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Supporting information for article:

Crystal structures and new perspectives on Y₃Au₄ and Y₁₄Au₅₁

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Included are a table of the interatomic distances as well as a figure displaying some of the coordination polyhedra for both Y_3Au_4 and $Y_{14}Au_{51}$.

Table S1 Interatomic distances (Å) for both Y_3Au_4 and $Y_{14}Au_{51}$ samples.

Y_3Au_4			
Au1—Y4 ⁱ	2.8810 (17)	Au2—Au3	2.9820 (4)
Au1—Au1 ⁱⁱ	2.9738 (12)	Au2—Au3 ^{xiii}	2.9820 (4)
Au1—Y4 ⁱⁱⁱ	2.9773 (17)	Au3—Au2 ^{xiv}	2.9820 (4)
Au1—Au1 ^{iv}	3.0577 (9)	Au3—Y4	3.0808 (17)
Au1—Au1 ^v	3.0578 (9)	Au3—Y4 ^{xv}	3.0808 (17)
Au1—Y4 ⁱⁱ	3.0596 (17)	Au3—Y4 ^{xii}	3.0808 (17)
Au1—Y4 ^{vi}	3.0651 (17)	Au3—Y4 ^{xvi}	3.0808 (17)
Au1—Y4 ^{vii}	3.1590 (17)	Au3—Y4 ⁱ	3.0808 (17)
Au1—Y4 ^{viii}	3.1688 (18)	Au3—Y4 ^{xvii}	3.0808 (17)
Au1—Y4 ^{ix}	3.2754 (17)	Y4—Au1 ^{xii}	2.8810 (17)
Au2—Y4 ^x	2.9425 (16)	Y4—Au1 ^{xviii}	2.9773 (17)
Au2—Y4 ^{xi}	2.9425 (16)	Y4—Au1 ⁱⁱ	3.0596 (17)
Au2—Y4 ⁱ	2.9425 (16)	Y4—Au1 ^{xix}	3.0651 (17)
Au2—Y4 ^{ix}	2.9425 (16)	Y4—Au1 ^{xx}	3.1590 (17)
Au2—Y4 ^{xii}	2.9425 (16)	Y4—Au1 ^{xxi}	3.1688 (18)
Au2—Y4	2.9425 (16)	Y4—Au1 ^{xi}	3.2755 (17)
$Y_{14}Au_{51}$			
Au1—Au3 ^{xxiii}	2.7542 (7)	Au5—Y3 ^x	3.188 (2)
Au1—Au4	2.7769 (7)	Au5—Y3	3.188 (2)
Au1—Au6	2.8654 (6)	Au5—Au5 ^x	3.196 (2)
Au1—Au3 ^{xii}	2.9686 (7)	Au6—Au7	2.8358 (9)
Au1—Au2 ^{xii}	2.9735 (7)	Au6—Au1 ^{xxxv}	2.8653 (6)
Au1—Au1 ^{xxiv}	2.9933 (9)	Au6—Au1 ^{xxxvi}	2.8654 (6)
Au1—Y1 ^{xxv}	3.0393 (14)	Au6—Au3 ^{xxiii}	2.8818 (6)
Au1—Y1 ^{xxvi}	3.0429 (14)	Au6—Au3 ^{xxxvii}	2.8818 (6)

