Table 1   Atomic coordinates and isotropic displacement parameters in $KHoF_4$ at ambient pressure.

Atom	x	y	z	U_{iso}
Ho1	0.13092(3)	0.89028(4)	0.32997(5)	0.00647(8)
Ho2	0.28333(4)	0.73244(4)	0.31985(6)	0.00601(8)
Ho3	0.77991(5)	0.20619(4)	0.33963(4)	0.00640(8)
Ho4	0.94280(4)	0.05934(5)	0.32538(7)	0.00682(8)
Ho5	0.45263(5)	0.54464(6)	0.32348(4)	0.00677(7)
Ho6	0.60445(4)	0.38679(4)	0.34418(3)	0.00634(8)
K1	0.7812(2)	0.71865(19)	0.3212(2)	0.0188(7)
K2	0.26731(18)	0.22010(18)	0.3473(2)	0.0158(6)
K3	0.10348(19)	0.3955(2)	0.3126(2)	0.0178(5)
K4	0.6114(2)	0.87697(17)	0.3469(2)	0.0171(6)
K5	0.9492(2)	0.56257(20)	0.3449(2)	0.0194(6)
K6	0.45537(17)	0.06479(14)	0.3138(2)	0.0158(5)
F1	0.1314(4)	0.9341(3)	0.1128(4)	0.0158(9)
F2	0.0694(4)	0.8779(4)	0.5400(4)	0.0176(10)
F3	0.2103(4)	0.5940(3)	0.4670(5)	0.0224(7)
F4	0.3341(4)	0.7293(3)	0.6513(7)	0.0305(8)
F5	0.7379(4)	0.2035(4)	0.5577(5)	0.0176(10)
F6	0.7885(3)	0.2679(4)	0.1307(5)	0.0158(9)
F7	-0.0034(4)	0.0602(3)	0.6599(6)	0.0305(8)
F8	-0.1221(4)	-0.0774(3)	0.4741(4)	0.0224(7)
F9	0.3905(4)	0.5374(4)	0.5331(4)	0.0176(10)
F10	0.4569(4)	0.5886(3)	0.1062(5)	0.0158(9)
F11	0.5463(4)	0.2904(4)	0.5350(5)	0.0224(7)
F12	0.7361(4)	0.3949(3)	0.6776(6)	0.0305(8)
F13	0.7675(4)	0.7281(3)	0.0649(5)	0.0162(7)
F14	0.8078(4)	0.7233(3)	0.5753(5)	0.0150(7)
F15	0.2479(3)	0.2233(3)	0.6072(5)	0.0155(7)
F16	0.8086(4)	0.0749(4)	0.4302(5)	0.0147(8)
F17	0.1306(3)	0.3946(3)	0.5673(5)	0.0150(7)
F18	0.0917(3)	0.4027(3)	0.0612(4)	0.0162(7)
F19	0.1539(3)	0.7554(3)	0.4241(4)	0.0147(8)
F20	0.5892(3)	0.8837(3)	0.6032(4)	0.0155(7)
F21	0.9377(3)	0.5758(3)	0.6002(5)	0.0155(7)
F22	-0.5325(4)	0.4106(4)	0.4255(5)	0.0147(8)
F23	0.4846(3)	0.0702(3)	0.5686(4)	0.0150(7)
F24	0.4535(4)	0.0868(3)	0.0582(5)	0.0162(7)

Table 2   Atomic coordinates and isotropic displacement parameters in KErF$_4$ at ambient pressure.

Atom	x	y	z	U_{iso}
Er1	0.12924(4)	0.88850(5)	0.33061(6)	0.00773(10)
Er2	0.28257(4)	0.73204(5)	0.32051(6)	0.00657(9)
Er3	0.77948(5)	0.20594(5)	0.33866(5)	0.00651(9)
Er4	0.94245(6)	0.05903(6)	0.32607(9)	0.00784(10)
Er5	0.45238(7)	0.54450(7)	0.32453(6)	0.00737(9)
Er6	0.60496(4)	0.38766(4)	0.34247(4)	0.00627(10)
K1	0.7818(2)	0.7210(2)	0.3192(2)	0.0168(7)
K2	0.2670(2)	0.2202(2)	0.3480(3)	0.0188(7)
K3	0.1042(2)	0.3948(2)	0.3134(3)	0.0168(6)
K4	0.6111(3)	0.8773(2)	0.3460(3)	0.0213(8)
K5	0.9493(3)	0.5620(2)	0.3450(3)	0.0223(8)
K6	0.4543(2)	0.06467(16)	0.3149(2)	0.0161(6)
F1	0.1313(4)	0.9347(4)	0.1132(5)	0.0153(10)
F2	0.0689(5)	0.8763(5)	0.5408(5)	0.0184(12)
F3	0.2094(4)	0.5943(4)	0.4685(5)	0.0234(9)
F4	0.3359(6)	0.7290(3)	0.6540(8)	0.0341(6)
F5	0.7363(5)	0.2032(5)	0.5553(6)	0.0184(12)
F6	0.7880(4)	0.2676(4)	0.1295(5)	0.0153(10)
F7	0.0004(5)	0.0602(3)	0.6622(7)	0.0341(6)
F8	-0.1241(4)	-0.0762(4)	0.4772(5)	0.0234(9)
F9	0.3907(4)	0.5368(5)	0.5339(5)	0.0184(12)
F10	0.4571(5)	0.5899(4)	0.1081(5)	0.0153(10)
F11	0.5466(5)	0.2887(4)	0.5306(5)	0.0234(9)
F12	-0.2666(6)	-0.6056(4)	0.6751(7)	0.0341(6)
F13	0.7678(5)	0.7290(4)	0.0628(6)	0.0183(9)
F14	0.8088(5)	0.7239(3)	0.5720(6)	0.0165(10)
F15	0.2484(4)	0.2237(4)	0.6052(5)	0.0171(9)
F16	0.8082(5)	0.0743(5)	0.4283(6)	0.0154(10)
F17	0.1319(4)	0.3933(4)	0.5656(6)	0.0165(10)
F18	0.0922(4)	0.4018(4)	0.0584(5)	0.0183(9)
F19	0.1535(4)	0.7551(4)	0.4228(5)	0.0154(10)
F20	0.5883(4)	0.8836(4)	0.6029(5)	0.0171(9)
F21	0.9365(4)	0.5741(4)	0.5987(5)	0.0171(9)
F22	-0.5311(5)	0.4112(4)	0.4238(5)	0.0154(10)
F23	0.4842(4)	0.0682(4)	0.5660(5)	0.0165(10)
F24	0.4519(5)	0.0857(4)	0.0570(6)	0.0183(9)

Table 3   Atomic coordinates and isotropic displacement parameters in $KTmF_4$ at ambient pressure.

