)	110.1
C(25)	C(30)	H(35)	109.7	C(25)	C(30)	H(36)	109.7

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Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
H(34)	C(30)	H(35)	111.0	H(34)	C(30)	H(36)	108.4
H(35)	C(30)	H(36)	107.9	C(26)	C(31)	H(37)	107.5
C(26)	C(31)	H(38)	106.6	C(26)	C(31)	H(39)	111.2
H(37)	C(31)	H(38)	108.5	H(37)	C(31)	H(39)	111.9
H(38)	C(31)	H(39)	110.8	C(27)	C(32)	H(40)	108.9
C(27)	C(32)	H(41)	108.4	C(27)	C(32)	H(42)	109.0
H(40)	C(32)	H(41)	109.0	H(40)	C(32)	H(42)	111.5
H(41)	C(32)	H(42)	109.9	C(28)	C(33)	H(43)	108.6
C(28)	C(33)	H(44)	109.4	C(28)	C(33)	H(45)	109.8
H(43)	C(33)	H(44)	108.1	H(43)	C(33)	H(45)	108.9
H(44)	C(33)	H(45)	112.0				

Table 5. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Ru(1)	Ru(2)	N(1)	C(1)	-176.9(6)	Ru(1)	Ru(2)	C(6)	C(4)	0.2(3)
Ru(1)	Ru(2)	C(6)	C(7)	114.6(3)	Ru(1)	Ru(2)	C(7)	C(6)	-59.8(3)
Ru(1)	Ru(2)	C(7)	C(13)	55.6(5)	Ru(1)	Ru(2)	C(24)	C(25)	153.2(5)
Ru(1)	Ru(2)	C(24)	C(28)	-90.2(4)	Ru(1)	Ru(2)	C(24)	C(29)	33(1)
Ru(1)	Ru(2)	C(25)	C(24)	-53.7(7)	Ru(1)	Ru(2)	C(25)	C(26)	-168.3(5)
Ru(1)	Ru(2)	C(25)	C(30)	72(1)	Ru(1)	Ru(2)	C(26)	C(25)	150(1)
Ru(1)	Ru(2)	C(26)	C(27)	32(1)	Ru(1)	Ru(2)	C(26)	C(31)	-87(1)
Ru(1)	Ru(2)	C(27)	C(26)	-171.8(6)	Ru(1)	Ru(2)	C(27)	C(28)	70.7(5)
Ru(1)	Ru(2)	C(27)	C(32)	-48(1)	Ru(1)	Ru(2)	C(28)	C(24)	110.8(4)
Ru(1)	Ru(2)	C(28)	C(27)	-131.3(5)	Ru(1)	Ru(2)	C(28)	C(33)	-10.9(10)
Ru(1)	N(1)	Ru(2)	C(6)	58.3(2)	Ru(1)	N(1)	Ru(2)	C(7)	94.6(2)
Ru(1)	N(1)	Ru(2)	C(24)	-84.4(4)	Ru(1)	N(1)	Ru(2)	C(25)	-171.7(8)
Ru(1)	N(1)	Ru(2)	C(26)	-172.5(3)	Ru(1)	N(1)	Ru(2)	C(27)	-140.3(3)
Ru(1)	N(1)	Ru(2)	C(28)	-104.4(2)	Ru(1)	N(1)	C(1)	C(2)	1(1)
Ru(1)	C(4)	C(5)	C(8)	113.4(5)	Ru(1)	C(4)	C(6)	Ru(2)	-0.3(4)
Ru(1)	C(4)	C(6)	C(7)	-79.4(5)	Ru(1)	C(5)	C(4)	C(6)	-100.9(4)
Ru(1)	C(5)	C(8)	C(9)	-110.2(5)	Ru(1)	C(5)	C(8)	C(13)	70.7(6)
Ru(1)	C(14)	C(15)	C(16)	62.5(4)	Ru(1)	C(14)	C(15)	C(21)	-126.1(6)
Ru(1)	C(14)	C(18)	C(17)	-59.9(4)	Ru(1)	C(14)	C(18)	C(19)	129.0(6)
Ru(1)	C(15)	C(14)	C(18)	-60.8(4)	Ru(1)	C(15)	C(14)	C(20)	122.5(6)
Ru(1)	C(15)	C(16)	C(17)	62.7(4)	Ru(1)	C(15)	C(16)	C(22)	-123.8(6)
Ru(1)	C(16)	C(15)	C(14)	-64.8(4)	Ru(1)	C(16)	C(15)	C(21)	123.6(6)
Ru(1)	C(16)	C(17)	C(18)	64.5(4)	Ru(1)	C(16)	C(17)	C(23)	-122.7(6)
Ru(1)	C(17)	C(16)	C(15)	-62.7(4)	Ru(1)	C(17)	C(16)	C(22)	123.8(6)

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Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Ru(1)	C(17)	C(18)	C(14)	61.8(4)	Ru(1)	C(17)	C(18)	C(19)	-127.1(5)
