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Table S1. Atomic coordinates and equivalent isotropic displacement parameters [$Å^2$] for 2. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Re(1) | .86418(2) | .17021(2) | .278643(8) | .01940(7) |
| Re(2) | .73003(2) | .29460(2) | .323198(8) | .01665(7) |
| Re(3) | .78380(2) | .255894(14) | .425822(8) | .01298(7) |
| Re(4) | .57285(2) | .15996(2) | .451690(8) | .01415(7) |
| C(11) | .9114(5) | .2602(5) | .2421(2) | .030(2) |
| C(12) | .7492(6) | .1535(5) | .2394(2) | .029(2) |
| C(13) | .7999(5) | .0935(4) | .3178(2) | .026(2) |
| C(14) | .9632(5) | .2050(4) | .3222(2) | .026(2) |
| C(15) | .9527(5) | .0870(5) | .2558(2) | .029(2) |
| C(21) | .8503(5) | .3689(4) | .3248(2) | .024(2) |
| C(22) | .6947(6) | .3292(5) | .2674(2) | .033(2) |
| C(23) | .6332(5) | .3695(4) | .3456(2) | .025(2) |
| C(24) | .6261(5) | .2071(5) | .3217(2) | .024(2) |
| C(31) | .8552(5) | .1504(4) | .4216(2) | .022(2) |
| C(32) | .9129(5) | .3103(4) | .4221(2) | .0175(14) |
| C(33) | .7942(5) | .2499(4) | .4866(2) | .0180(14) |
| C(34) | .7085(5) | .3600(4) | .4340(2) | .022(2) |
| C(42) | .4777(5) | .2028(4) | .4094(2) | .021(2) |
| C(43) | .4671(5) | .1037(4) | .4812(2) | .020(2) |
| C(44) | .6104(5) | .0579(4) | .4223(2) | .019(2) |
| C(41) | .5552(5) | .2526(4) | .4901(2) | .021(2) |
| O(11) | .9350(4) | .3128(4) | .2216(2) | .048(2) |
| O(12) | .6833(4) | .1460(4) | .2158(2) | .050(2) |
| O(13) | .7617(5) | .0495(3) | .3406(2) | .046(2) |
| O(14) | 1.0198(4) | .2238(4) | .3472(2) | .0410(14) |
| O(15) | 1.0053(4) | .0364(3) | .2451(2) | .0424(14) |
| O(22) | .6750(5) | .3512(4) | .2340(2) | .051(2) |
| O(23) | .5701(4) | .4138(3) | .3566(2) | .0388(14) |
| O(24) | .5681(4) | .1571(3) | .3214(2) | .0361(13) |
| O(21) | .9202(4) | .4095(3) | .3252(2) | .0422(14) |
| O(31) | .8987(4) | .0913(3) | .4204(2) | .0381(13) |
| O(32) | .9908(4) | .3432(3) | .41966(14) | .0283(11) |
| O(33) | .8017(4) | .2486(3) | .52222(14) | .0263(11) |
| O(34) | .6681(4) | .4184(3) | .4420(2) | .0402(14) |
| O(41) | .5455(4) | .3035(3) | .5132(2) | .0319(12) |
| O(42) | .4217(4) | .2283(3) | .3854(2) | .0377(13) |
| O(43) | .4005(4) | .0695(3) | .49721(14) | .0275(11) |
| O(44) | .6308(4) | -.0024(3) | .4081(2) | .0377(13) |
| H(1) | .7802 | .2382 | .3686 | .060 |
| H(2) | .6643 | .2024 | .4133 | .060 |
| H(3) | .6654 | .1219 | .4910 | .060 |
| N | .7684(4) | .0264(3) | .6058(2) | .0170(12) |
| C(51) | .7958(5) | .0934(4) | .6358(2) | .024(2) |
| C(52) | .7273(6) | .1665(4) | .6330(2) | .032(2) |
| C(53) | .8375(5) | -.0441(4) | .6165(2) | .025(2) |
| C(54) | .8207(6) | -.1191(4) | .5899(3) | .037(2) |
| C(55) | .6567(5) | .0034(4) | .6106(2) | .019(2) |
| C(56) | .6258(5) | -.0238(4) | .6546(2) | .032(2) |
| C(57) | .7824(5) | .0516(4) | .5600(2) | .025(2) |
| C(58) | .8916(6) | .0679(5) | .5475(3) | .043(2) |
| H(51A) | .8669(5) | .1103(4) | .6303(2) | .028 |

