Supplementary data

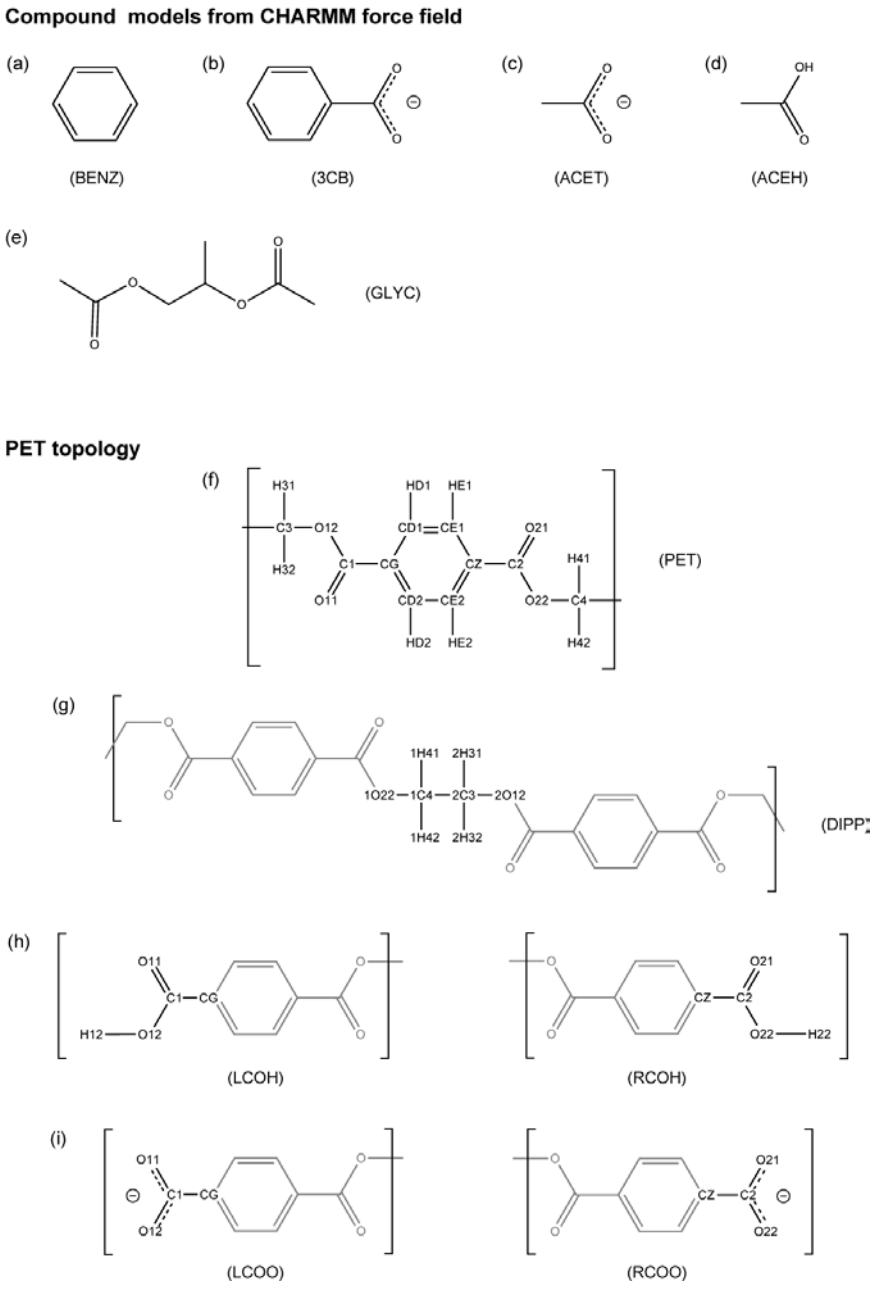
Atomic coordinates for PET monomers as well as topology and parameter files needed to perform MD simulations of PET polymers are provided. Topology files can be used to generate PET polymers with the plugin *psfgen* available in the VMD program (1). Parameter files comply with the functional form of CHARMM force field (2).

