Electronic Supporting Information

Unraveling the aggregation effect on amorphous phase AIE luminogens: A computational study

Xiaoyan Zheng[a], Qian Peng[b,*] Lizhe Zhu[a], Yujun Xie[c], Xuhui Huang[a,*], Zhigang Shuai[d,*]

[a]Department of Chemistry, The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong

[b]Key Laboratory of Organic Solids, Beijing National Laboratory for Molecular Science (BNLMS), Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, P. R. China

[c]Department of Chemistry, Wuhan University, Wuhan 430072, P.R. China

[d]Key Laboratory of Organic OptoElectronics and Molecular Engineering, Department of Chemistry, Tsinghua University, Beijing 100084, P. R. China

Corresponding Author

* qpeng@iccas.ac.cn

* xuhuihuang@ust.hk

* zgshuai@tsinghua.edu.cn

Contents

I. Supplementary methods

1.1 Details of force field setup

All our MD simulations in this work were performed by GROMACS-4.5.4 package[1]. Excepting for Si atom in HPS molecule, all atom types and their structural parameters were taken from the general amber force field (GAFF)[2]. Due to the absent parameters for Si in GAFF, the force field parameters for Si atom were dealt separately as follows. We took the equilibrium bond lengths and bond angles involved Si atom from HPS crystal structure directly[3]. And the corresponding force constants of the bond stretching and angle bending were borrowed from the sp^3-hybridized carbon[4,5]. Due to the key roles of dihedral angles in AIE effects, we fitted the related dihedral angles by using quantum mechanism (QM) and molecular mechanism (MM) methods as follows. First, we truncated the representative fragment from HPS molecule (see Fig. S2a) and performed geometry optimization at B3LYP/6-31G* level[6] using Gaussian09 package[7]. Second, we scanned the dihedral angle C1-Si2-C3-C4 of this fragment at 5° interval and did geometry optimization at each step by QM method to obtain the QM energy profile (see Fig. S2b, blue). Third, we used the MM method to calculate the corresponding MM energy profile with each optimized structure obtained from QM calculation. Fourth, we fitted the energy difference between QM and MM energy profiles versus the dihedral angle using the Ryckaert-Bellemans function[8] to obtain new parameters of the dihedral angle. Then, we repeated steps 3 and 4 iteratively to optimize the dihedral angle parameters until the difference between QM and MM energy profiles within a threshold. It is obvious that the final obtained MM energy profile could well reproduce the QM energy profile, as shown in Fig. S2b. In addition, the non-bonded Lennard-Jones parameters of radius and well-depth for Si atom were assigned as 2.220 Å and 0.320 kcal/mol, respectively[9]. Here, the partial charge of all atoms in for both the fragment and HPS molecule were obtained by using the restrained electrostatic potential (RESP) fit method[10,11] at HF/6-31G* level[12]. The force field parameters for water were TIP3P[13].

1.2 Details of Force field validation

To validate the force filed parameters used here, we performed MD simulations of HPS molecular crystal[3]. The parameters of HPS unit cell were a = 9.53 Å, b = 10.04 Å, c = 16.31 Å, α = 77.150, β = 79.580, γ = 71.981. We constructed the triclinic supercell of HPS with size 5 × 5 × 5 in the a, b, and c dimensions by a replication of the original unit cell and used this supercell as the initial configuration for HPS crystal simulations (see Figure S3a). Then, we performed energy

minimization, followed by 2 ns equilibrium simulations with position restrains in three dimensions for all heavy atoms in the HPS supercell under NVT (T = 300 K) ensemble with temperature annealed from 50 to 300 K in the first 1 ns. Finally, we performed five independent 20 ns production MD simulations with different initial velocities under the NPT (T = 300 K and P = 1 bar) ensemble. The temperature and pressure were controlled by the velocity rescaling thermostat[14] and Berendsen barostat[15,16] respectively. The time constants of couplings for both temperature and pressure were 1.0 ps. For the electrostatic interactions, the reciprocal space summation was evaluated by the particle mesh Ewald (PME) method[17,18]. The direct space summation was computed at a cutoff distance of 1.2 nm. The cutoff distance for VDW interactions was 1.1 nm. All bond lengths were constrained via the LINCS algorithm[19]. Periodic boundary condition was applied in all three directions to minimize the edge effects in a finite system. Here, the time step of the HPS supercell simulation was 0.5 fs. The configurations were stored at a time interval 20 ps for the packing density calculations. In total, we collected 5000 MD conformations and calculated the packing density of each conformation. The obtained average packing density of HPS molecular crystal by MD simulations was 1260 g/L, with standard error of 6 g/L, which is highly similar to the experimental measurement (1246 g/L), see details in Figure S3b. These results demonstrated the applicability of our force field to the current study of amorphous HPS aggregates.

1.3 Definition of asphericity parameter (Ap)

To describe the aggregates morphology, we defined the asphericity parameter (Ap)[20-24]. The definition of Ap is: $Ap = \frac{\left(\lambda_1^2 - \lambda_2^2\right)^2 + \left(\lambda_1^2 - \lambda_3^2\right)^2 + \left(\lambda_3^2 - \lambda_2^2\right)^2}{2\left(\lambda_1^2 + \lambda_2^2 + \lambda_3^2\right)^2}$, where λ_1, λ_2, λ_3 are three eigenvalues of the radius of gyration tensor A of the aggregate. The radius of gyration tensor A was $A = \begin{bmatrix} S_{xx} & S_{xy} & S_{xz} \\ S_{yx} & S_{yy} & S_{yz} \\ S_{zx} & S_{zy} & S_{zz} \end{bmatrix}$, where $S_{xx} = \frac{1}{n}\sum_i \left(x_i - x_c\right)^2$, $S_{xy} = \frac{1}{n}\sum_i \left(x_i - x_c\right)\left(y_i - y_c\right)$. And, n represents the total number of atoms of the aggregate; x_i and x_c represent the coordinates of the ith atom and the center of mass of the aggregate, respectively. When Ap equals to 0, the aggregate morphology is a perfect sphere, while Ap is 1, it denotes a rod.

1.4 Details of QM/MM calculations

During the QM/MM calculations, the force field parameters for MM part were the same as those in

MD simulations. In QM region, the geometry optimization and frequency calculations for the ground (S_0) and excited (S_1) states of HPS molecule in QM region were performed at DFT/B3LYP/SV(P)[25] and TDDFT/B3LYP/SV(P) levels, respectively. Here, the electrostatic embedding scheme[26,27] was used in the QM/MM calculation. Specifically, the partial charge of each atom in MM region was incorporated into the one-electron part of the QM Hamiltonian and the QM/MM electrostatic interactions can be evaluated by the electrostatic potential of QM region and the partial charge in MM region. Thus, QM region could reflect the electronic states properties while MM region could take into account the environment effects. Here, the intermolecular charge transfer was neglected due to the larger intermolecular distances in amorphous HPS aggregates[5]. In addition, during the QM/MM geometry optimization, only atoms in QM region were free to relax, the others in MM region were frozen. We chose the numerical two-point displacement method to calculate the vibrational frequency, and the polarization effect of environment was included. Here, the absence of imaginary frequency for all conformations was carefully checked. No symmetric constraints were imposed during optimization.

1.5 Reorganization energy (λ) calculations

The reorganization energy (λ) is calculated by normal mode analysis[28,29], which is proved to be reasonable for describing HPS molecule[4,5]. Based on harmonic oscillator approximation, we used a summation over all normal modes: $\lambda_{gs} = \sum_{k=1}^{3n} \lambda_{gs,k} = \sum_{k=1}^{3n} \frac{1}{2} \omega_{gs,k}^2 \Delta D_k^2$ and $\lambda_{es} = \sum_{k=1}^{3n} \lambda_{es,k} = \sum_{k=1}^{3n} \frac{1}{2} \omega_{es,k}^2 \Delta D_k^2$ to describe λ of the ground/excited states (λ_{gs}/λ_{es}), where $\omega_{gs(es),k}$ is frequency of the k^{th} normal mode at ground (excited) state, and ΔD_k represents the displacement of the k^{th} normal mode along coordinates between minima of two states.

II. Supplementary discussions

Amorphous HPS aggregates formation process

To mimic amorphous HPS aggregates, we first performed the large-scale MD simulations to obtain the various conformations in aqueous solution. Our MD simulations are sufficiently long for HPS to reach stable amorphous states. The aggregation processes of HPS are illustrated by the representative snapshots extracted from one of each five MD trajectories for systems at different concentrations (see Fig. S3). Take the system with 60 HPS molecules for example, we observed that within 1 ns HPS monomers cluster into small and loosely packed aggregates, which further merge quickly into a large loosely packed aggregate (see the snapshot at 5 ns of Fig. S3a). Then, this large aggregate undergoes slow structural rearrangement to achieve densely packing (see Fig. S3a). Similar behaviors were observed for all other four systems (see Fig. S3b-S3e). These results demonstrate three characteristic stages of the aggregation: (i) formation of small aggregates at $t < 1$ ns; (ii) growth of small aggregates into one large aggregate at 1 ns $< t <$ 5 ns; (iii) structural reorganization process of each largest aggregate at $t >$ 5 ns.

