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Experimental

Crystallographic Studies

Crystal, data collection, and refinement parameters are given in Table I. A suitable crystal was selected and mounted in a thin-walled, nitrogen-flushed, glass capillary. The unit-cell parameters were obtained by the least-squares refinement of the angular settings of 24 reflections ($20° \leq 2\theta \leq 24°$).

The systematic absences in the diffraction data are uniquely consistent for the reported space group. The structure was solved using direct methods, completed by subsequent difference Fourier syntheses and refined by full-matrix least-squares procedures. Semi-empirical absorption corrections were applied. All non-hydrogen atoms were refined with anisotropic displacement coefficients. Hydrogen atoms were treated as idealized contributions.

All software and sources of the scattering factors are contained in the SHELXTL (5.3) program library (G. Sheldrick, Siemens XRD, Madison, WI).

Table 1. Crystal data and structure refinement for 1.

Identification code	rabg
Empirical formula	$C_{40}H_{88}EuLi_2O_2P_4$
Formula weight	890.82
Temperature	248(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	*a* = 21.740(3) Å alpha = 90° *b* = 12.345(1) Å beta = 109.136(6)° *c* = 20.633(2) Å gamma = 90°
Volume, Z	5231.5(8) $Å^3$, 4
Density (calculated)	1.131 g/cm^3
Absorption coefficient	1.348 mm^{-1}
F(000)	1892
Crystal size	0.40 x 0.40 x 0.30 mm
Crystal color	Orange block
θ range for data collection	2.03 to 22.50°
Limiting indices	$-23 \leq h \leq 22$, $-13 \leq k \leq 1$, $-1 \leq l \leq 22$
Reflections collected	8345
Independent reflections	6842 (R_{int} = 0.0296)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6841 / 0 / 443
Goodness-of-fit on F^2	1.029
Final R indices [I>2σ(I)]	R1 = 0.0329, wR2 = 0.0746
R indices (all data)	R1 = 0.0468, wR2 = 0.0782
Extinction coefficient	0.00216(11)
Largest diff. peak and hole	0.602 and -0.386 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Eu	2524.6(1)	1134.7(2)	2216.6(1)	37(1)
P(1)	3820.5(6)	1599(1)	3319.8(6)	50(1)
P(2)	2499.5(6)	3581(1)	2069.9(6)	45(1)
P(3)	2285.8(6)	-313(1)	965(6)	53(1)
P(4)	1444.5(6)	-248(1)	2452.7(6)	48(1)
Li(1)	3533(4)	3572(7)	3063(4)	62(2)
Li(2)	1424(4)	-1206(7)	1362(4)	58(2)
O(1)	3962(2)	4831(3)	3536(2)	90(1)
O(2)	814(2)	-2249(3)	841(2)	82(1)
C(1)	3678(4)	5786(7)	3651(6)	202(6)
C(2)	4159(5)	6501(10)	4025(8)	227(7)
C(3)	4722(6)	6171(10)	3937(7)	236(8)
C(4)	4629(3)	4996(7)	3757(4)	132(3)
C(5)	224(3)	-2525(7)	948(4)	131(3)
C(6)	-115(4)	-3284(7)	410(5)	142(4)
C(7)	283(5)	-3403(8)	-20(4)	149(4)
C(8)	866(4)	-2842(6)	280(4)	124(3)
C(9)	4656(2)	1083(5)	3384(3)	71(2)
C(10)	4760(3)	1487(6)	2736(3)	116(3)
C(11)	5205(2)	1542(5)	3993(3)	101(2)
C(12)	4708(3)	-144(5)	3401(4)	116(3)
C(13)	3673(2)	1454(4)	4169(2)	62(1)
C(14)	4050(3)	2296(6)	4701(3)	114(3)
C(15)	3802(3)	339(6)	4490(3)	101(2)
C(16)	2940(3)	1691(5)	3990(3)	77(2)
C(17)	2824(3)	3968(4)	1352(3)	64(1)
C(18)	3266(3)	4954(5)	1531(4)	107(2)
C(19)	3247(3)	2990(5)	1305(3)	94(2)
C(20)	2302(3)	4136(5)	661(3)	97(2)
C(21)	1824(2)	4519(4)	2092(2)	56(1)
C(22)	1764(3)	4365(6)	2796(3)	97(2)
C(23)	1969(3)	5722(4)	1999(3)	91(2)
C(24)	1170(2)	4219(5)	1549(3)	78(2)
C(25)	3004(3)	-1191(5)	1016(3)	75(2)
C(26)	3597(3)	-564(7)	960(5)	152(4)
C(27)	3198(3)	-1691(6)	1730(4)	125(3)
C(28)	2866(4)	-2111(6)	502(4)	139(3)
C(29)	1916(3)	287(5)	80(3)	79(2)
C(30)	1431(5)	1089(7)	173(4)	178(4)
C(31)	2390(4)	921(6)	-182(4)	140(3)
C(32)	1568(4)	-528(6)	-458(3)	149(4)
C(33)	1603(3)	-1205(4)	3202(3)	61(1)
C(34)	1644(3)	-676(5)	3882(3)	94(2)
C(35)	2276(3)	-1689(5)	3272(3)	98(2)
C(36)	1124(3)	-2147(4)	3062(3)	91(2)
C(37)	698(3)	603(5)	2367(3)	72(2)
C(38)	836(4)	1516(6)	2899(4)	127(3)