Atom	x	y	z	U_{iso}
Tm1	0.12764(4)	0.88686(4)	0.66930(5)	0.00854(8)
Tm2	0.28098(4)	0.73088(4)	0.67972(5)	0.00683(8)
Tm3	0.77849(4)	0.20520(4)	0.66356(4)	0.00623(6)
Tm4	0.94085(6)	0.05764(6)	0.67311(8)	0.00832(8)
Tm5	0.45217(6)	0.54475(6)	0.67551(4)	0.00666(6)
Tm6	0.60485(4)	0.38809(4)	0.66008(4)	0.00624(8)
K1	0.26504(19)	0.22064(19)	0.6510(2)	0.0169(5)
K2	0.7811(2)	0.7188(2)	0.6814(2)	0.0214(6)
K3	0.6068(2)	0.87666(16)	0.65505(17)	0.0152(5)
K4	0.1039(2)	0.3920(2)	0.6833(2)	0.0182(6)
K5	0.45351(19)	0.06488(19)	0.68443(18)	0.0183(5)
K6	0.9447(2)	0.55911(19)	0.6549(2)	0.0185(6)
F1	0.1340(4)	0.9396(4)	0.8845(4)	0.0190(11)
F2	0.0712(3)	0.8783(3)	0.4580(4)	0.0149(9)
F3	0.2087(4)	0.5951(3)	0.5294(4)	0.0217(7)
F4	0.3375(5)	0.7291(3)	0.3462(6)	0.0315(7)
F5	0.7366(3)	0.2044(4)	0.4468(4)	0.0149(9)
F6	0.7911(4)	0.2707(4)	0.8717(4)	0.0190(11)
F7	0.0083(4)	0.0603(3)	0.3377(5)	0.0315(7)
F8	-0.1255(3)	-0.0729(3)	0.5168(4)	0.0217(7)
F9	0.3947(3)	0.5392(3)	0.4648(4)	0.0149(9)
F10	0.4609(5)	0.5942(4)	0.8912(4)	0.0190(11)
F11	0.5450(4)	0.2867(3)	0.4740(4)	0.0217(7)
F12	-0.2698(5)	-0.6070(3)	0.3294(6)	0.0315(7)
F13	0.7687(4)	0.7317(3)	0.9380(4)	0.0170(7)
F14	0.8109(4)	0.7241(3)	0.4293(5)	0.0174(9)
F15	0.2503(3)	0.2258(3)	0.3962(4)	0.0161(7)
F16	0.8065(4)	0.0739(4)	0.5735(4)	0.0143(8)
F17	0.1331(4)	0.3930(3)	0.4342(4)	0.0174(9)
F18	0.0930(3)	0.4030(3)	0.9398(4)	0.0170(7)
F19	0.1512(3)	0.7534(3)	0.5782(4)	0.0143(8)
F20	0.5879(3)	0.8837(3)	0.3982(4)	0.0161(7)
F21	0.9366(3)	0.5724(3)	0.4017(4)	0.0161(7)
F22	-0.5311(3)	0.4113(4)	1.5780(4)	0.0143(8)
F23	0.4834(4)	0.0667(3)	0.4339(4)	0.0174(9)
F24	0.4513(3)	0.0869(3)	0.9442(4)	0.0170(7)

Table 4   Atomic coordinates and isotropic displacement parameters in Er:KYbF$_4$ at ambient pressure.

Atom	x	y	z	U_{iso}
Yb1	0.13032(3)	0.88970(4)	0.67154(8)	0.00581(10)
Yb2	0.27742(5)	0.72800(5)	0.67585(10)	0.00714(17)
Yb3	0.78381(7)	0.21038(6)	0.66442(6)	0.00503(14)
Yb4	0.93987(8)	0.05710(8)	0.67429(12)	0.00646(15)
Yb5	0.45319(9)	0.54605(10)	0.67458(8)	0.00765(18)
Yb6	0.60253(5)	0.38535(5)	0.65929(5)	0.00495(11)
K1	0.2668(3)	0.2173(3)	0.6549(4)	0.0154(9)
K2	0.7787(3)	0.7165(3)	0.6877(4)	0.0223(12)
K3	0.6052(3)	0.8798(3)	0.6585(4)	0.0179(10)
K4	0.1049(3)	0.3975(3)	0.6896(3)	0.0160(8)
K5	0.4542(3)	0.0614(3)	0.6859(4)	0.0195(11)
K6	0.9458(3)	0.5596(3)	0.6625(3)	0.0095(7)
F1	0.1328(6)	0.9374(6)	0.8843(9)	0.0176(16)
F2	0.0690(6)	0.8783(6)	0.4594(6)	0.0135(13)
F3	0.2067(5)	0.5985(5)	0.5200(7)	0.0199(10)
F4	0.3440(7)	0.7280(4)	0.3414(9)	0.0316(11)
F5	0.7372(6)	0.2048(6)	0.4470(8)	0.0135(13)
F6	0.7919(6)	0.2713(6)	0.8699(7)	0.0176(16)
F7	0.0015(7)	0.0602(4)	0.3368(10)	0.0316(11)
F8	-0.1236(5)	-0.0746(5)	0.5235(7)	0.0199(10)
F9	0.3948(6)	0.5382(6)	0.4599(7)	0.0135(13)
F10	0.4593(7)	0.5949(7)	0.8885(8)	0.0176(16)
F11	0.5449(6)	0.2842(5)	0.4762(8)	0.0199(10)
F12	-0.2745(7)	-0.6061(5)	0.3272(11)	0.0316(11)
F13	0.7665(6)	0.7312(5)	0.9371(8)	0.0157(13)
F14	0.8053(6)	0.7234(5)	0.4265(8)	0.0119(11)
F15	0.2483(5)	0.2220(5)	0.3936(8)	0.0167(14)
F16	0.8101(6)	0.0775(6)	0.5701(8)	0.0164(15)
F17	0.1328(5)	0.3939(5)	0.4313(8)	0.0119(11)
F18	0.0961(6)	0.4070(5)	0.9390(8)	0.0157(13)
F19	0.1509(5)	0.7547(6)	0.5748(7)	0.0164(15)
F20	0.5896(5)	0.8865(6)	0.3969(8)	0.0167(14)
F21	0.9339(6)	0.5726(7)	0.3975(10)	0.0167(14)
F22	-0.5272(7)	0.4133(7)	0.5734(9)	0.0164(15)
F23	0.4844(5)	0.0678(5)	0.4283(8)	0.0119(11)
F24	0.4492(6)	0.0844(6)	0.9417(8)	0.0157(13)

Table 5   Atomic coordinates and isotropic displacement parameters in KYF$_4$ at ambient pressure.

