Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information to "Insight into Conformationally-Dependent Binding of 1-n-Alkyl-3-Methylimidazolium Cations to Porphyrin Molecules using Quantum Mechanical Calculations"

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March 18, 2019

Table S1 Binding Energy contributions to tail up $[C_n mim]^+$ FBP complexes (kcal/mol)

Cation	B3LYP-D2					M06				
	Conformation		Interaction	Counterpoise	Binding	Conformation		Interaction	Counterpoise	Binding
	Cation	FBP				Cation	FBP			
$[C_2mim]^+$	0.6	-2.6	-34.1	4.5	-31.6	0.3	1.3	-28.0	3.5	-22.9
$[C_4mim]^+$	0.6	-2.6	-33.9	4.5	-31.4	0.2	1.5	-27.8	3.5	-22.6
$[C_6mim]^+$	1.3	-3.0	-33.7	4.7	-30.7	1.3	1.0	-28.8	3.8	-22.7
$[C_8mim]^+$	0.4	-3.1	-32.8	4.5	-30.9	0.2	1.1	-28.9	5.2	-22.4
$[C_{10}mim]^+$	1.5	-3.1	-37.3	6.0	-32.9	1.4	1.3	-30.3	4.6	-23.0

Table S2 Binding Energy contributions to tail down $[C_n mim]^+$ FBP complexes (kcal/mol)

Cation	B3LYP-D2					M06				
	Conformation		Interaction	Counterpoise	Binding	Conformation		Interaction	Counterpoise	Binding
	Cation	FBP				Cation	FBP			
$[C_2mim]^+$	1.1	-3.1	-33.4	4.8	-30.7	1.0	1.5	-28.2	3.7	-22.0
$[C_4mim]^+$	1.4	-2.5	-35.7	5.3	-31.4	1.4	1.3	-29.3	4.1	-22.6
$[C_6mim]^+$	1.5	-2.7	-37.3	6.0	-32.5	1.5	1.2	-30.7	4.6	-23.4
$[C_8mim]^+$	1.3	-3.6	-31.0	5.9	-27.4	0.6	0.7	-23.8	4.1	-18.5
$[C_{10}mim]^+$	0.1	-3.8	-19.6	4.8	-18.5	0.2	0.2	-14.9	3.8	-10.7

Table S3 Binding Energy contributions to interplanar $[C_n mim]^+$ FBP complexes (kcal/mol)

Cation	B3LYP-D2					M06				
	Conformation		Interaction	Counterpoise	Binding	Conformation		Interaction	Counterpoise	Binding
	Cation	FBP				Cation	FBP			
$[C_2mim]^+$	1.3	-2.8	-34.9	4.8	-31.6	1.2	1.4	-28.8	3.7	-22.6
$[C_4mim]^+$	1.3	-3.3	-34.2	5.1	-31.1	1.1	0.8	-28.0	4.1	-21.9
$[C_6mim]^+$	1.1	-2.4	-37.8	4.6	-34.5	0.8	1.7	-31.1	3.6	-25.1
$[C_8mim]^+$	1.3	-2.4	-38.3	4.8	-34.6	1.1	1.9	-31.8	3.7	-25.1
$[C_{10}mim]^+$	1.4	-2.4	-38.5	4.8	-34.8	1.1	1.8	-31.6	3.7	-25.1

Table S4 Binding Energy contributions to tail up $[C_n mim]^+$ FeP complexes (kcal/mol)

Cation	B3LYP-D2					M06				
	Conformation		Interaction	Counterpoise	Binding	Conformation		Interaction	Counterpoise	Binding
	Cation	FeP				Cation	FeP			
$[C_2mim]^+$	0.7	0.6	-28.7	4.3	-23.2	0.4	0.3	-20.3	3.4	-16.2
$[C_4mim]^+$	0.4	1.1	-29.1	4.4	-23.2	0.3	0.5	-19.4	3.4	-15.2
$[C_6mim]^+$	1.3	1.3	-30.2	5.0	-22.7	1.6	0.6	-20.2	4.0	-14.0
$[C_8mim]^+$	0.4	0.8	-26.3	4.2	-20.8	0.3	0.4	-16.5	3.3	-12.4
$[C_{10}mim]^+$	0.3	0.9	-26.1	4.4	-20.4	0.2	0.6	-15.1	3.4	-10.9

