

Table B1. Bond lengths [Å] and angles [°] for C1

| | | | |
|-----------------|----------|-----------------|----------|
| Mo(1)-O(1) | 1.954(2) | C(2)-C(1) | 1.404(4) |
| Mo(1)-O(2) | 1.711(2) | O(1)-C(1) | 1.354(4) |
| Mo(1)-N(1) | 2.284(3) | C(3)-C(2) | 1.408(4) |
| Mo(1)-S(1) | 2.437(8) | C(4)-C(3) | 1.377(4) |
| Mo(1)-O(3) | 1.695(2) | C(4)-C(5) | 1.390(4) |
| Mo(1)-O(4) | 2.312(2) | C(6)-C(1) | 1.388(4) |
| Cl(1)-C(4) | 1.738(3) | C(6)-C(5) | 1.391(4) |
| S(1)-C(8) | 1.749(3) | C(7)-C(2) | 1.447(4) |
| S(2)-O(4) | 1.538(2) | C(7)-N(1) | 1.295(4) |
| S(2)-C(9) | 1.777(3) | C(8)-N(2) | 1.309(4) |
| S(2)-C(10) | 1.776(3) | N(1)-N(2) | 1.395(3) |
| N(3)-C(8) | 1.347(4) | | |
| | | | |
| O(2)-Mo(1)-O(1) | 107.6(1) | O(4)-S(2)-C(10) | 105.0(2) |
| O(3)-Mo(1)-O(1) | 96.7(1) | O(4)-S(2)-C(9) | 102.8(1) |
| O(3)-Mo(1)-O(2) | 105.5(1) | C(10)-S(2)-C(9) | 98.3(2) |
| O(1)-Mo(1)-N(1) | 81.7(9) | C(8)-N(3)-H(1) | 119.0(3) |
| O(2)-Mo(1)-N(1) | 159.4(1) | N(1)-C(7)-C(2) | 124.9(3) |
| O(3)-Mo(1)-N(1) | 91.1(1) | N(2)-C(8)-N(3) | 118.9(3) |
| O(1)-Mo(1)-O(4) | 77.1(8) | N(2)-C(8)-S(1) | 125.6(2) |
| O(2)-Mo(1)-O(4) | 85.2(9) | N(3)-C(8)-S(1) | 115.5(2) |
| O(3)-Mo(1)-O(4) | 168.9(9) | C(1)-C(2)-C(3) | 118.8(3) |
| O(1)-Mo(1)-S(1) | 151.5(7) | C(1)-C(2)-C(7) | 124.0(3) |
| O(2)-Mo(1)-S(1) | 89.5(8) | C(3)-C(2)-C(7) | 117.2(3) |
| O(3)-Mo(1)-S(1) | 100.4(8) | C(4)-C(5)-C(6) | 119.4(3) |
| N(1)-Mo(1)-S(1) | 75.4(6) | C(7)-N(1)-N(2) | 113.7(3) |
| N(1)-Mo(1)-O(4) | 79.0(8) | C(7)-N(1)-Mo(1) | 122.5(2) |
| O(4)-Mo(1)-S(1) | 82.1(6) | N(2)-N(1)-Mo(1) | 123.7(2) |
| C(1)-O(1)-Mo(1) | 126.7(2) | C(8)-N(2)-N(1) | 113.6(2) |
| C(8)-S(1)-Mo(1) | 101.3(1) | O(1)-C(1)-C(6) | 118.7(3) |
| S(2)-O(4)-Mo(1) | 122.9(1) | O(1)-C(1)-C(2) | 120.8(3) |
| C(4)-C(3)-C(2) | 119.9(3) | C(6)-C(1)-C(2) | 120.5(3) |

Table B2. Bond lengths [Å] and angles [°] for C2

| | | | |
|------------------|----------|-------------------|----------|
| Mo(1)-O(1) | 1.951(2) | C(1)-N(3) | 1.346(3) |
| Mo(1)-O(2) | 1.702(2) | N(3)-C(3) | 1.452(3) |
| Mo(1)-O(3) | 1.712(2) | C(3)-C(4) | 1.515(3) |
| Mo(1)-N(1) | 2.290(2) | N(2)-N(1) | 1.397(2) |
| Mo(1)-S(1) | 2.416(6) | N(1)-C(7) | 1.287(3) |
| Mo(1)-O(4) | 2.263(2) | C(7)-C(8) | 1.459(3) |
| Cl(1)-C(10) | 1.744(2) | C(8)-C(13) | 1.405(3) |
| S(1)-C(1) | 1.759(2) | C(8)-C(9) | 1.407(3) |
| S(2)-O(4) | 1.535(2) | C(9)-C(10) | 1.370(3) |
| S(2)-C(16) | 1.788(2) | C(10)-C(11) | 1.392(4) |
| S(2)-C(17) | 1.777(2) | C(11)-C(12) | 1.385(3) |
| O(1)-C(13) | 1.342(3) | C(12)-C(13) | 1.396(3) |
| C(1)-N(2) | 1.307(3) | | |
| | | | |
| O(2)-Mo(1)-O(1) | 96.8(7) | N(1)-C(7)-C(8) | 126.3(2) |
| O(2)-Mo(1)-O(3) | 105.2(9) | N(2)-C(1)-N(3) | 119.9(2) |
| O(3)-Mo(1)-O(1) | 106.4(7) | N(2)-C(1)-S(1) | 126.1(2) |
| O(1)-Mo(1)-O(4) | 75.0(6) | N(3)-C(1)-S(1) | 114.0(2) |
| O(2)-Mo(1)-O(4) | 165.6(7) | N(3)-C(3)-C(4) | 109.2(2) |
| O(3)-Mo(1)-O(4) | 88.6(7) | C(1)-N(3)-C(3) | 124.1(2) |
| O(1)-Mo(1)-N(1) | 84.05(6) | C(1)-N(2)-N(1) | 113.1(2) |
| O(2)-Mo(1)-N(1) | 89.84(8) | C(7)-N(1)-N(2) | 113.4(2) |
| O(3)-Mo(1)-N(1) | 160.2(7) | C(9)-C(8)-C(7) | 117.1(2) |
| O(4)-Mo(1)-N(1) | 77.7(6) | C(9)-C(10)-C(11) | 121.0(2) |
| O(1)-Mo(1)-S(1) | 153.9(5) | C(9)-C(10)-Cl(1) | 120.0(2) |
| O(2)-Mo(1)-S(1) | 99.8(6) | C(10)-C(9)-C(8) | 120.6(2) |
| O(3)-Mo(1)-S(1) | 88.5(6) | C(11)-C(10)-Cl(1) | 119.1(2) |
| O(4)-Mo(1)-S(1) | 84.4(4) | C(11)-C(12)-C(13) | 120.6(2) |
| N(1)-Mo(1)-S(1) | 76.5(5) | C(12)-C(11)-C(10) | 119.3(2) |
| C(1)-S(1)-Mo(1) | 101.1(8) | C(12)-C(13)-C(8) | 120.0(2) |
| C(13)-O(1)-Mo(1) | 133.1(1) | C(13)-C(8)-C(9) | 118.5(2) |
| C(7)-N(1)-Mo(1) | 123.3(2) | C(13)-C(8)-C(7) | 124.4(2) |
| N(2)-N(1)-Mo(1) | 123.3(1) | C(17)-S(2)-C(16) | 98.9(1) |
| S(2)-O(4)-Mo(1) | 129.3(9) | O(1)-C(13)-C(12) | 117.2(2) |
| O(4)-S(2)-C(17) | 102.1(1) | O(1)-C(13)-C(8) | 122.8(2) |
| O(4)-S(2)-C(16) | 104.9(1) | | |

Table B3. Bond lengths [Å] and angles [°] for C3

| | | | |
|-----------------|----------|------------------|----------|
| Mo(1)-O(1) | 1.926(1) | C(1)-C(2) | 1.406(3) |
| Mo(1)-O(2) | 1.717(1) | C(1)-C(6) | 1.398(3) |
| Mo(1)-O(3) | 1.696(1) | C(2)-C(7) | 1.443(3) |
| Mo(1)-N(1) | 2.270(2) | C(3)-C(2) | 1.411(3) |
| Mo(1)-S(1) | 2.446(5) | C(3)-C(4) | 1.375(3) |
| Mo(1)-O(4) | 2.336(2) | C(4)-C(5) | 1.393(3) |
| S(1)-C(8) | 1.760(2) | C(4)-Cl(1) | 1.739(2) |
| S(2)-O(4) | 1.537(2) | C(6)-C(5) | 1.381(3) |
| S(2)-C(16) | 1.777(2) | C(9)-C(14) | 1.399(3) |
| S(2)-C(15) | 1.778(2) | C(9)-N(3) | 1.417(2) |
| O(1)-C(1) | 1.341(2) | C(10)-C(9) | 1.393(3) |
| N(1)-C(7) | 1.297(3) | C(10)-C(11) | 1.394(3) |
| N(2)-C(8) | 1.296(3) | C(13)-C(12) | 1.387(3) |
| N(2)-N(1) | 1.393(2) | C(14)-C(13) | 1.387(3) |
| C(8)-N(3) | 1.367(2) | | |
| O(2)-Mo(1)-O(1) | 105.5(6) | C(1)-O(1)-Mo(1) | 135.2(1) |
| O(3)-Mo(1)-O(1) | 99.0(7) | S(2)-O(4)-Mo(1) | 116.3(8) |
| O(3)-Mo(1)-O(2) | 106.3(7) | N(2)-N(1)-Mo(1) | 123.6(1) |
| O(1)-Mo(1)-N(1) | 83.0(6) | C(7)-N(1)-Mo(1) | 123.5(3) |
| O(2)-Mo(1)-N(1) | 159.3(6) | C(1)-C(2)-C(3) | 118.8(2) |
| O(3)-Mo(1)-N(1) | 90.5(6) | C(1)-C(2)-C(7) | 123.9(2) |
| O(1)-Mo(1)-O(4) | 77.3(6) | C(3)-C(2)-C(7) | 117.1(2) |
| O(2)-Mo(1)-O(4) | 85.5(6) | C(6)-C(1)-C(2) | 120.1(2) |
| O(3)-Mo(1)-O(4) | 168.1(6) | C(7)-N(1)-N(2) | 112.1(2) |
| N(1)-Mo(1)-O(4) | 77.9(5) | C(8)-N(2)-N(1) | 114.1(2) |
| O(1)-Mo(1)-S(1) | 153.5(5) | C(9)-C(10)-C(11) | 119.7(2) |
| O(2)-Mo(1)-S(1) | 90.2(5) | C(16)-S(2)-C(15) | 99.0(1) |
| O(3)-Mo(1)-S(1) | 96.7(5) | N(2)-C(8)-N(3) | 120.9(2) |
| N(1)-Mo(1)-S(1) | 75.6(4) | N(2)-C(8)-S(1) | 125.5(2) |
| O(4)-Mo(1)-S(1) | 83.0(4) | N(3)-C(8)-S(1) | 113.6(1) |
| O(4)-S(2)-C(15) | 103.4(1) | C(4)-C(3)-C(2) | 119.9(2) |
| O(4)-S(2)-C(16) | 104.5(1) | O(1)-C(1)-C(2) | 121.7(2) |
| C(8)-S(1)-Mo(1) | 100.3(7) | O(1)-C(1)-C(6) | 118.1(2) |

Table B4. Bond lengths [Å] and angles [°] for C4

| | | | |
|------------------|----------|-------------------|----------|
| Mo(1)-O(1) | 1.915(4) | C(2)-C(9) | 1.443(7) |
| Mo(1)-O(2) | 1.699(4) | C(3)-C(2) | 1.422(7) |
| Mo(1)-O(3) | 1.693(5) | C(5)-C(4) | 1.401(8) |
| Mo(1)-O(4) | 1.994(4) | C(4)-C(3) | 1.374(7) |
| Mo(1)-O(6) | 2.336(4) | C(6)-C(5) | 1.382(7) |
| Mo(1)-N(1) | 2.261(4) | C(7)-C(8) | 1.514(9) |
| O(4)-C(10) | 1.310(6) | C(10)-C(11) | 1.485(7) |
| O(5)-C(6) | 1.369(6) | C(11)-C(12) | 1.389(8) |
| O(5)-C(7) | 1.422(6) | C(11)-C(16) | 1.404(8) |
| N(1)-N(2) | 1.385(6) | C(12)-C(13) | 1.397(8) |
| N(1)-C(9) | 1.292(6) | C(13)-O(7) | 1.345(8) |
| N(2)-C(10) | 1.308(7) | C(13)-C(14) | 1.392(9) |
| O(1)-C(1) | 1.343(6) | C(14)-C(15) | 1.369(1) |
| C(1)-C(6) | 1.399(7) | C(15)-C(16) | 1.404(9) |
| C(1)-C(2) | 1.403(7) | O(6)-C(18) | 1.590(2) |
| O(7)-C(17) | 1.419(9) | | |
| | | | |
| O(2)-Mo(1)-O(1) | 103.2(2) | C(6)-C(1)-C(2) | 120.8(4) |
| O(3)-Mo(1)-O(1) | 98.8(2) | C(6)-C(5)-C(4) | 119.9(5) |
| O(3)-Mo(1)-O(2) | 106.1(2) | C(11)-C(12)-C(13) | 118.9(5) |
| O(1)-Mo(1)-O(4) | 149.9(2) | C(11)-C(16)-C(15) | 118.7(6) |
| O(2)-Mo(1)-O(4) | 97.0(2) | C(12)-C(11)-C(10) | 121.5(5) |
| O(1)-Mo(1)-N(1) | 82.0(2) | C(12)-C(11)-C(16) | 121.0(5) |
| O(2)-Mo(1)-N(1) | 157.7(2) | C(14)-C(13)-C(12) | 120.5(6) |
| O(3)-Mo(1)-N(1) | 94.3(2) | C(14)-C(15)-C(16) | 120.5(6) |
| O(3)-Mo(1)-O(4) | 96.7(2) | C(15)-C(14)-C(13) | 120.5(6) |
| O(4)-Mo(1)-N(1) | 71.2(2) | C(16)-C(11)-C(10) | 117.5(5) |
| O(1)-Mo(1)-O(6) | 81.4(2) | C(6)-O(5)-C(7) | 118.1(4) |
| O(2)-Mo(1)-O(6) | 83.0(2) | C(9)-N(1)-N(2) | 117.6(4) |
| O(3)-Mo(1)-O(6) | 170.5(2) | C(10)-N(2)-N(1) | 109.5(4) |
| O(4)-Mo(1)-O(6) | 79.2(2) | C(13)-O(7)-C(17) | 116.6(5) |
| N(1)-Mo(1)-O(6) | 76.3(1) | O(1)-C(1)-C(6) | 116.6(5) |
| C(1)-O(1)-Mo(1) | 136.1(4) | O(1)-C(1)-C(2) | 122.5(4) |
| N(2)-N(1)-Mo(1) | 115.0(3) | O(4)-C(10)-C(11) | 115.4(4) |
| C(9)-N(1)-Mo(1) | 127.3(3) | O(5)-C(6)-C(1) | 115.2(5) |
| C(10)-O(4)-Mo(1) | 121.2(3) | O(5)-C(6)-C(5) | 124.7(5) |
| C(18)-O(6)-Mo(1) | 120.8(4) | O(5)-C(7)-C(8) | 107.1(5) |
| C(1)-C(2)-C(3) | 118.0(4) | O(7)-C(13)-C(12) | 124.5(6) |
| C(1)-C(2)-C(9) | 123.5(4) | O(7)-C(13)-C(14) | 114.9(6) |
| C(3)-C(2)-C(9) | 118.5(4) | N(1)-C(9)-C(2) | 124.2(4) |
| C(3)-C(4)-C(5) | 120.6(5) | N(2)-C(10)-O(4) | 122.7(4) |
| C(4)-C(3)-C(2) | 120.6(5) | N(2)-C(10)-C(11) | 121.9(5) |
| C(5)-C(6)-C(1) | 120.1(5) | | |

Table B5. Bond lengths [Å] and angles [°] for C6.

