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Phosphoramides bearing isoxazole derivative: Spectroscopic and structural characterization, study of hydrogen bonding interactions, and two lanthanide complexes (Ln^{III} = Ce and Eu)

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Table S1 Selected geometrical parameters for **7**

7A		**7B**	
Bond lengths (Å)			
Ce(1A)–O(11A)	2.441(3)	Ce(1B)–O(11B)	2.443(3)
Ce(1A)–O(12A)	2.450(3)	Ce(1B)–O(12B)	2.431(3)
Ce(1A)–N(4A)	2.712(3)	Ce(1B)–N(4B)	2.744(3)
Ce(1A)–O(10A)	2.514(3)	Ce(1B)–O(10B)	2.513(3)
Ce(1A)–O(1A)	2.593(3)	Ce(1B)–O(1B)	2.607(3)
P(1A)–O(11A)	1.498(3)	P(1B)–O(11B)	1.489(3)
P(2A)–O(12A)	1.492(3)	P(2B)–O(12B)	1.488(3)
P(1A)–N(5A)	1.655(3)	P(1B)–N(5B)	1.655(3)
P(2A)–N(7A)	1.651(4)	P(2B)–N(7B)	1.653(4)
Bond angles (°)			
O(11A)–Ce(1A)–O(12A)	139.65(9)	O(12B)–Ce(1B)–O(11B)	140.75(9)
O(11A)–Ce(1A)–N(4A)	68.17(9)	O(11B)–Ce(1B)–N(4B)	68.07(9)
O(12A)–Ce(1A)–N(4A)	75.72(9)	O(12B)–Ce(1B)–N(4B)	76.43(9)
O(11A)–P(1A)–N(5A)	112.36(17)	O(11B)–P(1B)–N(5B)	112.82(16)
O(12A)–P(2A)–N(7A)	115.42(17)	O(12B)–P(2B)–N(7B)	115.23(17)
Torsion angles (°)			
N(5A)–P(1A)–O(11A)–Ce(1A)	17.4(3)	N(5B)–P(1B)–O(11B)–Ce(1B)	–9.4(3)
N(4A)–Ce(1A)–O(11A)–P(1A)	16.4(2)	N(4B)–Ce(1B)–O(11B)–P(1B)	–23.4(2)
N(7A)–P(2A)–O(12A)–Ce(1A)	85.3(11)	N(7B)–P(2B)–O(12B)–Ce(1B)	–53.5(11)
N(4A)–Ce(1A)–O(12A)–P(2A)	–95.2(11)	N(4B)–Ce(1B)–O(12B)–P(2B)	57.9(11)
Ce(1A)–N(4A)–C(3A)–N(5A)	25.5(5)	Ce(1B)–N(4B)–C(3B)–N(5B)	–21.2(5)
C(11A)–P(1A)–O(11A)–Ce(1A)	–101.3(3)	C(11B)–P(1B)–O(11B)–Ce(1B)	–124.6(2)
O(11A)–P(1A)–N(5A)–C(3A)	–56.3(3)	O(11B)–P(1B)–N(5B)–C(3B)	56.1(3)