Ru(1)	C(18)	C(14)	C(15)	59.4(4)	Ru(1)	C(18)	C(14)	C(20)	-123.9(5)
Ru(1)	C(18)	C(17)	C(16)	-62.6(4)	Ru(1)	C(18)	C(17)	C(23)	124.7(6)
Ru(2)	Ru(1)	N(1)	C(1)	176.2(7)	Ru(2)	Ru(1)	C(4)	C(5)	-115.4(3)
Ru(2)	Ru(1)	C(4)	C(6)	0.2(3)	Ru(2)	Ru(1)	C(5)	C(4)	59.4(3)
Ru(2)	Ru(1)	C(5)	C(8)	-55.8(5)	Ru(2)	Ru(1)	C(14)	C(15)	163.1(3)
Ru(2)	Ru(1)	C(14)	C(18)	-77.5(4)	Ru(2)	Ru(1)	C(14)	C(20)	42.4(7)
Ru(2)	Ru(1)	C(15)	C(14)	-47.5(7)	Ru(2)	Ru(1)	C(15)	C(16)	-163.1(4)
Ru(2)	Ru(1)	C(15)	C(21)	76.9(8)	Ru(2)	Ru(1)	C(16)	C(15)	166.2(3)
Ru(2)	Ru(1)	C(16)	C(17)	48.6(6)	Ru(2)	Ru(1)	C(16)	C(22)	-72.0(8)
Ru(2)	Ru(1)	C(17)	C(16)	-160.0(3)	Ru(2)	Ru(1)	C(17)	C(18)	84.4(3)
Ru(2)	Ru(1)	C(17)	C(23)	-39.4(7)	Ru(2)	Ru(1)	C(18)	C(14)	124.1(3)
Ru(2)	Ru(1)	C(18)	C(17)	-117.3(3)	Ru(2)	Ru(1)	C(18)	C(19)	2.2(7)
Ru(2)	N(1)	Ru(1)	C(4)	-58.6(2)	Ru(2)	N(1)	Ru(1)	C(5)	-94.9(2)
Ru(2)	N(1)	Ru(1)	C(14)	133.2(2)	Ru(2)	N(1)	Ru(1)	C(15)	169.5(2)
Ru(2)	N(1)	Ru(1)	C(16)	-177.6(4)	Ru(2)	N(1)	Ru(1)	C(17)	81.5(4)
Ru(2)	N(1)	Ru(1)	C(18)	97.7(2)	Ru(2)	N(1)	C(1)	C(2)	176.3(5)
Ru(2)	C(6)	C(4)	C(5)	78.9(5)	Ru(2)	C(6)	C(7)	C(13)	-113.5(5)
Ru(2)	C(7)	C(6)	C(4)	101.5(4)	Ru(2)	C(7)	C(13)	C(8)	-71.5(6)
Ru(2)	C(7)	C(13)	C(12)	109.2(5)	Ru(2)	C(24)	C(25)	C(26)	64.1(6)
Ru(2)	C(24)	C(25)	C(30)	-123.2(9)	Ru(2)	C(24)	C(28)	C(27)	-63.7(5)
Ru(2)	C(24)	C(28)	C(33)	125.1(6)	Ru(2)	C(25)	C(24)	C(28)	-63.5(4)
Ru(2)	C(25)	C(24)	C(29)	122.2(7)	Ru(2)	C(25)	C(26)	C(27)	63.7(6)
Ru(2)	C(25)	C(26)	C(31)	-121.2(9)	Ru(2)	C(26)	C(25)	C(24)	-63.9(5)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Ru(2)	C(26)	C(25)	C(30)	122.8(8)	Ru(2)	C(26)	C(27)	C(28)	61.9(5)
Ru(2)	C(26)	C(27)	C(32)	-121.0(8)	Ru(2)	C(27)	C(26)	C(25)	-62.1(6)
Ru(2)	C(27)	C(26)	C(31)	122.7(9)	Ru(2)	C(27)	C(28)	C(24)	62.0(4)
Ru(2)	C(27)	C(28)	C(33)	-126.5(6)	Ru(2)	C(28)	C(24)	C(25)	63.0(5)
Ru(2)	C(28)	C(24)	C(29)	-123.0(7)	Ru(2)	C(28)	C(27)	C(26)	-61.4(6)
Ru(2)	C(28)	C(27)	C(32)	121.4(7)	N(1)	Ru(1)	Ru(2)	C(6)	-117.1(2)
N(1)	Ru(1)	Ru(2)	C(7)	-83.2(2)	N(1)	Ru(1)	Ru(2)	C(24)	139.4(3)
N(1)	Ru(1)	Ru(2)	C(25)	174.4(5)	N(1)	Ru(1)	Ru(2)	C(26)	34(1)
N(1)	Ru(1)	Ru(2)	C(27)	60.2(4)	N(1)	Ru(1)	Ru(2)	C(28)	97.5(3)
N(1)	Ru(1)	C(4)	C(5)	-75.4(3)	N(1)	Ru(1)	C(4)	C(6)	40.2(4)
N(1)	Ru(1)	C(5)	C(4)	105.0(3)	N(1)	Ru(1)	C(5)	C(8)	-10.2(5)
N(1)	Ru(1)	C(14)	C(15)	120.5(3)	N(1)	Ru(1)	C(14)	C(18)	-120.1(3)
N(1)	Ru(1)	C(14)	C(20)	-0.2(6)	N(1)	Ru(1)	C(15)	C(14)	-72.9(4)
N(1)	Ru(1)	C(15)	C(16)	171.5(3)	N(1)	Ru(1)	C(15)	C(21)	51.5(6)
