Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


Supporting information

# Magnetic resonance imaging: An innovative approach to observe rare metal extraction using ionic liquid

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**Table S1: Nomenclature of the prepared samples.**

| Nomenclature | Sample Description |
|---|---|
| TTPB | Ionic liquid |
| DIW | Ionic liquid + water |
| Nd5 | Ionic liquid + 5 mg $NdCl_3$ |
| Nd10 | Ionic liquid + 10 mg $NdCl_3$ |
| Nd25 | Ionic liquid + 25 mg $NdCl_3$ |
| Nd50 | Ionic liquid + 50 mg $NdCl_3$ |
| Nd75 | Ionic liquid + 75 mg $NdCl_3$ |
| Nd100 | Ionic liquid + 100 mg $NdCl_3$ |
| Nd300 | Ionic liquid + 300 mg $NdCl_3$ |
| Nd500 | Ionic liquid + 500 mg $NdCl_3$ |

**Table S2: $^1$H NMR peak position for TTPB ionic liquid and Nd containing complexes.**

| Sample | Peak Position (ppm) | | | | | |
|---|---|---|---|---|---|---|
| | *$CH_3$* | *$CH_{(2\text{-}all)}$* | *$CH_{2(1)}$* | *$H_2O$* | *Meta, Para (m,p)* | *Ortho (o)* |
| TTPB | 0.97 | 1.38 | 2.57 | 4.69 | 7.19 | 8.07 |
| DIW | 0.94 | 1.39 | 2.25 | 4.69 | 7.27 | 8.12 |
| Nd5 | 1.16 | 1.61 | 2.45 | 4.89 | 7.49 | 8.35 |
| Nd10 | 1.26 | 1.70 | 2.55 | 4.98 | 7.59 | 8.46 |
| Nd25 | 1.74 | 2.18 | 3.01 | 5.40 | 8.09 | 8.99 |
| Nd50 | 2.50 | 2.94 | 3.74 | 6.05 | 8.88 | 9.86 |
| Nd75 | 3.32 | 3.76 | 4.52 | 6.76 | 9.73 | 10.76 |
| Nd100 | 4.06 | 4.47 | 5.18 | 7.36 | 10.48 | 11.57 |
| Nd300 | 4.34 | 4.75 | 5.60 | 7.36 | 10.86 | 12.06 |

**Table S3. $T_1$ relaxation time for the neodymium containing complexes.**

| Sample Code | $T_1$ relaxation time (s) | | | | | |
|---|---|---|---|---|---|---|
| | Cation | | | | Anion | |
| | t-$CH_3$ | $CH_{2(2\text{-}all)}$ | $CH_{2(1)}$ | $H_2O$ | Meta, Para | Ortho |
| TTPB | 0.47 | 0.40 | 0.38 | 0.32 | 0.5 | 0.48 |
| DIW | 0.56 | 0.39 | 0.31 | 0.31 | 0.62 | 0.64 |
| Nd5 | 0.54 | 0.38 | 0.27 | 0.23 | 0.57 | 0.47 |
| Nd10 | 0.53 | 0.38 | 0.28 | 0.24 | 0.56 | 0.49 |
| Nd25 | 0.53 | 0.38 | 0.27 | 0.19 | 0.54 | 0.39 |
| Nd50 | 0.49 | 0.36 | 0.26 | 0.13 | 0.46 | 0.28 |
| Nd75 | 0.44 | 0.34 | 0.25 | 0.10 | 0.39 | 0.23 |
| Nd100 | 0.40 | 0.32 | 0.24 | 0.08 | 0.34 | 0.20 |
| Nd300 | 0.41 | 0.33 | 0.23 | 0.06 | 0.28 | |

**Table S4. $T_2$ relaxation time for the neodymium containing complexes.**

| Sample Code | $T_2$ relaxation time (ms) | | | | | |
|---|---|---|---|---|---|---|
| | Cation | | | | Anion | |
| | t-$CH_3$ | $CH_{2(2\text{-all})}$ | $CH_{2(1)}$ | $H_2O$ | Meta, Para | Ortho |
| TTPB | 37.82 | 22.57 | 5.16 | - | 25.00 | 20.35 |
| DIW | 119.50 | 73.60 | 32.14 | 169.83 | 134.60 | 130.00 |
| Nd5 | 71.81 | 47.65 | 18.43 | 22.02 | 50.30 | 25.40 |
| Nd10 | 47.36 | 34.07 | 16.99 | 27.32 | 44.04 | 30.63 |
| Nd25 | 51.75 | 35.29 | 12.25 | 15.92 | 32.30 | 13.68 |
| Nd50 | 37.25 | 25.41 | 6.60 | 7.80 | 19.54 | 6.14 |
| Nd75 | 28.18 | 20.19 | 4.12 | 5.44 | 13.94 | 3.45 |
| Nd100 | 16.85 | 12.64 | 3.11 | 3.68 | 8.84 | 2.43 |
| Nd300 | 22.45 | 16.32 | 3.37 | 3.37 | 5.56 | 1.71 |

