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Table S1. Crystal Data and Intensity Collection for $CsTaQ_3$ (Q = S, Se, Te).

| | | | |
|---|---|---|---|
| Formula | $CsTaS_3$ | $CsTaSe_3$ | $CsTaTe_3$ |
| Formula mass (amu) | 410.04 | 550.74 | 696.66 |
| Space group | $D^4_{6h}$–$P6_3/mmc$ | $D^4_{6h}$–$P6_3/mmc$ | $D^4_{6h}$–$P6_3/mmc$ |
| $a$ (Å)[a] | 7.266(2) | 7.500(1) | 7.992(4) |
| $c$ | 5.961(2) | 6.182(1) | 6.496(4) |
| $V$ (Å$^3$) | 272.55(1) | 301.15(7) | 359.3(4) |
| $Z$ | 2 | 2 | 2 |
| $\rho_c$ (g cm$^{-3}$) | 4.996 | 6.074 | 6.439 |
| $T$ of data collection (K)[b] | 115(2) | 115(2) | 115(2) |
| Crystal shape | Needle ≈ 0.048 x 0.030 x 0.034 x 0.307 mm | Needle ≈ 0.020 x 0.017 x 0.020 x 0.307 mm | Needle ≈ 0.034 x 0.036 x 0.036 x 0.294 mm |
| | | bounded by {100},{001} | |
| Crystal volume (mm$^3$) | 0.341 x $10^{-3}$ | 0.941 x $10^{-4}$ | 0.318 x $10^{-3}$ |
| Radiation | graphite monochromated MoK ($\lambda(K\alpha_1)$ = 0.7093 Å) | | |
| Detector aperture (mm) | Horizontal, 6.5; vertical 6.5; 32 cm from crystal | | |
| Scan type | θ–2θ | θ–2θ | θ–2θ |
| Scan speed (deg min$^{-1}$) | 3 | 3 | 2 |
| Scan width (deg) | 2.3 | 2.1 | 1.7 |
| Takeoff angle (deg) | 2.5 | 2.5 | 2.5 |
| $\lambda^{-1}$ sinθ limits (Å$^{-1}$) | 0.079-0.595 | 0.077-0.571 | 0.072–0.628 |
| Background measurement | 13.4 sec | 14 sec | 20 sec |
| Number of data collected | 212 | 1822 | 1750 |
| Number of unique data | 114 | 112 | 111 |
| Number of unique data with $F_o^2 > 2\sigma(F_o^2)$ | 98 | 98 | 87 |
| Number of variables | 11 | 11 | 10 |
| $R_{ave}$ | 0.042 | 0.137 | 0.113 |

| | | | |
|---|---|---|---|
| $R_w(F^2)^c$ | 0.072 | 0.106 | 0.131 |
| $R_1{}^c$ | 0.034 | 0.036 | 0.038 |
| Extinction coefficient | 0.004(2) | 0.013(3) | – |
| Error in observation of unit weight | 1.033 | 1.672 | 2.208 |
| Linear absorption coefficient ($cm^{-1}$) | 277 | 422 | 321 |
| Transmission factors[d] | 0.309-0.487 | 0.448-0.529 | 0.343–0.392 |

[a] Obtained from a refinement with the constraints $a = b$, $\alpha = \beta = 90°$, $\gamma = 120°$. [b] The low temperature system is based on a design by Huffman. [c] $R_w(F_o{}^2) = [\Sigma[w(F_o{}^2-F_c{}^2)^2]/\Sigma wF_o{}^4]^{1/2}$; $w^{-1} = \sigma^2(F_o{}^2) + (0.04F_o{}^2)^2$ for $F_o{}^2 \geq 0$; $w^{-1} = \sigma^2(F_o{}^2)$ for $F_o{}^2 \leq 0$; $R_1(F) = \Sigma|\,|F_o| - |F_c|\,|/\Sigma|F_o|$. [d] The analytical method as employed in the Northwestern absorption program AGNOST was used for the absorption correction.

Table S2. Bond lengths (Å) and angles (deg.) for $CsTaS_3$.

| | |
|---|---|
| Ta(1)-S(1)#2 | 2.339(5) |
| Ta(1)-S(1) | 2.339(5) |
| Ta(1)-S(1)#1 | 2.339(5) |
| Ta(1)-Ta(1)#3 | 2.579(12) |
| Ta(1)-S(1)#1 | 2.582(6) |
| Ta(1)-S(1)#4 | 2.582(6) |
| Ta(1)-S(1)#5 | 2.582(6) |
| Ta(1)-Cs(1)#7 | 4.389(2) |
| Ta(1)-Cs(1)#8 | 4.389(2) |
| Cs(1)-S(1)#9 | 3.6360(10) |
| Cs(1)-S(1)#7 | 3.6360(10) |
| Cs(1)-S(1)#10 | 3.6360(10) |
| Cs(1)-S(1)#11 | 3.6360(10) |
| Cs(1)-S(1)#12 | 3.6359(10) |
| Cs(1)-S(1)#8 | 3.6359(10) |
| Cs(1)-S(1)#7 | 3.731(3) |
| Cs(1)-S(1)#13 | 3.731(3) |
| Cs(1)-S(1)#14 | 3.731(3) |
| Cs(1)-S(1)#15 | 3.731(3) |
| Cs(1)-S(1) | 3.731(3) |
| Cs(1)-S(1)#16 | 3.731(3) |
| S(1)-Ta(1)#3 | 2.339(5) |
| S(1)-Ta(1)#1 | 2.582(6) |
| S(1)-Ta(1)#4 | 2.582(6) |
| S(1)-S(1)#2 | 3.379(9) |
| S(1)-S(1)#1 | 3.379(9) |
| S(1)-S(1)#12 | 3.562(3) |
| S(1)-S(1)#11 | 3.562(3) |
| S(1)-S(1)#4 | 3.562(3) |
| S(1)-S(1)#5 | 3.562(3) |
| S(1)-Cs(1)#7 | 3.6359(10) |
| S(1)-Cs(1)#8 | 3.6360(10) |
| S(1)-Cs(1)#17 | 3.731(3) |
| S(1)-S(1)#13 | 3.887(9) |
| S(1)-S(1)#16 | 3.887(9) |
| | |
| S(1)#2-Ta(1)-S(1) | 92.5(2) |
| S(1)#2-Ta(1)-S(1)#1 | 92.5(2) |
| S(1)-Ta(1)-S(1)#1 | 92.5(2) |
| S(1)#2-Ta(1)-S(1)#1 | 92.64(11) |
| S(1)-Ta(1)-S(1)#1 | 172.5(2) |
| S(1)#1-Ta(1)-S(1)#1 | 92.64(11) |
| S(1)#2-Ta(1)-S(1)#4 | 172.5(2) |
| S(1)-Ta(1)-S(1)#4 | 92.64(11) |
| S(1)#1-Ta(1)-S(1)#4 | 92.64(11) |
| S(1)#1-Ta(1)-S(1)#4 | 81.7(2) |
| S(1)#2-Ta(1)-S(1)#5 | 92.64(11) |
| S(1)-Ta(1)-S(1)#5 | 92.64(11) |
| S(1)#1-Ta(1)-S(1)#5 | 172.5(2) |
| S(1)#1-Ta(1)-S(1)#5 | 81.7(2) |
| S(1)#4-Ta(1)-S(1)#5 | 81.7(2) |
| S(1)#2-Ta(1)-Cs(1)#7 | 55.89(3) |
| S(1)-Ta(1)-Cs(1)#7 | 55.89(3) |
| S(1)#1-Ta(1)-Cs(1)#7 | 129.4(2) |
| S(1)#1-Ta(1)-Cs(1)#7 | 123.61(6) |
| S(1)#4-Ta(1)-Cs(1)#7 | 123.61(6) |
| S(1)#5-Ta(1)-Cs(1)#7 | 58.00(8) |
| S(1)#2-Ta(1)-Cs(1)#8 | 129.4(2) |
| S(1)-Ta(1)-Cs(1)#8 | 55.89(3) |
| S(1)#1-Ta(1)-Cs(1)#8 | 55.89(3) |
| S(1)#1-Ta(1)-Cs(1)#8 | 123.61(6) |
| S(1)#4-Ta(1)-Cs(1)#8 | 58.01(8) |
| S(1)#5-Ta(1)-Cs(1)#8 | 123.61(6) |
| Cs(1)#7-Ta(1)-Cs(1)#8 | 111.75(7) |
| S(1)#9-Cs(1)-S(1)#7 | 55.4(2) |
| S(1)#9-Cs(1)-S(1)#10 | 64.6(2) |