The hydrophobic interactions play an important role in the aggregation process of HPS molecules. The time evolution of the number of water molecules around HPS aggregates (within 5 Å) averaged by five MD trajectories, at each concentration, are displayed in Fig. S4. It is clear that, for all five systems, the number of water molecules first decrease suddenly, and then reduce regularly until reach a platform. For system with 60 HPS molecules, the number of water molecules first decrease by 1070 within 1 ns, and then by 252 in the following 4 ns, finally reduce by only 158 within the last 20 ns production simulations. For system with 30 HPS molecules, the number of water molecules first decrease by 760 ($t < 1$ ns), and then by 281 (1 ns $< t <$ 5 ns), finally reduce by only 38 within the last 20 ns. It is clear that the number of water molecules for systems with higher HPS concentration decrease much faster than the lower ones. In addition, both the exposed surface area and volume of HPS aggregates at each concentration had a sharp decrease in the initial stage, and then reduce slowly to achieve equilibrium with almost constant surface area and volume, as shown in Fig. S5 and Fig. S6, respectively. What's more, the average volume of aggregates from Agg-60 to Agg-10 are 54.0, 36.3, 27.5, 18.7 and 9.6 nm^3, respectively. It is clear that the aggregate size and volume of HPS aggregates have a linear relationship.

The aggregation process can be divided into three characteristic stages: the first stage, $t < 1$ ns, is small aggregates formation process; the second stage, 1 ns $< t <$ 5 ns, is small aggregates growth process; and the final stage is the equilibrium process. During the aggregation process, the HPS molecules cluster first, and the size of aggregates grow accordingly. Due to the hydrophobic interactions, both the number of water molecules around HPS aggregates, the exposed surface areas

and volume of HPS aggregates reduce continuously. In addition, systems with higher concentration aggregate faster than the lower ones. Thus, the dynamics of the aggregation process and the size of the aggregates are heavily concentration dependent.

III. Supplementary Tables S1-S6

Table S1. The optimized bond lengths (in Å), bond angles (in degree), and dihedral angles (in degree) of one representative embedded HPS molecule of the amorphous HPS aggregate, at each size. S_0/S_1, and Δ represent the geometric parameters extracted from the ground/excited state, and the difference between two states, respectively. The index of each atom shown here is labeled in Figure S1.

	geometric	Agg-60			Agg-40			Agg-30			Agg-20			Agg-10			crystal (cal.)[a]			crystal (exper.)[b]
	parameter	S_0	S_1	Δ|	S_0	S_1	Δ	S_0	S_1	Δ	S_0	S_1	Δ	S_0	S_1	Δ	S_0	S_1	Δ	S_0
	Si-C2	1.901	1.882	-0.019	1.896	1.880	-0.016	1.895	1.886	-0.009	1.903	1.883	-0.020	1.885	1.871	-0.014	1.893	1.876	-0.017	1.862
	Si-C5	1.883	1.870	-0.013	1.902	1.887	-0.015	1.903	1.884	-0.019	1.903	1.891	-0.012	1.895	1.881	-0.014	1.902	1.888	-0.015	1.874
	Si-C30	1.898	1.907	0.009	1.896	1.905	0.009	1.898	1.909	0.011	1.898	1.909	0.011	1.901	1.908	0.007	1.9	1.909	0.009	1.864
	Si-C31	1.892	1.903	0.011	1.904	1.912	0.008	1.904	1.911	0.007	1.898	1.905	0.007	1.891	1.900	0.009	1.905	1.917	0.012	1.875
	C2-C3	1.376	1.444	0.068	1.372	1.436	0.064	1.375	1.437	0.062	1.376	1.449	0.073	1.372	1.441	0.069	1.371	1.445	0.074	1.358
	C4-C5	1.370	1.434	0.064	1.376	1.444	0.068	1.376	1.444	0.068	1.375	1.438	0.063	1.372	1.440	0.068	1.371	1.444	0.073	1.358
	C2-C19	1.479	1.452	-0.027	1.479	1.452	-0.027	1.481	1.454	-0.027	1.482	1.449	-0.033	1.473	1.443	-0.030	1.479	1.448	-0.03	1.479
	C5-C18	1.477	1.448	-0.029	1.482	1.451	-0.031	1.479	1.450	-0.029	1.483	1.457	-0.026	1.481	1.456	-0.025	1.481	1.453	-0.028	1.480
	C3-C4	1.513	1.444	-0.069	1.512	1.441	-0.071	1.515	1.446	-0.069	1.510	1.437	-0.073	1.512	1.440	-0.072	1.509	1.432	-0.077	1.501
	C3-C6	1.496	1.482	-0.014	1.496	1.483	-0.013	1.494	1.482	-0.012	1.496	1.481	-0.015	1.493	1.480	-0.013	1.497	1.484	-0.014	1.494
	C4-C7	1.489	1.474	-0.015	1.491	1.477	-0.014	1.496	1.479	-0.017	1.499	1.492	-0.007	1.494	1.481	-0.013	1.498	1.495	-0.003	1.487
	C5-Si-C2	93.03	91.53	-1.5	92.92	91.27	-1.65	92.32	90.66	-1.66	93.22	91.51	-1.71	92.52	90.83	-1.69	92.97	91.50	-1.46	93.21
	C30-Si-C31	115.09	112.88	-2.21	114.07	112.14	-1.93	113.76	111.97	-1.79	108.00	106.33	-1.67	114.07	112.17	-1.91	111.62	109.67	-1.95	111.65
	Si-C2-C3	106.55	108.67	2.12	106.79	108.52	1.73	107.26	108.99	1.73	105.90	107.72	1.78	107.11	108.66	1.55	106.87	108.46	1.59	106.33
	C2-C3-C4	116.41	114.74	-1.67	116.78	116.04	-0.74	116.77	115.88	-0.89	117.00	115.89	-1.10	116.15	115.35	-0.79	116.59	115.57	-1.02	117.02
	C3-C2-C19	129.69	128.33	-1.36	127.37	126.10	-1.27	128.52	127.30	-1.22	128.50	126.20	-2.34	129.07	127.37	-1.70	128.15	126.74	-1.41	127.46
	C4-C5-C18	127.97	126.65	-1.32	129.92	128.17	-1.75	129.54	127.80	-1.74	128.30	126.20	-2.07	127.51	126.87	-0.64	129.66	128.39	-1.27	129.30
2-	C3-C2-C19-C24	32.67	27.92	4.75	-31.29	-24.33	6.96	23.56	18.48	5.08	-20.78	-17.64	3.14	-43.36	-32.63	10.73	40.46	33.62	6.84	39.40
5-	C4-C5-C18-C25	20.26	17.13	3.13	-14.38	-14.07	0.31	24.72	23.14	1.58	-11.17	-9.11	2.06	-24.01	-19.02	4.99	-4.40	-1.87	2.53	3.95
3-	C2-C3-C6-C8	57.67	52.66	5.01	-55.56	-52.41	3.15	49.83	45.49	4.34	-63.97	-54.02	9.95	-56.39	-52.78	3.61	62.83	55.52	7.31	58.63
4-	C5-C4-C7-C17	56.96	50.81	6.15	-61.92	-58.02	3.9	56.16	54.33	1.83	-72.08	-70.85	1.23	-62.63	-53.80	8.83	83.89	85.82	1.93	79.75

[a]: ref.[5]; [b]: ref.[3]

Table S2. The optimized bond lengths (in Å), bond angles (in degree), and dihedral angles (in degree) of one representative exposed HPS molecule of the amorphous HPS aggregate, at each size. S_0/S_1, and Δ represent the geometric parameters extracted from the ground/excited state, and the difference between two states, respectively. The index of each atom shown here is labeled in Figure S1.