C(39)	535(3)	1118(6)	1655(4)	120(3)
C(40)	107(3)	-28(6)	2382(4)	124(3)

Table 3. Bond lengths [Å] and angles [°] for 1.

Eu-P(2)	3.0337(13)	Eu-P(1)	3.0401(12)
Eu-P(3)	3.0417(13)	Eu-P(4)	3.0680(12)
Eu-Li(1)	3.794(8)	Eu-Li(2)	3.796(8)
P(1)-C(9)	1.888(5)	P(1)-C(13)	1.890(5)
P(1)-Li(1)	2.528(9)	P(2)-C(21)	1.883(5)
P(2)-C(17)	1.899(5)	P(2)-Li(1)	2.495(8)
P(3)-C(25)	1.875(6)	P(3)-C(29)	1.888(5)
P(3)-Li(2)	2.530(8)	P(4)-C(33)	1.885(5)
P(4)-C(37)	1.892(5)	P(4)-Li(2)	2.530(8)
Li(1)-O(1)	1.909(9)	Li(2)-O(2)	1.908(9)
O(1)-C(4)	1.385(7)	O(1)-C(1)	1.386(8)
O(2)-C(8)	1.406(7)	O(2)-C(5)	1.411(7)
C(1)-C(2)	1.392(10)	C(2)-C(3)	1.359(13)
C(3)-C(4)	1.495(12)	C(5)-C(6)	1.455(9)
C(6)-C(7)	1.435(10)	C(7)-C(8)	1.399(9)
C(9)-C(10)	1.512(8)	C(9)-C(12)	1.518(8)
C(9)-C(11)	1.530(7)	C(13)-C(15)	1.513(8)
C(13)-C(14)	1.540(7)	C(13)-C(16)	1.542(7)
C(17)-C(20)	1.517(7)	C(17)-C(18)	1.519(7)
C(17)-C(19)	1.539(7)	C(21)-C(22)	1.511(7)
C(21)-C(24)	1.539(6)	C(21)-C(23)	1.543(7)
C(25)-C(28)	1.515(8)	C(25)-C(27)	1.524(9)
C(25)-C(26)	1.541(8)	C(29)-C(30)	1.505(9)
C(29)-C(32)	1.506(8)	C(29)-C(31)	1.528(8)
C(33)-C(34)	1.523(7)	C(33)-C(36)	1.525(7)
C(33)-C(35)	1.542(7)	C(37)-C(40)	1.512(7)
C(37)-C(39)	1.532(8)	C(37)-C(38)	1.532(8)