Table S5 Binding Energy contributions to tail down $[C_n mim]^+$ FeP complexes (kcal/mol)

Cation	B3LYP-D2					M06				
	Conformation		Interaction	Counterpoise	Binding	Conformation		Interaction	Counterpoise	Binding
	Cation	FeP				Cation	FeP			
$[C_2mim]^+$	1.3	1.0	-30.8	4.4	-24.1	1.1	0.9	-22.5	3.7	-16.8
$[C_4mim]^+$	0.4	0.9	-29.4	4.6	-23.2	1.3	0.7	-19.8	3.7	-14.9
$[C_6mim]^+$	1.3	1.0	-29.2	5.5	-21.6	0.4	0.4	-18.9	4.2	-12.9
$[C_8mim]^+$	0.4	0.6	-24.0	4.5	-17.4	1.3	0.8	-14.9	3.7	-9.6
$[C_{10}mim]^+$	0.3	0.5	-23.7	4.6	-17.8	0.3	0.4	-12.7	3.7	-7.8

Table S6 Binding Energy contributions to interplanar $[C_n mim]^+$ FeP complexes (kcal/mol)

Cation	B3LYP-D2					M06				
	Conformation		Interaction	Counterpoise	Binding	Conformation		Interaction	Counterpoise	Binding
	Cation	FeP				Cation	FeP			
$[C_2mim]^+$	1.2	1.1	-31.2	4.6	-24.3	1.1	0.9	-22.5	3.7	-16.8
$[C_4mim]^+$	1.4	0.4	-30.8	5.3	-23.6	1.3	0.7	-21.8	4.0	-15.8
$[C_6mim]^+$	0.5	1.4	-28.7	4.5	-22.3	0.4	0.4	-17.4	3.4	-13.1
$[C_8mim]^+$	1.4	1.1	-30.7	5.4	-22.8	1.3	0.8	-22.0	4.1	-15.8
$[C_{10}mim]^+$	0.3	1.0	-26.6	4.9	-20.4	0.3	0.4	-15.0	3.3	-11.0

Table S7 Electrophilicity indexes of FBP in $[C_n mim]^+$ FBP complexes (kcal/mol)

Cation	B3LYP-D2				M06			
	Gas Phase	Tail Up	Tail Down	Interplanar	Gas Phase	Tail Up	Tail Down	Interplanar
$[C_2mim]^+$	53.9	170.2	167.9	170.0	51.5	155.7	154.8	155.7
$[C_4mim]^+$	53.9	168.7	167.3	166.8	51.5	154.6	152.0	153.2
$[C_6mim]^+$	53.9	165.9	167.2	165.1	51.5	153.2	152.7	152.3
$[C_8mim]^+$	53.9	165.4	151.9	164.1	51.5	151.3	136.6	151.1
$[C_{10}mim]^+$	53.9	167.6	110.8	164.1	51.5	153.7	120.4	151.1

Table S8 Electrophilicity indexes of FeP in $[C_n mim]^+$ FeP complexes (kcal/mol)

Cation	B3LYP-D2				M06			
	Gas Phase	Tail Up	Tail Down	Interplanar	Gas Phase	Tail Up	Tail Down	Interplanar
$[C_2mim]^+$	49.5	159.4	160.3	161.6	48.0	145.9	148.6	148.6
$[C_4mim]^+$	49.5	159.4	154.1	159.2	48.0	145.9	143.7	146.9
$[C_6mim]^+$	49.5	159.6	154.3	159.4	48.0	148.1	143.4	145.3
$[C_8mim]^+$	49.5	156.2	148.9	160.4	48.0	145.1	137.9	148.6
$[C_{10}mim]^+$	49.5	157.9	149.4	157.9	48.0	145.5	139.1	145.1

