Supporting information

Syntheses, Raman spectroscopy and crystal structures of alkali hexafluoridorhenates(IV) – revisited

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Synopsis

Geometry.

Anisotropic displacement parameters [Å²] for K₂ReF₆

| Atom | U₁₁       | U₂₂       | U₃₃       | U₁₂       | U₁₃       | U₂₃       |
|------|-----------|-----------|-----------|-----------|-----------|-----------|
| Re1  | 0.00883(16)| 0.00883(16)| 0.0082(2) | 0.00441(8)| 0.00000   | 0.00000   |
| F1   | 0.0119(13) | 0.0162(10) | 0.0117(12)| 0.0060(6) | -0.0012(10)| -0.0006(5)|
| K1   | 0.0118(5)  | 0.0118(5)  | 0.0096(6) | 0.0059(2) | 0.00000   | 0.00000   |
| Bond/Angle | Value (Å or °) |
|-----------|---------------|
| Re1—F1    | 1.948(3)      |
| F1—K1     | 2.9325(10)    |
| Re1—F1\(^i\) | 1.948(3)  |
| F1—K1\(^i\) | 2.946(3)  |
| Re1—F1\(^ii\) | 1.948(3) |
| F1—K1\(^vi\) | 2.762(3)  |
| Re1—F1\(^iii\) | 1.948(3) |
| K1—F1\(^x\) | 2.762(3)  |
| Re1—F1\(^iv\) | 1.948(3) |
| K1—F1\(^xii\) | 2.762(3) |
| Re1—F1\(^v\) | 1.948(3) |
| K1—F1\(^xiii\) | 2.9325(11) |
| Re1—K1\(^i\) | 3.6263(13) |
| K1—F1\(^xiv\) | 2.9325(10) |
| Re1—K1\(^vi\) | 3.6263(13) |
| K1—F1\(^iv\) | 2.9325(11) |
| Re1—K1\(^vii\) | 3.6263(13) |
| K1—F1\(^xv\) | 2.9325(11) |
| Re1—K1\(^i\) | 3.6263(13) |
| K1—F1\(^xvi\) | 2.9325(11) |
| Re1—K1\(^viii\) | 3.6263(13) |
| K1—F1\(^xvii\) | 2.946(3)  |
| Re1—K1\(^ix\) | 3.6263(13) |
| K1—F1\(^ix\) | 2.946(3)  |
| F1—K1\(^x\) | 2.762(3) |
| K1—F1\(^vi\) | 2.946(3)  |
| F1—K1    | 2.9325(11) |
| F1—Re1—F1\(^i\) | 180.000 |
| K1—F1—K1\(^viii\) | 168.22(13) |
| F1—Re1—F1\(^ii\) | 86.08(12) |
| Re1—F1—K1\(^vi\) | 93.38(11)  |
| F1\(^i\)—Re1—F1\(^i\) | 93.92(12) |
| K1\(^i\)—F1—K1\(^vi\) | 105.55(10) |
| F1\(^i\)—Re1—F1\(^iii\) | 93.92(12) |
| K1\(^i\)—F1—K1\(^vi\) | 94.27(6)  |
| F1\(^i\)—Re1—F1\(^iv\) | 86.08(12) |
| K1\(^viii\)—F1—K1\(^vi\) | 94.27(6)  |
| F1\(^i\)—Re1—F1\(^ii\) | 180.00(19) |
| F1\(^xi\)—K1—F1\(^x\) | 65.46(11) |
| F1—Re1—F1\(^iv\) | 93.92(12) |
| F1\(^xi\)—K1—F1\(^xii\) | 65.46(11) |
| F1\(^i\)—Re1—F1\(^iv\) | 86.08(12) |
