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# 咪唑类离子液体与酪氨酸相互作用及机理的密度泛函理论研究

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# Interaction and Mechanism between Imidazolium Ionic Liquids and Zwitterionic Amino Acid Tyr: a DFT study

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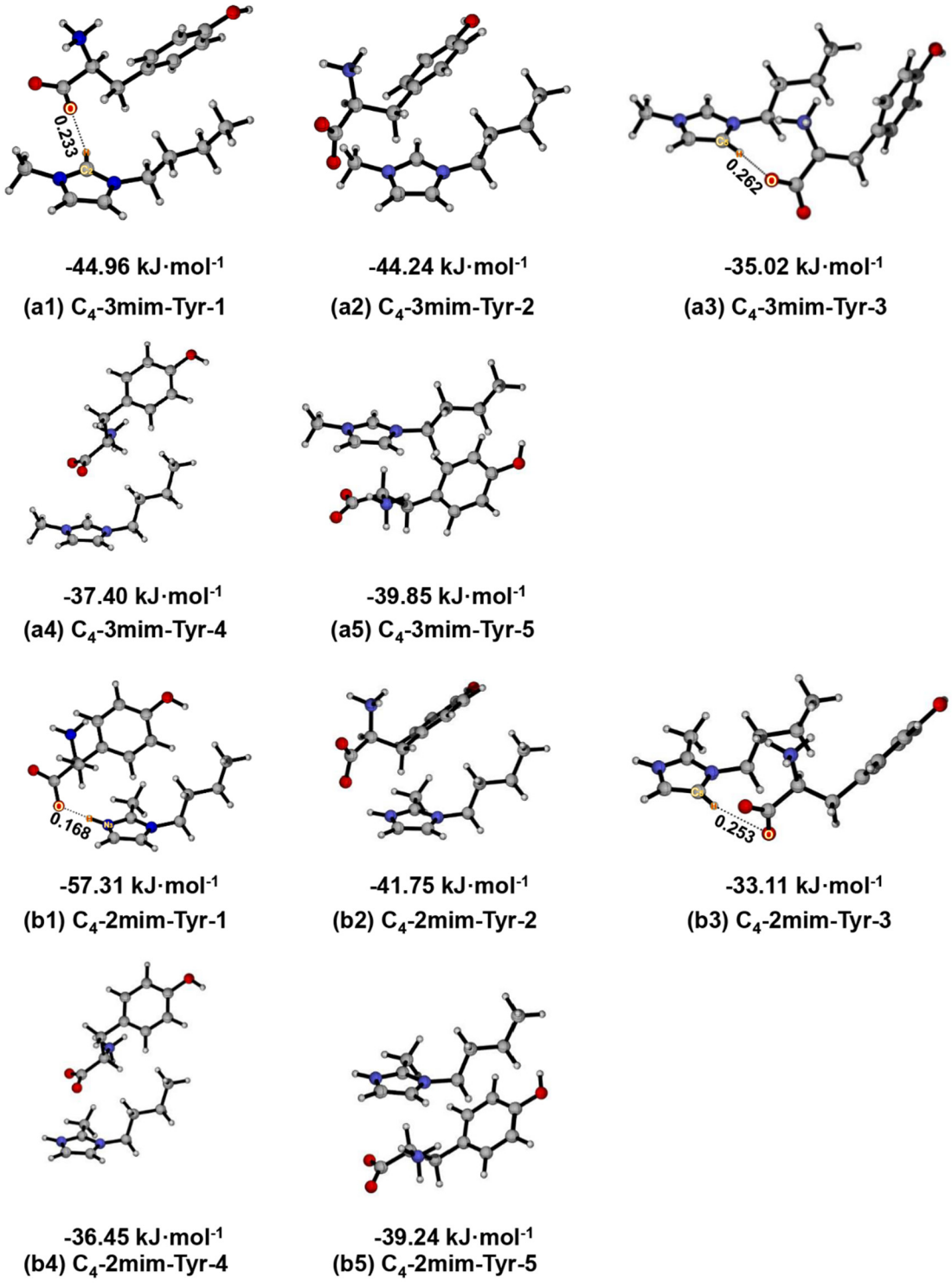


**Fig. S1 The optimized conformers of $C_4$-3mim-Tyr/$C_4$-2mim-Tyr complexes.**

The unit of the distances of H-bond labeled in picture is nm.

