

## **Supporting Information**

### **Physicochemical properties of air and water stable rhenium ionic liquids**

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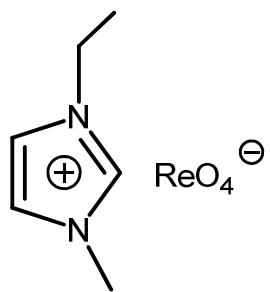
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b: Shu-Liang Zang, [slzang@lnu.edu.cn](mailto:slzang@lnu.edu.cn)

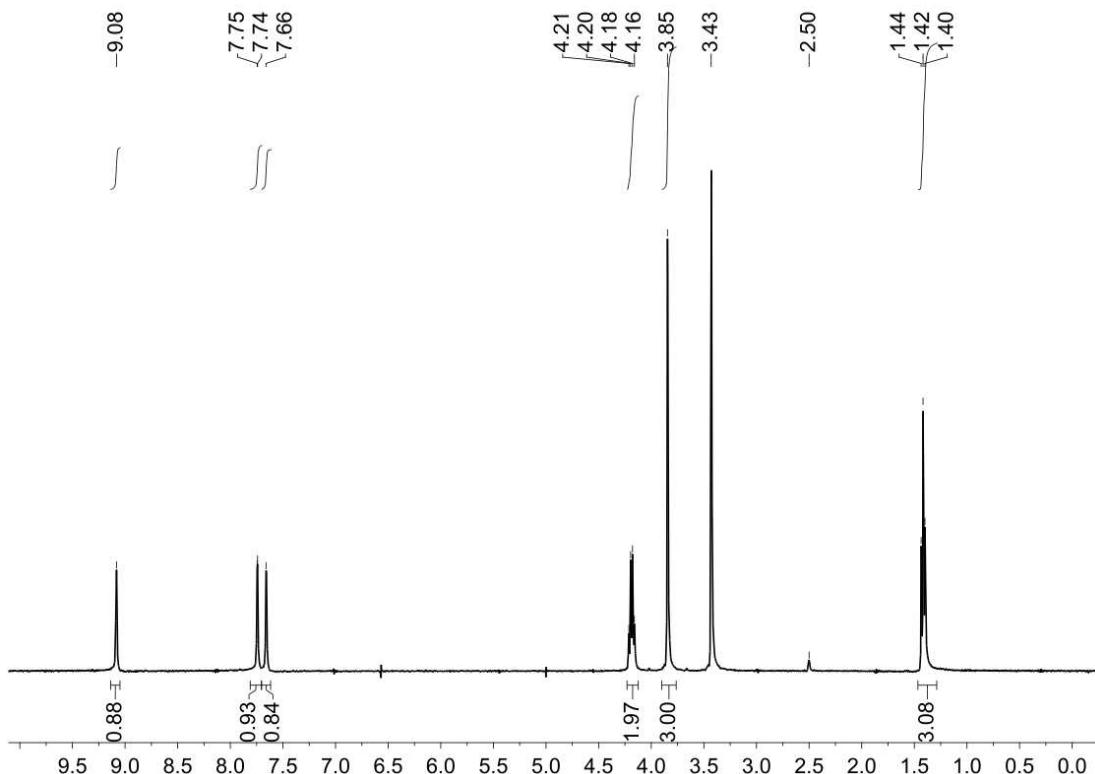
#### **General Remarks:**

<sup>1</sup>H, <sup>13</sup>C NMR and <sup>17</sup>O NMR are measured in DMSO with a mercury-VX 300 spectrometer and a 400-MHz Bruker Avance DPX-400 spectrometer. IR spectra are recorded on a JASCO FT/IR-4100 spectrometer. ESI-MS spectra are measured on a Finnigan LCQ Classic mass spectrometer. Raman spectrum are measured on a Microscopic Confocal Raman Spectrometer (RM2000) produced by Renishaw.

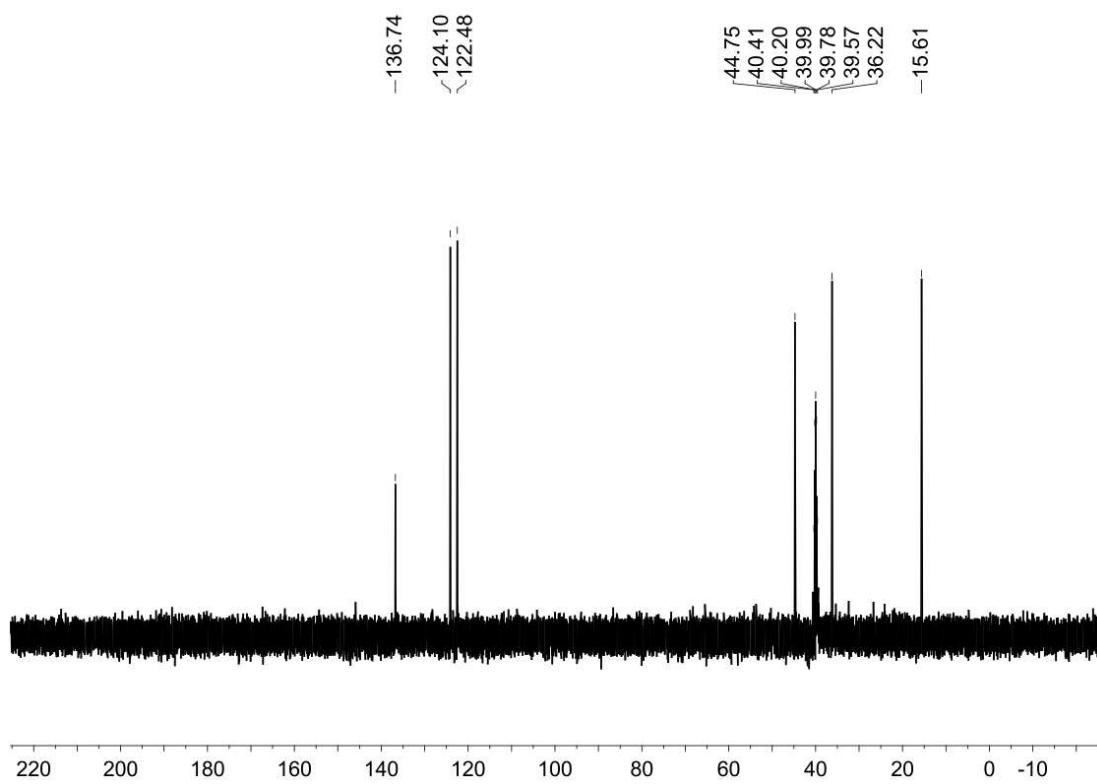
[C<sub>2</sub>mim][ReO<sub>4</sub>]:



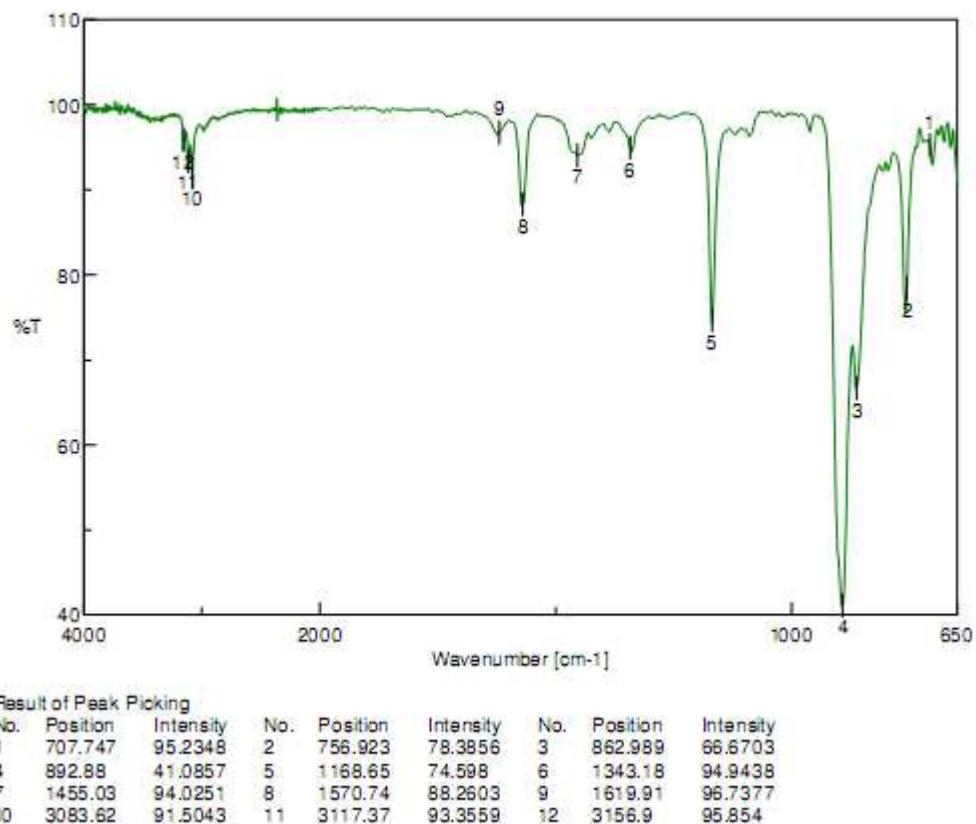
C<sub>6</sub>H<sub>11</sub>N<sub>2</sub>O<sub>4</sub>Re (361.37), elemental analysis calcd.: C, 19.94, H, 3.07, N, 7.75; found: C, 19.85, H, 2.98, N, 7.71; IR (cm<sup>-1</sup>):  $\nu$  = 893 (Re=O), 863 (Re=O); <sup>1</sup>H-NMR (DMSO, 400Hz, r.t., ppm):  $\delta$  = 9.08 (1H, s, mz-H<sup>2</sup>), 7.75 (1H, d, mz-H<sup>4</sup>), 7.66 (1H, d, mz-H<sup>5</sup>), 4.21 - 4.16 (2H, q, -CH<sub>2</sub>-), 3.85 (3H, s, N-CH<sub>3</sub>), 1.42 (3H, t, -CH<sub>3</sub>); <sup>13</sup>C-NMR (DMSO, 100Hz, r.t., ppm):  $\delta$  = 136.84 (mz-C<sup>2</sup>), 124.52 (mz-C<sup>4</sup>), 122.52 (mz-C<sup>5</sup>), 44.76 (-CH<sub>2</sub>-), 36.34 (N-CH<sub>3</sub>), 15.61 (-CH<sub>3</sub>). ESI-MS (methanol, m/z, %): cation, 111.0 (C<sub>6</sub>H<sub>11</sub>N<sub>2</sub><sup>+</sup>, 100%).



**Figure S1-1** <sup>1</sup>H NMR spectra of [C<sub>2</sub>mim][ReO<sub>4</sub>]



**Figure S1-2**  $^{13}\text{C}$  NMR spectra of  $[\text{C}_2\text{mim}][\text{ReO}_4]$



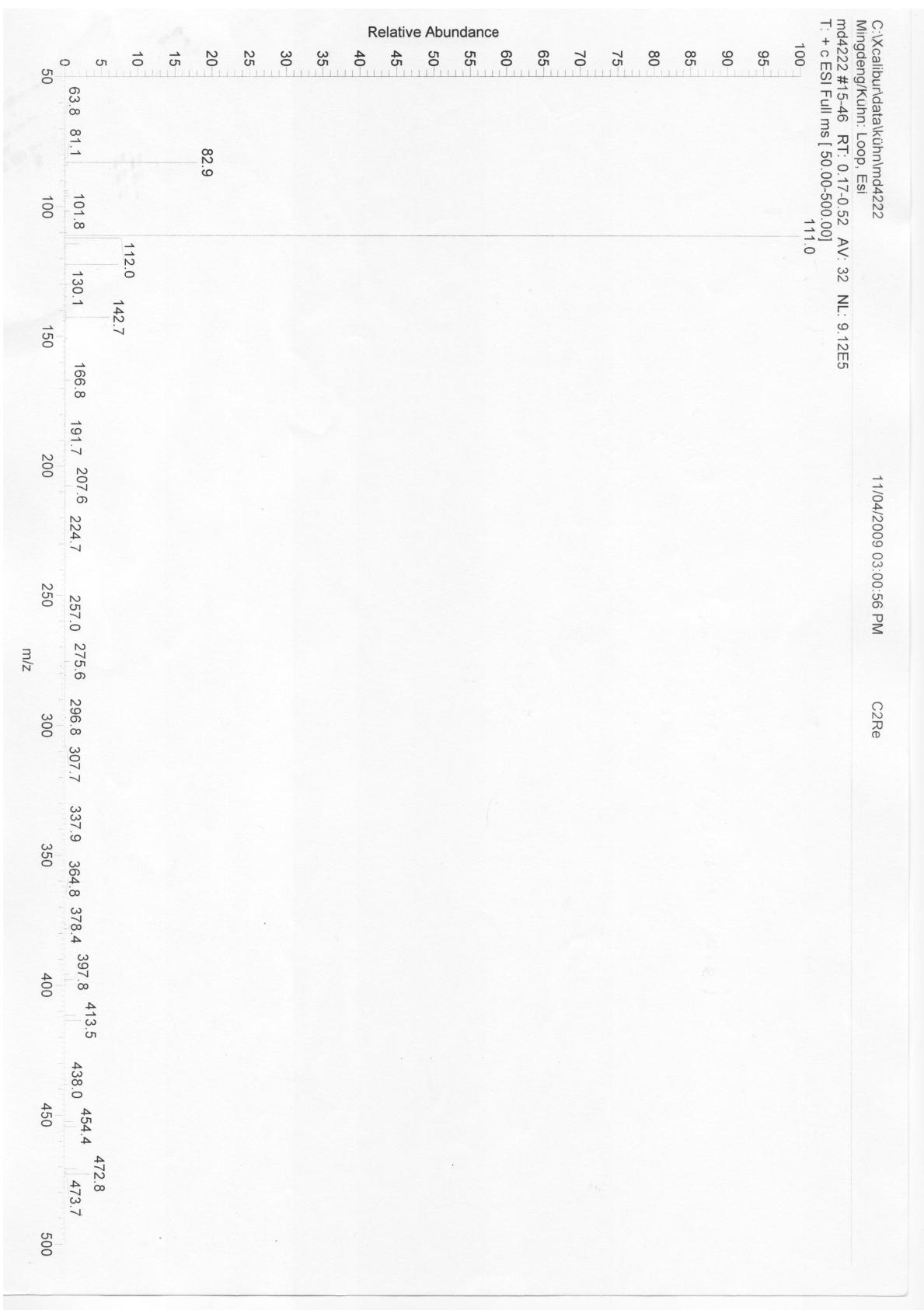
**Figure S1-3** IR spectra of  $[\text{C}_2\text{mim}][\text{ReO}_4]$

C:\Xcaliburn\data\kühn\md4222

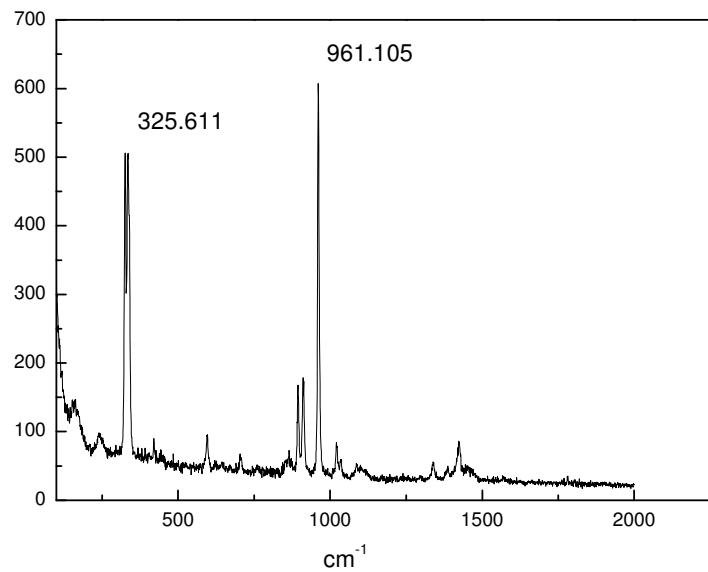
11/04/2009 03:00:56 PM

C2Re

Mingdeng\Kuhn: Loop, Esi  
md4222 #15-46 RT: 0.17-0.52 AV: 32 NL: 9.12E5  
T. + c ESI Full ms [ 50.00-500.00]  
111.0