N(1)	Ru(1)	C(16)	C(15)	-18.5(6)	N(1)	Ru(1)	C(16)	C(17)	-136.1(4)
N(1)	Ru(1)	C(16)	C(22)	103.2(7)	N(1)	Ru(1)	C(17)	C(16)	139.3(4)
N(1)	Ru(1)	C(17)	C(18)	23.8(6)	N(1)	Ru(1)	C(17)	C(23)	-100.1(7)
N(1)	Ru(1)	C(18)	C(14)	72.8(4)	N(1)	Ru(1)	C(18)	C(17)	-168.6(3)
N(1)	Ru(1)	C(18)	C(19)	-49.0(7)	N(1)	Ru(2)	Ru(1)	C(4)	116.9(2)
N(1)	Ru(2)	Ru(1)	C(5)	83.5(2)	N(1)	Ru(2)	Ru(1)	C(14)	-66.9(3)
N(1)	Ru(2)	Ru(1)	C(15)	-31.7(5)	N(1)	Ru(2)	Ru(1)	C(16)	177.3(4)
N(1)	Ru(2)	Ru(1)	C(17)	-148.2(3)	N(1)	Ru(2)	Ru(1)	C(18)	-106.3(2)
N(1)	Ru(2)	C(6)	C(4)	-40.2(4)	N(1)	Ru(2)	C(6)	C(7)	74.2(3)
N(1)	Ru(2)	C(7)	C(6)	-106.1(3)	N(1)	Ru(2)	C(7)	C(13)	9.4(5)

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Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
N(1)	Ru(2)	C(24)	C(25)	-148.2(6)	N(1)	Ru(2)	C(24)	C(28)	-31.6(6)
N(1)	Ru(2)	C(24)	C(29)	92.1(10)	N(1)	Ru(2)	C(25)	C(24)	113(1)
N(1)	Ru(2)	C(25)	C(26)	-1(1)	N(1)	Ru(2)	C(25)	C(30)	-119(1)
N(1)	Ru(2)	C(26)	C(25)	179.6(5)	N(1)	Ru(2)	C(26)	C(27)	61.7(7)
N(1)	Ru(2)	C(26)	C(31)	-58(1)	N(1)	Ru(2)	C(27)	C(26)	-131.7(7)
N(1)	Ru(2)	C(27)	C(28)	110.9(5)	N(1)	Ru(2)	C(27)	C(32)	-8(1)
N(1)	Ru(2)	C(28)	C(24)	161.8(4)	N(1)	Ru(2)	C(28)	C(27)	-80.4(5)
N(1)	Ru(2)	C(28)	C(33)	40.1(10)	N(1)	C(1)	C(2)	C(3)	136.6(8)
C(1)	N(1)	Ru(1)	C(4)	117.6(6)	C(1)	N(1)	Ru(1)	C(5)	81.3(6)
C(1)	N(1)	Ru(1)	C(14)	-50.6(6)	C(1)	N(1)	Ru(1)	C(15)	-14.3(7)
C(1)	N(1)	Ru(1)	C(16)	-1.3(9)	C(1)	N(1)	Ru(1)	C(17)	-102.3(7)
C(1)	N(1)	Ru(1)	C(18)	-86.1(6)	C(1)	N(1)	Ru(2)	C(6)	-118.6(5)
C(1)	N(1)	Ru(2)	C(7)	-82.3(5)	C(1)	N(1)	Ru(2)	C(24)	98.7(6)
C(1)	N(1)	Ru(2)	C(25)	11(1)	C(1)	N(1)	Ru(2)	C(26)	10.6(6)
C(1)	N(1)	Ru(2)	C(27)	42.8(6)	C(1)	N(1)	Ru(2)	C(28)	78.7(5)
C(4)	Ru(1)	Ru(2)	C(6)	-0.2(2)	C(4)	Ru(1)	Ru(2)	C(7)	33.8(2)
C(4)	Ru(1)	Ru(2)	C(24)	-103.6(3)	C(4)	Ru(1)	Ru(2)	C(25)	-68.7(5)
C(4)	Ru(1)	Ru(2)	C(26)	151(1)	C(4)	Ru(1)	Ru(2)	C(27)	177.1(4)
C(4)	Ru(1)	Ru(2)	C(28)	-145.6(3)	C(4)	Ru(1)	C(5)	C(8)	-115.2(6)
C(4)	Ru(1)	C(14)	C(15)	-26.6(7)	C(4)	Ru(1)	C(14)	C(18)	92.8(6)
C(4)	Ru(1)	C(14)	C(20)	-147.3(6)	C(4)	Ru(1)	C(15)	C(14)	168.6(3)
C(4)	Ru(1)	C(15)	C(16)	52.9(4)	C(4)	Ru(1)	C(15)	C(21)	-67.1(6)
C(4)	Ru(1)	C(16)	C(15)	-137.4(4)	C(4)	Ru(1)	C(16)	C(17)	105.0(4)
C(4)	Ru(1)	C(16)	C(22)	-15.6(6)	C(4)	Ru(1)	C(17)	C(16)	-81.9(4)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(4)	Ru(1)	C(17)	C(18)	162.6(3)	C(4)	Ru(1)	C(17)	C(23)	38.7(6)
C(4)	Ru(1)	C(18)	C(14)	-145.0(4)	C(4)	Ru(1)	C(18)	C(17)	-26.5(5)
C(4)	Ru(1)	C(18)	C(19)	93.1(7)	C(4)	C(5)	Ru(1)	C(14)	-151.4(3)
