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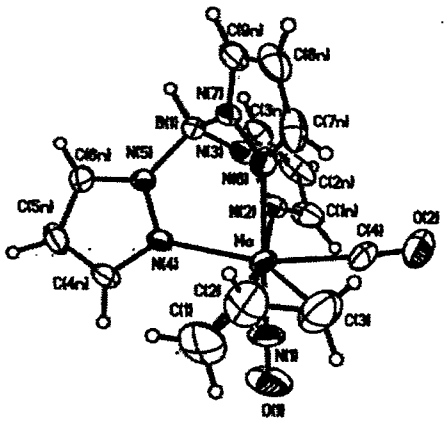

**Figure 1. ORTEP of *exo*-[TpMo(CO)(NO)($\eta^3$-$C_3H_5$)][(3,5-$(CF_3)_2C_6H_3)_4$B], 9a.**

**Table S-I. Bond lengths (Å) and angles (deg) for [TpMo(CO)(NO)($\eta^3$-$C_3H_5$)][(3,5-$(CF_3)_2C_6H_3)_4B$] 9a.**

| | | | |
|---|---|---|---|
| Mo-N(1) | 1.833(9) | C(11)-C(61) | 1.419(9) |
| Mo-C(4) | 2.011(10) | C(21)-C(31) | 1.39(2) |
| Mo-N(2) | 2.175(9) | C(31)-C(41) | 1.411(10) |
| Mo-N(6) | 2.198(7) | C(31)-C(71) | 1.46(2) |
| Mo-N(4) | 2.196(6) | C(41)-C(51) | 1.331(14) |
| Mo-C(3) | 2.34(2) | C(51)-C(61) | 1.419(14) |
| Mo-C(2) | 2.35(2) | C(51)-C(81) | 1.506(11) |
| Mo-C(1) | 2.47(2) | C(71)-F(2) | 1.297(10) |
| O(1)-N(1) | 1.143(11) | C(71)-F(1) | 1.32(2) |
| O(2)-C(4) | 1.161(11) | C(71)-F(3) | 1.381(12) |
| N(2)-C(1N) | 1.314(14) | C(81)-F(4) | 1.210(11) |
| N(2)-N(3) | 1.376(9) | C(81)-F(6) | 1.308(14) |
| N(3)-C(3N) | 1.349(13) | C(81)-F(5) | 1.35(2) |
| N(3)-B(1) | 1.507(14) | C(12)-C(22) | 1.396(10) |
| N(4)-C(4N) | 1.347(9) | C(12)-C(62) | 1.385(11) |
| N(4)-N(5) | 1.355(8) | C(22)-C(32) | 1.40(2) |
| N(5)-C(6N) | 1.336(9) | C(32)-C(42) | 1.37(2) |
| N(5)-B(1) | 1.551(10) | C(32)-C(72A) | 1.40(2) |
| N(6)-N(7) | 1.352(10) | C(42)-C(52) | 1.379(11) |
| N(6)-C(7N) | 1.376(13) | C(52)-C(62) | 1.394(12) |
| N(7)-C(9N) | 1.358(12) | C(52)-C(82) | 1.469(14) |
| N(7)-B(1) | 1.540(14) | C(72)-F(7) | 0.57(3) |
| C(1N)-C(2N) | 1.39(2) | C(72)-F(7A) | 1.04(3) |
| C(2N)-C(3N) | 1.34(2) | C(72)-C(72A) | 1.14(4) |
| C(4N)-C(5N) | 1.366(13) | C(72)-F(9) | 1.42(3) |
| C(5N)-C(6N) | 1.382(11) | C(72)-F(7AA) | 1.76(4) |
| C(7N)-C(8N) | 1.34(2) | C(72A)-F(9) | 0.94(2) |
| C(8N)-C(9N) | 1.34(2) | C(72A)-F(7A) | 1.09(2) |
| C(1)-C(2) | 1.32(2) | C(72A)-F(9A) | 1.43(3) |
| C(2)-C(3) | 1.43(2) | C(72A)-F(8) | 1.55(3) |
| B(2)-C(12) | 1.629(12) | C(72A)-F(7) | 1.62(3) |
| B(2)-C(11) | 1.671(13) | C(72A)-F(7AA) | 1.71(3) |
| B(2)-C(14) | 1.651(9) | C(82)-F(10) | 1.321(10) |
| B(2)-C(13) | 1.655(10) | | |
| C(11)-C(21) | 1.357(13) | | |