| | | | | |
|---|---|---|---|---|
| H(51B) | .7930(5) | .0723(4) | .6649(2) | .028 |
| H(52A) | .7499(6) | .2070(4) | .6533(2) | .049 |
| H(52B) | .6568(6) | .1509(4) | .6392(2) | .049 |
| H(52C) | .7308(6) | .1890(4) | .6046(2) | .049 |
| H(53A) | .8272(5) | -.0583(4) | .6464(2) | .030 |
| H(53B) | .9094(5) | -.0268(4) | .6132(2) | .030 |
| H(54A) | .8682(6) | -.1613(4) | .5989(3) | .055 |
| H(54B) | .8328(6) | -.1063(4) | .5603(3) | .055 |
| H(54C) | .7504(6) | -.1380(4) | .5935(3) | .055 |
| H(55A) | .6413(5) | -.0404(4) | .5906(2) | .023 |
| H(55B) | .6142(5) | .0502(4) | .6027(2) | .023 |
| H(56A) | .5530(5) | -.0374(4) | .6548(2) | .048 |
| H(56B) | .6387(5) | .0196(4) | .6747(2) | .048 |
| H(56C) | .6658(5) | -.0712(4) | .6625(2) | .048 |
| H(57A) | .7550(5) | .0086(4) | .5417(2) | .030 |
| H(57B) | .7416(5) | .1007(4) | .5548(2) | .030 |
| H(58A) | .8941(6) | .0836(5) | .5179(3) | .064 |
| H(58B) | .9325(6) | .0193(5) | .5517(3) | .064 |
| H(58C) | .9191(6) | .1115(5) | .5648(3) | .064 |

Table S2. Anisotropic displacement parameters [Å$^2$] for 2. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Re(1) | .01692(14) | .0267(2) | .01458(14) | -.00364(11) | .00216(11) | -.00021(12) |
| Re(2) | .01517(13) | .0215(2) | .01324(13) | .00187(11) | .00145(11) | .00072(11) |
| Re(3) | .01228(12) | .01464(13) | .01203(13) | .00009(10) | -.00003(10) | -.00153(10) |
| Re(4) | .01323(13) | .01642(13) | .01279(13) | .00014(10) | .00029(11) | -.00168(11) |
| C(11) | .020(4) | .041(5) | .028(4) | -.002(4) | .009(3) | .000(3) |
| C(12) | .028(4) | .044(5) | .016(4) | -.005(3) | .006(3) | .002(4) |
| C(13) | .024(4) | .029(4) | .024(4) | -.010(3) | .002(3) | .002(3) |
| C(14) | .022(4) | .029(4) | .028(4) | -.006(3) | .006(3) | .000(3) |
| C(15) | .024(4) | .037(4) | .024(4) | -.012(3) | .002(3) | .004(4) |
| C(21) | .027(4) | .028(4) | .017(4) | -.002(3) | .009(3) | -.004(3) |
| C(22) | .034(4) | .043(5) | .024(4) | .000(4) | -.001(4) | .011(4) |
| C(23) | .022(4) | .029(4) | .024(4) | .001(3) | -.001(3) | -.001(3) |
| C(24) | .020(4) | .038(4) | .013(3) | -.001(3) | -.002(3) | .001(3) |
| C(31) | .023(4) | .026(4) | .017(4) | .001(3) | -.004(3) | -.003(3) |
| C(32) | .021(4) | .023(4) | .008(3) | -.003(3) | .000(3) | .003(3) |
| C(33) | .014(3) | .023(4) | .018(4) | -.004(3) | -.004(3) | -.002(3) |
| C(34) | .022(4) | .023(4) | .020(4) | .004(3) | .002(3) | -.003(3) |
| C(42) | .017(3) | .023(4) | .022(4) | -.001(3) | .009(3) | .002(3) |
| C(43) | .023(4) | .021(4) | .016(3) | -.003(3) | .002(3) | -.002(3) |
| C(44) | .019(3) | .023(4) | .016(3) | .004(3) | .001(3) | -.002(3) |
| C(41) | .017(3) | .021(4) | .025(4) | .002(3) | .006(3) | -.003(3) |
| O(11) | .048(4) | .048(4) | .049(4) | .015(3) | .019(3) | -.003(3) |
| O(12) | .031(3) | .081(5) | .039(4) | -.019(3) | -.013(3) | .003(3) |
| O(13) | .056(4) | .034(3) | .049(4) | .006(3) | .018(3) | -.006(3) |
| O(14) | .026(3) | .060(4) | .036(3) | -.016(3) | -.010(3) | -.001(3) |
| O(15) | .041(3) | .048(4) | .037(3) | -.012(3) | .005(3) | .009(3) |
| O(22) | .060(4) | .073(5) | .020(3) | .013(3) | -.004(3) | .017(3) |
| O(23) | .030(3) | .044(3) | .043(3) | -.007(3) | .002(3) | .016(3) |
| O(24) | .031(3) | .046(3) | .031(3) | -.005(3) | -.002(3) | -.019(3) |
| O(21) | .044(3) | .042(3) | .041(3) | -.004(3) | .010(3) | -.020(3) |
| O(31) | .041(3) | .024(3) | .050(4) | -.006(3) | -.003(3) | .011(3) |
| O(32) | .022(3) | .034(3) | .028(3) | -.003(2) | .004(2) | -.012(2) |
| O(33) | .027(3) | .038(3) | .014(3) | -.002(2) | -.003(2) | -.007(2) |
| O(34) | .048(3) | .022(3) | .051(4) | -.001(3) | .004(3) | .014(3) |
| O(41) | .031(3) | .030(3) | .035(3) | -.013(3) | .010(2) | -.003(2) |
| O(42) | .031(3) | .050(4) | .031(3) | .004(3) | -.008(3) | .015(3) |
| O(43) | .029(3) | .035(3) | .018(3) | -.002(2) | .009(2) | -.010(2) |
| O(44) | .058(4) | .018(3) | .037(3) | -.004(2) | .012(3) | .003(3) |
| N | .017(3) | .016(3) | .018(3) | .004(2) | -.002(2) | .000(2) |
| C(51) | .022(4) | .023(4) | .025(4) | -.004(3) | .001(3) | -.005(3) |
| C(52) | .037(4) | .024(4) | .037(4) | -.009(4) | .005(4) | .001(3) |
| C(53) | .020(4) | .030(4) | .024(4) | .006(3) | -.001(3) | .010(3) |
| C(54) | .038(4) | .020(4) | .053(5) | -.003(4) | .001(4) | .007(4) |
| C(55) | .013(3) | .020(4) | .025(4) | .001(3) | -.002(3) | -.002(3) |
| C(56) | .023(4) | .031(4) | .041(5) | .002(4) | .006(4) | -.005(3) |
| C(57) | .035(4) | .026(4) | .013(3) | .006(3) | .000(3) | -.003(3) |
| C(58) | .045(5) | .046(5) | .037(5) | .010(4) | .019(4) | -.002(4) |