(1) W. Humphrey *et al.*, *J. Mol. Graphics*, 1996, **14**, 3338.

(2) A. MacKerell Jr. *et al.*, *J. Phys. Chem. B*, 1998,**102**, 35863616.

PET atomic model

Figure S1. The figure shows the CHARMM compound models (a) benzene, (b) deprotonated benzoic acid, (c) deprotonated acetic acid, (d) protonated acetic acid, and (e) propane-1,2-diyl diacetate. These compound models were used to build models for (f) PET monomer, (g) juncture between PET monomers, (h) protonated terminal residues, and (g) deprotonated terminal residues. CHARMM abbreviations are shown in parenthesis.



Atomic coordinates for PET monomer

REMARK	Coordinates for PET monomer in TRANS conformation										
REMARK	For CIS isomer, change the following coordinates										
REMARK		O12				27.653	-4.733	0.000			
REMARK		O11				30.840	-4.733	0.000			
REMARK		C3				27.653	-2.893	0.000			
REMARK		H31				28.223	-2.564	0.931			
REMARK		H32				28.107	-2.564	-1.012			
ATOM	1	CD1	PET	T	1	30.840	-8.412	0.000	1.00	0.00	TR	C
ATOM	2	HD1	PET	T	1	31.794	-7.862	0.000	1.00	0.00	TR	H
ATOM	3	CE1	PET	T	1	30.840	-10.252	0.000	1.00	0.00	TR	C
ATOM	4	HE1	PET	T	1	31.794	-10.803	0.000	1.00	0.00	TR	H
ATOM	5	CD2	PET	T	1	27.653	-8.412	0.000	1.00	0.00	TR	C
ATOM	6	HD2	PET	T	1	26.699	-7.862	0.000	1.00	0.00	TR	H
ATOM	7	CE2	PET	T	1	27.653	-10.252	0.000	1.00	0.00	TR	C
ATOM	8	HE2	PET	T	1	26.699	-10.803	0.000	1.00	0.00	TR	H
ATOM	9	CG	PET	T	1	29.246	-7.492	0.000	1.00	0.00	TR	C
ATOM	10	C1	PET	T	1	29.246	-5.653	0.000	1.00	0.00	TR	C
ATOM	11	O12	PET	T	1	30.840	-4.733	0.000	1.00	0.00	TR	O
ATOM	12	O11	PET	T	1	27.653	-4.733	0.000	1.00	0.00	TR	O
ATOM	13	C3	PET	T	1	30.840	-2.893	0.000	1.00	0.00	TR	C
ATOM	14	H31	PET	T	1	31.700	-2.564	0.931	1.00	0.00	TR	H
ATOM	15	H32	PET	T	1	31.700	-2.564	-1.012	1.00	0.00	TR	H
ATOM	16	CZ	PET	T	1	29.246	-11.172	0.000	1.00	0.00	TR	C
ATOM	17	C2	PET	T	1	29.246	-13.012	0.000	1.00	0.00	TR	C
ATOM	18	O21	PET	T	1	30.840	-13.932	0.000	1.00	0.00	TR	O
ATOM	19	O22	PET	T	1	27.653	-13.932	0.000	1.00	0.00	TR	O
ATOM	20	C4	PET	T	1	27.653	-15.772	0.000	1.00	0.00	TR	C
ATOM	21	H41	PET	T	1	27.153	-16.101	0.931	1.00	0.00	TR	H
ATOM	22	H42	PET	T	1	27.153	-16.034	-1.012	1.00	0.00	TR	H