	geometric	Agg-60			Agg-40			Agg-30			Agg-20			Agg-10			crystal (cal.)[a]			crystal (exper.)[b]
	parameters	S_0	S_1	Δ	S_0	S_1	Δ	S_0	S_1	Δ	S_0	S_1	Δ	S_0	S_1	Δ	S_0	S_1	Δ	S_0
	Si-C2	1.893	1.879	-0.014	1.894	1.878	-0.016	1.898	1.886	-0.012	1.893	1.876	-0.017	1.895	1.874	-0.021	1.893	1.876	-0.017	1.862
	Si-C5	1.898	1.883	-0.015	1.893	1.880	-0.013	1.893	1.872	-0.021	1.897	1.882	-0.015	1.898	1.887	-0.011	1.902	1.888	-0.015	1.874
	Si-C30	1.894	1.905	0.011	1.893	1.909	0.016	1.896	1.908	0.012	1.894	1.906	0.012	1.900	1.909	0.009	1.900	1.909	0.009	1.864
	Si-C31	1.896	1.906	0.010	1.898	1.904	0.006	1.892	1.904	0.012	1.897	1.908	0.011	1.895	1.905	0.01	1.905	1.917	0.012	1.875
	C2-C3	1.373	1.444	0.071	1.372	1.439	0.067	1.373	1.437	0.064	1.374	1.444	0.07	1.374	1.446	0.072	1.371	1.445	0.074	1.358
	C4-C5	1.374	1.439	0.065	1.372	1.445	0.073	1.370	1.444	0.074	1.373	1.441	0.068	1.373	1.439	0.066	1.371	1.444	0.073	1.358
	C2-C19	1.481	1.451	-0.03	1.477	1.450	-0.027	1.481	1.455	-0.026	1.479	1.449	-0.03	1.479	1.448	-0.031	1.479	1.448	-0.03	1.479
	C5-C18	1.479	1.452	-0.027	1.483	1.453	-0.03	1.479	1.447	-0.032	1.480	1.454	-0.026	1.480	1.456	-0.024	1.481	1.453	-0.028	1.480
	C3-C4	1.512	1.440	-0.072	1.511	1.438	-0.073	1.509	1.437	-0.072	1.513	1.442	-0.071	1.509	1.437	-0.072	1.509	1.432	-0.077	1.501
	C3-C6	1.491	1.475	-0.016	1.490	1.484	-0.006	1.490	1.482	-0.008	1.494	1.479	-0.015	1.497	1.480	-0.017	1.497	1.484	-0.014	1.494
	C4-C7	1.496	1.485	-0.011	1.496	1.475	-0.021	1.495	1.478	-0.017	1.496	1.484	-0.012	1.495	1.484	-0.011	1.498	1.495	-0.003	1.487
	C5-Si-C2	92.72	91.10	-1.62	92.414	90.988	-1.426	93.10	91.32	-1.78	92.90	91.16	-1.74	93.22	91.19	-2.03	92.97	91.50	-1.46	93.21
	C30-Si-C31	111.18	108.96	-2.22	109.81	107.50	-2.31	112.16	109.74	-2.42	110.84	108.13	-2.71	110.67	108.35	-2.32	111.62	109.67	-1.95	111.65
	Si-C2-C3	107.02	108.73	1.71	107.32	109.11	1.79	106.18	108.07	1.89	106.82	108.78	1.96	106.19	108.42	2.23	106.87	108.46	1.59	106.33
	C2-C3-C4	116.72	115.66	-1.06	116.23	115.36	-0.87	117.22	116.26	-0.96	116.70	115.61	-1.09	117.07	115.57	-1.5	116.59	115.57	-1.02	117.02
	C3-C2-C19	126.85	125.59	-1.26	126.76	125.89	-0.87	128.58	127.43	-1.15	128.10	126.38	-1.72	129.12	126.46	-2.66	128.15	126.74	-1.41	127.46
	C4-C5-C18	128.13	126.65	-1.48	125.78	125.57	-0.21	127.34	126.25	-1.09	127.75	126.52	-1.23	128.58	127.31	-1.27	129.66	128.39	-1.27	129.30
2-	C3-C2-C19-C24	-36.13	-26.21	9.92	-45.09	-28.12	16.97	39.45	22.98	16.47	29.80	21.47	8.33	-28.10	-25.42	2.68	40.46	33.62	6.84	39.40
5-	C4-C5-C18-C25	-25.37	-18.86	6.51	-35.81	-24.88	10.93	24.32	20.10	4.22	27.45	20.74	6.71	-18.06	-18.83	0.77	-4.40	-1.87	2.53	3.95
3-	C2-C3-C6-C8	-49.59	-46.00	3.59	-51.25	-47.48	3.77	58.31	45.99	12.32	58.64	50.27	8.37	-62.49	-61.05	1.44	62.83	55.52	7.31	58.63
4-	C5-C4-C7-C17	-64.77	-57.42	7.35	-57.48	-54.19	3.29	66.02	65.24	0.78	60.77	54.37	6.4	-68.17	-49.98	18.19	83.89	85.82	1.93	79.75

[a]: ref.[5]; [b]: ref.[3]

Table S3. The averaged energies of HOMO and LUMO, and the corresponding energy gap (ΔE_{L-H}) at S_0 for five embedded and one exposed HPS molecules in amorphous HPS aggregates, at each size. The error bars are included in parenthesis.

system	HOMO (eV)	LUMO (eV)	ΔE_{L-H} (eV)
		embedded	
Agg-60	-4.97 (0.03)	-1.59 (0.06)	3.37 (0.04)
Agg-40	-5.10 (0.07)	-1.73 (0.06)	3.37 (0.07)
Agg-30	-4.90 (0.10)	-1.61 (0.10)	3.33 (0.08)
Agg-20	-4.97 (0.08)	-1.62 (0.08)	3.35 (0.05)
Agg-10	-5.07 (0.06)	-1.66 (0.04)	3.41 (0.06)
		exposed	
Agg-60	-5.33	-1.92	3.41
Agg-40	-5.29	-1.76	3.52
Agg-30	-5.34	-1.85	3.50
Agg-20	-5.09	-1.62	3.47
Agg-10	-5.29	-1.90	3.40

Table S4. The calculated peak values (in nm) of the vibrationally resolved absorption and emission spectra for five embedded and one exposed HPS molecules in amorphous HPS aggregates, at each size. The corresponding peak values for HPS crystal are included for comparison. The error bars are included in parenthesis.

system	absorption	emission	Stokes shift
		embedded	
Agg-60	437 (8)	550 (11)	113 (9)
Agg-40	447 (12)	552 (9)	105 (5)
Agg-30	455 (6)	559 (5)	104 (8)
Agg-20	444 (9)	553 (6)	108 (7)
Agg-10	425 (21)	564 (7)	139 (18)
		exposed	
Agg-60	408	581	173
Agg-40	389	605	216
Agg-30	355	625	270
Agg-20	414	561	147
Agg-10	395	590	195

[a]: ref.[5].

Table S5. The calculated adiabatic excitation energy (ΔE), oscillator strength (*f*), the electric transition dipole moment (EDM) and the assignment of S_1 for both five embedded (average) and one exposed HPS of the amorphous aggregates. The corresponding parameters for HPS in crystal are included for comparison. The error bars are included in parenthesis.

system	ΔE (eV)	*f*	EDM (D)	assignment
crystal (cal.)[a]	2.70	0.311	5.908	HOMO → LUMO 98.3%
		embedded		
Agg-60	2.60 (0.04)	0.28 (0.03)	5.69 (0.34)	HOMO → LUMO (98.6 ± 0.2)%
Agg-40	2.58 (0.05)	0.25 (0.03)	5.59 (0.32)	HOMO → LUMO (98.6 ± 0.1)%
Agg-30	2.54 (0.09)	0.27 (0.08)	5.66 (0.67)	HOMO → LUMO (98.5 ± 0.1)%
Agg-20	2.59 (0.03)	0.27 (0.02)	5.65 (0.18)	HOMO → LUMO (98.6 ± 0.1)%
Agg-10	2.60 (0.05)	0.25 (0.02)	4.65 (1.61)	HOMO → LUMO (98.6 ± 0.1)%
		exposed		
Agg-60	2.57	0.23	5.25	HOMO → LUMO (98.7%)
Agg-40	2.61	0.22	5.09	HOMO → LUMO (98.8%)
Agg-30	2.62	0.24	5.49	HOMO → LUMO (98.6%)
Agg-20	2.67	0.24	5.48	HOMO → LUMO (98.7%)
Agg-10	2.59	0.24	5.42	HOMO → LUMO (98.6%)

[a]: ref.[5].

IV. Supplementary Figures S1-S7

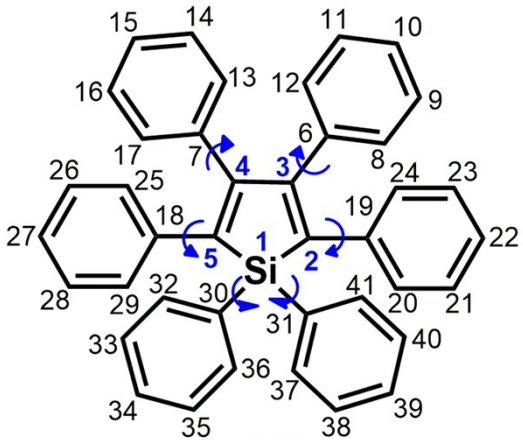

Figure S1. The molecular structure of HPS. The dihedral angles between the phenyl groups at 1,1,2,3,4,5-positions and the central silole ring are highlighted by arrows. And the atom index of all heavy atoms are labeled in the figure.