Table S3. Bond lengths [Å] and angles [deg] for 2.

| | | | |
|---|---|---|---|
| Re(1)-Re(2) | 3.0641(4) | C(14)-O(14) | 1.132(8) |
| Re(2)-Re(3) | 3.4040(4) | C(15)-O(15) | 1.140(8) |
| Re(3)-Re(4) | 3.2968(3) | C(21)-O(21) | 1.139(8) |
| Re(1)-C(11) | 1.994(8) | C(22)-O(22) | 1.154(8) |
| Re(1)-C(12) | 1.976(8) | C(23)-O(23) | 1.160(8) |
| Re(1)-C(13) | 1.972(8) | C(24)-O(24) | 1.127(8) |
| Re(1)-C(14) | 1.986(8) | C(31)-O(31) | 1.137(8) |
| Re(1)-C(15) | 1.948(7) | C(32)-O(32) | 1.161(7) |
| Re(2)-C(21) | 2.003(7) | C(33)-O(33) | 1.138(7) |
| Re(2)-C(22) | 1.924(8) | C(34)-O(34) | 1.136(8) |
| Re(2)-C(23) | 1.918(7) | C(42)-O(42) | 1.143(8) |
| Re(2)-C(24) | 1.994(7) | C(43)-O(43) | 1.160(7) |
| Re(3)-C(31) | 1.994(7) | C(44)-O(44) | 1.133(8) |
| Re(3)-C(32) | 1.922(7) | C(41)-O(41) | 1.130(8) |
| Re(3)-C(33) | 1.943(7) | N-C(51) | 1.511(8) |
| Re(3)-C(34) | 2.010(7) | N-C(55) | 1.521(7) |
| Re(4)-C(41) | 1.982(7) | N-C(53) | 1.521(8) |
| Re(4)-C(42) | 1.968(7) | N-C(57) | 1.529(8) |
| Re(4)-C(43) | 1.919(7) | C(51)-C(52) | 1.515(9) |
| Re(4)-C(44) | 2.001(7) | C(53)-C(54) | 1.524(9) |
| C(11)-O(11) | 1.137(9) | C(55)-C(56) | 1.525(9) |
| C(12)-O(12) | 1.152(9) | C(57)-C(58) | 1.509(10) |
| C(13)-O(13) | 1.147(8) | | |