PET topology

* <CHARMM22 topology file for PET>

27 1

MASS	1	H	1.008	H	! nonpolar H
MASS	2	HAL2	1.008	H	! nonpolar H
MASS	3	HP	1.008	H	! aromatic H
MASS	4	CAP	12.011	C	! aromatic C
MASS	5	CC	12.011	C	! carbonyl C, asn,asp,gln,glu,cter,ct2
MASS	6	CD	12.011	C	! carbonyl C, pres aspp,glup,ct1
MASS	7	CL	12.011	C	! carbonyl C (acetic acid/methyl acetate)
MASS	8	CTL2	12.011	C	! aliphatic sp3 C for CH2
MASS	9	OC	15.999	O	! carboxylate oxygen
MASS	10	OB	15.999	O	! carbonyl oxygen in acetic acid
MASS	11	OBL	15.999	O	! acetic acid carboxyl oxygen (e. to protein OB)
MASS	12	OH1	15.999	O	! hydroxyl oxygen
MASS	13	OSL	15.999	O	! ester oxygen

AUTO ANGLES DIHE

RESI PET		0.0	! topology for PET			
GROUP						
ATOM	CD1	CAP	-0.115			
ATOM	HD1	HP	0.115			
GROUP						
ATOM	CE1	CAP	-0.115			
ATOM	HE1	HP	0.115			
GROUP						
ATOM	CD2	CAP	-0.115			
ATOM	HD2	HP	0.115			
GROUP						
ATOM	CE2	CAP	-0.115			
ATOM	HE2	HP	0.115			
GROUP						
ATOM	CG	CAP	0.10			
ATOM	C1	CL	0.63			
ATOM	O11	OBL	-0.52			
ATOM	O12	OSL	-0.34			
ATOM	C3	CTL2	-0.05			
ATOM	H31	HAL2	0.09			
ATOM	H32	HAL2	0.09			
GROUP						
ATOM	CZ	CAP	0.10			
ATOM	C2	CL	0.63			
ATOM	O21	OBL	-0.52			
ATOM	O22	OSL	-0.34			
ATOM	C4	CTL2	-0.05			
ATOM	H41	HAL2	0.09			
ATOM	H42	HAL2	0.09			
BOND	C3	H31	C3	H32	C3	O12
BOND	O12	C1	C1	CG		
BOND	C4 H41	C4	H42	C4	O22	
BOND	O22	C2	C2	CZ		
BOND	CD1	HD1	CD2	HD2		
BOND	CE1	HE1	CE2	HE2		
BOND	CD1	CE1	CG	CD2	CE2	CZ
DOUBLE	O11	C1	C2	O21		
DOUBLE	CG	CD1	CE1	CZ	CD2	CE2
IMPR	C1	CG	O12	O11		
IMPR	C2	CZ	O22	O21		

PRES DIPP	0.0	! patch for two PET molecules. Patch must be 1-PET and 2-PET				
		! use in a patch statement				
		! follow with AUTOgenerate ANGLes DIHEdrals command				
BOND	1C4	2C3				
ANGLE	1H41	1C4	2C3	1H42	1C4	2C3
ANGLE	2H31	2C3	1C4	2H32	2C3	1C4
ANGLE	2O12	2C3	1C4	1O22	1C4	2C3
DIHE	1H41	1C4	2C3	2H31		
DIHE	1H41	1C4	2C3	2H32		
DIHE	1H41	1C4	2C3	2O12		
DIHE	1O22	1C4	2C3	2H31		
DIHE	1O22	1C4	2C3	2H32		
DIHE	1O22	1C4	2C3	2O12		
DIHE	1H42	1C4	2C3	2H31		
DIHE	1H42	1C4	2C3	2H32		
DIHE	1H42	1C4	2C3	2O12		

PRES LCOH		0.0	! protonated carboxyl group						
GROUP									
ATOM	C1	CD	0.75						
ATOM	O11	OB	-0.55						
ATOM	O12	OH1	-0.61						
ATOM	CG	CAP	-0.03						
ATOM	H12	H	0.44						
DELETE	ATOM	H31							
DELETE	ATOM	H32							
DELETE	ATOM	C3							
BOND	O12	H12							
ANGLE	H12	O12	C1						
DIHE	H12	O12	C1	O11					
DIHE	H12	O12	C1	CG					
IC	H12	O12	C1	O11	0.0000	0.0000	0.0000	0.0000	0.0000

