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Supplementary Information

Towards the origin of effective An(III)/Ln(III) separation by tridentate N-donor ligands: A theoretical study on atomic charges and polarizabilities for Cm(III)/Gd(III) separation.

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Figure 1. Contour map of ΔE_{pol} from the MD trajectory [kcal/mol] based on the unscaled Hirshfeld charges of BTP.

Table 1. Molecular structures and acronyms of all studied ligands.

Compound	Acronym
Terpy	2,2':6',2''-terpyridine
BDP	2,6-bis(1,2-diazin-3-yl)pyridine
EtBDP4	2,6-bis(4-ethyl-1,2-diazin-3-yl)pyridine
EtBDP5	2,6-bis(5-ethyl-1,2-diazin-3-yl)pyridine
EtBDP6	2,6-bis(6-ethyl-1,2-diazin-3-yl)pyridine
EtBDP56	2,6-bis(5,6-diethyl-1,2-diazin-3-yl)pyridine
BTP	2,6-bis(1,2,4-triazin-3-yl)pyridine
nPrBTP	2,6-bis(5,6-dipropyl-1,2,4-triazin-3-yl)pyridine
iPrBTP	2,6-bis(5,6-diisopropyl-1,2,4-triazin-3-yl)pyridine
mBTP5	2,6-bis(5-methyl-1,2,4-triazin-3-yl)pyridine

Table 1. Molecular structures and acronyms of all studied ligands.

Compound	Acronym
mBTP6	2,6-bis(6-methyl-1,2,4-triazin-3-yl)pyridine
mBTP56	2,6-bis(5,6-dimethyl-1,2,4-triazin-3-yl)pyridine
mBTPp4	2,6-bis(1,2,4-triazin-3-yl)4-methyl-pyridine
BQP	2,6-bis(1,2,4,5-tetrazin-3-yl)pyridine
nPrBQP	2,6-bis(3-propyl-1,2,4,5-tetrazin-3-yl)pyridine