| | |
|---|---|
| S(1)#7-Cs(1)-S(1)#10 | 120.0 |
| S(1)#9-Cs(1)-S(1)#11 | 119.999(1) |
| S(1)#7-Cs(1)-S(1)#11 | 64.6(2) |
| S(1)#10-Cs(1)-S(1)#11 | 175.4(2) |
| S(1)#9-Cs(1)-S(1)#12 | 175.4(2) |
| S(1)#7-Cs(1)-S(1)#12 | 120.0 |
| S(1)#10-Cs(1)-S(1)#12 | 120.0 |
| S(1)#11-Cs(1)-S(1)#12 | 55.4(2) |
| S(1)#9-Cs(1)-S(1)#8 | 120.0 |
| S(1)#7-Cs(1)-S(1)#8 | 175.4(2) |
| S(1)#10-Cs(1)-S(1)#8 | 55.4(2) |
| S(1)#11-Cs(1)-S(1)#8 | 120.0 |
| S(1)#12-Cs(1)-S(1)#8 | 64.6(2) |
| S(1)#9-Cs(1)-S(1)#7 | 57.82(8) |
| S(1)#7-Cs(1)-S(1)#7 | 57.82(8) |
| S(1)#10-Cs(1)-S(1)#7 | 91.39(5) |
| S(1)#11-Cs(1)-S(1)#7 | 91.39(5) |
| S(1)#12-Cs(1)-S(1)#7 | 120.55(2) |
| S(1)#8-Cs(1)-S(1)#7 | 120.56(2) |
| S(1)#9-Cs(1)-S(1)#13 | 57.82(8) |
| S(1)#7-Cs(1)-S(1)#13 | 57.82(8) |
| S(1)#10-Cs(1)-S(1)#13 | 91.39(5) |
| S(1)#11-Cs(1)-S(1)#13 | 91.39(5) |
| S(1)#12-Cs(1)-S(1)#13 | 120.55(2) |
| S(1)#8-Cs(1)-S(1)#13 | 120.55(2) |
| S(1)#7-Cs(1)-S(1)#13 | 106.04(12) |
| S(1)#9-Cs(1)-S(1)#14 | 91.39(5) |
| S(1)#7-Cs(1)-S(1)#14 | 120.56(2) |
| S(1)#10-Cs(1)-S(1)#14 | 57.82(8) |
| S(1)#11-Cs(1)-S(1)#14 | 120.56(2) |
| S(1)#12-Cs(1)-S(1)#14 | 91.39(5) |
| S(1)#8-Cs(1)-S(1)#14 | 57.82(8) |
| S(1)#7-Cs(1)-S(1)#14 | 62.79(10) |
| S(1)#13-Cs(1)-S(1)#14 | 144.99(5) |
| S(1)#9-Cs(1)-S(1)#15 | 120.56(2) |
| S(1)#7-Cs(1)-S(1)#15 | 91.39(5) |
| S(1)#10-Cs(1)-S(1)#15 | 120.56(2) |
| S(1)#11-Cs(1)-S(1)#15 | 57.82(8) |
| S(1)#12-Cs(1)-S(1)#15 | 57.82(8) |
| S(1)#8-Cs(1)-S(1)#15 | 91.39(5) |
| S(1)#7-Cs(1)-S(1)#15 | 62.79(10) |
| S(1)#13-Cs(1)-S(1)#15 | 144.99(5) |
| S(1)#14-Cs(1)-S(1)#15 | 62.79(10) |
| S(1)#9-Cs(1)-S(1) | 120.55(2) |
| S(1)#7-Cs(1)-S(1) | 91.39(5) |
| S(1)#10-Cs(1)-S(1) | 120.56(2) |
| S(1)#11-Cs(1)-S(1) | 57.82(8) |
| S(1)#12-Cs(1)-S(1) | 57.82(8) |
| S(1)#8-Cs(1)-S(1) | 91.39(5) |
| S(1)#7-Cs(1)-S(1) | 144.99(5) |
| S(1)#13-Cs(1)-S(1) | 62.79(10) |
| S(1)#14-Cs(1)-S(1) | 144.99(5) |
| S(1)#15-Cs(1)-S(1) | 106.04(13) |
| S(1)#9-Cs(1)-S(1)#16 | 91.39(5) |
| S(1)#7-Cs(1)-S(1)#16 | 120.55(2) |
| S(1)#10-Cs(1)-S(1)#16 | 57.82(8) |
| S(1)#11-Cs(1)-S(1)#16 | 120.55(2) |
| S(1)#12-Cs(1)-S(1)#16 | 91.39(5) |
| S(1)#8-Cs(1)-S(1)#16 | 57.82(8) |
| S(1)#7-Cs(1)-S(1)#16 | 144.99(5) |
| S(1)#13-Cs(1)-S(1)#16 | 62.79(10) |
| S(1)#14-Cs(1)-S(1)#16 | 106.04(13) |
| S(1)#15-Cs(1)-S(1)#16 | 144.99(5) |
| S(1)-Cs(1)-S(1)#16 | 62.79(10) |
| Ta(1)-S(1)-S(1)#2 | 43.74(10) |
| Ta(1)#3-S(1)-S(1)#2 | 43.74(10) |
| Ta(1)#1-S(1)-S(1)#2 | 49.12(9) |
| Ta(1)#4-S(1)-S(1)#2 | 49.13(9) |
| Ta(1)-S(1)-S(1)#1 | 43.74(10) |