| | | | |
|-------------------|----------|-------------------|----------|
| Mo(1)-O(1) | 1.934(2) | C(7)-C(1) | 1.459(3) |
| Mo(1)-O(2) | 1.699(2) | C(8)-C(9) | 1.471(3) |
| Mo(1)-O(3) | 1.697(2) | C(10)-C(9) | 1.403(3) |
| Mo(1)-O(4) | 1.996(2) | C(11)-C(10) | 1.380(3) |
| Mo(1)-O(6) | 2.279(2) | C(13)-C(12) | 1.367(4) |
| Mo(1)-N(1) | 2.258(2) | C(14)-C(9) | 1.388(3) |
| Cl(1)-C(5) | 1.738(3) | C(14)-C(13) | 1.404(4) |
| O(6)-S(1) | 1.514(2) | C(11)-O(5) | 1.370(3) |
| C(2)-C(1) | 1.408(4) | C(11)-C(12) | 1.387(4) |
| C(3)-C(2) | 1.398(3) | C(16)-S(1) | 1.777(3) |
| C(4)-C(3) | 1.384(4) | N(1)-C(7) | 1.280(3) |
| C(4)-C(5) | 1.373(4) | N(1)-N(2) | 1.401(3) |
| C(6)-C(1) | 1.401(4) | S(1)-C(15) | 1.783(3) |
| C(6)-C(5) | 1.385(4) | O(5)-C(17) | 1.420(3) |
| C(2)-O(1) | 1.343(3) | C(8)-O(4) | 1.321(3) |
| C(8)-N(2) | 1.302(3) | | |
| O(1)-Mo(1)-O(4) | 148.9(8) | C(2)-O(1)-Mo(1) | 134.7(2) |
| O(2)-Mo(1)-O(1) | 98.6(9) | C(7)-N(1)-Mo(1) | 128.3(2) |
| O(2)-Mo(1)-O(3) | 104.9(1) | C(8)-O(4)-Mo(1) | 121.1(1) |
| O(2)-Mo(1)-O(4) | 98.3(9) | N(2)-N(1)-Mo(1) | 115.4(1) |
| O(3)-Mo(1)-O(1) | 103.9(9) | C(1)-C(2)-C(3) | 119.1(2) |
| O(3)-Mo(1)-O(4) | 96.7(9) | C(2)-C(1)-C(6) | 119.3(2) |
| O(1)-Mo(1)-N(1) | 82.3(7) | C(2)-C(1)-C(7) | 123.3(2) |
| O(2)-Mo(1)-N(1) | 91.7(9) | C(3)-C(4)-C(5) | 119.3(2) |
| O(3)-Mo(1)-N(1) | 161.0(1) | C(4)-C(3)-C(2) | 121.0(3) |
| O(4)-Mo(1)-N(1) | 71.3(7) | C(5)-C(6)-C(1) | 119.7(3) |
| O(1)-Mo(1)-O(6) | 77.8(7) | C(6)-C(1)-C(7) | 117.3(2) |
| O(2)-Mo(1)-O(6) | 168.1(1) | C(6)-C(5)-C(4) | 121.5(3) |
| O(3)-Mo(1)-O(6) | 87.0(9) | C(10)-C(9)-C(8) | 120.4(2) |
| O(4)-Mo(1)-O(6) | 80.2(7) | C(10)-C(11)-C(12) | 120.6(2) |
| N(1)-Mo(1)-O(6) | 76.6(7) | C(11)-C(10)-C(9) | 119.3(2) |
| S(1)-O(6)-Mo(1) | 126.6(1) | C(11)-C(12)-C(13) | 120.1(3) |
| C(13)-C(14)-C(9) | 118.8(2) | C(4)-C(5)-Cl(1) | 119.8(2) |
| C(14)-C(13)-C(12) | 120.8(2) | C(6)-C(5)-Cl(1) | 118.7(2) |
| C(14)-C(9)-C(8) | 119.2(2) | C(7)-N(1)-N(2) | 116.3(2) |
| C(14)-C(9)-C(10) | 120.4(2) | C(8)-N(2)-N(1) | 108.9(2) |
| C(11)-O(5)-C(17) | 118.0(2) | O(6)-S(1)-C(15) | 103.3(1) |
| C(15)-S(1)-C(16) | 99.8(2) | O(6)-S(1)-C(16) | 106.2(2) |
| O(1)-C(2)-C(1) | 123.7(2) | N(1)-C(7)-C(1) | 123.3(2) |
| O(1)-C(2)-C(3) | 117.2(2) | N(2)-C(8)-O(4) | 123.1(2) |
| O(5)-C(11)-C(10) | 124.0(2) | N(2)-C(8)-C(9) | 120.8(2) |
| O(5)-C(11)-C(12) | 115.4(2) | O(4)-C(8)-C(9) | 116.1(2) |

Table B6. Bond lengths [\AA] and angles [$^\circ$] for C7.

| | | | |
|-----------------|-----------|-------------------|----------|
| Mo(1)-O(1) | 1.939(2) | C(9)-C(12) | 1.347(3) |
| Mo(1)-O(3) | 1.696(2) | C(10)-C(11) | 1.321(5) |
| Mo(1)-O(2) | 1.712(2) | C(11)-C(12) | 1.399(4) |
| Mo(1)-O(4) | 2.010(2) | C(7)-N(1) | 1.296(3) |
| Mo(1)-O(6) | 2.267(2) | C(8)-N(2) | 1.300(3) |
| Mo(1)-N(1) | 2.242(2) | C(8)-O(4) | 1.325(3) |
| C(2)-C(1) | 1.410(3) | C(9)-O(5) | 1.338(3) |
| C(3)-C(2) | 1.415(3) | C(10)-O(5) | 1.403(4) |
| C(4)-C(3) | 1.372(4) | Cl(1)-C(4) | 1.752(3) |
| C(4)-C(5) | 1.391(4) | O(1)-C(1) | 1.345(3) |
| C(5)-C(6) | 1.380(3) | O(6)-S(1) | 1.530(8) |
| C(6)-C(1) | 1.394(3) | N(1)-N(2) | 1.390(3) |
| C(7)-C(2) | 1.437(3) | S(1)-C(14) | 1.773(3) |
| C(9)-C(8) | 1.452(3) | S(1)-C(13) | 1.789(3) |
| | | | |
| O(1)-Mo(1)-O(4) | 149.87(7) | C(4)-C(3)-C(2) | 119.6(2) |
| O(2)-Mo(1)-O(1) | 104.68(7) | C(5)-C(6)-C(1) | 121.1(2) |
| O(2)-Mo(1)-O(4) | 95.68(7) | C(6)-C(1)-C(2) | 119.4(2) |
| O(3)-Mo(1)-O(1) | 97.78(8) | C(6)-C(5)-C(4) | 119.2(2) |
| O(3)-Mo(1)-O(2) | 104.7(9) | C(9)-C(12)-C(11) | 105.6(2) |
| O(3)-Mo(1)-O(4) | 98.26(8) | C(10)-C(11)-C(12) | 108.6(3) |
| O(1)-Mo(1)-N(1) | 82.15(7) | C(12)-C(9)-C(8) | 124.6(2) |
| O(2)-Mo(1)-N(1) | 160.1(8) | C(3)-C(4)-Cl(1) | 118.5(1) |
| O(3)-Mo(1)-N(1) | 92.64(8) | C(5)-C(4)-Cl(1) | 120.0(2) |
| O(4)-Mo(1)-N(1) | 71.78(7) | C(11)-C(10)-O(5) | 108.9(3) |
| O(1)-Mo(1)-O(6) | 77.66(7) | C(9)-O(5)-C(10) | 105.4(2) |
| O(2)-Mo(1)-O(6) | 86.07(7) | C(8)-N(2)-N(1) | 108.7(2) |
| O(3)-Mo(1)-O(6) | 169.1(7) | C(7)-N(1)-N(2) | 115.9(2) |
| O(4)-Mo(1)-O(6) | 81.90(6) | N(1)-C(7)-C(2) | 123.4(2) |
| N(1)-Mo(1)-O(6) | 77.04(6) | N(2)-C(8)-O(4) | 124.2(2) |
| C(1)-O(1)-Mo(1) | 134.9(1) | N(2)-C(8)-C(9) | 119.3(2) |
| C(7)-N(1)-Mo(1) | 128.2(2) | O(1)-C(1)-C(6) | 118.1(2) |
| C(8)-O(4)-Mo(1) | 119.1(2) | O(1)-C(1)-C(2) | 122.4(2) |
| S(1)-O(6)-Mo(1) | 127.0(1) | O(4)-C(8)-C(9) | 116.5(2) |
| N(2)-N(1)-Mo(1) | 116.0(1) | O(5)-C(9)-C(12) | 111.6(2) |
| C(1)-C(2)-C(3) | 119.1(2) | O(5)-C(9)-C(8) | 123.8(2) |
| C(1)-C(2)-C(7) | 124.1(2) | O(6)-S(1)-C(14) | 102.7(1) |
| C(3)-C(2)-C(7) | 116.9(2) | O(6)-S(1)-C(13) | 105.8(1) |
| C(3)-C(4)-C(5) | 121.5(2) | | |

Table B7. Bond lengths [Å] and angles [°] for C8

| | | | |
|------------------|----------|------------------|----------|
| Mo(1)-O(1) | 1.933(2) | C(10)-C(11) | 1.393(5) |
| Mo(1)-O(2) | 1.711(3) | C(11)-C(12) | 1.377(5) |
| Mo(1)-O(3) | 1.691(3) | C(12)-C(13) | 1.400(5) |
| Mo(1)-O(4) | 2.009(2) | C(13)-C(14) | 1.375(5) |
| Mo(1)-O(6) | 2.336(3) | Cl(1)-C(4) | 1.735(4) |
| Mo(1)-N(1) | 2.242(3) | S(1)-O(6) | 1.518(3) |
| C(1)-C(6) | 1.399(5) | S(1)-C(15) | 1.785(4) |
| C(2)-C(1) | 1.412(5) | S(1)-C(16) | 1.785(4) |
| C(2)-C(3) | 1.396(5) | O(1)-C(1) | 1.347(4) |
| C(2)-C(7) | 1.447(5) | O(4)-C(8) | 1.327(4) |
| C(4)-C(3) | 1.378(5) | O(5)-C(10) | 1.346(4) |
| C(5)-C(4) | 1.395(5) | O(7)-C(12) | 1.373(4) |
| C(6)-C(5) | 1.375(5) | N(1)-C(7) | 1.284(5) |
| C(8)-C(9) | 1.457(5) | N(2)-C(8) | 1.303(5) |
| C(9)-C(10) | 1.412(5) | N(1)-N(2) | 1.392(4) |
| C(9)-C(14) | 1.405(5) | | |
| O(1)-Mo(1)-O(4) | 148.2(1) | C(1)-C(2)-C(7) | 123.0(3) |
| O(2)-Mo(1)-O(1) | 104.6(1) | C(8)-N(2)-N(1) | 110.3(3) |
| O(2)-Mo(1)-O(4) | 97.5(1) | C(3)-C(2)-C(1) | 119.4(3) |
| O(3)-Mo(1)-O(1) | 99.1(1) | C(3)-C(2)-C(7) | 117.7(3) |
| O(3)-Mo(1)-O(2) | 104.1(1) | C(3)-C(4)-C(5) | 120.3(3) |
| O(3)-Mo(1)-O(4) | 97.4(1) | C(4)-C(3)-C(2) | 120.5(3) |
| O(1)-Mo(1)-N(1) | 80.7(1) | C(5)-C(6)-C(1) | 120.7(3) |
| O(2)-Mo(1)-N(1) | 163.1(1) | C(6)-C(1)-C(2) | 119.1(3) |
| O(3)-Mo(1)-N(1) | 90.6(1) | C(6)-C(5)-C(4) | 120.0(3) |
| O(4)-Mo(1)-N(1) | 72.2(1) | C(10)-C(9)-C(8) | 121.3(3) |
| O(1)-Mo(1)-O(6) | 80.9(1) | C(14)-C(9)-C(8) | 120.5(3) |
| O(2)-Mo(1)-O(6) | 79.4(1) | C(14)-C(9)-C(10) | 118.3(3) |
| O(3)-Mo(1)-O(6) | 176.3(1) | C(3)-C(4)-Cl(1) | 119.7(3) |
| O(4)-Mo(1)-O(6) | 81.0(1) | C(5)-C(4)-Cl(1) | 120.0(3) |
| C(1)-O(1)-Mo(1) | 135.2(2) | O(1)-C(1)-C(6) | 118.6(3) |
| C(8)-O(4)-Mo(1) | 119.4(2) | O(1)-C(1)-C(2) | 122.3(3) |
| S(1)-O(6)-Mo(1) | 149.3(2) | O(4)-C(8)-C(9) | 118.9(3) |
| C(7)-N(1)-Mo(1) | 129.4(2) | O(5)-C(10)-C(9) | 123.4(3) |
| N(1)-Mo(1)-O(6) | 85.7(1) | O(5)-C(10)-C(11) | 116.6(3) |
| N(2)-N(1)-Mo(1) | 114.7(2) | N(1)-C(7)-C(2) | 123.0(3) |
| O(6)-S(1)-C(15) | 106.5(2) | N(2)-C(8)-C(9) | 118.4(3) |
| O(6)-S(1)-C(16) | 106.8(2) | N(2)-C(8)-O(4) | 122.7(3) |
| C(15)-S(1)-C(16) | 99.0(2) | | |
| C(7)-N(1)-N(2) | 115.5(3) | | |

Table B8. Bond lengths [Å] and angles [°] for C9

| | | | |
|-----------------|----------|-------------------|----------|
| Mo(1)-O(1) | 1.941(3) | C(14)-N(3) | 1.428(1) |
| Mo(1)-O(3) | 1.700(4) | C(17)-N(5) | 1.530(2) |
| Mo(1)-O(2) | 1.701(4) | C(19)-N(6) | 1.328(8) |
| Mo(1)-O(4) | 2.022(3) | C(20)-N(6) | 1.436(9) |
| Mo(1)-O(6) | 2.189(4) | C(21)-N(6) | 1.435(9) |
| Mo(1)-N(1) | 2.251(4) | C(9)-O(5) | 1.355(7) |
| C(1)-C(2) | 1.408(6) | C(10)-O(5) | 1.428(7) |
| C(1)-C(6) | 1.400(7) | P(1)-O(6) | 1.490(4) |
| C(2)-C(7) | 1.447(6) | P(1)-N(4) | 1.621(1) |
| C(3)-C(2) | 1.415(6) | P(1)-N(5) | 1.500(1) |
| C(4)-C(3) | 1.374(6) | N(2)-C(8) | 1.305(6) |
| C(4)-C(5) | 1.383(7) | N(2)-N(1) | 1.389(5) |
| C(5)-C(6) | 1.384(7) | N(1)-C(7) | 1.293(6) |
| C(9)-C(8) | 1.454(6) | N(4)-C(15) | 1.590(2) |
| C(11)-C(10) | 1.338(8) | N(4)-C(16) | 1.510(2) |
| C(11)-C(12) | 1.373(6) | N(5)-C(18) | 1.690(9) |
| C(13)-N(3) | 1.488(1) | | |
| O(1)-Mo(1)-O(4) | 150.7(2) | C(6)-C(1)-C(2) | 119.3(4) |
| O(1)-Mo(1)-O(6) | 81.4(2) | C(9)-C(12)-C(11) | 106.2(4) |
| O(2)-Mo(1)-O(1) | 104.9(2) | C(10)-C(11)-C(12) | 110.4(5) |
| O(2)-Mo(1)-O(4) | 97.0(2) | C(12)-C(9)-C(8) | 117.6(4) |
| O(2)-Mo(1)-O(6) | 89.4(2) | C(3)-C(4)-Cl(1) | 118.9(4) |
| O(3)-Mo(1)-O(1) | 97.1(2) | C(5)-C(4)-Cl(1) | 119.0(4) |
| O(3)-Mo(1)-O(2) | 104.6(2) | C(11)-C(10)-O(5) | 107.0(5) |
| O(3)-Mo(1)-O(4) | 95.7(2) | C(14)-N(3)-C(13) | 116.9(7) |
| O(3)-Mo(1)-O(6) | 165.7(1) | C(14)-N(3)-P(1) | 117.2(6) |
| O(4)-Mo(1)-O(6) | 79.7(1) | C(13)-N(3)-P(1) | 121.4(6) |
| O(1)-Mo(1)-N(1) | 82.3(1) | C(15)-N(4)-P(1) | 113.8(2) |
| O(2)-Mo(1)-N(1) | 163.3(1) | C(16)-N(4)-P(1) | 115.7(9) |
| O(3)-Mo(1)-N(1) | 89.1(2) | C(16)-N(4)-C(15) | 130.0(1) |
| O(4)-Mo(1)-N(1) | 71.7(1) | C(9)-O(5)-C(10) | 105.7(5) |
| O(6)-Mo(1)-N(1) | 76.7(1) | C(17)-N(5)-C(18) | 116.3(1) |
| C(1)-O(1)-Mo(1) | 131.7(3) | O(1)-C(1)-C(6) | 117.4(4) |
| C(7)-N(1)-Mo(1) | 127.1(3) | O(1)-C(1)-C(2) | 123.3(4) |
| C(8)-O(4)-Mo(1) | 118.8(3) | O(4)-C(8)-C(9) | 114.5(4) |
| C(8)-N(2)-N(1) | 108.5(4) | O(5)-C(9)-C(8) | 131.8(4) |
| C(7)-N(1)-N(2) | 116.6(4) | O(5)-C(9)-C(12) | 110.6(4) |
| N(2)-N(1)-Mo(1) | 115.8(3) | O(6)-P(1)-N(5) | 113.1(4) |
| P(1)-O(6)-Mo(1) | 156.1(3) | O(6)-P(1)-N(4) | 113.7(5) |
| C(1)-C(2)-C(3) | 118.9(4) | O(6)-P(1)-N(3) | 106.6(3) |
| C(1)-C(2)-C(7) | 124.3(4) | O(7)-C(19)-N(6) | 126.4(6) |
| C(3)-C(2)-C(7) | 116.8(4) | N(2)-C(8)-O(4) | 125.0(4) |
| C(3)-C(4)-C(5) | 122.1(4) | N(2)-C(8)-C(9) | 120.4(4) |
| C(4)-C(3)-C(2) | 119.7(4) | N(4)-P(1)-N(3) | 104.4(5) |
| C(4)-C(5)-C(6) | 118.7(5) | N(5)-P(1)-N(4) | 103.0(1) |
| C(5)-C(6)-C(1) | 121.3(5) | N(5)-P(1)-N(3) | 115.8(1) |

