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Supporting information for article:

High-pressure study of a 3*d*–4*f* heterometallic CuEu–organic skeleton

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Table S1 Summary of Crystal Data and Structure Results for NBU-8.

CCDC	1561729
Empirical formula	$C_{66}H_{44}Cu_3Eu_2N_{18}O_{31}$
structural formula	$\{Eu_2Cu_3(PBA)_6(NO_3)_6{\bullet}H_2O\}_n$(NBU-8)
fw	2079.73
Crystal system	trigonal
Space group	R-3c
Temperature (K)	296(2)
Λ (Mo Kα), Å	0.71073
a / Å	14.0021(3)
b / Å	14.0021(3)
c / Å	63.523(3)
α / °	90
β / °	90
γ / °	120
V / $Å^3$	10785.7(5)
Z	6
2θ max (deg)	52.14
μ(Mo-Kα) mm^{-1}	2.697
D, g/cm^3	1.921
F (000)	6162
Crystal size (mm^3)	0.25×0.23×0.20
Reflections collected / unique	21300/2373 [R_{int} = 0.0472]
Final R indices [I > 2σ(I)]	[a] R_1 = 0.0296, [b] wR_2 = 0.0856
R indices (all data)	[a] R_1 = 0.0377, [b] wR_2 = 0.0912
GOF	1.075

[a] $R_1 = \Sigma||F_o|-|F_c||/å|F_o|$, [b] $wR_2 = \{\Sigma w[(F_o)^2-(F_c)^2]^2/\Sigma w[(F_o)^2]^2\}^{1/2}$

Table S2 The indexed and refined structural parameters of NBU-8 at high pressure. The R_p and wR_p factors values are also given.

Pressure (GPa)	Cell parameters					
	a(Å)	b(Å)	c(Å)	V(Å^3)	R_p	wR_p
0.292	14.067	13.960	63.575	10816.681	0.18%	0.53%
0.958	13.937	13.941	63.433	10743.547	0.20%	0.60%
2.063	13.673	13.751	63.950	10389.757	0.46%	1.61%
3.048	13.667	13.664	63.855	10252.480	0.23%	0.66%
4.220	13.472	13.576	63.781	10156.080	0.20%	0.48%
5.128	13.461	13.506	63.201	9876.693	0.19%	0.63%

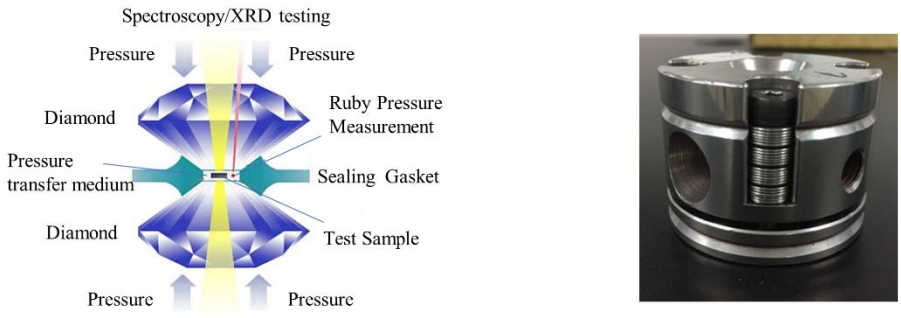

Figure S1 The schematic diagram of the diamond anvil cell and the experimental setup.

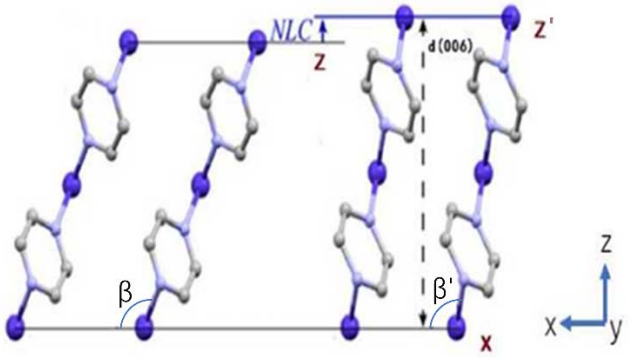

Figure S2 Linear rotation of the negative linear compression occurs when the rotation of the ligand causes the d-spacing to increase.

As shown in Figure S2, under pressure, the plane slides along the x-axis of the central axis, and the lattice parameter β, i.e., the obtuse angle between the x-axis and the z-axis, decreases, leading to a corresponding increase in sin β, which affects the change in the length of d(0 0 6) as shown in equation (1). As pressure rises from P to P ', we obtain the following relationships:

$d(006) = z \bullet \sin \beta$.

$d'(006) = z' \bullet \sin \beta'$.

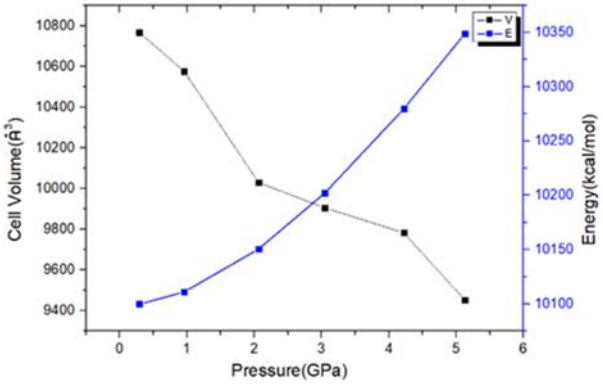

Figure S3 Unit cell volume and total system energy with pressure.