| | |
|---|---|
| Ta(1)#3-S(1)-S(1)#1 | 43.74(10) |
| Ta(1)#1-S(1)-S(1)#1 | 49.12(9) |
| Ta(1)#4-S(1)-S(1)#1 | 49.13(9) |
| S(1)#2-S(1)-S(1)#1 | 60.0 |
| Ta(1)-S(1)-S(1)#12 | 103.5(2) |
| Ta(1)#3-S(1)-S(1)#12 | 46.38(11) |
| Ta(1)#1-S(1)-S(1)#12 | 109.94(14) |
| Ta(1)#4-S(1)-S(1)#12 | 40.98(9) |
| S(1)#2-S(1)-S(1)#12 | 90.0 |
| S(1)#1-S(1)-S(1)#12 | 61.69(6) |
| Ta(1)-S(1)-S(1)#11 | 103.5(2) |
| Ta(1)#3-S(1)-S(1)#11 | 46.38(11) |
| Ta(1)#1-S(1)-S(1)#11 | 109.94(14) |
| Ta(1)#4-S(1)-S(1)#11 | 40.98(9) |
| S(1)#2-S(1)-S(1)#11 | 61.69(6) |
| S(1)#1-S(1)-S(1)#11 | 90.0 |
| S(1)#12-S(1)-S(1)#11 | 56.63(11) |
| Ta(1)-S(1)-S(1)#4 | 46.38(11) |
| Ta(1)#3-S(1)-S(1)#4 | 103.5(2) |
| Ta(1)#1-S(1)-S(1)#4 | 40.98(9) |
| Ta(1)#4-S(1)-S(1)#4 | 109.94(14) |
| S(1)#2-S(1)-S(1)#4 | 90.0 |
| S(1)#1-S(1)-S(1)#4 | 61.69(6) |
| S(1)#12-S(1)-S(1)#4 | 113.59(14) |
| S(1)#11-S(1)-S(1)#4 | 148.22(6) |
| Ta(1)-S(1)-S(1)#5 | 46.39(11) |
| Ta(1)#3-S(1)-S(1)#5 | 103.5(2) |
| Ta(1)#1-S(1)-S(1)#5 | 40.98(9) |
| Ta(1)#4-S(1)-S(1)#5 | 109.94(14) |
| S(1)#2-S(1)-S(1)#5 | 61.69(6) |
| S(1)#1-S(1)-S(1)#5 | 90.0 |
| S(1)#12-S(1)-S(1)#5 | 148.22(6) |
| S(1)#11-S(1)-S(1)#5 | 113.59(14) |
| S(1)#4-S(1)-S(1)#5 | 56.63(11) |
| Ta(1)-S(1)-Cs(1)#7 | 91.93(6) |
| Ta(1)#3-S(1)-Cs(1)#7 | 91.93(6) |
| Ta(1)#1-S(1)-Cs(1)#7 | 91.75(6) |
| Ta(1)#4-S(1)-Cs(1)#7 | 91.75(6) |
| S(1)#2-S(1)-Cs(1)#7 | 62.31(8) |
| S(1)#1-S(1)-Cs(1)#7 | 122.31(8) |
| S(1)#12-S(1)-Cs(1)#7 | 119.01(4) |
| S(1)#11-S(1)-Cs(1)#7 | 62.43(8) |
| S(1)#4-S(1)-Cs(1)#7 | 119.01(4) |
| S(1)#5-S(1)-Cs(1)#7 | 62.43(8) |
| Ta(1)-S(1)-Cs(1)#8 | 91.93(6) |
| Ta(1)#3-S(1)-Cs(1)#8 | 91.93(6) |
| Ta(1)#1-S(1)-Cs(1)#8 | 91.75(6) |
| Ta(1)#4-S(1)-Cs(1)#8 | 91.75(6) |
| S(1)#2-S(1)-Cs(1)#8 | 122.31(8) |
| S(1)#1-S(1)-Cs(1)#8 | 62.31(8) |
| S(1)#12-S(1)-Cs(1)#8 | 62.43(8) |
| S(1)#11-S(1)-Cs(1)#8 | 119.01(4) |
| S(1)#4-S(1)-Cs(1)#8 | 62.43(8) |
| S(1)#5-S(1)-Cs(1)#8 | 119.01(4) |
| Cs(1)#7-S(1)-Cs(1)#8 | 175.4(2) |
| Ta(1)-S(1)-Cs(1) | 160.4(2) |
| Ta(1)#3-S(1)-Cs(1) | 93.51(13) |
| Ta(1)#1-S(1)-Cs(1) | 167.9(2) |
| Ta(1)#4-S(1)-Cs(1) | 86.06(10) |
| S(1)#2-S(1)-Cs(1) | 121.39(5) |
| S(1)#1-S(1)-Cs(1) | 121.39(5) |
| S(1)#12-S(1)-Cs(1) | 59.75(2) |
| S(1)#11-S(1)-Cs(1) | 59.75(2) |
| S(1)#4-S(1)-Cs(1) | 146.421(14) |
| S(1)#5-S(1)-Cs(1) | 146.420(13) |
| Cs(1)#7-S(1)-Cs(1) | 88.61(5) |
| Cs(1)#8-S(1)-Cs(1) | 88.61(5) |
| Ta(1)-S(1)-Cs(1)#17 | 93.51(12) |
| Ta(1)#3-S(1)-Cs(1)#17 | 160.4(2) |

| | |
|---|---|
| Ta(1)#1-S(1)-Cs(1)#17 | 86.06(10) |
| Ta(1)#4-S(1)-Cs(1)#17 | 167.9(2) |
| S(1)#2-S(1)-Cs(1)#17 | 121.39(5) |
| S(1)#1-S(1)-Cs(1)#17 | 121.39(5) |
| S(1)#12-S(1)-Cs(1)#17 | 146.421(13) |
| S(1)#11-S(1)-Cs(1)#17 | 146.420(14) |
| S(1)#4-S(1)-Cs(1)#17 | 59.75(2) |
| S(1)#5-S(1)-Cs(1)#17 | 59.75(2) |
| Cs(1)#7-S(1)-Cs(1)#17 | 88.61(5) |
| Cs(1)#8-S(1)-Cs(1)#17 | 88.61(5) |
| Cs(1)-S(1)-Cs(1)#17 | 106.04(12) |
| Ta(1)-S(1)-S(1)#13 | 136.26(10) |
| Ta(1)#3-S(1)-S(1)#13 | 136.26(10) |
| Ta(1)#1-S(1)-S(1)#13 | 130.87(9) |
| Ta(1)#4-S(1)-S(1)#13 | 130.88(9) |
| S(1)#2-S(1)-S(1)#13 | 120.0 |
| S(1)#1-S(1)-S(1)#13 | 180.0(2) |
| S(1)#12-S(1)-S(1)#13 | 118.31(6) |
| S(1)#11-S(1)-S(1)#13 | 90.0 |
| S(1)#4-S(1)-S(1)#13 | 118.31(6) |
| S(1)#5-S(1)-S(1)#13 | 90.0 |
| Cs(1)#7-S(1)-S(1)#13 | 57.69(8) |
| Cs(1)#8-S(1)-S(1)#13 | 117.69(8) |
| Cs(1)-S(1)-S(1)#13 | 58.61(5) |
| Cs(1)#17-S(1)-S(1)#13 | 58.61(5) |
| Ta(1)-S(1)-S(1)#16 | 136.26(10) |
| Ta(1)#3-S(1)-S(1)#16 | 136.26(10) |
| Ta(1)#1-S(1)-S(1)#16 | 130.87(9) |
| Ta(1)#4-S(1)-S(1)#16 | 130.87(9) |
| S(1)#2-S(1)-S(1)#16 | 179.999(3) |
| S(1)#1-S(1)-S(1)#16 | 120.0 |
| S(1)#12-S(1)-S(1)#16 | 90.0 |
| S(1)#11-S(1)-S(1)#16 | 118.31(6) |
| S(1)#4-S(1)-S(1)#16 | 90.0 |
| S(1)#5-S(1)-S(1)#16 | 118.31(6) |
| Cs(1)#7-S(1)-S(1)#16 | 117.69(8) |
| Cs(1)#8-S(1)-S(1)#16 | 57.69(8) |
| Cs(1)-S(1)-S(1)#16 | 58.61(5) |
| Cs(1)#17-S(1)-S(1)#16 | 58.61(5) |
| S(1)#13-S(1)-S(1)#16 | 60.0 |