Table B9. Bond lengths [Å] and angles [°] for C10

| | | | |
|-----------------|----------|-------------------|----------|
| Mo(1)-O(1) | 1.943(5) | C(9)-C(10) | 1.488(2) |
| Mo(1)-O(2) | 1.702(8) | C(11)-C(10) | 1.388(2) |
| Mo(1)-O(3) | 1.702(8) | C(12)-C(11) | 1.374(3) |
| Mo(1)-O(4) | 2.022(1) | C(7)-N(1) | 1.293(8) |
| Mo(1)-O(6) | 2.190(1) | C(8)-N(2) | 1.303(1) |
| Mo(1)-N(1) | 2.252(4) | C(8)-O(6) | 1.313(2) |
| C(2)-C(1) | 1.500(2) | C(9)-O(5) | 1.355(3) |
| C(3)-C(2) | 1.412(2) | C(12)-O(5) | 1.428(5) |
| C(4)-C(3) | 1.372(2) | Cl(1)-C(4) | 1.744(1) |
| C(4)-C(5) | 1.382(2) | N(1)-N(2) | 1.388(5) |
| C(5)-C(6) | 1.385(2) | O(1)-C(1) | 1.347(1) |
| C(6)-C(1) | 1.400(2) | O(6)-S(1) | 1.514(8) |
| C(7)-C(6) | 1.508(4) | S(1)-C(14) | 1.777(8) |
| C(9)-C(8) | 1.454(2) | S(1)-C(13) | 1.774(4) |
| <hr/> | | | |
| O(1)-Mo(1)-O(2) | 105.0(1) | N(2)-N(1)-Mo(1) | 115.4(1) |
| O(1)-Mo(1)-O(6) | 81.5(1) | C(1)-C(6)-C(5) | 121.4(1) |
| O(3)-Mo(1)-O(1) | 97.0(1) | C(1)-C(6)-C(7) | 119.4(1) |
| O(3)-Mo(1)-O(2) | 104.7(1) | C(2)-C(1)-C(6) | 119.3(1) |
| O(3)-Mo(1)-O(6) | 162.9(1) | C(2)-C(3)-C(4) | 119.7(1) |
| O(4)-Mo(1)-O(1) | 150.7(1) | C(3)-C(2)-C(1) | 118.9(1) |
| O(4)-Mo(1)-O(2) | 97.3(1) | C(4)-C(5)-C(6) | 118.7(1) |
| O(4)-Mo(1)-O(3) | 95.7(1) | C(5)-C(4)-C(3) | 122.1(1) |
| O(4)-Mo(1)-O(6) | 79.6(3) | C(5)-C(6)-C(7) | 117.0(1) |
| O(6)-Mo(1)-O(2) | 89.3(1) | C(9)-C(10)-C(11) | 115.6(1) |
| O(1)-Mo(1)-N(1) | 82.3(1) | C(10)-C(9)-C(8) | 117.1(1) |
| O(3)-Mo(1)-N(1) | 89.2(3) | C(12)-C(11)-C(10) | 110.4(1) |
| O(4)-Mo(1)-N(1) | 72.0(1) | C(3)-C(4)-Cl(1) | 118.9(1) |
| O(6)-Mo(1)-N(1) | 76.4(1) | C(5)-C(4)-Cl(1) | 118.8(1) |
| N(1)-Mo(1)-O(2) | 163.6(1) | C(11)-C(12)-O(5) | 107.5(1) |
| C(1)-O(1)-Mo(1) | 131.7(1) | C(7)-N(1)-N(2) | 116.6(2) |
| C(7)-N(1)-Mo(1) | 127.1(2) | C(8)-N(2)-N(1) | 108.5(1) |
| C(8)-O(6)-Mo(1) | 118.8(1) | C(9)-O(5)-C(12) | 105.7(1) |
| S(1)-O(2)-Mo(1) | 113.0(1) | C(14)-S(1)-C(13) | 99.7(1) |

Table B10. Bond lengths [\AA] and angles [$^\circ$] for C12

| | | | |
|------------------|----------|------------------|----------|
| Mo(1)-O(1) | 1.924(1) | C(13)-C(14) | 1.389(3) |
| Mo(1)-O(2) | 1.708(1) | C(14)-C(15) | 1.393(3) |
| Mo(1)-O(3) | 1.703(2) | C(15)-C(16) | 1.383(3) |
| Mo(1)-O(4) | 2.021(1) | C(1)-O(1) | 1.335(2) |
| Mo(1)-O(6) | 2.295(1) | N(1)-C(9) | 1.284(3) |
| Mo(1)-N(1) | 2.229(2) | N(1)-N(2) | 1.400(2) |
| C(2)-C(1) | 1.407(3) | N(2)-C(10) | 1.298(3) |
| C(2)-C(3) | 1.412(3) | N(3)-C(18) | 1.311(3) |
| C(3)-C(4) | 1.373(3) | N(3)-C(19) | 1.455(3) |
| C(4)-C(5) | 1.396(3) | N(3)-C(20) | 1.461(3) |
| C(5)-C(6) | 1.383(3) | O(4)-C(10) | 1.324(2) |
| C(6)-C(1) | 1.413(3) | O(5)-C(6) | 1.366(2) |
| C(9)-C(2) | 1.446(3) | O(5)-C(7) | 1.435(2) |
| C(10)-C(11) | 1.481(2) | O(6)-C(18) | 1.246(3) |
| C(11)-C(12) | 1.388(3) | O(7)-C(13) | 1.370(2) |
| C(11)-C(16) | 1.401(3) | O(7)-C(17) | 1.428(2) |
| C(12)-C(13) | 1.401(3) | C(7)-C(8) | 1.503(3) |
| O(1)-Mo(1)-O(4) | 151.1(6) | C(3)-C(4)-C(5) | 120.2(2) |
| O(1)-Mo(1)-O(6) | 78.8(6) | C(4)-C(3)-C(2) | 120.1(2) |
| O(2)-Mo(1)-O(1) | 105.0(6) | C(5)-C(6)-C(1) | 119.9(2) |
| O(2)-Mo(1)-O(4) | 94.1(6) | C(6)-C(5)-C(4) | 120.9(2) |
| O(2)-Mo(1)-O(6) | 85.0(6) | C(9)-N(1)-N(2) | 115.6(2) |
| O(3)-Mo(1)-O(1) | 98.9(7) | C(10)-N(2)-N(1) | 109.2(2) |
| O(3)-Mo(1)-O(2) | 105.4(7) | C(18)-N(3)-C(19) | 120.8(2) |
| O(3)-Mo(1)-O(4) | 96.4(6) | C(18)-N(3)-C(20) | 121.5(2) |
| O(3)-Mo(1)-O(6) | 169.6(6) | C(19)-N(3)-C(20) | 117.7(2) |
| O(4)-Mo(1)-O(6) | 81.6(6) | C(6)-O(5)-C(7) | 116.5(2) |
| O(1)-Mo(1)-N(1) | 82.5(6) | C(13)-O(7)-C(17) | 116.9(2) |
| O(2)-Mo(1)-N(1) | 156.3(7) | N(1)-C(9)-C(2) | 124.3(2) |
| O(3)-Mo(1)-N(1) | 95.3(7) | N(2)-C(10)-O(4) | 123.5(2) |
| O(4)-Mo(1)-N(1) | 71.8(6) | N(2)-C(10)-C(11) | 118.9(2) |
| N(1)-Mo(1)-O(6) | 74.3(6) | N(2)-N(1)-Mo(1) | 115.7(2) |
| C(1)-O(1)-Mo(1) | 137.4(1) | O(1)-C(1)-C(2) | 123.4(2) |
| C(9)-N(1)-Mo(1) | 128.6(1) | O(1)-C(1)-C(6) | 117.6(2) |
| C(10)-O(4)-Mo(1) | 118.9(1) | O(4)-C(10)-C(11) | 117.6(2) |
| C(18)-O(6)-Mo(1) | 123.3(1) | O(5)-C(7)-C(8) | 107.5(2) |
| C(1)-C(2)-C(3) | 120.0(2) | O(6)-C(18)-N(3) | 124.6(2) |
| C(1)-C(2)-C(9) | 122.9(2) | O(7)-C(13)-C(14) | 124.0(2) |
| C(2)-C(1)-C(6) | 119.0(2) | O(7)-C(13)-C(12) | 115.5(2) |
| C(3)-C(2)-C(9) | 117.1(2) | | |

Table B11. Bond lengths [Å] and angles [°] for C13

| | | | |
|------------------|----------|-------------------|----------|
| Mo(1)-O(1) | 1.944(2) | C(14)-C(13) | 1.387(3) |
| Mo(1)-O(2) | 1.707(2) | C(15)-C(14) | 1.392(4) |
| Mo(1)-O(3) | 1.707(2) | C(16)-C(15) | 1.385(3) |
| Mo(1)-O(4) | 2.014(2) | C(18)-C(19) | 1.351(4) |
| Mo(1)-N(1) | 2.247(2) | C(13)-O(6) | 1.369(3) |
| Mo(1)-N(3) | 2.351(2) | C(19)-N(4) | 1.377(4) |
| C(2)-C(1) | 1.406(3) | O(1)-C(1) | 1.349(3) |
| C(2)-C(3) | 1.408(3) | O(4)-C(10) | 1.326(3) |
| C(3)-C(4) | 1.370(3) | O(5)-C(6) | 1.368(3) |
| C(4)-C(5) | 1.402(3) | O(5)-C(7) | 1.442(3) |
| C(5)-C(6) | 1.385(3) | O(6)-C(17) | 1.428(3) |
| C(6)-C(1) | 1.410(3) | O(7)-C(21) | 1.332(4) |
| C(7)-C(8) | 1.504(3) | N(1)-C(9) | 1.291(3) |
| C(9)-C(2) | 1.447(3) | N(1)-N(2) | 1.393(3) |
| C(10)-C(11) | 1.483(3) | N(2)-C(10) | 1.298(3) |
| C(11)-C(12) | 1.383(3) | N(3)-C(20) | 1.325(3) |
| C(11)-C(16) | 1.401(3) | N(3)-C(18) | 1.372(3) |
| C(13)-C(12) | 1.392(3) | N(4)-C(20) | 1.338(4) |
| O(1)-Mo(1)-O(4) | 149.1(7) | C(6)-C(5)-C(4) | 120.3(2) |
| O(2)-Mo(1)-O(1) | 105.0(7) | C(11)-C(12)-C(13) | 120.0(2) |
| O(2)-Mo(1)-O(4) | 96.8(7) | C(12)-C(11)-C(10) | 120.5(2) |
| O(3)-Mo(1)-O(1) | 97.0(8) | C(12)-C(11)-C(16) | 119.9(2) |
| O(3)-Mo(1)-O(2) | 105.5(8) | C(13)-C(14)-C(15) | 118.8(2) |
| O(3)-Mo(1)-O(4) | 97.9(7) | C(14)-C(13)-C(12) | 120.7(2) |
| O(1)-Mo(1)-N(1) | 81.5(7) | C(15)-C(16)-C(11) | 119.4(2) |
| O(2)-Mo(1)-N(1) | 162.1(8) | C(16)-C(11)-C(10) | 119.6(2) |
| O(3)-Mo(1)-N(1) | 89.9(7) | C(16)-C(15)-C(14) | 121.2(2) |
| O(4)-Mo(1)-N(1) | 71.6(6) | C(19)-C(18)-N(3) | 109.7(3) |
| O(1)-Mo(1)-N(3) | 79.9(7) | C(18)-C(19)-N(4) | 105.9(3) |
| O(2)-Mo(1)-N(3) | 83.8(8) | C(20)-N(3)-C(18) | 105.9(2) |
| O(3)-Mo(1)-N(3) | 170.7(7) | C(20)-N(4)-C(19) | 107.7(2) |
| O(4)-Mo(1)-N(3) | 81.0(7) | C(9)-N(1)-N(2) | 116.2(2) |
| N(1)-Mo(1)-N(3) | 80.9(7) | C(10)-N(2)-N(1) | 108.8(2) |
| C(1)-O(1)-Mo(1) | 132.6(1) | C(6)-O(5)-C(7) | 116.3(2) |
| C(10)-O(4)-Mo(1) | 119.3(1) | N(1)-C(9)-C(2) | 123.8(2) |
| C(9)-N(1)-Mo(1) | 127.1(2) | N(2)-C(10)-O(4) | 124.0(2) |
| C(18)-N(3)-Mo(1) | 124.3(2) | N(2)-C(10)-C(11) | 119.0(2) |
| C(20)-N(3)-Mo(1) | 129.8(2) | O(1)-C(1)-C(2) | 123.5(2) |
| N(2)-N(1)-Mo(1) | 115.9(1) | O(1)-C(1)-C(6) | 117.0(2) |
| C(1)-C(2)-C(3) | 119.4(2) | O(4)-C(10)-C(11) | 117.0(2) |
| C(1)-C(2)-C(9) | 122.9(2) | O(6)-C(13)-C(12) | 114.8(2) |
| C(2)-C(1)-C(6) | 119.4(2) | O(6)-C(13)-C(14) | 124.4(2) |
| C(3)-C(2)-C(9) | 117.7(2) | O(5)-C(6)-C(1) | 115.0(2) |
| C(3)-C(4)-C(5) | 120.2(2) | O(5)-C(6)-C(5) | 125.0(2) |
| C(4)-C(3)-C(2) | 120.7(2) | O(5)-C(7)-C(8) | 107.6(2) |
| C(5)-C(6)-C(1) | 120.0(2) | | |

Table B12. Bond lengths [\AA] and angles [$^\circ$] for C14

| | | | |
|-----------------|----------|-----------------|----------|
| Mo(1)-O(6) | 1.705(1) | C(5)-C(4) | 1.531(3) |
| Mo(1)-O(5) | 1.712(1) | C(6)-C(5) | 1.537(3) |
| Mo(1)-O(3) | 1.917(1) | C(7)-C(8) | 1.411(3) |
| Mo(1)-O(4) | 1.997(1) | C(8)-C(9) | 1.370(3) |
| Mo(1)-N(2) | 2.239(2) | C(10)-C(7) | 1.444(3) |
| Mo(1)-O(7) | 2.308(1) | C(10)-N(4) | 1.288(2) |
| S(2)-C(3) | 1.801(2) | O(7)-S(1) | 1.536(1) |
| S(2)-C(6) | 1.818(2) | | |
| O(3)-Mo(1)-O(4) | 151.2(5) | O(6)-Mo(1)-O(7) | 167.2(6) |
| O(3)-Mo(1)-O(7) | 80.8(5) | O(3)-Mo(1)-N(2) | 82.7(5) |
| O(4)-Mo(1)-O(7) | 78.9(5) | O(4)-Mo(1)-N(2) | 71.8(5) |
| O(5)-Mo(1)-O(3) | 101.9(6) | O(5)-Mo(1)-N(2) | 157.4(6) |
| O(5)-Mo(1)-O(4) | 97.0(6) | O(6)-Mo(1)-N(2) | 94.9(6) |
| O(5)-Mo(1)-O(7) | 86.4(6) | N(2)-Mo(1)-O(7) | 72.4(5) |
| O(6)-Mo(1)-O(3) | 99.3(6) | C(3)-S(2)-C(6) | 92.2(9) |
| O(6)-Mo(1)-O(4) | 96.0(6) | C(5)-C(6)-S(2) | 108.1(1) |
| O(6)-Mo(1)-O(5) | 106.1(7) | N(4)-C(10)-C(7) | 123.7(2) |

Table B13. Bond lengths [\AA] and angles [$^\circ$] for C15

| | | | |
|------------------|----------|-------------------|----------|
| Mo(1)-O(1) | 1.920(1) | C(11)-C(16) | 1.406(2) |
| Mo(1)-O(2) | 1.713(1) | C(13)-C(12) | 1.406(2) |
| Mo(1)-O(3) | 1.706(1) | C(14)-C(13) | 1.381(2) |
| Mo(1)-O(4) | 2.030(1) | C(15)-C(14) | 1.393(2) |
| Mo(1)-O(6) | 2.293(1) | C(16)-C(15) | 1.379(2) |
| Mo(1)-N(1) | 2.234(1) | C(9)-N(1) | 1.286(2) |
| C(1)-C(2) | 1.407(2) | C(12)-O(7) | 1.354(2) |
| C(1)-C(6) | 1.412(2) | O(1)-C(1) | 1.343(2) |
| C(2)-C(3) | 1.408(2) | O(4)-C(10) | 1.318(2) |
| C(2)-C(9) | 1.445(2) | O(5)-C(6) | 1.358(2) |
| C(3)-C(4) | 1.370(2) | O(5)-C(7) | 1.443(2) |
| C(4)-C(5) | 1.391(2) | O(6)-S(1) | 1.528(1) |
| C(5)-C(6) | 1.389(2) | N(1)-N(2) | 1.390(2) |
| C(7)-C(8) | 1.505(2) | N(2)-C(10) | 1.307(2) |
| C(10)-C(11) | 1.459(2) | S(1)-C(17) | 1.784(2) |
| C(11)-C(12) | 1.407(2) | S(1)-C(18) | 1.789(2) |
| | | | |
| O(1)-Mo(1)-O(4) | 150.9(5) | C(1)-C(2)-C(3) | 119.4(2) |
| O(1)-Mo(1)-O(6) | 81.6(5) | C(1)-C(2)-C(9) | 122.9(1) |
| O(2)-Mo(1)-O(1) | 103.3(5) | C(2)-C(1)-C(6) | 119.4(1) |
| O(2)-Mo(1)-O(4) | 96.9(5) | C(3)-C(2)-C(9) | 117.6(2) |
| O(2)-Mo(1)-O(6) | 85.1(5) | C(3)-C(4)-C(5) | 120.2(2) |
| O(3)-Mo(1)-O(1) | 99.2(5) | C(4)-C(3)-C(2) | 120.7(2) |
| O(3)-Mo(1)-O(2) | 105.3(6) | C(5)-C(6)-C(1) | 119.5(1) |
| O(3)-Mo(1)-O(6) | 168.9(5) | C(6)-C(5)-C(4) | 120.8(2) |
| O(3)-Mo(1)-O(4) | 95.2(5) | C(12)-C(11)-C(10) | 121.1(1) |
| O(4)-Mo(1)-O(6) | 79.5(4) | C(13)-C(12)-C(11) | 119.8(1) |
| O(1)-Mo(1)-N(1) | 81.7(5) | C(13)-C(14)-C(15) | 120.8(2) |
| O(2)-Mo(1)-N(1) | 158.2(5) | C(14)-C(13)-C(12) | 120.1(2) |
| O(3)-Mo(1)-N(1) | 94.6(5) | C(9)-N(1)-N(2) | 115.8(2) |
| O(4)-Mo(1)-N(1) | 72.1(5) | C(10)-N(2)-N(1) | 110.7(1) |
| N(1)-Mo(1)-O(6) | 74.6(4) | N(1)-C(9)-C(2) | 123.9(1) |
| C(1)-O(1)-Mo(1) | 138.0(1) | N(2)-C(10)-O(4) | 122.6(1) |
| C(9)-N(1)-Mo(1) | 129.0(1) | N(2)-C(10)-C(11) | 119.1(1) |
| C(10)-O(4)-Mo(1) | 119.5(1) | O(1)-C(1)-C(6) | 117.7(1) |
| N(2)-N(1)-Mo(1) | 115.2(1) | O(4)-C(10)-C(11) | 118.4(1) |
| S(1)-O(6)-Mo(1) | 119.3(6) | O(7)-C(12)-C(13) | 116.6(1) |
| C(6)-O(5)-C(7) | 116.9(1) | O(7)-C(12)-C(11) | 123.5(2) |
| O(1)-C(1)-C(2) | 122.9(1) | | |