C(4)	C(5)	Ru(1)	C(15)	-136.7(3)	C(4)	C(5)	Ru(1)	C(16)	-98.9(3)
C(4)	C(5)	Ru(1)	C(17)	-73.2(4)	C(4)	C(5)	Ru(1)	C(18)	-100.4(6)
C(4)	C(5)	C(8)	C(9)	166.3(5)	C(4)	C(5)	C(8)	C(13)	-12.8(8)
C(4)	C(6)	Ru(2)	C(7)	-114.3(5)	C(4)	C(6)	Ru(2)	C(24)	118.9(4)
C(4)	C(6)	Ru(2)	C(25)	154.0(5)	C(4)	C(6)	Ru(2)	C(26)	-173.8(5)
C(4)	C(6)	Ru(2)	C(27)	-175.3(5)	C(4)	C(6)	Ru(2)	C(28)	109.4(5)
C(4)	C(6)	C(7)	C(13)	-12.0(7)	C(5)	Ru(1)	Ru(2)	C(6)	-33.6(2)
C(5)	Ru(1)	Ru(2)	C(7)	0.3(2)	C(5)	Ru(1)	Ru(2)	C(24)	-137.1(3)
C(5)	Ru(1)	Ru(2)	C(25)	-102.1(5)	C(5)	Ru(1)	Ru(2)	C(26)	117(1)
C(5)	Ru(1)	Ru(2)	C(27)	143.7(4)	C(5)	Ru(1)	Ru(2)	C(28)	-179.0(3)
C(5)	Ru(1)	C(4)	C(6)	115.6(5)	C(5)	Ru(1)	C(14)	C(15)	24.7(5)
C(5)	Ru(1)	C(14)	C(18)	144.1(4)	C(5)	Ru(1)	C(14)	C(20)	-96.1(6)
C(5)	Ru(1)	C(15)	C(14)	-161.7(4)	C(5)	Ru(1)	C(15)	C(16)	82.7(4)
C(5)	Ru(1)	C(15)	C(21)	-37.3(6)	C(5)	Ru(1)	C(16)	C(15)	-100.1(4)
C(5)	Ru(1)	C(16)	C(17)	142.3(4)	C(5)	Ru(1)	C(16)	C(22)	21.7(6)
C(5)	Ru(1)	C(17)	C(16)	-44.9(4)	C(5)	Ru(1)	C(17)	C(18)	-160.4(3)
C(5)	Ru(1)	C(17)	C(23)	75.7(6)	C(5)	Ru(1)	C(18)	C(14)	-78.1(6)
C(5)	Ru(1)	C(18)	C(17)	40.5(7)	C(5)	Ru(1)	C(18)	C(19)	160.0(6)
C(5)	C(4)	Ru(1)	C(14)	72.5(7)	C(5)	C(4)	Ru(1)	C(15)	53.8(4)
C(5)	C(4)	Ru(1)	C(16)	83.6(4)	C(5)	C(4)	Ru(1)	C(17)	121.3(3)
C(5)	C(4)	Ru(1)	C(18)	137.6(3)	C(5)	C(4)	C(6)	C(7)	-0.2(7)

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Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(5)	C(8)	C(9)	C(10)	-179.1(6)	C(5)	C(8)	C(13)	C(7)	0.5(8)
C(5)	C(8)	C(13)	C(12)	179.8(5)	C(6)	Ru(2)	Ru(1)	C(14)	176.0(2)
C(6)	Ru(2)	Ru(1)	C(15)	-148.8(5)	C(6)	Ru(2)	Ru(1)	C(16)	60.2(4)
C(6)	Ru(2)	Ru(1)	C(17)	94.7(3)	C(6)	Ru(2)	Ru(1)	C(18)	136.7(2)
C(6)	Ru(2)	C(7)	C(13)	115.4(6)	C(6)	Ru(2)	C(24)	C(25)	72.0(6)
C(6)	Ru(2)	C(24)	C(28)	-171.5(4)	C(6)	Ru(2)	C(24)	C(29)	-47.7(10)
C(6)	Ru(2)	C(25)	C(24)	-116.5(5)	C(6)	Ru(2)	C(25)	C(26)	128.9(7)
C(6)	Ru(2)	C(25)	C(30)	10(1)	C(6)	Ru(2)	C(26)	C(25)	-61.0(7)
C(6)	Ru(2)	C(26)	C(27)	-178.8(5)	C(6)	Ru(2)	C(26)	C(31)	61(1)
C(6)	Ru(2)	C(27)	C(26)	2(1)	C(6)	Ru(2)	C(27)	C(28)	-115.1(8)
C(6)	Ru(2)	C(27)	C(32)	125(1)	C(6)	Ru(2)	C(28)	C(24)	14.9(7)
C(6)	Ru(2)	C(28)	C(27)	132.7(6)	C(6)	Ru(2)	C(28)	C(33)	-106.8(9)
C(6)	C(4)	Ru(1)	C(14)	-171.9(5)	C(6)	C(4)	Ru(1)	C(15)	169.4(3)
C(6)	C(4)	Ru(1)	C(16)	-160.8(4)	C(6)	C(4)	Ru(1)	C(17)	-123.1(4)
C(6)	C(4)	Ru(1)	C(18)	-106.8(4)	C(6)	C(4)	C(5)	C(8)	12.6(7)
C(6)	C(7)	Ru(2)	C(24)	73.3(4)	C(6)	C(7)	Ru(2)	C(25)	92.5(5)