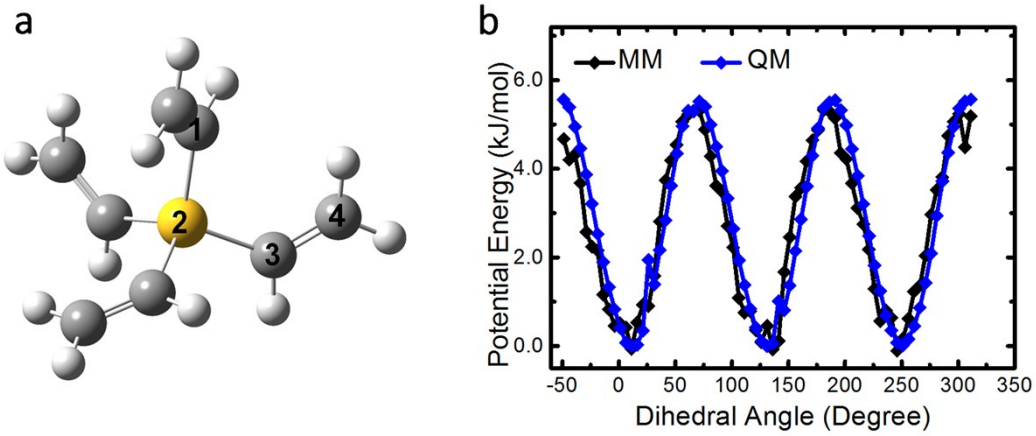

Figure S2 (a) The fragment truncated from HPS molecule for dihedral angles parameters fitting. One specific dihedral angle is labeled on the 3D structure. Atoms for Si, C and H are displayed in yellow, gray and white, respectively. (b) The calculated QM (blue) and MM (black) energy profiles of the dihedral angle C1-Si2-C3-C4.

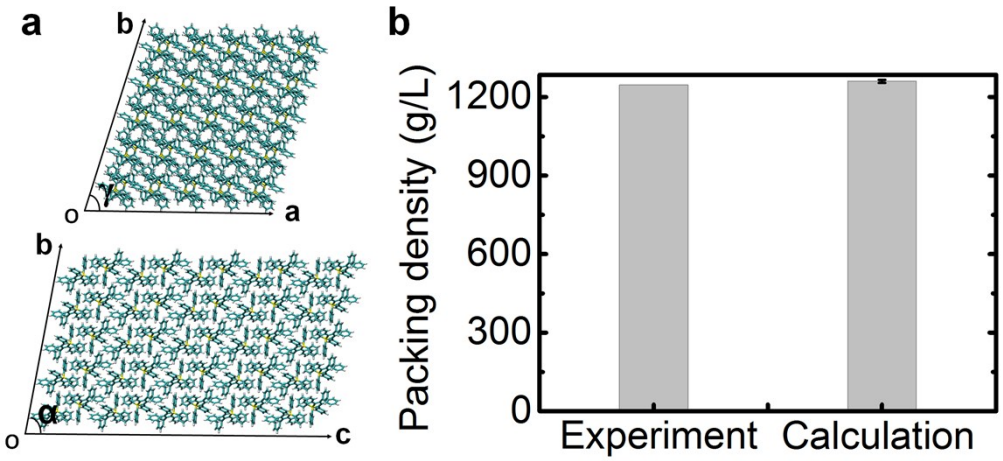

Figure S3. (a) Initial configuration of HPS molecular crystal for use in the MD simulations, with size 5 × 5 × 5 in the *a*, *b*, and *c* dimensions generated by a replication of the original unit cell. The *aob* (upper) and *boc* (lower) planes of the HPS supercell were displayed in the upper and lower panels of a. (b) The comparison of the packing density between the experimental measurement and MD calculations.

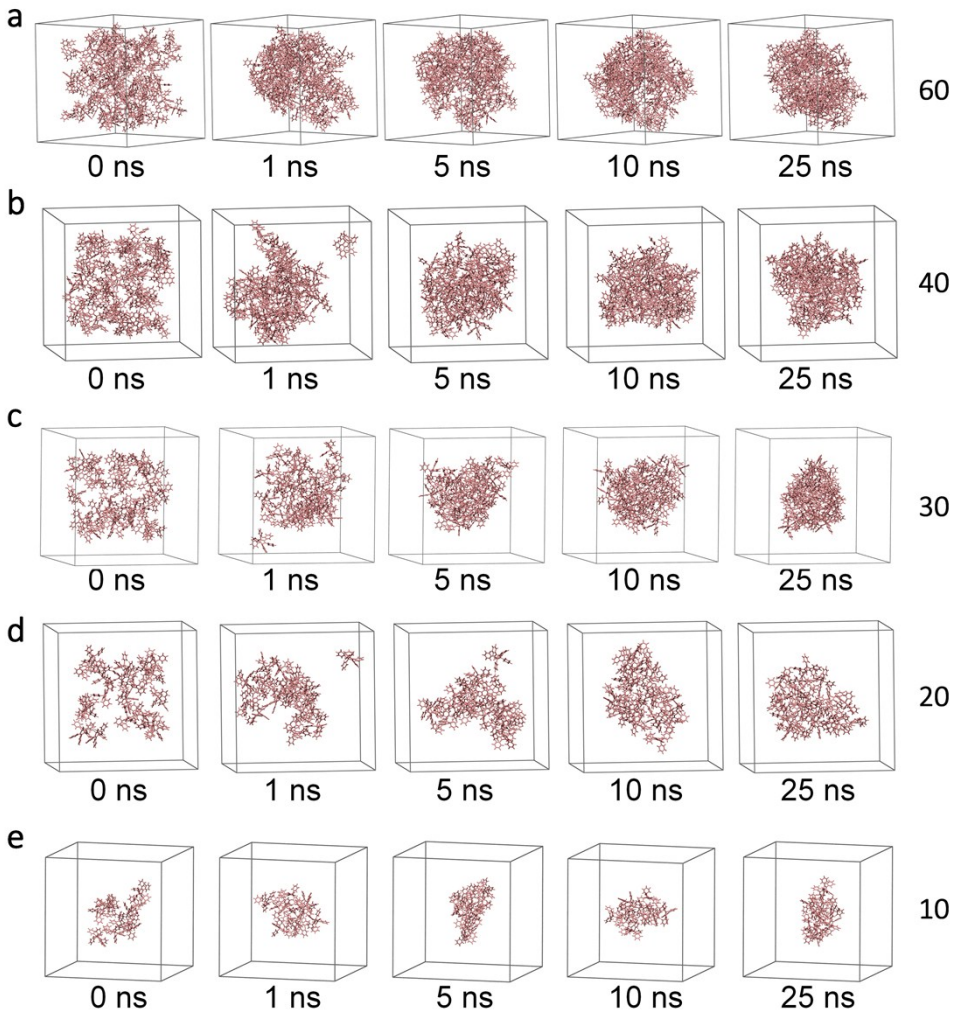

Figure S4 The representative snapshots extracted from one of the five MD trajectories, at each concentration, to show the aggregation process. Water molecules are not shown for clarity.

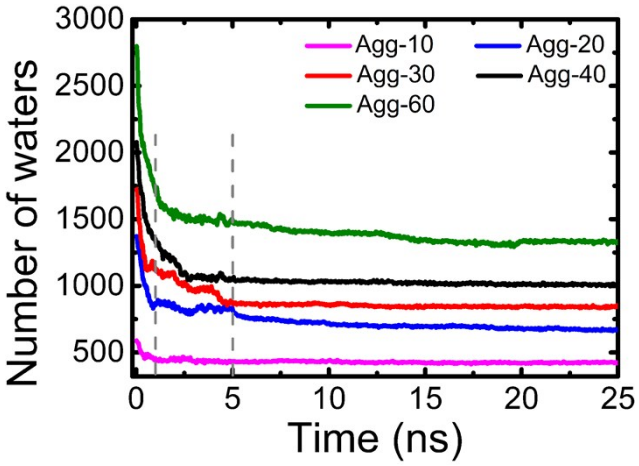

Figure S5 The time evolution of the number of water molecules (within 5 Å) around all amorphous HPS aggregates averaged by five MD trajectories, at each concentration. The different stages of the aggregation process are divided by the dashed lines.

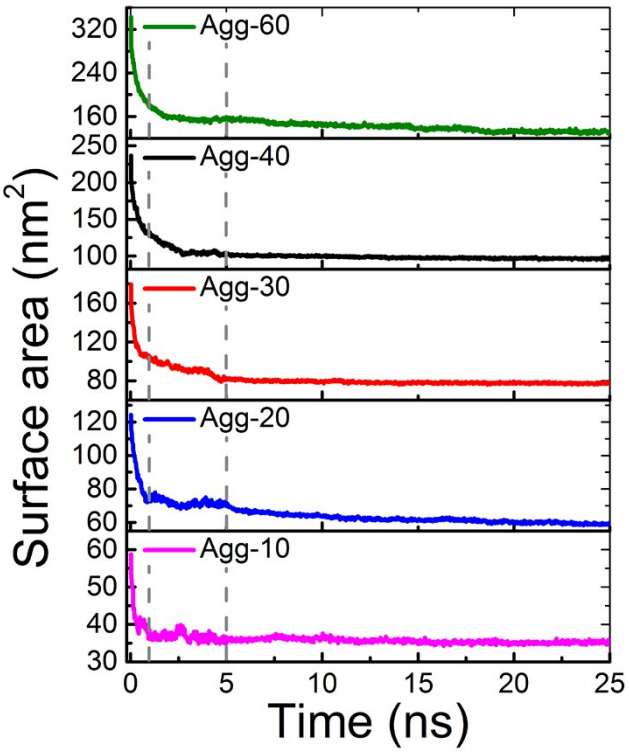

Figure S6 The time evolution of the exposed surface area of HPS aggregates averaged by five MD trajectories, at each concentration. The different stages of the aggregation process are divided by the dashed lines.