**Table S-I. Bond lengths (Å) and angles (deg) for [TpMo(CO)(NO)($\eta^3$-$C_3H_5$)][(3,5-$(CF_3)_2C_6H_3)_4$B] 9a (cont.).**

| | | | |
|---|---|---|---|
| C(82)-F(12) | 1.344(12) | N(1)-Mo-N(4) | 95.3(3) |
| C(82)-F(11) | 1.354(10) | C(4)-Mo-N(4) | 160.2(4) |
| C(13)-C(23) | 1.398(9) | N(2)-Mo-N(4) | 80.5(3) |
| C(13)-C(63) | 1.389(10) | N(6)-Mo-N(4) | 85.1(2) |
| C(23)-C(33) | 1.398(10) | N(1)-Mo-C(3) | 94.0(6) |
| C(33)-C(43) | 1.386(10) | C(4)-Mo-C(3) | 66.1(6) |
| C(33)-C(73) | 1.495(11) | N(2)-Mo-C(3) | 146.0(4) |
| C(43)-C(53) | 1.371(11) | N(6)-Mo-C(3) | 90.4(5) |
| C(53)-C(63) | 1.407(10) | N(4)-Mo-C(3) | 132.2(5) |
| C(53)-C(83) | 1.503(11) | N(1)-Mo-C(2) | 102.5(6) |
| C(73)-F(14) | 1.30(2) | C(4)-Mo-C(2) | 100.6(6) |
| C(73)-F(15) | 1.299(9) | N(2)-Mo-C(2) | 166.6(5) |
| C(73)-F(13) | 1.344(13) | N(6)-Mo-C(2) | 83.7(5) |
| C(83)-F(18) | 1.256(13) | N(4)-Mo-C(2) | 96.9(4) |
| C(83)-F(17) | 1.287(11) | C(3)-Mo-C(2) | 35.5(5) |
| C(83)-F(16) | 1.34(2) | N(1)-Mo-C(1) | 79.1(6) |
| C(14)-C(64) | 1.399(10) | C(4)-Mo-C(1) | 121.7(5) |
| C(14)-C(24) | 1.415(10) | N(2)-Mo-C(1) | 155.4(4) |
| C(24)-C(34) | 1.384(10) | N(6)-Mo-C(1) | 107.1(5) |
| C(34)-C(44) | 1.369(11) | N(4)-Mo-C(1) | 78.1(4) |
| C(34)-C(74) | 1.515(13) | C(3)-Mo-C(1) | 58.0(5) |
| C(44)-C(54) | 1.378(10) | C(2)-Mo-C(1) | 31.7(5) |
| C(54)-C(64) | 1.382(9) | O(1)-N(1)-Mo | 177.8(12) |
| C(54)-C(84) | 1.516(12) | O(2)-C(4)-Mo | 174.4(9) |
| C(74)-F(20) | 1.321(13) | C(1N)-N(2)-N(3) | 106.7(9) |
| C(74)-F(19) | 1.330(12) | C(1N)-N(2)-Mo | 133.0(7) |
| C(74)-F(21) | 1.339(11) | N(3)-N(2)-Mo | 120.3(7) |
| C(84)-F(24) | 1.270(10) | C(3N)-N(3)-N(2) | 108.3(9) |
| C(84)-F(22) | 1.297(11) | C(3N)-N(3)-B(1) | 130.7(8) |
| C(84)-F(23) | 1.348(11) | N(2)-N(3)-B(1) | 120.9(8) |
| N(1)-Mo-C(4) | 89.8(4) | C(4N)-N(4)-N(5) | 105.5(6) |
| N(1)-Mo-N(2) | 90.8(4) | C(4N)-N(4)-Mo | 134.8(5) |
| C(4)-Mo-N(2) | 80.3(4) | C(21)-C(11)-B(2) | 120.6(6) |
| N(1)-Mo-N(6) | 173.6(4) | C(61)-C(11)-B(2) | 123.0(9) |
| C(4)-Mo-N(6) | 87.8(4) | C(11)-C(21)-C(31) | 124.8(7) |
| N(2)-Mo-N(6) | 83.0(3) | C(21)-C(31)-C(41) | 117.3(11) |