PRES RCOH		0.0	! protonated carboxyl group						
GROUP									
ATOM	C2	CD	0.75						
ATOM	O21	OB	-0.55						
ATOM	O22	OH1	-0.61						
ATOM	CZ	CAP	-0.03						
ATOM	H22	H	0.44						
DELETE	ATOM	H41							
DELETE	ATOM	H42							
DELETE	ATOM	C4							
BOND	O22	H22							
ANGLE	H22	O22	C2						
DIHE	H22	O22	C2	O21					
DIHE	H22	O22	C2	CZ					
IC	H22	O22	C2	O21	0.0000	0.0000	0.0000	0.0000	0.0000

PRES LCOO		-1.0	! deprotonated carboxyl group
GROUP			
ATOM	C1	CC	0.62
ATOM	O11	OC	-0.76
ATOM	O12	OC	-0.76
ATOM	CG	CAP	-0.10
DELETE	ATOM	H31	
DELETE	ATOM	H32	
DELETE	ATOM	C3	

PRES RCOO		-1.0	! deprotonated carboxyl group
GROUP			
ATOM	C2	CC	0.62
ATOM	O21	OC	-0.76
ATOM	O22	OC	-0.76
ATOM	CZ	CAP	-0.10
DELETE	ATOM	H41	
DELETE	ATOM	H42	
DELETE	ATOM	C4	

PET parameters

BONDS

!V(bond) = Kb(b - b0)**2
!Kb: kcal/mole/A**2
!b0: A
!atom types Kb b0

CAP	CAP	370.000	1.3600	! from 3CB
CAP	HP	340.000	1.0800	! from 3CB
CAP	CC	200.000	1.5000	! from 3CB
CAP	CD	200.000	1.5000	! from 3CB
CAP	CL	200.000	1.5000	! from 3CB
CC	OC	525.000	1.2600	! from ACET
CD	OB	750.000	1.2200	! from ACEH
CD	OH1	230.000	1.4000	! from ACEH
CL	OBL	750.000	1.2200	! from GLYC
CL	OSL	150.000	1.3340	! from GLYC
CTL2	CTL2	222.500	1.5300	! from GLYC
CTL2	HAL2	309.000	1.1110	! from GLYC
CTL2	OSL	340.000	1.4300	! from GLYC
H	OH1	545.000	0.9600	! from ACEH

ANGLES

!V(angle) = Ktheta(Theta - Theta0)**2
!Ktheta: kcal/mole/rad**2
!Theta0: degrees
!Kub: kcal/mole/A**2 (Urey-Bradley)
!S0: A

!atom types			Ktheta	Theta0	Kub	S0	
CAP	CAP	CAP	90.00	122.00	30.00	2.38800	! from 3CB
CAP	CAP	HP	30.00	119.00	22.00	2.15250	! from 3CB
CAP	CAP	CC	40.00	119.00	35.00	2.41620	! from 3CB
CAP	CAP	CD	40.00	119.00	35.00	2.41620	! from 3CB
CAP	CAP	CL	40.00	119.00	35.00	2.41620	! from 3CB
CAP	CC	OC	40.00	118.00	50.00	2.38800	! from 3CB
CAP	CD	OB	70.000	125.00	20.00	2.44200	! from ACEH
CAP	CD	OH1	55.000	110.50			! from ACEH
CAP	CL	OBL	70.000	125.00	20.00	2.44200	! from GLYC
CAP	CL	OSL	55.000	109.00	20.00	2.32600	! from GLYC
CD	OH1	H	55.000	115.00			! from ACEH
CL	OSL	CTL2	40.000	109.60	30.00	2.26510	! from GLYC
CTL2	CTL2	HAL2	26.500	110.10	22.53	2.17900	! from GLYC
CTL2	CTL2	OSL	75.700	110.10			! from GLYC
HAL2	CTL2	HAL2	35.500	109.00	5.40	1.80200	! from GLYC
HAL2	CTL2	OSL	60.000	109.50			! from GLYC
OBL	CL	OSL	90.000	125.90	160.00	2.25760	! from GLYC
OB	CD	OH1	50.000	123.00	210.00	2.26200	! from ACEH
OC	CC	OC	100.000	124.00	70.00	2.22500	! from ACET