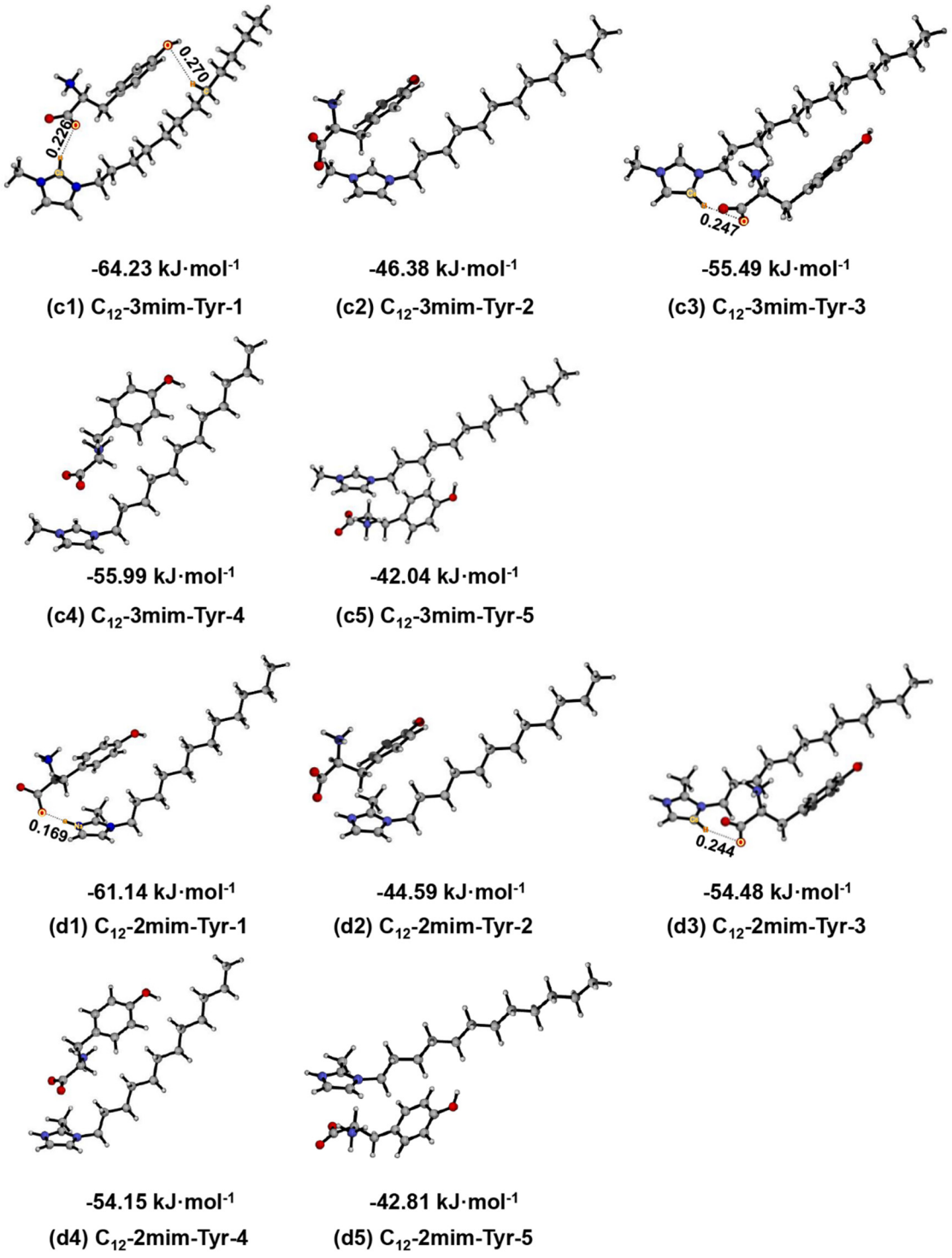


**Fig. S2 The optimized conformers of $C_{12}$-3mim-Tyr/$C_{12}$-2mim-Tyr complexes.**

The unit of the distances of H-bond labeled in picture is nm.