Table B14. Bond lengths [Å] and angles [°] for C16

| | | | |
|--------------|----------|--------------|----------|
| Mo(1)—O(1) | 2.011(3) | N(1) – C(7) | 1.311(5) |
| Mo(1) – O(4) | 1.918(3) | N(2) – C(8) | 1.292(5) |
| Mo(1) – O(5) | 1.707(3) | N(3) – C(16) | 1.338(5) |
| Mo(1) – O(6) | 1.705(3) | N(3) – C(20) | 1.341(6) |
| Mo(1) – O(7) | 2.289(3) | N(4) – C(21) | 1.337(5) |
| Mo(1) – N(2) | 2.238(3) | N(4) – C(25) | 1.340(6) |
| O(1) – C(7) | 1.326(5) | C(1) – C(2) | 1.408(5) |
| O(2) – C(6) | 1.355(5) | C(1) – C(6) | 1.410(5) |
| O(3) – C(4) | 1.352(5) | C(8) – C(9) | 1.448(5) |
| O(7) – C(15) | 1.436(5) | | |

| | | | |
|---------------------|----------|----------------------|----------|
| O(1) - Mo(1) - O(7) | 79.1(1) | O(4) – Mo(1) – N(2) | 82.0(1) |
| O(4) – Mo(1) - O(1) | 151.1(1) | O(5) – Mo(1) – N(2) | 160.0(1) |
| O(5) – Mo(1) – O(1) | 98.1(1) | O(6) – Mo(1) – N(2) | 93.5(1) |
| O(6) – Mo(1) – O(1) | 94.6(1) | N(2) – Mo(1) – O(7) | 76.7(1) |
| O(5) – Mo(1) – O(4) | 101.7(1) | C(7) – O(1) – Mo(1) | 119.7(1) |
| O(6) – Mo(1) – O(4) | 99.5(1) | C(14) – O(4) – Mo(1) | 138.0(2) |
| O(6) – Mo(1) – O(5) | 105.1(1) | C(15) – O(7) – Mo(1) | 122.4(2) |
| O(4) – Mo(1) – O(7) | 82.9(1) | C(7) – N(2) – Mo(1) | 128.6(3) |
| O(5) – Mo(1) – O(7) | 84.1(1) | N(1) – N(2) – Mo(1) | 115.2(2) |
| O(6) – Mo(1) – O(7) | 169.6(2) | | |

Table B15. Bond lengths [Å] and angles [°] for C17

| | | | |
|---------------------|----------|----------------------|----------|
| Mo(1)—O(1) | 2.250(2) | O(4) – C(13) | 1.431(3) |
| Mo(1) – O(2) | 2.027(2) | N(1) – C(5) | 1.292(5) |
| Mo(1) – O(3) | 1.926(2) | N(2) – C(6) | 1.291(3) |
| Mo(1) – O(5) | 1.709(2) | N(3) – C(15) | 1.288(4) |
| Mo(1) – O(6) | 1.707(2) | N(3) – C(19') | 1.291(5) |
| Mo(1) – N(2) | 2.250(2) | N(3) – C(15') | 1.454(4) |
| O(1) – C(1) | 1.371(3) | N(3) – C(19) | 1.371(6) |
| O(2) – C(5) | 1.313(2) | N(1) – N(2) | 1.398(2) |
| O(3) – C(12) | 1.345(3) | C(1) – C(2) | 1.344(4) |
| O(4) – C(11) | 1.365(3) | | |
| | | | |
| O(2) – Mo(1) – O(1) | 80.3(6) | O(3) – Mo(1) – N(2) | 81.2(6) |
| O(3) – Mo(1) – O(1) | 84.9(6) | O(5) – Mo(1) – N(2) | 157.5(7) |
| O(5) – Mo(1) – O(1) | 82.9(6) | O(6) – Mo(1) – N(2) | 96.0(7) |
| O(6) – Mo(1) – O(1) | 170.7(7) | O(2) – Mo(1) – N(2) | 72.0(6) |
| O(3) – Mo(1) – O(2) | 151.8(6) | O(1) – Mo(1) – N(2) | 75.4(6) |
| O(5) – Mo(1) – O(2) | 98.7(7) | C(5) – O(2) – Mo(1) | 119.0(1) |
| O(6) – Mo(1) – O(2) | 93.9(7) | C(12) – O(3) – Mo(1) | 134.5(2) |
| O(5) – Mo(1) – O(3) | 103.1(7) | C(6) – N(2) – Mo(1) | 128.8(1) |
| O(6) – Mo(1) – O(3) | 97.4(4) | N(1) – N(2) – Mo(1) | 115.2(1) |
| O(6) – Mo(1) – O(5) | 105.2(7) | | |

Table B16: Bond lengths [Å] and angles [°] for C18

| | | | |
|------------------|----------|------------------|----------|
| Mo(1)-O(1) | 1.923(2) | C(9)-C(2) | 1.450(4) |
| Mo(1)-O(2) | 1.707(2) | C(1)-O(1) | 1.343(3) |
| Mo(1)-O(3) | 1.692(2) | C(6)-O(5) | 1.361(4) |
| Mo(1)-O(4) | 2.026(2) | N(1)-N(2) | 1.411(3) |
| Mo(1)-O(6) | 2.327(2) | N(1)-C(9) | 1.286(3) |
| Mo(1)-N(1) | 2.234(2) | N(2)-C(10) | 1.296(4) |
| C(1)-C(6) | 1.411(4) | O(4)-C(10) | 1.312(3) |
| C(2)-C(1) | 1.408(4) | O(6)-C(13) | 1.436(4) |
| C(2)-C(3) | 1.411(4) | O(5)-C(7) | 1.445(3) |
| C(6)-C(5) | 1.385(4) | | |
| | | | |
| O(1)-Mo(1)-O(4) | 149.7(8) | C(13)-O(6)-Mo(1) | 127.1(2) |
| O(1)-Mo(1)-O(6) | 81.9(8) | C(9)-N(1)-Mo(1) | 126.9(2) |
| O(2)-Mo(1)-O(1) | 103.8(9) | C(1)-C(2)-C(3) | 119.4(3) |
| O(3)-Mo(1)-O(1) | 97.4(1) | C(1)-C(2)-C(9) | 122.5(2) |
| O(2)-Mo(1)-O(4) | 97.3(9) | C(2)-C(1)-C(6) | 119.7(3) |
| O(2)-Mo(1)-O(6) | 85.0(9) | C(3)-C(2)-C(9) | 118.1(3) |
| O(3)-Mo(1)-O(2) | 106.1(1) | C(5)-C(6)-C(1) | 119.2(3) |
| O(3)-Mo(1)-O(4) | 97.4(9) | N(2)-N(1)-Mo(1) | 115.8(2) |
| O(3)-Mo(1)-O(6) | 168.7(9) | C(9)-N(1)-N(2) | 116.9(2) |
| O(4)-Mo(1)-O(6) | 78.5(8) | C(10)-N(2)-N(1) | 109.1(2) |
| O(1)-Mo(1)-N(1) | 81.6(8) | N(1)-C(9)-C(2) | 123.3(3) |
| O(2)-Mo(1)-N(1) | 158.7(9) | O(1)-C(1)-C(2) | 122.9(2) |
| O(3)-Mo(1)-N(1) | 93.5(9) | O(1)-C(1)-C(6) | 117.3(3) |
| O(4)-Mo(1)-N(1) | 71.3(8) | O(5)-C(6)-C(5) | 125.8(3) |
| N(1)-Mo(1)-O(6) | 75.3(8) | O(5)-C(6)-C(1) | 115.0(3) |
| C(1)-O(1)-Mo(1) | 130.3(2) | C(6)-O(5)-C(7) | 117.1(2) |
| C(10)-O(4)-Mo(1) | 120.4(2) | | |

Table B17: Bond lengths [Å] and angles [°] for C19

| | | | |
|------------------|------------|------------------|------------|
| Mo(1)-O(1) | 1.931(1) | C(7)-C(2) | 1.450(2) |
| Mo(1)-O(2) | 1.698(1) | C(8)-C(9) | 1.498(2) |
| Mo(1)-O(3) | 1.701(1) | C(10)-C(9) | 1.534(2) |
| Mo(1)-O(4) | 2.016(1) | C(12)-C(11) | 1.499(3) |
| Mo(1)-O(5) | 2.279(1) | Cl(1)-C(6) | 1.729(2) |
| Mo(1)-N(1) | 2.259(1) | Cl(2)-C(4) | 1.736(2) |
| C(1)-C(2) | 1.412(2) | O(1)-C(1) | 1.327(2) |
| C(1)-C(6) | 1.406(2) | O(4)-C(8) | 1.312(2) |
| C(3)-C(2) | 1.405(2) | N(1)-C(7) | 1.286(2) |
| C(4)-C(3) | 1.377(2) | N(1)-N(2) | 1.404(2) |
| C(4)-C(5) | 1.397(2) | N(2)-C(8) | 1.303(2) |
| C(5)-C(6) | 1.382(2) | | |
| | | | |
| O(1)-Mo(1)-O(4) | 150.32(5) | C(1)-C(2)-C(7) | 122.76(15) |
| O(1)-Mo(1)-O(5) | 81.78(5) | C(3)-C(2)-C(1) | 119.87(16) |
| O(2)-Mo(1)-O(1) | 102.36(5) | C(3)-C(4)-C(5) | 121.28(16) |
| O(2)-Mo(1)-O(3) | 105.47(6) | C(3)-C(4)-Cl(2) | 119.77(14) |
| O(2)-Mo(1)-O(5) | 84.97(5) | C(3)-C(2)-C(7) | 117.36(15) |
| O(3)-Mo(1)-O(1) | 99.03(6) | C(4)-C(3)-C(2) | 119.95(16) |
| O(2)-Mo(1)-O(4) | 99.00(5) | C(5)-C(6)-C(1) | 121.84(16) |
| O(3)-Mo(1)-O(4) | 94.84(5) | C(6)-C(1)-C(2) | 118.25(16) |
| O(3)-Mo(1)-O(5) | 168.99(5) | C(6)-C(5)-C(4) | 118.75(16) |
| O(4)-Mo(1)-O(5) | 79.80(5) | C(8)-C(9)-C(10) | 115.37(14) |
| O(1)-Mo(1)-N(1) | 81.42(5) | C(5)-C(4)-Cl(2) | 118.94(14) |
| O(2)-Mo(1)-N(1) | 159.60(6) | C(8)-N(2)-N(1) | 110.00(13) |
| O(3)-Mo(1)-N(1) | 93.55(5) | N(1)-C(7)-C(2) | 123.60(15) |
| O(4)-Mo(1)-N(1) | 71.59(5) | N(2)-C(8)-O(4) | 123.04(15) |
| N(1)-Mo(1)-O(5) | 75.66(5) | N(2)-C(8)-C(9) | 119.28(14) |
| C(1)-O(1)-Mo(1) | 138.07(11) | O(1)-C(1)-C(2) | 123.77(15) |
| C(7)-N(1)-Mo(1) | 128.92(11) | O(1)-C(1)-C(6) | 117.98(15) |
| C(8)-O(4)-Mo(1) | 120.58(11) | O(4)-C(8)-C(9) | 117.68(15) |
| C(11)-O(5)-Mo(1) | 127.85(11) | O(5)-C(11)-C(12) | 110.92(15) |
| N(2)-N(1)-Mo(1) | 114.56(10) | C(5)-C(6)-Cl(1) | 119.65(13) |
| C(7)-N(1)-N(2) | 116.46(13) | C(1)-C(6)-Cl(1) | 118.50(13) |

Table B18: Bond lengths [Å] and angles [°] for C20

| | | | |
|-----------------|-----------|------------------|----------|
| Mo(1)-O(1) | 1.948(1) | C(1)-O(1) | 1.338(2) |
| Mo(1)-O(2) | 1.708(1) | C(16)-O(4) | 1.344(2) |
| Mo(1)-O(3) | 1.711(1) | C(4)-Cl(1) | 1.742(2) |
| Mo(2)-O(4) | 1.951(1) | C(19)-Cl(2) | 1.740(1) |
| Mo(2)-O(5) | 1.712(1) | C(11)-N(4) | 1.336(2) |
| Mo(2)-O(6) | 1.705(1) | C(12)-N(4) | 1.341(2) |
| Mo(1)-N(1) | 2.293(1) | C(24)-N(7) | 1.456(2) |
| Mo(1)-N(4) | 2.457(1) | C(8)-S(1) | 1.761(2) |
| Mo(2)-N(5) | 2.269(1) | N(5)-N(6) | 1.380(2) |
| Mo(2)-N(8) | 2.427(1) | N(1)-C(7) | 1.297(2) |
| Mo(1)-S(1) | 2.412(4) | N(3)-C(8) | 1.342(2) |
| Mo(2)-S(2) | 2.425(4) | N(3)-C(9) | 1.458(2) |
| N(8)-C(27) | 1.337(2) | N(5)-C(22) | 1.295(2) |
| N(8)-C(26) | 1.343(2) | N(6)-C(23) | 1.308(2) |
| N(2)-N(1) | 1.384(2) | N(7)-C(23) | 1.338(2) |
| | | | |
| O(3)-Mo(1)-O(1) | 100.2(5) | S(1)-Mo(1)-N(4) | 80.4(3) |
| O(5)-Mo(2)-O(4) | 106.3(5) | O(2)-Mo(1)-O(1) | 105.0(5) |
| O(6)-Mo(2)-O(4) | 98.0(5) | O(2)-Mo(1)-O(3) | 105.9(5) |
| O(6)-Mo(2)-O(5) | 106.3(5) | O(4)-Mo(2)-N(5) | 80.7(4) |
| O(1)-Mo(1)-N(1) | 80.7(4) | O(4)-Mo(2)-N(8) | 76.8(4) |
| O(2)-Mo(1)-N(1) | 160.4(5) | O(5)-Mo(2)-N(8) | 83.0(5) |
| O(3)-Mo(1)-N(1) | 91.1(5) | O(6)-Mo(2)-N(8) | 170.5(5) |
| O(1)-Mo(1)-S(1) | 149.6 (3) | O(5)-Mo(2)-S(2) | 90.7(4) |
| O(2)-Mo(1)-S(1) | 91.2(4) | O(6)-Mo(2)-S(2) | 101.3(4) |
| O(3)-Mo(1)-S(1) | 99.7(4) | O(4)-Mo(2)-S(2) | 149.5(3) |
| O(1)-Mo(1)-N(4) | 77.3(4) | N(5)-Mo(2)-N(8) | 82.0(4) |
| O(2)-Mo(1)-N(4) | 80.5(5) | N(5)-Mo(2)-S(2) | 76.2(3) |
| O(3)-Mo(1)-N(4) | 173.5(5) | S(2)-Mo(2)-N(8) | 80.5(3) |
| O(5)-Mo(2)-N(5) | 161.4(5) | C(27)-N(8)-C(26) | 117.0(1) |
| O(6)-Mo(2)-N(5) | 89.3(5) | C(27)-N(8)-Mo(2) | 124.0(1) |
| N(1)-Mo(1)-N(4) | 82.6(4) | C(26)-N(8)-Mo(2) | 118.9(9) |
| N(1)-Mo(1)-S(1) | 76.2(3) | C(8)-N(2)-N(1) | 113.4(1) |