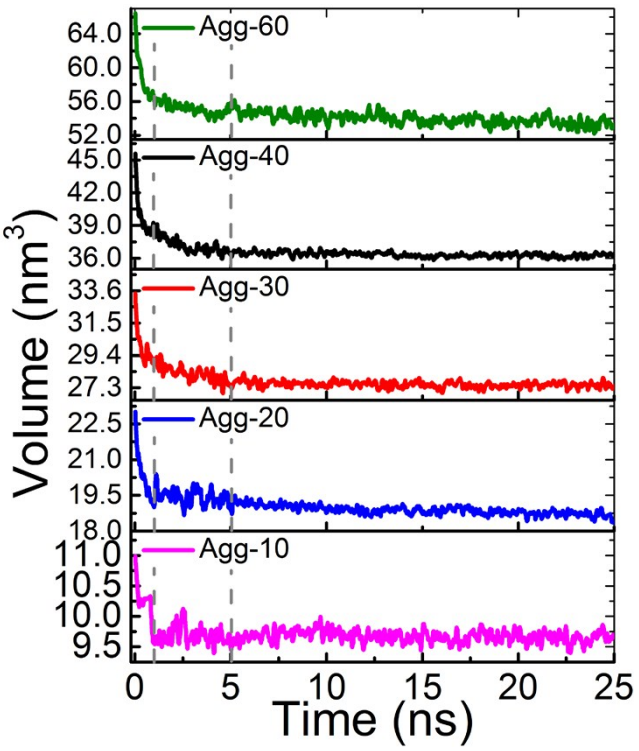

Figure. S7 The time evolution of the volume of HPS aggregates averaged by five MD trajectories, at each concentration. The different stages of the aggregation process are divided by the dashed lines.

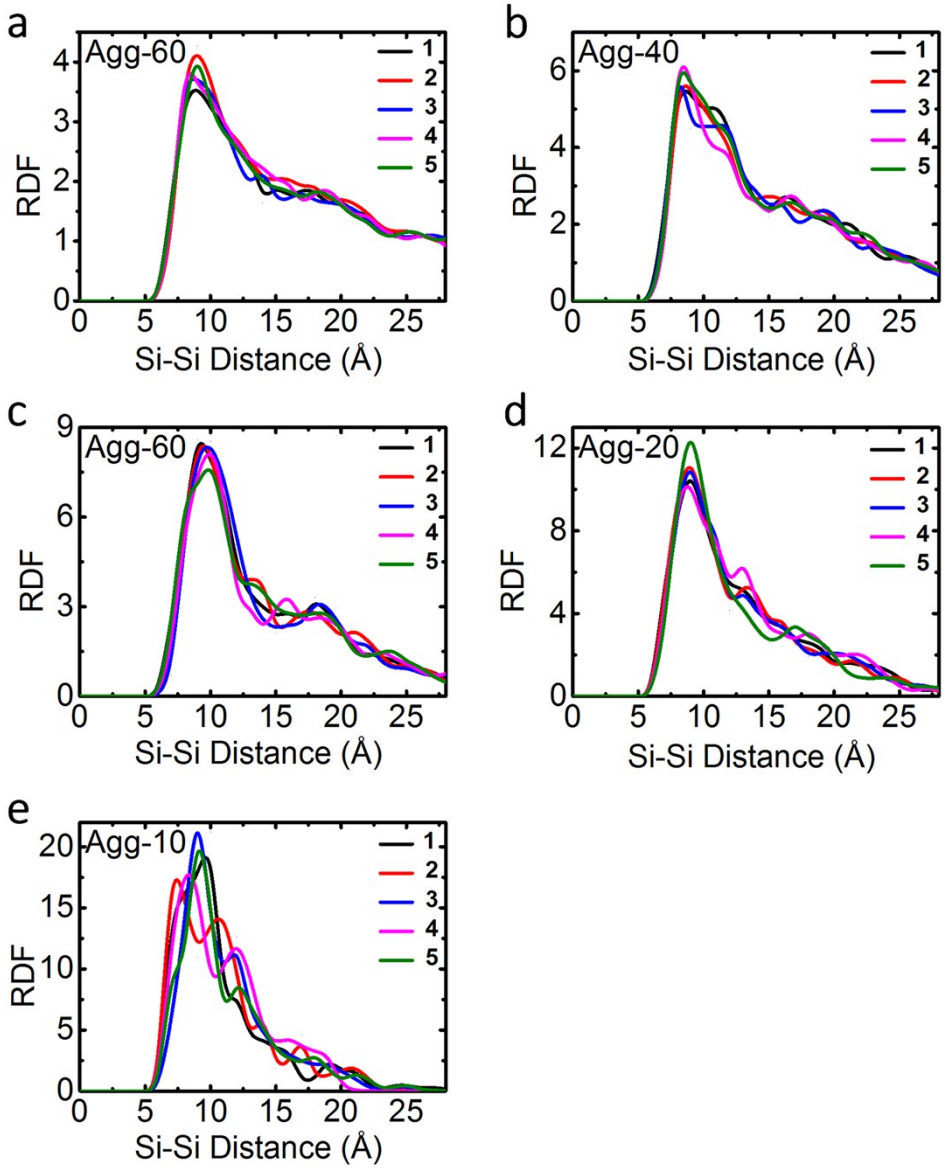

Figure. S8 The radical distribution functions (RDFs) *vs* the intermolecular Si-Si distance for each separate MD trajectory for systems (a) Agg-60, (b) Agg-40, (c) Agg-30, (d) Agg-20 and (e) Agg-10, respectively.

V. Supplementary force filed parameters of HPS

The force field parameters of HPS molecule in Gromacs format:

; HPS.itp

[moleculetype]

; name nrexcl

HPS 3

[atoms]

; nr	type	resi	res	atom	cgnr	charge	mass
1	Si	1	MOL	SI1	1	0.886633	28.08500
2	ce	1	MOL	C1	2	-0.417819	12.01000
3	ca	1	MOL	C2	3	0.190061	12.01000
4	ca	1	MOL	C3	4	-0.167300	12.01000
5	ha	1	MOL	H1	5	0.152041	1.00800
6	ca	1	MOL	C4	6	-0.197748	12.01000
7	ha	1	MOL	H2	7	0.159639	1.00800
8	ca	1	MOL	C5	8	-0.117471	12.01000
9	ha	1	MOL	H3	9	0.140432	1.00800
10	ca	1	MOL	C6	10	-0.197748	12.01000
11	ha	1	MOL	H4	11	0.159639	1.00800
12	ca	1	MOL	C7	12	-0.167300	12.01000
13	ha	1	MOL	H5	13	0.152041	1.00800
14	cf	1	MOL	C8	14	0.021750	12.01000
15	ca	1	MOL	C9	15	0.160900	12.01000
16	ca	1	MOL	C10	16	-0.199923	12.01000
17	ha	1	MOL	H6	17	0.152918	1.00800
18	ca	1	MOL	C11	18	-0.144689	12.01000
19	ha	1	MOL	H7	19	0.147962	1.00800
20	ca	1	MOL	C12	20	-0.154776	12.01000
21	ha	1	MOL	H8	21	0.145188	1.00800
22	ca	1	MOL	C13	22	-0.144689	12.01000
23	ha	1	MOL	H9	23	0.147962	1.00800
24	ca	1	MOL	C14	24	-0.199923	12.01000
25	ha	1	MOL	H10	25	0.152918	1.00800
26	cf	1	MOL	C15	26	0.021750	12.01000
27	ca	1	MOL	C16	27	0.160900	12.01000
28	ca	1	MOL	C17	28	-0.199923	12.01000
29	ha	1	MOL	H11	29	0.152918	1.00800
30	ca	1	MOL	C18	30	-0.144689	12.01000
31	ha	1	MOL	H12	31	0.147962	1.00800
32	ca	1	MOL	C19	32	-0.154776	12.01000
33	ha	1	MOL	H13	33	0.145188	1.00800
34	ca	1	MOL	C20	34	-0.144689	12.01000
35	ha	1	MOL	H14	35	0.147962	1.00800
36	ca	1	MOL	C21	36	-0.199923	12.01000

