**Title:** Research data supporting publication "Probing the influence of Zn and water on solvation and dynamics in ethaline and reline deep eutectic solvents by 1H nuclear magnetic resonance"

The data record contains the following files:

**Figure 1**

|  |  |
| --- | --- |
| **Directory No.** | **Experiment description** |
| 6 | 1H NMR spectrum for dry neat ethaline |
| 10 | 1H NMR spectrum for dry neat reline |

**Figure 2**

|  |  |  |
| --- | --- | --- |
| **Directory name** | **Directory No.** | **Experiment description** |
| **Ethaline** | 6 | 1H NMR spectrum for dry ethaline + 0.0 M ZnCl2 |
| 21 | 1H NMR spectrum for dry ethaline + 0.1 M ZnCl2 |
| 36 | 1H NMR spectrum for dry ethaline + 0.2 M ZnCl2 |
| 51 | 1H NMR spectrum for dry ethaline + 0.3 M ZnCl2 |
| **Reline** | 10 | 1H NMR spectrum for dry reline + 0.0 M ZnCl2 |
| 28 | 1H NMR spectrum for dry reline + 0.3 M ZnCl2 |

**Figure 3**

|  |  |  |
| --- | --- | --- |
|  | **Directory No.** | **Experiment description** |
| **Ethaline\_A** | 6\_1 | 1H NMR spectrum for pure ethaline + 0.0 wt.% water |
| 5 | 1H NMR spectrum for pure ethaline + 2.7 wt.% water |
| 13 | 1H NMR spectrum for pure ethaline + 5.5 wt.% water |
| 6 | 1H NMR spectrum for pure ethaline + 8.3 wt.% water |
| 21 | 1H NMR spectrum for pure ethaline + 16.0 wt.% water |
| 36 | 1H NMR spectrum for pure ethaline + 29.2 wt.% water |
| **Ethaline\_B** | 51 | 1H NMR spectrum for 0.3 M ZnCl2 ethaline + 0.0 wt.% water |
| 21\_1 | 1H NMR spectrum for 0.3 M ZnCl2 ethaline + 2.7 wt.% water |
| 29 | 1H NMR spectrum for 0.3 M ZnCl2 ethaline + 5.5 wt.% water |
| 6 | 1H NMR spectrum for 0.3 M ZnCl2 ethaline + 8.3 wt.% water |
| 21 | 1H NMR spectrum for 0.3 M ZnCl2 ethaline + 16 wt.% water |
| 36 | 1H NMR spectrum for 0.3 M ZnCl2 ethaline + 29.2 wt.% water |

**Figure 4**

|  |  |  |
| --- | --- | --- |
|  | **Directory No.** | **Experiment description** |
| **Reline\_A** | 10 | 1H NMR spectrum for pure reline + 0.0 wt.% water |
| 36 | 1H NMR spectrum for pure reline + 5.5 wt.% water |
| 26 | 1H NMR spectrum for pure reline + 8.3 wt.% water |
| 18 | 1H NMR spectrum for pure reline + 26.2 wt.% water |
| **Reline\_B** | 28 | 1H NMR spectrum for 0.3 M ZnCl2 reline + 0.0 wt.% water |
| 16 | 1H NMR spectrum for 0.3 M ZnCl2 reline + 5.5 wt.% water |
| 6 | 1H NMR spectrum for 0.3 M ZnCl2 reline + 8.3 wt.% water |
| 36 | 1H NMR spectrum for 0.3 M ZnCl2 reline + 26.2 wt.% water |

**Figure 5**

|  |  |
| --- | --- |
| **Directory No.** | **Experiment description** |
| 19 | 1H-1H NOESY NMR spectrum for dry ethaline, in the absence of ZnCl2, at mixing time = 300 ms |
| 1 | 1H-1H NOESY NMR spectrum for dry ethaline, in the presence of 0.3 M ZnCl2, at mixing time = 300 ms |