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -y,x-y,z #3 x,y,-z+1/2
#4 y,-x+y,-z #5 x-y,x,-z #6 -x,-y,z-1/2
#7 -x,-y+1,-z+1 #8 -x+1,-y+1,-z+1 #9 y,-x+y+1,-z+1
#10 x-y+1,x+1,-z+1 #11 x-y,x,-z+1 #12 y,-x+y,-z+1
#13 -x+y,-x+1,z #14 -y+1,x-y+1,z+1 #15 x,y,z+1
#16 -y+1,x-y+1,z #17 x,y,z-1

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Table S3. Bond lengths (Å) and angles (deg.) for $CsTaSe_3$.

| | |
|---|---|
| Ta(1)-Se(1)#1 | 2.440(2) |
| Ta(1)-Se(1)#2 | 2.440(2) |
| Ta(1)-Se(1) | 2.440(2) |
| Ta(1)-Ta(1)#3 | 2.540(5) |
| Ta(1)-Se(1)#1 | 2.767(2) |
| Ta(1)-Se(1)#4 | 2.767(2) |
| Ta(1)-Se(1)#5 | 2.767(2) |
| Ta(1)-Cs(1)#7 | 4.5125(9) |
| Ta(1)-Cs(1)#8 | 4.5125(9) |
| Cs(1)-Se(1)#7 | 3.7509(5) |
| Cs(1)-Se(1)#9 | 3.7509(5) |
| Cs(1)-Se(1)#10 | 3.7509(5) |
| Cs(1)-Se(1)#11 | 3.7509(5) |
| Cs(1)-Se(1)#12 | 3.7509(5) |
| Cs(1)-Se(1)#8 | 3.7509(5) |
| Cs(1)-Se(1)#7 | 3.8211(12) |
| Cs(1)-Se(1)#13 | 3.8212(12) |
| Cs(1)-Se(1)#14 | 3.8211(12) |
| Cs(1)-Se(1)#15 | 3.8211(12) |
| Cs(1)-Se(1) | 3.8212(12) |
| Cs(1)-Se(1)#16 | 3.8212(12) |
| Se(1)-Ta(1)#3 | 2.440(2) |
| Se(1)-Ta(1)#1 | 2.767(2) |
| Se(1)-Ta(1)#5 | 2.767(2) |
| Se(1)-Se(1)#2 | 3.609(3) |
| Se(1)-Se(1)#1 | 3.609(3) |
| Se(1)-Se(1)#12 | 3.7277(12) |
| Se(1)-Se(1)#11 | 3.7277(12) |
| Se(1)-Se(1)#4 | 3.7277(12) |
| Se(1)-Se(1)#5 | 3.7277(12) |
| Se(1)-Cs(1)#7 | 3.7509(5) |
| Se(1)-Cs(1)#8 | 3.7509(5) |
| Se(1)-Cs(1)#17 | 3.8212(12) |
| Se(1)-Se(1)#13 | 3.891(3) |
| Se(1)-Se(1)#16 | 3.891(3) |
| | |
| Se(1)#1-Ta(1)-Se(1)#2 | 95.38(7) |
| Se(1)#1-Ta(1)-Se(1) | 95.38(7) |
| Se(1)#2-Ta(1)-Se(1) | 95.38(7) |
| Se(1)#1-Ta(1)-Se(1)#1 | 91.20(4) |
| Se(1)#2-Ta(1)-Se(1)#1 | 91.20(4) |
| Se(1)-Ta(1)-Se(1)#1 | 170.21(9) |
| Se(1)#1-Ta(1)-Se(1)#4 | 170.21(9) |
| Se(1)#2-Ta(1)-Se(1)#4 | 91.20(4) |
| Se(1)-Ta(1)-Se(1)#4 | 91.20(4) |
| Se(1)#1-Ta(1)-Se(1)#4 | 81.40(7) |
| Ta(1)#1-Ta(1)-Se(1)#5 | 48.85(5) |
| Se(1)#1-Ta(1)-Se(1)#5 | 91.20(4) |
| Se(1)#2-Ta(1)-Se(1)#5 | 170.21(9) |
| Se(1)-Ta(1)-Se(1)#5 | 91.21(4) |
| Se(1)#1-Ta(1)-Se(1)#5 | 81.40(7) |
| Se(1)#4-Ta(1)-Se(1)#5 | 81.40(7) |
| Se(1)#1-Ta(1)-Cs(1)#7 | 132.29(8) |
| Se(1)#2-Ta(1)-Cs(1)#7 | 56.209(14) |
| Se(1)-Ta(1)-Cs(1)#7 | 56.210(14) |
| Se(1)#1-Ta(1)-Cs(1)#7 | 123.12(2) |
| Se(1)#4-Ta(1)-Cs(1)#7 | 57.50(3) |
| Se(1)#5-Ta(1)-Cs(1)#7 | 123.12(2) |
| Se(1)#1-Ta(1)-Cs(1)#8 | 56.210(14) |
| Se(1)#2-Ta(1)-Cs(1)#8 | 132.29(8) |
| Se(1)-Ta(1)-Cs(1)#8 | 56.210(14) |
| Se(1)#1-Ta(1)-Cs(1)#8 | 123.12(2) |
| Se(1)#4-Ta(1)-Cs(1)#8 | 123.12(2) |
| Se(1)#5-Ta(1)-Cs(1)#8 | 57.50(3) |
| Cs(1)#7-Ta(1)-Cs(1)#8 | 112.41(3) |
| Se(1)#7-Cs(1)-Se(1)#9 | 120.0 |

