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Supporting information for article:

Tb₃Pd₂, Er₃Pd₂ and Er₆Co_{5-x}: structural variations and bonding in rare-earth-richer binary intermetallics

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Table S1 Selected geometric parameters (\AA)

Tb₃Pd₂			
Tb1—Pd1 ⁱ	2.9415 (9)	Tb3—Pd2	2.9375 (9)
Tb1—Pd1	2.9415 (9)	Tb3—Pd1 ^{xii}	2.9950 (9)
Tb1—Pd2 ⁱⁱ	2.9953 (9)	Tb3—Pd1 ^{xi}	2.9950 (9)
Tb1—Pd2 ⁱⁱⁱ	2.9953 (9)	Tb3—Pd2 ^{xi}	3.1126 (9)
Tb1—Pd1 ^{iv}	3.1087 (9)	Tb3—Pd2 ^{xii}	3.1126 (9)
Tb1—Pd1 ^v	3.1087 (9)	Tb3—Tb2 ^{xiii}	3.4916 (8)
Tb1—Tb2 ^v	3.5089 (8)	Tb3—Tb2 ^{xiv}	3.4916 (8)
Tb1—Tb2 ^{iv}	3.5089 (8)	Tb3—Tb2 ^{xi}	3.5338 (8)
Tb1—Tb2 ⁱⁱⁱ	3.5175 (8)	Tb3—Tb2 ^{xii}	3.5338 (8)
Tb1—Tb2 ⁱⁱ	3.5175 (8)	Tb3—Tb3 ^{xii}	3.6476 (12)
Tb1—Tb1 ^{iv}	3.6399 (13)	Tb3—Tb3 ^{vi}	3.8810 (9)
Tb1—Tb1 ^{vi}	3.8810 (9)	Pd1—Pd1 ^v	2.8848 (18)
Tb2—Pd2	2.8999 (11)	Pd1—Tb1 ^{vi}	2.9415 (9)
Tb2—Pd1	2.9137 (12)	Pd1—Tb3 ^{xii}	2.9950 (9)
Tb2—Pd1 ^{vii}	3.2193 (12)	Pd1—Tb3 ^{xi}	2.9950 (9)
Tb2—Pd2 ^{viii}	3.2382 (12)	Pd1—Tb1 ^{iv}	3.1087 (9)
Tb2—Tb3 ^{ix}	3.4916 (8)	Pd1—Tb1 ^v	3.1087 (9)
Tb2—Tb3 ^{viii}	3.4916 (8)	Pd1—Tb2 ⁱⁱ	3.2194 (12)
Tb2—Tb1 ^v	3.5089 (8)	Pd2—Pd2 ^{xi}	2.8752 (19)
Tb2—Tb1 ^{iv}	3.5089 (8)	Pd2—Tb3 ^{vi}	2.9375 (9)
Tb2—Tb1 ^{vii}	3.5174 (8)	Pd2—Tb1 ^{vii}	2.9953 (9)
Tb2—Tb1 ^x	3.5174 (8)	Pd2—Tb1 ^x	2.9953 (9)
Tb2—Tb3 ^{xi}	3.5338 (8)	Pd2—Tb3 ^{xi}	3.1125 (9)
Tb2—Tb3 ^{xii}	3.5338 (8)	Pd2—Tb3 ^{xii}	3.1125 (9)