| | | | |
|---|---|---|---|
| Re(1)-Re(2)-Re(3) | 101.41(1) | C(31)-Re(3)-Re(4) | 89.1(2) |
| Re(2)-Re(3)-Re(4) | 99.084(9) | C(32)-Re(3)-Re(4) | 169.0(2) |
| C(15)-Re(1)-C(13) | 91.7(3) | C(33)-Re(3)-Re(4) | 77.6(2) |
| C(15)-Re(1)-C(12) | 96.8(3) | C(34)-Re(3)-Re(4) | 88.5(2) |
| C(13)-Re(1)-C(12) | 89.0(3) | C(43)-Re(4)-C(42) | 93.1(3) |
| C(15)-Re(1)-C(14) | 94.5(3) | C(43)-Re(4)-C(41) | 89.6(3) |
| C(13)-Re(1)-C(14) | 91.5(3) | C(42)-Re(4)-C(41) | 93.8(3) |
| C(12)-Re(1)-C(14) | 168.7(3) | C(43)-Re(4)-C(44) | 89.5(3) |
| C(15)-Re(1)-C(11) | 97.6(3) | C(42)-Re(4)-C(44) | 98.3(3) |
| C(13)-Re(1)-C(11) | 170.6(3) | C(41)-Re(4)-C(44) | 167.9(3) |
| C(12)-Re(1)-C(11) | 88.5(3) | C(41)-Re(4)-Re(3) | 82.8(2) |
| C(14)-Re(1)-C(11) | 89.1(3) | C(42)-Re(4)-Re(3) | 100.7(2) |
| C(11)-Re(1)-Re(2) | 86.6(2) | C(43)-Re(4)-Re(3) | 164.7(2) |
| C(12)-Re(1)-Re(2) | 87.1(2) | C(44)-Re(4)-Re(3) | 95.1(2) |
| C(13)-Re(1)-Re(2) | 84.3(2) | O(11)-C(11)-Re(1) | 177.5(7) |
| C(14)-Re(1)-Re(2) | 81.6(2) | O(12)-C(12)-Re(1) | 177.6(7) |
| C(15)-Re(1)-Re(2) | 174.3(2) | O(13)-C(13)-Re(1) | 179.3(6) |
| C(23)-Re(2)-C(22) | 89.4(3) | O(14)-C(14)-Re(1) | 179.0(6) |
| C(23)-Re(2)-C(24) | 91.8(3) | O(15)-C(15)-Re(1) | 175.5(7) |
| C(22)-Re(2)-C(24) | 91.8(3) | O(21)-C(21)-Re(2) | 178.1(6) |
| C(23)-Re(2)-C(21) | 96.3(3) | O(22)-C(22)-Re(2) | 178.5(7) |
| C(22)-Re(2)-C(21) | 91.6(3) | O(23)-C(23)-Re(2) | 174.8(6) |
| C(24)-Re(2)-C(21) | 171.2(3) | O(24)-C(24)-Re(2) | 178.8(6) |
| C(21)-Re(2)-Re(1) | 88.7(2) | O(31)-C(31)-Re(3) | 177.2(6) |
| C(22)-Re(2)-Re(1) | 85.0(2) | O(32)-C(32)-Re(3) | 179.8(5) |
| C(23)-Re(2)-Re(1) | 172.6(2) | O(33)-C(33)-Re(3) | 177.9(6) |
| C(24)-Re(2)-Re(1) | 83.5(2) | O(34)-C(34)-Re(3) | 174.5(6) |
| C(21)-Re(2)-Re(3) | 86.0(2) | O(42)-C(42)-Re(4) | 178.9(6) |
| C(22)-Re(2)-Re(3) | 173.1(2) | O(43)-C(43)-Re(4) | 176.6(6) |
| C(23)-Re(2)-Re(3) | 84.4(2) | O(44)-C(44)-Re(4) | 175.6(6) |
| C(24)-Re(2)-Re(3) | 91.5(2) | O(41)-C(41)-Re(4) | 177.5(6) |
| C(32)-Re(3)-C(33) | 91.4(3) | C(51)-N-C(55) | 110.5(5) |

| | | | |
|---|---|---|---|
| C(32)-Re(3)-C(31) | 89.8(3) | C(51)-N-C(53) | 106.7(5) |
| C(33)-Re(3)-C(31) | 89.3(3) | C(55)-N-C(53) | 110.8(5) |
| C(32)-Re(3)-C(34) | 92.0(3) | C(51)-N-C(57) | 111.9(5) |
| C(33)-Re(3)-C(34) | 87.1(3) | C(55)-N-C(57) | 106.3(5) |
| C(31)-Re(3)-C(34) | 176.0(3) | C(53)-N-C(57) | 110.7(5) |
| C(31)-Re(3)-Re(2) | 101.5(2) | N-C(51)-C(52) | 114.5(5) |
| C(32)-Re(3)-Re(2) | 91.9(2) | N-C(53)-C(54) | 115.0(6) |
| C(33)-Re(3)-Re(2) | 168.7(2) | N-C(55)-C(56) | 115.1(5) |
| C(34)-Re(3)-Re(2) | 82.0(2) | C(58)-C(57)-N | 114.5(6) |

Table S4. Least-squares planes for 2.

Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane)

9.840 (0.001) x + 10.978 (0.002) y - 1.016 (0.003) z = 10.089 (0.001)

| | | |
|---|---|---|
| * | 0.000 (0.000) | Re1 |
| * | 0.000 (0.000) | Re2 |
| * | 0.000 (0.000) | Re3 |
| | -0.171 (0.000) | H1 |

Rms deviation of fitted atoms = 0.000

- 5.542 (0.002) x + 14.437 (0.001) y + 8.348 (0.003) z = 2.906 (0.002)

Angle to previous plane (with approximate esd) = 75.75 ( 0.01 )

| | | |
|---|---|---|
| * | 0.000 (0.000) | Re2 |
| * | 0.000 (0.000) | Re3 |
| * | 0.000 (0.000) | Re4 |
| | -0.215 (0.000) | H2 |