C(6)	C(7)	Ru(2)	C(26)	130.0(5)	C(6)	C(7)	Ru(2)	C(27)	151.9(4)
C(6)	C(7)	Ru(2)	C(28)	118.8(6)	C(6)	C(7)	C(13)	C(8)	11.9(8)
C(6)	C(7)	C(13)	C(12)	-167.4(5)	C(7)	Ru(2)	Ru(1)	C(14)	-150.0(3)
C(7)	Ru(2)	Ru(1)	C(15)	-114.9(5)	C(7)	Ru(2)	Ru(1)	C(16)	94.2(4)
C(7)	Ru(2)	Ru(1)	C(17)	128.7(3)	C(7)	Ru(2)	Ru(1)	C(18)	170.6(2)
C(7)	Ru(2)	C(24)	C(25)	33.1(6)	C(7)	Ru(2)	C(24)	C(28)	149.6(4)
C(7)	Ru(2)	C(24)	C(29)	-86.6(10)	C(7)	Ru(2)	C(25)	C(24)	-154.6(5)
C(7)	Ru(2)	C(25)	C(26)	90.8(7)	C(7)	Ru(2)	C(25)	C(30)	-28(1)

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Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(7)	Ru(2)	C(26)	C(25)	-93.0(7)	C(7)	Ru(2)	C(26)	C(27)	149.1(6)
C(7)	Ru(2)	C(26)	C(31)	29(1)	C(7)	Ru(2)	C(27)	C(26)	-38.8(8)
C(7)	Ru(2)	C(27)	C(28)	-156.3(4)	C(7)	Ru(2)	C(27)	C(32)	84(1)
C(7)	Ru(2)	C(28)	C(24)	-67.7(8)	C(7)	Ru(2)	C(28)	C(27)	50.2(9)
C(7)	Ru(2)	C(28)	C(33)	170.7(8)	C(7)	C(6)	Ru(2)	C(24)	-126.8(4)
C(7)	C(6)	Ru(2)	C(25)	-91.7(5)	C(7)	C(6)	Ru(2)	C(26)	-59.4(5)
C(7)	C(6)	Ru(2)	C(27)	-61.0(7)	C(7)	C(6)	Ru(2)	C(28)	-136.3(4)
C(7)	C(13)	C(8)	C(9)	-178.6(5)	C(7)	C(13)	C(12)	C(11)	178.1(6)
C(8)	C(5)	Ru(1)	C(14)	93.4(5)	C(8)	C(5)	Ru(1)	C(15)	108.1(5)
C(8)	C(5)	Ru(1)	C(16)	145.9(5)	C(8)	C(5)	Ru(1)	C(17)	171.6(4)
C(8)	C(5)	Ru(1)	C(18)	144.4(5)	C(8)	C(9)	C(10)	C(11)	0(1)
C(8)	C(13)	C(12)	C(11)	-1.2(9)	C(9)	C(8)	C(13)	C(12)	0.7(8)
C(9)	C(10)	C(11)	C(12)	0(1)	C(10)	C(9)	C(8)	C(13)	-0.1(9)
C(10)	C(11)	C(12)	C(13)	1(1)	C(13)	C(7)	Ru(2)	C(24)	-171.3(4)
C(13)	C(7)	Ru(2)	C(25)	-152.1(6)	C(13)	C(7)	Ru(2)	C(26)	-114.5(6)
C(13)	C(7)	Ru(2)	C(27)	-92.7(5)	C(13)	C(7)	Ru(2)	C(28)	-125.8(7)
C(14)	Ru(1)	Ru(2)	C(24)	72.6(3)	C(14)	Ru(1)	Ru(2)	C(25)	107.5(5)
C(14)	Ru(1)	Ru(2)	C(26)	-32(1)	C(14)	Ru(1)	Ru(2)	C(27)	-6.7(4)
C(14)	Ru(1)	Ru(2)	C(28)	30.6(3)	C(14)	Ru(1)	C(15)	C(16)	-115.6(5)
C(14)	Ru(1)	C(15)	C(21)	124.4(8)	C(14)	Ru(1)	C(16)	C(15)	38.0(3)
C(14)	Ru(1)	C(16)	C(17)	-79.6(4)	C(14)	Ru(1)	C(16)	C(22)	159.7(7)
C(14)	Ru(1)	C(17)	C(16)	79.6(4)	C(14)	Ru(1)	C(17)	C(18)	-35.9(3)
C(14)	Ru(1)	C(17)	C(23)	-159.8(7)	C(14)	Ru(1)	C(18)	C(17)	118.6(5)
C(14)	Ru(1)	C(18)	C(19)	-121.9(8)	C(14)	C(15)	Ru(1)	C(16)	115.6(5)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(14)	C(15)	Ru(1)	C(17)	78.2(4)	C(14)	C(15)	Ru(1)	C(18)	35.7(3)
C(14)	C(15)	C(16)	C(17)	-2.1(6)	C(14)	C(15)	C(16)	C(22)	171.3(5)
C(14)	C(18)	Ru(1)	C(15)	-36.5(3)	C(14)	C(18)	Ru(1)	C(16)	-79.9(4)
C(14)	C(18)	Ru(1)	C(17)	-118.6(5)	C(14)	C(18)	C(17)	C(16)	-0.8(6)