**Table S-I. Bond lengths (Å) and angles (deg) for [TpMo(CO)(NO)($\eta^3$-$C_3H_5$)][(3,5-$(CF_3)_2C_6H_3)_4$B] 9a (cont.).**

| | | | |
|---|---|---|---|
| N(5)-N(4)-Mo | 119.7(4) | C(51)-C(41)-C(31) | 120.2(9) |
| C(6N)-N(5)-N(4) | 110.4(5) | C(41)-C(51)-C(61) | 121.7(7) |
| C(6N)-N(5)-B(1) | 128.0(6) | C(41)-C(51)-C(81) | 121.8(9) |
| N(4)-N(5)-B(1) | 121.3(5) | C(61)-C(51)-C(81) | 116.5(10) |
| N(7)-N(6)-C(7N) | 105.0(7) | C(11)-C(61)-C(51) | 119.6(9) |
| N(7)-N(6)-Mo | 119.5(6) | F(2)-C(71)-F(1) | 110.9(13) |
| C(7N)-N(6)-Mo | 135.5(7) | F(2)-C(71)-F(3) | 100.6(9) |
| N(6)-N(7)-C(9N) | 108.2(8) | F(1)-C(71)-F(3) | 101.8(10) |
| N(6)-N(7)-B(1) | 121.7(6) | F(2)-C(71)-C(31) | 115.7(9) |
| C(9N)-N(7)-B(1) | 130.1(8) | F(1)-C(71)-C(31) | 114.3(10) |
| N(3)-B(1)-N(7) | 107.6(6) | F(3)-C(71)-C(31) | 111.8(10) |
| N(3)-B(1)-N(5) | 107.7(6) | F(4)-C(81)-F(6) | 108.0(12) |
| N(7)-B(1)-N(5) | 108.3(8) | F(4)-C(81)-F(5) | 108.7(10) |
| N(2)-C(1N)-C(2N) | 110.3(10) | F(6)-C(81)-F(5) | 98.6(8) |
| C(3N)-C(2N)-C(1N) | 105.6(11) | F(4)-C(81)-C(51) | 115.2(8) |
| C(2N)-C(3N)-N(3) | 109.1(9) | F(6)-C(81)-C(51) | 114.6(8) |
| N(4)-C(4N)-C(5N) | 111.0(7) | F(5)-C(81)-C(51) | 110.4(11) |
| C(4N)-C(5N)-C(6N) | 105.1(6) | C(22)-C(12)-C(62) | 116.1(8) |
| N(5)-C(6N)-C(5N) | 108.0(7) | C(22)-C(12)-B(2) | 118.8(8) |
| C(8N)-C(7N)-N(6) | 111.3(10) | C(62)-C(12)-B(2) | 124.8(6) |
| C(9N)-C(8N)-C(7N) | 105.3(9) | C(32)-C(22)-C(12) | 122.1(10) |
| C(8N)-C(9N)-N(7) | 110.3(9) | C(22)-C(32)-C(42) | 119.8(9) |
| C(2)-C(1)-Mo | 68.8(8) | C(22)-C(32)-C(72A) | 117(2) |
| C(1)-C(2)-C(3) | 117(2) | C(42)-C(32)-C(72A) | 124(2) |
| C(1)-C(2)-Mo | 79.6(10) | C(32)-C(42)-C(52) | 119.6(10) |
| C(3)-C(2)-Mo | 72.1(10) | C(62)-C(52)-C(42) | 119.9(9) |
| C(2)-C(3)-Mo | 72.5(9) | C(62)-C(52)-C(82) | 120.7(7) |
| C(12)-B(2)-C(11) | 114.2(5) | F(9)-C(72A)-F(7AA) | 125(2) |
| C(12)-B(2)-C(14) | 105.0(6) | F(7A)-C(72A)-F(7AA) | 25.7(13) |
| C(11)-B(2)-C(14) | 108.2(7) | C(72)-C(72A)-F(7AA) | 73(2) |
| C(12)-B(2)-C(13) | 113.0(7) | C(32)-C(72A)-F(7AA) | 104(2) |
| C(11)-B(2)-C(13) | 104.1(6) | F(9A)-C(72A)-F(7AA) | 84(2) |
| C(14)-B(2)-C(13) | 112.3(5) | F(8)-C(72A)-F(7AA) | 143(2) |
| C(21)-C(11)-C(61) | 116.4(8) | F(7)-C(72A)-F(7AA) | 74.3(12) |
| C(21)-C(31)-C(71) | 120.7(7) | C(72)-F(7)-C(72A) | 27(3) |
| C(41)-C(31)-C(71) | 121.9(10) | C(72)-F(7A)-C(72A) | 65(2) |