Au1—Au2 ^{xxvi}	3.0640 (7)	Au6—Au3 ^{xxvi}	2.8818 (6)
Au1—Y1 ^{xxiii}	3.1036 (14)	Au6—Y1 ^{xxiii}	3.0189 (13)
Au1—Y2	3.1532 (7)	Au6—Y1 ^{xxxviii}	3.0189 (13)
Au2—Au3	2.7337 (7)	Au6—Y1 ^{xxvi}	3.0189 (13)
Au2—Au5 ^{xxvii}	2.7381 (9)	Au7—Au6 ^{xxxix}	2.8358 (9)
Au2—Au5 ^{xxviii}	2.8229 (10)	Au7—Au3 ^{xl}	2.8488 (5)
Au2—Au4 ^{xxix}	2.8630 (6)	Au7—Au3 ^{xxxvii}	2.8488 (5)
Au2—Au4 ^{xxviii}	2.8708 (6)	Au7—Au3 ^{xxiii}	2.8488 (5)
Au2—Au1 ⁱ	2.9735 (7)	Au7—Au3 ^{xxxii}	2.8488 (5)
Au2—Au2 ^{xxvi}	2.9872 (6)	Au7—Au3 ^{xi}	2.8488 (5)
Au2—Au2 ^{xxviii}	2.9872 (6)	Au7—Au3 ^{xxvi}	2.8488 (5)
Au2—Y3	3.0537 (8)	Au7—Y2	3.1572 (18)
Au2—Au1 ^{xxviii}	3.0639 (7)	Au7—Y2 ^{xxxix}	3.1572 (18)
Au2—Y2 ^{xxviii}	3.0723 (13)	Au7—Y2 ^{xli}	3.1572 (18)
Au2—Y2 ^{xxvii}	3.2509 (14)	Y1—Au6 ^{xxxviii}	3.0190 (13)
Au3—Au1 ^{xxx}	2.7542 (7)	Y1—Au6 ^{xxx}	3.0190 (13)
Au3—Au3 ^{xxxi}	2.7692 (9)	Y1—Au1 ⁱ	3.0393 (14)
Au3—Au7 ^{xxxii}	2.8489 (5)	Y1—Au1 ^{xxix}	3.0393 (14)
Au3—Au6 ^{xxx}	2.8818 (6)	Y1—Au1 ^{xv}	3.0429 (14)
Au3—Au1 ⁱ	2.9686 (7)	Y1—Au1 ^{xxviii}	3.0429 (14)
Au3—Au3 ^{xxxiii}	3.0024 (10)	Y1—Au1 ^{xlii}	3.1037 (14)
Au3—Y2 ^{xxvii}	3.1167 (15)	Y1—Au1 ^{xxx}	3.1037 (14)
Au3—Y2 ^{xxx}	3.1852 (17)	Y1—Au4 ^{xxviii}	3.1174 (16)
Au3—Y2 ^{xxviii}	3.2096 (16)	Y1—Au4 ^{xxix}	3.1837 (16)
Au3—Y1	3.2373 (7)	Y1—Au3 ^{xxiv}	3.2374 (7)
Au4—Au4 ^{xxvi}	2.6942 (7)	Y2—Au2 ^{xi}	3.0723 (13)
Au4—Au4 ^{xxviii}	2.6942 (7)	Y2—Au2 ^{xxvi}	3.0723 (13)
Au4—Au1 ^{xxiv}	2.7769 (7)	Y2—Au3 ^{xxxiv}	3.1167 (15)
Au4—Au2 ^{xii}	2.8630 (6)	Y2—Au3 ^{xii}	3.1167 (15)
Au4—Au2 ^{xxv}	2.8630 (6)	Y2—Au1 ^{xxxi}	3.1532 (7)
Au4—Au2 ^{xxvi}	2.8709 (6)	Y2—Au3 ^{xxiii}	3.1852 (16)

Au4—Au2 ^{xxvi}	2.8709 (6)	Y2—Au3 ^{xl}	3.1852 (17)
Au4—Y1 ^{xxvi}	3.1175 (17)	Y2—Au3 ^{xxvi}	3.2096 (15)
Au4—Y1 ^{xxv}	3.1837 (16)	Y2—Au3 ^{xi}	3.2096 (15)
Au4—Y3	3.2463 (15)	Y3—Au2 ⁱ	3.0537 (8)
Au4—Y3 ^{xvii}	3.2463 (15)	Y3—Au2 ^{xliii}	3.0537 (8)
Au5—Au5 ^{xxviii}	1.5982 (12)	Y3—Au2 ^{xxvi}	3.0537 (8)
Au5—Au5 ^{xxvi}	1.5983 (12)	Y3—Au2 ^{xxviii}	3.0537 (8)
Au5—Au2 ^{xxxiv}	2.7381 (9)	Y3—Au2 ^{xii}	3.0537 (8)
Au5—Au2 ^{xii}	2.7381 (9)	Y3—Au5 ^{xxxiv}	3.188 (2)
Au5—Au5 ^{xxvii}	2.768 (2)	Y3—Au5 ^x	3.188 (2)
Au5—Au5 ^{xxxiv}	2.768 (2)	Y3—Au5 ^{xxvi}	3.188 (2)
Au5—Y2	2.799 (2)	Y3—Au5 ^{xxvii}	3.188 (2)
Au5—Au2 ^{xxvi}	2.8228 (10)	Y3—Au5 ^{xxviii}	3.188 (2)
Au5—Au2 ^{xi}	2.8228 (10)		

Symmetry code(s): (i) $-x+y, -x, z$; (ii) $-x+2/3, -y+1/3, -z+1/3$; (iii) $-y+2/3, x-y+1/3, z-2/3$; (iv) $-x+y+2/3, -x+1/3, z+1/3$; (v) $-y+1/3, x-y-1/3, z-1/3$; (vi) $x-y+2/3, x+1/3, -z+1/3$; (vii) $-y+2/3, x-y+1/3, z+1/3$; (viii) $x+1/3, y-1/3, z-1/3$; (ix) $y, -x+y, -z$; (x) $-x, -y, -z$; (xi) $x-y, x, -z$; (xii) $-y, x-y, z$; (xiii) $x, y, z-1$; (xiv) $x, y, z+1$; (xv) $y, -x+y, -z+1$; (xvi) $x-y, x, -z+1$; (xvii) $-x, -y, -z+1$; (xviii) $-x+y+1/3, -x+2/3, z+2/3$; (xix) $y-1/3, -x+y+1/3, -z+1/3$; (xx) $-x+y+1/3, -x+2/3, z-1/3$; (xxi) $x-1/3, y+1/3, z+1/3$; (xxii) $-x+1/3, -y+2/3, -z+2/3$; (xxiii) $y, -x+y+1, z$; (xxiv) $x, y, -z+1$; (xxv) $-y, x-y, -z+1$; (xxvi) $x-y, x, z$; (xxvii) $-x+y, -x, -z$; (xxviii) $y, -x+y, z$; (xxix) $-x+y, -x, -z+1$; (xxx) $x-y+1, x, z$; (xxxii) $-x+1, -y+1, -z$; (xxxiii) $-x+1, -y, z$; (xxxiv) $-y, x-y, -z$; (xxxv) $-y+1, x-y+1, z$; (xxxvi) $-x+y, -x+1, z$; (xxxvii) $-x+1, -y+1, z$; (xxxviii) $-x+1, -y+1, -z+1$; (xxxix) $-x+y, -x+1, -z$; (xl) $y, -x+y+1, -z$; (xli) $-y+1, x-y+1, -z$; (xlii) $x-y+1, x, -z+1$; (xliii) $-x, -y, z$.