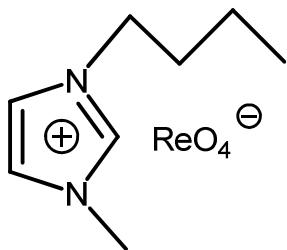


**Figure S1-4** ESI-MS spectra of  $[C_2mim][ReO_4]$



**Figure S1-6** Raman spectrum of  $[\text{C}_2\text{mim}][\text{ReO}_4]$

[C<sub>4</sub>mim][ReO<sub>4</sub>]:



C<sub>8</sub>H<sub>15</sub>N<sub>2</sub>O<sub>4</sub>Re (389.42), elemental analysis calcd.: C, 24.67, H, 3.88, N, 7.19; found: C, 25.21, H, 4.12, N, 7.17; IR (cm<sup>-1</sup>):  $\nu$  = 898 (Re=O), 863 (Re=O); <sup>1</sup>H-NMR (DMSO, 400Hz, r.t., ppm):  $\delta$  = 9.04 (1H, s, mz-H<sup>2</sup>), 7.71 (1H, d, mz-H<sup>4</sup>), 7.65 (1H, d, mz-H<sup>5</sup>), 4.17 - 4.14 (2H, t, -CH<sub>2</sub>-), 3.85 (3H, s, N-CH<sub>3</sub>), 1.80-1.73 (2H, m, -CH<sub>2</sub>-), 1.29-1.23 (2H, m, -CH<sub>2</sub>-), 0.89 (3H, t, -CH<sub>3</sub>); <sup>13</sup>C-NMR (DMSO, 100Hz, r.t., ppm):  $\delta$  = 137.00 (mz-C<sup>2</sup>), 124.11 (mz-C<sup>4</sup>), 122.76 (mz-C<sup>5</sup>), 49.17 (-CH<sub>2</sub>-), 36.22 (N-CH<sub>3</sub>), 31.93, 19.36 (-CH<sub>2</sub>-), 13.77 (-CH<sub>3</sub>). ESI-MS (methanol, m/z, %): cation, 139.1 (C<sub>8</sub>H<sub>15</sub>N<sub>2</sub><sup>+</sup>, 100%).

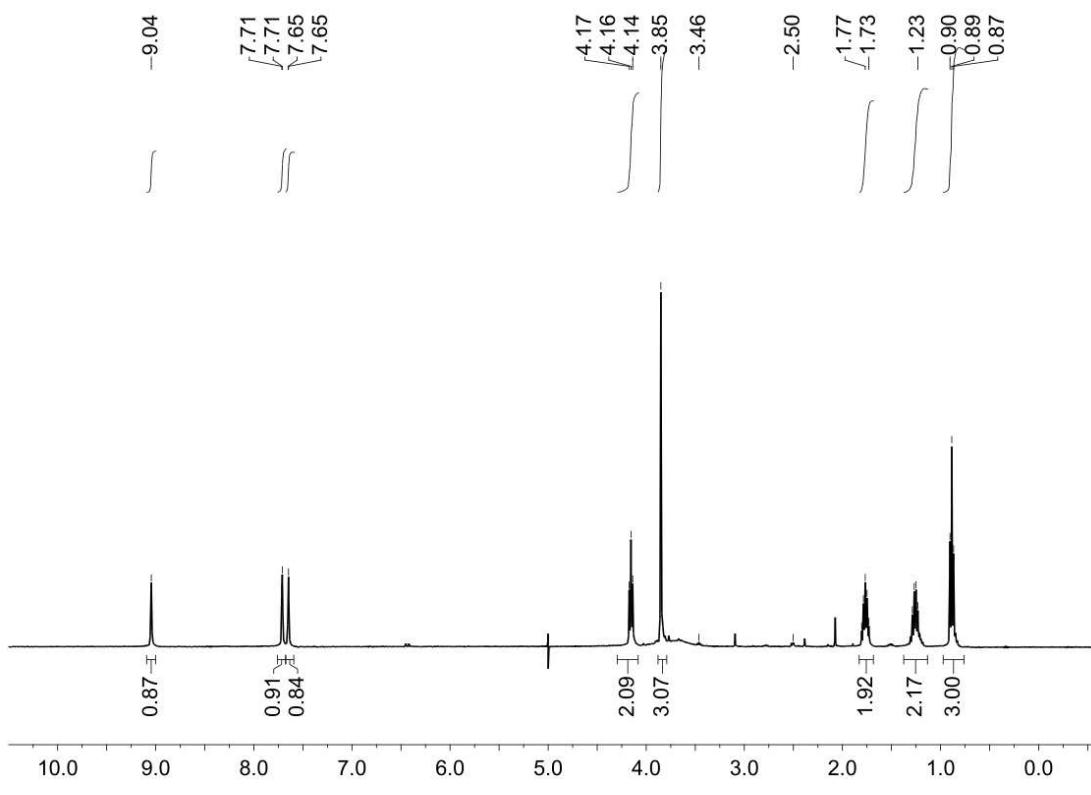
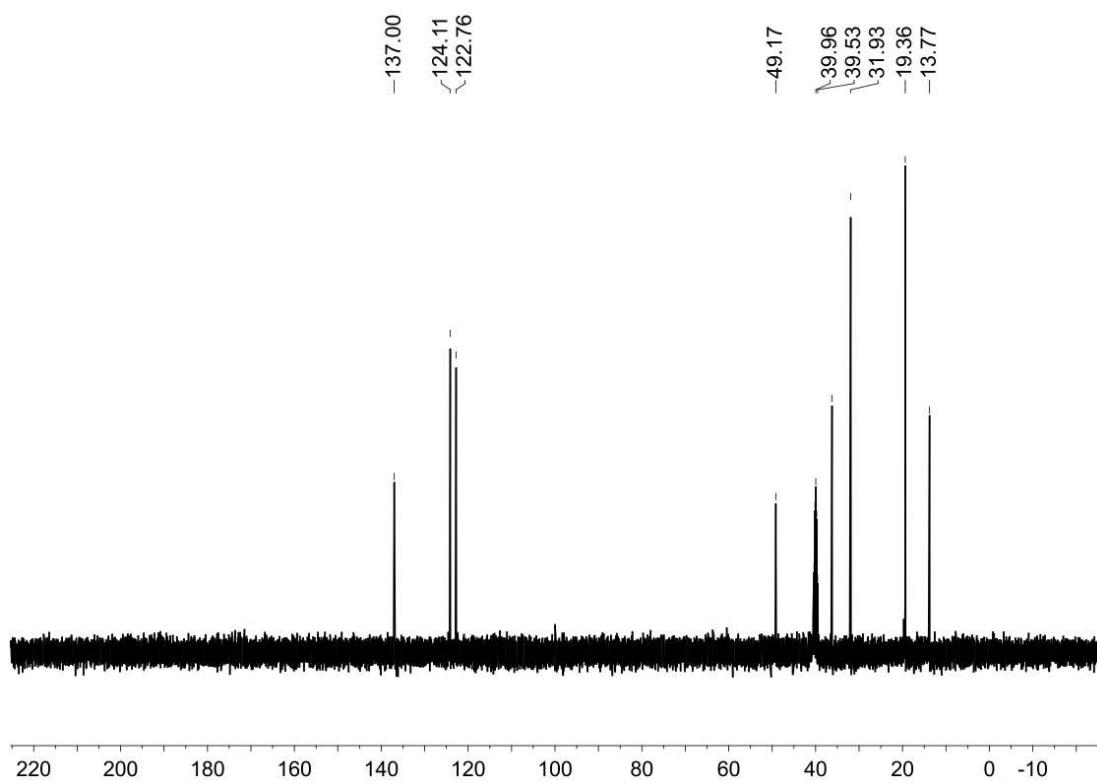
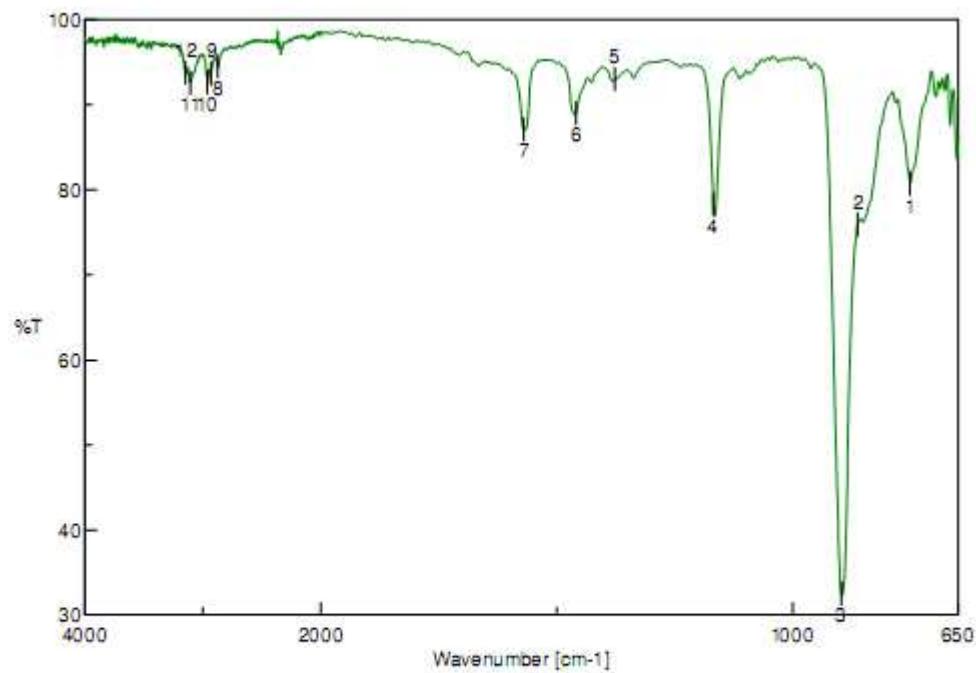