Table B19: Bond lengths [Å] and angles [°] for C21

| | | | |
|-----------------|----------|-------------------|----------|
| Mo(1)-O(1) | 1.952(2) | C(13)-C(12) | 1.373(4) |
| Mo(1)-O(2) | 1.711(2) | C(13)-C(14) | 1.399(4) |
| Mo(1)-O(3) | 1.708(2) | C(14)-C(15) | 1.400(4) |
| Mo(1)-O(4) | 2.294(2) | C(7)-N(1) | 1.301(4) |
| Mo(1)-N(1) | 2.286(2) | C(8)-N(3) | 1.341(4) |
| Mo(1)-S(1) | 2.416(7) | S(1)-C(8) | 1.755(3) |
| C(1)-C(6) | 1.402(4) | Cl(1)-C(4) | 1.749(3) |
| C(2)-C(1) | 1.407(4) | Cl(2)-C(6) | 1.733(3) |
| C(3)-C(2) | 1.410(4) | O(1)-C(1) | 1.333(4) |
| C(3)-C(4) | 1.370(4) | N(2)-C(8) | 1.313(4) |
| C(5)-C(4) | 1.391(4) | N(2)-N(1) | 1.379(3) |
| C(5)-C(6) | 1.376(4) | N(3)-C(9) | 1.464(4) |
| C(7)-C(2) | 1.446(4) | N(4)-C(12) | 1.342(4) |
| C(9)-C(10) | 1.508(4) | N(4)-C(11) | 1.351(4) |
| C(11)-C(15) | 1.373(4) | N(4)-O(4) | 1.346(3) |
| | | | |
| O(1)-Mo(1)-O(4) | 75.0(8) | C(1)-C(2)-C(7) | 122.8(3) |
| O(2)-Mo(1)-O(4) | 85.0(9) | C(3)-C(2)-C(7) | 117.4(3) |
| O(3)-Mo(1)-O(4) | 169.1(9) | C(3)-C(4)-C(5) | 121.9(3) |
| O(2)-Mo(1)-O(1) | 108.8(9) | C(4)-C(3)-C(2) | 119.6(3) |
| O(3)-Mo(1)-O(1) | 96.3(1) | C(6)-C(5)-C(4) | 118.5(3) |
| O(3)-Mo(1)-O(2) | 104.2(1) | C(12)-C(13)-C(14) | 121.2(3) |
| O(3)-Mo(1)-N(1) | 89.2(9) | C(3)-C(4)-Cl(1) | 119.8(2) |
| O(2)-Mo(1)-N(1) | 161.5(1) | C(5)-C(4)-Cl(1) | 118.3(2) |
| O(1)-Mo(1)-N(1) | 81.8(9) | C(12)-N(4)-O(4) | 119.6(2) |
| O(1)-Mo(1)-S(1) | 150.7(7) | C(12)-N(4)-C(11) | 121.4(3) |
| O(2)-Mo(1)-S(1) | 88.9(7) | C(8)-N(2)-N(1) | 114.2(2) |
| O(3)-Mo(1)-S(1) | 101.9(8) | C(7)-N(1)-N(2) | 113.5(2) |
| O(4)-Mo(1)-S(1) | 83.8(5) | O(4)-N(4)-C(11) | 119.1(2) |
| N(1)-Mo(1)-O(4) | 83.3(8) | N(4)-O(4)-Mo(1) | 117.4(2) |
| N(1)-Mo(1)-S(1) | 75.7(6) | N(1)-C(7)-C(2) | 126.5(3) |
| C(1)-O(1)-Mo(1) | 131.9(2) | N(2)-C(8)-N(3) | 117.9(2) |
| C(7)-N(1)-Mo(1) | 122.1(2) | N(2)-C(8)-S(1) | 124.9(2) |
| C(8)-S(1)-Mo(1) | 101.5(1) | N(3)-C(8)-S(1) | 117.2(2) |
| N(2)-N(1)-Mo(1) | 123.6(2) | N(3)-C(9)-C(10) | 109.8(2) |
| C(1)-C(2)-C(3) | 119.6(3) | | |

Table B20: Bond lengths [Å] and angles [°] for C22

| | | | |
|------------------|----------|-------------------|----------|
| Mo(1)-O(1) | 1.929(2) | O(5)-C(6) | 1.362(4) |
| Mo(1)-O(2) | 1.713(2) | O(5)-C(7) | 1.432(4) |
| Mo(1)-O(3) | 1.700(2) | O(1)-C(1) | 1.341(4) |
| Mo(1)-O(4) | 2.022(2) | O(4)-C(10) | 1.318(4) |
| Mo(1)-O(6) | 2.205(2) | C(13)-N(3) | 1.462(5) |
| Mo(1)-N(1) | 2.243(3) | C(15)-N(4) | 1.460(5) |
| C(1)-C(2) | 1.411(5) | C(16)-N(4) | 1.458(5) |
| C(1)-C(6) | 1.416(5) | C(17)-N(5) | 1.463(4) |
| C(2)-C(3) | 1.403(5) | C(18)-N(5) | 1.464(4) |
| C(4)-C(3) | 1.366(6) | P(1)-O(6) | 1.503(2) |
| C(5)-C(4) | 1.396(6) | P(1)-N(4) | 1.631(3) |
| C(5)-C(6) | 1.382(5) | P(1)-N(5) | 1.642(3) |
| C(7)-C(8) | 1.507(5) | P(1)-N(3) | 1.644(3) |
| C(9)-C(2) | 1.440(5) | N(1)-N(2) | 1.404(4) |
| C(11)-C(10) | 1.496(5) | N(2)-C(10) | 1.296(5) |
| C(11)-C(12) | 1.521(5) | N(3)-C(14) | 1.469(5) |
| C(9)-N(1) | 1.286(5) | | |
| O(1)-Mo(1)-O(4) | 150.6(1) | C(6)-O(5)-C(7) | 116.8(3) |
| O(1)-Mo(1)-O(6) | 83.3(1) | C(10)-C(11)-C(12) | 111.8(3) |
| O(2)-Mo(1)-O(1) | 104.3(1) | C(13)-N(3)-C(14) | 112.4(3) |
| O(3)-Mo(1)-O(1) | 98.3(1) | C(16)-N(4)-C(15) | 113.8(3) |
| O(2)-Mo(1)-O(4) | 97.5(1) | C(9)-N(1)-N(2) | 116.1(3) |
| O(2)-Mo(1)-O(6) | 88.0(1) | C(10)-N(2)-N(1) | 108.8(3) |
| O(3)-Mo(1)-O(2) | 105.0(1) | C(17)-N(5)-C(18) | 114.1(3) |
| O(3)-Mo(1)-O(4) | 94.8(1) | C(13)-N(3)-P(1) | 118.6(3) |
| O(3)-Mo(1)-O(6) | 166.0(1) | C(14)-N(3)-P(1) | 119.0(3) |
| O(4)-Mo(1)-O(6) | 77.9(9) | C(15)-N(4)-P(1) | 119.9(2) |
| O(1)-Mo(1)-N(1) | 81.8(1) | C(16)-N(4)-P(1) | 125.5(3) |
| O(2)-Mo(1)-N(1) | 162.2(1) | C(17)-N(5)-P(1) | 120.8(2) |
| O(3)-Mo(1)-N(1) | 90.4(1) | C(18)-N(5)-P(1) | 122.1(2) |
| O(4)-Mo(1)-N(1) | 71.8(1) | N(1)-C(9)-C(2) | 123.5(3) |
| O(6)-Mo(1)-N(1) | 76.0(9) | N(4)-P(1)-N(3) | 103.3(2) |
| C(1)-O(1)-Mo(1) | 134.2(2) | N(4)-P(1)-N(5) | 111.7(2) |
| C(10)-O(4)-Mo(1) | 119.2(2) | N(5)-P(1)-N(3) | 109.0(2) |
| C(9)-N(1)-Mo(1) | 128.1(2) | O(1)-C(1)-C(2) | 123.9(3) |
| N(2)-N(1)-Mo(1) | 115.7(2) | O(1)-C(1)-C(6) | 116.8(3) |
| C(1)-C(2)-C(9) | 122.8(3) | O(5)-C(6)-C(1) | 114.8(3) |
| C(2)-C(1)-C(6) | 119.3(3) | O(5)-C(6)-C(5) | 125.3(3) |
| C(3)-C(4)-C(5) | 120.5(3) | O(5)-C(7)-C(8) | 107.1(3) |
| C(3)-C(2)-C(1) | 119.1(3) | O(6)-P(1)-N(3) | 116.6(2) |
| C(3)-C(2)-C(9) | 118.1(3) | O(6)-P(1)-N(4) | 111.1(2) |
| C(5)-C(6)-C(1) | 119.8(3) | O(6)-P(1)-N(5) | 105.4(1) |
| C(6)-C(5)-C(4) | 120.3(4) | P(1)-O(6)-Mo(1) | 140.5(1) |

Table B21: Bond lengths [Å] and angles [°] for C23

| | | | |
|------------------|----------|-------------------|----------|
| Mo(1)-O(1) | 1.941(1) | C(10)-C(11) | 1.496(2) |
| Mo(1)-O(2) | 1.717(1) | C(11)-C(12) | 1.531(3) |
| Mo(1)-O(3) | 1.703(1) | O(1)-C(1) | 1.350(2) |
| Mo(1)-O(4) | 2.014(1) | O(4)-C(10) | 1.324(2) |
| Mo(1)-O(6) | 2.285(1) | O(5)-C(6) | 1.362(2) |
| Mo(1)-N(1) | 2.224(2) | O(5)-C(7) | 1.437(2) |
| C(2)-C(1) | 1.408(2) | O(6)-C(13) | 1.252(2) |
| C(2)-C(3) | 1.409(3) | N(1)-C(9) | 1.285(2) |
| C(3)-C(4) | 1.381(3) | N(1)-N(2) | 1.403(2) |
| C(4)-C(5) | 1.397(3) | N(2)-C(10) | 1.296(2) |
| C(5)-C(6) | 1.387(3) | N(3)-C(13) | 1.301(2) |
| C(6)-C(1) | 1.415(2) | N(3)-C(15) | 1.456(2) |
| C(7)-C(8) | 1.506(3) | N(3)-C(14) | 1.461(2) |
| C(9)-C(2) | 1.448(3) | | |
| O(1)-Mo(1)-O(4) | 147.4(6) | C(3)-C(2)-C(9) | 118.0(2) |
| O(1)-Mo(1)-O(6) | 79.0(5) | C(3)-C(4)-C(5) | 120.0(2) |
| O(2)-Mo(1)-O(1) | 106.8(6) | C(4)-C(3)-C(2) | 120.5(2) |
| O(2)-Mo(1)-O(4) | 94.8(6) | C(5)-C(6)-C(1) | 119.6(2) |
| O(2)-Mo(1)-O(6) | 84.9(6) | C(6)-C(5)-C(4) | 120.8(2) |
| O(3)-Mo(1)-O(1) | 97.1(6) | C(10)-C(11)-C(12) | 111.6(2) |
| O(3)-Mo(1)-O(2) | 105.1(7) | C(9)-N(1)-N(2) | 117.5(2) |
| O(3)-Mo(1)-O(4) | 100.4(6) | C(6)-O(5)-C(7) | 116.6(1) |
| O(3)-Mo(1)-O(6) | 169.9(6) | C(13)-N(3)-C(15) | 120.7(2) |
| O(4)-Mo(1)-O(6) | 79.0(5) | C(13)-N(3)-C(14) | 121.5(2) |
| O(1)-Mo(1)-N(1) | 81.1(5) | C(15)-N(3)-C(14) | 117.7(2) |
| O(2)-Mo(1)-N(1) | 160.9(6) | C(10)-N(2)-N(1) | 108.2(2) |
| O(3)-Mo(1)-N(1) | 90.7(6) | N(1)-C(9)-C(2) | 122.7(2) |
| O(4)-Mo(1)-N(1) | 71.5(5) | N(2)-C(10)-O(4) | 123.8(2) |
| N(1)-Mo(1)-O(6) | 79.5(5) | N(2)-C(10)-C(11) | 119.8(2) |
| C(1)-O(1)-Mo(1) | 127.8(1) | O(1)-C(1)-C(2) | 123.0(2) |
| C(10)-O(4)-Mo(1) | 119.5(1) | O(1)-C(1)-C(6) | 117.4(2) |
| C(13)-O(6)-Mo(1) | 117.9(1) | O(4)-C(10)-C(11) | 116.5(2) |
| C(9)-N(1)-Mo(1) | 125.3(1) | O(5)-C(6)-C(5) | 125.1(2) |
| N(2)-N(1)-Mo(1) | 116.5(1) | O(5)-C(6)-C(1) | 115.3(2) |
| C(1)-C(2)-C(3) | 119.4(2) | O(5)-C(7)-C(8) | 107.3(2) |
| C(1)-C(2)-C(9) | 122.4(2) | O(6)-C(13)-N(3) | 124.7(2) |
| C(2)-C(1)-C(6) | 119.5(2) | | |

Table B22: Bond lengths [Å] and angles [°] for C24

| | | | |
|------------------|----------|-------------------|----------|
| Mo(1)-O(1) | 1.933(3) | C(9)-C(10) | 1.523(6) |
| Mo(1)-O(2) | 1.729(3) | C(11)-C(12) | 1.384(7) |
| Mo(1)-O(3) | 1.696(3) | C(12)-C(13) | 1.381(6) |
| Mo(1)-O(4) | 2.001(3) | C(13)-C(14) | 1.384(6) |
| Mo(1)-N(1) | 2.217(4) | C(14)-C(15) | 1.372(7) |
| Mo(1)-N(3) | 2.391(4) | O(1)-C(1) | 1.360(5) |
| C(1)-C(2) | 1.410(6) | O(4)-C(8) | 1.315(5) |
| C(1)-C(6) | 1.384(6) | O(5)-C(5) | 1.353(5) |
| C(2)-C(3) | 1.409(5) | O(6)-C(16) | 1.362(8) |
| C(2)-C(7) | 1.438(6) | N(1)-C(7) | 1.292(5) |
| C(3)-C(4) | 1.377(6) | N(1)-N(2) | 1.403(5) |
| C(4)-C(5) | 1.403(7) | N(2)-C(8) | 1.292(5) |
| C(5)-C(6) | 1.402(6) | N(3)-C(11) | 1.336(6) |
| C(8)-C(9) | 1.484(6) | | |
| O(1)-Mo(1)-O(4) | 149.1(1) | C(3)-C(2)-C(1) | 118.1(4) |
| O(2)-Mo(1)-O(1) | 107.3(1) | C(3)-C(2)-C(7) | 118.0(4) |
| O(2)-Mo(1)-O(4) | 93.7(1) | C(3)-C(4)-C(5) | 119.1(4) |
| O(3)-Mo(1)-O(1) | 97.3(1) | C(4)-C(3)-C(2) | 121.8(4) |
| O(3)-Mo(1)-O(2) | 106.3(2) | C(6)-C(1)-C(2) | 120.7(4) |
| O(3)-Mo(1)-O(4) | 98.1(2) | C(6)-C(5)-C(4) | 120.3(4) |
| O(1)-Mo(1)-N(1) | 81.8(1) | C(8)-C(9)-C(10) | 112.0(4) |
| O(2)-Mo(1)-N(1) | 159.6(1) | C(12)-C(13)-C(14) | 116.5(4) |
| O(3)-Mo(1)-N(1) | 90.1(2) | C(13)-C(12)-C(11) | 120.2(4) |
| O(1)-Mo(1)-N(3) | 80.6(1) | C(15)-C(14)-C(13) | 120.4(4) |
| O(2)-Mo(1)-N(3) | 84.2(1) | C(7)-N(1)-N(2) | 116.7(4) |
| O(3)-Mo(1)-N(3) | 169.4(2) | C(8)-N(2)-N(1) | 108.5(4) |
| O(4)-Mo(1)-N(3) | 79.4(1) | C(11)-N(3)-C(15) | 116.4(4) |
| O(4)-Mo(1)-N(1) | 71.7(1) | O(1)-C(1)-C(2) | 121.5(4) |
| N(1)-Mo(1)-N(3) | 79.3(1) | O(1)-C(1)-C(6) | 117.8(4) |
| C(1)-O(1)-Mo(1) | 130.7(3) | O(4)-C(8)-C(9) | 116.3(4) |
| C(8)-O(4)-Mo(1) | 120.1(3) | O(5)-C(5)-C(4) | 122.2(4) |
| C(7)-N(1)-Mo(1) | 126.0(3) | O(5)-C(5)-C(6) | 117.5(4) |
| C(11)-N(3)-Mo(1) | 124.7(3) | N(1)-C(7)-C(2) | 123.3(4) |
| C(15)-N(3)-Mo(1) | 118.9(3) | N(2)-C(8)-C(9) | 120.2(4) |
| N(2)-N(1)-Mo(1) | 116.1(2) | N(2)-C(8)-O(4) | 123.5(4) |
| C(1)-C(2)-C(7) | 123.9(4) | N(3)-C(11)-C(12) | 123.3(4) |
| C(1)-C(6)-C(5) | 120.0(4) | N(3)-C(15)-C(14) | 123.2(4) |

Table B23. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **C1**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | U(eq) |
|-------|----------|---------|---------|-------|
| Mo(1) | 10526(1) | 4934(1) | 2522(1) | 12(1) |
| Cl(1) | 7338(1) | -353(1) | -390(1) | 17(1) |
| N(1) | 9569(4) | 2479(4) | 3070(2) | 13(1) |
| N(2) | 9868(4) | 1651(4) | 3945(2) | 14(1) |
| N(3) | 11440(4) | 1473(4) | 5232(2) | 15(1) |
| O(1) | 8422(3) | 5390(3) | 1696(1) | 17(1) |
| O(2) | 10975(3) | 7011(3) | 2495(2) | 18(1) |
| O(3) | 12408(3) | 3391(3) | 1891(2) | 19(1) |
| O(4) | 7669(3) | 6623(3) | 3358(1) | 16(1) |
| S(1) | 11895(1) | 4009(1) | 4005(1) | 15(1) |
| S(2) | 5615(1) | 6667(1) | 3168(1) | 15(1) |
| C(1) | 8161(4) | 4047(4) | 1230(2) | 14(1) |
| C(2) | 8283(4) | 2260(4) | 1650(2) | 13(1) |
| C(3) | 7960(4) | 923(5) | 1143(2) | 15(1) |
| C(4) | 7571(4) | 1368(5) | 248(2) | 15(1) |
| C(5) | 7423(4) | 3149(5) | -164(2) | 16(1) |
| C(6) | 7707(5) | 4494(5) | 333(2) | 17(1) |
| C(7) | 8758(4) | 1676(4) | 2578(2) | 14(1) |
| C(8) | 10937(4) | 2271(4) | 4400(2) | 13(1) |
| C(9) | 4214(5) | 7442(5) | 4185(2) | 23(1) |
| C(10) | 4489(5) | 8833(5) | 2486(2) | 25(1) |