37	ha	1	MOL	H15	37	0.152918	1.00800
38	ce	1	MOL	C22	38	-0.417819	12.01000
39	ca	1	MOL	C23	39	0.190061	12.01000
40	ca	1	MOL	C24	40	-0.167300	12.01000
41	ha	1	MOL	H16	41	0.152041	1.00800
42	ca	1	MOL	C25	42	-0.197748	12.01000
43	ha	1	MOL	H17	43	0.159639	1.00800
44	ca	1	MOL	C26	44	-0.117471	12.01000
45	ha	1	MOL	H18	45	0.140432	1.00800
46	ca	1	MOL	C27	46	-0.197748	12.01000
47	ha	1	MOL	H19	47	0.159639	1.00800
48	ca	1	MOL	C28	48	-0.167300	12.01000
49	ha	1	MOL	H20	49	0.152041	1.00800
50	ca	1	MOL	C29	50	-0.262672	12.01000
51	ca	1	MOL	C30	51	-0.097514	12.01000
52	ha	1	MOL	H21	52	0.115976	1.00800
53	ca	1	MOL	C31	53	-0.133910	12.01000
54	ha	1	MOL	H22	54	0.134201	1.00800
55	ca	1	MOL	C32	55	-0.129414	12.01000
56	ha	1	MOL	H23	56	0.137199	1.00800
57	ca	1	MOL	C33	57	-0.133910	12.01000
58	ha	1	MOL	H24	58	0.134201	1.00800
59	ca	1	MOL	C34	59	-0.097514	12.01000
60	ha	1	MOL	H25	60	0.115976	1.00800
61	ca	1	MOL	C35	61	-0.262672	12.01000
62	ca	1	MOL	C36	62	-0.097514	12.01000
63	ha	1	MOL	H26	63	0.115976	1.00800
64	ca	1	MOL	C37	64	-0.133910	12.01000
65	ha	1	MOL	H27	65	0.134201	1.00800
66	ca	1	MOL	C38	66	-0.129414	12.01000
67	ha	1	MOL	H28	67	0.137199	1.00800
68	ca	1	MOL	C39	68	-0.133910	12.01000
69	ha	1	MOL	H29	69	0.134201	1.00800
70	ca	1	MOL	C40	70	-0.097514	12.01000
71	ha	1	MOL	H30	71	0.115976	1.00800

[bonds]

; ai	aj	funct	r	k	
1	2	1	1.8680e-01	2.7723e+05 ;	SI1 - C1
1	38	1	1.8680e-01	2.7723e+05 ;	SI1 - C22
1	50	1	1.8700e-01	2.7070e+05 ;	SI1 - C29
1	61	1	1.8700e-01	2.7070e+05 ;	SI1 - C35
2	3	1	1.4720e-01	3.0627e+05 ;	C1 - C2
2	14	1	1.3380e-01	4.7062e+05 ;	C1 - C8
3	4	1	1.3870e-01	4.0033e+05 ;	C2 - C3

3	12	1	1.3870e-01	4.0033e+05 ;	C2 - C7
4	5	1	1.0870e-01	2.8811e+05 ;	C3 - H1
4	6	1	1.3870e-01	4.0033e+05 ;	C3 - C4
6	7	1	1.0870e-01	2.8811e+05 ;	C4 - H2
6	8	1	1.3870e-01	4.0033e+05 ;	C4 - C5
8	9	1	1.0870e-01	2.8811e+05 ;	C5 - H3
8	10	1	1.3870e-01	4.0033e+05 ;	C5 - C6
10	11	1	1.0870e-01	2.8811e+05 ;	C6 - H4
10	12	1	1.3870e-01	4.0033e+05 ;	C6 - C7
12	13	1	1.0870e-01	2.8811e+05 ;	C7 - H5
14	15	1	1.4720e-01	3.0627e+05 ;	C8 - C9
14	26	1	1.4510e-01	3.2677e+05 ;	C8 - C15
15	16	1	1.3870e-01	4.0033e+05 ;	C9 - C10
15	24	1	1.3870e-01	4.0033e+05 ;	C9 - C14
16	17	1	1.0870e-01	2.8811e+05 ;	C10 - H6
16	18	1	1.3870e-01	4.0033e+05 ;	C10 - C11
18	19	1	1.0870e-01	2.8811e+05 ;	C11 - H7
18	20	1	1.3870e-01	4.0033e+05 ;	C11 - C12
20	21	1	1.0870e-01	2.8811e+05 ;	C12 - H8
20	22	1	1.3870e-01	4.0033e+05 ;	C12 - C13
22	23	1	1.0870e-01	2.8811e+05 ;	C13 - H9
22	24	1	1.3870e-01	4.0033e+05 ;	C13 - C14
24	25	1	1.0870e-01	2.8811e+05 ;	C14 - H10
26	27	1	1.4720e-01	3.0627e+05 ;	C15 - C16
26	38	1	1.3380e-01	4.7062e+05 ;	C15 - C22
27	28	1	1.3870e-01	4.0033e+05 ;	C16 - C17
27	36	1	1.3870e-01	4.0033e+05 ;	C16 - C21
28	29	1	1.0870e-01	2.8811e+05 ;	C17 - H11
28	30	1	1.3870e-01	4.0033e+05 ;	C17 - C18
30	31	1	1.0870e-01	2.8811e+05 ;	C18 - H12
30	32	1	1.3870e-01	4.0033e+05 ;	C18 - C19
32	33	1	1.0870e-01	2.8811e+05 ;	C19 - H13
32	34	1	1.3870e-01	4.0033e+05 ;	C19 - C20
34	35	1	1.0870e-01	2.8811e+05 ;	C20 - H14
34	36	1	1.3870e-01	4.0033e+05 ;	C20 - C21
36	37	1	1.0870e-01	2.8811e+05 ;	C21 - H15
38	39	1	1.4720e-01	3.0627e+05 ;	C22 - C23
39	40	1	1.3870e-01	4.0033e+05 ;	C23 - C24
39	48	1	1.3870e-01	4.0033e+05 ;	C23 - C28
40	41	1	1.0870e-01	2.8811e+05 ;	C24 - H16
40	42	1	1.3870e-01	4.0033e+05 ;	C24 - C25
42	43	1	1.0870e-01	2.8811e+05 ;	C25 - H17
42	44	1	1.3870e-01	4.0033e+05 ;	C25 - C26
44	45	1	1.0870e-01	2.8811e+05 ;	C26 - H18
44	46	1	1.3870e-01	4.0033e+05 ;	C26 - C27

46	47	1	1.0870e-01	2.8811e+05 ;	C27 - H19
46	48	1	1.3870e-01	4.0033e+05 ;	C27 - C28
48	49	1	1.0870e-01	2.8811e+05 ;	C28 - H20
50	51	1	1.3870e-01	4.0033e+05 ;	C29 - C30
50	59	1	1.3870e-01	4.0033e+05 ;	C29 - C34
51	52	1	1.0870e-01	2.8811e+05 ;	C30 - H21
51	53	1	1.3870e-01	4.0033e+05 ;	C30 - C31
53	54	1	1.0870e-01	2.8811e+05 ;	C31 - H22
53	55	1	1.3870e-01	4.0033e+05 ;	C31 - C32
55	56	1	1.0870e-01	2.8811e+05 ;	C32 - H23
55	57	1	1.3870e-01	4.0033e+05 ;	C32 - C33
57	58	1	1.0870e-01	2.8811e+05 ;	C33 - H24
57	59	1	1.3870e-01	4.0033e+05 ;	C33 - C34
59	60	1	1.0870e-01	2.8811e+05 ;	C34 - H25
61	62	1	1.3870e-01	4.0033e+05 ;	C35 - C36
61	70	1	1.3870e-01	4.0033e+05 ;	C35 - C40
62	63	1	1.0870e-01	2.8811e+05 ;	C36 - H26
62	64	1	1.3870e-01	4.0033e+05 ;	C36 - C37
64	65	1	1.0870e-01	2.8811e+05 ;	C37 - H27
64	66	1	1.3870e-01	4.0033e+05 ;	C37 - C38
66	67	1	1.0870e-01	2.8811e+05 ;	C38 - H28
66	68	1	1.3870e-01	4.0033e+05 ;	C38 - C39
68	69	1	1.0870e-01	2.8811e+05 ;	C39 - H29
68	70	1	1.3870e-01	4.0033e+05 ;	C39 - C40
70	71	1	1.0870e-01	2.8811e+05 ;	C40 - H30

[pairs]

;ai	aj	funct	
1	4	1 ;	SI1 - C3
1	12	1 ;	SI1 - C7
1	15	1 ;	SI1 - C9
1	27	1 ;	SI1 - C16
1	40	1 ;	SI1 - C24
1	48	1 ;	SI1 - C28
1	52	1 ;	SI1 - H21
1	53	1 ;	SI1 - C31
1	57	1 ;	SI1 - C33
1	60	1 ;	SI1 - H25
1	63	1 ;	SI1 - H26
1	64	1 ;	SI1 - C37
1	68	1 ;	SI1 - C39
1	71	1 ;	SI1 - H30
2	5	1 ;	C1 - H1
2	6	1 ;	C1 - C4
2	10	1 ;	C1 - C6
2	13	1 ;	C1 - H5