Figure S2-1 <sup>1</sup>H NMR spectra of [C<sub>4</sub>mim][ReO<sub>4</sub>]

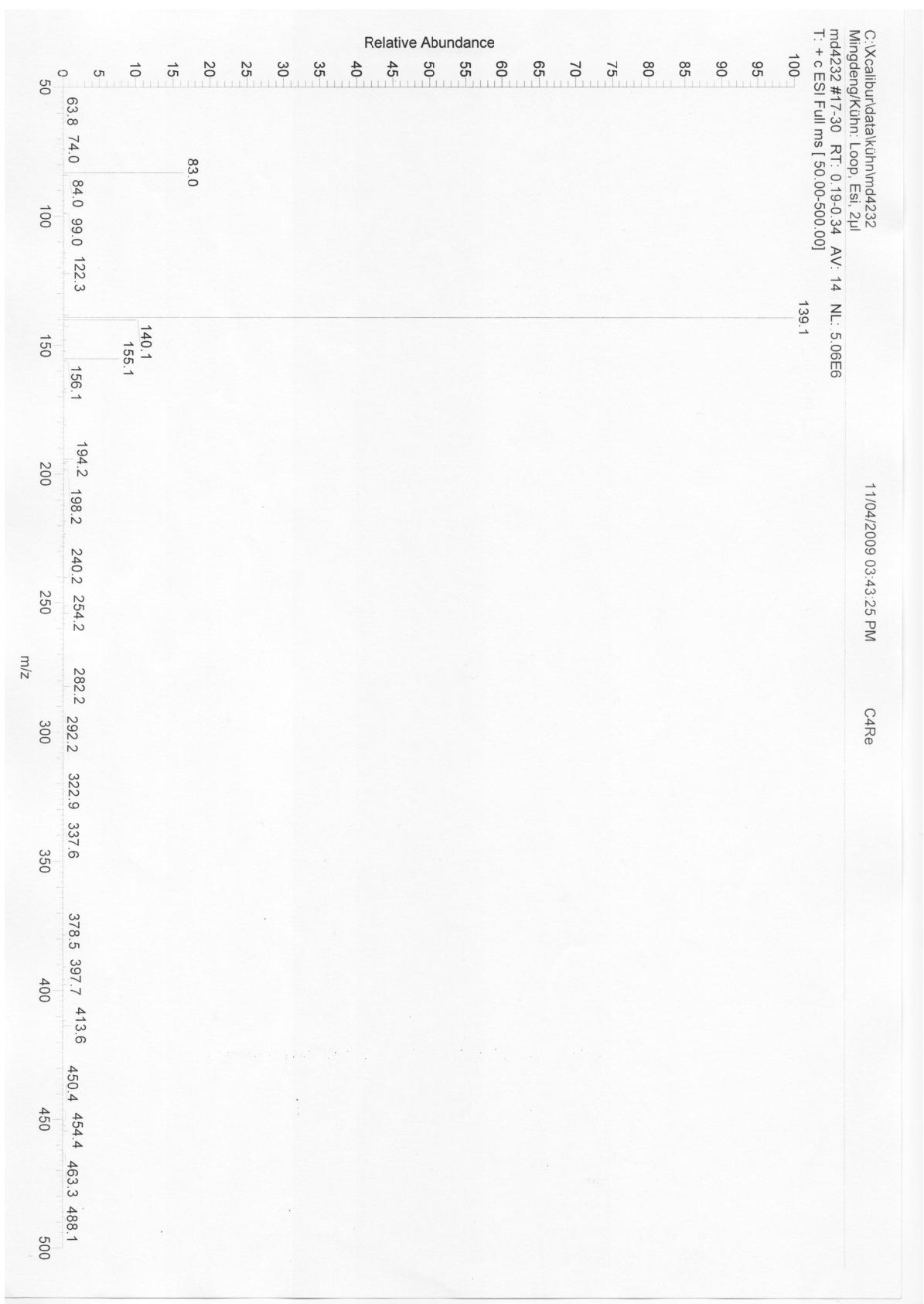


**Figure S2-2**  $^{13}\text{C}$  NMR spectra of  $[\text{C}_4\text{mim}][\text{ReO}_4]$

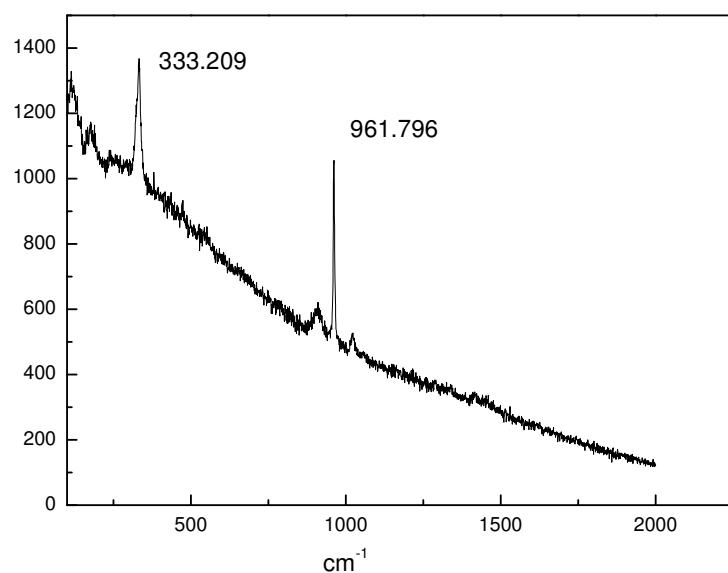


Result of Peak Picking								
No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	752.102	80.7176	2	862.989	75.9011	3	897.701	32.4728
4	1168.65	78.251	5	1376.93	92.9947	6	1459.85	89.0124
7	1570.74	87.0752	8	2875.34	94.5336	9	2933.2	93.6445
10	2962.13	92.6191	11	3107.72	92.5301	12	3146.29	93.7434