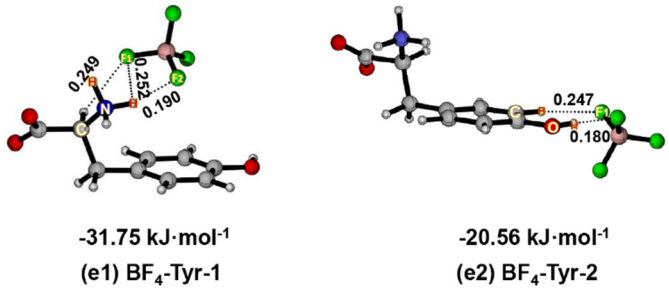


**Fig. S3 The optimized conformers of $BF_4$-Tyr complexes.**

The unit of the distances of H-bond labeled in picture is nm.

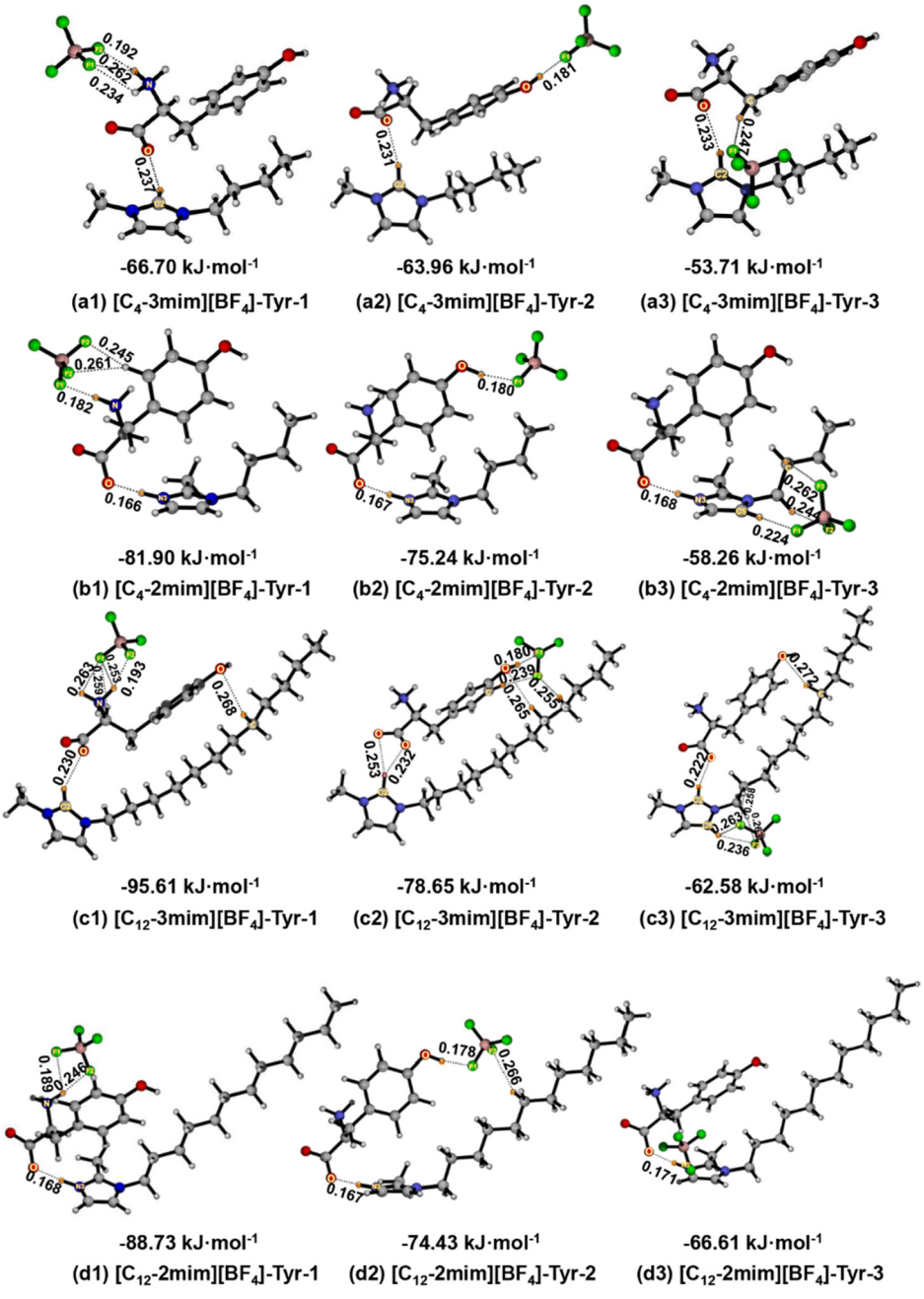


**Fig. S4 The optimized conformers of ILs-Tyr complexes.**

The unit of the distances of H-bond labeled in picture is nm.