**Table S-I. Bond lengths (Å) and angles (deg) for [TpMo(CO)(NO)($\eta^3$-$C_3H_5$)][(3,5-$(CF_3)_2C_6H_3)_4$B] 9a (cont.).**

| | | | |
|---|---|---|---|
| C(42)-C(52)-C(82) | 119.3(9) | F(10)-C(82)-F(11) | 103.2(6) |
| C(52)-C(62)-C(12) | 122.5(6) | F(12)-C(82)-F(11) | 102.7(9) |
| F(7)-C(72)-F(7A) | 129(5) | F(10)-C(82)-C(52) | 114.8(9) |
| F(7)-C(72)-C(72A) | 140(4) | F(12)-C(82)-C(52) | 113.7(7) |
| F(7A)-C(72)-C(72A) | 60(3) | F(11)-C(82)-C(52) | 112.7(6) |
| F(7)-C(72)-F(9) | 152(5) | C(23)-C(13)-C(63) | 116.4(6) |
| F(7A)-C(72)-F(9) | 78(3) | C(23)-C(13)-B(2) | 118.9(5) |
| C(72A)-C(72)-F(9) | 41.3(14) | C(63)-C(13)-B(2) | 124.6(6) |
| F(7)-C(72)-F(7AA) | 109(4) | C(13)-C(23)-C(33) | 121.9(6) |
| F(7A)-C(72)-F(7AA) | 21.1(13) | C(43)-C(33)-C(23) | 120.4(7) |
| C(72A)-C(72)-F(7AA) | 69(3) | C(43)-C(33)-C(73) | 119.5(6) |
| F(9)-C(72)-F(7AA) | 96(3) | C(23)-C(33)-C(73) | 120.0(6) |
| F(9)-C(72A)-F(7A) | 102(2) | C(33)-C(43)-C(53) | 118.8(7) |
| F(9)-C(72A)-C(72) | 86(3) | C(63)-C(53)-C(43) | 120.6(7) |
| F(7A)-C(72A)-C(72) | 55(2) | C(63)-C(53)-C(83) | 118.5(7) |
| F(9)-C(72A)-C(32) | 130(2) | C(43)-C(53)-C(83) | 120.9(7) |
| F(7A)-C(72A)-C(32) | 129(2) | C(53)-C(63)-C(13) | 121.9(7) |
| C(72)-C(72A)-C(32) | 124(2) | F(14)-C(73)-F(15) | 107.3(9) |
| F(9)-C(72A)-F(9A) | 68(2) | F(14)-C(73)-F(13) | 101.2(8) |
| F(7A)-C(72A)-F(9A) | 83(2) | F(10)-C(82)-F(12) | 108.7(8) |
| C(72)-C(72A)-F(9A) | 124(2) | F(10)-C(82)-F(11) | 103.2(6) |
| C(32)-C(72A)-F(9A) | 110(2) | F(12)-C(82)-F(11) | 102.7(9) |
| F(9)-C(72A)-F(8) | 18.8(14) | F(10)-C(82)-C(52) | 114.8(9) |
| F(7A)-C(72A)-F(8) | 119(2) | F(12)-C(82)-C(52) | 113.7(7) |
| C(72)-C(72A)-F(8) | 90(2) | F(11)-C(82)-C(52) | 112.7(6) |
| C(32)-C(72A)-F(8) | 112.6(14) | C(23)-C(13)-C(63) | 116.4(6) |
| F(9A)-C(72A)-F(8) | 79.4(13) | C(23)-C(13)-B(2) | 118.9(5) |
| F(9)-C(72A)-F(7) | 95(2) | C(63)-C(13)-B(2) | 124.6(6) |
| F(7A)-C(72A)-F(7) | 62(2) | C(13)-C(23)-C(33) | 121.9(6) |
| C(72)-C(72A)-F(7) | 13(2) | C(43)-C(33)-C(23) | 120.4(7) |
| C(32)-C(72A)-F(7) | 111(2) | C(43)-C(33)-C(73) | 119.5(6) |
| F(7A)-C(72A)-F(7AA) | 25.7(13) | C(23)-C(33)-C(73) | 120.0(6) |
| C(72)-C(72A)-F(7AA) | 73(2) | C(33)-C(43)-C(53) | 118.8(7) |
| C(72A)-F(7AA)-C(72) | 38.5(13) | C(63)-C(53)-C(43) | 120.6(7) |
| C(72A)-F(9)-C(72) | 53(2) | C(63)-C(53)-C(83) | 118.5(7) |
| F(10)-C(82)-F(12) | 108.7(8) | C(43)-C(53)-C(83) | 120.9(7) |

