**New mercury(II) and cadmium(II) complexes with (*p*-methylbenzoyl)methylene triphenylphosphorane: synthesis, spectroscopic and structural characterization**

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Table **S1**. Atomic coordinates (× 104) and equivalent isotropic displacement parameters (A2 × 103) for *U*(eq) is defined as one third of the trace of the orthogonalized *Uij* tensor. \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ *x y z* *U*(eq) \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

C(1) 10654(5) 9627(6) 3093(4) 42(2)

C(2) 11043(5) 10874(6) 3403(4) 43(2)

C(3) 10824(5) 11483(7) 4011(4) 49(2)

C(4) 11401(6) 12360(7) 4506(4) 60(2)

C(5) 11217(8) 12956(9) 5067(6) 82(3)

C(6) 10456(9) 12747(9) 5148(6) 81(3)

C(7) 10205(11) 13430(13) 5723(8) 134(6)

C(8) 9876(8) 11893(11) 4645(7) 97(4)

C(9) 10067(7) 11245(9) 4100(5) 75(3)

C(10) 12528(5) 8839(6) 3566(4) 48(2)

C(11) 12722(6) 9113(8) 4353(4) 64(2)

C(12) 13608(8) 9128(10) 4915(6) 91(4)

C(13) 14259(8) 8846(10) 4702(7) 89(3)

C(14) 14063(7) 8578(10) 3932(8) 87(3)

C(15) 13202(6) 8600(8) 3351(6) 66(2)

C(16) 11081(5) 7088(6) 2919(4) 45(2)

C(17) 11651(6) 6316(8) 3533(5) 66(2)

C(18) 11414(7) 5104(8) 3542(7) 87(3)

C(19) 10643(7) 4645(8) 2985(6) 72(2)

C(20) 10071(6) 5400(8) 2388(5) 67(2)

C(21) 10290(6) 6616(7) 2357(5) 60(2)

C(22) 11297(5) 8867(6) 1869(4) 44(2)

C(23) 11442(6) 7874(7) 1480(5) 56(2)

C(24) 11392(6) 8038(9) 725(5) 67(2)

C(25) 11203(6) 9163(9) 367(5) 67(2)

C(26) 11075(6) 10142(8) 753(5) 62(2)

C(27) 11117(5) 10019(7) 1507(4) 49(2)

C(28) 7160(17) 9340(30) 2259(11) 340(20)

C(29) 7640(12) 9751(15) 3669(9) 146(7)

O(1) 11552(4) 11370(5) 3173(3) 53(1)

O(2) 8594(7) 9361(15) 2914(5) 188(6)

P(1) 11378(1) 8670(2) 2856(1) 40(1)

Hg(1) 9362(1) 9867(1) 2036(1) 53(1)

S(1) 7852(3) 8862(6) 2986(3) 165(2)

Br(1) 8997(1) 12183(1) 1601(1) 79(1)

Br(2) 8259(1) 8581(1) 916(1) 82(1)

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Table **S2**. Bond lengths (Å) and angles (º) for **6**.\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

C(1)–C(2) 1.498(10)

C(1)–P(1) 1.788(7)

C(1)–Hg(1) 2.221(7)

C(1)–H(1) 0.9800

C(2)–O(1) 1.230(8)

C(2)–C(3) 1.488(10)

C(3)–C(9) 1.371(12)

C(3)–C(4) 1.381(10)

C(4)–C(5) 1.372(12)

C(4)–H(4) 0.9300

C(5)–C(6) 1.363(14)

C(5)–H(5) 0.9300

C(6)–C(8) 1.372(15)

C(6)–C(7) 1.505(14)

C(7)–H(7A) 0.9600

C(7)–H(7B) 0.9600

C(7)–H(7C) 0.9600

C(8)–C(9) 1.380(12)

C(8)–H(8) 0.9300

C(9)–H(9) 0.9300

C(10)–C(15) 1.373(12)

C(10)–C(11) 1.390(10)

C(10)–P(1) 1.811(7)

C(11)–C(12) 1.396(13)

C(11)–H(11) 0.9300

C(12)–C(13) 1.343(16)

C(12)–H(12) 0.9300

C(13)–C(14) 1.359(16)

C(13)–H(13) 0.9300

C(14)–C(15) 1.377(14)

C(14)–H(14) 0.9300

C(15)–H(15) 0.9300

C(16)–C(21) 1.381(10)

C(16)–C(17) 1.402(10)

