**Supplementary Material**

**Investigation of physicochemical properties of aggregated models of [MIM+]2[C(CN)3-]2 ionic liquid: A theoretical study**

Batoul Makiabadi1, Mohammad Zakarianezhad\*2

1Department of Chemical Engineering, Sirjan University of Technology, Sirjan, Iran

2Department of Chemistry, Payame Noor University, Tehran, Iran



**Fig. S1.** Molecular graphs of A–D clusters. The critical points of bonds and rings are represented by small red spheres and small yellow spheres, respectively.

|  |
| --- |
| **Table S1**. NBO results calculated at the MP2/6-311++G(2d,2p) level of theory |
|  | **A** | **B** | **C** | **D** | **Cation** | **Anion** |
| **Natural Charge** |  |  |  |  |  |  |
| C1(C3) | 0.290 | 0.290 | 0.277 | 0.276 | 0.29542(-0.016) |  |
| N2(C4) | -0.523 | -0.523 | -0.370 | -0.511 | -0.487(-0.019) |  |
| H10(H12) | 0.283 | 0.287 | 0.295 | 0.305 | 0.25251(0.262) |  |
| H11(H13) | 0.484 | 0.484 | 0.295 | 0.486 | 0.4553(0.260) |  |
| N14 | -0.554 | -0.540 | -0.509 | -0.539 |  | -0.457 |
| C15 | 0.458 | 0.451 | 0.386 | 0.452 |  | -0.618 |
| C16 | -0.598 | -0.594 | -0.597 | -0.595 |  | -0.618 |
| C17 | 0.399 | 0.451 | 0.457 | 0.452 |  | 0.330 |
| N18 | -0.526 | -0.540 | -0.560 | -0.539 |  | -0.457 |
| C21(C24) | 0.290 | 0.290 | 0.286 | (-0.019) |  |  |
| N25 | -0.523 | -0.523 | -0.523 | -0.511 |  |  |
| H27(H32) | 0.283 | 0.287 | 0.286 | (0.305) |  |  |
| H33 | 0.484 | 0.484 | 0.484 | 0.486 |  |  |
| N34 | -0.554 | -0.542 | -0.538 | -0.521 |  |  |
| C35 | 0.458 | 0.404 | 0.395 | 0.395 |  |  |
| C36 | -0.598 | -0.603 | -0.603 | -0.606 |  |  |
| C37 | 0.399 | 0.404 | 0.394 | 0.395 |  |  |
| N38 | -0.526 | -0.542 | -0.522 | -0.521 |  |  |
| **Charge Transfer** | -1.779 | -1.790 | -1.838 | -1.870 |  |  |
| **Occupancy** |  |  |  |  |  |  |
| σ\*(N2-H) | 0.0954 | 0.0883 |  | 0.0883 | 0.0119 |  |
| σ\*(C1-H) | 0.0235 | 0.0251 | 0.0362 |  | 0.0099 |  |
| σ\*(C3(C4)-H) |  |  | (0.0195) | 0.0315 | 0.0080(0.0083) |  |
| σ\*(C21(C24)-H) | 0.0235 | 0.0251 | 0.0255 | (0.0315) | 0.0080 |  |
| σ\*(C15-N) | 0.0180 | 0.0132 | 0.0122 | 0.0123 |  | 0.0118 |
| σ\*(C17-N) | 0.0123 | 0.0132 | 0.0135 | 0.0123 |  | 0.0118 |
| σ\*(N25-H) | 0.0954 | 0.0883 | 0.0955 | 0.0883 | 0.0119 | 0.0118 |
| σ\*(C37-N) | 0.0123 | 0.0125 | 0.0123 | 0.0132 |  | 0.0118 |
| σ\*(C35-N) | 0.0180 | 0.0125 | 0.0126 | 0.0132 |  | 0.0118 |
| **E(2)(kJ /mol)** |  |  |  |  |  |  |
| LP N→σ\* (N2 - H) | 200.46 | 181.79 | - | 96.61 |  |  |
| LP N→σ\*(N25 - H) | 200.46 | 181.79 | 26.78 | 96.61 |  |  |
| LP N→σ\* (C1(C3) - H) | 27.11 | 30.79 | (58.37) |  |  |  |
| LP N→σ\* (C21(C24) - H) | 26.90 | 30.79 | 36.40 | (54.52) |  |  |
| LP N→σ\* (C4 (C3)- H) | - | - | 200.33 | (54.52) |  |  |