P(2)-Eu-P(1)	82.47(3)	P(2)-Eu-P(3)	120.50(3)
P(1)-Eu-P(3)	127.21(4)	P(2)-Eu-P(4)	125.44(3)
P(1)-Eu-P(4)	123.75(4)	P(3)-Eu-P(4)	83.20(3)
P(2)-Eu-Li(1)	40.99(13)	P(1)-Eu-Li(1)	41.61(13)
P(3)-Eu-Li(1)	140.23(14)	P(4)-Eu-Li(1)	136.44(14)
P(2)-Eu-Li(2)	136.33(13)	P(1)-Eu-Li(2)	141.20(13)
P(3)-Eu-Li(2)	41.62(12)	P(4)-Eu-Li(2)	41.58(12)
Li(1)-Eu-Li(2)	176.5(2)	C(9)-P(1)-C(13)	110.8(2)
C(9)-P(1)-Li(1)	120.4(3)	C(13)-P(1)-Li(1)	100.4(3)
C(9)-P(1)-Eu	128.6(2)	C(13)-P(1)-Eu	106.2(2)
Li(1)-P(1)-Eu	85.4(2)	C(21)-P(2)-C(17)	110.9(2)
C(21)-P(2)-Li(1)	118.8(3)	C(17)-P(2)-Li(1)	100.2(3)
C(21)-P(2)-Eu	126.8(2)	C(17)-P(2)-Eu	109.2(2)
Li(1)-P(2)-Eu	86.1(2)	C(25)-P(3)-C(29)	111.3(3)
C(25)-P(3)-Li(2)	114.9(3)	C(29)-P(3)-Li(2)	111.0(3)
C(25)-P(3)-Eu	112.6(2)	C(29)-P(3)-Eu	119.4(2)
Li(2)-P(3)-Eu	85.4(2)	C(33)-P(4)-C(37)	110.2(2)
C(33)-P(4)-Li(2)	112.4(3)	C(37)-P(4)-Li(2)	114.4(3)
C(33)-P(4)-Eu	122.3(2)	C(37)-P(4)-Eu	110.7(2)
Li(2)-P(4)-Eu	84.8(2)	O(1)-Li(1)-P(2)	125.0(4)
O(1)-Li(1)-P(1)	129.2(4)	P(2)-Li(1)-P(1)	105.7(3)
O(1)-Li(1)-Eu	173.2(4)	P(2)-Li(1)-Eu	52.9(2)
P(1)-Li(1)-Eu	53.0(2)	O(2)-Li(2)-P(4)	128.5(4)
O(2)-Li(2)-P(3)	124.3(4)	P(4)-Li(2)-P(3)	106.6(3)
O(2)-Li(2)-Eu	172.5(4)	P(4)-Li(2)-Eu	53.6(2)
P(3)-Li(2)-Eu	53.0(2)	C(4)-O(1)-C(1)	107.2(5)

