Additional material to deposit for the paper of F. Liebau & X. Wang, "A bond-valence investigation of two series of isostructural lanthanide compounds".

Table 3. Values of calculated bond-valence sums $(BVS)_{Ln}$ and bond valences s_{ij}(LnO, N), both measured in v.u., for the $[LnO_8N_3]$ coordination polyhedra in the lanthanide chelates $[Ln_3(C_{36}H_{32}N_7O_{10})\cdot H_2O]$ described by Seitz *et al.* (2007a, b).

Ln	Z_{Ln}	$(BVS)_{Ln}$	O(1)	O(2)	O(3)	O(4)	O(5)	O(6)	O(7)	O(10)	N(3)	N(5)	N(7)
La	57	3.643	0.481	0.476	0.454	0.442	0.436	0.433	0.395	0.331	0.067	0.066	0.063
Ce	58	3.660	0.477	0.468	0.452	0.452	0.446	0.425	0.413	0.320	0.071	0.069	0.068
Pr	59	3.656	0.486	0.479	0.457	0.449	0.443	0.425	0.401	0.319	0.068	0.066	0.063
Nd	60	3.650	0.474	0.473	0.469	0.447	0.443	0.425	0.394	0.323	0.068	0.068	0.066
Sm	62	3.594	0.462	0.458	0.458	0.454	0.435	0.435	0.393	0.313	0.063	0.063	0.061
Eu	63	3.615	0.469	0.463	0.455	0.454	0.434	0.434	0.395	0.317	0.066	0.065	0.064
Gd	64	3.626	0.472	0.465	0.459	0.453	0.435	0.431	0.401	0.316	0.066	0.064	0.063
Tb	65	3.641	0.465	0.464	0.462	0.458	0.436	0.430	0.408	0.328	0.066	0.063	0.061
Dy66		3.583	0.462	0.457	0.453	0.446	0.440	0.422	0.400	0.319	0.062	0.062	0.061
Ho	67	3.607	0.458	0.458	0.457	0.451	0.440	0.433	0.410	0.311	0.064	0.063	0.063
Er	68	3.538	0.448	0.447	0.446	0.441	0.440	0.421	0.396	0.311	0.063	0.063	0.062
Tm	69	3.533	0.452	0.447	0.444	0.440	0.435	0.415	0.401	0.319	0.061	0.060	0.059
Yb	70	3.529	0.468	0.453	0.448	0.443	0.427	0.426	0.390	0.295	0.061	0.059	0.059
Lu	71	3.366	0.431	0.426	0.425	0.420	0.418	0.390	0.380	0.298	0.058	0.057	0.057

The bonds LnO(1-6) are strained chelate bonds to oxygen atoms of the organic anion forming the complex molecule. LnO(7) is a bond to an oxygen atom of the organic anion of a neighbouring complex. O(10) is part of a H_2O molecule complementing the coordination sphere of the Ln cation. The weak LnN (3, 5, 7) bonds to nitrogen atoms of the organic anion complete the coordination sphere of Ln to $[LnO_8N_3]$.