| F1\(^x\)—K1—F1\(^xi\) | 65.46(11) |
| F1\(^ii\)—Re1—F1\(^iv\) | 86.08(12) |
| F1\(^xi\)—K1—F1\(^xiii\) | 62.44(10) |
| F1\(^iii\)—Re1—F1\(^iv\) | 93.92(12) |
| F1\(^x\)—K1—F1\(^xii\) | 127.81(6) |
| F1—Re1—F1\(^v\) | 86.08(12) |
| F1\(^xii\)—K1—F1\(^xiii\) | 95.05(6)  |
| F1\(^i\)—Re1—F1\(^v\) | 93.92(12) |
| F1\(^x\)—K1—F1\(^xiv\) | 62.44(10) |
| F1\(^ii\)—Re1—F1\(^v\) | 93.92(12) |
| F1\(^x\)—K1—F1\(^xv\) | 95.05(6)  |
| F1\(^iii\)—Re1—F1\(^v\) | 86.08(12) |
| F1\(^xii\)—K1—F1\(^xv\) | 127.81(6) |
| F1\(^iv\)—Re1—F1\(^v\) | 180.00(7) |
| F1\(^xiii\)—K1—F1\(^xiv\) | 58.10(11) |
| F1—Re1—K1\(^i\) | 126.206(14) |
| F1\(^xi\)—K1—F1\(^iv\) | 95.05(6)  |
| F1\(^i\)—Re1—K1\(^i\) | 53.794(14) |
| F1\(^x\)—K1—F1\(^iv\) | 127.81(6) |
| F1\(^ii\)—Re1—K1\(^i\) | 125.81(9) |
| F1\(^xii\)—K1—F1\(^iv\) | 62.44(10) |
| F1\(^iii\)—Re1—K1\(^i\) | 54.19(9) |
| F1\(^xiii\)—K1—F1\(^iv\) | 61.22(12) |
| F1\(^iv\)—Re1—K1\(^i\) | 126.205(14) |
| F1\(^xiv\)—K1—F1\(^iv\) | 118.98(2)  |
| F1\(^v\)—Re1—K1\(^i\) | 53.795(14) |
| F1\(^x\)—K1—F1\(^v\) | 95.05(6)  |
| F1—Re1—K1\(^v\) | 54.19(9) |
| F1\(^x\)—K1—F1\(^v\) | 62.44(10) |
| F1\(^i\)—Re1—K1\(^v\) | 125.81(9) |
| F1\(^xii\)—K1—F1\(^v\) | 127.81(6) |
| F1\(^ii\)—Re1—K1\(^v\) | 53.794(14) |
| F1\(^xiii\)—K1—F1\(^v\) | 118.98(2)  |
| F1\(^iii\)—Re1—K1\(^v\) | 126.206(14) |
| F1\(^xiv\)—K1—F1\(^v\) | 61.22(12) |
| F1\(^iv\)—Re1—K1\(^v\) | 126.205(14) |
| F1\(^iv\)—K1—F1\(^v\) | 168.22(13) |
| F1\(^v\)—Re1—K1\(^v\) | 53.795(14) |
| F1\(^x\)—K1—F1\(^vi\) | 127.81(6) |
| K1'—Rel—K1 vi | 107.11(3) | F1'x—K1—F1 xvi | 62.44(10) |
| F1—Rel—K1 vii | 125.81(9) | F1'xiv—K1—F1 xvi | 95.05(6) |
| F1'i—Rel—K1 vii | 54.19(9) | F1'xivii—K1—F1 xvi | 168.22(13) |
| F1''i—Rel—K1 vii | 126.206(14) | F1'xiv—K1—F1 xvi | 118.98(2) |
| F1''i—Rel—K1 vii | 53.794(14) | F1'iv—K1—F1 xvi | 118.98(2) |
| F1''iv—Rel—K1 vii | 53.795(14) | F1'iv—K1—F1 xvi | 58.10(11) |
| F1''v—Rel—K1 vii | 126.205(14) | F1'iv—K1—F1 | 127.81(6) |
| K1'i—Rel—K1 vii | 72.89(3) | F1'iv—K1—F1 | 95.05(6) |
| K1'i—Rel—K1 vii | 180.000 | F1'ivii—K1—F1 | 62.44(10) |