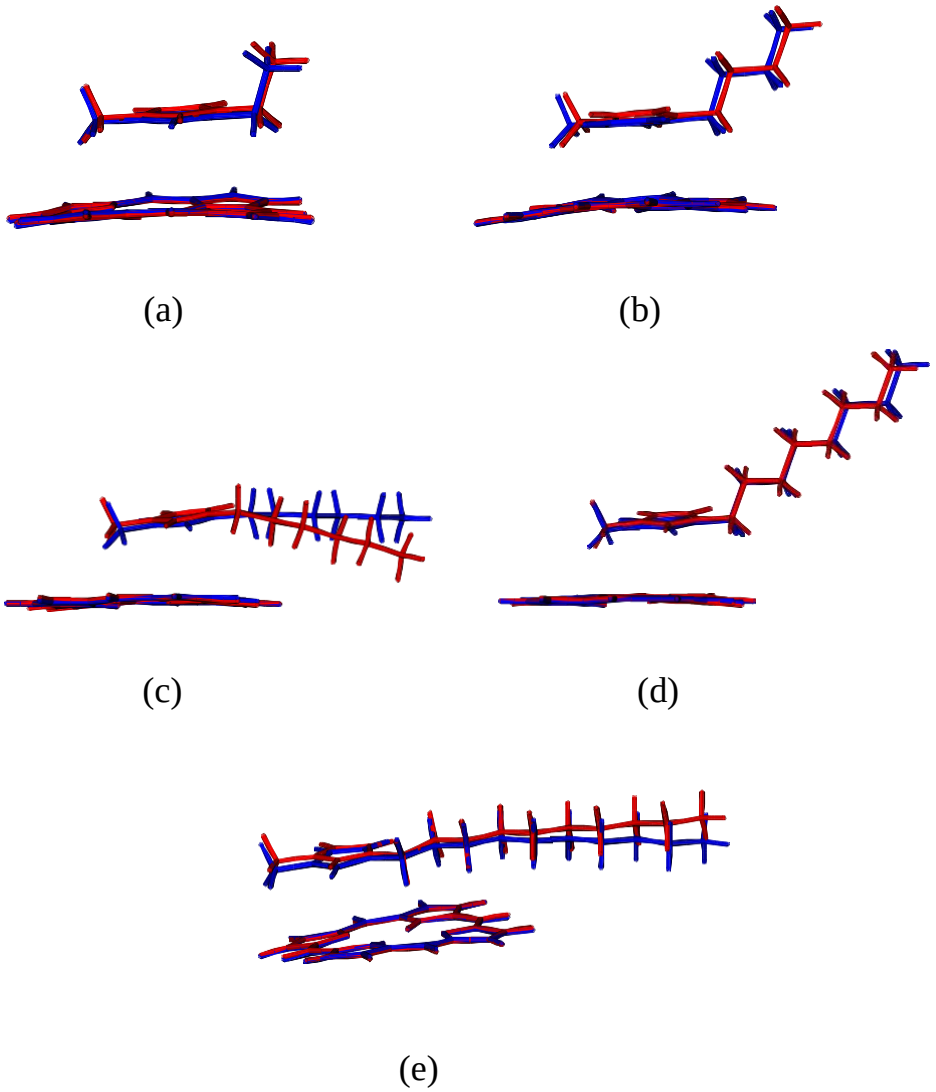

Figure S1 Alignment of $[C_n mim]^+$ FBP tail up (TU) optimized complexes at B3LYP-D2 (Blue) and M06 (Red) theories consisting of cations (a) $[C_2 mim]^+$ (b) $[C_4 mim]^+$ (c) $[C_6 mim]^+$ (d) $[C_8 mim]^+$ (e) $[C_{10} mim]^+$