**Figure S2-3** IR spectra of  $[\text{C}_4\text{mim}][\text{ReO}_4]$

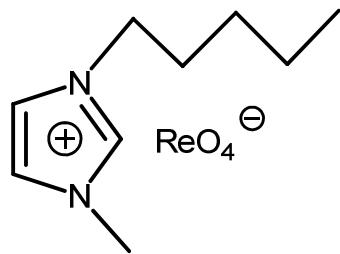


**Figure S2-4** ESI-MS spectra of [C<sub>4</sub>mim][ReO<sub>4</sub>]

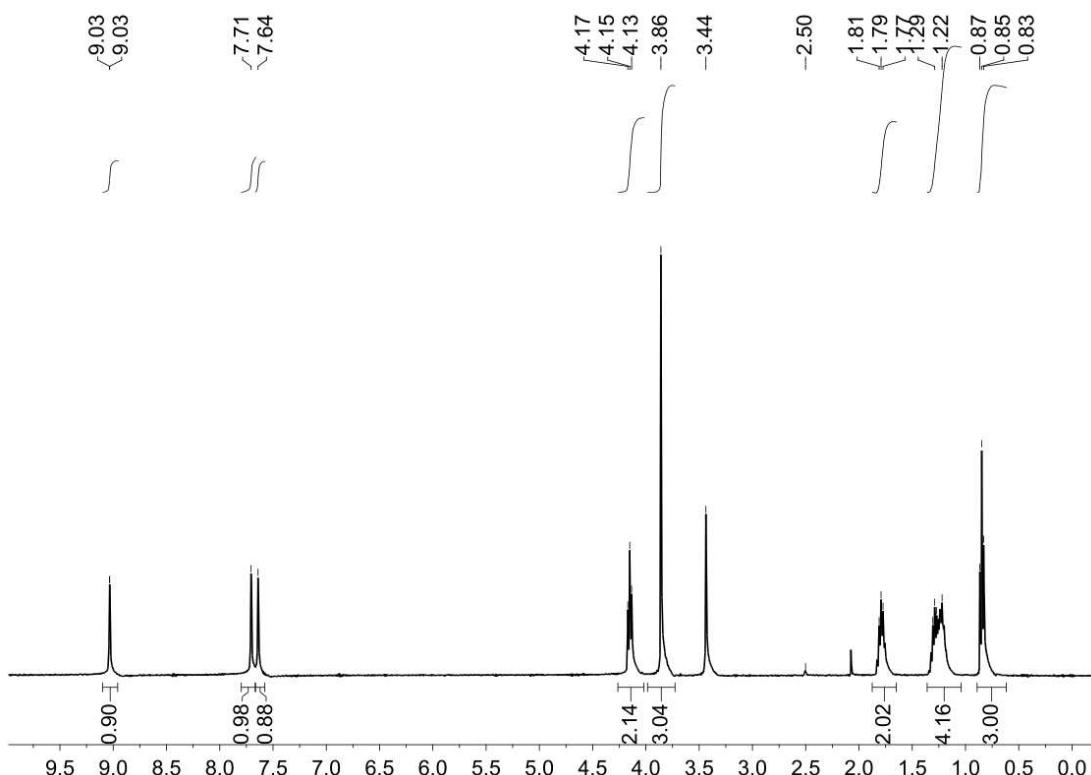


**Figure S2-6** Raman spectrum of  $[\text{C}_4\text{mim}][\text{ReO}_4]$

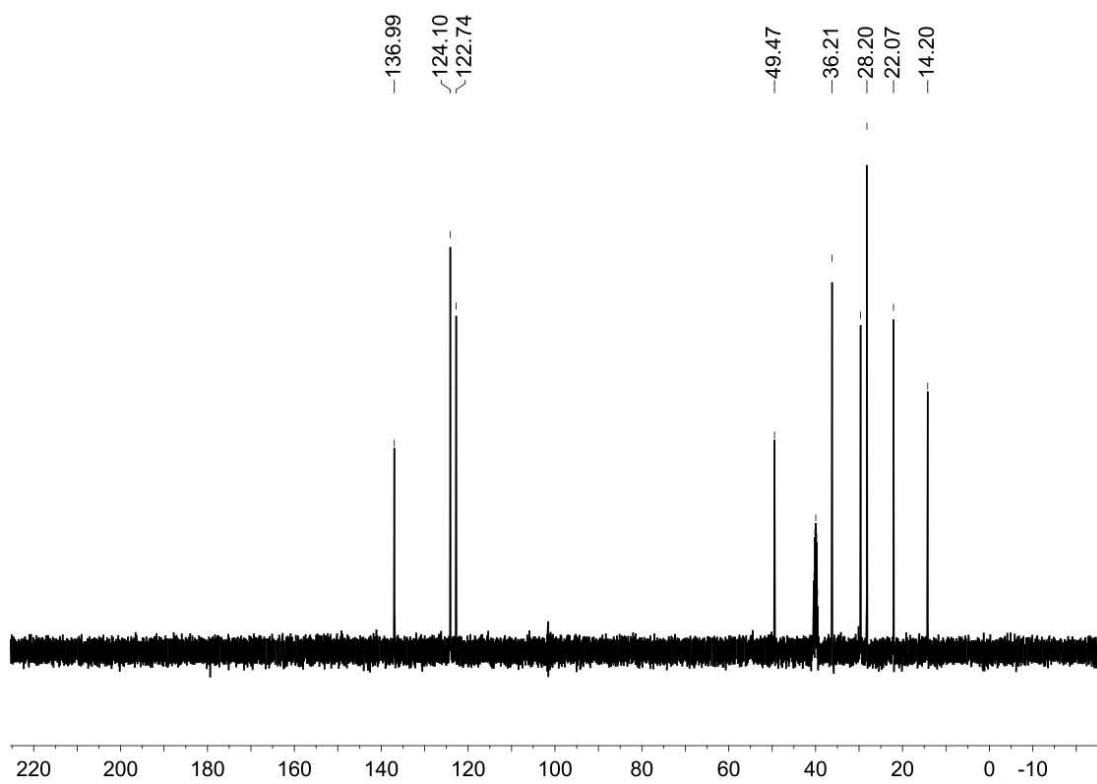
[C<sub>5</sub>mim][ReO<sub>4</sub>]:



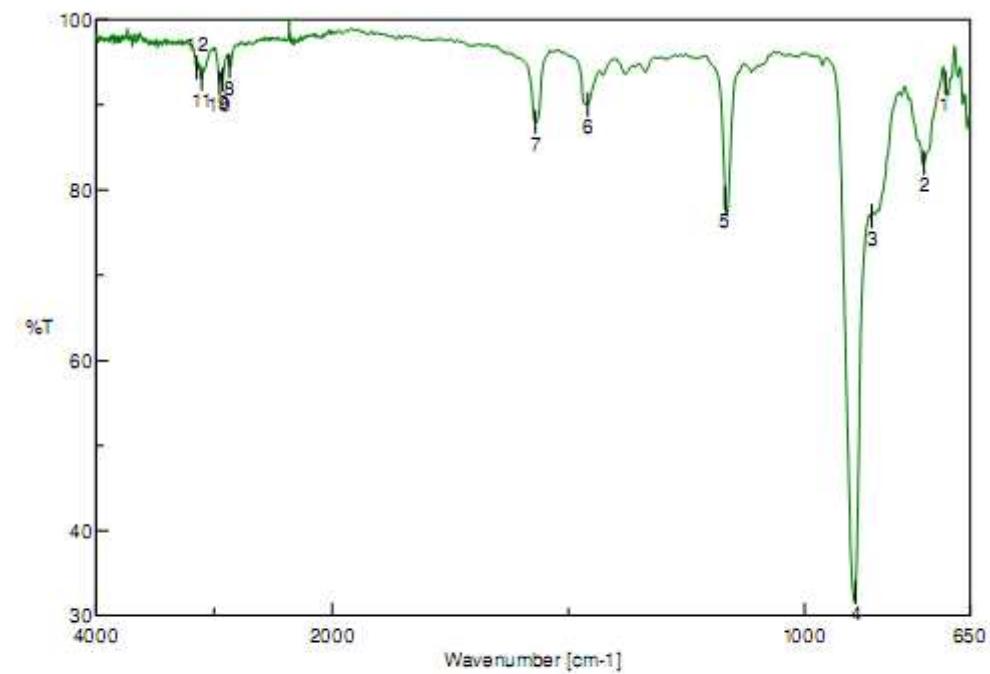
C<sub>9</sub>H<sub>17</sub>N<sub>2</sub>O<sub>4</sub>Re (403.45), elemental analysis calcd.: C, 26.79, H, 4.25, N, 6.94; found: C, 26.48, H, 4.24, N, 6.90; IR (cm<sup>-1</sup>):  $\nu$  = 893 (Re=O), 858 (Re=O); <sup>1</sup>H-NMR (DMSO, 400Hz, r.t., ppm):  $\delta$  = 9.03 (1H, s, mz-H<sup>2</sup>), 7.71 (1H, d, mz-H<sup>4</sup>), 7.64 (1H, d, mz-H<sup>5</sup>), 4.17 - 4.13 (2H, t, -CH<sub>2</sub>-), 3.86 (3H, s, N-CH<sub>3</sub>), 1.81-1.77 (2H, m, -CH<sub>2</sub>-), 1.33-1.18, (4H, m, 2x-CH<sub>2</sub>-), 0.85 (3H, t, -CH<sub>3</sub>); <sup>13</sup>C-NMR (DMSO, 100Hz, r.t., ppm):  $\delta$  = 136.99 (mz-C<sup>2</sup>), 124.10 (mz-C<sup>4</sup>), 122.74 (mz-C<sup>5</sup>), 49.47 (-CH<sub>2</sub>-), 36.21 (N-CH<sub>3</sub>), 29.64, 28.20, 22.07 (-CH<sub>2</sub>-), 14.20 (-CH<sub>3</sub>). ESI-MS (methanol, m/z, %): cation, 153.1 (C<sub>9</sub>H<sub>17</sub>N<sub>2</sub><sup>+</sup>, 100%).