C(16)–P(1) 1.797(7)

C(17)–C(18) 1.369(12)

C(17)–H(17) 0.9300

C(18)–C(19) 1.351(13)

C(18)–H(18) 0.9300

C(19)–C(20) 1.378(12)

C(19)–H(19) 0.9300

C(20)–C(21) 1.370(11)

C(20)–H(20) 0.9300

C(21)–H(21) 0.9300

C(22)–C(23) 1.374(10)

C(22)–C(27) 1.384(10)

C(22)–P(1) 1.799(7)

C(23)–C(24) 1.385(11)

C(23)–H(23) 0.9300

C(24)–C(25) 1.355(13)

C(24)–H(24) 0.9300

C(25)–C(26) 1.346(12)

C(25)–H(25) 0.9300

C(26)–C(27) 1.384(10)

C(26)–H(26) 0.9300

C(27)–H(27) 0.9300

C(28)–S(1) 1.446(16)

C(28)–H(28A) 0.9600

C(28)–H(28B) 0.9600

C(28)–H(28C) 0.9600

C(29)–S(1) 1.750(14)

C(29)–H(29A) 0.9600

C(29)–H(29B) 0.9600

C(29)–H(29C) 0.9600

O(2)–S(1) 1.412(8)

O(2)–Hg(1) 2.540(7)

Hg(1)–Br(2) 2.5204(9)

Hg(1)–Br(1) 2.6166(10)

C(2)–C(1)–P(1) 112.8(5)

C(2)–C(1)–Hg(1) 109.3(4)

P(1)–C(1)–Hg(1) 110.5(3)

C(2)–C(1)–H(1) 108.0

P(1)–C(1)–H(1) 108.0

Hg(1)–C(1)–H(1) 108.0

O(1)–C(2)–C(3) 120.7(6)

O(1)–C(2)–C(1) 120.5(6)

C(3)–C(2)–C(1) 118.8(6)

C(9)–C(3)–C(4) 117.5(7)

C(9)–C(3)–C(2) 123.7(7)

C(4)–C(3)–C(2) 118.8(7)

C(5)–C(4)–C(3) 120.6(9)

C(5)–C(4)–H(4) 119.7

C(3)–C(4)–H(4) 119.7

C(6)–C(5)–C(4) 122.3(9)

C(6)–C(5)–H(5) 118.8

C(4)–C(5)–H(5) 118.8

C(5)–C(6)–C(8) 116.9(9)

C(5)–C(6)–C(7) 124.0(11)

C(8)–C(6)–C(7) 119.0(11)

C(6)–C(7)–H(7A) 109.5

C(6)–C(7)–H(7B) 109.5

H(7A)–C(7)–H(7B) 109.5

C(6)–C(7)–H(7C) 109.5

H(7A)–C(7)–H(7C) 109.5

H(7B)–C(7)–H(7C) 109.5

C(6)–C(8)–C(9) 121.6(10)

C(6)–C(8)–H(8) 119.2

C(9)–C(8)–H(8) 119.2

C(3)–C(9)–C(8) 121.0(9)

C(3)–C(9)–H(9) 119.5

C(8)–C(9)–H(9) 119.5

C(15)–C(10)–C(11) 120.1(8)

C(15)–C(10)–P(1) 120.8(6)

C(11)–C(10)–P(1) 118.8(6)

C(10)–C(11)–C(12) 118.8(10)

C(10)–C(11)–H(11) 120.6

C(12)–C(11)–H(11) 120.6

C(13)–C(12)–C(11) 120.5(10)

C(13)–C(12)–H(12) 119.8

C(11)–C(12)–H(12) 119.7

C(12)–C(13)–C(14) 120.3(10)

C(12)–C(13)–H(13) 119.9

C(14)–C(13)–H(13) 119.9

C(13)–C(14)–C(15) 121.3(11)

C(13)–C(14)–H(14) 119.3

C(15)–C(14)–H(14) 119.3

C(10)–C(15)–C(14) 118.9(9)

C(10)–C(15)–H(15) 120.6

C(14)–C(15)–H(15) 120.6

C(21)–C(16)–C(17) 119.3(7)

C(21)–C(16)–P(1) 120.1(5)

C(17)–C(16)–P(1) 120.7(6)

C(18)–C(17)–C(16) 118.7(8)

C(18)–C(17)–H(17) 120.7

C(16)–C(17)–H(17) 120.7

C(19)–C(18)–C(17) 121.8(9)