Table B24. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **C2**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | $U(\text{eq})$ |
|-------|----------|----------|----------|----------------|
| Mo(1) | 2924(1) | 1377(1) | 2530(1) | 14(1) |
| Cl(1) | 6616(1) | -5366(1) | 1465(1) | 28(1) |
| N(1) | 2462(2) | 523(2) | 713(2) | 15(1) |
| N(2) | 1540(2) | 1272(2) | -377(2) | 16(1) |
| N(3) | -10(3) | 3325(2) | -1207(2) | 20(1) |
| O(1) | 3645(2) | -517(2) | 3335(2) | 16(1) |
| O(2) | 4779(2) | 1733(2) | 1932(2) | 23(1) |
| O(3) | 2568(2) | 2228(2) | 3792(2) | 22(1) |
| O(4) | 583(2) | 479(2) | 3045(2) | 17(1) |
| S(1) | 1141(1) | 3194(1) | 1154(1) | 19(1) |
| S(2) | -1208(1) | 1158(1) | 2824(1) | 16(1) |
| C(1) | 917(3) | 2491(2) | -237(2) | 18(1) |
| C(3) | -215(3) | 3035(2) | -2502(2) | 19(1) |
| C(4) | -1326(3) | 4205(3) | -3333(2) | 25(1) |
| C(7) | 3090(3) | -672(2) | 569(2) | 18(1) |
| C(8) | 4076(3) | -1701(2) | 1541(2) | 16(1) |
| C(9) | 4798(3) | -2886(2) | 1132(2) | 19(1) |
| C(10) | 5719(3) | -3910(2) | 1993(2) | 20(1) |
| C(11) | 5943(3) | -3814(2) | 3293(2) | 20(1) |
| C(12) | 5237(3) | -2658(2) | 3716(2) | 18(1) |
| C(13) | 4308(3) | -1597(2) | 2851(2) | 14(1) |
| C(16) | -1591(3) | 2108(3) | 4096(2) | 22(1) |
| C(17) | -2306(3) | -203(2) | 3462(2) | 21(1) |

Table B25. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **C3**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | U(eq) |
|-------|----------|----------|----------|-------|
| Mo(1) | 525(1) | 4520(1) | 7515(1) | 10(1) |
| Cl(1) | 8399(1) | 1532(1) | 4333(1) | 25(1) |
| N(1) | 654(2) | 2367(2) | 7093(1) | 12(1) |
| N(2) | -850(2) | 1495(2) | 7334(1) | 13(1) |
| N(3) | -3968(2) | 1314(2) | 8087(1) | 13(1) |
| O(1) | 3227(2) | 4362(2) | 7042(1) | 15(1) |
| O(2) | 231(2) | 5750(2) | 8228(1) | 15(1) |
| O(3) | -371(2) | 5400(2) | 6491(1) | 14(1) |
| O(4) | 1896(2) | 2902(2) | 8773(1) | 16(1) |
| S(1) | -2445(1) | 3531(1) | 8335(1) | 13(1) |
| S(2) | 1194(1) | 3173(1) | 9774(1) | 15(1) |
| C(1) | 4324(3) | 3740(2) | 6381(1) | 12(1) |
| C(2) | 3760(3) | 2568(2) | 6097(1) | 13(1) |
| C(3) | 5032(3) | 1913(2) | 5438(2) | 16(1) |
| C(4) | 6791(3) | 2416(2) | 5092(2) | 16(1) |
| C(5) | 7342(3) | 3584(2) | 5368(1) | 14(1) |
| C(6) | 6103(3) | 4248(2) | 6004(1) | 13(1) |
| C(7) | 2009(3) | 1914(2) | 6492(1) | 14(1) |
| C(8) | -2328(3) | 1997(2) | 7850(1) | 12(1) |
| C(9) | -4362(3) | 39(2) | 7849(1) | 13(1) |
| C(10) | -3121(3) | -716(2) | 7251(2) | 17(1) |
| C(11) | -3625(3) | -1990(2) | 7093(2) | 20(1) |
| C(12) | -5346(3) | -2519(2) | 7516(2) | 23(1) |
| C(13) | -6600(3) | -1747(3) | 8092(2) | 25(1) |
| C(14) | -6122(3) | -479(2) | 8262(2) | 18(1) |
| C(15) | 1365(4) | 1404(3) | 10518(2) | 29(1) |
| C(16) | 3171(3) | 3834(3) | 10098(2) | 30(1) |

Table B26. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters

($\text{\AA}^2 \times 10^3$) for **C4**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | $U(\text{eq})$ |
|-------|---------|----------|---------|----------------|
| Mo(1) | 965(1) | 5837(1) | 1673(1) | 20(1) |
| N(1) | 2161(2) | 5890(5) | 1723(2) | 17(1) |
| N(2) | 2429(2) | 6647(6) | 2147(2) | 19(1) |
| O(1) | 1166(2) | 4401(7) | 1111(2) | 32(1) |
| O(2) | 122(2) | 5264(6) | 1821(2) | 26(1) |
| O(3) | 909(2) | 7812(7) | 1387(2) | 38(1) |
| O(4) | 1243(2) | 6758(5) | 2332(1) | 25(1) |
| O(5) | 850(2) | 3151(6) | 255(1) | 26(1) |
| O(6) | 1241(2) | 3223(5) | 2081(2) | 28(1) |
| O(7) | 3423(3) | 8897(7) | 3826(2) | 43(1) |
| C(1) | 1711(3) | 4203(7) | 798(2) | 18(1) |
| C(2) | 2412(3) | 4597(7) | 929(2) | 17(1) |
| C(3) | 2957(3) | 4211(6) | 584(2) | 19(1) |
| C(4) | 2794(3) | 3491(7) | 134(2) | 23(1) |
| C(5) | 2090(3) | 3132(7) | 7(2) | 22(1) |
| C(6) | 1553(3) | 3484(7) | 338(2) | 20(1) |
| C(7) | 648(3) | 2499(8) | -215(2) | 28(1) |
| C(8) | -152(4) | 2357(9) | -216(2) | 38(2) |
| C(9) | 2609(3) | 5383(7) | 1393(2) | 18(1) |
| C(10) | 1908(3) | 7039(6) | 2444(2) | 19(1) |
| C(11) | 2033(3) | 7819(7) | 2937(2) | 22(1) |
| C(12) | 2713(3) | 8027(8) | 3123(2) | 28(1) |
| C(13) | 2796(4) | 8703(8) | 3598(2) | 33(1) |
| C(14) | 2207(4) | 9126(8) | 3882(2) | 35(2) |
| C(15) | 1538(4) | 8927(9) | 3695(3) | 42(2) |
| C(16) | 1436(4) | 8290(9) | 3216(2) | 35(1) |
| C(17) | 4038(4) | 8633(14) | 3536(3) | 53(2) |
| C(18) | 650(7) | 1772(19) | 2177(6) | 175(11) |

Table B27. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters

(Å²x 10³) for **C6**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | U(eq) |
|-------|----------|----------|----------|-------|
| Mo(1) | 7312(1) | 7638(1) | 9041(1) | 37(1) |
| Cl(1) | 3394(1) | 8021(1) | 15030(1) | 77(1) |
| N(1) | 7537(2) | 9243(2) | 9721(2) | 35(1) |
| N(2) | 8466(2) | 10277(2) | 8897(2) | 38(1) |
| O(1) | 6502(2) | 6728(2) | 10779(2) | 42(1) |
| O(2) | 7820(3) | 6440(2) | 8487(2) | 59(1) |
| O(3) | 5530(2) | 8275(2) | 8498(2) | 60(1) |
| O(4) | 8769(2) | 8960(2) | 7759(2) | 43(1) |
| O(5) | 11557(2) | 14262(2) | 5756(2) | 54(1) |
| O(6) | 9624(2) | 7090(2) | 9960(2) | 44(1) |
| S(1) | 11316(1) | 7475(1) | 9319(1) | 43(1) |
| C(1) | 5954(3) | 8316(2) | 11748(2) | 38(1) |
| C(2) | 5802(3) | 7084(2) | 11729(2) | 38(1) |
| C(3) | 4922(3) | 6163(2) | 12735(2) | 48(1) |
| C(4) | 4174(3) | 6448(3) | 13751(3) | 54(1) |
| C(5) | 4315(3) | 7654(3) | 13756(2) | 49(1) |
| C(6) | 5204(3) | 8589(2) | 12789(2) | 46(1) |
| C(7) | 6909(3) | 9326(2) | 10770(2) | 40(1) |
| C(8) | 9050(3) | 10033(2) | 7900(2) | 35(1) |
| C(9) | 10124(3) | 10946(2) | 6885(2) | 37(1) |
| C(10) | 10315(3) | 12182(2) | 6856(2) | 37(1) |
| C(11) | 11305(3) | 13027(2) | 5877(2) | 42(1) |
| C(12) | 12107(3) | 12652(3) | 4930(2) | 50(1) |
| C(13) | 11952(3) | 11433(3) | 4978(2) | 54(1) |
| C(14) | 10942(3) | 10557(2) | 5946(2) | 46(1) |
| C(15) | 10702(4) | 14723(3) | 6657(3) | 58(1) |
| C(16) | 11911(5) | 6492(4) | 8433(3) | 76(1) |
| C(17) | 12524(3) | 6737(3) | 10548(3) | 55(1) |

Table B28. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **C7**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | $U(\text{eq})$ |
|-------|----------|----------|----------|----------------|
| Mo(1) | 3027(1) | 2263(1) | 1287(1) | 14(1) |
| Cl(1) | 5950(1) | 2096(1) | -5497(1) | 36(1) |
| N(1) | 2524(2) | 665(2) | 195(2) | 16(1) |
| N(2) | 1657(2) | -450(2) | 901(2) | 18(1) |
| O(1) | 3645(2) | 3297(2) | -464(2) | 18(1) |
| O(2) | 2697(2) | 3472(2) | 2195(2) | 20(1) |
| O(3) | 4874(2) | 1561(2) | 1697(2) | 23(1) |
| O(4) | 1664(2) | 828(2) | 2481(2) | 18(1) |
| O(5) | -204(3) | -1158(3) | 4181(2) | 42(1) |
| O(6) | 598(2) | 2964(2) | 448(2) | 18(1) |
| S(1) | -1064(1) | 2797(1) | 1180(1) | 20(1) |
| C(1) | 4189(3) | 2968(2) | -1588(2) | 16(1) |
| C(2) | 3854(3) | 1708(2) | -1880(2) | 16(1) |
| C(3) | 4414(3) | 1458(2) | -3106(2) | 19(1) |
| C(4) | 5297(3) | 2428(3) | -3977(2) | 22(1) |
| C(5) | 5660(3) | 3662(3) | -3684(2) | 22(1) |
| C(6) | 5095(3) | 3924(2) | -2498(2) | 19(1) |
| C(7) | 2940(3) | 649(2) | -1012(2) | 16(1) |
| C(8) | 1298(3) | -274(2) | 2076(2) | 17(1) |
| C(9) | 425(3) | -1324(2) | 3021(2) | 18(1) |
| C(10) | -935(4) | -2402(4) | 4778(3) | 42(1) |
| C(11) | -760(4) | -3236(3) | 3969(4) | 40(1) |
| C(12) | 118(3) | -2571(2) | 2834(2) | 20(1) |
| C(13) | -1242(3) | 4113(3) | 2078(3) | 26(1) |
| C(14) | -2396(3) | 3517(3) | -72(3) | 27(1) |

Table B29. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **C8**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | U(eq) |
|-------|---------|----------|---------|-------|
| Mo(1) | 2630(1) | 10966(1) | 3493(1) | 11(1) |
| Cl(1) | 1753(1) | 6308(1) | 5990(1) | 24(1) |
| N(1) | 3957(3) | 9701(2) | 3583(2) | 11(1) |
| N(2) | 5144(3) | 9875(2) | 3262(3) | 14(1) |
| O(1) | 1431(2) | 9987(2) | 3767(2) | 14(1) |
| O(2) | 1650(2) | 11913(2) | 3034(2) | 17(1) |
| O(3) | 3284(2) | 11257(2) | 4779(2) | 18(1) |
| O(4) | 4170(2) | 11334(2) | 2833(2) | 15(1) |
| O(5) | 7646(2) | 9710(2) | 3318(2) | 15(1) |
| O(6) | 1830(3) | 10490(2) | 1722(2) | 20(1) |
| O(7) | 9556(2) | 11911(2) | 1250(2) | 24(1) |
| S(1) | 1678(1) | 9722(1) | 864(1) | 19(1) |
| C(1) | 1548(3) | 9147(3) | 4288(3) | 12(1) |
| C(2) | 2685(3) | 8581(3) | 4385(3) | 13(1) |
| C(3) | 2718(3) | 7697(3) | 4892(3) | 15(1) |
| C(5) | 556(4) | 7958(3) | 5249(3) | 16(1) |
| C(4) | 1674(4) | 7395(3) | 5332(3) | 15(1) |
| C(6) | 488(3) | 8815(3) | 4719(3) | 14(1) |
| C(7) | 3834(3) | 8872(3) | 3978(3) | 14(1) |
| C(8) | 5176(3) | 10742(3) | 2905(3) | 13(1) |
| C(9) | 6349(3) | 11059(3) | 2535(3) | 12(1) |
| C(10) | 7512(4) | 10517(3) | 2736(3) | 13(1) |
| C(11) | 8600(3) | 10814(3) | 2327(3) | 14(1) |
| C(12) | 8535(4) | 11635(3) | 1727(3) | 16(1) |
| C(13) | 7412(4) | 12205(3) | 1545(3) | 16(1) |
| C(14) | 6343(4) | 11911(3) | 1954(3) | 15(1) |
| C(15) | 3282(4) | 9278(3) | 849(4) | 27(1) |
| C(16) | 1014(4) | 8704(3) | 1413(4) | 27(1) |

Table B30. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **C9**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | U(eq) |
|-------|----------|----------|----------|---------|
| Mo(1) | 3863(1) | 2135(1) | 7102(1) | 20(1) |
| Cl(1) | 5031(2) | 572(1) | 11956(1) | 34(1) |
| N(1) | 3217(4) | 1165(2) | 7298(3) | 18(1) |
| N(2) | 2356(4) | 881(2) | 6439(3) | 23(1) |
| N(3) | 7820(7) | 974(3) | 6906(5) | 56(2) |
| N(4) | 7653(11) | 2086(6) | 6147(12) | 59(4) |
| N(5) | 6125(11) | 1322(17) | 5056(7) | 210(18) |
| N(6) | 506(6) | 9081(2) | 9712(4) | 40(1) |
| O(1) | 5234(4) | 1986(2) | 8408(3) | 30(1) |
| O(2) | 4482(5) | 2777(2) | 6667(3) | 35(1) |
| O(3) | 2462(5) | 2381(2) | 7524(3) | 37(1) |
| O(4) | 2609(4) | 1830(2) | 5760(2) | 25(1) |
| O(5) | 669(6) | 1429(3) | 3850(4) | 55(1) |
| O(6) | 5458(4) | 1595(2) | 6614(3) | 35(1) |
| O(7) | 1447(5) | 9883(2) | 9054(3) | 46(1) |
| P(1) | 6657(2) | 1488(1) | 6148(1) | 41(1) |
| C(1) | 5140(5) | 1644(2) | 9190(3) | 24(1) |
| C(2) | 4292(5) | 1110(2) | 9085(3) | 20(1) |
| C(3) | 4290(5) | 775(2) | 9957(3) | 23(1) |
| C(4) | 5094(6) | 980(2) | 10884(3) | 26(1) |
| C(5) | 5946(6) | 1500(2) | 10998(4) | 35(1) |
| C(6) | 5969(7) | 1826(3) | 10148(4) | 37(1) |
| C(7) | 3418(5) | 870(2) | 8134(3) | 20(1) |
| C(8) | 2089(5) | 1272(2) | 5699(3) | 23(1) |
| C(9) | 1114(6) | 1112(2) | 4722(3) | 26(1) |
| C(10) | -351(6) | 1043(3) | 3168(4) | 36(1) |
| C(11) | -452(7) | 529(3) | 3665(4) | 43(2) |
| C(12) | 449(5) | 557(2) | 4629(3) | 20(1) |
| C(13) | 9375(9) | 936(5) | 6924(7) | 73(2) |
| C(14) | 7189(12) | 439(4) | 7197(10) | 36(3) |
| C(15) | 8150(30) | 2156(9) | 5150(20) | 241(16) |
| C(16) | 8124(10) | 2435(5) | 7124(13) | 114(5) |
| C(17) | 4852(15) | 1647(13) | 4311(8) | 99(9) |
| C(18) | 6538(19) | 617(9) | 4724(9) | 69(5) |
| C(19) | 1550(7) | 9467(3) | 9665(5) | 41(1) |
| C(20) | 728(11) | 8602(4) | 10449(6) | 64(2) |
| C(21) | -916(7) | 9114(3) | 9011(6) | 50(2) |