**Figure 6**

|  |  |
| --- | --- |
| **Directory No.** | **Experiment description** |
| 20 | 1H-1H NOESY NMR spectrum for ethaline with an addition of 8.3 wt.% water,in the absenceof ZnCl2, at mixing time = 300 ms |
| 8 | 1H-1H NOESY NMR spectrum for ethaline with an addition of 8.3 wt.% water,in the presenceof 0.3 M ZnCl2, at mixing time = 300 ms |

**Figure 7**

|  |  |
| --- | --- |
| **Directory No.** | **Experiment description** |
| 6 | 1H-1H NOESY NMR spectrum for dry reline,in the absenceof ZnCl2, at mixing time = 100 ms |
| 8 | 1H-1H NOESY NMR spectrum for dry reline,in the presenceof ZnCl2, at mixing time = 100 ms |

**Figure 8**

|  |  |
| --- | --- |
| **Directory No.** | **Experiment description** |
| 7 | 1H-1H NOESY NMR spectrum for reline with an addition of 8.3 wt.% water,in the absenceof ZnCl2, at mixing time = 300 ms |
| 13 | 1H-1H NOESY NMR spectrum for reline with an addition of 8.3 wt.% water,in the presenceof 0.3 M ZnCl2, at mixing time = 300 ms |

**Figure 9**

|  |  |
| --- | --- |
| **Directory No.** | **Experiment description** |
| 4 | 1H-1H NOESY NMR spectrum for reline with an addition of 26.2 wt.% water,in the absenceof ZnCl2, at mixing time = 100 ms |
| 2 | 1H-1H NOESY NMR spectrum for reline with an addition of 26.2 wt.% water,in the presenceof 0.3 M ZnCl2, at mixing time = 100 ms |

**Figure 10**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **Directory No.** | | | | **Experiment description** |
| **Ethaline\_A** | **A** | 2 | 7 | 12 | 1H *T*1 NMR relaxation time data for pure ethaline + 0.0 wt.% water |
| **B** | 2 | 6 |  | 1H *T*1 NMR relaxation time data for pure ethaline + 2.7 wt.% water |
| **C** | 10 | 14 |  | 1H *T*1 NMR relaxation time data for pure ethaline + 5.5 wt.% water |
| **D** | 2 | 7 | 12 | 1H *T*1 NMR relaxation time data for pure ethaline + 8.3 wt.% water |
| **E** | 17 | 22 | 27 | 1H *T*1 NMR relaxation time data for pure ethaline + 16.0 wt.% water |
| **F** | 32 | 37 | 42 | 1H *T*1 NMR relaxation time data for pure ethaline + 29.2 wt.% water |
| **Ethaline\_B** | **A** | 47 | 52 | 57 | 1H *T*1 NMR relaxation time data for 0.3 M ZnCl2 ethaline + 0.0 wt.% water |
| **B** | 18 | 22 |  | 1H *T*1 NMR relaxation time data for 0.3 M ZnCl2 ethaline + 2.7 wt.% water |
| **C** | 26 | 30 |  | 1H *T*1 NMR relaxation time data for 0.3 M ZnCl2 ethaline + 5.5 wt.% water |
| **D** | 2 | 7 | 12 | 1H *T*1 NMR relaxation time data for 0.3 M ZnCl2 ethaline + 8.3 wt.% water |
| **E** | 17 | 22 | 27 | 1H *T*1 NMR relaxation time data for 0.3 M ZnCl2 ethaline + 16.0 wt.% water |
| **F** | 32 | 37 | 42 | 1H *T*1 NMR relaxation time data for 0.3 M ZnCl2 ethaline + 29.2 wt.% water |
| **Reline\_A** | **A** | 11\_1 | 11 | 15 | 1H *T*1 NMR relaxation time data for pure reline + 0.0 wt.% water |
| **B** | 32 | 37 |  | 1H *T*1 NMR relaxation time data for pure reline + 5.5 wt.% water |
| **C** | 22 | 27 |  | 1H *T*1 NMR relaxation time data for pure reline + 8.3 wt.% water |
| **D** | 8 | 19 | 24 | 1H *T*1 NMR relaxation time data for pure reline + 26.2 wt.% water |
| **Reline\_B** | **A** | 2 | 29 | 33 | 1H *T*1 NMR relaxation time data for 0.3 M ZnCl2 reline + 0.0 wt.% water |
| **B** | 12 | 17 |  | 1H *T*1 NMR relaxation time data for 0.3 M ZnCl2 reline + 5.5 wt.% water |
| **C** | 2 | 7 |  | 1H *T*1 NMR relaxation time data for 0.3 M ZnCl2 reline + 8.3 wt.% water |
| **D** | 5 | 37 | 42 | 1H *T*1 NMR relaxation time data for 0.3 M ZnCl2 reline + 26.2 wt.% water |