C(19)–C(18)–H(18) 119.1

C(17)–C(18)–H(18) 119.1

C(18)–C(19)–C(20) 120.0(8)

C(18)–C(19)–H(19) 120.0

C(20)–C(19)–H(19) 120.0

C(21)–C(20)–C(19) 119.7(8)

C(21)–C(20)–H(20) 120.1

C(19)–C(20)–H(20) 120.1

C(20)–C(21)–C(16) 120.5(8)

C(20)–C(21)–H(21) 119.8

C(16)–C(21)–H(21) 119.8

C(23)–C(22)–C(27) 119.6(6)

C(23)–C(22)–P(1) 119.8(5)

C(27)–C(22)–P(1) 120.6(5)

C(22)–C(23)–C(24) 119.4(7)

C(22)–C(23)–H(23) 120.3

C(24)–C(23)–H(23) 120.3

C(25)–C(24)–C(23) 120.9(8)

C(25)–C(24)–H(24) 119.6

C(23)–C(24)–H(24) 119.6

C(26)–C(25)–C(24) 119.9(7)

C(26)–C(25)–H(25) 120.1

C(24)–C(25)–H(25) 120.1

C(25)–C(26)–C(27) 121.2(8)

C(25)–C(26)–H(26) 119.4

C(27)–C(26)–H(26) 119.4

C(26)–C(27)–C(22) 119.1(7)

C(26)–C(27)–H(27) 120.4

C(22)–C(27)–H(27) 120.4

S(1)–C(28)–H(28A) 109.5

S(1)–C(28)–H(28B) 109.5

H(28A)–C(28)–H(28B) 109.5

S(1)–C(28)–H(28C) 109.5

H(28A)–C(28)–H(28C) 109.5

H(28B)–C(28)–H(28C) 109.5

S(1)–C(29)–H(29A) 109.5

S(1)–C(29)–H(29B) 109.5

H(29A)–C(29)–H(29B) 109.5

S(1)–C(29)–H(29C) 109.5

H(29A)–C(29)–H(29C) 109.5

H(29B)–C(29)–H(29C) 109.5

S(1)–O(2)–Hg(1) 148.6(5)

C(1)–P(1)–C(16) 107.3(3)

C(1)–P(1)–C(22) 115.3(3)

C(16)–P(1)–C(22) 106.2(3)

C(1)–P(1)–C(10) 112.3(3)

C(16)–P(1)–C(10) 106.4(3)

C(22)–P(1)–C(10) 108.8(3)

C(1)–Hg(1)–Br(2) 138.80(17)

C(1)–Hg(1)–O(2) 88.3(3)

Br(2)–Hg(1)–O(2) 91.4(2)

C(1)–Hg(1)–Br(1) 113.13(17)

Br(2)–Hg(1)–Br(1) 106.33(3)

O(2)–Hg(1)–Br(1) 106.9(4)

O(2)–S(1)–C(28) 98.8(13)

O(2)–S(1)–C(29) 108.9(7)

C(28)–S(1)–C(29) 98.8(11)

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ Symmetry transformations used to generate equivalent atoms:

Table **S3**. Anisotropic displacement parameters (Å2 x 103) for **6**. The anisotropic displacement factor exponent takes the form following equation: -2π2[ h2 a\*2 U11 + ... + 2 h k a\* b\* U12 ]

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

*U*11 *U*22 *U*33 *U*23 *U*13 *U*12\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

C(1) 43(4) 43(4) 41(3) 0(3) 20(3) -5(3)

C(2) 40(4) 45(4) 40(3) 3(3) 13(3) 2(3)

C(3) 59(5) 48(4) 40(3) -4(3) 21(3) -3(4)

C(4) 71(6) 54(5) 57(4) -9(4) 29(4) -12(4)

C(5) 115(9) 63(6) 71(6) -17(5) 43(6) -21(6)

C(6) 111(9) 69(6) 79(6) -12(5) 56(6) -2(6)

C(7) 194(16) 130(11) 119(10) -60(9) 108(11) -33(11)

C(8) 102(9) 107(9) 117(8) -27(7) 80(8) -11(7)

C(9) 78(7) 84(7) 80(6) -30(5) 49(5) -11(5)

C(10) 43(4) 39(4) 55(4) 6(3) 15(3) -1(3)

C(11) 54(5) 71(6) 50(4) 1(4) 8(4) 1(4)

C(12) 79(8) 78(7) 70(6) 6(5) -12(5) -21(6)