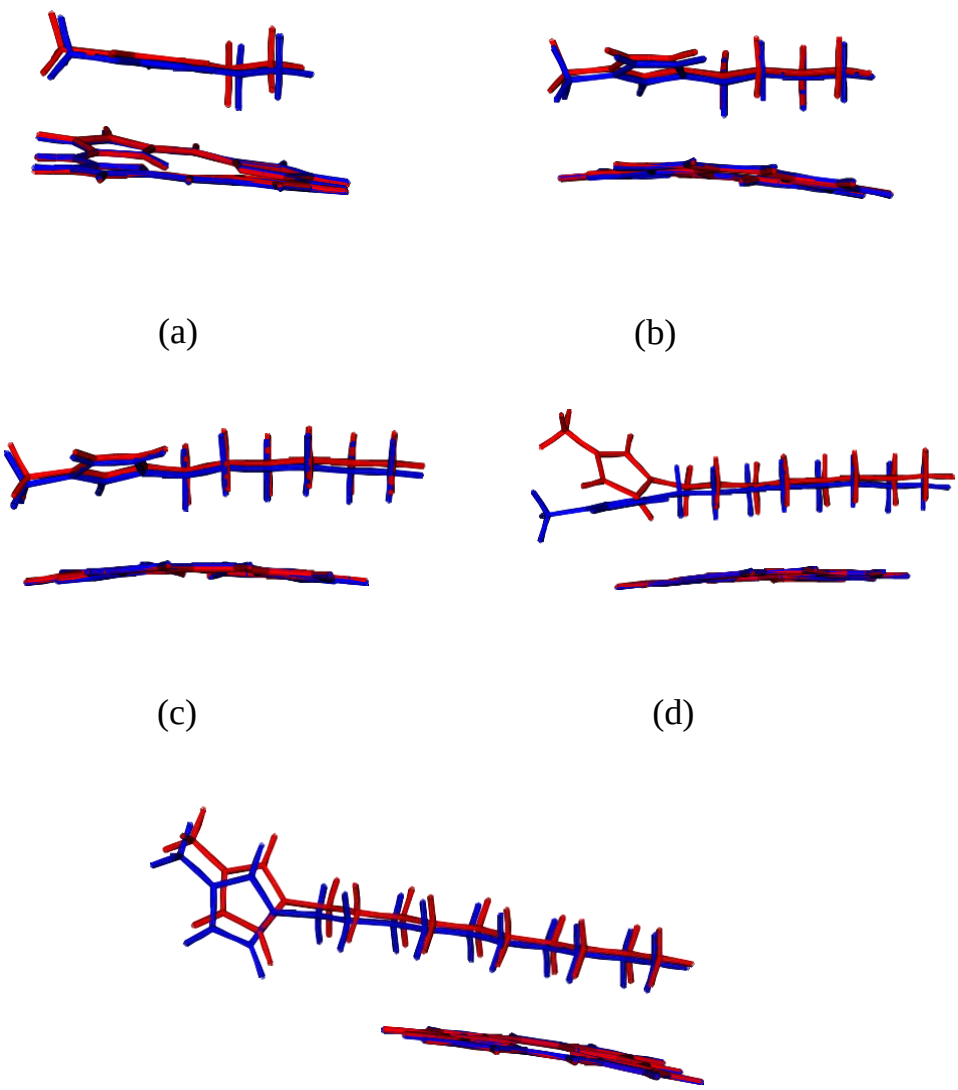

Figure S2 Alignment of $[C_n mim]^+$ FBP tail down (TD) optimized complexes at B3LYP-D2 (Blue) and M06 (Red) theories consisting of cations (a) $[C_2 mim]^+$ (b) $[C_4 mim]^+$ (c) $[C_6 mim]^+$ (d) $[C_8 mim]^+$ (e) $[C_{10} mim]^+$