Table B31. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **C10**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | U(eq) |
|-------|---------|---------|----------|-------|
| Mo(1) | 3010(1) | 2270(1) | 1300(8) | 39(2) |
| Cl(1) | 6100(3) | 2200(2) | -5460(2) | 24(5) |
| N(1) | 3000(3) | 2010(3) | 3000(5) | 18(3) |
| N(2) | 2000(1) | 300(8) | 1000(9) | 26(2) |
| O(1) | 4200(8) | 3400(7) | 600(5) | 36(2) |
| O(2) | 400(1) | 2700(8) | 300(7) | 45(2) |
| O(3) | 2900(1) | 3300(9) | 2200(5) | 20(5) |
| O(4) | 4900(1) | 1900(1) | 1700(9) | 40(2) |
| O(5) | 2000(4) | 3000(3) | 4000(3) | 25(2) |
| O(6) | 1600(2) | 1100(1) | 2500(7) | 10(4) |
| S(1) | 1200(3) | 3000(3) | 900(2) | 17(6) |
| C(1) | 3800(2) | 2600(1) | 1900(8) | 40(3) |
| C(2) | 4600(1) | 3900(1) | 2600(8) | 40(2) |
| C(3) | 7000(2) | 2000(2) | 2100(2) | 17(9) |
| C(4) | 2900(2) | 2700(2) | 4400(1) | 20(4) |
| C(5) | 3500(2) | 1700(1) | 2000(2) | 30(7) |
| C(6) | 3300(1) | 1500(9) | 2500(7) | 40(2) |
| C(7) | 3000(2) | 2020(3) | 3000(6) | 25(3) |
| C(8) | 1400(1) | 1440(1) | 2200(7) | 30(2) |
| C(9) | 2340(2) | 2300(2) | 3600(1) | 30(3) |
| C(10) | 600(2) | 3100(1) | 3100(1) | 20(4) |
| C(11) | 1500(2) | 3600(2) | 5300(1) | 30(6) |
| C(12) | 1230(2) | 3000(4) | 5500(2) | 50(2) |
| C(13) | 5000(2) | 4000(3) | 3000(2) | 19(2) |
| C(14) | 1600(1) | 2800(9) | 1400(7) | 40(2) |

Table B32. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **C12**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | U(eq) |
|-------|----------|----------|---------|-------|
| Mo(1) | 3598(1) | 4841(1) | 2741(1) | 12(1) |
| N(1) | 3391(2) | 3963(2) | 1278(1) | 14(1) |
| N(2) | 3966(2) | 2699(2) | 1180(1) | 15(1) |
| N(3) | -1372(2) | 2971(2) | 4430(1) | 17(1) |
| O(1) | 2356(2) | 6210(1) | 2218(1) | 17(1) |
| O(2) | 3181(2) | 5012(1) | 4096(1) | 18(1) |
| O(3) | 5638(2) | 5389(1) | 2157(1) | 19(1) |
| O(4) | 4239(2) | 2976(1) | 2873(1) | 15(1) |
| O(5) | 965(2) | 8475(1) | 2092(1) | 19(1) |
| O(6) | 880(2) | 4003(1) | 3219(1) | 19(1) |
| O(7) | 6080(2) | -1306(1) | 4099(1) | 20(1) |
| C(1) | 1903(2) | 6542(2) | 1321(2) | 15(1) |
| C(2) | 2112(2) | 5737(2) | 477(2) | 15(1) |
| C(3) | 1569(3) | 6149(2) | -437(2) | 18(1) |
| C(4) | 829(3) | 7332(2) | -502(2) | 20(1) |
| C(5) | 623(3) | 8137(2) | 331(2) | 20(1) |
| C(6) | 1150(2) | 7759(2) | 1233(2) | 16(1) |
| C(7) | 558(3) | 9800(2) | 1930(2) | 18(1) |
| C(8) | 432(3) | 10402(2) | 2963(2) | 23(1) |
| C(9) | 2832(2) | 4466(2) | 506(2) | 15(1) |
| C(10) | 4401(2) | 2289(2) | 2038(2) | 13(1) |
| C(11) | 5095(2) | 977(2) | 2105(2) | 14(1) |
| C(12) | 5284(2) | 414(2) | 3073(2) | 15(1) |
| C(13) | 5917(2) | -837(2) | 3113(2) | 15(1) |
| C(14) | 6315(3) | -1526(2) | 2202(2) | 18(1) |
| C(15) | 6113(3) | -948(2) | 1238(2) | 19(1) |
| C(16) | 5528(3) | 296(2) | 1178(2) | 17(1) |
| C(17) | 6742(3) | -2573(2) | 4168(2) | 22(1) |
| C(18) | 221(3) | 3376(2) | 4099(2) | 18(1) |
| C(19) | -2549(3) | 3298(2) | 3791(2) | 26(1) |
| C(20) | -2022(3) | 2168(2) | 5440(2) | 24(1) |

Table B33. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **C13**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | U(eq) |
|-------|----------|---------|---------|-------|
| Mo(1) | 2748(1) | 3719(1) | 2608(1) | 15(1) |
| N(1) | 3264(2) | 5686(2) | 1690(2) | 16(1) |
| N(2) | 1938(2) | 6883(2) | 1441(2) | 18(1) |
| N(3) | 2811(2) | 5034(2) | 4004(2) | 20(1) |
| N(4) | 3273(3) | 6516(3) | 4999(2) | 39(1) |
| O(1) | 5037(2) | 3137(2) | 2767(1) | 22(1) |
| O(2) | 2045(2) | 2627(2) | 3556(1) | 21(1) |
| O(3) | 2828(2) | 2964(2) | 1473(1) | 22(1) |
| O(4) | 667(2) | 5328(2) | 2417(1) | 18(1) |
| O(5) | 7824(2) | 1224(2) | 3063(1) | 20(1) |
| O(6) | -5030(2) | 8230(2) | 2563(2) | 27(1) |
| O(7) | 4664(6) | 8745(4) | 5286(3) | 53(2) |
| C(1) | 6263(3) | 3367(2) | 2135(2) | 16(1) |
| C(2) | 6113(3) | 4609(3) | 1400(2) | 17(1) |
| C(3) | 7475(3) | 4785(3) | 805(2) | 18(1) |
| C(4) | 8941(3) | 3770(3) | 944(2) | 20(1) |
| C(5) | 9106(3) | 2547(3) | 1693(2) | 18(1) |
| C(6) | 7785(3) | 2348(2) | 2289(2) | 16(1) |
| C(7) | 9378(3) | 214(3) | 3283(2) | 20(1) |
| C(8) | 9150(3) | -920(3) | 4150(2) | 27(1) |
| C(9) | 4613(3) | 5753(2) | 1241(2) | 18(1) |
| C(10) | 658(3) | 6567(2) | 1828(2) | 16(1) |
| C(11) | -925(3) | 7639(2) | 1611(2) | 16(1) |
| C(12) | -2292(3) | 7469(2) | 2158(2) | 18(1) |
| C(13) | -3764(3) | 8513(2) | 1976(2) | 18(1) |
| C(14) | -3882(3) | 9724(3) | 1242(2) | 20(1) |
| C(15) | -2504(3) | 9873(3) | 683(2) | 23(1) |
| C(16) | -1030(3) | 8847(3) | 857(2) | 20(1) |
| C(17) | -6553(3) | 9316(3) | 2474(2) | 30(1) |
| C(18) | 2016(3) | 4906(3) | 4959(2) | 25(1) |
| C(19) | 2278(4) | 5819(3) | 5582(2) | 36(1) |
| C(20) | 3574(3) | 6006(3) | 4063(2) | 30(1) |

Table B34. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **C14**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | U(eq) |
|-------|----------|---------|----------|-------|
| Mo(1) | 317(1) | 2390(1) | 3190(1) | 11(1) |
| Mo(2) | 9738(1) | 7800(1) | 1903(1) | 11(1) |
| N(1) | 2409(1) | 3869(1) | 3028(1) | 14(1) |
| N(2) | 1151(1) | 3790(1) | 3311(1) | 13(1) |
| N(3) | 7768(1) | 6237(1) | 1979(1) | 16(1) |
| N(4) | 9017(1) | 6379(1) | 1710(1) | 14(1) |
| O(1) | 6161(1) | 959(1) | 1719(1) | 22(1) |
| O(2) | -3309(1) | 2984(1) | 4505(1) | 19(1) |
| O(3) | -1039(1) | 2859(1) | 3847(1) | 17(1) |
| O(4) | 2148(1) | 2262(1) | 2836(1) | 15(1) |
| O(5) | 127(1) | 1071(1) | 3395(1) | 18(1) |
| O(6) | -275(1) | 3060(1) | 2194(1) | 20(1) |
| O(7) | 1319(1) | 1831(1) | 4491(1) | 20(1) |
| O(8) | 3592(1) | 8896(1) | 3207(1) | 21(1) |
| O(10) | 10434(1) | 7040(1) | 2847(1) | 19(1) |
| O(11) | 9880(1) | 9098(1) | 1818(1) | 15(1) |
| O(12) | 8646(1) | 8481(1) | 659(1) | 17(1) |
| O(13) | 7925(1) | 7786(1) | 2295(1) | 14(1) |
| O(19) | 13426(1) | 7423(1) | 640(1) | 18(1) |
| S(1) | 848(1) | 885(1) | 5196(1) | 15(1) |
| S(2) | 9221(1) | 9080(1) | -201(1) | 15(1) |
| C(1) | 2810(2) | -247(2) | 6242(1) | 25(1) |
| C(2) | -5159(2) | 2138(2) | 4648(1) | 23(1) |
| C(3) | 9314(2) | 8157(2) | -794(1) | 20(1) |
| C(4) | 7935(2) | 8077(2) | -936(1) | 21(1) |
| C(5) | 7302(2) | 9245(2) | -1280(1) | 23(1) |
| C(6) | 7806(2) | 9881(2) | -771(1) | 21(1) |
| C(7) | 10903(2) | 5726(1) | 1060(1) | 15(1) |
| C(8) | 11494(2) | 4857(2) | 805(1) | 19(1) |
| C(9) | 12727(2) | 4836(2) | 509(1) | 25(1) |
| C(10) | 9613(2) | 5688(1) | 1384(1) | 15(1) |
| C(11) | -1133(2) | 5442(2) | 4238(1) | 17(1) |
| C(12) | -655(2) | 4556(1) | 3968(1) | 14(1) |
| C(15) | 15151(2) | 8409(2) | 502(1) | 21(1) |

Table B35. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **C15**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | U(eq) |
|-------|----------|----------|---------|-------|
| Mo(1) | 3477(1) | 9424(1) | 2509(1) | 11(1) |
| N(1) | 3161(2) | 10203(1) | 3686(1) | 13(1) |
| N(2) | 3554(2) | 10826(1) | 3386(1) | 14(1) |
| O(1) | 2289(2) | 8923(1) | 3432(1) | 14(1) |
| O(2) | 3095(2) | 8997(1) | 1326(1) | 16(1) |
| O(3) | 5597(2) | 9253(1) | 3092(1) | 17(1) |
| O(4) | 4037(2) | 10286(1) | 1876(1) | 14(1) |
| O(5) | 918(2) | 7903(1) | 4171(1) | 19(1) |
| O(6) | 698(2) | 9825(1) | 1941(1) | 15(1) |
| O(7) | 3642(2) | 12080(1) | 3423(1) | 28(1) |
| S(1) | -535(1) | 9488(1) | 1020(1) | 14(1) |
| C(1) | 1871(2) | 8976(1) | 4411(1) | 13(1) |
| C(2) | 2087(2) | 9555(1) | 5011(1) | 14(1) |
| C(3) | 1605(2) | 9573(1) | 6029(1) | 17(1) |
| C(4) | 923(2) | 9035(1) | 6435(1) | 19(1) |
| C(5) | 698(2) | 8463(1) | 5843(1) | 20(1) |
| C(6) | 1139(2) | 8428(1) | 4830(1) | 16(1) |
| C(7) | 258(2) | 7320(1) | 4585(1) | 19(1) |
| C(8) | 207(2) | 6815(1) | 3720(2) | 20(1) |
| C(9) | 2673(2) | 10153(1) | 4599(1) | 13(1) |
| C(10) | 3984(2) | 10822(1) | 2436(1) | 14(1) |
| C(11) | 4365(2) | 11436(1) | 1955(1) | 15(1) |
| C(12) | 4164(2) | 12031(1) | 2464(1) | 19(1) |
| C(13) | 4469(3) | 12616(1) | 1960(1) | 23(1) |
| C(14) | 4938(2) | 12608(1) | 959(2) | 21(1) |
| C(15) | 5142(2) | 12023(1) | 445(1) | 18(1) |
| C(16) | 4873(2) | 11448(1) | 946(1) | 15(1) |
| C(17) | -2453(2) | 9984(1) | 839(1) | 19(1) |
| C(18) | -1346(2) | 8786(1) | 1596(1) | 22(1) |

Table B36. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **C16**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | $U(\text{eq})$ |
|-----|-----------|-----------|----------|----------------|
| Mo1 | 1018 (4) | 7200 (4) | 4160 (7) | 16 (1) |
| C11 | 2540 (1) | -3400 (1) | 5010 (2) | 19 (2) |
| O1 | 9736 (4) | 1896 (4) | 3779 (6) | 16 (5) |
| O2 | 4441 (4) | 1634 (4) | 3311 (6) | 21 (6) |
| O3 | 7322 (5) | 4673 (5) | 2555 (6) | 31 (8) |
| O4 | 9260 (4) | 1010 (4) | 4522 (6) | 16 (5) |
| O5 | 1226 (4) | 1843 (4) | 4262 (6) | 17 (6) |
| O6 | 1087 (4) | -1250 (4) | 4032 (6) | 19 (6) |
| O7 | 8759 (4) | 3422 (4) | 4283 (6) | 16 (5) |
| N1 | 6590 (5) | 904 (4) | 3758 (7) | 15 (6) |
| N2 | 7088 (5) | 358 (4) | 4030 (6) | 13 (6) |
| N3 | 4092 (5) | 3848 (5) | 2232 (7) | 22 (7) |
| N4 | -1397 (5) | 211 (5) | 1076 (7) | 19 (7) |
| C1 | 7832 (6) | 2412 (5) | 3357 (8) | 15 (7) |
| C2 | 9404 (6) | 3226 (5) | 3228 (8) | 18 (8) |
| C3 | 9220 (7) | 3981 (6) | 2963 (9) | 23 (9) |
| C4 | 7447 (6) | 3896 (6) | 2813 (8) | 21 (8) |
| C5 | 5880 (6) | 3080 (6) | 2936 (9) | 22 (8) |
| C6 | 6056 (6) | 2349 (5) | 3204 (8) | 16 (7) |
| C7 | 8056 (5) | 1687 (5) | 3641 (8) | 13 (7) |
| C8 | 5761 (5) | 460 (5) | 4165 (8) | 14 (7) |
| C9 | 5994 (5) | 1073 (5) | 4455 (8) | 13 (7) |
| C10 | 4417 (5) | -1914 (5) | 4577 (8) | 15 (7) |
| C11 | 4521 (5) | -2421 (5) | 4857 (8) | 14 (7) |
| C12 | 6185 (6) | -2137 (5) | 5024 (8) | 15 (7) |
| C13 | 7755 (5) | -1333 (5) | 4907 (8) | 12 (7) |
| C14 | 7686 (5) | -786 (5) | 4623 (8) | 13 (7) |
| C15 | 9788 (6) | 4819 (6) | 4335 (9) | 22 (8) |
| C16 | 4737 (6) | 3877 (5) | 1968 (8) | 18 (8) |
| C17 | 3700 (6) | 3215 (5) | 1734 (8) | 17 (8) |
| C18 | 1891 (6) | 2466 (5) | 1772 (9) | 18 (8) |
| C19 | 1193 (6) | 2480 (6) | 2045 (9) | 23 (9) |
| C20 | 2334 (7) | 3156 (7) | 2264 (9) | 28 (1) |
| C21 | 510 (6) | 1000 (6) | 1098 (8) | 19 (8) |
| C22 | 1631 (6) | 724 (6) | 1317 (9) | 19 (8) |
| C23 | 753 (6) | 1701 (5) | 1529 (8) | 16 (7) |
| C24 | -1230 (6) | 1915 (5) | 1507 (9) | 18 (8) |
| C25 | -2235 (6) | 1164 (6) | 1278 (9) | |

Table B37. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **C17**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | U(eq) |
|------|----------|-----------|-----------|--------|
| Mo1 | 7459(2) | 3042(2) | 1700(1) | 17 (7) |
| O1 | 1135(2) | 3026 (2) | 2048 (1) | 24 (3) |
| O2 | 9252 (2) | 2143 (1) | 5147 (1) | 19 (3) |
| O3 | 6036 (2) | 4657 (1) | 2393 (1) | 22 (3) |
| O4 | 3337 (2) | 5786 (2) | 3756 (1) | 30 (4) |
| O5 | 8232 (2) | 1763 (2) | 2694(1) | 22 (3) |
| O6 | 5697 (2) | 2680 (2) | 1397 (1) | 22 (3) |
| N1 | 8802 (2) | 4322 (2) | -5053 (1) | 17 (3) |
| N2 | 7547 (2) | 4758(2) | 3625 (1) | 16 (3) |
| N3 | 1183 (3) | 2227 (2) | 3351 (2) | 31 (5) |
| C1 | 1265 (3) | 2079 (3) | -2636 (2) | 27 (5) |
| C2 | 1300 (3) | 757 (3) | 2131 (2) | 27 (5) |
| C3 | 1188 (3) | 854 (2) | -1156 (2) | 23 (4) |
| C4 | 1091 (3) | 2245 (2) | -1144 (2) | 19 (4) |
| C5 | 9575 (3) | 2954 (2) | -3452 (2) | 17 (4) |
| C6 | 6621 (3) | 6087 (2) | 2969 (2) | 18 (4) |
| C7 | 5219 (3) | 6710 (2) | 1106 (2) | 19 (4) |
| C8 | 4088 (3) | 8115 (2) | 8794 (2) | 24 (4) |
| C9 | 2662 (3) | 8737 (3) | 1600 (2) | 29 (5) |
| C10 | 2339 (3) | 7978 (3) | 2571 (2) | 30 (5) |
| C11 | 3482 (3) | 6612 (3) | 2825 (2) | 25 (5) |
| C12 | 4943 (3) | 5964 (2) | 2092 (2) | 20 (4) |
| C13 | 1903 (3) | 6364 (3) | 4549 (2) | 34 (6) |
| C14 | 2070 (4) | 5235 (4) | 5478 (2) | 38 (6) |
| C15 | 1202 (5) | 903 (4) | 3618 (3) | 21 (8) |
| C16 | 1328 (5) | -2800 (4) | 4216 (3) | 20 (8) |
| C15' | 1132 (6) | 1138 (4) | 4102 (3) | 19 (8) |
| C16' | 1251 (5) | 266 (4) | 4794 (3) | 21 (8) |
| C17 | 1433 (4) | 471 (2) | 4655 (2) | 34 (6) |
| C18 | 1434 (8) | 1850 (6) | 4256 (5) | 22 (2) |
| C19 | 1306 (8) | 2709 (7) | 3637 (4) | 28 (2) |
| C18' | 1450 (8) | 1689 (6) | 4113 (5) | 14 (1) |
| C19' | 1322 (6) | 2528 (5) | 3477 (4) | 11 (1) |