Atom	x	y	z	U$_{iso}$
Y1	0.13055(3)	0.89040(3)	0.66619(4)	0.00575(7)
Y2	0.28078(4)	0.73037(4)	0.67411(5)	0.00745(10)
Y3	0.78105(4)	0.20748(4)	0.65710(4)	0.00633(8)
Y4	0.94103(4)	0.05768(4)	0.66979(6)	0.00663(8)
Y5	0.45274(4)	0.54494(5)	0.67143(4)	0.00674(8)
Y6	0.60289(3)	0.38552(4)	0.65198(3)	0.00522(7)
K1	0.26672(10)	0.21929(11)	0.64643(12)	0.0158(3)
K2	0.78083(12)	0.71936(12)	0.67589(13)	0.0202(4)
K3	0.61130(12)	0.87785(10)	0.65016(11)	0.0180(3)
K4	0.10466(11)	0.39538(12)	0.67984(12)	0.0167(3)
K5	0.45608(9)	0.06437(9)	0.68040(11)	0.0151(3)
K6	0.94765(11)	0.56221(12)	0.65014(11)	0.0182(3)
F1	0.1309(2)	0.9354(2)	0.8839(2)	0.0152(5)
F2	0.0702(2)	0.8784(2)	0.4569(2)	0.0176(6)
F3	0.20735(19)	0.59552(19)	0.5238(3)	0.0199(3)
F4	0.3388(3)	0.72858(17)	0.3409(3)	0.0296(4)
F5	0.7377(2)	0.2036(2)	0.4403(3)	0.0176(6)
F6	0.78924(19)	0.2701(2)	0.8667(3)	0.0152(5)
F7	-0.0014(3)	0.05974(17)	0.3346(3)	0.0296(4)
F8	0.0761(2)	-0.04768(18)	0.1866(3)	0.0199(3)
F9	0.3917(2)	0.5369(2)	0.4623(2)	0.0176(6)
F10	0.4571(2)	0.5913(2)	0.8881(2)	0.0152(5)
F11	0.54783(19)	0.29041(19)	0.4623(3)	0.0199(3)
F12	-0.2663(2)	-0.60517(18)	0.3190(4)	0.0296(4)
F13	0.7667(2)	0.72828(18)	0.9313(3)	0.0159(4)
F14	0.8094(2)	0.72448(15)	0.4231(3)	0.0156(4)
F15	0.24799(17)	0.22319(18)	0.3903(3)	0.0152(4)
F16	0.8089(2)	0.0749(2)	0.5653(3)	0.0144(4)
F17	0.13261(19)	0.39378(16)	0.4279(2)	0.0156(4)
F18	0.09371(19)	0.40422(19)	0.9355(2)	0.0159(4)
F19	0.15200(18)	0.75538(18)	0.5735(2)	0.0144(4)
F20	0.59000(17)	0.88469(18)	0.3935(2)	0.0152(4)
F21	0.93653(19)	0.5753(2)	0.3960(3)	0.0152(4)
F22	-0.4102(2)	-0.94313(19)	0.2380(2)	0.0144(4)
F23	0.4854(2)	0.06895(16)	0.4277(2)	0.0156(4)
F24	0.4524(2)	0.08634(19)	0.9383(3)	0.0159(4)

Table 6   Selected distances and geometrical parameters (all in Å) in the structure of $KHoF_4$ at ambient conditions.

Ho-F distances

Ho1-F1	2.300(4)	Ho3-F5	2.298(5)	Ho5-F4	2.243(8)
Ho1-F2	2.287(4)	Ho3-F6	2.284(5)	Ho5-F9	2.295(5)
Ho1-F7	2.242(8)	Ho3-F12	2.243(8)	Ho5-F10	2.295(5)
Ho1-F13	2.176(4)	Ho3-F14	2.262(7)	Ho5-F18	2.175(4)
Ho1-F15	2.171(4)	Ho3-F16	2.291(6)	Ho5-F20	2.163(4)
Ho1-F17	2.274(7)	Ho3-F21	2.158(4)	Ho5-F22	2.269(6)
Ho1-F19	2.306(5)	Ho3-F24	2.176(5)	Ho5-F23	2.307(7)
<Ho1-F>	2.25	<Ho3-F>	2.24	<Ho5-F>	2.25
range Ho1-F	0.14	range Ho3-F	0.14	range Ho5-F	0.15
Ho2-F3	2.270(4)	Ho4-F1	2.232(5)	Ho6-F5	2.241(5)
Ho2-F3	2.266(5)	Ho4-F2	2.225(5)	Ho6-F6	2.224(5)
Ho2-F4	2.216(9)	Ho4-F7	2.220(8)	Ho6-F11	2.283(5)
Ho2-F9	2.218(5)	Ho4-F8	2.264(4)	Ho6-F11	2.249(6)
Ho2-F10	2.237(5)	Ho4-F8	2.268(5)	Ho6-F12	2.232(8)
Ho2-F17	2.270(6)	Ho4-F14	2.271(6)	Ho6-F22	2.288(6)
Ho2-F19	2.282(5)	Ho4-F16	2.289(6)	Ho6-F23	2.264(6)
<Ho2-F>	2.25	<Ho4-F>	2.25	<Ho6-F>	2.25
range Ho2-F	0.06	range Ho4-F	0.07	range Ho6-F	0.07