**Table S5: TR dependence of MRI signal intensity at different Nd concentrations with fixed TE of 5.7ms**

| | Repetition Time (TR) | | | | | |
|---|---|---|---|---|---|---|
| | 300 ms | 500 ms | 1000 ms | 1500 ms | 5000 ms | 50000 ms |
| Nd 10mg |  |  |  |  |  |  |
| Nd 25mg |  |  |  |  |  |  |
| Nd 75mg |  |  |  |  |  |  |

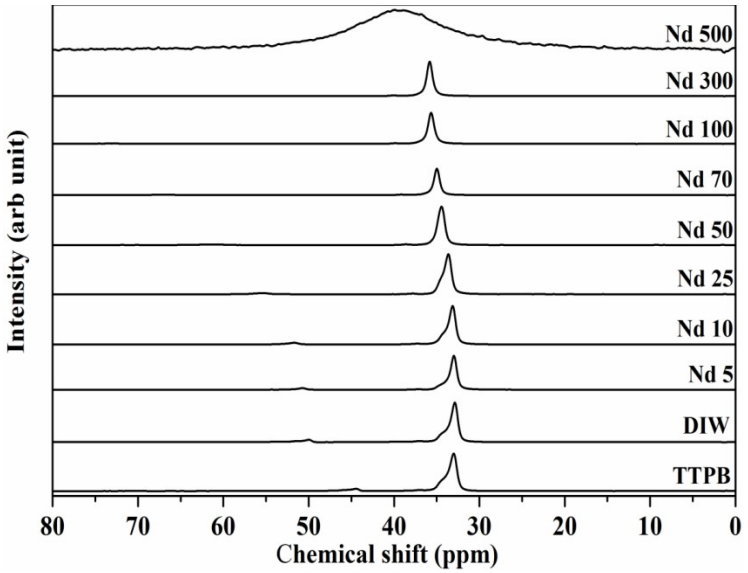


**Figure S1. $^{31}$P NMR spectra of neodymium containing complexes.**

$^{31}$P NMR spectra for the neodymium containing ionic liquid complexes are shown in Fig. S1. A small amount of phosphonium impurities were observed in the samples along with the TTP cation as reported earlier[35]. The peaks are shifted down field similar to the $^{1}$H NMR signals due to the very strong dipolar interaction exerted by neodymium ion on the cation.