Rms deviation of fitted atoms = 0.000

Table S5. Atomic coordinates and equivalent isotropic displacement parameters [$Å^2$] for 3. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| Re(1) | .69885(5) | .04037(3) | .28242(3) | .04860(13) |
| Re(2) | .87154(5) | .18984(3) | .13347(3) | .04301(12) |
| Re(3) | .92674(5) | .37934(3) | .22758(3) | .04659(12) |
| Re(4) | 1.04468(5) | .30220(3) | .41132(3) | .04828(13) |
| O(11) | .8915(12) | -.1261(7) | .1738(7) | .095(3) |
| O(12) | .4842(11) | .0708(9) | .1443(7) | .100(3) |
| O(13) | .5150(11) | .2289(7) | .3629(7) | .080(3) |
| O(14) | .9534(11) | .0131(8) | .3921(7) | .090(3) |
| O(15) | .5137(13) | -.0977(8) | .4334(8) | .112(4) |
| O(21) | 1.1552(10) | .0441(7) | .1673(7) | .075(3) |
| O(22) | .8146(11) | .0638(7) | -.0010(6) | .082(3) |
| O(23) | 1.0361(11) | .3117(7) | -.0436(7) | .088(3) |
| O(24) | .5656(10) | .3225(7) | .1361(7) | .084(3) |
| O(31) | 1.2512(10) | .3254(8) | .1190(7) | .088(3) |
| O(32) | .8086(11) | .4916(6) | .0539(7) | .082(3) |
| O(33) | .9979(13) | .5794(7) | .2545(7) | .095(3) |
| O(34) | .6202(10) | .4152(7) | .3621(7) | .083(3) |
| O(41) | 1.2398(11) | .1255(8) | .3165(8) | .098(3) |
| O(42) | .7692(10) | .1901(7) | .4772(7) | .090(3) |
| O(43) | .8330(12) | .4842(8) | .4838(8) | .105(4) |
| O(44) | 1.2948(10) | .4340(7) | .3154(7) | .085(3) |
| O(45) | 1.1572(12) | .2358(8) | .5964(7) | .095(3) |
| C(11) | .822(2) | -.0671(9) | .2144(9) | .062(3) |
| C(12) | .5607(14) | .0624(10) | .1945(9) | .063(3) |
| C(13) | .5864(13) | .1610(10) | .3354(9) | .059(3) |
| C(14) | .858(2) | .0275(9) | .3553(8) | .058(3) |
| C(15) | .585(2) | -.0475(9) | .3769(10) | .069(4) |
| C(21) | 1.0523(14) | .0980(10) | .1550(9) | .060(3) |
| C(22) | .8353(14) | .1091(9) | .0506(9) | .058(3) |
| C(23) | .9770(14) | .2676(9) | .0253(9) | .066(3) |
| C(24) | .6747(14) | .2741(8) | .1343(9) | .059(3) |
| C(31) | 1.134(2) | .3454(9) | .1599(9) | .061(3) |
| C(32) | .8544(13) | .4466(8) | .1176(10) | .059(3) |
| C(33) | .9712(14) | .5046(9) | .2458(9) | .065(3) |
| C(34) | .731(2) | .4003(8) | .3124(10) | .062(3) |
| C(41) | 1.1685(14) | .1896(10) | .3497(10) | .067(3) |
| C(42) | .8706(14) | .2307(8) | .4512(9) | .060(3) |
| C(43) | .9120(14) | .4186(9) | .4578(9) | .063(3) |
| C(44) | 1.2061(13) | .3857(9) | .3489(9) | .060(3) |
| C(45) | 1.115(2) | .2600(9) | .5253(9) | .068(3) |
| H | .8920 | .2500 | .2321 | .060 |
| N | .4402(12) | .7198(7) | .1939(8) | .066(3) |
| C(51) | .354(3) | .812(2) | .226(2) | .164(10) |
| C(52) | .203(2) | .797(2) | .286(2) | .200(14) |
| C(53) | .584(3) | .747(2) | .136(2) | .183(11) |
| C(54) | .593(3) | .822(2) | .059(2) | .166(10) |
| C(55) | .469(3) | .6427(14) | .274(2) | .146(8) |
| C(56) | .549(3) | .673(2) | .341(2) | .197(14) |
| C(57) | .359(2) | .6813(14) | .137(2) | .137(8) |
| C(58) | .418(2) | .5881(12) | .1001(12) | .124(7) |

| | | | | |
|---|---|---|---|---|
| H(51A) | .342(3) | .861(2) | .172(2) | .197 |
| H(51B) | .410(3) | .837(2) | .263(2) | .197 |
| H(52A) | .152(2) | .859(2) | .305(2) | .301 |
| H(52B) | .214(2) | .750(2) | .342(2) | .301 |
| H(52C) | .146(2) | .773(2) | .250(2) | .301 |
| H(53A) | .637(3) | .764(2) | .179(2) | .220 |
| H(53B) | .639(3) | .686(2) | .113(2) | .220 |
| H(54A) | .695(3) | .828(2) | .032(2) | .248 |
| H(54B) | .544(3) | .884(2) | .079(2) | .248 |
| H(54C) | .546(3) | .807(2) | .013(2) | .248 |
| H(55A) | .527(3) | .5842(14) | .249(2) | .175 |
| H(55B) | .375(3) | .6237(14) | .310(2) | .175 |
| H(56A) | .562(3) | .618(2) | .391(2) | .296 |
| H(56B) | .491(3) | .729(2) | .369(2) | .296 |
| H(56C) | .644(3) | .689(2) | .308(2) | .296 |
| H(57A) | .261(2) | .6741(14) | .175(2) | .165 |
| H(57B) | .346(2) | .7321(14) | .084(2) | .165 |
| H(58A) | .352(2) | .5735(12) | .0647(12) | .186 |
| H(58B) | .428(2) | .5354(12) | .1515(12) | .186 |
| H(58C) | .513(2) | .5937(12) | .0597(12) | .186 |