| | |
|---|---|
| Se(1)#7-Cs(1)-Se(1)#10 | 57.51(6) |
| Se(1)#9-Cs(1)-Se(1)#10 | 62.49(6) |
| Se(1)#7-Cs(1)-Se(1)#11 | 120.0 |
| Se(1)#9-Cs(1)-Se(1)#11 | 120.0 |
| Se(1)#10-Cs(1)-Se(1)#11 | 177.51(6) |
| Se(1)#7-Cs(1)-Se(1)#12 | 62.49(6) |
| Se(1)#9-Cs(1)-Se(1)#12 | 177.51(6) |
| Se(1)#10-Cs(1)-Se(1)#12 | 120.0 |
| Se(1)#11-Cs(1)-Se(1)#12 | 57.51(6) |
| Se(1)#7-Cs(1)-Se(1)#8 | 177.51(6) |
| Se(1)#9-Cs(1)-Se(1)#8 | 57.51(6) |
| Se(1)#10-Cs(1)-Se(1)#8 | 120.0 |
| Se(1)#11-Cs(1)-Se(1)#8 | 62.49(6) |
| Se(1)#12-Cs(1)-Se(1)#8 | 120.0 |
| Se(1)#7-Cs(1)-Se(1)#7 | 58.97(3) |
| Se(1)#9-Cs(1)-Se(1)#7 | 90.73(2) |
| Se(1)#10-Cs(1)-Se(1)#7 | 58.97(3) |
| Se(1)#11-Cs(1)-Se(1)#7 | 120.176(10) |
| Se(1)#12-Cs(1)-Se(1)#7 | 90.73(2) |
| Se(1)#8-Cs(1)-Se(1)#7 | 120.176(10) |
| Se(1)#7-Cs(1)-Se(1)#13 | 58.97(3) |
| Se(1)#9-Cs(1)-Se(1)#13 | 90.73(2) |
| Se(1)#10-Cs(1)-Se(1)#13 | 58.97(3) |
| Se(1)#11-Cs(1)-Se(1)#13 | 120.175(9) |
| Se(1)#12-Cs(1)-Se(1)#13 | 90.73(2) |
| Se(1)#8-Cs(1)-Se(1)#13 | 120.175(9) |
| Se(1)#7-Cs(1)-Se(1)#13 | 107.98(5) |
| Se(1)#7-Cs(1)-Se(1)#14 | 120.176(9) |
| Se(1)#9-Cs(1)-Se(1)#14 | 58.97(3) |
| Se(1)#10-Cs(1)-Se(1)#14 | 90.73(2) |
| Se(1)#11-Cs(1)-Se(1)#14 | 90.73(2) |
| Se(1)#12-Cs(1)-Se(1)#14 | 120.176(10) |
| Se(1)#8-Cs(1)-Se(1)#14 | 58.97(3) |
| Se(1)#7-Cs(1)-Se(1)#14 | 61.22(4) |
| Se(1)#13-Cs(1)-Se(1)#14 | 145.81(2) |
| Se(1)#7-Cs(1)-Se(1)#15 | 90.73(2) |
| Se(1)#9-Cs(1)-Se(1)#15 | 120.176(10) |
| Se(1)#10-Cs(1)-Se(1)#15 | 120.176(9) |
| Se(1)#11-Cs(1)-Se(1)#15 | 58.97(3) |
| Se(1)#12-Cs(1)-Se(1)#15 | 58.97(3) |
| Se(1)#8-Cs(1)-Se(1)#15 | 90.73(2) |
| Se(1)#7-Cs(1)-Se(1)#15 | 61.22(4) |
| Se(1)#13-Cs(1)-Se(1)#15 | 145.81(2) |
| Se(1)#14-Cs(1)-Se(1)#15 | 61.22(4) |
| Se(1)#7-Cs(1)-Se(1) | 90.73(2) |
| Se(1)#9-Cs(1)-Se(1) | 120.175(10) |
| Se(1)#10-Cs(1)-Se(1) | 120.175(9) |
| Se(1)#11-Cs(1)-Se(1) | 58.97(3) |
| Se(1)#12-Cs(1)-Se(1) | 58.97(3) |
| Se(1)#8-Cs(1)-Se(1) | 90.73(2) |
| Se(1)#7-Cs(1)-Se(1) | 145.81(2) |
| Se(1)#13-Cs(1)-Se(1) | 61.21(4) |
| Se(1)#14-Cs(1)-Se(1) | 145.81(2) |
| Se(1)#15-Cs(1)-Se(1) | 107.98(5) |
| Se(1)#7-Cs(1)-Se(1)#16 | 120.175(10) |
| Se(1)#9-Cs(1)-Se(1)#16 | 58.97(3) |
| Se(1)#10-Cs(1)-Se(1)#16 | 90.73(2) |
| Se(1)#11-Cs(1)-Se(1)#16 | 90.73(2) |
| Se(1)#12-Cs(1)-Se(1)#16 | 120.175(10) |
| Se(1)#8-Cs(1)-Se(1)#16 | 58.97(3) |
| Se(1)#7-Cs(1)-Se(1)#16 | 145.81(2) |
| Se(1)#13-Cs(1)-Se(1)#16 | 61.21(4) |
| Se(1)#14-Cs(1)-Se(1)#16 | 107.98(5) |
| Se(1)#15-Cs(1)-Se(1)#16 | 145.81(2) |
| Se(1)-Cs(1)-Se(1)#16 | 61.22(4) |
| Ta(1)-Se(1)-Se(1)#2 | 42.31(4) |
| Ta(1)#3-Se(1)-Se(1)#2 | 42.31(4) |
| Ta(1)#1-Se(1)-Se(1)#2 | 49.30(4) |
| Ta(1)#5-Se(1)-Se(1)#2 | 49.30(4) |