C(4)-O(1)-Li(1)	124.8(5)	C(1)-O(1)-Li(1)	127.6(5)
C(8)-O(2)-C(5)	109.0(5)	C(8)-O(2)-Li(2)	125.8(5)
C(5)-O(2)-Li(2)	125.1(5)	O(1)-C(1)-C(2)	109.8(7)
C(3)-C(2)-C(1)	106.3(9)	C(2)-C(3)-C(4)	105.6(8)
O(1)-C(4)-C(3)	105.5(8)	O(2)-C(5)-C(6)	107.2(6)
C(7)-C(6)-C(5)	106.3(7)	C(8)-C(7)-C(6)	108.6(7)
C(7)-C(8)-O(2)	108.4(7)	C(10)-C(9)-C(12)	108.6(6)
C(10)-C(9)-C(11)	107.5(5)	C(12)-C(9)-C(11)	108.6(5)
C(10)-C(9)-P(1)	104.2(4)	C(12)-C(9)-P(1)	113.6(4)
C(11)-C(9)-P(1)	114.0(4)	C(15)-C(13)-C(14)	108.9(5)
C(15)-C(13)-C(16)	107.8(5)	C(14)-C(13)-C(16)	108.0(5)
C(15)-C(13)-P(1)	115.4(4)	C(14)-C(13)-P(1)	112.6(4)
C(16)-C(13)-P(1)	103.7(3)	C(20)-C(17)-C(18)	109.8(5)
C(20)-C(17)-C(19)	109.1(5)	C(18)-C(17)-C(19)	107.5(5)
C(20)-C(17)-P(2)	114.3(4)	C(18)-C(17)-P(2)	112.2(4)
C(19)-C(17)-P(2)	103.5(4)	C(22)-C(21)-C(24)	108.7(5)
C(22)-C(21)-C(23)	109.0(5)	C(24)-C(21)-C(23)	108.6(4)
C(22)-C(21)-P(2)	105.1(4)	C(24)-C(21)-P(2)	112.1(3)
C(23)-C(21)-P(2)	113.3(4)	C(28)-C(25)-C(27)	107.6(6)
C(28)-C(25)-C(26)	107.6(6)	C(27)-C(25)-C(26)	107.6(6)
C(28)-C(25)-P(3)	115.1(4)	C(27)-C(25)-P(3)	104.5(4)
C(26)-C(25)-P(3)	114.0(5)	C(30)-C(29)-C(32)	109.3(7)
C(30)-C(29)-C(31)	106.9(6)	C(32)-C(29)-C(31)	108.4(5)
C(30)-C(29)-P(3)	103.2(4)	C(32)-C(29)-P(3)	113.8(4)
C(31)-C(29)-P(3)	114.8(5)	C(34)-C(33)-C(36)	109.3(5)
C(34)-C(33)-C(35)	108.2(5)	C(36)-C(33)-C(35)	106.9(5)
C(34)-C(33)-P(4)	115.2(4)	C(36)-C(33)-P(4)	113.1(4)
C(35)-C(33)-P(4)	103.5(4)	C(40)-C(37)-C(39)	107.6(5)
C(40)-C(37)-C(38)	109.4(5)	C(39)-C(37)-C(38)	108.1(6)
C(40)-C(37)-P(4)	114.9(4)	C(39)-C(37)-P(4)	103.9(4)
C(38)-C(37)-P(4)	112.4(4)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for 1.