K-F distances

K1-F2	3.065(6)	K3-F1	2.923(7)	K5-F6	3.080(6)
K1-F6	2.923(7)	K3-F3	2.906(5)	K5-F9	2.938(7)
K1-F8	2.953(5)	K3-F9	3.009(6)	K5-F11	2.915(6)
K1-F13	2.629(5)	K3-F14	2.873(5)	K5-F15	2.626(6)
K1-F14	2.616(5)	K3-F17	2.627(5)	K5-F19	2.937(4)
K1-F15	2.597(7)	K3-F18	2.575(5)	K5-F21	2.622(5)
K1-F18	2.540(6)	K3-F20	2.645(7)	K5-F22	2.607(5)
K1-F23	2.964(5)	K3-F24	2.646(6)	K5-F24	2.606(7)
<K1-F>	2.79	<K3-F>	2.78	<K5-F>	2.79
range K1-F	0.52	range K3-F	0.43	range K5-F	0.47
K2-F1	2.892(6)	K4-F2	2.885(7)	K6-F5	2.879(7)
K2-F5	2.857(8)	K4-F4	3.047(5)	K6-F10	2.841(7)
K2-F7	2.995(5)	K4-F10	2.934(7)	K6-F12	2.874(5)
K2-F13	2.649(8)	K4-F16	2.929(4)	K6-F13	2.590(6)
K2-F15	2.668(5)	K4-F18	2.618(7)	K6-F17	2.863(4)
K2-F16	2.585(5)	K4-F19	2.641(5)	K6-F21	2.655(8)
K2-F20	2.655(5)	K4-F20	2.641(5)	K6-F23	2.627(5)
K2-F22	2.887(4)	K4-F21	2.594(6)	K6-F24	2.628(5)
<K2-F>	2.77	<K4-F>	2.79	<K6-F>	2.74
range K2-F	0.42	range K4-F	0.46	range K6-F	0.29

Table 7 Selected distances and geometrical parameters (all in Å) in the structure of KErF$_4$ at ambient conditions.

Er-F distances

Er1-F1	2.299(5)	Er3-F5	2.279(6)	Er5-F4	2.230(11)
Er1-F2	2.274(5)	Er3-F6	2.277(6)	Er5-F9	2.280(5)
Er1-F7	2.229(10)	Er3-F12	2.230(11)	Er5-F10	2.281(6)
Er1-F13	2.170(5)	Er3-F14	2.268(8)	Er5-F18	2.171(5)
Er1-F15	2.149(5)	Er3-F16	2.281(7)	Er5-F20	2.144(5)
Er1-F17	2.260(8)	Er3-F21	2.143(5)	Er5-F22	2.248(7)
Er1-F19	2.279(6)	Er3-F24	2.172(6)	Er5-F23	2.290(8)
<Er1-F>	2.24	<Er3-F>	2.24	<Er5-F>	2.24
range Er1-F	0.15	range Er3-F	0.14	range Er5-F	0.15

Er2-F3	2.259(5)	Er4-F1	2.217(5)	Er6-F5	2.226(6)
Er2-F3	2.264(6)	Er4-F2	2.215(6)	Er6-F6	2.208(5)
Er2-F4	2.205(11)	Er4-F7	2.201(10)	Er6-F11	2.266(5)
Er2-F9	2.207(6)	Er4-F8	2.257(5)	Er6-F11	2.234(7)
Er2-F10	2.228(6)	Er4-F8	2.263(6)	Er6-F12	2.215(10)
Er2-F17	2.272(7)	Er4-F14	2.269(8)	Er6-F22	2.265(7)
Er2-F19	2.259(6)	Er4-F16	2.266(7)	Er6-F23	2.268(7)
<Er2-F>	2.24	<Er4-F>	2.24	<Er6-F>	2.24
range Er2-F	0.06	range E4r-F	0.07	range Er6-F	0.06

K-F distances

K1-F2	3.026(8)	K3-F1	2.905(9)	K5-F6	3.061(8)
K1-F6	2.945(8)	K3-F3	2.905(6)	K5-F9	2.910(9)
K1-F8	2.957(6)	K3-F9	3.009(7)	K5-F11	2.947(8)
K1-F13	2.618(6)	K3-F14	2.882(6)	K5-F15	2.622(7)
K1-F14	2.594(7)	K3-F17	2.592(7)	K5-F19	2.919(5)
K1-F15	2.590(9)	K3-F18	2.601(6)	K5-F21	2.595(6)
K1-F18	2.518(7)	K3-F20	2.626(9)	K5-F22	2.616(6)
K1-F23	2.980(6)	K3-F24	2.624(8)	K5-F24	2.597(10)
<K1-F>	2.74	<K3-F>	2.77	<K5-F>	2.78
range K1-F	0.51	range K3-F	0.42	range K5-F	0.46

K2-F1	2.878(8)	K4-F2	2.854(9)	K6-F5	2.885(8)
K2-F5	2.873(10)	K4-F4	3.056(7)	K6-F10	2.843(9)
K2-F7	3.032(6)	K4-F10	2.936(8)	K6-F12	2.900(7)
K2-F13	2.637(10)	K4-F16	2.907(5)	K6-F13	2.564(7)
K2-F15	2.629(6)	K4-F18	2.596(9)	K6-F17	2.877(5)
K2-F16	2.600(6)	K4-F19	2.634(6)	K6-F21	2.646(10)
K2-F20	2.652(7)	K4-F20	2.636(6)	K6-F23	2.582(6)
K2-F22	2.884(5)	K4-F21	2.597(8)	K6-F24	2.639(6)
<K2-F>	2.77	<K4-F>	2.78	<K6-F>	2.74
range K2-F	0.43	range K4-F	0.46	range K6-F	0.44

Table 8   Selected distances and geometrical parameters (all in Å) in the structure of KTmF$_4$ at ambient conditions.