Table S2 Selected geometrical parameters for **8**

8A		**8B**	
Bond lengths (Å)			
Eu(1A)–O(11A)	2.3721(15)	Eu(1B)–O(11B)	2.3697(15)
Eu(1A)–O(12A)	2.3945(16)	Eu(1B)–O(12B)	2.3724(15)
Eu(1A)–N(4A)	2.6364(19)	Eu(1B)–N(4B)	2.6716(19)
Eu(1A)–O(10A)	2.4391(16)	Eu(1B)–O(10B)	2.4338(16)
Eu(1A)–O(1A)	2.5386(16)	Eu(1B)–O(1B)	2.5449(16)
P(1A)–O(11A)	1.4949(16)	P(1B)–O(11B)	1.4947(16)
P(2A)–O(12A)	1.4892(16)	P(2B)–O(12B)	1.4906(16)
P(1A)–N(5A)	1.660(2)	P(1B)–N(5B)	1.657(2)
P(2A)–N(7A)	1.661(2)	P(2B)–N(7B)	1.652(2)
Bond angles (°)			
O(11A)–Eu(1A)–O(12A)	141.18(5)	O(12B)–Eu(1B)–O(11B)	141.72(5)
O(11A)–Eu(1A)–N(4A)	69.64(6)	O(11B)–Eu(1B)–N(4B)	69.18(5)
O(12A)–Eu(1A)–N(4A)	69.64(6)	O(12B)–Eu(1B)–N(4B)	76.31(6)
O(11A)–P(1A)–N(5A)	112.30(10)	O(11B)–P(1B)–N(5B)	112.58(10)
O(12A)–P(2A)–N(7A)	115.67(10)	O(12B)–P(2B)–N(7B)	115.74(10)
Torsion angles (°)			
N(5A)–P(1A)–O(11A)–Eu(1A)	–16.88(18)	N(5B)–P(1B)–O(11B)–Eu(1B)	–9.39(17)
N(4A)–Eu(1A)–O(11A)–P(1A)	–16.03(14)	N(4B)–Eu(1B)–O(11B)–P(1B)	–22.97(13)
N(7A)–P(2A)–O(12A)–Eu(1A)	–79.1(7)	N(7B)–P(2B)–O(12B)–Eu(1B)	–50.1(7)
N(4A)–Eu(1A)–O(12A)–P(2A)	87.9(6)	N(4B)–Eu(1B)–O(12B)–P(2B)	54.3(6)
Eu(1A)–N(4A)–C(3A)–N(5A)	–22.2(3)	Eu(1B)–N(4B)–C(3B)–N(5B)	–19.4(3)
C(11A)–P(1A)–O(11A)–Eu(1A)	101.52(15)	C(11B)–P(1B)–O(11B)–Eu(1B)	–125.03(14)
O(11A)–P(1A)–N(5A)–C(3A)	55.0(2)	O(11B)–P(1B)–N(5B)–C(3B)	54.7(2)

Table S3 Hydrogen bond data for **7** and **8** (distances in Å and angles in °)

Compound	D–H…A	d(D–H)	d(H…A)	d(D…A)	<DHA
7	N(5A)–H(5A)...O(9B) [x,y–1,z]	0.80(5)	2.13(5)	2.914(4)	168(5)
	N(5B)–H(5B)...O(9A)	0.87(5)	2.01(5)	2.877(4)	173(6)
	N(7A)–H(7A)...O(1S)	0.79(4)	2.07(5)	2.838(5)	165(5)
	N(7B)–H(7B)...O(2S)	0.76(5)	2.08(5)	2.830(5)	167(5)
	O(10A)–H(10V)...N(6A)	0.73(6)	2.06(6)	2.786(4)	179(9)
	O(10B)–H(10W)...N(6B)	0.71(5)	2.15(5)	2.858(4)	170(5)
	O(1S)–H(1S)...O(5B) [x–1,y–1,z]	0.82(6)	2.14(6)	2.919(4)	161(5)
	O(1S)–H(1S)...O(6B) [x–1,y–1,z]	0.82(6)	2.51(6)	3.166(5)	138(5)
	O(2S)–H(2S)...O(4A) [x+1,y,z]	0.82(6)	2.43(6)	3.209(5)	159(6)
	O(2S)–H(2S)...O(6A) [x+1,y,z]	0.82(6)	2.33(6)	2.983(6)	137(5)
8	O(1S)–H(1S)...O(5B) [–x+1,–y+2,–z+1]	0.88	2.12	2.941(3)	155
	O(1S)–H(1S)...O(6B) [–x+1,–y+2,–z+1]	0.88	2.37	3.145(3)	148
	O(2S)–H(2S)...O(4A) [–x+1,–y+1,–z+1]	0.82	2.47	3.252(3)	159
	O(2S)–H(2S)...O(6A) [–x+1,–y+1,–z+1]	0.82	2.31	2.997(3)	142
	N(5A)–H(5A)...O(9B) [–x+1,–y+2,–z+1]	0.78(3)	2.12(3)	2.883(3)	168(3)
	N(5B)–H(5B)...O(9A) [–x+1,–y+1,–z+1]	0.79(3)	2.07(3)	2.855(3)	174(3)
	N(7A)–H(7A)...O(1S) [x+1,y,z]	0.84	2.02	2.842(3)	163
	N(7B)–H(7B)...O(2S) [x+1,y,z]	0.77(3)	2.07(3)	2.822(3)	169(3)
	O(10B)–H(1OB)...N(6B)	0.80	2.05	2.841(2)	170
	O(10A)–H(1OA)...N(6A)	0.86	1.91	2.775(3)	174