Table S6. Anisotropic displacement parameters [$Å^2$] for 3. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| Re(1) | .0466(3) | .0466(3) | .0526(3) | -.0086(2) | -.0021(2) | -.0157(2) |
| Re(2) | .0420(2) | .0450(2) | .0425(2) | -.0074(2) | -.0052(2) | -.0106(2) |
| Re(3) | .0464(3) | .0404(2) | .0546(3) | -.0066(2) | -.0119(2) | -.0088(2) |
| Re(4) | .0463(3) | .0515(3) | .0513(3) | -.0150(2) | -.0094(2) | -.0113(2) |
| O(11) | .111(8) | .073(6) | .093(8) | -.032(6) | -.002(6) | .002(6) |
| O(12) | .067(7) | .159(10) | .091(8) | -.031(7) | -.032(6) | -.024(6) |
| O(13) | .087(7) | .064(6) | .090(7) | -.024(5) | -.019(6) | .005(5) |
| O(14) | .080(7) | .098(8) | .098(8) | -.005(6) | -.040(6) | -.008(6) |
| O(15) | .112(9) | .096(8) | .112(9) | -.013(7) | .033(7) | -.050(7) |
| O(21) | .053(5) | .080(6) | .096(7) | -.026(5) | -.023(5) | .007(5) |
| O(22) | .098(7) | .096(7) | .064(6) | -.036(5) | -.014(5) | -.025(6) |
| O(23) | .103(8) | .092(7) | .065(6) | -.001(5) | .002(5) | -.042(6) |
| O(24) | .061(6) | .075(6) | .111(8) | -.001(6) | -.029(6) | .006(5) |
| O(31) | .052(6) | .126(9) | .083(7) | -.026(6) | .002(5) | -.012(5) |
| O(32) | .093(7) | .064(6) | .091(7) | .007(5) | -.042(6) | -.007(5) |
| O(33) | .141(9) | .053(5) | .105(8) | -.013(5) | -.037(7) | -.036(6) |
| O(34) | .058(6) | .084(7) | .103(8) | -.032(6) | -.002(5) | -.002(5) |
| O(41) | .066(6) | .099(8) | .135(10) | -.068(7) | -.012(6) | .009(5) |
| O(42) | .068(6) | .106(7) | .100(8) | -.030(6) | .009(5) | -.045(6) |
| O(43) | .087(7) | .105(8) | .137(10) | -.082(8) | -.024(7) | .011(6) |
| O(44) | .066(6) | .083(6) | .108(8) | -.006(6) | -.009(5) | -.036(5) |
| O(45) | .112(8) | .107(8) | .070(7) | -.001(6) | -.042(6) | -.010(6) |
| C(11) | .076(9) | .061(8) | .051(7) | -.007(6) | -.010(7) | -.021(7) |
| C(12) | .047(7) | .082(9) | .058(8) | -.017(7) | .003(6) | -.017(6) |
| C(13) | .053(7) | .064(8) | .065(8) | -.006(7) | -.010(6) | -.027(6) |
| C(14) | .066(8) | .055(7) | .056(8) | -.013(6) | -.015(7) | -.010(6) |
| C(15) | .072(9) | .055(7) | .077(9) | -.009(7) | .004(7) | -.023(7) |
| C(21) | .045(7) | .078(9) | .065(8) | -.029(7) | -.005(6) | -.017(6) |
| C(22) | .070(8) | .054(7) | .054(7) | -.003(6) | -.015(6) | -.017(6) |
| C(23) | .075(9) | .054(7) | .068(9) | -.002(6) | -.004(7) | -.028(6) |
| C(24) | .057(8) | .048(7) | .072(8) | .007(6) | -.027(7) | -.003(6) |
| C(31) | .061(8) | .066(8) | .064(8) | -.006(6) | -.023(7) | -.020(6) |
| C(32) | .057(7) | .045(7) | .077(9) | -.004(6) | -.026(7) | -.004(5) |
| C(33) | .064(8) | .059(8) | .076(9) | -.017(7) | -.004(7) | -.023(6) |
| C(34) | .061(8) | .048(7) | .086(10) | -.028(7) | -.023(7) | -.002(6) |
| C(41) | .053(8) | .074(9) | .082(9) | -.022(7) | -.020(7) | -.012(7) |
| C(42) | .060(8) | .055(7) | .067(8) | -.022(6) | -.007(6) | -.009(6) |
| C(43) | .055(7) | .065(8) | .078(9) | -.037(7) | -.010(6) | -.013(6) |
| C(44) | .049(7) | .063(8) | .068(8) | -.015(6) | -.009(6) | -.008(6) |
| C(45) | .076(9) | .068(8) | .051(8) | -.006(6) | .000(7) | -.012(7) |
| N | .068(7) | .046(6) | .085(8) | -.001(5) | -.021(6) | -.009(5) |
| C(51) | .14(2) | .13(2) | .17(2) | .00(2) | .01(2) | .056(14) |
| C(52) | .13(2) | .20(3) | .18(2) | .01(2) | .06(2) | .06(2) |
| C(53) | .14(2) | .19(3) | .21(3) | -.03(2) | .00(2) | -.05(2) |
| C(54) | .15(2) | .18(2) | .11(2) | .03(2) | .036(14) | -.03(2) |
| C(55) | .19(2) | .102(14) | .17(2) | -.002(14) | -.11(2) | -.013(14) |
| C(56) | .27(3) | .11(2) | .28(3) | -.09(2) | -.22(3) | .05(2) |
| C(57) | .16(2) | .12(2) | .17(2) | -.05(2) | -.07(2) | -.039(14) |
| C(58) | .22(2) | .078(11) | .091(12) | -.023(9) | -.046(14) | -.029(12) |