Tm-F distances

Tm1-F1	2.294(4)	Tm3-F5	2.276(4)	Tm5-F4	2.213(9)
Tm1-F2	2.269(4)	Tm3-F6	2.276(4)	Tm5-F9	2.273(4)
Tm1-F7	2.212(8)	Tm3-F12	2.228(9)	Tm5-F10	2.281(4)
Tm1-F13	2.153(4)	Tm3-F14	2.256(7)	Tm5-F18	2.160(4)
Tm1-F15	2.136(4)	Tm3-F16	2.268(6)	Tm5-F20	2.133(4)
Tm1-F17	2.251(7)	Tm3-F21	2.131(4)	Tm5-F22	2.238(6)
Tm1-F19	2.264(5)	Tm3-F24	2.159(5)	Tm5-F23	2.273(7)
<Tm1-F>	2.23	<Tm3-F>	2.23	<Tm5-F>	2.22
range Tm1-F	0.15	range Tm3-F	0.15	range Tm5-F	0.15
Tm2-F3	2.252(4)	Tm4-F1	2.199(5)	Tm6-F5	2.215(5)
Tm2-F3	2.261(5)	Tm4-F2	2.205(4)	Tm6-F6	2.192(5)
Tm2-F4	2.204(9)	Tm4-F7	2.183(8)	Tm6-F11	2.260(4)
Tm2-F9	2.206(4)	Tm4-F8	2.247(4)	Tm6-F11	2.240(5)
Tm2-F10	2.217(5)	Tm4-F8	2.261(4)	Tm6-F12	2.192(8)
Tm2-F17	2.263(7)	Tm4-F14	2.265(7)	Tm6-F22	2.257(6)
Tm2-F19	2.255(5)	Tm4-F16	2.256(6)	Tm6-F23	2.258(6)
<Tm2-F>	2.24	<Tm4-F>	2.23	<Tm6-F>	2.23
range Tm2-F	0.06	range Tm4-F	0.08	range Tm6-F	0.07

K-F distances

K1-F1	2.899(7)	K3-F2	2.887(7)	K5-F5	2.870(6)
K1-F5	2.918(7)	K3-F4	3.034(6)	K5-F10	2.832(8)
K1-F7	3.126(5)	K3-F10	2.935(7)	K5-F12	2.927(6)
K1-F13	2.653(8)	K3-F16	2.916(4)	K5-F13	2.567(6)
K1-F15	2.598(5)	K3-F18	2.610(7)	K5-F17	2.885(5)
K1-F16	2.626(5)	K3-F19	2.628(5)	K5-F21	2.629(8)
K1-F20	2.638(6)	K3-F20	2.626(5)	K5-F23	2.574(5)
K1-F22	2.880(4)	K3-F21	2.583(6)	K5-F24	2.656(5)
<K1-F>	2.79	<K3-F>	2.78	<K5-F>	2.74
range K1-F	0.53	range K3-F	0.45	range K5-F	0.36
K2-F2	3.007(6)	K4-F1	2.866(8)	K6-F6	3.041(7)
K2-F6	2.900(7)	K4-F3	2.930(5)	K6-F9	2.937(7)
K2-F8	3.044(5)	K4-F9	2.999(6)	K6-F11	2.921(6)
K2-F13	2.622(5)	K4-F14	2.891(5)	K6-F15	2.608(6)
K2-F14	2.587(5)	K4-F17	2.560(5)	K6-F19	2.931(4)
K2-F15	2.594(7)	K4-F18	2.616(4)	K6-F21	2.583(5)
K2-F18	2.533(6)	K4-F20	2.620(7)	K6-F22	2.629(5)
K2-F23	2.950(5)	K4-F24	2.622(6)	K6-F24	2.588(7)
<K2-F>	2.78	<K4-F>	2.76	<K6-F>	2.78
range K2-F	0.51	range K4-F	0.44	range K6-F	0.46

Table 9   Selected distances and geometrical parameters (all in Å) in the structure of Er:KYbF$_4$ at ambient conditions.

Yb-F distances

Yb1-F1	2.250(9)	Yb3-F5	2.286(8)	Yb5-F4	2.194(13)
Yb1-F2	2.288(7)	Yb3-F6	2.229(8)	Yb5-F9	2.304(7)
Yb1-F7	2.207(13)	Yb3-F12	2.210(14)	Yb5-F10	2.259(9)
Yb1-F13	2.108(7)	Yb3-F14	2.224(11)	Yb5-F18	2.103(7)
Yb1-F15	2.153(7)	Yb3-F16	2.282(10)	Yb5-F20	2.137(7)
Yb1-F17	2.221(11)	Yb3-F21	2.138(8)	Yb5-F22	2.259(11)
Yb1-F19	2.274(9)	Yb3-F24	2.103(8)	Yb5-F23	2.252(11)
<Yb1-F>	2.21	<Yb3-F>	2.21	<Yb5-F>	2.22
range Yb1-F	0.18	range Yb3-F	0.19	range Yb5-F	0.20
Yb2-F3	2.229(7)	Yb4-F1	2.223(9)	Yb6-F5	2.186(8)
Yb2-F3	2.274(8)	Yb4-F2	2.163(7)	Yb6-F6	2.217(7)
Yb2-F4	2.183(13)	Yb4-F7	2.197(14)	Yb6-F11	2.225(8)
Yb2-F9	2.162(7)	Yb4-F8	2.211(7)	Yb6-F11	2.252(9)
Yb2-F10	2.220(8)	Yb4-F8	2.279(8)	Yb6-F12	2.170(14)
Yb2-F17	2.262(9)	Yb4-F14	2.271(10)	Yb6-F22	2.221(11)
Yb2-F19	2.236(9)	Yb4-F16	2.242(10)	Yb6-F23	2.230(9)
<Yb2-F>	2.22	<Yb4-F>	2.23	<Yb6-F>	2.21
range Yb2-F	0.11	range Yb4-F	0.12	range Yb6-F	0.08

K-F distances

K1-F1	2.920(11)	K3-F2	2.915(11)	K5-F5	2.898(11)
K1-F5	2.855(12)	K3-F4	3.125(8)	K5-F10	2.822(13)
K1-F7	3.001(8)	K3-F10	2.901(12)	K5-F12	3.007(9)
K1-F13	2.617(13)	K3-F16	2.962(7)	K5-F13	2.577(9)
K1-F15	2.661(9)	K3-F18	2.648(12)	K5-F17	2.831(7)
K1-F16	2.544(9)	K3-F19	2.561(9)	K5-F21	2.595(14)
K1-F20	2.637(9)	K3-F20	2.662(9)	K5-F23	2.635(9)
K1-F22	2.940(8)	K3-F21	2.521(10)	K5-F24	2.614(9)
<K1-F>	2.77	<K3-F>	2.79	<K5-F>	2.75
range K1-F	0.46	range K3-F	0.60	range K5-F	0.43
K2-F2	3.012(10)	K4-F1	2.945(13)	K6-F6	3.087(9)
K2-F6	2.907(11)	K4-F3	2.985(7)	K6-F9	2.841(11)
K2-F8	3.034(8)	K4-F9	2.882(10)	K6-F11	2.916(9)
K2-F13	2.546(9)	K4-F14	2.829(7)	K6-F15	2.605(9)
K2-F14	2.664(9)	K4-F17	2.646(8)	K6-F19	2.947(6)
K2-F15	2.556(12)	K4-F18	2.534(9)	K6-F21	2.699(10)
K2-F18	2.572(10)	K4-F20	2.640(12)	K6-F22	2.507(9)
K2-F23	2.878(7)	K4-F24	2.592(10)	K6-F24	2.605(12)
<K2-F>	2.77	<K4-F>	2.76	<K6-F>	2.78
range K2-F	0.49	range K4-F	0.45	range K6-F	0.58

Table 10   Selected distances and geometrical parameters (all in Å) in the structure of
KYF$_4$ at ambient conditions.