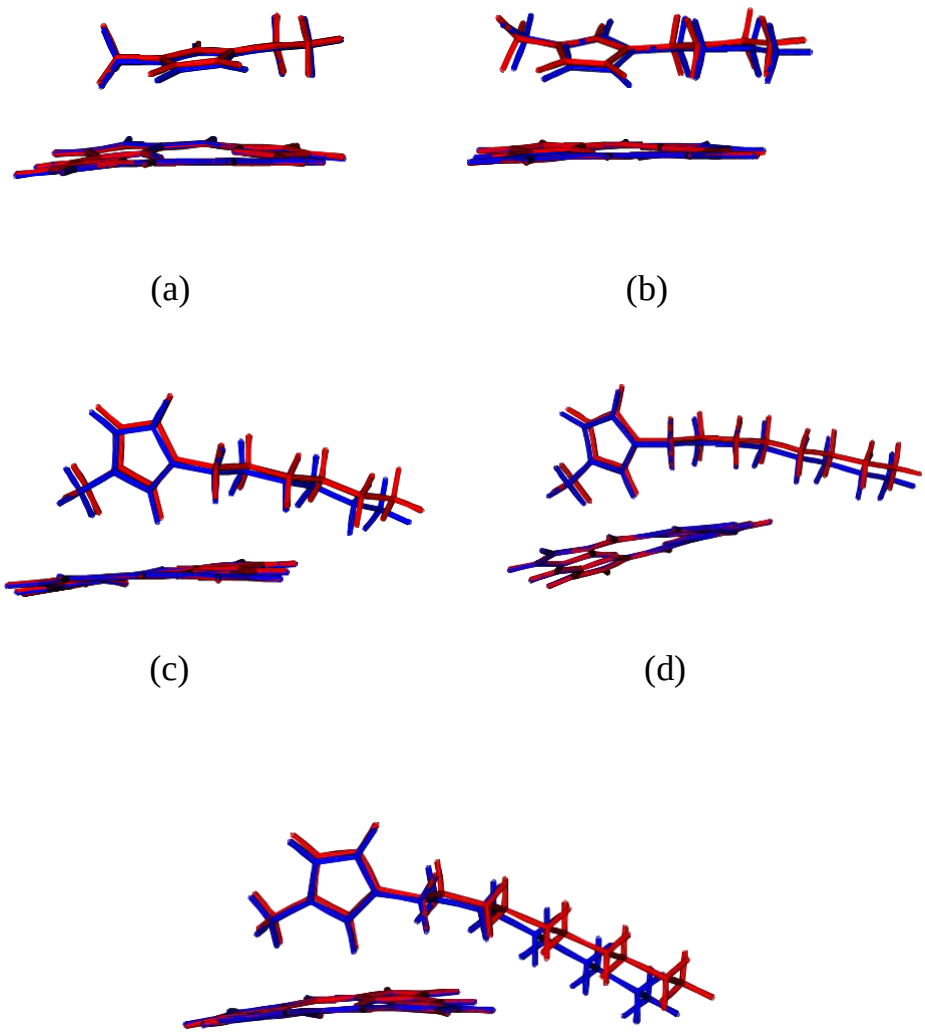

Figure S3 Alignment of $[C_n mim]^+$ FBP interplanar (IP) optimized complexes at B3LYP-D2 (Blue) and M06 (Red) theories consisting of cations (a) $[C_2 mim]^+$ (b) $[C_4 mim]^+$ (c) $[C_6 mim]^+$ (d) $[C_8 mim]^+$ (e) $[C_{10} mim]^+$