**Figure S3-1** <sup>1</sup>H NMR spectra of [C<sub>5</sub>mim][ReO<sub>4</sub>]

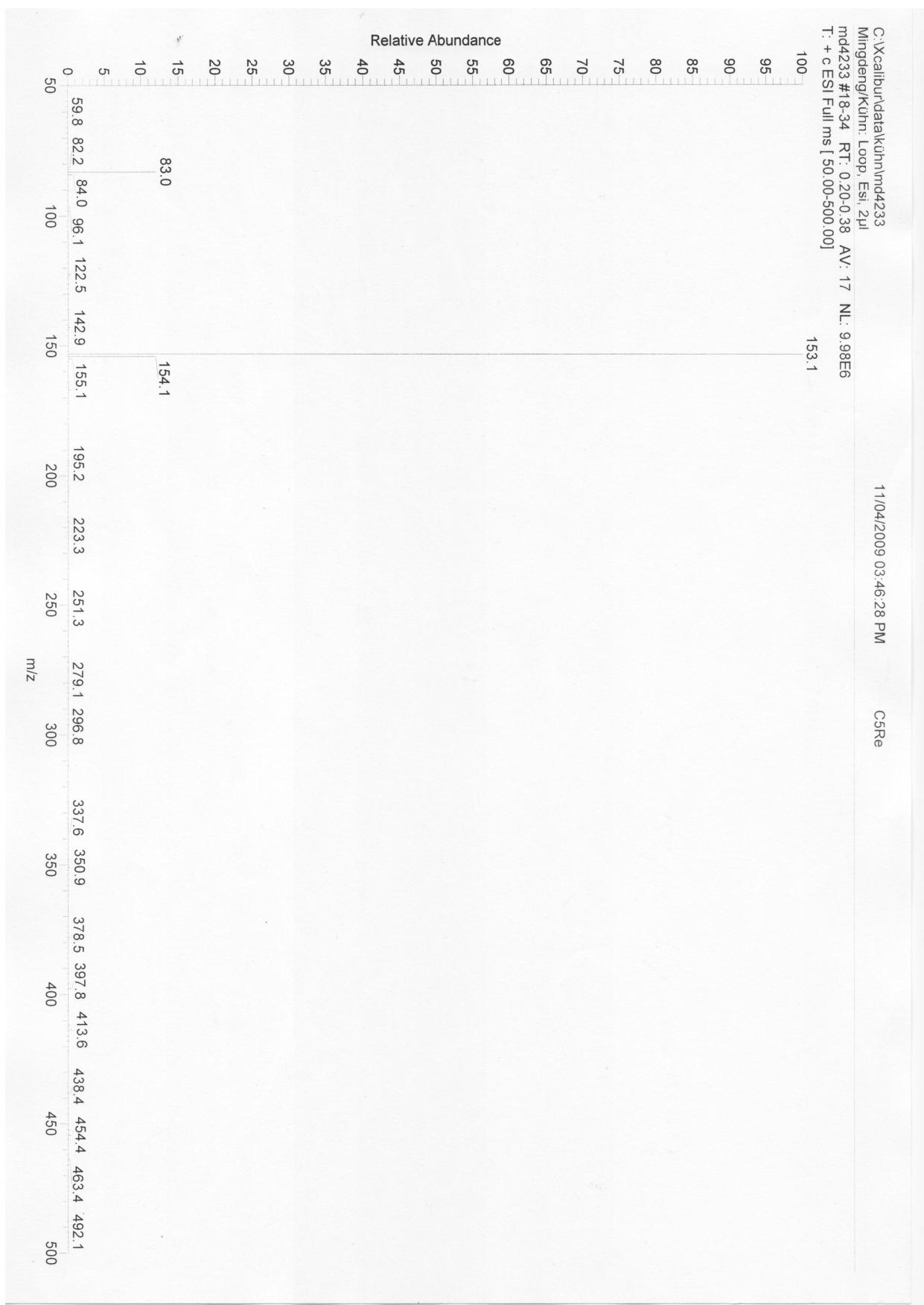


**Figure S3-2**  $^{13}\text{C}$  NMR spectra of  $[\text{C}_5\text{mim}][\text{ReO}_4]$

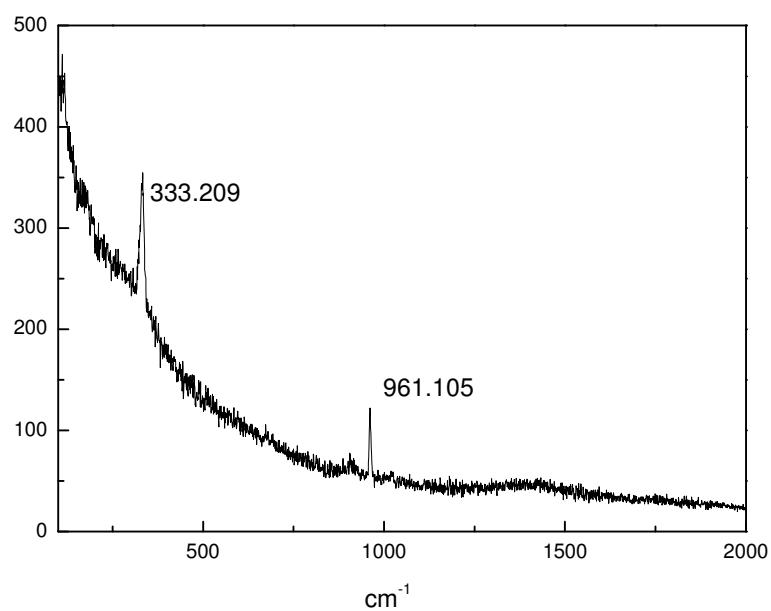


**Figure S3-3** IR spectra of  $[\text{C}_5\text{mim}][\text{ReO}_4]$

Result of Peak Picking								
No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	702.926	92.552	2	747.281	83.1754	3	858.168	76.9289
4	892.88	32.7182	5	1168.65	79.0223	6	1459.85	90.0306
7	1570.74	87.988	8	2870.52	94.5176	9	2928.38	92.9554
10	2957.3	92.5573	11	3107.72	93.0351	12	3146.29	94.3366