Y-F distances

Y1-F1	2.307(2)	Y3-F5	2.286(3)	Y5-F4	2.231(5)
Y1-F2	2.273(3)	Y3-F6	2.293(3)	Y5-F9	2.281(3)
Y1-F7	2.232(5)	Y3-F12	2.235(5)	Y5-F10	2.295(3)
Y1-F13	2.164(2)	Y3-F14	2.267(4)	Y5-F18	2.155(2)
Y1-F15	2.171(2)	Y3-F16	2.302(3)	Y5-F20	2.169(2)
Y1-F17	2.252(4)	Y3-F21	2.157(2)	Y5-F22	2.260(4)
Y1-F19	2.285(3)	Y3-F24	2.153(3)	Y5-F23	2.291(4)
<Y1-F>	2.24	<Y3-F>	2.24	<Y5-F>	2.24
range Y1-F	0.14	range Y3-F	0.15	range Y5-F	0.14

Y2-F3	2.256(3)	Y4-F1	2.221(3)	Y6-F5	2.227(3)
Y2-F3	2.286(3)	Y4-F2	2.217(3)	Y6-F6	2.207(3)
Y2-F4	2.203(5)	Y4-F7	2.210(5)	Y6-F11	2.260(3)
Y2-F9	2.212(3)	Y4-F8	2.289(2)	Y6-F11	2.254(3)
Y2-F10	2.228(3)	Y4-F8	2.242(3)	Y6-F12	2.219(4)
Y2-F17	2.274(3)	Y4-F14	2.270(4)	Y6-F22	2.274(4)
Y2-F19	2.269(3)	Y4-F16	2.270(3)	Y6-F23	2.270(3)
<Y2-F>	2.25	<Y4-F>	2.24	<Y6-F>	2.24
range Y2-F	0.08	range Y4-F	0.08	range Y6-F	0.07

K-F distances

K1-F1	2.880(4)	K3-F2	2.882(4)	K5-F5	2.896(4)
K1-F5	2.879(5)	K3-F4	3.113(3)	K5-F10	2.849(4)
K1-F7	3.011(3)	K3-F10	2.953(4)	K5-F12	2.896(3)
K1-F13	2.645(4)	K3-F16	2.925(3)	K5-F13	2.588(3)
K1-F15	2.627(3)	K3-F18	2.611(4)	K5-F17	2.895(2)
K1-F16	2.600(3)	K3-F19	2.643(3)	K5-F21	2.642(4)
K1-F20	2.656(3)	K3-F20	2.640(3)	K5-F23	2.604(3)
K1-F22	2.877(3)	K3-F21	2.587(3)	K5-F24	2.650(3)
<K1-F>	2.77	<K3-F>	2.79	<K5-F>	2.75
range K1-F	0.41	range K3-F	0.53	range K5-F	0.31

K2-F2	3.039(4)	K4-F1	2.910(4)	K6-F6	3.069(3)
K2-F6	2.937(4)	K4-F3	2.925(3)	K6-F9	2.937(4)
K2-F8	2.971(3)	K4-F9	3.013(4)	K6-F11	2.922(3)
K2-F13	2.618(3)	K4-F14	2.905(3)	K6-F15	2.625(3)
K2-F14	2.603(3)	K4-F17	2.599(3)	K6-F19	2.924(2)
K2-F15	2.599(4)	K4-F18	2.617(3)	K6-F21	2.606(3)
K2-F18	2.550(3)	K4-F20	2.638(4)	K6-F22	2.622(3)
K2-F23	2.978(3)	K4-F24	2.636(3)	K6-F24	2.612(4)
<K2-F>	2.79	<K4-F>	2.78	<K6-F>	2.79
range K2-F	0.49	range K4-F	0.41	range K6-F	0.46

Table 11 Atomic coordinates and isotropic displacement parameters in Er:KYbF$_4$ at 3.98 GPa.

Atom	x	y	z	U_{iso}
Yb1	0.13433(12)	0.89287(13)	0.6710(2)	0.0121(2)
Yb2	0.28475(16)	0.73326(14)	0.6809(2)	0.0125(2)
Yb3	0.77966(18)	0.20538(15)	0.65941(18)	0.0121(2)
Yb4	0.94283(17)	0.05946(19)	0.6763(3)	0.0125(2)
Yb5	0.45111(19)	0.5417(2)	0.67879(18)	0.0121(2)
Yb6	0.60383(13)	0.38564(16)	0.65423(16)	0.0125(2)
K1	0.2653(8)	0.2183(7)	0.6523(13)	0.027(2)
K2	0.7829(7)	0.7152(7)	0.6807(9)	0.0181(14)
K3	0.6122(10)	0.8752(7)	0.6507(11)	0.027(2)
K4	0.1056(6)	0.3982(7)	0.6909(9)	0.0181(14)
K5	0.4586(7)	0.0656(6)	0.6892(9)	0.0181(14)
K6	0.9516(9)	0.5702(6)	0.6555(10)	0.027(2)
F1	0.1361(13)	0.9343(12)	0.8961(17)	0.0118(16)
F2	0.068(2)	0.877(2)	0.466(3)	0.032(3)
F3	0.2038(14)	0.5934(14)	0.537(2)	0.0231(17)
F4	0.3352(18)	0.7318(17)	0.347(3)	0.0290(17)
F5	0.750(2)	0.211(2)	0.443(3)	0.032(3)
F6	0.7839(12)	0.2650(13)	0.873(2)	0.0118(16)
F7	-0.0105(18)	0.0584(16)	0.341(3)	0.0290(17)
F8	-0.1237(14)	-0.0765(14)	0.526(2)	0.0231(17)
F9	0.3881(18)	0.5320(18)	0.470(3)	0.032(3)
F10	0.4597(15)	0.5890(13)	0.8981(19)	0.0118(16)
F11	0.5482(14)	0.2997(14)	0.452(2)	0.0231(17)
F12	-0.2601(17)	-0.6055(19)	0.314(3)	0.0290(17)
F13	0.7702(16)	0.7268(13)	0.943(2)	0.0185(19)
F14	0.7999(14)	0.7213(14)	0.416(2)	0.0172(17)
F15	0.2463(13)	0.2225(12)	0.398(2)	0.0161(18)
F16	0.8053(14)	0.0696(15)	0.572(2)	0.0139(16)
F17	0.1232(13)	0.3959(17)	0.425(2)	0.0172(17)
F18	0.0901(13)	0.4034(15)	0.9489(18)	0.0185(19)
F19	0.1534(13)	0.7531(14)	0.5748(19)	0.0139(16)
F20	0.5921(13)	0.8853(13)	0.3986(19)	0.0161(18)
F21	0.9430(14)	0.5837(15)	0.406(2)	0.0161(18)
F22	-0.5286(13)	0.4121(13)	0.5645(18)	0.0139(16)
F23	0.4913(15)	0.0706(15)	0.436(2)	0.0172(17)
F24	0.4612(14)	0.0895(14)	0.947(2)	0.0185(19)