**Table S-I. Bond lengths (Å) and angles (deg) for [TpMo(CO)(NO)($\eta^3$-$C_3H_5$)][(3,5-$(CF_3)_2C_6H_3)_4$B] 9a (cont.).**

| | | | |
|---|---|---|---|
| C(53)-C(63)-C(13) | 121.9(7) | C(44)-C(34)-C(74) | 118.9(7) |
| F(14)-C(73)-F(15) | 107.3(9) | C(54)-C(44)-C(34) | 118.7(6) |
| F(14)-C(73)-F(13) | 101.2(8) | C(44)-C(54)-C(64) | 120.7(7) |
| F(15)-C(73)-F(13) | 107.2(9) | C(44)-C(54)-C(84) | 118.2(6) |
| F(14)-C(73)-C(33) | 113.3(8) | C(64)-C(54)-C(84) | 121.1(6) |
| F(15)-C(73)-C(33) | 115.3(6) | C(14)-C(64)-C(54) | 122.2(6) |
| F(13)-C(73)-C(33) | 111.6(9) | F(20)-C(74)-F(19) | 109.5(8) |
| F(18)-C(83)-F(17) | 110.5(11) | F(20)-C(74)-F(21) | 106.3(10) |
| F(18)-C(83)-F(16) | 104.3(9) | F(19)-C(74)-F(21) | 104.8(7) |
| F(17)-C(83)-F(16) | 102.2(9) | F(20)-C(74)-C(34) | 113.3(7) |
| F(18)-C(83)-C(53) | 115.4(8) | F(19)-C(74)-C(34) | 110.8(10) |
| F(17)-C(83)-C(53) | 113.7(8) | F(21)-C(74)-C(34) | 111.7(7) |
| F(16)-C(83)-C(53) | 109.4(11) | F(24)-C(84)-F(22) | 109.0(11) |
| C(64)-C(14)-C(24) | 115.6(6) | F(24)-C(84)-F(23) | 105.0(6) |
| C(64)-C(14)-B(2) | 123.4(6) | F(22)-C(84)-F(23) | 104.8(7) |
| C(24)-C(14)-B(2) | 120.5(7) | F(24)-C(84)-C(54) | 113.8(6) |
| C(34)-C(24)-C(14) | 121.4(8) | F(22)-C(84)-C(54) | 113.8(6) |
| C(24)-C(34)-C(44) | 121.3(7) | F(23)-C(84)-C(54) | 109.7(9) |
| C(24)-C(34)-C(74) | 119.8(8) | | |