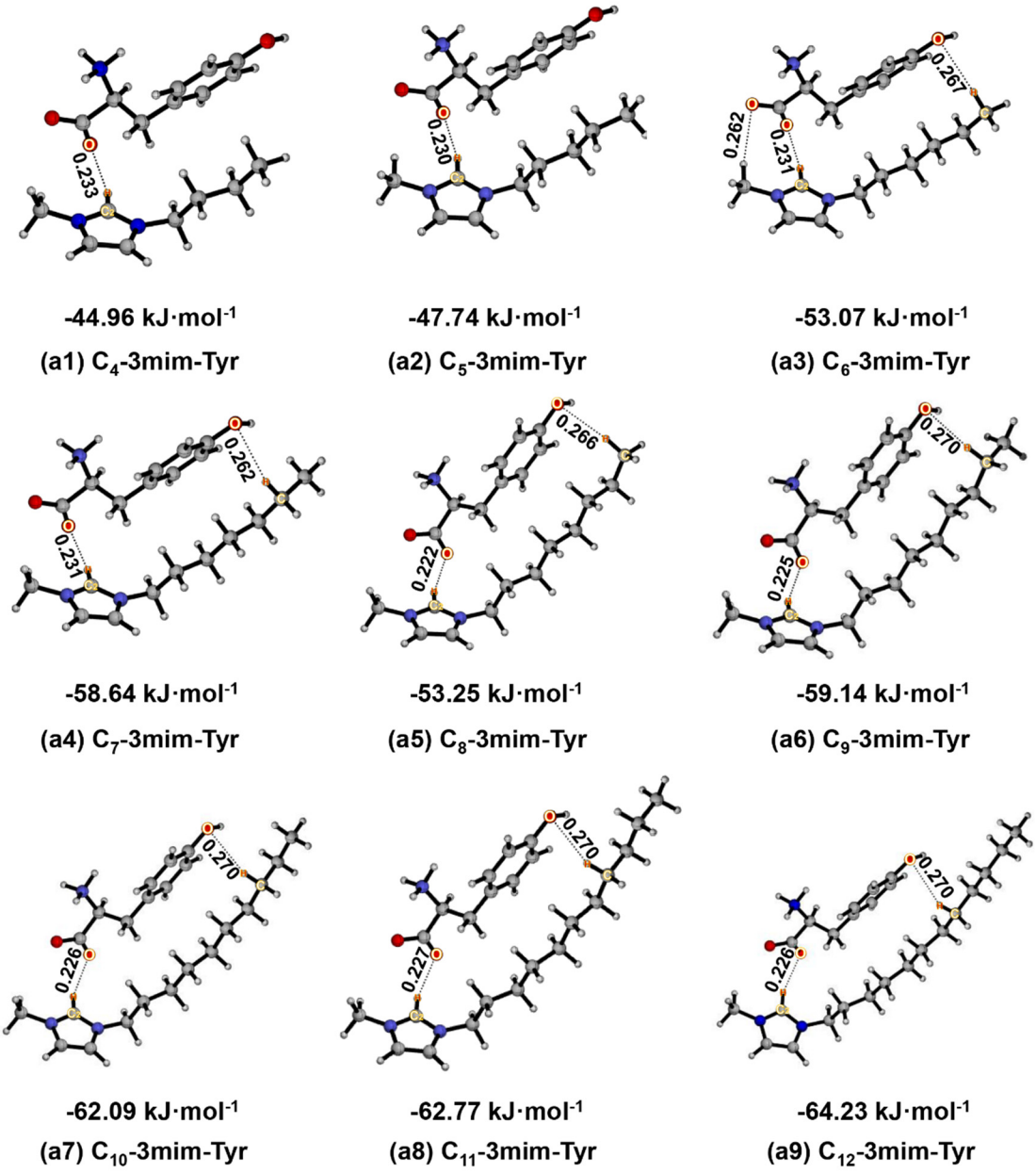


**Fig. S5 The optimized conformers of C*n*-3mim complexes.**

Chain length *n* increase from 4 to 12, the unit of the distances of H-bond labeled in picture is nm.