| | |
|---|---|
| Ta(1)-Se(1)-Se(1)#1 | 42.31(4) |
| Ta(1)#3-Se(1)-Se(1)#1 | 42.31(4) |
| Ta(1)#1-Se(1)-Se(1)#1 | 49.30(4) |
| Ta(1)#5-Se(1)-Se(1)#1 | 49.30(4) |
| Se(1)#2-Se(1)-Se(1)#1 | 60.0 |
| Ta(1)-Se(1)-Se(1)#12 | 101.12(6) |
| Ta(1)#3-Se(1)-Se(1)#12 | 47.92(4) |
| Ta(1)#1-Se(1)-Se(1)#12 | 109.59(5) |
| Ta(1)#5-Se(1)-Se(1)#12 | 40.88(3) |
| Se(1)#2-Se(1)-Se(1)#12 | 61.05(2) |
| Se(1)#1-Se(1)-Se(1)#12 | 90.0 |
| Ta(1)-Se(1)-Se(1)#11 | 101.12(6) |
| Ta(1)#3-Se(1)-Se(1)#11 | 47.92(4) |
| Ta(1)#1-Se(1)-Se(1)#11 | 109.59(5) |
| Ta(1)#5-Se(1)-Se(1)#11 | 40.88(3) |
| Se(1)#2-Se(1)-Se(1)#11 | 90.0 |
| Se(1)#1-Se(1)-Se(1)#11 | 61.05(2) |
| Se(1)#12-Se(1)-Se(1)#11 | 57.90(4) |
| Ta(1)-Se(1)-Se(1)#4 | 47.92(4) |
| Ta(1)#3-Se(1)-Se(1)#4 | 101.12(6) |
| Ta(1)#1-Se(1)-Se(1)#4 | 40.88(3) |
| Ta(1)#5-Se(1)-Se(1)#4 | 109.59(5) |
| Se(1)#2-Se(1)-Se(1)#4 | 61.05(2) |
| Se(1)#1-Se(1)-Se(1)#4 | 90.0 |
| Se(1)#12-Se(1)-Se(1)#4 | 112.03(5) |
| Se(1)#11-Se(1)-Se(1)#4 | 147.54(2) |
| Ta(1)-Se(1)-Se(1)#5 | 47.92(4) |
| Ta(1)#3-Se(1)-Se(1)#5 | 101.12(6) |
| Ta(1)#1-Se(1)-Se(1)#5 | 40.88(3) |
| Ta(1)#5-Se(1)-Se(1)#5 | 109.59(5) |
| Se(1)#2-Se(1)-Se(1)#5 | 90.0 |
| Se(1)#1-Se(1)-Se(1)#5 | 61.05(2) |
| Se(1)#12-Se(1)-Se(1)#5 | 147.54(2) |
| Se(1)#11-Se(1)-Se(1)#5 | 112.03(5) |
| Se(1)#4-Se(1)-Se(1)#5 | 57.90(4) |
| Ta(1)-Se(1)-Cs(1)#7 | 91.06(2) |
| Ta(1)#3-Se(1)-Cs(1)#7 | 91.06(2) |
| Ta(1)#1-Se(1)-Cs(1)#7 | 90.94(2) |
| Ta(1)#5-Se(1)-Cs(1)#7 | 90.94(2) |
| Se(1)#2-Se(1)-Cs(1)#7 | 61.24(3) |
| Se(1)#1-Se(1)-Cs(1)#7 | 121.24(3) |
| Se(1)#12-Se(1)-Cs(1)#7 | 61.45(3) |
| Se(1)#11-Se(1)-Cs(1)#7 | 119.342(12) |
| Se(1)#4-Se(1)-Cs(1)#7 | 61.45(3) |
| Se(1)#5-Se(1)-Cs(1)#7 | 119.341(12) |
| Ta(1)-Se(1)-Cs(1)#8 | 91.06(2) |
| Ta(1)#3-Se(1)-Cs(1)#8 | 91.06(2) |
| Ta(1)#1-Se(1)-Cs(1)#8 | 90.94(2) |
| Ta(1)#5-Se(1)-Cs(1)#8 | 90.94(2) |
| Se(1)#2-Se(1)-Cs(1)#8 | 121.24(3) |
| Se(1)#1-Se(1)-Cs(1)#8 | 61.24(3) |
| Se(1)#12-Se(1)-Cs(1)#8 | 119.342(12) |
| Se(1)#11-Se(1)-Cs(1)#8 | 61.45(3) |
| Se(1)#4-Se(1)-Cs(1)#8 | 119.341(12) |
| Se(1)#5-Se(1)-Cs(1)#8 | 61.45(3) |
| Cs(1)#7-Se(1)-Cs(1)#8 | 177.51(6) |
| Ta(1)-Se(1)-Cs(1) | 157.37(7) |
| Ta(1)#3-Se(1)-Cs(1) | 94.65(5) |
| Ta(1)#1-Se(1)-Cs(1) | 167.16(6) |
| Ta(1)#5-Se(1)-Cs(1) | 84.86(4) |
| Se(1)#2-Se(1)-Cs(1) | 120.61(2) |
| Se(1)#1-Se(1)-Cs(1) | 120.61(2) |
| Se(1)#12-Se(1)-Cs(1) | 59.572(9) |
| Se(1)#11-Se(1)-Cs(1) | 59.573(9) |
| Se(1)#4-Se(1)-Cs(1) | 146.622(5) |
| Se(1)#5-Se(1)-Cs(1) | 146.623(5) |
| Cs(1)#7-Se(1)-Cs(1) | 89.27(2) |
| Cs(1)#8-Se(1)-Cs(1) | 89.27(2) |
| Ta(1)-Se(1)-Cs(1)#17 | 94.65(5) |

| | |
|---|---|
| Ta(1)#3-Se(1)-Cs(1)#17 | 157.37(7) |
| Ta(1)#1-Se(1)-Cs(1)#17 | 84.86(4) |
| Ta(1)#5-Se(1)-Cs(1)#17 | 167.16(6) |
| Se(1)#2-Se(1)-Cs(1)#17 | 120.61(2) |
| Se(1)#1-Se(1)-Cs(1)#17 | 120.61(2) |
| Se(1)#12-Se(1)-Cs(1)#17 | 146.622(5) |
| Se(1)#11-Se(1)-Cs(1)#17 | 146.623(5) |
| Se(1)#4-Se(1)-Cs(1)#17 | 59.572(9) |
| Se(1)#5-Se(1)-Cs(1)#17 | 59.573(9) |
| Cs(1)#7-Se(1)-Cs(1)#17 | 89.27(2) |
| Cs(1)#8-Se(1)-Cs(1)#17 | 89.27(2) |
| Cs(1)-Se(1)-Cs(1)#17 | 107.98(5) |
| Ta(1)-Se(1)-Se(1)#13 | 137.69(4) |
| Ta(1)#3-Se(1)-Se(1)#13 | 137.69(4) |
| Ta(1)#1-Se(1)-Se(1)#13 | 130.70(4) |
| Ta(1)#5-Se(1)-Se(1)#13 | 130.70(4) |
| Se(1)#2-Se(1)-Se(1)#13 | 120.0 |
| Se(1)#1-Se(1)-Se(1)#13 | 180.00(6) |
| Se(1)#12-Se(1)-Se(1)#13 | 90.0 |
| Se(1)#11-Se(1)-Se(1)#13 | 118.95(2) |
| Se(1)#4-Se(1)-Se(1)#13 | 90.0 |
| Se(1)#5-Se(1)-Se(1)#13 | 118.95(2) |
| Cs(1)#7-Se(1)-Se(1)#13 | 58.76(3) |
| Cs(1)#8-Se(1)-Se(1)#13 | 118.76(3) |
| Cs(1)-Se(1)-Se(1)#13 | 59.39(2) |
| Cs(1)#17-Se(1)-Se(1)#13 | 59.39(2) |
| Ta(1)-Se(1)-Se(1)#16 | 137.69(4) |
| Ta(1)#3-Se(1)-Se(1)#16 | 137.69(4) |
| Ta(1)#1-Se(1)-Se(1)#16 | 130.70(4) |
| Ta(1)#5-Se(1)-Se(1)#16 | 130.70(4) |
| Se(1)#2-Se(1)-Se(1)#16 | 179.999(2) |
| Se(1)#1-Se(1)-Se(1)#16 | 120.0 |
| Se(1)#12-Se(1)-Se(1)#16 | 118.95(2) |
| Se(1)#11-Se(1)-Se(1)#16 | 90.0 |
| Se(1)#4-Se(1)-Se(1)#16 | 118.95(2) |
| Se(1)#5-Se(1)-Se(1)#16 | 90.0 |
| Cs(1)#7-Se(1)-Se(1)#16 | 118.76(3) |
| Cs(1)#8-Se(1)-Se(1)#16 | 58.76(3) |
| Cs(1)-Se(1)-Se(1)#16 | 59.39(2) |
| Cs(1)#17-Se(1)-Se(1)#16 | 59.39(2) |
| Se(1)#13-Se(1)-Se(1)#16 | 60.0 |