**Figure 11**

* **1H *T*1 NMR relaxation time data:**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **Directory No.** | | | | **Experiment description** |
| **Ethaline\_A** | **A** | 2 | 7 | 12 | 1H *T*1 NMR relaxation time data for pure ethaline + 0.0 wt.% water |
| **B** | 2 | 6 |  | 1H *T*1 NMR relaxation time data for pure ethaline + 2.7 wt.% water |
| **C** | 10 | 14 |  | 1H *T*1 NMR relaxation time data for pure ethaline + 5.5 wt.% water |
| **D** | 2 | 7 | 12 | 1H *T*1 NMR relaxation time data for pure ethaline + 8.3 wt.% water |
| **E** | 17 | 22 | 27 | 1H *T*1 NMR relaxation time data for pure ethaline + 16.0 wt.% water |
| **F** | 32 | 37 | 42 | 1H *T*1 NMR relaxation time data for pure ethaline + 29.2 wt.% water |
| **Ethaline\_B** | **A** | 47 | 52 | 57 | 1H *T*1 NMR relaxation time data for 0.3 M ZnCl2 ethaline + 0.0 wt.% water |
| **B** | 18 | 22 |  | 1H *T*1 NMR relaxation time data for 0.3 M ZnCl2 ethaline + 2.7 wt.% water |
| **C** | 26 | 30 |  | 1H *T*1 NMR relaxation time data for 0.3 M ZnCl2 ethaline + 5.5 wt.% water |
| **D** | 2 | 7 | 12 | 1H *T*1 NMR relaxation time data for 0.3 M ZnCl2 ethaline + 8.3 wt.% water |
| **E** | 17 | 22 | 27 | 1H *T*1 NMR relaxation time data for 0.3 M ZnCl2 ethaline + 16.0 wt.% water |
| **F** | 32 | 37 | 42 | 1H *T*1 NMR relaxation time data for 0.3 M ZnCl2 ethaline + 29.2 wt.% water |
| **Reline\_A** | **A** | 11\_1 | 11 | 15 | 1H *T*1 NMR relaxation time data for pure reline + 0.0 wt.% water |
| **B** | 32 | 37 |  | 1H *T*1 NMR relaxation time data for pure reline + 5.5 wt.% water |
| **C** | 22 | 27 |  | 1H *T*1 NMR relaxation time data for pure reline + 8.3 wt.% water |
| **D** | 8 | 19 | 24 | 1H *T*1 NMR relaxation time data for pure reline + 26.2 wt.% water |
| **Reline\_B** | **A** | 2 | 29 | 33 | 1H *T*1 NMR relaxation time data for 0.3 M ZnCl2 reline + 0.0 wt.% water |
| **B** | 12 | 17 |  | 1H *T*1 NMR relaxation time data for 0.3 M ZnCl2 reline + 5.5 wt.% water |
| **C** | 2 | 7 |  | 1H *T*1 NMR relaxation time data for 0.3 M ZnCl2 reline + 8.3 wt.% water |
| **D** | 5 | 37 | 42 | 1H *T*1 NMR relaxation time data for 0.3 M ZnCl2 reline + 26.2 wt.% water |