Tb3—Pd2 ⁱ	2.9375 (9)	Pd2—Tb2 ^{xiv}	3.2382 (12)
Er₃Pd₂			
Er1—Pd1	2.9918 (11)	Er2—Pd1 ^{xx}	3.0096 (9)
Er1—Pd1 ^{xi}	2.9918 (11)	Er2—Pd1 ^{xvii}	3.0096 (10)
Er1—Pd1 ^{xv}	2.9918 (11)	Er2—Pd1 ^{xv}	3.0096 (9)
Er1—Pd1 ^{xvi}	2.9918 (11)	Er2—Er1 ^{xxi}	3.4756 (10)
Er1—Er2 ^{xii}	3.4756 (10)	Er2—Er1 ⁱ	3.4756 (10)
Er1—Er2 ^{vi}	3.4756 (10)	Er2—Er1 ^{xxii}	3.4756 (10)
Er1—Er2 ^{xvii}	3.4756 (10)	Er2—Er2 ^{iv}	3.5359 (16)
Er1—Er2 ^{xviii}	3.4756 (10)	Er2—Er2 ⁱ	3.9169 (17)
Er1—Er2	3.4756 (10)	Pd1—Pd1 ^{xxix}	2.8959 (19)
Er1—Er2 ^{xi}	3.4756 (10)	Pd1—Er2 ^{vi}	2.9511 (11)
Er1—Er2 ^{xvi}	3.4756 (10)	Pd1—Er1 ^{xxi}	2.9918 (11)
Er1—Er2 ^{xv}	3.4756 (10)	Pd1—Er2 ^{xxiv}	3.0096 (9)
Er2—Pd1	2.9511 (11)	Pd1—Er2 ^{xxv}	3.0096 (10)
Er2—Pd1 ⁱ	2.9511 (11)	Pd1—Er2 ^{xvi}	3.0096 (9)
Er2—Pd1 ^{ix}	3.0096 (9)	Pd1—Er2 ^{xviii}	3.0096 (9)
Er₆Co₅			
Er1—Co3 ^{vi}	2.8519 (5)	Er2—Er1 ^{xxxiii}	3.4687 (8)
Er1—Co3	2.8519 (5)	Co3—Co4 ^{xxx}	2.323 (2)
Er1—Co4 ^{xxvi}	2.9491 (15)	Co3—Co4 ^{xxvii}	2.323 (2)
Er1—Co4 ^{xxvii}	2.9491 (15)	Co3—Co4	2.323 (2)
Er1—Co4 ^{vi}	2.9763 (14)	Co3—Er1 ^{xxxiv}	2.8519 (5)
Er1—Co4	2.9763 (14)	Co3—Er1 ^{xxvii}	2.8519 (5)
Er1—Co4 ^{xxviii}	3.0470 (19)	Co3—Er1 ^{xxx}	2.8519 (5)
Er1—Er2 ^{xxviii}	3.4687 (8)	Co3—Er1 ^{xxv}	2.8519 (5)
Er1—Er2 ^{xxix}	3.4687 (8)	Co3—Er1 ⁱ	2.8519 (5)

Er1—Er1 ^{xi}	3.5203 (10)	Co4—Er2 ⁱ	2.7988 (15)
Er1—Er1 ^{xii}	3.5203 (10)	Co4—Er1 ^{xxx}	2.9490 (15)
Er1—Er1 ^{xxx}	3.5434 (11)	Co4—Er1 ^{xxxiv}	2.9490 (15)
Er2—Co4 ^{vi}	2.7988 (15)	Co4—Er1 ⁱ	2.9763 (14)
Er2—Co4	2.7988 (15)	Co4—Er1 ^{xxxii}	3.0469 (19)
Er2—Co5	2.8716 (7)	Co4—Er2 ^{xxviii}	3.074 (2)
Er2—Co5 ^{xxxi}	2.8716 (7)	Co5—Co5 ^{xxxii}	1.9870 (4)
Er2—Co4 ^{xxxii}	3.074 (2)	Co5—Co5 ^{xxxvi}	1.9870 (4)
Er2—Er2 ^{xxix}	3.3477 (6)	Co5—Er2 ^{xxxvii}	2.8716 (7)
Er2—Er2 ^{xxviii}	3.3477 (6)	Co5—Er2 ^{xxxviii}	2.8716 (7)
Er2—Er2 ^{xxxii}	3.3477 (6)	Co5—Er2 ^{xxviii}	2.8716 (7)
Er2—Er2 ^{xxxiii}	3.3477 (6)	Co5—Er2 ^{xxxix}	2.8716 (7)
Er2—Er1 ^{xxxii}	3.4687 (8)	Co5—Er2 ^{xxxii}	2.8716 (7)