**Table S-II. Hydrogen atom coordinates ($x10^4$) and temperature factors ($Å^2$ $x10^3$) for $[TpMo(CO)(NO)(\eta^3\text{-}C_3H_5)][(3,5\text{-}(CF_3)_2C_6H_3)_4B]$ 9a.**

| *atom* | *x* | *y* | *z* | $U_{11}$ |
|---|---|---|---|---|
| H(2B) | 4214(3) | 8054(7) | 2327(5) | 50 |
| H(1NA) | 4723(3) | 4499(9) | 1639(5) | 50 |
| H(2NA) | 5158(3) | 5991(11) | 1374(5) | 50 |
| H(3NA) | 4859(3) | 7547(8) | 1842(5) | 50 |
| H(4NA) | 3161(3) | 5673(7) | 1417(5) | 50 |
| H(5NA) | 3073(3) | 7517(7) | 1153(5) | 50 |
| H(6NA) | 3606(3) | 8475(6) | 1679(4) | 50 |
| H(7NA) | 3908(4) | 5163(9) | 3985(4) | 50 |
| H(8NA) | 4044(4) | 6856(10) | 4453(5) | 50 |
| H(9NA) | 4161(3) | 8056(8) | 3609(5) | 50 |
| H(1B) | 3145(5) | 3632(13) | 2240(9) | 50 |
| H(1A) | 3025(5) | 4817(13) | 2317(9) | 50 |
| H(2A) | 3256(4) | 4686(11) | 3277(9) | 50 |
| H(3A) | 3762(5) | 3527(9) | 3454(9) | 50 |
| H(3B) | 3613(5) | 2879(9) | 2882(9) | 50 |
| H(21A) | 3034(3) | 10271(5) | 883(4) | 50 |
| H(41A) | 3366(3) | 10474(6) | 2643(4) | 50 |
| H(61A) | 4140(3) | 10625(5) | 1293(3) | 50 |
| H(22) | 4116(3) | 12055(6) | 626(4) | 50 |
| H(42) | 5067(3) | 11889(6) | -389(4) | 50 |
| H(62) | 4229(2) | 9801(5) | -594(3) | 50 |
| H(23) | 4047(2) | 8686(5) | 341(3) | 50 |
| H(43) | 3347(3) | 6579(6) | -425(4) | 50 |
| H(63) | 3068(2) | 9600(5) | -408(4) | 50 |
| H(24) | 3438(2) | 10836(5) | -952(4) | 50 |
| H(44) | 2846(2) | 13491(5) | -863(4) | 50 |
| H(64) | 3299(2) | 12254(5) | 655(3) | 50 |

**Table S-III. Temperature factors ($Å^2$ x$10^3$) for [TpMo(CO)(NO)($\eta^3$-$C_3H_5$)][(3,5-$(CF_3)_2C_6H_3)_4B$] 9a (cont.).**

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| C(82) | 39(6) | 57(5) | 53(7) | -9(4) | 1(7) | 11(4) |
| F(10) | 110(6) | 52(3) | 107(5) | -23(3) | 57(6) | 10(3) |
| F(11) | 57(4) | 93(4) | 48(3) | -12(3) | 5(4) | 15(3) |
| F(12) | 33(4) | 143(5) | 72(5) | -29(4) | 4(5) | 23(4) |
| C(73) | 54(7) | 38(5) | 75(7) | -14(5) | 8(8) | 1(4) |
| F(13) | 69(5) | 52(4) | 304(14) | 65(5) | 32(9) | 8(3) |
| F(14) | 116(7) | 141(6) | 104(6) | -62(5) | -28(7) | 79(6) |
| F(15) | 84(5) | 55(3) | 91(4) | -11(3) | -30(5) | 26(3) |
| C(83) | 70(9) | 60(6) | 86(8) | -13(5) | -33(9) | -9(6) |
| F(16) | 113(8) | 239(10) | 88(6) | 9(6) | -52(7) | -58(7) |
| F(17) | 118(6) | 93(5) | 195(9) | 0(5) | -90(7) | -50(4) |
| F(18) | 58(4) | 137(6) | 250(12) | -96(7) | -73(7) | 20(4) |
| C(74) | 74(9) | 66(6) | 53(7) | 2(5) | -22(8) | 3(6) |
| F(19) | 80(5) | 181(6) | 43(4) | -2(4) | -15(5) | -31(5) |
| F(20) | 130(7) | 74(4) | 41(3) | -9(3) | -2(5) | 21(4) |
| F(21) | 88(5) | 82(4) | 48(3) | 22(3) | 10(4) | 15(3) |
| C(84) | 58(7) | 37(4) | 55(6) | 3(4) | -21(7) | 0(4) |
| F(22) | 168(10) | 81(4) | 66(4) | -15(3) | 4(6) | 65(5) |
| F(23) | 88(6) | 53(3) | 166(8) | -35(4) | 52(7) | -24(4) |
| F(24) | 65(5) | 85(4) | 124(6) | -43(4) | -26(6) | 35(3) |

The anisotropic temperature factor exponent takes the form: $-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23})$.