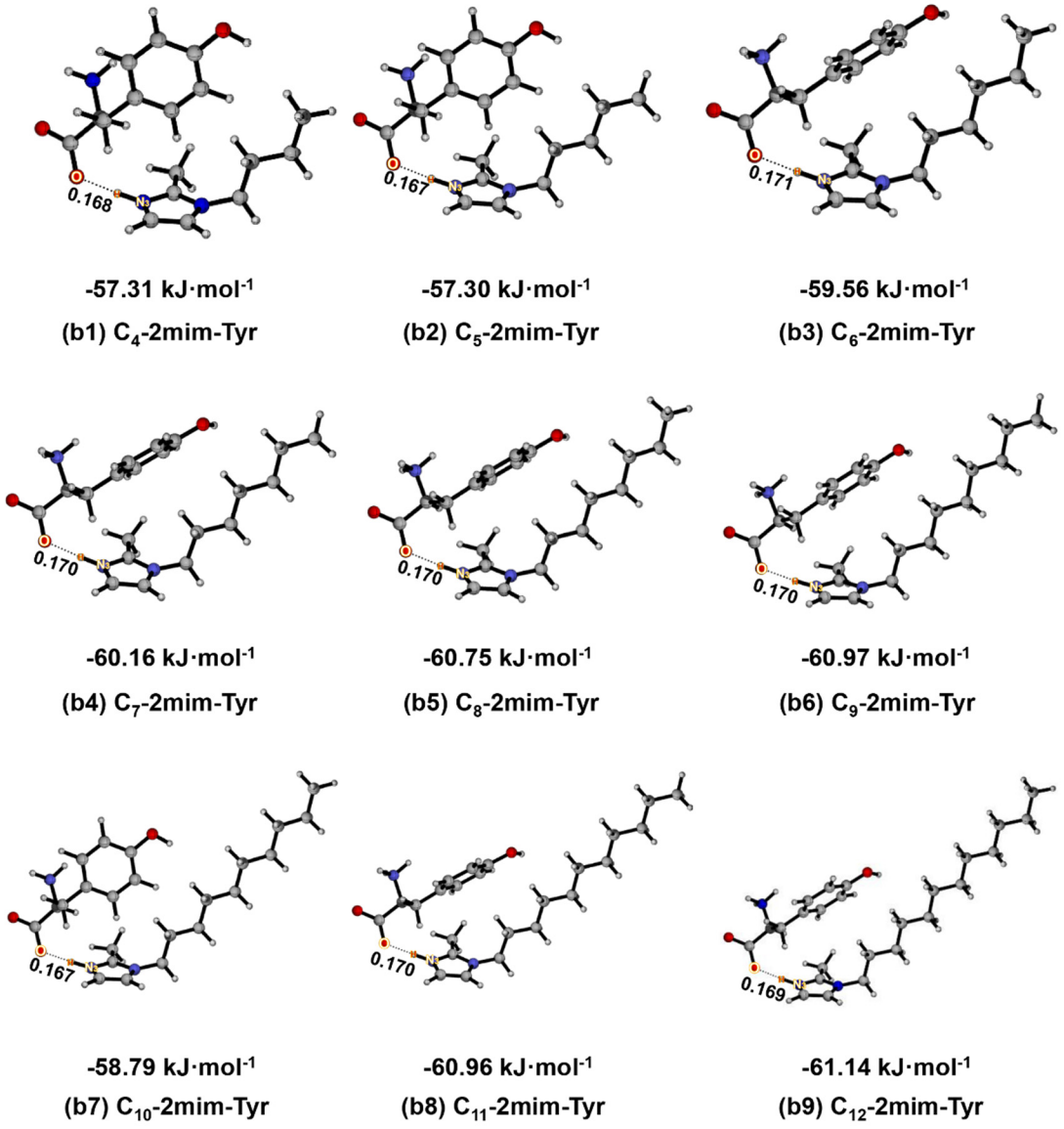


**Fig. S6 The optimized conformers of $C_n$-2mim complexes.**

Chain length *n* increase from 4 to 12, the unit of the distances of H-bond labeled in picture is nm.