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -y,x-y,z #3 x,y,-z+1/2
#4 x-y,x,-z #5 y,-x+y,-z #6 -x,-y,z-1/2
#7 -x,-y+1,-z+1 #8 -x+1,-y+1,-z+1 #9 x-y+1,x+1,-z+1
#10 y,-x+y+1,-z+1 #11 y,-x+y,-z+1 #12 x-y,x,-z+1
#13 -x+y,-x+1,z #14 -y+1,x-y+1,z+1 #15 x,y,z+1
#16 -y+1,x-y+1,z #17 x,y,z-1

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Table S4. Bond lengths (Å) and angles (deg.) for $CsTaTe_3$.

| | |
|---|---|
| Ta(1)-Ta(1)#2 | 2.590(6) |
| Ta(1)-Te(1)#3 | 2.616(3) |
| Ta(1)-Te(1)#1 | 2.616(3) |
| Ta(1)-Te(1) | 2.616(3) |
| Ta(1)-Te(1)#1 | 2.997(3) |
| Ta(1)-Te(1)#4 | 2.997(3) |
| Ta(1)-Te(1)#5 | 2.997(3) |
| Cs(1)-Te(1)#7 | 3.996(2) |
| Cs(1)-Te(1)#8 | 3.996(2) |
| Cs(1)-Te(1)#9 | 3.996(2) |
| Cs(1)-Te(1)#10 | 3.996(2) |
| Cs(1)-Te(1)#11 | 3.996(2) |
| Cs(1)-Te(1)#12 | 3.996(2) |
| Cs(1)-Te(1)#13 | 4.004(2) |
| Cs(1)-Te(1)#7 | 4.004(2) |
| Cs(1)-Te(1) | 4.004(2) |
| Cs(1)-Te(1)#14 | 4.004(2) |
| Cs(1)-Te(1)#15 | 4.004(2) |
| Cs(1)-Te(1)#16 | 4.004(2) |
| Te(1)-Ta(1)#2 | 2.616(3) |
| Te(1)-Ta(1)#5 | 2.997(3) |
| Te(1)-Ta(1)#1 | 2.997(3) |
| Te(1)-Cs(1)#7 | 3.996(2) |
| Te(1)-Cs(1)#12 | 3.996(2) |
| Te(1)-Cs(1)#17 | 4.004(2) |
| | |
| Te(1)#3-Ta(1)-Te(1)#1 | 97.60(8) |
| Ta(1)#1-Ta(1)-Te(1) | 119.67(6) |
| Ta(1)#2-Ta(1)-Te(1) | 60.33(6) |
| Te(1)#3-Ta(1)-Te(1) | 97.61(8) |
| Te(1)#1-Ta(1)-Te(1) | 97.61(8) |
| Te(1)#3-Ta(1)-Te(1)#1 | 89.61(5) |
| Te(1)#1-Ta(1)-Te(1)#1 | 89.61(5) |
| Te(1)-Ta(1)-Te(1)#1 | 169.01(10) |
| Ta(1)#1-Ta(1)-Te(1)#4 | 49.33(6) |
| Ta(1)#2-Ta(1)-Te(1)#4 | 130.67(6) |
| Te(1)#3-Ta(1)-Te(1)#4 | 89.61(5) |
| Te(1)#1-Ta(1)-Te(1)#4 | 169.01(10) |
| Te(1)-Ta(1)-Te(1)#4 | 89.61(5) |
| Te(1)#1-Ta(1)-Te(1)#4 | 82.12(8) |
| Te(1)#3-Ta(1)-Te(1)#5 | 169.01(10) |
| Te(1)#1-Ta(1)-Te(1)#5 | 89.61(5) |
| Te(1)-Ta(1)-Te(1)#5 | 89.61(5) |
| Te(1)#1-Ta(1)-Te(1)#5 | 82.12(8) |
| Te(1)#4-Ta(1)-Te(1)#5 | 82.12(9) |
| Te(1)#7-Cs(1)-Te(1)#8 | 120.0 |
| Te(1)#7-Cs(1)-Te(1)#9 | 59.02(7) |
| Te(1)#8-Cs(1)-Te(1)#9 | 60.98(6) |
| Te(1)#7-Cs(1)-Te(1)#10 | 120.0 |
| Te(1)#8-Cs(1)-Te(1)#10 | 120.0 |
| Te(1)#9-Cs(1)-Te(1)#10 | 179.02(7) |
| Te(1)#7-Cs(1)-Te(1)#11 | 60.98(7) |
| Te(1)#8-Cs(1)-Te(1)#11 | 179.02(6) |
| Te(1)#9-Cs(1)-Te(1)#11 | 120.0 |
| Te(1)#10-Cs(1)-Te(1)#11 | 59.02(7) |
| Te(1)#7-Cs(1)-Te(1)#12 | 179.02(7) |
| Te(1)#8-Cs(1)-Te(1)#12 | 59.02(7) |
| Te(1)#9-Cs(1)-Te(1)#12 | 120.0 |
| Te(1)#10-Cs(1)-Te(1)#12 | 60.98(7) |
| Te(1)#11-Cs(1)-Te(1)#12 | 120.0 |
| Te(1)#7-Cs(1)-Te(1)#13 | 59.41(4) |
| Te(1)#8-Cs(1)-Te(1)#13 | 90.29(2) |
| Te(1)#9-Cs(1)-Te(1)#13 | 59.41(4) |
| Te(1)#10-Cs(1)-Te(1)#13 | 120.26(2) |
| Te(1)#11-Cs(1)-Te(1)#13 | 90.29(2) |
| Te(1)#12-Cs(1)-Te(1)#13 | 120.26(2) |

