

Bond type	Atom 1	Atom 2
C3-C2'	-0.05	-0.01
	0.04	-0.04
	-0.06	-0.03
	0.08	-0.04
C3-O'	0.39	0.09
C3-N'	0.30	0.13
	0.33	0.16
	0.28	0.17

(a) *Pol-RC40*

Bond type	Atom 1	Atom 2
C3-C1'	-0.03	-0.42
C3-O'	0.44	0.02
	0.51	0.03
	0.45	0.04
	0.40	0.04
	0.40	0.07
C3-N'	0.30	0.08
	0.26	0.14
C2-C2'	-0.02	0.03
	0.02	-0.05
	-0.05	-0.00
	0.01	0.00
C1-O'	-0.00	0.09

(c) *Pol-RC60*

Bond type	Atom 1	Atom 2
C3-O'	0.43	0.06
	0.59	0.05
	0.46	0.05
C3-N'	0.32	0.17
	0.28	0.15
	0.32	0.11
	0.31	0.13
	0.46	0.00
C2-C2'	-0.05	0.06
	0.06	0.03
	0.00	0.01
	-0.02	-0.00
C1-O'	-0.01	0.15

(b) *Pol-RC50*

Bond type	Atom 1	Atom 2
C3-O'	0.36	-0.01
	0.36	0.01
	0.40	0.04
	0.38	0.03
	0.38	0.00
	0.39	-0.01
	0.39	0.02
	0.40	0.06
C2-C2'	0.00	-0.00
	-0.07	-0.04

(d) *Pol-III'*

Table 1: Difference between Bader charges before and after polymerization of the atoms which form bonds during polymerization for each of the polymers obtained from MD.