2	16	1 ;	C1 - C10
2	24	1 ;	C1 - C14
2	27	1 ;	C1 - C16
2	39	1 ;	C1 - C23
2	51	1 ;	C1 - C30
2	59	1 ;	C1 - C34
2	62	1 ;	C1 - C36
2	70	1 ;	C1 - C40
3	7	1 ;	C2 - H2
3	8	1 ;	C2 - C5
3	11	1 ;	C2 - H4
3	15	1 ;	C2 - C9
3	26	1 ;	C2 - C15
4	9	1 ;	C3 - H3
4	10	1 ;	C3 - C6
4	13	1 ;	C3 - H5
4	14	1 ;	C3 - C8
5	7	1 ;	H1 - H2
5	8	1 ;	H1 - C5
5	12	1 ;	H1 - C7
6	11	1 ;	C4 - H4
6	12	1 ;	C4 - C7
7	9	1 ;	H2 - H3
7	10	1 ;	H2 - C6
8	13	1 ;	C5 - H5
9	11	1 ;	H3 - H4
9	12	1 ;	H3 - C7
11	13	1 ;	H4 - H5
12	14	1 ;	C7 - C8
14	17	1 ;	C8 - H6
14	18	1 ;	C8 - C11
14	22	1 ;	C8 - C13
14	25	1 ;	C8 - H10
14	28	1 ;	C8 - C17
14	36	1 ;	C8 - C21
14	39	1 ;	C8 - C23
15	19	1 ;	C9 - H7
15	20	1 ;	C9 - C12
15	23	1 ;	C9 - H9
15	27	1 ;	C9 - C16
15	38	1 ;	C9 - C22
16	21	1 ;	C10 - H8
16	22	1 ;	C10 - C13
16	25	1 ;	C10 - H10
16	26	1 ;	C10 - C15

17 19 1 ; H6 - H7
17 20 1 ; H6 - C12
17 24 1 ; H6 - C14
18 23 1 ; C11 - H9
18 24 1 ; C11 - C14
19 21 1 ; H7 - H8
19 22 1 ; H7 - C13
20 25 1 ; C12 - H10
21 23 1 ; H8 - H9
21 24 1 ; H8 - C14
23 25 1 ; H9 - H10
24 26 1 ; C14 - C15
26 29 1 ; C15 - H11
26 30 1 ; C15 - C18
26 34 1 ; C15 - C20
26 37 1 ; C15 - H15
26 40 1 ; C15 - C24
26 48 1 ; C15 - C28
27 31 1 ; C16 - H12
27 32 1 ; C16 - C19
27 35 1 ; C16 - H14
27 39 1 ; C16 - C23
28 33 1 ; C17 - H13
28 34 1 ; C17 - C20
28 37 1 ; C17 - H15
28 38 1 ; C17 - C22
29 31 1 ; H11 - H12
29 32 1 ; H11 - C19
29 36 1 ; H11 - C21
30 35 1 ; C18 - H14
30 36 1 ; C18 - C21
31 33 1 ; H12 - H13
31 34 1 ; H12 - C20
32 37 1 ; C19 - H15
33 35 1 ; H13 - H14
33 36 1 ; H13 - C21
35 37 1 ; H14 - H15
36 38 1 ; C21 - C22
38 3 1 ; C22 - C2
38 41 1 ; C22 - H16
38 42 1 ; C22 - C25
38 46 1 ; C22 - C27
38 49 1 ; C22 - H20
38 51 1 ; C22 - C30
38 59 1 ; C22 - C34

38 62 1 ; C22 - C36
38 70 1 ; C22 - C40
39 43 1 ; C23 - H17
39 44 1 ; C23 - C26
39 47 1 ; C23 - H19
40 45 1 ; C24 - H18
40 46 1 ; C24 - C27
40 49 1 ; C24 - H20
41 43 1 ; H16 - H17
41 44 1 ; H16 - C26
41 48 1 ; H16 - C28
42 47 1 ; C25 - H19
42 48 1 ; C25 - C28
43 45 1 ; H17 - H18
43 46 1 ; H17 - C27
44 49 1 ; C26 - H20
45 47 1 ; H18 - H19
45 48 1 ; H18 - C28
47 49 1 ; H19 - H20
50 3 1 ; C29 - C2
50 14 1 ; C29 - C8
50 26 1 ; C29 - C15
50 39 1 ; C29 - C23
50 54 1 ; C29 - H22
50 55 1 ; C29 - C32
50 58 1 ; C29 - H24
50 62 1 ; C29 - C36
50 70 1 ; C29 - C40
51 56 1 ; C30 - H23
51 57 1 ; C30 - C33
51 60 1 ; C30 - H25
52 54 1 ; H21 - H22
52 55 1 ; H21 - C32
52 59 1 ; H21 - C34
53 58 1 ; C31 - H24
53 59 1 ; C31 - C34
54 56 1 ; H22 - H23
54 57 1 ; H22 - C33
55 60 1 ; C32 - H25
56 58 1 ; H23 - H24
56 59 1 ; H23 - C34
58 60 1 ; H24 - H25
61 3 1 ; C35 - C2
61 14 1 ; C35 - C8
61 26 1 ; C35 - C15

61 39 1 ; C35 - C23
61 51 1 ; C35 - C30
61 59 1 ; C35 - C34
61 65 1 ; C35 - H27
61 66 1 ; C35 - C38
61 69 1 ; C35 - H29
62 67 1 ; C36 - H28
62 68 1 ; C36 - C39
62 71 1 ; C36 - H30
63 65 1 ; H26 - H27
63 66 1 ; H26 - C38
63 70 1 ; H26 - C40
64 69 1 ; C37 - H29
64 70 1 ; C37 - C40
65 67 1 ; H27 - H28
65 68 1 ; H27 - C39
66 71 1 ; C38 - H30
67 69 1 ; H28 - H29
67 70 1 ; H28 - C40
69 71 1 ; H29 - H30

[angles]

; ai	aj	ak	funct	theta	cth	
1	2	3	1	1.2462e+02	5.2559e+02 ;	SI1 - C1 - C2
1	2	14	1	1.0674e+02	5.3982e+02 ;	SI1 - C1 - C8
1	38	26	1	1.0674e+02	5.3982e+02 ;	SI1 - C22- C15
1	38	39	1	1.2462e+02	5.2559e+02 ;	SI1 - C22- C23
1	50	51	1	1.2182e+02	5.3421e+02 ;	SI1 - C29- C30
1	50	59	1	1.2182e+02	5.3421e+02 ;	SI1 - C29- C34
1	61	62	1	1.2182e+02	5.3421e+02 ;	SI1 - C35- C36
1	61	70	1	1.2182e+02	5.3421e+02 ;	SI1 - C35- C40
2	1	38	1	9.3205e+01	5.3756e+02 ;	C1 - SI1- C22
2	1	50	1	1.1061e+02	5.3396e+02 ;	C1 - SI1- C29
2	1	61	1	1.1061e+02	5.3396e+02 ;	C1 - SI1- C35
2	3	4	1	1.2066e+02	5.4308e+02 ;	C1 - C2 - C3
2	3	12	1	1.2066e+02	5.4308e+02 ;	C1 - C2 - C7
2	14	15	1	1.2308e+02	5.4559e+02 ;	C1 - C8 - C9
2	14	26	1	1.3092e+02	5.3388e+02 ;	C1 - C8 - C15
3	2	14	1	1.2308e+02	5.4559e+02 ;	C2 - C1 - C8
3	4	5	1	1.2001e+02	4.0585e+02 ;	C2 - C3 - H1
3	4	6	1	1.1997e+02	5.6233e+02 ;	C2 - C3 - C4
3	12	10	1	1.1997e+02	5.6233e+02 ;	C2 - C7 - C6
3	12	13	1	1.2001e+02	4.0585e+02 ;	C2 - C7 - H5
4	3	12	1	1.1997e+02	5.6233e+02 ;	C3 - C2 - C7
4	6	7	1	1.2001e+02	4.0585e+02 ;	C3 - C4 - H2

