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 $\Delta E_{pol}$ 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       | 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|
| Compound | Acronym | Structure |
|----------|---------|-----------|
| 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 |