* **1H NMR diffusion data:**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **Directory No.** | | | | **Experiment description** |
| **Ethaline\_C** | **A** | 5 | 10 | 15 | 1H NMR diffusion data for pure ethaline + 0.0 wt.% water |
| **B** | 4 | 8 |  | 1H NMR diffusion data for pure ethaline + 2.7 wt.% water |
| **C** | 12 | 16 |  | 1H NMR diffusion data for pure ethaline + 5.5 wt.% water |
| **D** | 5 | 10 | 15 | 1H NMR diffusion data for pure ethaline + 8.3 wt.% water |
| **E** | 20 | 25 | 30 | 1H NMR diffusion data for pure ethaline + 16.0 wt.% water |
| **F** | 35 | 40 | 45 | 1H NMR diffusion data for pure ethaline + 29.2 wt.% water |
| **Ethaline\_D** | **A** | 50 | 55 | 60 | 1H NMR diffusion data for 0.3 M ZnCl2 ethaline + 0.0 wt.% water |
| **B** | 38 | 40 |  | 1H NMR diffusion data for 0.3 M ZnCl2 ethaline + 2.7 wt.% water |
| **C** | 42 | 44 |  | 1H NMR diffusion data for 0.3 M ZnCl2 ethaline + 5.5 wt.% water |
| **D** | 5 | 10 | 15 | 1H NMR diffusion data for 0.3 M ZnCl2 ethaline + 8.3 wt.% water |
| **E** | 20 | 25 | 30 | 1H NMR diffusion data for 0.3 M ZnCl2 ethaline + 16.0 wt.% water |
| **F** | 35 | 40 | 45 | 1H NMR diffusion data for 0.3 M ZnCl2 ethaline + 29.2 wt.% water |
| **Reline\_C** | **A** | 20 | 13 | 17 | 1H NMR diffusion data for pure reline + 0.0 wt.% water |
| **B** | 35 | 40 |  | 1H NMR diffusion data for pure reline + 5.5 wt.% water |
| **C** | 25 | 30 |  | 1H NMR diffusion data for pure reline + 8.3 wt.% water |
| **D** | 22\_1 | 22 | 27 | 1H NMR diffusion data for pure reline + 26.2 wt.% water |
| **Reline\_D** | **A** | 21 | 31 | 35 | 1H NMR diffusion data for 0.3 M ZnCl2 reline + 0.0 wt.% water |
| **B** | 15 | 20 |  | 1H NMR diffusion data for 0.3 M ZnCl2 reline + 5.5 wt.% water |
| **C** | 5 | 10 |  | 1H NMR diffusion data for 0.3 M ZnCl2 reline + 8.3 wt.% water |
| **D** | 24 | 40 | 45 | 1H NMR diffusion data for 0.3 M ZnCl2 reline + 26.2 wt.% water |

**Table 1**

|  |  |  |  |
| --- | --- | --- | --- |
|  | **Directory No.** | **Mixing time / ms** | **Experiment description** |
| Reline\_A | 9 | 0 | 1H-1H NOESY NMR spectrum for reline with an addition of 8.3 wt.% water,in the absenceof ZnCl2 |
| 10 | 20 |
| 11 | 50 |
| 12 | 100 |
| 13 | 300 |
| 14 | 400 |
| Reline\_B | 2 | 0 | 1H-1H NOESY NMR spectrum for reline with an addition of 8.3 wt.% water,in the presenceof 0.3 M ZnCl2 |
| 3 | 10 |
| 4 | 20 |
| 5 | 50 |
| 6 | 100 |
| 7 | 300 |
| Ethaline\_A | 6 | 0 | 1H-1H NOESY NMR spectrum for dry ethaline, in the absenceof ZnCl2 |
| 5 | 20 |
| 4 | 50 |
| 3 | 100 |
| 2 | 200 |
| 19 | 300 |
| Ethaline\_B | 25 | 0 | 1H-1H NOESY NMR spectrum for ethaline with an addition of 8.3 wt.% water,in the absenceof ZnCl2 |
| 24 | 20 |
| 23 | 50 |
| 22 | 100 |
| 21 | 200 |
| 20 | 300 |
| Ethaline\_C | 12 | 0 | 1H-1H NOESY NMR spectrum for ethaline with an addition of 29.2 wt.% water,in the absenceof ZnCl2 |
| 11 | 20 |
| 10 | 50 |
| 9 | 100 |
| 8 | 200 |
| 7 | 300 |
| Ethaline\_D | 14 | 0 | 1H-1H NOESY NMR spectrum for ethaline with an addition of 8.3 wt.% water,in the presenceof 0.3 M ZnCl2 |
| 13 | 20 |
| 12 | 50 |
| 11 | 80 |
| 10 | 100 |
| 9 | 200 |
| 8 | 300 |
| Ethaline\_E | 28 | 0 | 1H-1H NOESY NMR spectrum for ethaline with an addition of 29.2 wt.% water,in the presenceof 0.3 M ZnCl2 |
| 27 | 20 |
| 26 | 50 |
| 25 | 80 |
| 24 | 100 |
| 23 | 200 |
| 22 | 300 |