**Table 5. Atom coordinates ($x10^4$) and Equivalent Isotropic Displacement Parameters ($Å \times 10^3$) for $[TpMo(CO)(NO)(\eta^3\text{-}C_3H_5)][(3,5\text{-}(CF_3)_2C_6H_3)_4B]$, 9a.**

| *Atom* | *x* | *y* | *z* | *U(eq)* |
|---|---|---|---|---|
| Mo | 3883(1) | 4793(1) | 2385(1) | 52(1) |
| O(1) | 3837(3) | 3397(7) | 1320(6) | 148(6) |
| N(1) | 3857(3) | 3948(6) | 1722(5) | 93(4) |
| O(2) | 4544(3) | 3439(6) | 2937(6) | 137(5) |
| C(4) | 4289(4) | 3894(6) | 2742(6) | 86(5) |
| N(2) | 4382(2) | 5550(5) | 2019(4) | 54(3) |
| N(3) | 4430(2) | 6591(5) | 2090(3) | 47(2) |
| N(4) | 3611(2) | 6111(4) | 1942(3) | 43(2) |
| N(5) | 3755(2) | 7066(4) | 2022(3) | 42(2) |
| N(6) | 3976(2) | 5855(5) | 3145(3) | 55(3) |
| N(7) | 4069(2) | 6843(5) | 3031(3) | 48(3) |
| B(1) | 4127(3) | 7240(7) | 2380(5) | 46(3) |
| C(1N) | 4681(3) | 5211(9) | 1730(5) | 71(4) |
| C(2N) | 4926(3) | 6019(11) | 1600(5) | 75(4) |
| C(3N) | 4762(3) | 6858(8) | 1835(5) | 58(3) |
| C(4N) | 3314(3) | 6229(7) | 1564(5) | 65(3) |
| C(5N) | 3270(3) | 7235(7) | 1404(5) | 67(4) |
| C(6N) | 3556(3) | 7751(6) | 1702(4) | 52(3) |
| C(7N) | 3963(4) | 5783(9) | 3767(4) | 73(4) |
| C(8N) | 4038(4) | 6692(10) | 4029(5) | 95(5) |
| C(9N) | 4103(3) | 7340(8) | 3569(5) | 74(4) |
| C(1) | 3207(5) | 4291(13) | 2408(9) | 122(7) |
| C(2) | 3357(4) | 4271(11) | 2957(9) | 106(6) |
| C(3) | 3654(5) | 3546(9) | 3054(9) | 121(7) |
| B(2) | 3678(3) | 10508(6) | 224(4) | 31(3) |
| C(11) | 3591(2) | 10486(5) | 968(3) | 33(2) |
| C(21) | 3233(3) | 10354(5) | 1177(4) | 40(2) |
| C(31) | 3132(3) | 10335(6) | 1788(4) | 50(2) |
| C(41) | 3424(3) | 10456(6) | 2218(4) | 50(2) |
| C(51) | 3782(3) | 10553(6) | 2036(4) | 43(2) |
| C(61) | 3880(3) | 10564(5) | 1413(3) | 39(2) |
| C(71) | 2740(4) | 10154(8) | 1969(5) | 67(4) |