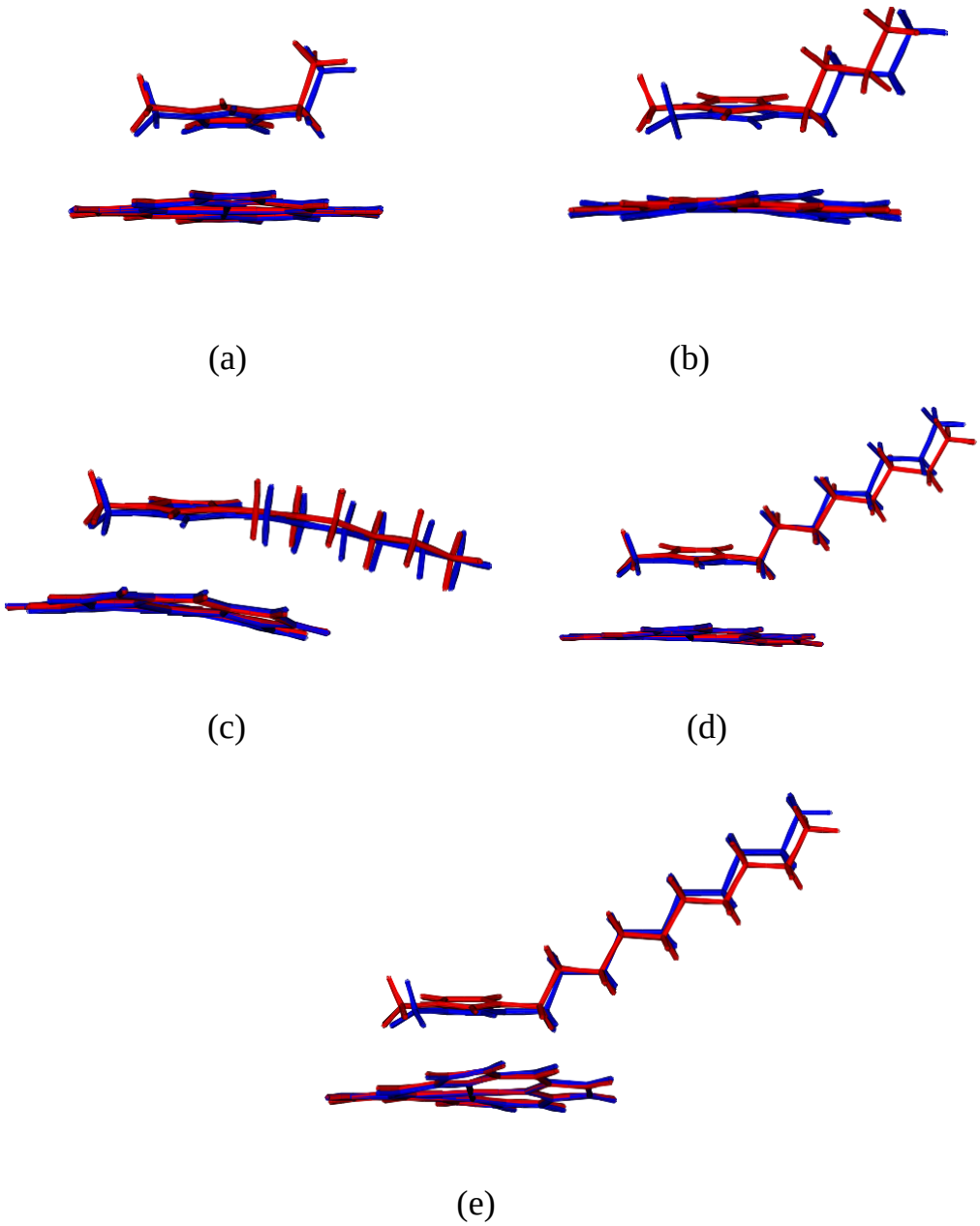

Figure S4 Alignment of $[C_n mim]^+$ FeP tail up (TU) optimized complexes at B3LYP-D2 (Blue) and M06 (Red) theories consisting of cations (a) $[C_2 mim]^+$ (b) $[C_4 mim]^+$ (c) $[C_6 mim]^+$ (d) $[C_8 mim]^+$ (e) $[C_{10} mim]^+$