C(14)	C(18)	C(17)	C(23)	-173.5(5)	C(15)	Ru(1)	Ru(2)	C(24)	107.7(6)
C(15)	Ru(1)	Ru(2)	C(25)	142.7(7)	C(15)	Ru(1)	Ru(2)	C(26)	2(1)
C(15)	Ru(1)	Ru(2)	C(27)	28.5(6)	C(15)	Ru(1)	Ru(2)	C(28)	65.8(6)
C(15)	Ru(1)	C(14)	C(18)	119.4(5)	C(15)	Ru(1)	C(14)	C(20)	-120.7(8)
C(15)	Ru(1)	C(16)	C(17)	-117.6(5)	C(15)	Ru(1)	C(16)	C(22)	121.8(8)
C(15)	Ru(1)	C(17)	C(16)	37.7(3)	C(15)	Ru(1)	C(17)	C(18)	-77.8(4)
C(15)	Ru(1)	C(17)	C(23)	158.3(7)	C(15)	Ru(1)	C(18)	C(17)	82.1(4)
C(15)	Ru(1)	C(18)	C(19)	-158.4(8)	C(15)	C(14)	Ru(1)	C(16)	-39.0(3)
C(15)	C(14)	Ru(1)	C(17)	-82.1(4)	C(15)	C(14)	Ru(1)	C(18)	-119.4(5)
C(15)	C(14)	C(18)	C(17)	-0.5(6)	C(15)	C(14)	C(18)	C(19)	-171.6(5)
C(15)	C(16)	Ru(1)	C(17)	117.6(5)	C(15)	C(16)	Ru(1)	C(18)	79.1(4)
C(15)	C(16)	C(17)	C(18)	1.8(6)	C(15)	C(16)	C(17)	C(23)	174.6(5)
C(16)	Ru(1)	Ru(2)	C(24)	-43.2(5)	C(16)	Ru(1)	Ru(2)	C(25)	-8.3(6)
C(16)	Ru(1)	Ru(2)	C(26)	-148(1)	C(16)	Ru(1)	Ru(2)	C(27)	-122.5(5)
C(16)	Ru(1)	Ru(2)	C(28)	-85.2(5)	C(16)	Ru(1)	C(14)	C(18)	80.4(4)
C(16)	Ru(1)	C(14)	C(20)	-159.8(7)	C(16)	Ru(1)	C(15)	C(21)	-120.0(7)
C(16)	Ru(1)	C(17)	C(18)	-115.5(5)	C(16)	Ru(1)	C(17)	C(23)	120.6(8)
C(16)	Ru(1)	C(18)	C(17)	38.7(3)	C(16)	Ru(1)	C(18)	C(19)	158.3(8)
C(16)	C(15)	Ru(1)	C(17)	-37.4(3)	C(16)	C(15)	Ru(1)	C(18)	-79.9(4)
C(16)	C(15)	C(14)	C(18)	1.6(6)	C(16)	C(15)	C(14)	C(20)	-175.0(5)

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Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(16)	C(17)	Ru(1)	C(18)	115.5(5)	C(16)	C(17)	C(18)	C(19)	170.3(5)
C(17)	Ru(1)	Ru(2)	C(24)	-8.7(3)	C(17)	Ru(1)	Ru(2)	C(25)	26.3(5)
C(17)	Ru(1)	Ru(2)	C(26)	-113(1)	C(17)	Ru(1)	Ru(2)	C(27)	-88.0(4)
C(17)	Ru(1)	Ru(2)	C(28)	-50.7(3)	C(17)	Ru(1)	C(14)	C(18)	37.3(3)
C(17)	Ru(1)	C(14)	C(20)	157.2(7)	C(17)	Ru(1)	C(15)	C(21)	-157.4(7)
C(17)	Ru(1)	C(16)	C(22)	-120.6(8)	C(17)	Ru(1)	C(18)	C(19)	119.5(8)
C(17)	C(16)	Ru(1)	C(18)	-38.5(3)	C(17)	C(16)	C(15)	C(21)	-173.7(5)
C(17)	C(18)	C(14)	C(20)	176.2(5)	C(18)	Ru(1)	Ru(2)	C(24)	33.2(3)
C(18)	Ru(1)	Ru(2)	C(25)	68.2(5)	C(18)	Ru(1)	Ru(2)	C(26)	-72(1)
C(18)	Ru(1)	Ru(2)	C(27)	-46.1(4)	C(18)	Ru(1)	Ru(2)	C(28)	-8.8(3)
C(18)	Ru(1)	C(14)	C(20)	119.9(8)	C(18)	Ru(1)	C(15)	C(21)	160.1(7)
C(18)	Ru(1)	C(16)	C(22)	-159.1(7)	C(18)	Ru(1)	C(17)	C(23)	-123.9(7)
C(18)	C(14)	C(15)	C(21)	173.1(5)	C(18)	C(17)	C(16)	C(22)	-171.7(5)
C(19)	C(18)	C(14)	C(20)	5.1(9)	C(19)	C(18)	C(17)	C(23)	-2.4(9)
C(20)	C(14)	C(15)	C(21)	-3.6(9)	C(21)	C(15)	C(16)	C(22)	-0.2(10)