|  |
| --- |
| **Table S2.** MP2/6-311++G(2d,2p)-calculated topological properties of the BCPs (au) in clusters. |
| **Bond** | **** | **r** | **H( r )** | **Bond** | **ρ** | **r** | **H( r )** |
|  |  | **A** |  |  |  | **B** |  |
| N14...HN | 0.0539 | 0.0065 | -0.0107 | N14...HN | 0.0507 | 0.0066 | -0.0088 |
| N34…HN | 0.0539 | 0.0065 | -0.0107 | N18...HN | 0.0507 | 0.0066 | -0.0088 |
| N18...HC | 0.0185 | 0.0040 | 0.0022 | N34…HC | 0.0198 | 0.0043 | 0.0021 |
| N38…HC | 0.0185 | 0.0040 | 0.0022 | N38…HC | 0.0198 | 0.0043 | 0.0021 |
| C1-H10 | 0.3014 | -0.0787 | -0.3395 | C1-H10 | 0.3009 | -0.0787 | -0.3392 |
| C21-H27 | 0.3014 | -0.0787 | -0.3395 | C21-H27 | 0.3009 | -0.0787 | -0.3392 |
| N2-H11 | 0.2977 | -0.1145 | -0.5003 | N2-H11 | 0.3026 | -0.1170 | -0.5096 |
| N25-H33 | 0.2977 | -0.1145 | -0.5003 | N25-H33 | 0.3026 | -0.1170 | -0.5096 |
| C14-N15 | 0.4823 | -0.0397 | -0.9044 | C14-N15 | 0.4835 | -0.0387 | -0.9081 |
| C37-N38 | 0.4823 | -0.0397 | -0.9044 | C37-N38 | 0.4839 | -0.0424 | -0.9085 |
|  |  | **C** |  |  |  | **D** |  |
| N18...HN | 0.0539 | 0.0065 | -0.0107 | N34…HN | 0.0508 | 0.0066 | -0.0089 |
| N14...HC | 0.0170 | 0.0037 | 0.0022 | N38…HN | 0.0508 | 0.0066 | -0.0089 |
| N34…HC | 0.0196 | 0.0042 | 0.0021 | N14...HC | 0.0238 | 0.0048 | 0.0014 |
| N38…HC | 0.0261 | 0.0052 | 0.0011 | N18...HC | 0.0238 | 0.0048 | 0.0014 |
| C1-H10 | 0.2959 | -0.0771 | -0.3320 | C3-H12 | 0.2959 | -0.0764 | -0.3306 |
| C4-H13 | 0.2989 | -0.0767 | -0.3339 | C24-H32 | 0.2959 | -0.0764 | -0.3306 |
| C21-H27 | 0.3006 | -0.0785 | -0.3384 | N2-H11 | 0.302018 | -0.1170 | -0.5095 |
| N25-H33 | 0.2976 | -0.1144 | -0.4999 | N25-H33 | 0.302018 | -0.1170 | -0.5095 |
| C14-N15 | 0.4848 | -0.0407 | -0.9113 | C14-N15 | 0.4843 | -0.0411 | -0.9098 |
| C37-N38 | 0.4837 | -0.0420 | -0.9080 | C37-N38 | 0.4838 | -0.0385 | -0.9091 |
|  |  | Ions |  |  |  |  |  |
| C1-H10 | 0.3040 | -0.0786 | -0.3425 |  |  |  |  |
| C37-N38 | 0.4916 | -0.0373 | -0.9317 |  |  |  |  |
| C4-H13 | 0.30169 | -0.07687 | -0.3390 |   |   |   |   |