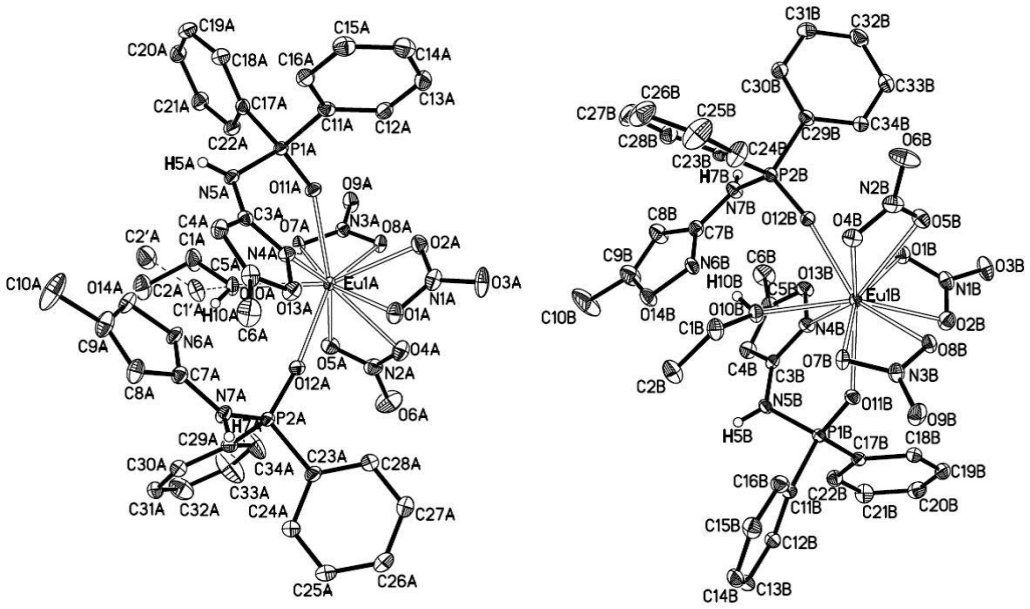
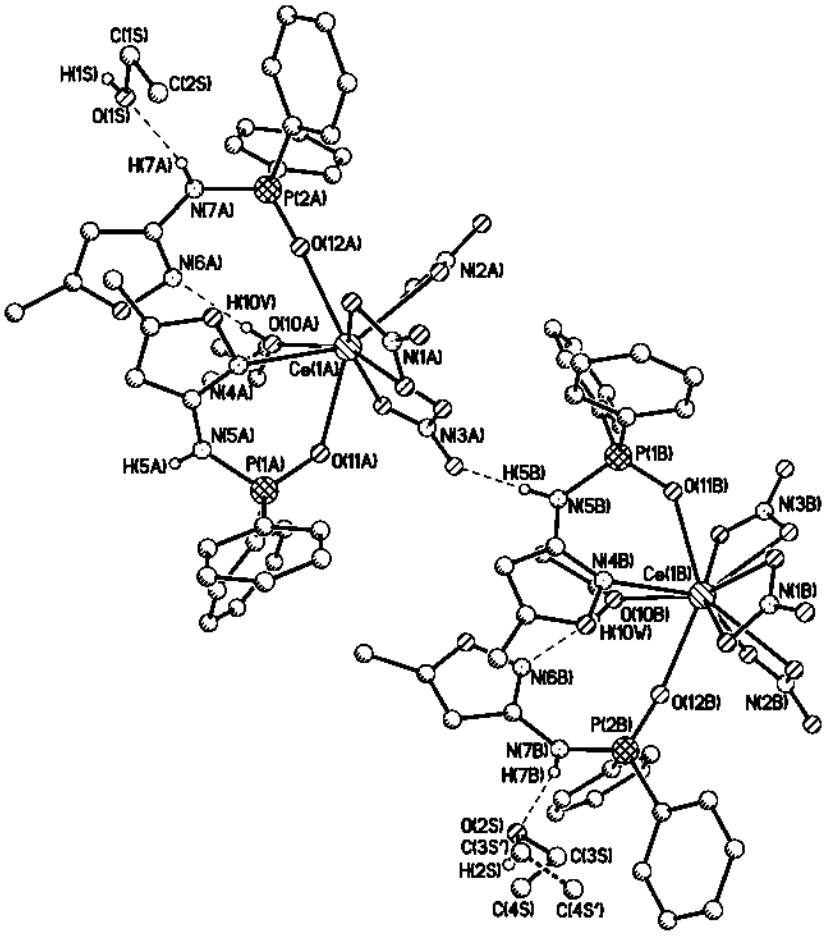
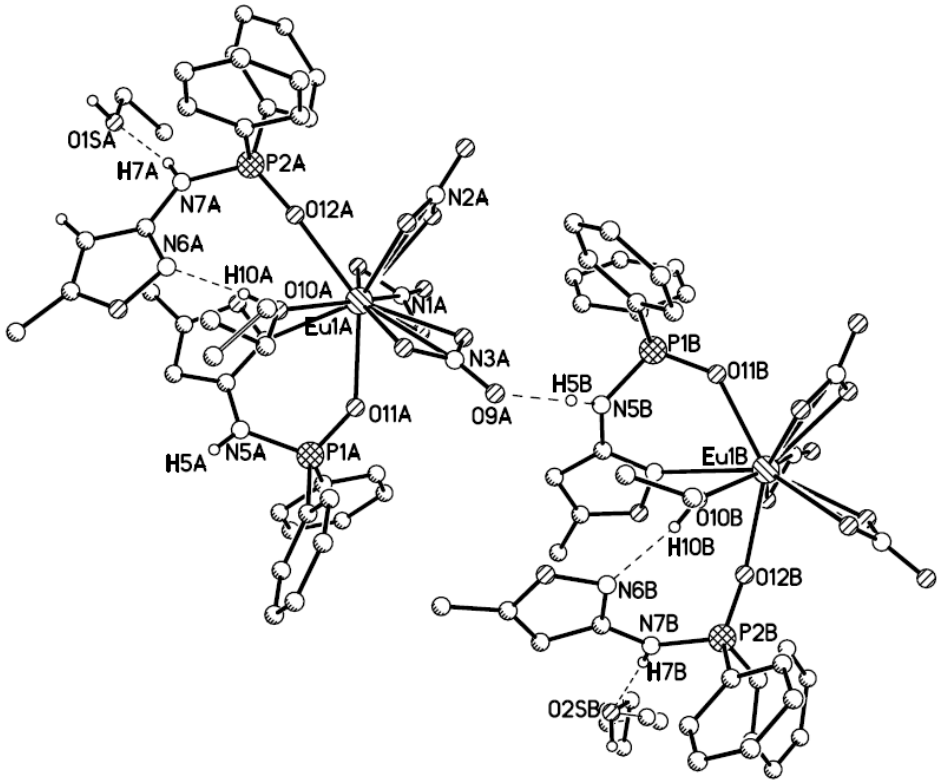


Figure S1 General view of two independent molecules (**A** and **B**) of **8** with numbering scheme. Thermal ellipsoids are shown at 50% probability level.


C(1S)
H(1S)
C(2S)
O(1S)
H(7A)
N(7A)
P(2A)
O(12A)
N(2A)
N(6A)
H(10V)
O(10A)
Ce(1A)
N(1A)
N(4A)
N(3A)
N(5A)
H(5A)
P(1A)
O(11A)
H(5B)
P(1B)
O(11B)
N(3B)
N(5B)
N(4B)
Ce(1B)
N(1B)
O(10B)
H(10W)
N(6B)
O(12B)
N(2B)
P(2B)
N(7B)
H(7B)
O(2S)
C(3S')
C(3S)
H(2S)
C(4S)
C(4S')

(a)



(b)

Figure S2 Independent part of the unit cell of **7** (a) and **8** (b) contains two independent molecules of complex and two solvate ethanol molecules. Carbon part of one of the two solvate ethanol molecules (O2SC3SC4S) is disordered over two positions with 0.7/0.3 occupancies for **7**, and (O2SBC3SBC4SB) is disordered over three positions with 0.45/0.35/0.20 occupancies for **8**.