**Table S1 H-bonds and interaction energy of cation/anion-Tyr complexes.**

| Structures | H-bond | Distance/nm | Angle/(°) | $\Delta E$/(kJ·mol$^{-1}$) | $\Delta\Delta E$/(kJ·mol$^{-1}$) |
|---|---|---|---|---|---|
| $C_4$-3mim-Tyr -1 | C2—H···$O_{COO}$ | 0.233 | 155.0 | −44.96 | 0.00 |
| $C_4$-3mim-Tyr -2 | N/A | N/A | N/A | −44.24 | 0.72 |
| $C_4$-3mim-Tyr -3 | C5—H···$O_{COO}$ | 0.262 | 167.0 | −35.02 | 9.94 |
| $C_4$-3mim-Tyr -4 | N/A | N/A | N/A | −37.40 | 7.56 |
| $C_4$-3mim-Tyr -5 | N/A | N/A | N/A | −39.85 | 5.11 |
| $C_4$-2mim-Tyr -1 | N3—H···$O_{COO}$ | 0.168 | 174.7 | −57.31 | 0.00 |
| $C_4$-2mim-Tyr -2 | N/A | N/A | N/A | −41.75 | 15.56 |
| $C_4$-2mim-Tyr -3 | C5—H···$O_{COO}$ | 0.253 | 155.0 | −33.11 | 24.20 |
| $C_4$-2mim-Tyr -4 | N/A | N/A | N/A | −36.45 | 20.86 |
| $C_4$-2mim-Tyr -5 | N/A | N/A | N/A | −39.24 | 18.07 |
| $C_{12}$-3mim-Tyr -1 | C2—H···$O_{COO}$ | 0.226 | 151.3 | −64.23 | 0.00 |
| | $C_{Alkyl}$—H···$O_{OH}$ | 0.270 | 132.7 | N/A | N/A |
| $C_{12}$-3mim-Tyr -2 | N/A | N/A | N/A | −46.38 | 17.85 |
| $C_{12}$-3mim-Tyr -3 | C5—H···$O_{COO}$ | 0.247 | 156.2 | −55.49 | 8.74 |
| $C_{12}$-3mim-Tyr -4 | N/A | N/A | N/A | −55.99 | 8.24 |
| $C_{12}$-3mim-Tyr -5 | N/A | N/A | N/A | −42.04 | 22.19 |
| $C_{12}$-2mim-Tyr -1 | N3—H···$O_{COO}$ | 0.169 | 168.9 | −61.14 | 0.00 |
| $C_{12}$-2mim-Tyr -2 | N/A | N/A | N/A | −44.59 | 16.55 |
| $C_{12}$-2mim-Tyr -3 | C5—H···$O_{COO}$ | 0.244 | 157.8 | −54.48 | 6.66 |
| $C_{12}$-2mim-Tyr -4 | N/A | N/A | N/A | −54.15 | 6.99 |
| $C_{12}$-2mim-Tyr -5 | N/A | N/A | N/A | −42.81 | 18.33 |
| $BF_4$-Tyr-1 | $N_{Tyr}$—H···F2 | 0.190 | 161.8 | −31.75 | N/A |
| | $C_{Amino}$—H···F1 | 0.249 | 124.6 | N/A | N/A |
| | $N_{Tyr}$—H···F1 | 0.252 | 106.9 | N/A | N/A |
| $BF_4$-Tyr-2 | $O_{OH}$—H···F1 | 0.180 | 170.2 | −20.56 | 11.19 |
| | $C_{Ben}$—H···F1 | 0.247 | 173.0 | N/A | N/A |