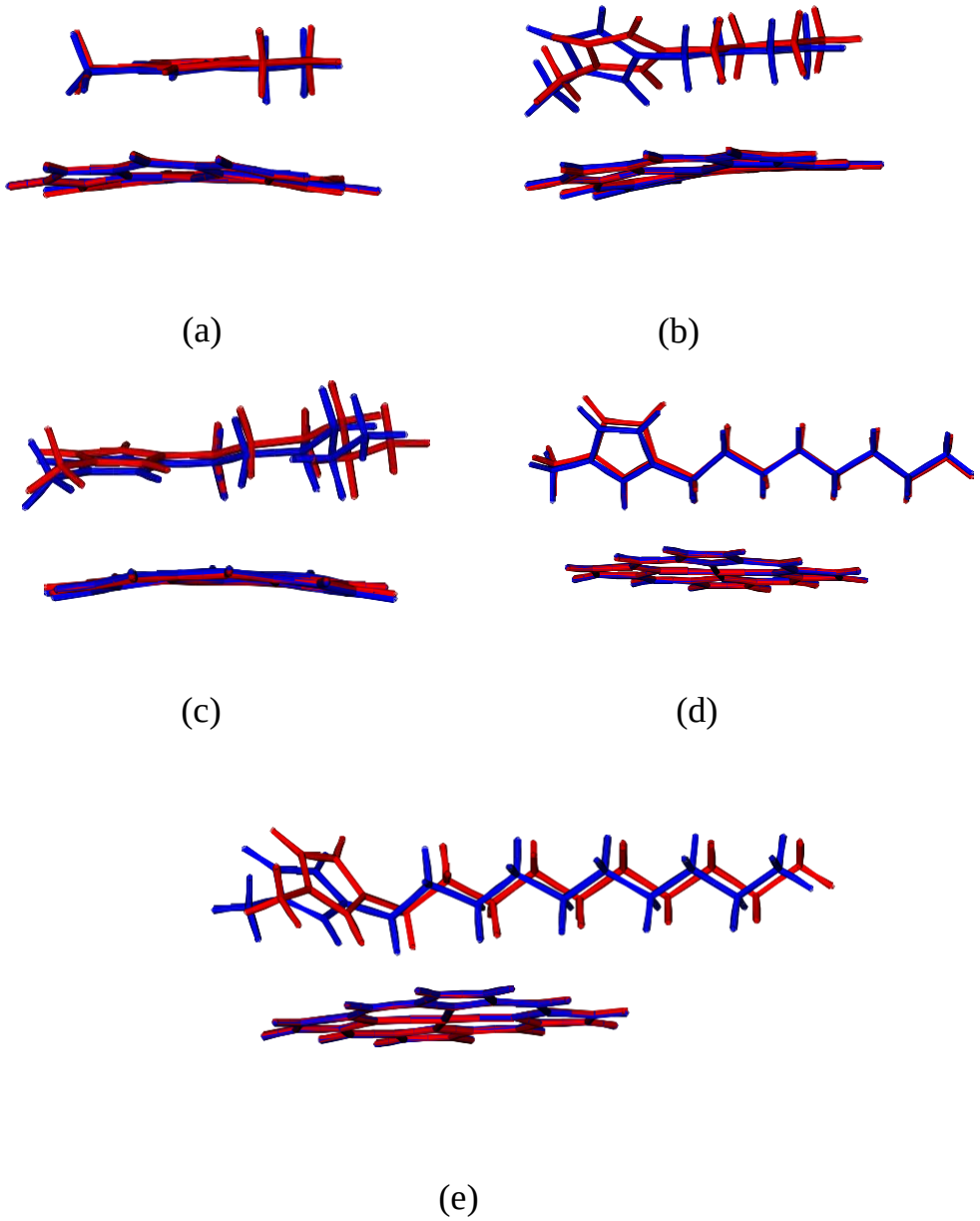

Figure S5 Alignment of $[C_n mim]^+$ FeP tail down (TD) optimized complexes at B3LYP-D2 (Blue) and M06 (Red) theories consisting of cations (a) $[C_2 mim]^+$ (b) $[C_4 mim]^+$ (c) $[C_6 mim]^+$ (d) $[C_8 mim]^+$ (e) $[C_{10} mim]^+$