Table 12   Selected distances and geometrical parameters (all in Å) in the structure of Er:KYbF$_4$ at 3.98 GPa.

Yb-F distances

Yb1-F1	2.296(17)	Yb3-F5	2.19(3)	Yb5-F4	2.17(3)
Yb1-F2	2.19(3)	Yb3-F6	2.25(2)	Yb5-F9	2.21(3)
Yb1-F7	2.21(3)	Yb3-F12	2.20(4)	Yb5-F10	2.251(19)
Yb1-F13	2.086(18)	Yb3-F14	2.18(3)	Yb5-F18	2.092(17)
Yb1-F15	2.141(17)	Yb3-F16	2.24(2)	Yb5-F20	2.094(18)
Yb1-F17	2.20(3)	Yb3-F21	2.132(17)	Yb5-F22	2.24(2)
Yb1-F19	2.27(2)	Yb3-F24	2.14(2)	Yb5-F23	2.22(3)
<Yb1-F>	2.20	<Yb3-F>	2.19	<Yb5-F>	2.18
range Yb1-F	0.21	range Yb3-F	0.12	range Yb5-F	0.14

Yb2-F3	2.193(18)	Yb4-F1	2.155(16)	Yb6-F5	2.27(3)
Yb2-F3	2.26(2)	Yb4-F2	2.17(3)	Yb6-F6	2.145(17)
Yb2-F4	2.17(4)	Yb4-F7	2.15(4)	Yb6-F11	2.258(19)
Yb2-F9	2.19(2)	Yb4-F8	2.202(18)	Yb6-F11	2.19(2)
Yb2-F10	2.150(17)	Yb4-F8	2.20(2)	Yb6-F12	2.16(3)
Yb2-F17	2.20(2)	Yb4-F14	2.22(3)	Yb6-F22	2.21(2)
Yb2-F19	2.22(2)	Yb4-F16	2.22(2)	Yb6-F23	2.20(3)
<Yb2-F>	2.20	<Yb4-F>	2.19	<Yb6-F>	2.20
range Yb2-F	0.11	range Yb4-F	0.07	range Yb6-F	0.13

K-F distances

K1-F1	2.78(2)	K3-F2	2.83(4)	K5-F5	2.66(3)
K1-F5	2.79(4)	K3-F4	2.94(2)	K5-F10	2.72(3)
K1-F7	2.79(2)	K3-F10	2.87(3)	K5-F12	2.72(2)
K1-F13	2.50(3)	K3-F16	2.776(17)	K5-F13	2.54(2)
K1-F15	2.54(2)	K3-F18	2.52(3)	K5-F17	2.666(19)
K1-F16	2.52(2)	K3-F19	2.57(2)	K5-F21	2.61(3)
K1-F20	2.56(2)	K3-F20	2.52(2)	K5-F23	2.54(2)
K1-F22	2.888(16)	K3-F21	2.49(2)	K5-F24	2.56(2)
<K1-F>	2.67	<K3-F>	2.69	<K5-F>	2.63
range K1-F	0.39	range K3-F	0.42	range K5-F	0.18

K2-F2	3.06(3)	K4-F1	2.78(2)	K6-F6	2.93(2)
K2-F6	2.81(3)	K4-F3	2.78(2)	K6-F9	2.82(4)
K2-F8	2.92(2)	K4-F9	2.93(3)	K6-F11	2.72(2)
K2-F13	2.61(2)	K4-F14	2.698(18)	K6-F15	2.49(2)
K2-F14	2.62(2)	K4-F17	2.65(2)	K6-F19	2.773(16)
K2-F15	2.49(3)	K4-F18	2.57(2)	K6-F21	2.48(2)
K2-F18	2.48(2)	K4-F20	2.55(3)	K6-F22	2.45(2)
K2-F23	2.955(19)	K4-F24	2.64(2)	K6-F24	2.53(3)
<K2-F>	2.74	<K4-F>	2.70	<K6-F>	2.65
range K2-F	0.58	range K4-F	0.38	range K6-F	0.48

Table 13   Atomic coordinates and isotropic displacement parameters in KYF_4 at 2.04 GPa.