The anisotropic displacement factor exponent takes the form:
$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
Eu	38(1)	37(1)	37(1)	-1(1)	13(1)	-2(1)
P(1)	40(1)	60(1)	47(1)	-1(1)	10(1)	3(1)
P(2)	53(1)	39(1)	45(1)	3(1)	17(1)	4(1)
P(3)	65(1)	51(1)	46(1)	-7(1)	24(1)	-5(1)
P(4)	48(1)	48(1)	55(1)	-2(1)	25(1)	-7(1)
Li(1)	61(5)	54(5)	62(5)	-4(4)	8(4)	-3(4)
Li(2)	63(5)	65(6)	49(5)	-9(4)	22(4)	-7(5)
O(1)	69(3)	69(3)	114(3)	-26(3)	5(2)	-12(2)
O(2)	79(3)	82(3)	82(3)	-25(2)	23(2)	-28(2)
C(1)	95(6)	130(8)	347(16)	-133(10)	28(8)	-2(6)
C(2)	192(12)	174(11)	339(18)	-174(12)	119(12)	-78(10)
C(3)	269(15)	223(13)	286(15)	-177(12)	185(13)	-186(13)
C(4)	83(5)	144(8)	146(7)	-36(6)	8(5)	-26(5)
C(5)	63(4)	166(8)	159(7)	-69(6)	31(5)	-45(5)
C(6)	74(5)	113(6)	219(11)	-61(7)	21(6)	-28(5)
C(7)	140(8)	161(9)	124(7)	-59(7)	12(6)	-61(7)
C(8)	154(7)	128(7)	100(6)	-53(5)	55(5)	-59(6)
C(9)	47(3)	87(4)	75(4)	-5(4)	13(3)	7(3)
C(10)	81(4)	168(8)	115(6)	2(6)	54(4)	30(5)
C(11)	45(3)	102(5)	135(6)	-2(5)	1(4)	0(3)
C(12)	80(5)	88(5)	171(8)	-29(5)	30(5)	24(4)
C(13)	64(3)	70(4)	46(3)	2(3)	11(3)	-14(3)
C(14)	137(6)	155(7)	59(4)	-30(4)	42(4)	-58(5)
C(15)	98(5)	111(6)	88(5)	31(4)	24(4)	0(4)
C(16)	82(4)	95(4)	71(4)	8(4)	47(3)	-1(4)
C(17)	79(4)	58(3)	62(3)	5(3)	34(3)	6(3)
C(18)	124(6)	89(5)	137(6)	10(5)	81(5)	-33(4)
C(19)	115(5)	105(5)	84(4)	10(4)	63(4)	26(4)
C(20)	142(6)	102(5)	54(4)	22(4)	41(4)	35(4)
C(21)	52(3)	61(3)	53(3)	-2(3)	16(2)	10(3)
C(22)	80(4)	143(6)	78(4)	-1(4)	39(3)	27(4)
C(23)	99(5)	58(4)	103(5)	-20(4)	13(4)	23(3)
C(24)	60(3)	75(4)	89(4)	3(3)	10(3)	17(3)
C(25)	62(3)	69(4)	96(4)	-16(4)	29(3)	-2(3)
C(26)	84(5)	126(7)	271(12)	-12(8)	93(6)	-9(5)
C(27)	103(5)	114(6)	140(7)	22(6)	13(5)	37(5)
C(28)	126(6)	115(6)	169(8)	-81(6)	39(6)	23(5)
C(29)	111(5)	73(4)	51(3)	10(3)	24(3)	-10(4)
C(30)	195(9)	194(10)	133(8)	76(7)	38(7)	119(8)
C(31)	210(9)	140(7)	81(5)	4(5)	63(6)	-67(7)
C(32)	203(8)	130(7)	61(4)	11(5)	-29(5)	-79(7)
C(33)	76(3)	50(3)	59(3)	8(3)	23(3)	-7(3)
C(34)	139(6)	86(5)	62(4)	2(4)	39(4)	-17(4)
C(35)	94(5)	77(4)	105(5)	18(4)	6(4)	14(4)
C(36)	114(5)	54(4)	102(5)	16(4)	32(4)	-23(4)
C(37)	59(3)	72(4)	94(4)	10(4)	37(3)	7(3)
C(38)	143(7)	94(5)	155(7)	-14(5)	62(6)	48(5)

C(39)	104(5)	122(6)	136(7)	61(5)	43(5)	50(5)
C(40)	61(4)	151(7)	175(8)	42(6)	58(5)	14(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(1A)	3379(4)	5631(7)	3906(6)	242
H(1B)	3428(4)	6116(7)	3212(6)	242
H(2A)	4053(5)	7243(10)	3857(8)	273
H(2B)	4199(5)	6480(10)	4512(8)	273
H(3A)	5091(6)	6275(10)	4359(7)	284
H(3B)	4804(6)	6582(10)	3567(7)	284
H(4A)	4809(3)	4818(7)	3392(4)	158
H(4B)	4844(3)	4545(7)	4158(4)	158
H(5A)	-42(3)	-1876(7)	925(4)	157
H(5B)	311(3)	-2859(7)	1400(4)	157
H(6A)	-171(4)	-3983(7)	608(5)	171
H(6B)	-545(4)	-3002(7)	144(5)	171
H(7A)	374(5)	-4172(8)	-67(4)	179
H(7B)	56(5)	-3111(8)	-478(4)	179
H(8A)	948(4)	-2350(6)	-56(4)	148
H(8B)	1230(4)	-3353(6)	434(4)	148
H(10A)	4728(3)	2271(6)	2719(3)	175
H(10B)	4430(3)	1181(6)	2340(3)	175
H(10C)	5188(3)	1270(6)	2735(3)	175
H(11A)	5152(2)	1296(5)	4418(3)	151
H(11B)	5190(2)	2327(5)	3976(3)	151
H(11C)	5621(2)	1295(5)	3970(3)	151
H(12A)	4642(3)	-415(5)	3815(4)	173
H(12B)	5136(3)	-356(5)	3397(4)	173
H(12C)	4379(3)	-444(5)	3003(4)	173
H(14A)	3971(3)	3014(6)	4500(3)	172
H(14B)	4513(3)	2138(6)	4840(3)	172
H(14C)	3906(3)	2268(6)	5098(3)	172
H(15A)	3566(3)	-198(6)	4158(3)	151
H(15B)	3658(3)	315(6)	4888(3)	151
H(15C)	4265(3)	185(6)	4630(3)	151
H(16A)	2844(3)	2403(5)	3783(3)	116
H(16B)	2823(3)	1670(5)	4406(3)	116
H(16C)	2691(3)	1149(5)	3671(3)	116
H(18A)	3599(3)	4843(5)	1973(4)	161
H(18B)	3011(3)	5589(5)	1553(4)	161
H(18C)	3470(3)	5059(5)	1183(4)	161
H(19A)	3582(3)	2878(5)	1746(3)	141
H(19B)	3449(3)	3126(5)	958(3)	141
H(19C)	2976(3)	2348(5)	1183(3)	141
H(20A)	2021(3)	3505(5)	549(3)	145
H(20B)	2505(3)	4240(5)	312(3)	145
H(20C)	2045(3)	4770(5)	682(3)	145
H(22A)	2173(3)	4552(6)	3143(3)	145
H(22B)	1659(3)	3615(6)	2852(3)	145
H(22C)	1421(3)	4830(6)	2843(3)	145
H(23A)	2008(3)	5826(4)	1549(3)	137
H(23B)	2373(3)	5928(4)	2348(3)	137