C(22)	C(16)	C(17)	C(23)	1.1(9)	C(24)	Ru(2)	C(25)	C(26)	-114.6(8)
C(24)	Ru(2)	C(25)	C(30)	126(1)	C(24)	Ru(2)	C(26)	C(25)	38.6(5)
C(24)	Ru(2)	C(26)	C(27)	-79.3(6)	C(24)	Ru(2)	C(26)	C(31)	160(1)
C(24)	Ru(2)	C(27)	C(26)	79.8(6)	C(24)	Ru(2)	C(27)	C(28)	-37.6(4)
C(24)	Ru(2)	C(27)	C(32)	-157(1)	C(24)	Ru(2)	C(28)	C(27)	117.9(6)
C(24)	Ru(2)	C(28)	C(33)	-121(1)	C(24)	C(25)	Ru(2)	C(26)	114.6(8)
C(24)	C(25)	Ru(2)	C(27)	78.3(5)	C(24)	C(25)	Ru(2)	C(28)	37.8(4)
C(24)	C(25)	C(26)	C(27)	-0.2(10)	C(24)	C(25)	C(26)	C(31)	174.9(8)
C(24)	C(28)	Ru(2)	C(25)	-37.6(5)	C(24)	C(28)	Ru(2)	C(26)	-80.6(5)

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Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(24)	C(28)	Ru(2)	C(27)	-117.9(6)	C(24)	C(28)	C(27)	C(26)	0.6(8)
C(24)	C(28)	C(27)	C(32)	-176.6(7)	C(25)	Ru(2)	C(24)	C(28)	116.6(6)
C(25)	Ru(2)	C(24)	C(29)	-119(1)	C(25)	Ru(2)	C(26)	C(27)	-117.9(8)
C(25)	Ru(2)	C(26)	C(31)	121(2)	C(25)	Ru(2)	C(27)	C(26)	37.5(6)
C(25)	Ru(2)	C(27)	C(28)	-80.0(5)	C(25)	Ru(2)	C(27)	C(32)	160(1)
C(25)	Ru(2)	C(28)	C(27)	80.2(5)	C(25)	Ru(2)	C(28)	C(33)	-159(1)
C(25)	C(24)	Ru(2)	C(26)	-39.1(5)	C(25)	C(24)	Ru(2)	C(27)	-80.7(5)
C(25)	C(24)	Ru(2)	C(28)	-116.6(6)	C(25)	C(24)	C(28)	C(27)	-0.7(8)
C(25)	C(24)	C(28)	C(33)	-172.0(6)	C(25)	C(26)	Ru(2)	C(27)	117.9(8)
C(25)	C(26)	Ru(2)	C(28)	81.5(6)	C(25)	C(26)	C(27)	C(28)	-0.2(10)
C(25)	C(26)	C(27)	C(32)	176.9(7)	C(26)	Ru(2)	C(24)	C(28)	77.5(5)
C(26)	Ru(2)	C(24)	C(29)	-158(1)	C(26)	Ru(2)	C(25)	C(30)	-118(1)
C(26)	Ru(2)	C(27)	C(28)	-117.5(8)	C(26)	Ru(2)	C(27)	C(32)	122(1)
C(26)	Ru(2)	C(28)	C(27)	37.2(5)	C(26)	Ru(2)	C(28)	C(33)	157(1)
C(26)	C(25)	Ru(2)	C(27)	-36.4(5)	C(26)	C(25)	Ru(2)	C(28)	-76.8(6)
C(26)	C(25)	C(24)	C(28)	0.5(8)	C(26)	C(25)	C(24)	C(29)	-173.7(7)
C(26)	C(27)	Ru(2)	C(28)	117.5(8)	C(26)	C(27)	C(28)	C(33)	172.1(7)
C(27)	Ru(2)	C(24)	C(28)	35.9(4)	C(27)	Ru(2)	C(24)	C(29)	159(1)
C(27)	Ru(2)	C(25)	C(30)	-155(1)	C(27)	Ru(2)	C(26)	C(31)	-120(2)
C(27)	Ru(2)	C(28)	C(33)	120(1)	C(27)	C(26)	Ru(2)	C(28)	-36.4(5)
C(27)	C(26)	C(25)	C(30)	-173.5(7)	C(27)	C(28)	C(24)	C(29)	173.4(7)
C(28)	Ru(2)	C(24)	C(29)	123(1)	C(28)	Ru(2)	C(25)	C(30)	164(1)
C(28)	Ru(2)	C(26)	C(31)	-156(1)	C(28)	Ru(2)	C(27)	C(32)	-119(1)
C(28)	C(24)	C(25)	C(30)	173.3(8)	C(28)	C(27)	C(26)	C(31)	-175.5(7)

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Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(29)	C(24)	C(25)	C(30)	-1(1)	C(29)	C(24)	C(28)	C(33)	2(1)
C(30)	C(25)	C(26)	C(31)	1(1)	C(31)	C(26)	C(27)	C(32)	1(1)