C(13) 49(6) 67(6) 112(9) 10(6) -2(6) -7(5)

C(14) 57(7) 76(7) 119(9) 10(6) 28(6) -2(5)

C(15) 52(5) 68(5) 75(5) 3(4) 23(4) -8(4)

C(16) 51(5) 38(4) 42(3) -1(3) 18(3) -4(3)

C(17) 45(5) 56(5) 79(5) 17(4) 11(4) -6(4)

C(18) 70(7) 55(6) 112(8) 28(5) 17(6) 2(5)

C(19) 71(6) 41(4) 100(7) 4(5) 32(5) -8(5)

C(20) 61(6) 48(5) 75(5) -2(4) 12(4) -16(4)

C(21) 64(6) 38(4) 60(4) 2(3) 11(4) -6(4)

C(22) 43(4) 45(4) 47(3) 4(3) 22(3) -1(3)

C(23) 63(5) 49(4) 60(4) -3(3) 31(4) -2(4)

C(24) 72(6) 80(6) 61(5) -17(5) 39(5) -5(5)

C(25) 66(6) 93(7) 44(4) -1(4) 26(4) -12(5)

C(26) 64(5) 70(5) 52(4) 11(4) 25(4) 0(5)

C(27) 50(4) 47(4) 53(4) 1(3) 26(3) 3(4)

C(28) 360(30) 580(50) 152(15) 230(20) 200(20) 390(40)

C(29) 162(15) 178(15) 143(12) -58(11) 107(12) -69(12)

O(1) 59(3) 51(3) 56(3) -3(2) 32(3) -6(3)

O(2) 112(7) 385(18) 100(6) -73(9) 77(6) -133(10)

P(1) 41(1) 37(1) 40(1) 4(1) 16(1) -1(1)

Hg(1) 46(1) 63(1) 48(1) -4(1) 18(1) -2(1)

S(1) 101(3) 287(7) 121(3) -74(4) 60(2) -79(4)

Br(1) 86(1) 53(1) 88(1) -10(1) 26(1) 11(1)

Br(2) 89(1) 76(1) 61(1) -14(1) 14(1) -23(1)

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Table **S4**. Hydrogen coordinates (× 104) and isotropic displacement parameters (*A*2 × 103) for **6**.

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ *x y z* *U*(eq) \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

H(1) 10542 9209 3507 51

H(4) 11919 12548 4460 72

H(5) 11626 13523 5405 98

H(7A) 10185 14303 5620 160

H(7B) 10637 13267 6257 160

H(7C) 9632 13155 5660 160

H(8) 9342 11746 4673 116

H(9) 9676 10639 3789 91

H(11) 12270 9284 4501 76

H(12) 13750 9333 5440 109

H(13) 14846 8835 5084 107

H(14) 14519 8375 3795 105

H(15) 13078 8456 2822 80

H(17) 12179 6621 3925 79

H(18) 11793 4583 3941 104

H(19) 10498 3818 3006 87

H(20) 9538 5087 2006 81

H(21) 9903 7127 1955 71

H(23) 11573 7099 1721 67

H(24) 11489 7367 460 81

H(25) 11161 9259 -143 80

H(26) 10957 10915 509 74

H(27) 11025 10700 1767 58

H(28A) 7147 8882 1814 403

H(28B) 7275 10200 2201 403

H(28C) 6597 9268 2278 403

H(29A) 7475 10575 3464 176

H(29B) 8164 9784 4164 176

H(29C) 7164 9382 3752 176

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Table **S5**. Torsion angles [º] for **6.** \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ P(1)–C(1)–C(2)–O(1) 31.5(8)

Hg(1)–C(1)–C(2)–O(1) –91.8(7)

P(1)–C(1)–C(2)–C(3) –146.7(5)

Hg(1)–C(1)–C(2)–C(3) 90.0(6)

O(1)–C(2)–C(3)–C(9) 156.5(8)

C(1)–C(2)–C(3)–C(9) –25.2(11)

O(1)–C(2)–C(3)–C(4) –22.1(10)

C(1)–C(2)–C(3)–C(4) 156.2(7)

C(9)–C(3)–C(4)–C(5) 0.4(12)

C(2)–C(3)–C(4)–C(5) 179.1(8)

C(3)–C(4)–C(5)–C(6) –2.0(15)

C(4)–C(5)–C(6)–C(8) 0.8(16)

C(4)–C(5)–C(6)–C(7) –176.5(11)