**Table S2 H-bonds and interaction energy of ILs-Tyr complexes.**

| Structure | H-bond | Distance/nm | Angle/(°) | $\Delta E$/(kJ·mol$^{-1}$) | $\Delta\Delta E$/(kJ·mol$^{-1}$) |
|---|---|---|---|---|---|
| [$C_4$-3mim][$BF_4$]-Tyr-1 | C2−H···$O_{COO}$ | 0.237 | 153.2 | -66.70 | 0.00 |
| | $N_{Tyr}$−H···F1 | 0.234 | 115.3 | N/A | N/A |
| | $N_{Tyr}$−H···F1 | 0.262 | 96.6 | N/A | N/A |
| | $N_{Tyr}$−H···F2 | 0.192 | 155.2 | N/A | N/A |
| [$C_4$-3mim][$BF_4$]-Tyr-2 | C2−H···$O_{COO}$ | 0.231 | 156.3 | −63.96 | 2.74 |
| | $O_{OH}$−H···F1 | 0.181 | 175.4 | N/A | N/A |
| [$C_4$-3mim][$BF_4$]-Tyr-3 | C2−H···$O_{COO}$ | 0.233 | 158.5 | −53.71 | 12.99 |
| | $C_{Amino}$−H···F1 | 0.247 | 157.7 | N/A | N/A |
| [$C_4$-2mim][$BF_4$]-Tyr-1 | N3−H···$O_{COO}$ | 0.166 | 177.5 | −81.90 | 0.00 |
| | $N_{Tyr}$−H···F1 | 0.182 | 179.4 | N/A | N/A |
| | $C_{Ben}$−H···F2 | 0.261 | 151.0 | N/A | N/A |
| | $C_{Ben}$−H···F3 | 0.245 | 151.1 | N/A | N/A |
| [$C_4$-2mim][$BF_4$]-Tyr-2 | C2−H···$O_{COO}$ | 0.167 | 176.0 | −75.24 | 6.66 |
| | $O_{OH}$−H···F1 | 0.180 | 166.4 | N/A | N/A |
| [$C_4$-2mim][$BF_4$]-Tyr-3 | C2−H···$O_{COO}$ | 0.168 | 175.8 | −58.26 | 23.64 |
| | C5−H···F1 | 0.224 | 180.0 | N/A | N/A |
| | $C_{Alkyl}$−H···F2 | 0.244 | 150.5 | N/A | N/A |
| | $C_{Alkyl}$−H···F3 | 0.262 | 129.8 | N/A | N/A |
| [$C_{12}$-3mim][$BF_4$]-Tyr-1 | C2−H···$O_{COO}$ | 0.230 | 143.5 | −95.61 | 0.00 |
| | $C_{Alkyl}$−H···$O_{OH}$ | 0.268 | 137.2 | N/A | N/A |
| | $N_{Tyr}$−H···F2 | 0.193 | 158.7 | N/A | N/A |
| | $N_{Tyr}$−H···F1 | 0.253 | 100.4 | N/A | N/A |
| | $C_{Amino}$−H···F1 | 0.259 | 75.9 | N/A | N/A |
| | $N_{Tyr}$−H···F1 | 0.263 | 95.0 | N/A | N/A |
| [$C_{12}$-3mim][$BF_4$]-Tyr-2 | C2−H···$O_{COO}$ | 0.232 | 153.3 | −78.65 | 16.96 |
| | C2−H···$O_{COO}$ | 0.253 | 139.4 | N/A | N/A |
| | $O_{OH}$−H···F1 | 0.180 | 168.1 | N/A | N/A |
| [$C_{12}$-3mim][$BF_4$]-Tyr-2 | $C_{Ben}$−H···F2 | 0.239 | 168.6 | N/A | N/A |
| | $C_{Alkyl}$−H···F2 | 0.255 | 122.5 | N/A | N/A |
| | $C_{Alkyl}$−H···$O_{OH}$ | 0.265 | 156.1 | N/A | N/A |
| [$C_{12}$-3mim][$BF_4$]-Tyr-3 | C2−H···$O_{COO}$ | 0.222 | 156.5 | −62.58 | 33.03 |
| | $C_{Alkyl}$−H···$O_{OH}$ | 0.272 | 131.2 | N/A | N/A |
| | C5−H···F2 | 0.236 | 146.4 | N/A | N/A |
| | $C_{Alkyl}$−H···F1 | 0.258 | 157.4 | N/A | N/A |
| | C5−H···F1 | 0.263 | 130.0 | N/A | N/A |
| | $C_{Alkyl}$−H···F2 | 0.263 | 130.8 | N/A | N/A |
| [$C_{12}$-2mim][$BF_4$]-Tyr-1 | N3−H···$O_{COO}$ | 0.168 | 173.9 | −88.73 | 0.00 |
| | $N_{Tyr}$−H···F1 | 0.189 | 116.7 | N/A | N/A |
| | $N_{Tyr}$−H···F2 | 0.246 | 146.8 | N/A | N/A |
| [$C_{12}$-2mim][$BF_4$]-Tyr-2 | N3−H···$O_{COO}$ | 0.167 | 175.9 | −74.43 | 14.30 |
| | $O_{OH}$−H···F1 | 0.178 | 168.1 | N/A | N/A |
| | $C_{Alkyl}$−H···F2 | 0.266 | 138.2 | N/A | N/A |
| [$C_{12}$-2mim][$BF_4$]-Tyr-2 | N3−H···$O_{COO}$ | 0.171 | 168.2 | −66.61 | 22.12 |