Table S3. Force field parameters for HMBPP.

Atom Name	Charge	AMBER GAFF Atom type
O1	-0.905	o
O2	-0.905	o
O3	-0.905	o
P1	1.206	p5
O4	-0.568	os
O5	-0.893	o
O6	-0.893	o
P2	1.345	p5
O7	-0.651	os
C1	0.493	c3
H1	-0.056	h1
H2	-0.056	h1
C2	-0.408	c2
H3	0.128	ha
C3	0.009	c2
C4	-0.101	c3
H4	-0.004	hc
H5	-0.004	hc
H6	-0.004	hc
C5	0.563	c3
H7	-0.214	h1
H8	-0.214	h1
O8	-0.963	o