Table S7. Bond lengths [Å] and angles [deg] for 3.

| | | | |
|---|---|---|---|
| Re(1)-Re(2) | 3.0990(9) | O(14)-C(14) | 1.119(13) |
| Re(2)-Re(3) | 3.3244(11) | O(15)-C(15) | 1.148(14) |
| Re(3)-Re(4) | 3.0959(11) | O(21)-C(21) | 1.137(14) |
| Re(1)-C(11) | 1.976(14) | O(22)-C(22) | 1.130(13) |
| Re(1)-C(12) | 1.981(14) | O(23)-C(23) | 1.159(13) |
| Re(1)-C(13) | 1.984(14) | O(24)-C(24) | 1.115(13) |
| Re(1)-C(14) | 1.991(13) | O(31)-C(31) | 1.139(14) |
| Re(1)-C(15) | 1.928(13) | O(32)-C(32) | 1.153(13) |
| Re(2)-C(21) | 1.979(14) | O(33)-C(33) | 1.136(13) |
| Re(2)-C(22) | 1.905(13) | O(34)-C(34) | 1.130(14) |
| Re(2)-C(23) | 1.925(12) | O(41)-C(41) | 1.122(14) |
| Re(2)-C(24) | 1.996(12) | O(42)-C(42) | 1.141(13) |
| Re(3)-C(31) | 1.980(14) | O(43)-C(43) | 1.125(13) |
| Re(3)-C(32) | 1.920(13) | O(44)-C(44) | 1.124(13) |
| Re(3)-C(33) | 1.919(12) | O(45)-C(45) | 1.17(2) |
| Re(3)-C(34) | 1.974(14) | N-C(57) | 1.47(2) |
| Re(4)-C(41) | 1.987(14) | N-C(51) | 1.47(2) |
| Re(4)-C(42) | 1.973(12) | N-C(55) | 1.48(2) |
| Re(4)-C(43) | 1.969(13) | N-C(53) | 1.48(2) |
| Re(4)-C(44) | 2.012(13) | C(51)-C(52) | 1.51(3) |
| Re(4)-C(45) | 1.899(14) | C(53)-C(54) | 1.40(3) |
| O(11)-C(11) | 1.118(14) | C(55)-C(56) | 1.51(2) |
| O(12)-C(12) | 1.120(14) | C(57)-C(58) | 1.45(2) |
| O(13)-C(13) | 1.130(13) | | |