C(32)	C(27)	C(28)	C(33)	-5(1)					

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Table 6. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
C(1)	H(14)	3.26	56602	C(2)	H(22)	3.42	66602
C(2)	H(24)	3.48	66602	C(2)	H(23)	3.55	66602
C(2)	H(14)	3.57	56602	C(3)	H(22)	3.24	66602
C(3)	H(42)	3.35	56502	C(3)	H(13)	3.48	55401
C(4)	H(16)	3.39	55601	C(4)	H(17)	3.54	55601
C(5)	H(20)	3.55	55601	C(6)	H(44)	3.17	55601
C(6)	H(45)	3.30	55601	C(6)	H(30)	3.48	65602
C(6)	C(33)	3.541(9)	55601	C(7)	H(44)	3.16	55601
C(7)	H(45)	3.34	55601	C(8)	H(21)	3.43	55601
C(9)	H(21)	3.22	55601	C(9)	H(5)	3.52	55601
C(9)	H(20)	3.53	55601	C(10)	H(5)	2.86	55601
C(10)	H(23)	3.03	66602	C(10)	H(19)	3.55	66602
C(11)	H(5)	3.08	55601	C(11)	H(14)	3.38	56602
C(11)	H(6)	3.53	56602	C(11)	H(15)	3.58	56602
C(12)	H(14)	3.20	56602	C(12)	H(40)	3.50	55601
C(13)	H(45)	3.54	55601	C(14)	H(38)	3.06	65501
C(14)	H(39)	3.24	65501	C(14)	C(31)	3.53(1)	65501
C(15)	H(39)	3.05	65501	C(15)	H(38)	3.47	65501
C(15)	C(31)	3.57(1)	65501	C(16)	H(39)	3.10	65501
C(17)	H(39)	3.37	65501	C(18)	H(38)	3.36	65501
C(18)	H(39)	3.44	65501	C(19)	H(8)	3.26	55401
C(19)	H(29)	3.39	65502	C(20)	H(13)	3.22	66602
C(20)	H(38)	3.25	65501	C(20)	H(12)	3.26	55401
C(20)	H(9)	3.42	55401	C(21)	H(4)	3.05	66602

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Table 6. Non-bonded Contacts out to 3.60 Å (continued)

atom	atom	distance	ADC	atom	atom	distancei	ADC
C(21)	H(13)	3.24	66602	C(21)	H(7)	3.30	66602
C(21)	H(39)	3.56	65501	C(22)	H(41)	3.27	65601
C(22)	H(33)	3.31	65602	C(23)	H(10)	3.12	65602
C(23)	H(8)	3.18	65602	C(23)	H(35)	3.53	65501
C(23)	H(43)	3.59	65502	C(24)	H(31)	3.01	2
C(25)	H(31)	3.02	2	C(26)	H(31)	3.26	2
C(27)	H(31)	3.40	2	C(28)	H(31)	3.26	2
C(29)	H(25)	3.39	65602	C(29)	H(26)	3.49	65602
C(29)	H(35)	3.50	2	C(29)	H(31)	3.54	2
C(30)	H(36)	3.33	55602	C(30)	H(30)	3.54	45501
C(30)	H(34)	3.55	55602	C(30)	H(31)	3.57	2
C(31)	H(23)	3.40	45501	C(31)	H(20)	3.51	45501
C(32)	H(27)	3.38	45401	C(32)	H(6)	3.42	56502
C(33)	H(10)	3.12	55401	C(33)	H(11)	3.43	55401
C(33)	H(35)	3.51	2	H(2)	H(14)	2.45	56602
H(3)	H(24)	3.41	66602	H(4)	H(23)	2.75	66602
H(4)	H(24)	2.91	66602	H(4)	H(22)	2.95	66602
H(4)	H(14)	3.36	56602	H(5)	H(13)	2.88	55401
H(5)	H(14)	3.23	55401	H(6)	H(14)	2.86	56602
H(6)	H(42)	2.94	56502	H(6)	H(40)	3.31	56502
H(6)	H(6)	3.40	56502	H(6)	H(15)	3.44	56602
H(6)	H(22)	3.44	66602	H(6)	H(41)	3.51	56502
H(7)	H(22)	2.56	66602	H(7)	H(42)	3.01	56502
H(7)	H(12)	3.18	66602	H(7)	H(13)	3.27	55401