C(5)–C(6)–C(8)–C(9) 2.0(18)

C(7)–C(6)–C(8)–C(9) 179.4(12)

C(4)–C(3)–C(9)–C(8) 2.3(14)

C(2)–C(3)–C(9)–C(8) –176.3(9)

C(6)–C(8)–C(9)–C(3) –3.6(18)

C(15)–C(10)–C(11)–C(12) –0.7(12)

P(1)–C(10)–C(11)–C(12) 174.0(7)

C(10)–C(11)–C(12)–C(13) –1.9(15)

C(11)–C(12)–C(13)–C(14) 1.8(16)

C(12)–C(13)–C(14)–C(15) 0.8(16)

C(11)–C(10)–C(15)–C(14) 3.2(13)

P(1)–C(10)–C(15)–C(14) –171.4(7)

C(13)–C(14)–C(15)–C(10) –3.3(15)

C(21)–C(16)–C(17)–C(18) 1.7(13)

P(1)–C(16)–C(17)–C(18) –177.6(8)

C(16)–C(17)–C(18)–C(19) –1.1(17)

C(17)–C(18)–C(19)–C(20) 0.0(18)

C(18)–C(19)–C(20)–C(21) 0.4(16)

C(19)–C(20)–C(21)–C(16) 0.2(15)

C(17)–C(16)–C(21)–C(20) –1.3(13)

P(1)–C(16)–C(21)–C(20) 178.0(7)

C(27)–C(22)–C(23)–C(24) –1.0(12)

P(1)–C(22)–C(23)–C(24) –179.0(6)

C(22)–C(23)–C(24)–C(25) 0.1(13)

C(23)–C(24)–C(25)–C(26) 1.0(14)

C(24)–C(25)–C(26)–C(27) –1.2(14)

C(25)–C(26)–C(27)–C(22) 0.3(12)

C(23)–C(22)–C(27)–C(26) 0.8(11)

P(1)–C(22)–C(27)–C(26) 178.8(6)

C(2)–C(1)–P(1)–C(16) 155.3(5)

Hg(1)–C(1)–P(1)–C(16) –82.0(4)

C(2)–C(1)–P(1)–C(22) –86.6(5)

Hg(1)–C(1)–P(1)–C(22) 36.0(4)

C(2)–C(1)–P(1)–C(10) 38.7(5)

Hg(1)–C(1)–P(1)–C(10) 161.4(3)

C(21)–C(16)–P(1)–C(1) 70.5(7)

C(17)–C(16)–P(1)–C(1) –110.2(7)

C(21)–C(16)–P(1)–C(22) –53.3(7)

C(17)–C(16)–P(1)–C(22) 126.0(7)

C(21)–C(16)–P(1)–C(10) –169.2(7)

C(17)–C(16)–P(1)–C(10) 10.2(8)

C(23)–C(22)–P(1)–C(1) –147.7(6)

C(27)–C(22)–P(1)–C(1) 34.3(7)

C(23)–C(22)–P(1)–C(16) –29.1(7)

C(27)–C(22)–P(1)–C(16) 152.9(6)

C(23)–C(22)–P(1)–C(10) 85.2(7)

C(27)–C(22)–P(1)–C(10) –92.9(7)

C(15)–C(10)–P(1)–C(1) –154.3(6)

C(11)–C(10)–P(1)–C(1) 31.1(7)

C(15)–C(10)–P(1)–C(16) 88.7(7)

C(11)–C(10)–P(1)–C(16) –86.0(7)

C(15)–C(10)–P(1)–C(22) –25.4(7)

C(11)–C(10)–P(1)–C(22) 159.9(6)

C(2)–C(1)–Hg(1)–Br(2) 167.0(3)

P(1)–C(1)–Hg(1)–Br(2) 42.3(5)

C(2)–C(1)–Hg(1)–O(2) –102.9(6)

P(1)–C(1)–Hg(1)–O(2) 132.4(5)

C(2)–C(1)–Hg(1)–Br(1) 4.8(5)

P(1)–C(1)–Hg(1)–Br(1) –119.9(3)

S(1)–O(2)–Hg(1)–C(1) –151(2)

S(1)–O(2)–Hg(1)–Br(2) –12(2)

S(1)–O(2)–Hg(1)–Br(1) 96(2)

Hg(1)–O(2)–S(1)–C(28) –41(2)

Hg(1)–O(2)–S(1)–C(29) –143.1(18)

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Symmetry transformations used to generate equivalent atoms:

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