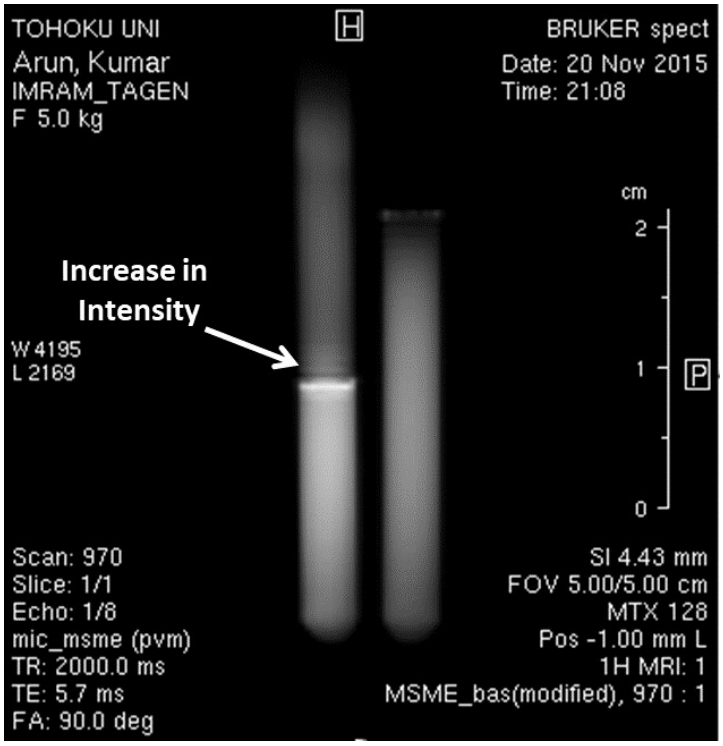


**Fig. S2. $^{1}$H MRI acquired after ~10h of 10mg Nd extraction using TTPB IL**

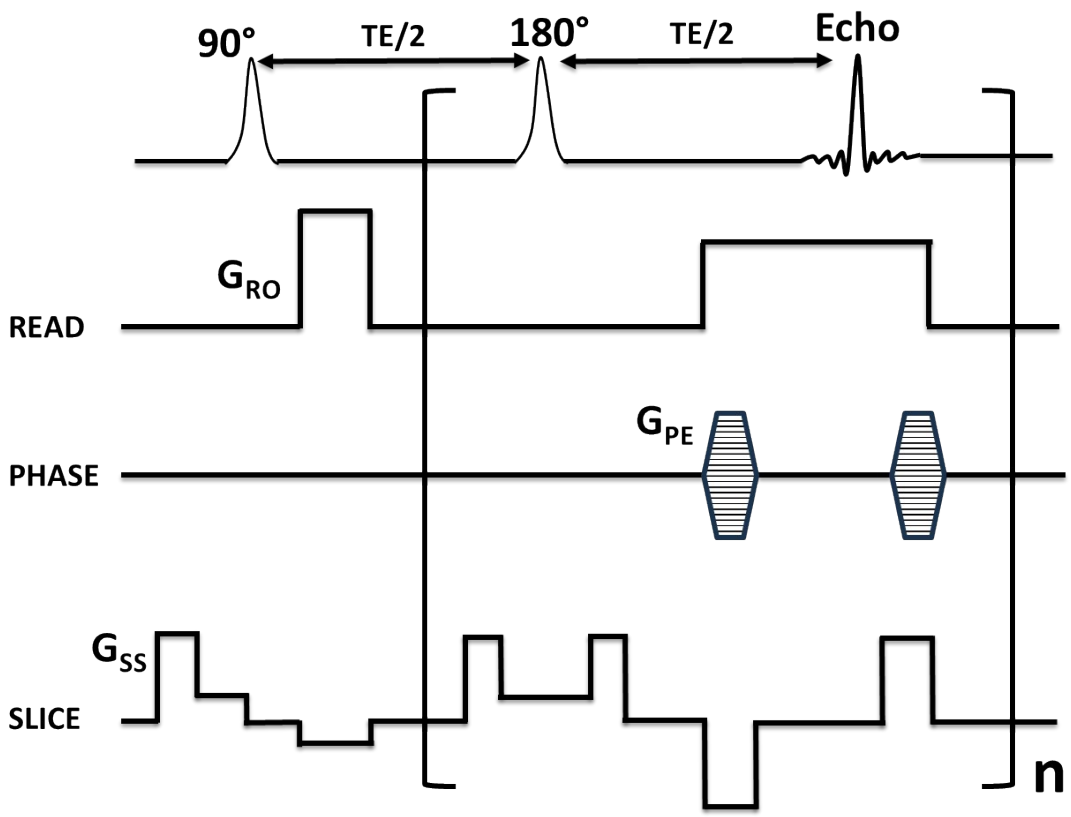


**Fig. S3. Pulse scheme for the MSME imaging pulse sequence used in this study. $G_{RO}$, $G_{PE}$ and $G_{SS}$ are the magnitudes of the read-out, phase-encoding and slice-selective gradients respectively. TE is the echo time and n is the number of echoes.**

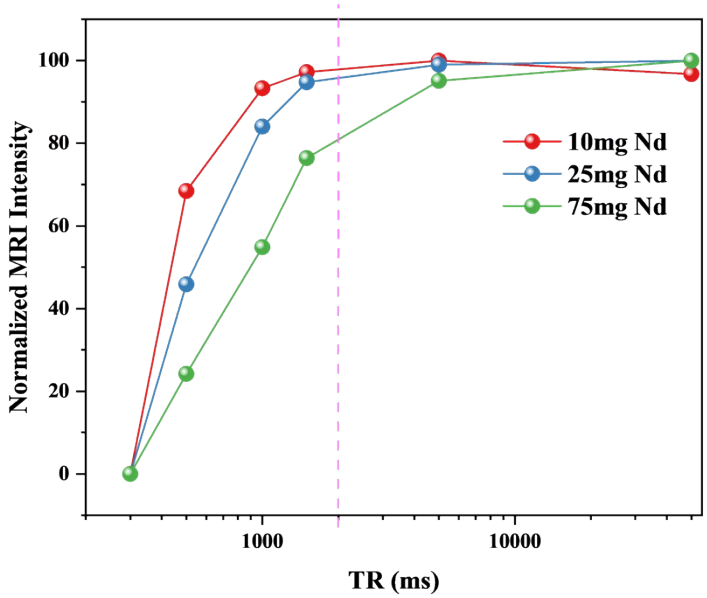


**Fig. S4. TR dependence of MRI signal intensity**