Figure S1 The coordination polyhedra for all crystallographic sites in Y_3Au_4 (a) as well as the coordination polyhedra for the Y sites in $Y_{14}Au_{51}$ (b).

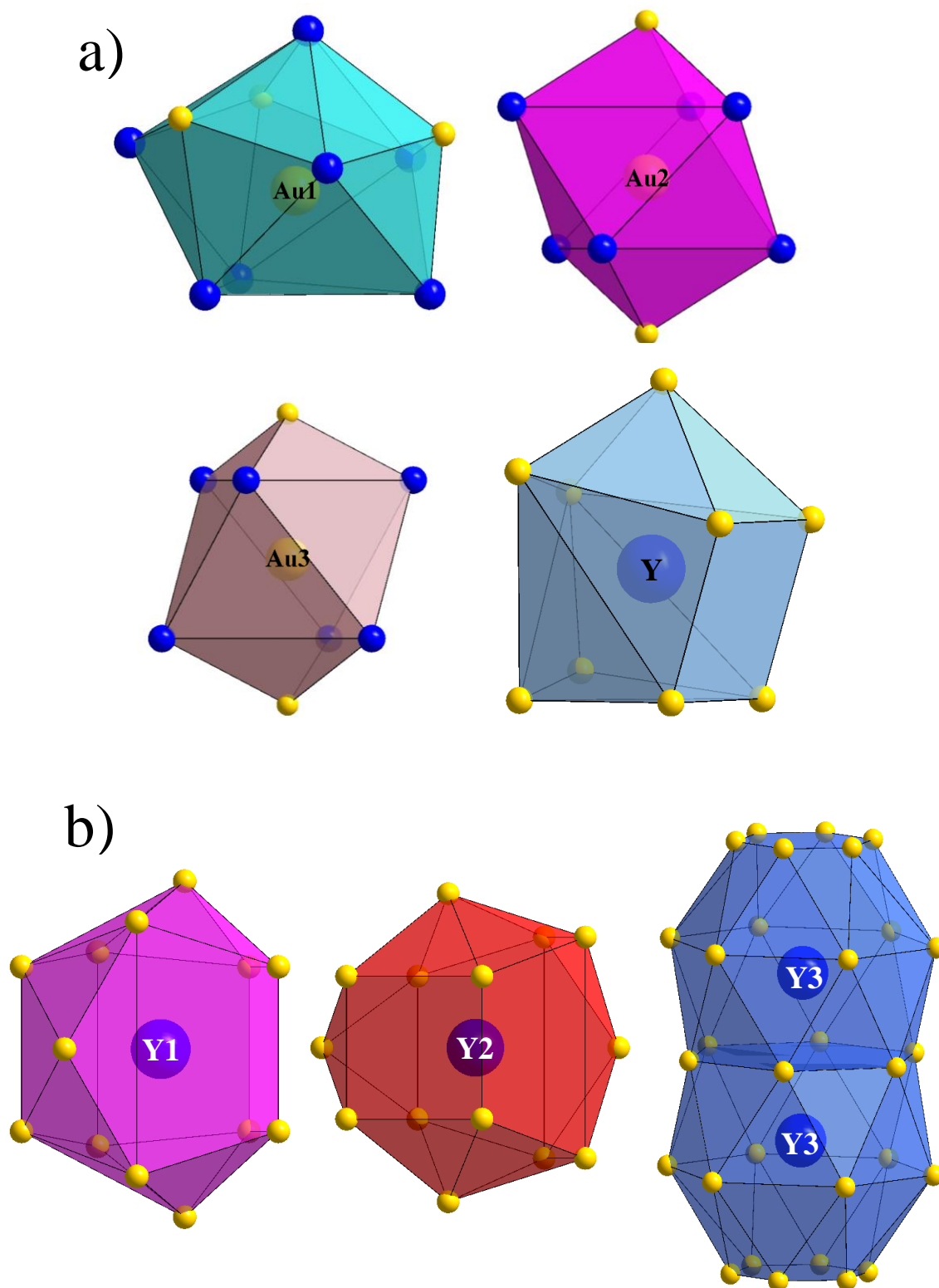


Figure S2 The crystal structures projections of Y_3Au_4 (a) and $Y_{14}Au_{51}$ (b) along the c axes including the anisotropic thermal displacement.