Table B38. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **C18**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | U(eq) |
|-------|----------|----------|---------|-------|
| Mo(1) | 1672(1) | 1159(1) | 4078(1) | 12(1) |
| Mo(2) | -1540(1) | 9040(1) | 1048(1) | 12(1) |
| Cl(1) | -3282(1) | -2283(1) | 3455(1) | 22(1) |
| Cl(2) | 3040(1) | 12878(1) | 1438(1) | 23(1) |
| N(1) | 193(1) | 1439(1) | 4507(1) | 12(1) |
| N(2) | 179(1) | 2200(1) | 4954(1) | 14(1) |
| N(3) | 1204(1) | 3462(1) | 5559(1) | 16(1) |
| N(4) | 958(1) | 2827(1) | 3515(1) | 14(1) |
| N(5) | -64(1) | 8715(1) | 640(1) | 12(1) |
| N(6) | 4(1) | 7854(1) | 253(1) | 14(1) |
| N(7) | -921(1) | 6439(1) | -270(1) | 17(1) |
| N(8) | -829(1) | 7434(1) | 1638(1) | 13(1) |
| O(1) | 549(1) | 536(1) | 3469(1) | 16(1) |
| O(2) | 2737(1) | 1436(1) | 3739(1) | 18(1) |
| O(3) | 2030(1) | -12(1) | 4494(1) | 18(1) |
| O(4) | -424(1) | 9696(1) | 1652(1) | 16(1) |
| O(5) | -2648(1) | 8822(1) | 1364(1) | 20(1) |
| O(6) | -1823(1) | 10199(1) | 618(1) | 20(1) |
| S(1) | 2264(1) | 2587(1) | 4801(1) | 14(1) |
| S(2) | -2123(1) | 7555(1) | 349(1) | 15(1) |
| C(1) | -318(1) | -107(1) | 3488(1) | 14(1) |
| C(2) | -906(1) | -20(1) | 3946(1) | 13(1) |
| C(3) | -1829(1) | -703(1) | 3933(1) | 15(1) |
| C(4) | -2140(1) | -1442(1) | 3477(1) | 16(1) |
| C(5) | -1570(1) | -1517(1) | 3022(1) | 18(1) |
| C(6) | -665(1) | -850(1) | 3027(1) | 17(1) |
| C(7) | -653(1) | 793(1) | 4414(1) | 13(1) |
| C(8) | 1096(1) | 2735(1) | 5112(1) | 13(1) |
| C(9) | 372(1) | 3637(1) | 5910(1) | 18(1) |
| C(10) | -466(1) | 4510(2) | 5652(1) | 24(1) |
| C(11) | -95(1) | 3046(1) | 3332(1) | 17(1) |
| C(12) | 1667(1) | 3535(1) | 3344(1) | 15(1) |
| C(13) | 1362(1) | 4446(1) | 2982(1) | 15(1) |
| C(14) | 260(1) | 4668(1) | 2784(1) | 12(1) |
| C(15) | -472(1) | 3946(1) | 2972(1) | 17(1) |
| C(16) | 362(1) | 10422(1) | 1584(1) | 14(1) |
| C(17) | 910(1) | 10337(1) | 1110(1) | 13(1) |
| C(18) | 1739(1) | 11110(1) | 1067(1) | 15(1) |
| C(19) | 2006(1) | 11931(1) | 1487(1) | 17(1) |
| C(20) | 1479(1) | 12001(1) | 1960(1) | 20(1) |
| C(21) | 665(1) | 11246(1) | 2010(1) | 18(1) |
| C(22) | 731(1) | 9423(1) | 691(1) | 13(1) |
| C(23) | -900(1) | 7289(1) | 107(1) | 14(1) |

Table B39. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **C19**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | U(eq) |
|-------|----------|----------|----------|-------|
| Mo(1) | 2470(1) | 8160(1) | 7687(1) | 15(1) |
| Cl(1) | -4543(1) | 3397(1) | 8588(1) | 22(1) |
| Cl(2) | 310(1) | 6927(1) | 5074(1) | 30(1) |
| N(1) | 321(3) | 7637(3) | 9336(2) | 16(1) |
| N(2) | 252(3) | 8047(3) | 10329(2) | 16(1) |
| N(3) | 1562(3) | 9212(3) | 11184(2) | 16(1) |
| N(4) | 2389(3) | 11712(3) | 6519(2) | 15(1) |
| O(1) | 947(2) | 7736(2) | 6969(2) | 20(1) |
| O(2) | 4119(2) | 9075(2) | 6571(2) | 21(1) |
| O(3) | 2915(3) | 6308(2) | 8180(2) | 22(1) |
| O(4) | 1405(2) | 10440(2) | 7113(2) | 18(1) |
| S(1) | 3203(1) | 9281(1) | 8997(1) | 18(1) |
| C(1) | -271(3) | 6700(3) | 7387(3) | 18(1) |
| C(2) | -1158(3) | 6159(3) | 8602(3) | 17(1) |
| C(3) | -2483(3) | 5128(3) | 8969(3) | 17(1) |
| C(4) | -2882(3) | 4651(3) | 8142(3) | 19(1) |
| C(5) | -2014(4) | 5157(4) | 6938(3) | 21(1) |
| C(6) | -733(4) | 6180(3) | 6577(3) | 21(1) |
| C(7) | -856(3) | 6716(3) | 9493(3) | 18(1) |
| C(8) | 1527(3) | 8792(3) | 10246(3) | 16(1) |
| C(9) | 2832(3) | 10143(3) | 11220(3) | 18(1) |
| C(10) | 2640(4) | 10043(4) | 12494(3) | 26(1) |
| C(11) | 2456(3) | 12752(3) | 7073(3) | 19(1) |
| C(12) | 3270(3) | 11931(4) | 5387(3) | 19(1) |
| C(13) | 4294(3) | 13214(3) | 4779(3) | 18(1) |
| C(14) | 4435(3) | 14315(3) | 5317(3) | 17(1) |
| C(15) | 3459(3) | 14053(3) | 6486(3) | 19(1) |

Table B40. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **C20**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | $U(\text{eq})$ |
|-------|----------|---------|----------|----------------|
| Mo(1) | 460(1) | 2430(1) | 9102(1) | 14(1) |
| N(1) | 314(2) | 3481(2) | 10329(2) | 13(1) |
| N(2) | -1098(2) | 4012(2) | 10315(2) | 13(1) |
| O(1) | 2621(2) | 2556(2) | 9576(1) | 17(1) |
| O(2) | 394(2) | 2066(2) | 7961(1) | 21(1) |
| O(3) | 142(2) | 1301(2) | 9681(2) | 21(1) |
| O(4) | -1695(2) | 3033(2) | 8965(1) | 16(1) |
| O(5) | 5253(2) | 1567(2) | 9874(2) | 21(1) |
| O(6) | 819(2) | 4150(2) | 8574(2) | 17(1) |
| C(1) | 3380(3) | 2556(2) | 10460(2) | 16(1) |
| C(2) | 2816(3) | 3066(2) | 11199(2) | 15(1) |
| C(3) | 3729(3) | 3091(2) | 12096(2) | 20(1) |
| C(4) | 5142(4) | 2611(2) | 12246(2) | 22(1) |
| C(5) | 5691(3) | 2090(3) | 11522(2) | 22(1) |
| C(6) | 4834(3) | 2058(2) | 10630(2) | 18(1) |
| C(7) | 6630(3) | 924(3) | 10038(2) | 24(1) |
| C(8) | 6799(4) | 410(3) | 9121(2) | 27(1) |
| C(9) | 1322(3) | 3576(2) | 11076(2) | 15(1) |
| C(10) | -2056(3) | 3708(2) | 9584(2) | 14(1) |
| C(11) | -3666(3) | 4136(2) | 9382(2) | 13(1) |
| C(12) | -4182(3) | 4800(2) | 10151(2) | 13(1) |
| C(13) | 1159(4) | 4452(3) | 7675(2) | 22(1) |
| C(14) | -247(4) | 4326(3) | 6944(2) | 28(1) |

Table B41. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **C21**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | U(eq) |
|-------|----------|---------|----------|-------|
| Mo(1) | 8306(1) | 3842(1) | -831(1) | 15(1) |
| Cl(1) | 6807(1) | 6584(1) | -2127(1) | 25(1) |
| Cl(2) | 9567(1) | 8724(1) | 835(1) | 28(1) |
| N(1) | 9597(1) | 4397(1) | 828(1) | 15(1) |
| N(2) | 10220(1) | 3728(1) | 1589(1) | 16(1) |
| O(1) | 8004(1) | 5109(1) | -946(1) | 19(1) |
| O(2) | 7365(1) | 3304(1) | -1616(1) | 21(1) |
| O(3) | 8492(1) | 3854(1) | -1912(1) | 21(1) |
| O(4) | 9082(1) | 2781(1) | 215(1) | 19(1) |
| O(5) | 8328(1) | 3877(1) | 911(1) | 21(1) |
| C(1) | 8390(1) | 5909(1) | -478(2) | 17(1) |
| C(2) | 9273(1) | 6007(1) | 495(2) | 17(1) |
| C(3) | 9631(1) | 6883(1) | 905(2) | 20(1) |
| C(4) | 9119(1) | 7643(1) | 371(2) | 21(1) |
| C(5) | 8242(1) | 7563(1) | -564(2) | 21(1) |
| C(6) | 7891(1) | 6701(1) | -970(2) | 19(1) |
| C(7) | 9841(1) | 5233(1) | 1128(2) | 17(1) |
| C(8) | 9885(1) | 2917(1) | 1194(2) | 17(1) |
| C(9) | 10437(1) | 2094(1) | 1861(2) | 20(1) |
| C(10) | 10015(1) | 1266(1) | 1941(2) | 22(1) |
| C(11) | 7618(1) | 3824(1) | 895(2) | 22(1) |
| C(12) | 7176(1) | 4727(1) | 533(2) | 29(1) |

Table B42. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **C22**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | U(eq) |
|-------|----------|----------|----------|-------|
| Mo(1) | -575(1) | 9766(1) | 7492(1) | 12(1) |
| N(1) | -395(4) | 12223(3) | 7805(2) | 15(1) |
| N(2) | -922(4) | 12649(4) | 8521(2) | 18(1) |
| N(3) | 4797(4) | 6931(4) | 7238(2) | 21(1) |
| N(4) | 3296(4) | 5699(4) | 8279(2) | 21(1) |
| N(5) | 4721(4) | 8013(4) | 8541(2) | 17(1) |
| O(1) | 869(3) | 10115(3) | 6665(1) | 18(1) |
| O(2) | -325(3) | 7651(3) | 7467(1) | 19(1) |
| O(3) | -2567(3) | 10862(3) | 7200(1) | 20(1) |
| O(4) | -1445(3) | 10118(3) | 8532(1) | 16(1) |
| O(5) | 2157(4) | 9747(3) | 5346(1) | 23(1) |
| O(6) | 1893(3) | 8941(3) | 7992(1) | 16(1) |
| P(1) | 3606(1) | 7458(1) | 8004(1) | 14(1) |
| C(1) | 1080(4) | 11499(4) | 6334(2) | 16(1) |
| C(2) | 665(4) | 13077(4) | 6665(2) | 18(1) |
| C(3) | 954(5) | 14438(5) | 6271(2) | 23(1) |
| C(4) | 1628(6) | 14253(5) | 5575(2) | 29(1) |
| C(5) | 2056(5) | 12693(5) | 5244(2) | 27(1) |
| C(6) | 1790(5) | 11322(5) | 5615(2) | 20(1) |
| C(7) | 2829(5) | 9525(5) | 4613(2) | 26(1) |
| C(8) | 3170(6) | 7693(5) | 4445(2) | 30(1) |
| C(9) | 32(4) | 13333(4) | 7405(2) | 18(1) |
| C(10) | -1450(4) | 11485(4) | 8839(2) | 16(1) |
| C(11) | -2080(5) | 11637(5) | 9612(2) | 21(1) |
| C(12) | -972(4) | 10123(5) | 10045(2) | 19(1) |
| C(13) | 5816(6) | 7970(6) | 6945(2) | 32(1) |
| C(14) | 4117(5) | 6280(5) | 6684(2) | 28(1) |
| C(15) | 1849(5) | 5770(5) | 8815(2) | 24(1) |
| C(16) | 4508(5) | 3965(5) | 8123(2) | 29(1) |
| C(17) | 6373(5) | 6783(5) | 8759(2) | 25(1) |
| C(18) | 4482(5) | 9806(5) | 8635(2) | 21(1) |

Table A43. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **C23**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | U(eq) |
|-------|---------|----------|----------|-------|
| Mo(1) | 5603(1) | 8418(1) | 7344(1) | 12(1) |
| N(1) | 3208(2) | 6534(2) | 5990(1) | 14(1) |
| N(2) | 1883(2) | 6849(2) | 5157(1) | 17(1) |
| N(3) | 1751(2) | 9313(2) | 8680(1) | 15(1) |
| O(1) | 5641(2) | 6895(1) | 8224(1) | 13(1) |
| O(2) | 6872(2) | 10043(1) | 8377(1) | 18(1) |
| O(3) | 7030(2) | 8288(2) | 6627(1) | 18(1) |
| O(4) | 4071(2) | 9178(1) | 6158(1) | 15(1) |
| O(5) | 7375(2) | 5743(1) | 9765(1) | 16(1) |
| O(6) | 3334(2) | 8194(1) | 8104(1) | 17(1) |
| C(1) | 5462(2) | 5559(2) | 7805(2) | 12(1) |
| C(2) | 4315(3) | 4756(2) | 6626(2) | 15(1) |
| C(3) | 4245(3) | 3384(2) | 6249(2) | 17(1) |
| C(4) | 5257(3) | 2815(2) | 7036(2) | 19(1) |
| C(5) | 6305(3) | 3572(2) | 8227(2) | 17(1) |
| C(6) | 6400(2) | 4925(2) | 8623(2) | 14(1) |
| C(7) | 8055(3) | 5031(2) | 10666(2) | 18(1) |
| C(8) | 9016(3) | 6117(2) | 11851(2) | 21(1) |
| C(9) | 3074(3) | 5230(2) | 5808(2) | 16(1) |
| C(10) | 2470(3) | 8251(2) | 5331(2) | 15(1) |
| C(11) | 1281(3) | 8897(2) | 4600(2) | 18(1) |
| C(12) | 589(2) | 9655(2) | 5373(2) | 15(1) |
| C(13) | 3084(3) | 9303(2) | 8338(2) | 17(1) |
| C(14) | 1530(3) | 10650(2) | 8917(2) | 20(1) |
| C(15) | 446(3) | 7987(2) | 8859(2) | 22(1) |

Table A44. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **C24**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

| | x | y | z | U(eq) |
|-------|----------|---------|---------|-------|
| Mo(1) | 2193(1) | 2200(1) | 6368(1) | 24(1) |
| N(1) | 721(4) | 3377(3) | 5607(3) | 25(1) |
| N(2) | 1204(4) | 4031(3) | 5019(3) | 28(1) |
| N(3) | 3243(4) | 3346(3) | 7819(3) | 25(1) |
| O(1) | 960(3) | 2062(2) | 7211(3) | 25(1) |
| O(2) | 3772(3) | 1600(2) | 7112(3) | 29(1) |
| O(3) | 1211(3) | 1536(2) | 5221(3) | 37(1) |
| O(4) | 3116(3) | 3022(2) | 5579(3) | 28(1) |
| O(5) | -3292(3) | 1212(2) | 7683(3) | 28(1) |
| O(6) | 8656(5) | 599(4) | 4399(4) | 79(2) |
| C(1) | -495(4) | 2162(3) | 6865(4) | 22(1) |
| C(2) | -1274(4) | 2812(3) | 6020(4) | 23(1) |
| C(3) | -2779(4) | 2877(3) | 5710(4) | 27(1) |
| C(4) | -3483(4) | 2350(3) | 6237(4) | 27(1) |
| C(5) | -2679(4) | 1727(3) | 7103(4) | 25(1) |
| C(6) | -1187(4) | 1629(3) | 7403(4) | 25(1) |
| C(7) | -616(4) | 3435(3) | 5481(4) | 26(1) |
| C(8) | 2445(4) | 3769(3) | 5044(4) | 25(1) |
| C(9) | 3197(4) | 4322(3) | 4458(4) | 28(1) |
| C(10) | 4585(4) | 4753(3) | 5310(4) | 24(1) |
| C(11) | 2529(5) | 3806(3) | 8349(4) | 33(1) |
| C(12) | 3175(5) | 4451(3) | 9204(4) | 32(1) |
| C(13) | 4626(4) | 4656(3) | 9542(4) | 23(1) |
| C(14) | 5363(5) | 4184(4) | 8987(4) | 35(1) |
| C(15) | 4659(5) | 3547(4) | 8151(4) | 33(1) |
| C(16) | 8481(7) | 511(6) | 3278(5) | 67(2) |