

Harnessing ionic interactions and hydrogen bonding for nucleophilic fluorination

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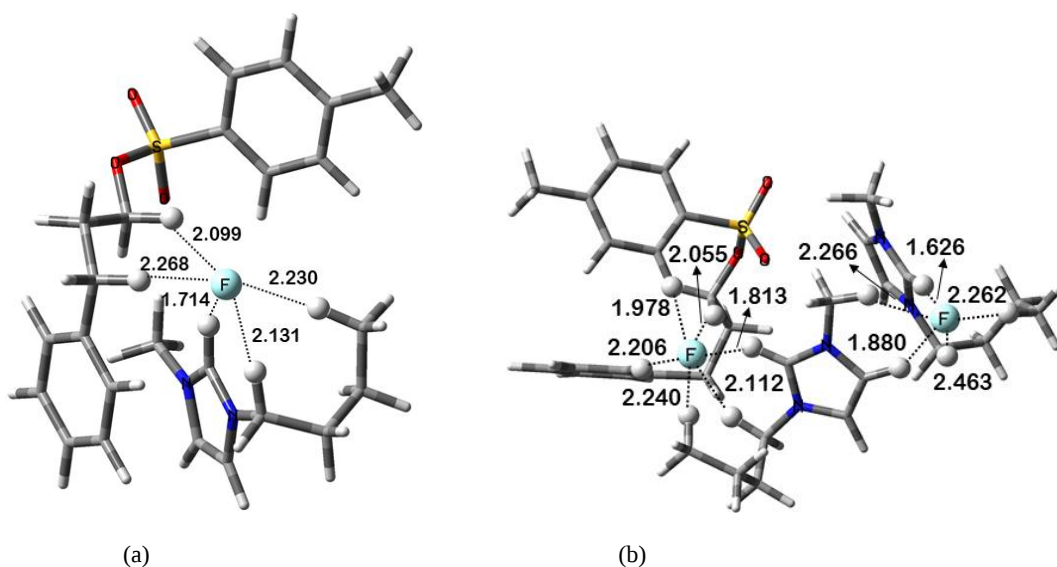


Figure 2S. Pre-reaction complexes of S_N2 fluorination in [bmim][F]. (a) equivalent of IL = 1 (b) equivalent of IL = 2. M06-2X /6-311G** method for C, H, O, N, S, F atoms, using Gaussian 09 set of programs.

Cartesian coordinates for conformers

(a)

```
C -3.50080600 0.54880000 2.24363100
C -3.85966900 1.50099600 1.34373000
C -1.92626800 0.64698500 0.69670800
N -2.29439000 0.03294300 1.82108200
H -3.98672900 0.19322500 3.13678400
H -4.72554800 2.14004900 1.29786000
H -1.03905000 0.50579900 0.05430000
N -2.86558500 1.54167500 0.39317300
C -1.53980600 -1.01132500 2.50730600
H -1.37195100 -0.70858700 3.54045300
H -2.10227000 -1.94407300 2.47971400
H -0.57936000 -1.13853200 2.01164300
C -2.82040300 2.40775900 -0.79331600
H -1.92354700 2.09886000 -1.33673100
H -3.70273400 2.18375800 -1.39647900
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C -2.78764400 3.88167500 -0.39915200
H -2.75949800 4.46124600 -1.32725600
H -3.72229500 4.14210200 0.10833100
C -1.59242500 4.25351000 0.47951400
H -1.69172200 5.30336800 0.77027800
H -1.63094500 3.67472900 1.40963100
C -0.24771000 4.03539900 -0.21312100
H 0.57431200 4.34088400 0.43913100
H -0.09324900 2.98953700 -0.49894000
H -0.18698900 4.63842700 -1.12500900
F -0.14349400 0.92679600 -1.34506300
C -2.30431600 -2.87320300 -0.70838100
C -2.11071800 -1.90287400 -1.69399000
C -3.11012800 -0.94068800 -1.87462400
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H 0.09127000 -1.86915300 0.02562000
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S 2.73392500 -1.89653600 1.00997200
O 3.78968700 -2.82959200 1.32555400
O 1.70310200 -1.61017400 1.99118000
C 3.43355400 -0.36902700 0.45827300
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C 2.74696100 0.81855600 0.67230200
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H 1.79885100 0.81974400 1.19622300
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H 4.50369800 4.14832400 -0.71772100
H 6.11960300 3.45425200 -0.50537400

(b)

C 3.23477400 1.66719400 -1.62556200
C 2.69906000 2.76285200 -1.02511400
C 1.03672100 1.39640000 -1.53584500
N 2.17849000 0.83543000 -1.93594500
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