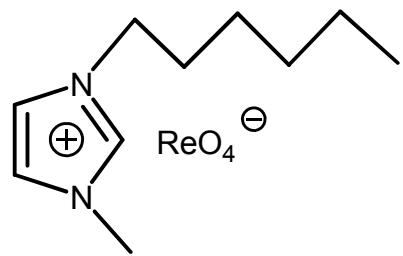


**Figure S3-4** ESI-MS spectra of  $[C_5mim][ReO_4]$

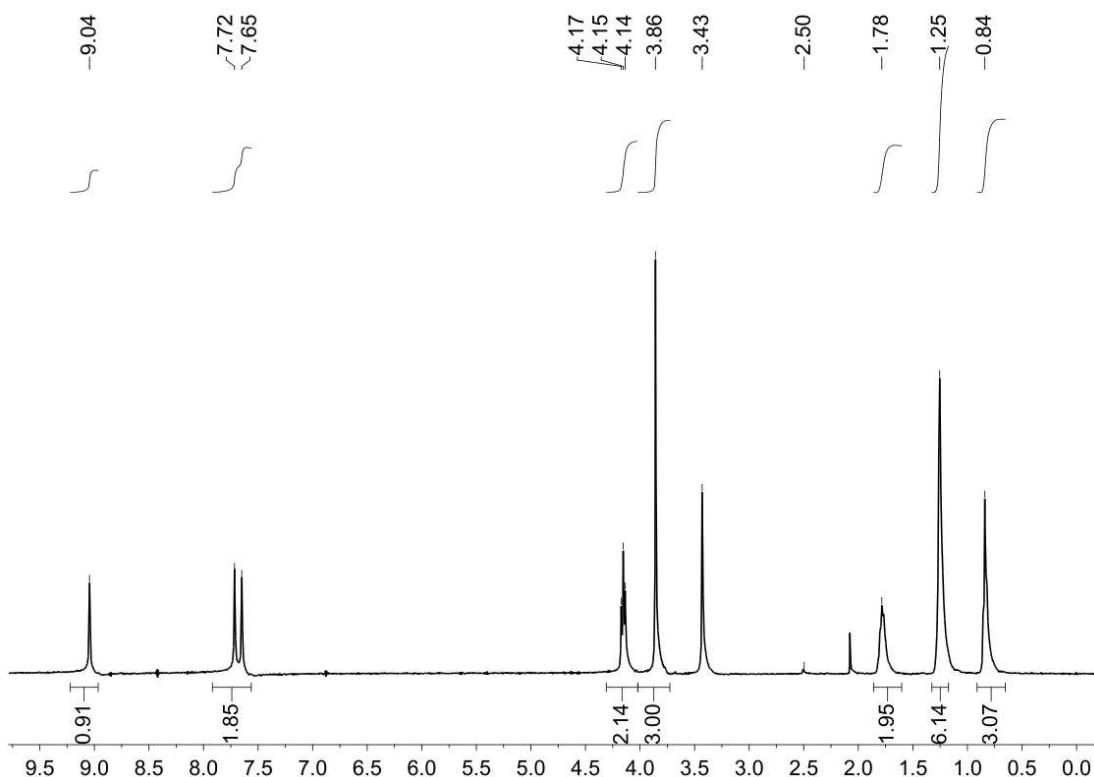


**Figure S3-6** Raman spectrum of  $[\text{C}_5\text{mim}][\text{ReO}_4]$

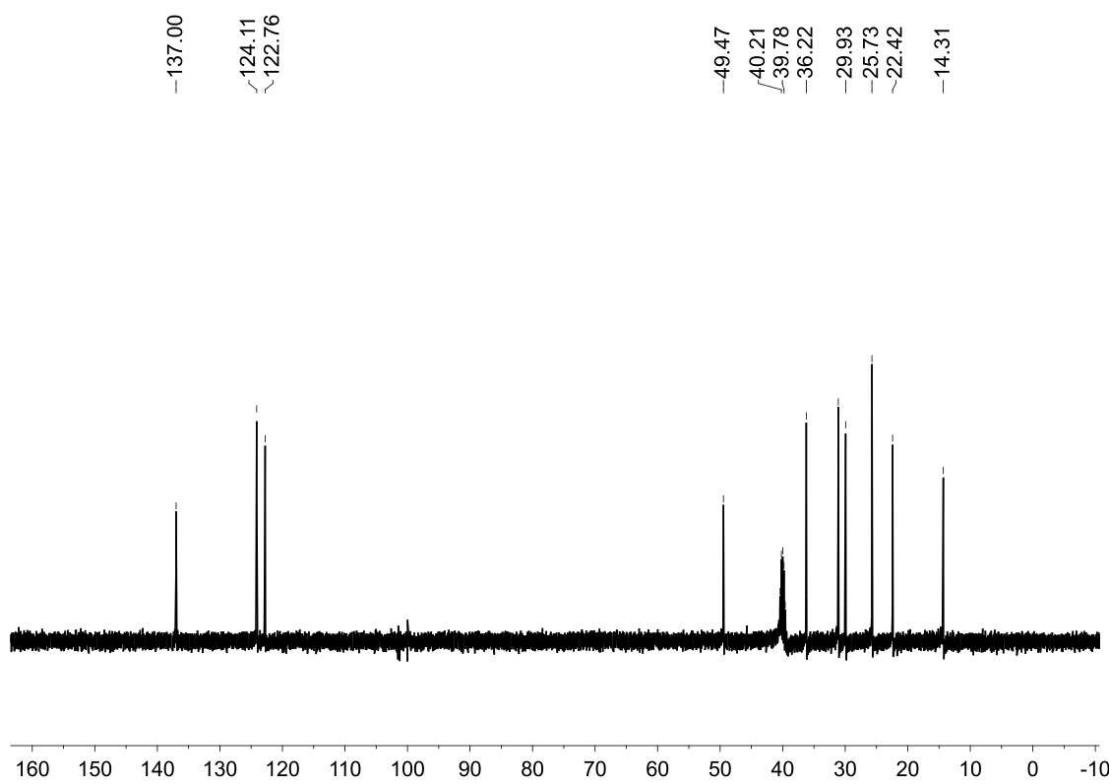
[C<sub>6</sub>mim][ReO<sub>4</sub>]:



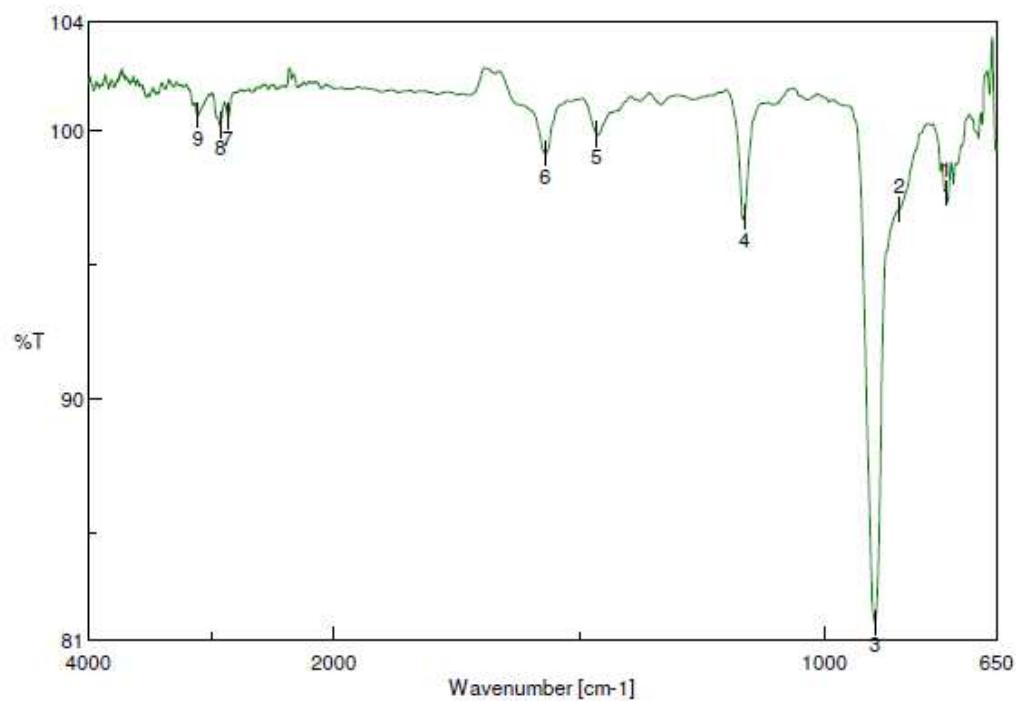
C<sub>10</sub>H<sub>19</sub>N<sub>2</sub>O<sub>4</sub>Re (417.48), elemental analysis calcd.: C, 28.77, H, 4.59, N, 6.71; found: C, 28.74, H, 4.69, N, 6.64; IR (cm<sup>-1</sup>):  $\nu$  = 893 (Re=O), 839 (Re=O); <sup>1</sup>H-NMR (DMSO, 400Hz, r.t., ppm):  $\delta$  = 9.53 (1H, s, mz-H<sup>2</sup>), 7.96 (1H, d, mz-H<sup>4</sup>), 7.87 (1H, d, mz-H<sup>5</sup>), 4.23 - 4.19 (2H, t, -CH<sub>2</sub>-), 3.89 (3H, s, N-CH<sub>3</sub>), 1.77-1.73 (2H, m, -CH<sub>2</sub>-), 1.19 (6H, m, 3x-CH<sub>2</sub>-), 0.77 (3H, t, -CH<sub>3</sub>); <sup>13</sup>C-NMR (DMSO, 100Hz, r.t., ppm):  $\delta$  = 137.00 (mz-C<sup>2</sup>), 124.11 (mz-C<sup>4</sup>), 122.76 (mz-C<sup>5</sup>), 49.47 (-CH<sub>2</sub>-), 36.22 (N-CH<sub>3</sub>), 31.11, 29.93, 25.73, 22.42 (-CH<sub>2</sub>-), 14.31 (-CH<sub>3</sub>). ESI-MS (methanol, m/z, %): cation, 167.1 (C<sub>10</sub>H<sub>19</sub>N<sub>2</sub><sup>+</sup>, 100%).