| K1'i—Rel—K1 vii | 53.794(14) | F1'xivii—K1—F1 vi | 118.98(2) |
| K1'i—Rel—K1 vii | 126.206(14) | F1'xiv—K1—F1 vii | 168.22(13) |
| K1'i—Rel—K1 vii | 54.19(9) | F1'xiv—K1—F1 | 58.09(11) |
| K1'i—Rel—K1 vii | 125.81(9) | F1'xiv—K1—F1 | 118.98(2) |
| K1'i—Rel—K1 vii | 126.206(14) | F1'xiv—K1—F1 vii | 118.98(2) |
| K1'i—Rel—K1 vii | 126.205(14) | F1'xiv—K1—F1 vii | 62.12(11) |
| K1'i—Rel—K1 vii | 180.000 | F1'xivii—K1—F1 vii | 105.55(10) |
| K1'i—Rel—K1 vii | 72.89(3) | F1'xivii—K1—F1 vii | 144.70(4) |
| K1'i—Rel—K1 vii | 107.11(3) | F1'xivii—K1—F1 xvi | 144.70(4) |
| K1'i—Rel—K1 vii | 53.794(14) | F1'xiv—K1—F1 vii | 53.8(1) |
| K1'i—Rel—K1 vii | 126.205(14) | F1'xiv—K1—F1 vii | 85.73(6) |
| K1'i—Rel—K1 vii | 126.206(14) | F1'xiv—K1—F1 vii | 85.73(6) |
| K1'i—Rel—K1 vii | 53.794(14) | F1'xiv—K1—F1 vii | 114.69(6) |
| K1'i—Rel—K1 vii | 125.81(9) | F1'xiv—K1—F1 vii | 114.69(6) |
| K1'i—Rel—K1 vii | 72.90(3) | F1'xiv—K1—F1 vii | 114.69(6) |
| K1'i—Rel—K1 vii | 107.10(3) | F1'xiv—K1—F1 vii | 114.69(6) |
| K1'i—Rel—K1 vii | 54.19(9) | F1'xiv—K1—F1 vii | 53.8(1) |
| K1'i—Rel—K1 vii | 126.205(14) | F1'xiv—K1—F1 vii | 85.73(6) |
| K1'i—Rel—K1 vii | 53.794(14) | F1'xiv—K1—F1 vii | 114.69(6) |
| K1'i—Rel—K1 vii | 126.206(14) | F1'xiv—K1—F1 vii | 114.69(6) |
| K1'i—Rel—K1 vii | 72.90(3) | F1'xiv—K1—F1 vii | 114.69(6) |
| K1'i—Rel—K1 vii | 107.10(3) | F1'xiv—K1—F1 vii | 114.69(6) |
| K1'i—Rel—K1 vii | 126.206(14) | F1'xiv—K1—F1 vii | 60.91(10) |
| K1'i—Rel—K1 vii | 125.81(9) | F1'xiv—K1—F1 vii | 60.91(10) |
| K1'i—Rel—K1 vii | 107.10(3) | F1'xiv—K1—F1 vii | 60.91(10) |
| K1'i—Rel—K1 vii | 107.10(3) | F1'xiv—K1—F1 vii | 60.91(10) |
| K1'i—Rel—K1 vii | 72.90(3) | F1'xiv—K1—F1 vii | 60.91(10) |
| K1'i—Rel—K1 vii | 180.000 | F1'xiv—K1—F1 vii | 60.91(10) |
Symmetry codes: (i) \(-x, -y, -z\); (ii) \(-y, x, -z\); (iii) \(-x+y, -x, z\); (iv) \(y, -x+y, -z\); (vi) \(1-x, 1-y, -z\); (vii) \(-1+x, -1+y, 0\); (viii) \(1-y, x, -z\); (ix) \(0, -x+y, 1-z\); (x) \(-y, x, 1-z\); (xi) \(1-x, -y, 0\); (xii) \(-x+y, 1-x, z\); (xiv) \(0, 1-y, z\); (xvi) \(-y, 1-x, 0\);
(xvii) \(1-x, 0, z\).