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

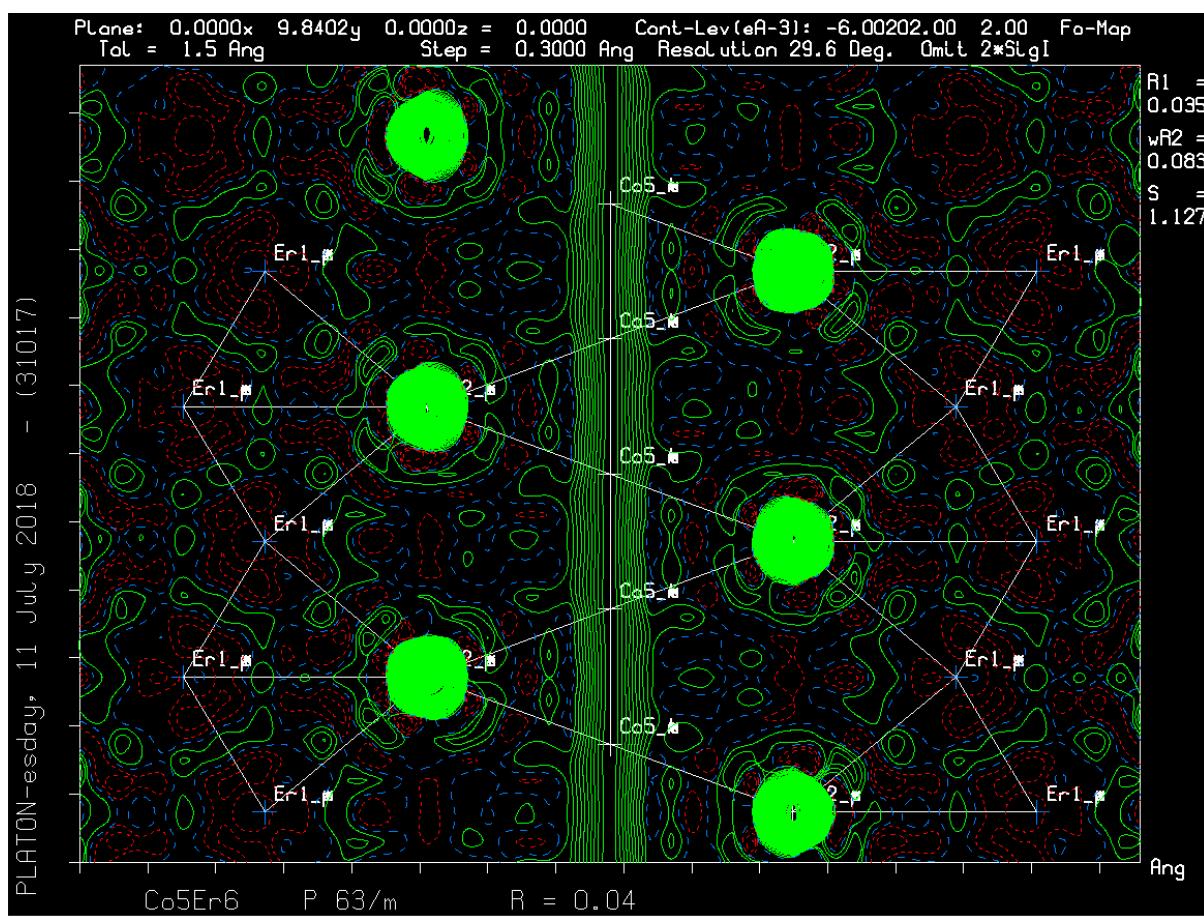


Figure S1. Observed electron density map for $\text{Er}_6\text{Co}_{5-x}$.