| Atom | x | y | z | U(eq) |
|---|---|---|---|---|
| F(1) | 2657(3) | 10479(7) | 2517(4) | 124(4) |
| F(2) | 2484(2) | 10440(7) | 1582(4) | 129(4) |
| F(3) | 2660(2) | 9119(5) | 2013(3) | 97(3) |
| C(81) | 4102(4) | 10686(7) | 2480(5) | 73(4) |
| F(4) | 4189(3) | 11567(6) | 2586(6) | 227(8) |
| F(5) | 4021(3) | 10213(9) | 3007(3) | 154(4) |
| F(6) | 4411(2) | 10183(6) | 2342(3) | 102(3) |
| C(12) | 4108(2) | 10849(5) | 49(3) | 31(2) |
| C(22) | 4261(3) | 11725(6) | 320(4) | 51(2) |
| C(32) | 4617(3) | 12114(7) | 157(5) | 61(2) |
| C(42) | 4826(3) | 11625(6) | -279(4) | 61(2) |
| C(52) | 4680(2) | 10770(5) | -564(4) | 40(2) |
| C(62) | 4326(2) | 10394(5) | -398(3) | 32(2) |
| C(72) | 4754(9) | 13044(17) | 987(14) | 55(6) |
| C(72A) | 4741(7) | 12984(16) | 471(10) | 64(5) |
| F(7) | 4724(5) | 12806(10) | 1197(7) | 73(4) |
| F(7A) | 5000(6) | 13086(11) | 731(8) | 88(4) |
| F(7AA) | 5194(6) | 12680(14) | 685(9) | 125(6) |
| F(8) | 4449(3) | 13874(7) | 454(5) | 49(2) |
| F(9) | 4636(6) | 13649(13) | 484(9) | 101(5) |
| F(9A) | 4926(4) | 13682(8) | 64(6) | 170(4) |
| C(82) | 4894(3) | 10294(6) | -1061(4) | 50(3) |
| F(10) | 4817(2) | 9315(4) | -1155(3) | 90(2) |
| F(11) | 4822(2) | 10733(4) | -1605(2) | 66(2) |
| F(12) | 5271(2) | 10402(5) | -1008(3) | 83(2) |
| C(13) | 3572(2) | 9333(5) | -6(3) | 35(2) |
| C(23) | 3818(2) | 8528(5) | 135(3) | 37(2) |
| C(33) | 3733(2) | 7508(5) | -10(4) | 42(2) |
| C(43) | 3404(3) | 7270(6) | -321(4) | 50(2) |
| C(53) | 3157(3) | 8045(6) | -463(4) | 46(2) |
| C(63) | 3240(2) | 9067(5) | -306(4) | 42(2) |
| C(73) | 4010(3) | 6676(6) | 138(5) | 56(3) |
| F(13) | 3836(2) | 5843(4) | 367(6) | 142(5) |
| F(14) | 4173(3) | 6290(6) | -336(4) | 120(4) |
| F(15) | 4276(2) | 6930(4) | 517(3) | 77(2) |
| C(83) | 2798(3) | 7828(7) | -805(5) | 72(4) |
| F(16) | 2857(3) | 7966(8) | -1400(4) | 147(4) |
| F(17) | 2694(2) | 6881(5) | -784(4) | 136(4) |
| F(18) | 2524(2) | 8409(6) | -685(5) | 148(5) |
| C(14) | 3403(2) | 11387(5) | -88(3) | 34(2) |
| C(24) | 3339(2) | 11391(5) | -721(4) | 41(2) |
| C(34) | 3128(2) | 12157(5) | -995(4) | 39(2) |
| C(44) | 2987(2) | 12963(5) | -668(4) | 40(2) |

| Atom | x | y | z | U(eq) |
|---|---|---|---|---|
| C(54) | 3053(2) | 12996(5) | -53(3) | 35(2) |
| C(64) | 3258(2) | 12228(5) | 230(3) | 31(2) |
| C(74) | 3063(3) | 12131(7) | -1674(5) | 65(4) |
| F(19) | 2700(2) | 11966(6) | -1799(3) | 101(3) |
| F(20) | 3272(2) | 11440(4) | -1956(2) | 82(2) |
| F(21) | 3142(2) | 13035(4) | -1933(2) | 73(2) |
| C(84) | 2903(3) | 13905(5) | 301(4) | 50(3) |
| F(22) | 2896(3) | 13761(4) | 883(3) | 105(3) |
| F(23) | 3133(2) | 14721(4) | 222(4) | 103(3) |
| F(24) | 2579(2) | 14208(4) | 128(3) | 91(3) |

* Equivalent isotropic U defined as one third of the trace of the orthogonalised $U_{ij}$ tensor.