Geometry.

| Atom | \(U_{11}\) | \(U_{22}\) | \(U_{33}\) | \(U_{12}\) | \(U_{13}\) | \(U_{23}\) |
|------|-------------|-------------|-------------|-------------|-------------|-------------|
| Re1  | 0.0133(6)   | 0.0133(6)   | 0.0205(8)   | 0.0066(3)   | 0.00000     | 0.00000     |
| F1   | 0.015(4)    | 0.017(3)    | 0.012(3)    | 0.0077(19)  | 0.001(3)    | 0.0007(14)  |
| Rb1  | 0.0131(8)   | 0.0131(8)   | 0.0152(12)  | 0.0065(4)   | 0.00000     | 0.00000     |

Geometric parameters, bond lengths [Å] and angles [°] for Rb\(_2\)ReF\(_6\).

| Bond | Length [Å] | Angle [°] |
|------|------------|-----------|
| Re1—F1\(^i\) | 1.945(7) | F1—Rb1\(^{viii}\) | 3.0181(11) |
| Re1—F1\(^{ii}\) | 1.945(7) | F1—Rb1\(^{vi}\) | 3.058(7) |
| Re1—F1\(^{iii}\) | 1.945(7) | Rb1—F1\(^{xi}\) | 2.907(7) |
| Re1—F1\(^{iv}\) | 1.945(7) | Rb1—F1\(^x\) | 2.907(7) |
| Re1—F1\(^{v}\) | 1.945(7) | Rb1—F1\(^{xii}\) | 2.907(7) |
| Re1—F1 | 1.945(7) | Rb1—F1\(^{xiii}\) | 3.0181(11) |
| Re1—Rb1\(^i\) | 3.733(1) | Rb1—F1\(^{xiv}\) | 3.0181(11) |
| Re1—Rb1\(^{vi}\) | 3.7330(11) | Rb1—F1\(^v\) | 3.0181(11) |
| Re1—Rb1\(^{vii}\) | 3.7330(11) | Rb1—F1\(^{xv}\) | 3.0181(11) |
| Re1—Rb1 | 3.733(1) | Rb1—F1\(^{xvi}\) | 3.0181(11) |
| Re1—Rb1\(^{viii}\) | 3.7330(11) | Rb1—F1\(^{xvii}\) | 3.058(7) |
| Re1—Rb1\(^{ix}\) | 3.7330(11) | Rb1—F1\(^{x}\) | 3.058(7) |
| F1—Rb1\(^x\) | 2.907(7) | Rb1—F1\(^{vi}\) | 3.058(7) |
| F1—Rb1 | 3.0181(11) | | |
| F1\(^{i}\)—Re1—F1\(^{ii}\) | 93.5(3) | Rb1—F1—Rb1\(^{viii}\) | 166.2(3) |
| F1\(^{i}\)—Re1—F1\(^{ii}\) | 86.5(3) | Re1—F1—Rb1\(^{vi}\) | 93.9(2) |
| F1\(^{ii}\)—Re1—F1\(^{iii}\) | 180.0(3) | Rb1\(^x\)—F1—Rb1\(^{vi}\) | 104.5(2) |
| F1\(^{i}\)—Re1—F1\(^{iv}\) | 93.5(3) | Rb1—F1—Rb1\(^{vi}\) | 94.26(14) |
| F1\(^{iv}\)—Re1—F1\(^{v}\) | 93.5(3) | Rb1\(^{vii}\)—F1—Rb1\(^{vi}\) | 94.26(14) |
| F1\(^{iii}\)—Re1—F1\(^{iv}\) | 86.5(3) | F1\(^{xi}\)—Rb1—F1\(^x\) | 65.8(2) |
| F1\(^{i}\)—Re1—F1\(^{v}\) | 86.5(3) | F1\(^{xi}\)—Rb1—F1\(^x\) | 65.8(2) |
| F1\(^{iv}\)—Re1—F1\(^{v}\) | 86.5(3) | F1\(^x\)—Rb1—F1\(^{xii}\) | 65.8(2) |
| F1\(^{iii}\)—Re1—F1\(^{v}\) | 93.5(3) | F1\(^{xi}\)—Rb1—F1\(^{xii}\) | 62.7(2) |
| F1\(^{iv}\)—Re1—F1\(^{v}\) | 180.000 | F1\(^{x}\)—Rb1—F1\(^{xiii}\) | 128.31(8) |
| F1\(^{i}\)—Re1—F1 | 180.000 | F1\(^{xi}\)—Rb1—F1\(^{xiii}\) | 96.30(14) |
| F1\(^{ii}\)—Re1—F1 | 86.5(3) | F1\(^{xi}\)—Rb1—F1\(^{xiv}\) | 62.7(2) |
Symmetry codes: (i) -x, -y, -z; (ii) x-y, x, -z; (iii) -x+y, -x, z; (iv) y, -x+y, -z; (v) -y, x-y, z; (vi) 1-x, 1-y, -z; (vii) 1-x, 1-y, 1-z; (viii) -y, 1+x-y, z; (ix) x-y, x, 1-z; (x) -x+y, 1-x, z; (xi) y, 1-x+y, -z.