| | | | |
|---|---|---|---|
| Re(1)-Re(2)-Re(3) | 111.96(3) | C(34)-Re(3)-Re(4) | 85.1(4) |
| Re(2)-Re(3)-Re(4) | 110.38(3) | C(45)-Re(4)-C(43) | 94.1(5) |
| C(15)-Re(1)-C(11) | 94.9(5) | C(45)-Re(4)-C(42) | 95.4(5) |
| C(15)-Re(1)-C(12) | 94.7(5) | C(43)-Re(4)-C(42) | 86.7(5) |
| C(11)-Re(1)-C(12) | 90.1(5) | C(45)-Re(4)-C(41) | 93.1(5) |
| C(15)-Re(1)-C(13) | 92.7(5) | C(43)-Re(4)-C(41) | 172.8(5) |
| C(11)-Re(1)-C(13) | 172.2(5) | C(42)-Re(4)-C(41) | 92.3(5) |
| C(12)-Re(1)-C(13) | 87.5(5) | C(45)-Re(4)-C(44) | 95.4(5) |
| C(15)-Re(1)-C(14) | 93.4(5) | C(43)-Re(4)-C(44) | 91.6(5) |
| C(11)-Re(1)-C(14) | 87.4(5) | C(42)-Re(4)-C(44) | 169.2(5) |
| C(12)-Re(1)-C(14) | 171.7(5) | C(41)-Re(4)-C(44) | 88.1(5) |
| C(13)-Re(1)-C(14) | 93.9(5) | C(41)-Re(4)-Re(3) | 89.0(4) |
| C(11)-Re(1)-Re(2) | 87.6(3) | C(42)-Re(4)-Re(3) | 85.4(4) |
| C(12)-Re(1)-Re(2) | 84.7(3) | C(43)-Re(4)-Re(3) | 83.9(4) |
| C(13)-Re(1)-Re(2) | 84.7(3) | C(44)-Re(4)-Re(3) | 83.8(4) |
| C(14)-Re(1)-Re(2) | 87.3(3) | C(45)-Re(4)-Re(3) | 177.7(4) |
| C(15)-Re(1)-Re(2) | 177.4(4) | O(11)-C(11)-Re(1) | 178.1(11) |
| C(22)-Re(2)-C(23) | 88.7(5) | O(12)-C(12)-Re(1) | 177.1(12) |
| C(22)-Re(2)-C(21) | 91.5(5) | O(13)-C(13)-Re(1) | 175.5(11) |
| C(23)-Re(2)-C(21) | 93.3(5) | O(14)-C(14)-Re(1) | 173.7(11) |
| C(22)-Re(2)-C(24) | 91.9(5) | O(15)-C(15)-Re(1) | 178.0(12) |
| C(23)-Re(2)-C(24) | 95.8(5) | O(21)-C(21)-Re(2) | 178.9(10) |
| C(21)-Re(2)-C(24) | 170.3(5) | O(22)-C(22)-Re(2) | 177.6(10) |
| C(21)-Re(2)-Re(1) | 85.9(3) | O(23)-C(23)-Re(2) | 175.5(11) |
| C(22)-Re(2)-Re(1) | 81.2(3) | O(24)-C(24)-Re(2) | 178.3(11) |
| C(23)-Re(2)-Re(1) | 169.8(4) | O(31)-C(31)-Re(3) | 178.2(11) |
| C(24)-Re(2)-Re(1) | 85.7(3) | O(32)-C(32)-Re(3) | 176.3(11) |
| C(21)-Re(2)-Re(3) | 98.0(3) | O(33)-C(33)-Re(3) | 178.5(12) |
| C(22)-Re(2)-Re(3) | 164.2(3) | O(34)-C(34)-Re(3) | 177.3(10) |
| C(23)-Re(2)-Re(3) | 78.2(4) | O(41)-C(41)-Re(4) | 178.5(12) |

| | | | |
|---|---|---|---|
| C(24)-Re(2)-Re(3) | 80.8(3) | O(42)-C(42)-Re(4) | 177.7(11) |
| C(33)-Re(3)-C(32) | 88.3(5) | O(43)-C(43)-Re(4) | 178.1(11) |
| C(33)-Re(3)-C(34) | 91.0(5) | O(44)-C(44)-Re(4) | 178.4(11) |
| C(32)-Re(3)-C(34) | 93.5(5) | O(45)-C(45)-Re(4) | 178.6(12) |
| C(33)-Re(3)-C(31) | 90.2(5) | C(57)-N-C(51) | 109(2) |
| C(32)-Re(3)-C(31) | 95.4(5) | C(57)-N-C(55) | 109.4(13) |
| C(34)-Re(3)-C(31) | 171.0(5) | C(51)-N-C(55) | 112(2) |
| C(31)-Re(3)-Re(2) | 82.8(3) | C(57)-N-C(53) | 111(2) |
| C(32)-Re(3)-Re(2) | 78.1(3) | C(51)-N-C(53) | 107(2) |
| C(33)-Re(3)-Re(2) | 164.1(4) | C(55)-N-C(53) | 109(2) |
| C(34)-Re(3)-Re(2) | 98.1(3) | N-C(51)-C(52) | 114(2) |
| C(31)-Re(3)-Re(4) | 86.2(3) | C(54)-C(53)-N | 123(2) |
| C(32)-Re(3)-Re(4) | 171.5(3) | N-C(55)-C(56) | 116(2) |
| C(33)-Re(3)-Re(4) | 83.3(4) | C(58)-C(57)-N | 120(2) |

Table S8. Least-squares planes for 3.

Least-squares planes (x,y,z in crystal coordinates) and deviations from them
(* indicates atom used to define plane)

7.952 (0.004) x - 4.602 (0.003) y + 4.602 (0.005) z = 6.672 (0.004)

| | | |
|---|---|---|
| * | 0.000 (0.000) | Re1 |
| * | 0.000 (0.000) | Re2 |
| * | 0.000 (0.000) | Re3 |
| | 0.340 (0.000) | H |

Rms deviation of fitted atoms = 0.000

7.836 (0.004) x + 0.178 (0.004) y - 4.955 (0.003) z = 6.202 (0.004)

Angle to previous plane (with approximate esd) = 47.47 ( 0.03 )

| | | |
|---|---|---|
| * | 0.000 (0.000) | Re2 |
| * | 0.000 (0.000) | Re3 |
| * | 0.000 (0.000) | Re4 |
| | -0.318 (0.000) | H |

Rms deviation of fitted atoms = 0.000