Atom	x	y	z	U_{iso}
Y1	0.13331(13)	0.89179(15)	0.6661(2)	0.0120(3)
Y2	0.28454(14)	0.73332(16)	0.6762(3)	0.0125(2)
Y3	0.77952(15)	0.20568(16)	0.6537(2)	0.0120(3)
Y4	0.94207(16)	0.0588(2)	0.6712(3)	0.0125(2)
Y5	0.45206(17)	0.5437(2)	0.6736(2)	0.0120(3)
Y6	0.60309(12)	0.38517(17)	0.6496(2)	0.0125(2)
K1	0.2681(4)	0.2190(4)	0.6451(7)	0.0174(8)
K2	0.7806(5)	0.7114(5)	0.6783(7)	0.0255(12)
K3	0.6117(5)	0.8763(4)	0.6499(5)	0.0174(8)
K4	0.1026(4)	0.3965(5)	0.6832(6)	0.0255(12)
K5	0.4585(4)	0.0652(4)	0.6831(7)	0.0255(12)
K6	0.9484(4)	0.5663(4)	0.6507(6)	0.0174(8)
F1	0.1287(10)	0.9292(10)	0.8867(17)	0.0197(15)
F2	0.0714(9)	0.8765(10)	0.4500(15)	0.0188(14)
F3	0.2065(8)	0.5927(9)	0.5287(14)	0.0237(9)
F4	0.3331(10)	0.7304(9)	0.3428(16)	0.0255(10)
F5	0.7385(10)	0.1997(10)	0.4338(17)	0.0188(14)
F6	0.7870(9)	0.2688(9)	0.8594(15)	0.0197(15)
F7	-0.0066(10)	0.0604(9)	0.3281(15)	0.0255(10)
F8	0.0789(9)	-0.0449(9)	0.1897(14)	0.0237(9)
F9	0.3901(9)	0.5338(9)	0.4573(15)	0.0188(14)
F10	0.4515(10)	0.5848(10)	0.8936(16)	0.0197(15)
F11	0.5506(9)	0.2963(9)	0.4539(15)	0.0237(9)
F12	-0.2600(9)	-0.6058(10)	0.3053(14)	0.0255(10)
F13	0.7708(8)	0.7285(8)	0.9359(15)	0.0155(12)
F14	0.8088(8)	0.7257(8)	0.4185(14)	0.0124(9)
F15	0.2460(9)	0.2233(8)	0.3949(14)	0.0174(12)
F16	0.8171(8)	0.0827(9)	0.5560(13)	0.0164(11)
F17	0.1252(8)	0.3952(9)	0.4301(13)	0.0124(9)
F18	0.0958(7)	0.4045(8)	0.9397(12)	0.0155(12)
F19	0.1623(7)	0.7643(7)	0.5642(11)	0.0164(11)
F20	0.5913(8)	0.8848(8)	0.4024(14)	0.0174(12)
F21	0.9440(8)	0.5822(8)	0.3982(14)	0.0174(12)
F22	-0.4084(10)	-0.9443(9)	0.2391(14)	0.0164(11)
F23	0.4766(7)	0.0706(7)	0.4222(12)	0.0124(9)
F24	0.4599(8)	0.0894(8)	0.9446(12)	0.0155(12)

Table 14   Selected distances and geometrical parameters (all in Å) in the structure of KYF$_4$ at 2.04 GPa.

Y-F distances

Y1-F1	2.289(17)	Y3-F5	2.277(17)	Y5-F4	2.21(2)
Y1-F2	2.311(15)	Y3-F6	2.233(15)	Y5-F9	2.322(15)
Y1-F7	2.223(19)	Y3-F12	2.24(2)	Y5-F10	2.288(16)
Y1-F13	2.125(11)	Y3-F14	2.259(17)	Y5-F18	2.148(10)
Y1-F15	2.163(11)	Y3-F16	2.262(14)	Y5-F20	2.168(11)
Y1-F17	2.266(17)	Y3-F21	2.185(11)	Y5-F22	2.230(17)
Y1-F19	2.265(12)	Y3-F24	2.155(11)	Y5-F23	2.297(15)
<Y1-F>	2.23	<Y3-F>	2.23	<Y5-F>	2.24
range Y1-F	0.19	range Y3-F	0.12	range Y5-F	0.17
Y2-F3	2.264(12)	Y4-F1	2.233(14)	Y6-F5	2.215(14)
Y2-F3	2.243(14)	Y4-F2	2.187(13)	Y6-F6	2.212(13)
Y2-F4	2.20(2)	Y4-F7	2.21(2)	Y6-F11	2.247(14)
Y2-F9	2.190(13)	Y4-F8	2.249(13)	Y6-F11	2.218(16)
Y2-F10	2.187(13)	Y4-F8	2.240(13)	Y6-F12	2.203(19)
Y2-F17	2.268(15)	Y4-F14	2.208(16)	Y6-F22	2.266(19)
Y2-F19	2.265(12)	Y4-F16	2.260(14)	Y6-F23	2.268(13)
<Y2-F>	2.23	<Y4-F>	2.23	<Y6-F>	2.23
range Y2-F	0.08	range Y4-F	0.07	range Y6-F	0.07

K-F distances

K1-F1	2.794(17)	K3-F2	2.773(19)	K5-F5	2.858(18)
K1-F5	2.75(2)	K3-F4	2.980(13)	K5-F10	2.82(2)
K1-F7	2.903(12)	K3-F10	2.835(18)	K5-F12	2.770(13)
K1-F13	2.535(18)	K3-F16	3.034(10)	K5-F13	2.604(15)
K1-F15	2.541(15)	K3-F18	2.524(17)	K5-F17	2.774(11)
K1-F16	2.505(15)	K3-F19	2.539(12)	K5-F21	2.630(19)
K1-F20	2.659(14)	K3-F20	2.516(15)	K5-F23	2.635(14)
K1-F22	2.797(12)	K3-F21	2.492(14)	K5-F24	2.652(14)
<K1-F>	2.69	<K3-F>	2.71	<K5-F>	2.72
range K1-F	0.40	range K3-F	0.54	range K5-F	0.25
K2-F2	3.073(17)	K4-F1	2.88(2)	K6-F6	3.038(15)
K2-F6	2.877(18)	K4-F3	2.843(13)	K6-F9	2.858(18)
K2-F8	2.987(14)	K4-F9	2.952(16)	K6-F11	2.825(15)
K2-F13	2.613(16)	K4-F14	2.835(11)	K6-F15	2.572(14)
K2-F14	2.637(15)	K4-F17	2.567(14)	K6-F19	3.019(9)
K2-F15	2.560(17)	K4-F18	2.587(13)	K6-F21	2.554(15)
K2-F18	2.568(14)	K4-F20	2.645(18)	K6-F22	2.597(16)
K2-F23	2.737(10)	K4-F24	2.629(14)	K6-F24	2.551(17)
<K2-F>	2.76	<K4-F>	2.74	<K6-F>	2.75
range K2-F	0.51	range K4-F	0.38	range K6-F	0.49