Geometry.

| Atom | U_{11}       | U_{22}       | U_{33}       | U_{12}       | U_{13}       | U_{23}       |
|------|--------------|--------------|--------------|--------------|--------------|--------------|
| Re1  | 0.00483(16)  | 0.00483(16)  | 0.0032(2)    | 0.00241(8)   | 0.00000      | 0.00000      |
| F1   | 0.0088(8)    | 0.0107(6)    | 0.0075(9)    | 0.0044(4)    | -0.0023(6)   | -0.0012(3)   |
| Cs1  | 0.00661(16)  | 0.00661(16)  | 0.0052(2)    | 0.00331(8)   | 0.00000      | 0.00000      |

Geometric parameters, bond lengths [Å] and angles [°] for Cs$_2$ReF$_6$

| Bond          | Length [Å] | Angle [°] |
|---------------|------------|-----------|
| Re1—F1$^i$    | 1.9594(18) |           |
| Re1—F1$^{ii}$ | 1.9594(18) |           |
| F1—Cs1$^{viii}$ | 3.1655(6)  |           |
| F1—Cs1$^v$    | 3.224(2)   |           |
| Bond          | Angle/Distance       |
|---------------|----------------------|
| Re1—F1<sup>iii</sup> | 1.9594(18)  | Cs1—F1<sup>xi</sup> | 3.0955(19) |
| Re1—F1<sup>iv</sup>  | 1.9594(18)  | Cs1—F1<sup>x</sup>  | 3.0955(19) |
| Re1—F1<sup>v</sup>   | 1.9594(18)  | Cs1—F1<sup>xii</sup>| 3.0955(19) |
| Re1—F1             | 1.9594(18)  | Cs1—F1<sup>xiii</sup>| 3.1655(6)  |
| Re1—Cs1<sup>i</sup> | 3.9100(6)   | Cs1—F1<sup>xiv</sup>| 3.1655(6)  |
| Re1—Cs1<sup>ii</sup>| 3.9100(6)   | Cs1—F1<sup>iii</sup> | 3.1655(6)  |
| Re1—Cs1<sup>iii</sup>| 3.9100(6)   | Cs1—F1<sup>iv</sup>  | 3.1655(6)  |
| Re1—Cs1<sup>iv</sup>| 3.9100(6)   | Cs1—F1<sup>v</sup>   | 3.1655(6)  |
| Re1—Cs1<sup>v</sup> | 3.9100(6)   | Cs1—F1<sup>xvi</sup>| 3.1655(6)  |
| Re1—Cs1<sup>vii</sup>| 3.9100(6)  | Cs1—F1<sup>xvii</sup> | 3.224(2)   |
| Re1—Cs1<sup>viii</sup>| 3.9100(6)  | Cs1—F1<sup>ix</sup>  | 3.224(2)   |
| F1—Cs1<sup>x</sup>  | 3.0955(19)  | Cs1—F1<sup>vi</sup>  | 3.224(2)   |