**Figure S4-1** <sup>1</sup>H NMR spectra of [C<sub>6</sub>mim][ReO<sub>4</sub>]



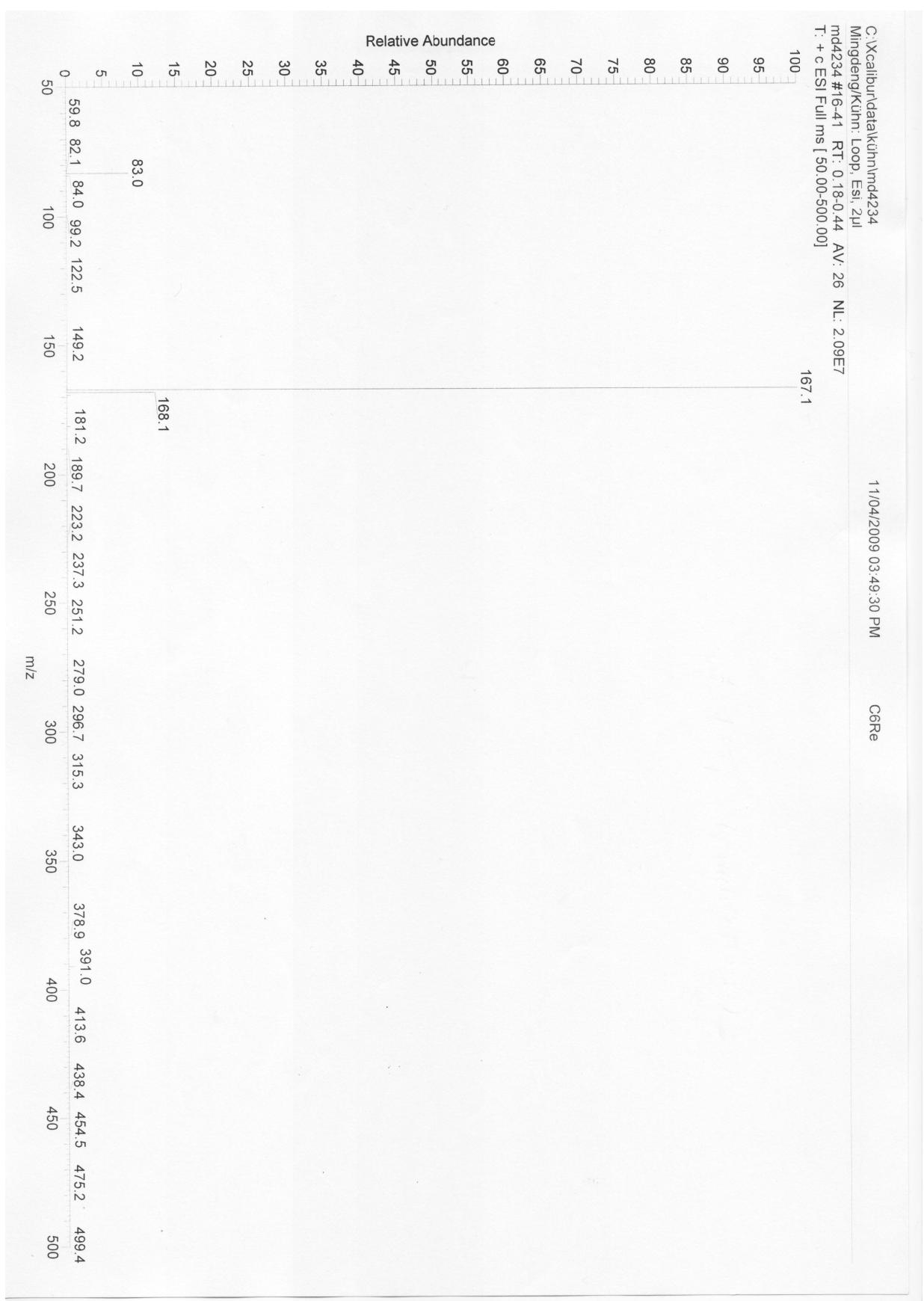
**Figure S4-2**  $^{13}\text{C}$  NMR spectra of  $[\text{C}_6\text{mim}][\text{ReO}_4]$



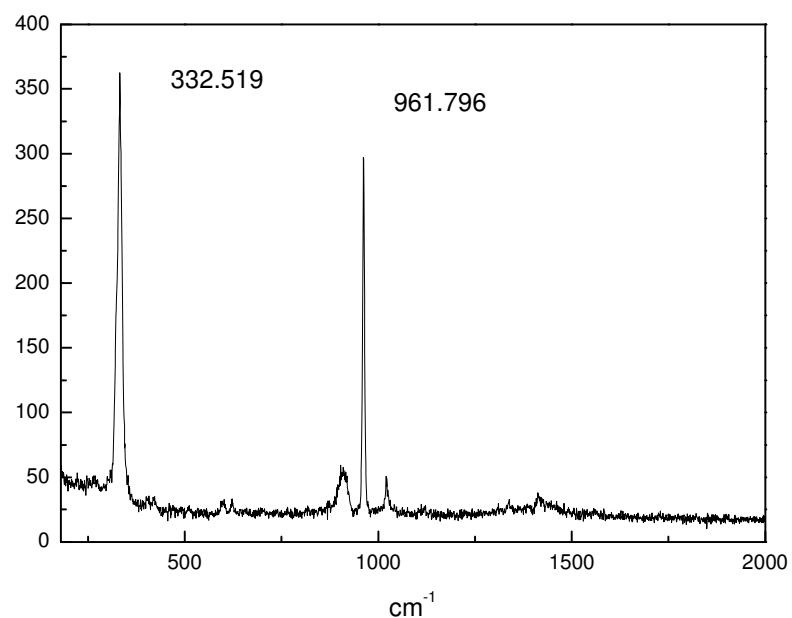
Result of Peak Picking

No.	Position	Intensity	No.	Position	Intensity	No.	Position	Intensity
1	752.102	97.6592	2	848.525	97.05	3	897.701	81.6841
4	1163.83	96.7432	5	1464.67	99.8519	6	1570.74	99.125
7	2860.88	100.518	8	2928.38	100.188	9	3107.72	100.533

**Figure S4-3** IR spectra of  $[\text{C}_6\text{mim}][\text{ReO}_4]$



**Figure S4-4** ESI-MS spectra of  $[C_6mim][ReO_4]$



**Figure S4-6** Raman spectrum of  $[\text{C}_6\text{mim}][\text{ReO}_4]$