DIHEDRALS

!V(dihedral) = Kchi(1 + cos(n(chi) - delta))
!Kchi: kcal/mole
!n: multiplicity
!delta: degrees

!atom types				Kchi	n	delta	
CAP	CAP	CAP	CAP	1.20	2	180.00	! from 3CB
CC	CAP	CAP	CAP	3.10	2	180.00	! from 3CB
CD	CAP	CAP	CAP	3.10	2	180.00	! from 3CB
CL	CAP	CAP	CAP	3.10	2	180.00	! from 3CB
OC	CC	CAP	CAP	3.10	2	180.00	! from 3CB
OSL	CL	CAP	CAP	3.10	2	180.00	! from 3CB
OBL	CL	CAP	CAP	3.10	2	180.00	! from 3CB
OH1	CD	CAP	CAP	3.10	2	180.00	! from 3CB
OB	CD	CAP	CAP	3.10	2	180.00	! from 3CB
HP	CAP	CAP	CAP	4.20	2	180.00	! from 3CB
HP	CAP	CAP	CC	4.20	2	180.00	! from 3CB
HP	CAP	CAP	CD	4.20	2	180.00	! from 3CB
HP	CAP	CAP	CL	4.20	2	180.00	! from 3CB
HP	CAP	CAP	HP	1.90	2	180.00	! from 3CB
OBL	CL	OSL	CTL2	3.85	2	180.00	! from GLYC
X	CD	OH1	X	2.05	2	180.00	! from ACEH
X	CL	OSL	X	2.05	2	180.00	! from GLYC
CTL2	CTL2	OSL	CL	0.07	1	180.00	! from GLYC
X	CTL2	OSL	X	0.00	3	0.00	! from GLYC
X	CTL2	CTL2	X	0.20	3	0.00	! from GLYC

IMPROPERS

!V(improper) = Kpsi(psi - psi0)**2
!Kpsi: kcal/mole/rad**2
!psi0: degrees
!note that the second column of numbers (0) is ignored

!atom types				Kpsi	psi0		
OC	X	X	CC	96.00	0	0.00	! from ACET
OBL	X	X	CL	100.00	0	0.00	! from GLYC
OB	X	X	CD	100.00	0	0.00	! from ACEH

NONBONDED

!V(Lennard-Jones) = Eps,i,j[(Rmin,i,j/ri,j)**12 - 2(Rmin,i,j/ri,j)**6]
!epsilon: kcal/mole, Eps,i,j = sqrt(eps,i * eps,j)
!Rmin/2: A, Rmin,i,j = Rmin/2,i + Rmin/2,j

!atom	ignored	epsilon	Rmin/2	ignored	eps,1-4	Rmin/2,1-4
H	0.0000	-0.0460	0.2245			
HAL2	0.0000	-0.0280	1.3400			
HP	0.0000	-0.0300	1.3582	0.0000	-0.0300	1.3582
CAP	0.0000	-0.0700	1.9924			
CC	0.0000	-0.0700	2.0000			
CD	0.0000	-0.0700	2.0000			
CL	0.0000	-0.0700	2.0000			
CTL2	0.0000	-0.0560	2.0100	0.0000	-0.0100	1.9000
OC	0.0000	-0.1200	1.7000			
OB	0.0000	-0.1200	1.7000	0.0000	-0.1200	1.4000
OBL	0.0000	-0.1200	1.7000	0.0000	-0.1200	1.4000
OH1	0.0000	-0.1521	1.7700			
OSL	0.0000	-0.1521	1.7700			