Supplementary material 1

Values of the parameters in CVFF and CLAYFF force fields are shown in Tables S1-S5 [45-46].

Table S1 Masses and Charges

Items	Species	Styles	Masses (g/mol)	Charges (e)
1	Hydrogen bonded to C	h	1.007970	0.1
2	Sp3 carbon in methyl (CH3) group	c3	12.011150	-0.3
3	Sp3 carbon bonded to 1 H, 3 C atoms	c1	12.011150	-0.1
4	Sp3 carbon bonded to 2 H, 2 C atoms	c2	12.011150	-0.2
5	Zeolite oxygen	oz	15.999400	-1.05
6	Hydroxyl oxygen	oh	15.999400	-0.95
7	Zeolite silicon	sz	28.086000	2.1
8	Hydroxyl hydrogen	ho	1.007970	0.425

Table S2 Pair Coefficients

Items	Styles	Constant values	
		ε (Kcal/mol)	σ (nm)
1	h	0.0380000011	0.24499714540
2	c3	0.0389999952	0.38754094636
3	c1	0.0380000011	0.38754094636
4	c2	0.0389999952	0.38754094636
5	oz	0.1554000000	0.31655413253
6	oh	0.1554000000	0.31655413253
7	sz	0.0000018405	0.33020270089
8	ho	0.0000000000	0.00000000000

Table S3 Bond Coefficients

Items	Styles	Constant values	
		k_b (Kcal/mol·Å^2)	r_0 (nm)
1	h-c3	340.6175	0.11050
2	c3-c1	322.7158	0.15260
3	h-c1	340.6175	0.11050
4	c1-c2	322.7158	0.15260
5	h-c2	340.6175	0.11050
6	c1-c1	322.7158	0.15260
7	c2-c2	322.7158	0.15260
8	oh-ho	554.1349	0.10000

Table S4 Angle Coefficients

Items	Styles	Constant values	
		$k_a\ (Kcal/mol)$	θ_0 (°)
1	h-c3-c1	44.4000	110.0000
2	h-c3-h	39.5000	106.4000
3	h-c1-c3	44.4000	110.0000
4	c3-c1-c3	46.6000	110.5000
5	c3-c1-c2	46.6000	110.5000
6	h-c1-c2	44.4000	110.0000
7	c1-c2-c1	46.6000	110.5000
8	h-c2-c1	44.4000	110.0000
9	h-c3-h	39.5000	106.4000
10	c2-c1-c2	46.6000	110.5000
11	c1-c1-c2	46.6000	110.5000
12	h-c1-c1	44.4000	110.0000
13	c3-c1-c1	46.6000	110.5000
14	c1-c2-c2	46.6000	110.5000
15	h-c1-c1	44.4000	110.0000
16	sz-oh-ho	30.0000	109.4700

Table S5 Torsion Coefficients

Items	Styles	Constant values		
		k_t (Kcal/mol)	n	ϕ_0 (°)
1	h-c3-c1-h	0.1581	3	180
2	h-c3-c1-c3	0.1581	3	180
3	h-c3-c1-c2	0.1581	3	180
4	c3-c1-c2-c1	0.1581	3	180
5	c3-c1-c2-h	0.1581	3	180
6	h-c1-c2-c1	0.1581	3	180
7	h-c1-c2-h	0.1581	3	180
8	c2-c1-c2-c1	0.1581	3	180
9	c2-c1-c2-h	0.1581	3	180
10	c1-c1-c2-c1	0.1581	3	180
11	c1-c1-c2-h	0.1581	3	180
12	h-c3-c1-c1	0.1581	3	180
13	c2-c1-c1-c2	0.1581	3	180
14	h-c1-c1-c2	0.1581	3	180
15	c3-c1-c1-c2	0.1581	3	180
16	h-c1-c1-h	0.1581	3	180
17	h-c1-c1-c3	0.1581	3	180
18	c3-c1-c1-c3	0.1581	3	180
19	c1-c1-c2-c2	0.1581	3	180
20	h-c1-c2-c2	0.1581	3	180

21	c3-c1-c2-c2	0.1581	3	180
22	c1-c2-c2-c1	0.1581	3	180
23	h-c2-c2-c1	0.1581	3	180
24	h-c2-c2-h	0.1581	3	180
25	c2-c1-c2-c2	0.1581	3	180