| F1—Cs1             | 3.1655(6)   |                       |            |
| F1<sup>i</sup>—Re1—F1<sup>ii</sup> | 93.14(7) | Cs1—F1—Cs1<sup>viii</sup>| 163.82(6) |
| F1<sup>i</sup>—Re1—F1<sup>iii</sup> | 86.86(7)  | Re1—F1—Cs1<sup>vi</sup>| 94.78(7)   |
| F1<sup>ii</sup>—Re1—F1<sup>iii</sup> | 180.00(4) | Cs1<sup>x</sup>—F1—Cs1<sup>vi</sup>| 102.55(5) |
| F1<sup>i</sup>—Re1—F1<sup>iv</sup> | 93.14(7)  | Cs1—F1—Cs1<sup>vi</sup>| 94.07(3)   |
| F1<sup>ii</sup>—Re1—F1<sup>iv</sup> | 93.14(7)  | Cs1<sup>viii</sup>—F1—Cs1<sup>vi</sup>| 94.07(3)   |
| F1<sup>iii</sup>—Re1—F1<sup>iv</sup> | 86.86(7)  | F1<sup>x</sup>—Cs1—F1<sup>x</sup>| 67.11(6)   |
| F1<sup>i</sup>—Re1—F1<sup>ix</sup> | 86.86(7)  | F1<sup>x</sup>—Cs1—F1<sup>ix</sup>| 67.11(6)   |
| F1<sup>ii</sup>—Re1—F1<sup>ix</sup> | 86.86(7)  | F1<sup>x</sup>—Cs1—F1<sup>xii</sup>| 67.11(6)   |
| F1<sup>iii</sup>—Re1—F1<sup>ix</sup> | 93.14(7)  | F1<sup>x</sup>—Cs1—F1<sup>xii</sup>| 67.11(6)   |
| F1<sup>iv</sup>—Re1—F1<sup>ix</sup> | 93.14(7)  | F1<sup>x</sup>—Cs1—F1<sup>xiii</sup>| 62.38(6)   |
| F1<sup>i</sup>—Re1—F1<sup>ix</sup> | 180.00(8) | F1<sup>x</sup>—Cs1—F1<sup>xiii</sup>| 129.122(17)|
| F1<sup>i</sup>—Re1—F1<sup>ix</sup> | 93.14(7)  | F1<sup>x</sup>—Cs1—F1<sup>ixiv</sup>| 97.70(3)   |
| F1<sup>iv</sup>—Re1—F1<sup>ix</sup> | 93.14(7)  | F1<sup>x</sup>—Cs1—F1<sup>ixiv</sup>| 129.122(17)|
| F1<sup>v</sup>—Re1—F1<sup>ix</sup> | 93.14(7)  | F1<sup>x</sup>—Cs1—F1<sup>ixiv</sup>| 97.70(3)   |
| F1<sup>i</sup>—Re1—Cs1<sup>i</sup> | 53.533(6) | F1<sup>x</sup>—Cs1—F1<sup>xix</sup>| 53.43(7)   |
| F1<sup>ii</sup>—Re1—Cs1<sup>i</sup> | 53.533(6) | F1<sup>x</sup>—Cs1—F1<sup>xii</sup>| 97.70(3)   |
| F1<sup>iii</sup>—Re1—Cs1<sup>i</sup> | 126.467(6)| F1<sup>x</sup>—Cs1—F1<sup>xii</sup>| 129.122(17)|
| F1<sup>iv</sup>—Re1—Cs1<sup>i</sup> | 124.74(6) | F1<sup>x</sup>—Cs1—F1<sup>xiii</sup>| 62.38(6)   |
