

**Text S1.**

[ bondtypes ]

;i	j	func	b0	kb
CTL	CTL	1	0.15350	253630.0
CTL	OHL	1	0.14260	262840.0
CTL	H1L	1	0.10930	281080.0
CTL	N3L	1	0.14990	245680.0
CTL	HPL	1	0.10910	283420.0
OHL	HOL	1	0.09740	309280.0

[ angletypes ]

;i	j	k	func	th0	cth
CTL	CTL	N3L	1	114.3200	539.3200
CTL	CTL	HPL	1	111.7400	385.1000
CTL	OHL	HOL	1	108.1600	394.0500
CTL	CTL	OHL	1	109.4300	566.6800
CTL	CTL	H1L	1	110.0700	387.9400
CTL	N3L	CTL	1	110.6400	525.8500
OHL	CTL	H1L	1	109.8800	426.5200
N3L	CTL	HPL	1	107.9100	410.2000
H1L	CTL	H1L	1	109.5500	327.8600
HPL	CTL	HPL	1	110.7400	326.6900

[ dihedraltypes ]

;i	j	k	l	func	phase	kd	pn
CTL	CTL	N3L	CTL	9	0.0	1.77466	2
CTL	CTL	N3L	CTL	9	0.0	0.395553	3
CTL	CTL	OHL	HOL	9	180.0	2.32803	1
CTL	CTL	OHL	HOL	9	0.0	2.56256	2
CTL	CTL	OHL	HOL	9	0.0	1.44623	3
CTL	N3L	CTL	HPL	9	0.0	0.898473	3
OHL	CTL	CTL	N3L	9	180.0	4.80502	1
OHL	CTL	CTL	N3L	9	0.0	1.13979	2
OHL	CTL	CTL	N3L	9	0.0	1.65992	3
OHL	CTL	CTL	HPL	9	0.0	0.829962	3
H1L	CTL	CTL	N3L	9	0.0	0.829962	3
H1L	CTL	CTL	HPL	9	0.0	0.141981	3
H1L	CTL	OHL	HOL	9	0.0	0.723115	3