H(23C)	1617(3)	6166(4)	2043(3)	137
H(24A)	1202(2)	4314(5)	1094(3)	117
H(24B)	829(2)	4684(5)	1600(3)	117
H(24C)	1067(2)	3469(5)	1609(3)	117
H(26A)	3697(3)	32(7)	1284(5)	228
H(26B)	3499(3)	-282(7)	498(5)	228
H(26C)	3969(3)	-1046(7)	1062(5)	228
H(27A)	3290(3)	-1119(6)	2071(4)	188
H(27B)	3583(3)	-2134(6)	1805(4)	188
H(27C)	2844(3)	-2137(6)	1769(4)	188
H(28A)	2740(4)	-1817(6)	41(4)	209
H(28B)	2515(4)	-2554(6)	549(4)	209
H(28C)	3254(4)	-2551(6)	586(4)	209
H(30A)	1654(5)	1615(7)	520(4)	266
H(30B)	1106(5)	711(7)	318(4)	266
H(30C)	1219(5)	1458(7)	-257(4)	266
H(31A)	2713(4)	430(6)	-249(4)	210
H(31B)	2606(4)	1470(6)	151(4)	210
H(31C)	2153(4)	1265(6)	-614(4)	210
H(32A)	1879(4)	-1047(6)	-519(3)	224
H(32B)	1356(4)	-158(6)	-888(3)	224
H(32C)	1243(4)	-904(6)	-313(3)	224
H(34A)	1949(3)	-77(5)	3972(3)	141
H(34B)	1792(3)	-1205(5)	4248(3)	141
H(34C)	1218(3)	-411(5)	3858(3)	141
H(35A)	2260(3)	-2030(5)	2843(3)	148
H(35B)	2391(3)	-2224(5)	3636(3)	148
H(35C)	2600(3)	-1117(5)	3380(3)	148
H(36A)	1097(3)	-2485(4)	2629(3)	137
H(36B)	697(3)	-1880(4)	3039(3)	137
H(36C)	1272(3)	-2675(4)	3428(3)	137
H(38A)	1215(4)	1922(6)	2890(4)	191
H(38B)	917(4)	1209(6)	3352(4)	191
H(38C)	462(4)	1996(6)	2792(4)	191
H(39A)	907(3)	1530(6)	1630(4)	179
H(39B)	164(3)	1597(6)	1575(4)	179
H(39C)	432(3)	554(6)	1309(4)	179
H(40A)	196(3)	-364(6)	2829(4)	186
H(40B)	7(3)	-584(6)	2031(4)	186
H(40C)	-261(3)	459(6)	2297(4)	186