| F1<sup>v</sup>—Re1—Cs1<sup>i</sup> | 55.26(6)  | F1<sup>x</sup>—Cs1—F1<sup>xiv</sup>| 118.323(15)|
| F1<sup>i</sup>—Re1—Cs1<sup>vi</sup> | 126.467(6)| F1<sup>x</sup>—Cs1—F1<sup>xv</sup>| 97.70(3)   |
| F1<sup>ii</sup>—Re1—Cs1<sup>vi</sup> | 124.74(6) | F1<sup>x</sup>—Cs1—F1<sup>xv</sup>| 62.38(6)   |
| F1<sup>iii</sup>—Re1—Cs1<sup>vi</sup> | 53.533(6) | F1<sup>x</sup>—Cs1—F1<sup>xv</sup>| 129.122(17)|
| F1<sup>iv</sup>—Re1—Cs1<sup>vi</sup> | 53.533(6) | F1<sup>x</sup>—Cs1—F1<sup>xv</sup>| 118.323(14)|
| F1<sup>v</sup>—Re1—Cs1<sup>vi</sup> | 126.467(6)| F1<sup>x</sup>—Cs1—F1<sup>xv</sup>| 65.44(7)   |
| F1<sup>i</sup>—Re1—Cs1<sup>vii</sup> | 126.467(6)| F1<sup>x</sup>—Cs1—F1<sup>xvi</sup>| 163.82(6) |
| F1<sup>ii</sup>—Re1—Cs1<sup>vii</sup> | 124.74(6) | F1<sup>x</sup>—Cs1—F1<sup>xvi</sup>| 129.123(17)|
| F1<sup>iii</sup>—Re1—Cs1<sup>vii</sup> | 55.26(6)  | F1<sup>x</sup>—Cs1—F1<sup>xvi</sup>| 62.38(6)   |
| F1<sup>iv</sup>—Re1—Cs1<sup>vii</sup> | 106.554(9)| F1<sup>x</sup>—Cs1—F1<sup>xvi</sup>| 97.70(3)   |
| F1<sup>v</sup>—Re1—Cs1<sup>vii</sup> | 55.26(6)  | F1<sup>x</sup>—Cs1—F1<sup>xvi</sup>| 62.38(6)   |
| F1<sup>i</sup>—Re1—Cs1<sup>viii</sup> | 126.467(6)| F1<sup>x</sup>—Cs1—F1<sup>xvii</sup>| 53.43(7)   |
| F1<sup>ii</sup>—Re1—Cs1<sup>viii</sup> | 124.74(6) | F1<sup>x</sup>—Cs1—F1<sup>xvii</sup>| 118.323(15)|
| F1<sup>iii</sup>—Re1—Cs1<sup>viii</sup> | 53.533(6) | F1<sup>x</sup>—Cs1—F1<sup>xvii</sup>| 163.82(6) |
| Symmetry codes: (i) -x, -y, -z; (ii) y, -x+y, -z; (iii) -y, x-y, z; (iv) x-y, x, -z; (v) -x+y, -x, z; (vi) 1-x, 1-y, -z; (vii) -1+x, -1+y, z; (viii) x, -1+y, z; (ix) -x, 1-y, -z; (x) 1-x, 1-y, 1-z; (xi) y, 1-x+y, 1-z; (xii) x-y, x, 1-z; (xiii) -x+y, 1-x, z; (xiv) x, 1+y, z; (xv) 1-y, 1-x+y, 1-z; (xvi) 1-x+y, 1-x, z; (xvii) y, 1-x+y, -z. |