| | |
|---|---|
| Te(1)#7-Cs(1)-Te(1)#7 | 59.41(4) |
| Te(1)#8-Cs(1)-Te(1)#7 | 90.29(2) |
| Te(1)#9-Cs(1)-Te(1)#7 | 59.41(4) |
| Te(1)#10-Cs(1)-Te(1)#7 | 120.26(2) |
| Te(1)#11-Cs(1)-Te(1)#7 | 90.29(2) |
| Te(1)#12-Cs(1)-Te(1)#7 | 120.26(2) |
| Te(1)#13-Cs(1)-Te(1)#7 | 108.43(7) |
| Te(1)#7-Cs(1)-Te(1) | 90.29(2) |
| Te(1)#8-Cs(1)-Te(1) | 120.26(2) |
| Te(1)#9-Cs(1)-Te(1) | 120.26(2) |
| Te(1)#10-Cs(1)-Te(1) | 59.41(4) |
| Te(1)#11-Cs(1)-Te(1) | 59.41(4) |
| Te(1)#12-Cs(1)-Te(1) | 90.29(2) |
| Te(1)#13-Cs(1)-Te(1) | 60.85(6) |
| Te(1)#7-Cs(1)-Te(1) | 146.00(3) |
| Te(1)#7-Cs(1)-Te(1)#14 | 120.26(2) |
| Te(1)#8-Cs(1)-Te(1)#14 | 59.41(4) |
| Te(1)#9-Cs(1)-Te(1)#14 | 90.29(2) |
| Te(1)#10-Cs(1)-Te(1)#14 | 90.29(2) |
| Te(1)#11-Cs(1)-Te(1)#14 | 120.26(2) |
| Te(1)#12-Cs(1)-Te(1)#14 | 59.41(4) |
| Te(1)#13-Cs(1)-Te(1)#14 | 60.85(6) |
| Te(1)#7-Cs(1)-Te(1)#14 | 146.00(3) |
| Te(1)-Cs(1)-Te(1)#14 | 60.85(6) |
| Te(1)#7-Cs(1)-Te(1)#15 | 120.26(2) |
| Te(1)#8-Cs(1)-Te(1)#15 | 59.41(4) |
| Te(1)#9-Cs(1)-Te(1)#15 | 90.29(2) |
| Te(1)#10-Cs(1)-Te(1)#15 | 90.29(2) |
| Te(1)#11-Cs(1)-Te(1)#15 | 120.26(2) |
| Te(1)#12-Cs(1)-Te(1)#15 | 59.41(4) |
| Te(1)#13-Cs(1)-Te(1)#15 | 146.00(3) |
| Te(1)#7-Cs(1)-Te(1)#15 | 60.85(6) |
| Te(1)-Cs(1)-Te(1)#15 | 146.00(3) |
| Te(1)#14-Cs(1)-Te(1)#15 | 108.43(7) |
| Te(1)#7-Cs(1)-Te(1)#16 | 90.29(2) |
| Te(1)#8-Cs(1)-Te(1)#16 | 120.26(2) |
| Te(1)#9-Cs(1)-Te(1)#16 | 120.26(2) |
| Te(1)#10-Cs(1)-Te(1)#16 | 59.41(4) |
| Te(1)#11-Cs(1)-Te(1)#16 | 59.41(4) |
| Te(1)#12-Cs(1)-Te(1)#16 | 90.29(2) |
| Te(1)#13-Cs(1)-Te(1)#16 | 146.00(3) |
| Te(1)#7-Cs(1)-Te(1)#16 | 60.85(6) |
| Te(1)-Cs(1)-Te(1)#16 | 108.43(7) |
| Te(1)#14-Cs(1)-Te(1)#16 | 146.00(3) |
| Te(1)#15-Cs(1)-Te(1)#16 | 60.85(6) |
| Ta(1)#2-Te(1)-Cs(1)#7 | 90.43(3) |
| Ta(1)-Te(1)-Cs(1)#7 | 90.43(3) |
| Ta(1)#5-Te(1)-Cs(1)#7 | 90.37(2) |
| Ta(1)#1-Te(1)-Cs(1)#7 | 90.37(2) |
| Ta(1)#2-Te(1)-Cs(1)#12 | 90.43(3) |
| Ta(1)-Te(1)-Cs(1)#12 | 90.43(3) |
| Ta(1)#5-Te(1)-Cs(1)#12 | 90.37(2) |
| Ta(1)#1-Te(1)-Cs(1)#12 | 90.37(2) |
| Cs(1)#7-Te(1)-Cs(1)#12 | 179.02(6) |
| Ta(1)#2-Te(1)-Cs(1)#17 | 155.46(7) |
| Ta(1)-Te(1)-Cs(1)#17 | 96.11(7) |
| Ta(1)#5-Te(1)-Cs(1)#17 | 166.45(7) |
| Ta(1)#1-Te(1)-Cs(1)#17 | 85.12(6) |
| Cs(1)#7-Te(1)-Cs(1)#17 | 89.71(2) |
| Cs(1)#12-Te(1)-Cs(1)#17 | 89.71(2) |
| Ta(1)#2-Te(1)-Cs(1) | 96.11(7) |
| Ta(1)-Te(1)-Cs(1) | 155.46(7) |
| Ta(1)#5-Te(1)-Cs(1) | 85.12(6) |
| Ta(1)#1-Te(1)-Cs(1) | 166.45(7) |
| Cs(1)#7-Te(1)-Cs(1) | 89.71(2) |
| Cs(1)#12-Te(1)-Cs(1) | 89.71(2) |
| Cs(1)#17-Te(1)-Cs(1) | 108.43(7) |

Symmetry transformations used to generate equivalent atoms:

| | | |
|---|---|---|
| #1 -x,-y,-z | #2 x,y,-z+1/2 | #3 -y,x-y,z |
| #4 x-y,x,-z | #5 y,-x+y,-z | #6 -x,-y,z-1/2 |
| #7 -x,-y+1,-z+1 | #8 x-y+1,x+1,-z+1 | #9 y,-x+y+1,-z+1 |
| #10 y,-x+y,-z+1 | #11 x-y,x,-z+1 | #12 -x+1,-y+1,-z+1 |
| #13 -x+y,-x+1,z | #14 -y+1,x-y+1,z | #15 -y+1,x-y+1,z+1 |
| #16 x,y,z+1 | #17 x,y,z-1 | |

Table S5. Anisotropic displacement parameters ($Å^2$) for $CsTaS_3$.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [ h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12} ]$

| atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| Ta(1) | 0.0304(8) | 0.0304(8) | 0.015(4) | 0.000 | 0.000 | 0.0152(4) |
| Cs(1) | 0.0109(7) | 0.0109(7) | 0.0210(11) | 0.000 | 0.000 | 0.0055(4) |
| S(1) | 0.019(2) | 0.021(3) | 0.021(2) | 0.000 | 0.000 | 0.0106(13) |

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Table S6. Anisotropic displacement parameters ($Å^2$) for $CsTaSe_3$.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [ h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12} ]$

| atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| Ta(1) | 0.0290(11) | 0.0290(11) | 0.017(3) | 0.000 | 0.000 | 0.0145(5) |
| Cs(1) | 0.0205(11) | 0.0205(11) | 0.020(2) | 0.000 | 0.000 | 0.0102(6) |
| Se(1) | 0.0239(12) | 0.0191(13) | 0.020(2) | 0.000 | 0.000 | 0.0096(7) |

Table S7. Anisotropic displacement parameters ($Å^2$) for $CsTaTe_3$.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [ h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12} ]$

| atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|
| Ta(1) | 0.0159(11) | 0.0159(11) | 0.031(4) | 0.000 | 0.000 | 0.0079(6) |
| Cs(1) | 0.024(2) | 0.024(2) | 0.028(3) | 0.000 | 0.000 | 0.0122(8) |
| Te(1) | 0.0278(14) | 0.026(2) | 0.030(2) | 0.000 | 0.000 | 0.0128(9) |