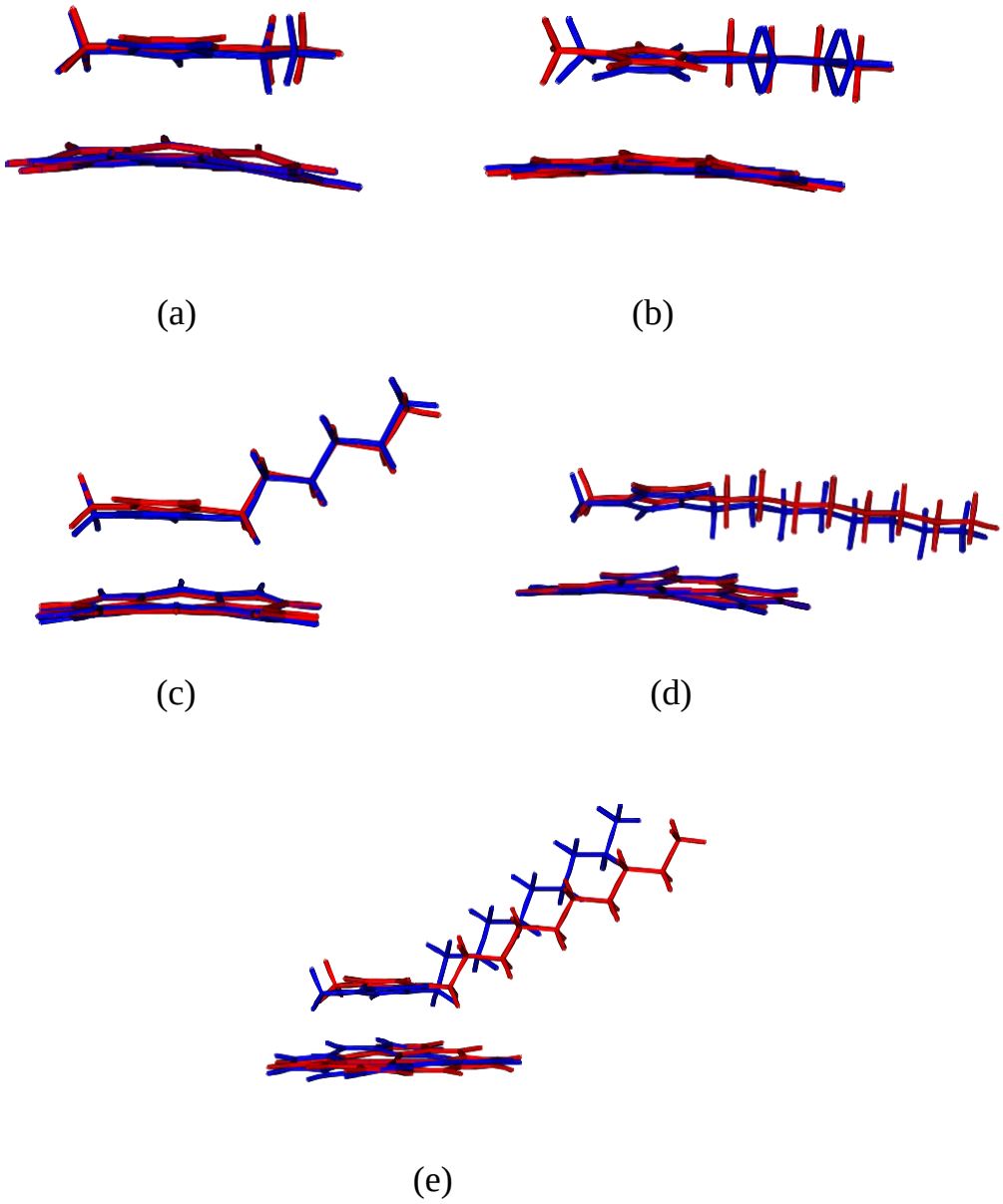

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Figure S6 Alignment of $[C_nmim]^+$ FeP interplanar (IP) optimized complexes at B3LYP-D2 (Blue) and M06 (Red) theories consisting of cations (a) $[C_2mim]^+$ (b) $[C_4mim]^+$ (c) $[C_6mim]^+$ (d) $[C_8mim]^+$ (e) $[C_{10}mim]^+$