**Table 2**

|  |  |  |
| --- | --- | --- |
|  | **Directory No.** | **Experiment description** |
| Ethaline\_A | 5 | 1H NMR diffusion data for dry ethaline |
| 10 |
| 15 |
| Ethaline\_B | 50 | 1H NMR diffusion data for dry ethaline + 0.3 M ZnCl2 |
| 55 |
| 60 |
| Reline\_A | 20 | 1H NMR diffusion data for dry reline |
| 13 |
| 17 |
| Reline\_B | 21 | 1H NMR Diffusion data for dry reline + 0.3 M ZnCl2 |
| 31 |
| 35 |

**Table 3**

|  |  |  |
| --- | --- | --- |
|  | **Directory No.** | **Experiment description** |
| Ethaline\_A | 12 | 1H NMR diffusion data for ethaline with addition of 5.5 wt.% water, in the absence of ZnCl2 |
| 16 |
| Ethaline\_B | 5 | 1H NMR diffusion data for ethaline with addition of 8.3 wt.% water, in the absence of ZnCl2 |
| 10 |
| 15 |
| Ethaline\_C | 35 | 1H NMR diffusion data for ethaline with addition of 29.2 wt.% water, in the absence of ZnCl2 |
| 40 |
| 45 |

**Table 4**

|  |  |  |
| --- | --- | --- |
|  | **Directory No.** | **Experiment description** |
| Ethaline\_A | 42 | 1H NMR diffusion data for ethaline with addition of 5.5 wt.% water, in the presence of 0.3 M ZnCl2 |
| 44 |
| Ethaline\_B | 5 | 1H NMR diffusion data for ethaline with addition of 8.3 wt.% water, in the presence of 0.3 M ZnCl2 |
| 10 |
| 15 |
| Ethaline\_C | 35 | 1H NMR diffusion data for ethaline with addition of 29.2 wt.% water, in the presence of 0.3 M ZnCl2 |
| 40 |
| 45 |

**Table 5**

|  |  |  |
| --- | --- | --- |
|  | **Directory No.** | **Experiment description** |
| Reline\_A | 35 | 1H NMR diffusion data for reline with addition of 5.5 wt.% water, in the absence of 0.3 M ZnCl2 |
| 40 |
| Reline\_B | 25 | 1H NMR diffusion data for reline with addition of 8.3 wt.% water, in the absence of 0.3 M ZnCl2 |
| 30 |
| Reline\_C | 22\_1 | 1H NMR diffusion data for reline with addition of 26.2 wt.% water, in the absence of 0.3 M ZnCl2 |
| 22 |
| 27 |

**Table 6**

|  |  |  |
| --- | --- | --- |
|  | **Directory No.** | **Experiment description** |
| Reline\_A | 15 | 1H NMR diffusion data for reline with addition of 5.5 wt.% water, in the presence of 0.3 M ZnCl2 |
| 20 |
| Reline\_B | 5 | 1H NMR diffusion data for reline with addition of 8.3 wt.% water, in the presence of 0.3 M ZnCl2 |
| 10 |
| Reline\_C | 24 | 1H NMR diffusion data for reline with addition of 26.2 wt.% water, in the presence of 0.3 M ZnCl2 |
| 40 |
| 45 |