4	6	8	1	1.1997e+02	5.6233e+02 ;	C3 - C4 - C5
5	4	6	1	1.2001e+02	4.0585e+02 ;	H1 - C3 - C4
6	8	9	1	1.2001e+02	4.0585e+02 ;	C4 - C5 - H3
6	8	10	1	1.1997e+02	5.6233e+02 ;	C4 - C5 - C6
7	6	8	1	1.2001e+02	4.0585e+02 ;	H2 - C4 - C5
8	10	11	1	1.2001e+02	4.0585e+02 ;	C5 - C6 - H4
8	10	12	1	1.1997e+02	5.6233e+02 ;	C5 - C6 - C7
9	8	10	1	1.2001e+02	4.0585e+02 ;	H3 - C5 - C6
10	12	13	1	1.2001e+02	4.0585e+02 ;	C6 - C7 - H5
11	10	12	1	1.2001e+02	4.0585e+02 ;	H4 - C6 - C7
14	15	16	1	1.2066e+02	5.4308e+02 ;	C8 - C9 - C10
14	15	24	1	1.2066e+02	5.4308e+02 ;	C8 - C9 - C14
14	26	27	1	1.1834e+02	5.3669e+02 ;	C8 - C15- C16
14	26	38	1	1.3092e+02	5.3388e+02 ;	C8 - C15- C22
15	14	26	1	1.1834e+02	5.3669e+02 ;	C9 - C8 - C15
15	16	17	1	1.2001e+02	4.0585e+02 ;	C9 - C10- H6
15	16	18	1	1.1997e+02	5.6233e+02 ;	C9 - C10- C11
15	24	22	1	1.1997e+02	5.6233e+02 ;	C9 - C14- C13
15	24	25	1	1.2001e+02	4.0585e+02 ;	C9 - C14- H10
16	15	24	1	1.1997e+02	5.6233e+02 ;	C10 - C9 - C14
16	18	19	1	1.2001e+02	4.0585e+02 ;	C10 - C11- H7
16	18	20	1	1.1997e+02	5.6233e+02 ;	C10 - C11- C12
17	16	18	1	1.2001e+02	4.0585e+02 ;	H6 - C10- C11
18	20	21	1	1.2001e+02	4.0585e+02 ;	C11 - C12- H8
18	20	22	1	1.1997e+02	5.6233e+02 ;	C11 - C12- C13
19	18	20	1	1.2001e+02	4.0585e+02 ;	H7 - C11- C12
20	22	23	1	1.2001e+02	4.0585e+02 ;	C12 - C13- H9
20	22	24	1	1.1997e+02	5.6233e+02 ;	C12 - C13- C14
21	20	22	1	1.2001e+02	4.0585e+02 ;	H8 - C12- C13
22	24	25	1	1.2001e+02	4.0585e+02 ;	C13 - C14- H10
23	22	24	1	1.2001e+02	4.0585e+02 ;	H9 - C13- C14
26	27	28	1	1.2066e+02	5.4308e+02 ;	C15 - C16- C17
26	27	36	1	1.2066e+02	5.4308e+02 ;	C15 - C16- C21
26	38	39	1	1.2308e+02	5.4559e+02 ;	C15 - C22- C23
27	26	38	1	1.2308e+02	5.4559e+02 ;	C16 - C15- C22
27	28	29	1	1.2001e+02	4.0585e+02 ;	C16 - C17- H11
27	28	30	1	1.1997e+02	5.6233e+02 ;	C16 - C17- C18
27	36	34	1	1.1997e+02	5.6233e+02 ;	C16 - C21- C20
27	36	37	1	1.2001e+02	4.0585e+02 ;	C16 - C21- H15
28	27	36	1	1.1997e+02	5.6233e+02 ;	C17 - C16- C21
28	30	31	1	1.2001e+02	4.0585e+02 ;	C17 - C18- H12
28	30	32	1	1.1997e+02	5.6233e+02 ;	C17 - C18- C19
29	28	30	1	1.2001e+02	4.0585e+02 ;	H11 - C17- C18
30	32	33	1	1.2001e+02	4.0585e+02 ;	C18 - C19- H13
30	32	34	1	1.1997e+02	5.6233e+02 ;	C18 - C19- C20

31	30	32	1	1.2001e+02	4.0585e+02 ;	H12 - C18- C19
32	34	35	1	1.2001e+02	4.0585e+02 ;	C19 - C20- H14
32	34	36	1	1.1997e+02	5.6233e+02 ;	C19 - C20- C21
33	32	34	1	1.2001e+02	4.0585e+02 ;	H13 - C19- C20
34	36	37	1	1.2001e+02	4.0585e+02 ;	C20 - C21- H15
35	34	36	1	1.2001e+02	4.0585e+02 ;	H14 - C20- C21
38	1	50	1	1.1061e+02	5.3396e+02 ;	C22 - SI1- C29
38	1	61	1	1.1061e+02	5.3396e+02 ;	C22 - SI1- C35
38	39	40	1	1.2066e+02	5.4308e+02 ;	C22 - C23- C24
38	39	48	1	1.2066e+02	5.4308e+02 ;	C22 - C23- C28
39	40	41	1	1.2001e+02	4.0585e+02 ;	C23 - C24- H16
39	40	42	1	1.1997e+02	5.6233e+02 ;	C23 - C24- C25
39	48	46	1	1.1997e+02	5.6233e+02 ;	C23 - C28- C27
39	48	49	1	1.2001e+02	4.0585e+02 ;	C23 - C28- H20
40	39	48	1	1.1997e+02	5.6233e+02 ;	C24 - C23- C28
40	42	43	1	1.2001e+02	4.0585e+02 ;	C24 - C25- H17
40	42	44	1	1.1997e+02	5.6233e+02 ;	C24 - C25- C26
41	40	42	1	1.2001e+02	4.0585e+02 ;	H16 - C24- C25
42	44	45	1	1.2001e+02	4.0585e+02 ;	C25 - C26- H18
42	44	46	1	1.1997e+02	5.6233e+02 ;	C25 - C26- C27
43	42	44	1	1.2001e+02	4.0585e+02 ;	H17 - C25- C26
44	46	47	1	1.2001e+02	4.0585e+02 ;	C26 - C27- H19
44	46	48	1	1.1997e+02	5.6233e+02 ;	C26 - C27- C28
45	44	46	1	1.2001e+02	4.0585e+02 ;	H18 - C26- C27
46	48	49	1	1.2001e+02	4.0585e+02 ;	C27 - C28- H20
47	46	48	1	1.2001e+02	4.0585e+02 ;	H19 - C27- C28
50	1	61	1	1.1165e+02	5.3271e+02 ;	C29 - SI1- C35
50	51	52	1	1.2001e+02	4.0585e+02 ;	C29 - C30- H21
50	51	53	1	1.1997e+02	5.6233e+02 ;	C29 - C30- C31
50	59	57	1	1.1997e+02	5.6233e+02 ;	C29 - C34- C33
50	59	60	1	1.2001e+02	4.0585e+02 ;	C29 - C34- H25
51	50	59	1	1.1997e+02	5.6233e+02 ;	C30 - C29- C34
51	53	54	1	1.2001e+02	4.0585e+02 ;	C30 - C31- H22
51	53	55	1	1.1997e+02	5.6233e+02 ;	C30 - C31- C32
52	51	53	1	1.2001e+02	4.0585e+02 ;	H21 - C30- C31
53	55	56	1	1.2001e+02	4.0585e+02 ;	C31 - C32- H23
53	55	57	1	1.1997e+02	5.6233e+02 ;	C31 - C32- C33
54	53	55	1	1.2001e+02	4.0585e+02 ;	H22 - C31- C32
55	57	58	1	1.2001e+02	4.0585e+02 ;	C32 - C33- H24
55	57	59	1	1.1997e+02	5.6233e+02 ;	C32 - C33- C34
56	55	57	1	1.2001e+02	4.0585e+02 ;	H23 - C32- C33
57	59	60	1	1.2001e+02	4.0585e+02 ;	C33 - C34- H25
58	57	59	1	1.2001e+02	4.0585e+02 ;	H24 - C33- C34
61	62	63	1	1.2001e+02	4.0585e+02 ;	C35 - C36- H26
61	62	64	1	1.1997e+02	5.6233e+02 ;	C35 - C36- C37

61	70	68	1	1.1997e+02	5.6233e+02 ;	C35 - C40- C39
61	70	71	1	1.2001e+02	4.0585e+02 ;	C35 - C40- H30
62	61	70	1	1.1997e+02	5.6233e+02 ;	C36 - C35- C40
62	64	65	1	1.2001e+02	4.0585e+02 ;	C36 - C37- H27
62	64	66	1	1.1997e+02	5.6233e+02 ;	C36 - C37- C38
63	62	64	1	1.2001e+02	4.0585e+02 ;	H26 - C36- C37
64	66	67	1	1.2001e+02	4.0585e+02 ;	C37 - C38- H28
64	66	68	1	1.1997e+02	5.6233e+02 ;	C37 - C38- C39
65	64	66	1	1.2001e+02	4.0585e+02 ;	H27 - C37- C38
66	68	69	1	1.2001e+02	4.0585e+02 ;	C38 - C39- H29
66	68	70	1	1.1997e+02	5.6233e+02 ;	C38 - C39- C40
67	66	68	1	1.2001e+02	4.0585e+02 ;	H28 - C38- C39
68	70	71	1	1.2001e+02	4.0585e+02 ;	C39 - C40- H30
69	68	70	1	1.2001e+02	4.0585e+02 ;	H29 - C39- C40

[dihedrals] ; propers

; treated as RBs in GROMACS to use combine multiple AMBER torsions per quartet

; i	j	k	l	func	C0	C1	C2	C3	C4	C5	
1	2	3	4	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000	; SI1- C1- C2- C3
1	2	3	12	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000	; SI1- C1- C2- C7
1	2	14	15	3	55.64720	0.00000	-55.64720	0.00000	0.00000	0.00000	; SI1- C1- C8- C9
1	2	14	26	3	55.64720	0.00000	-55.64720	0.00000	0.00000	0.00000	; SI1- C1- C8-C15
1	38	26	14	3	55.64720	0.00000	-55.64720	0.00000	0.00000	0.00000	; SI1-C22-C15- C8
1	38	26	27	3	55.64720	0.00000	-55.64720	0.00000	0.00000	0.00000	; SI1-C22-C15-C16
1	38	39	40	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000	; SI1-C22-C23-C24
1	38	39	48	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000	; SI1-C22-C23-C28
1	50	51	52	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	; SI1-C29-C30-H21
1	50	51	53	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	; SI1-C29-C30-C31
1	50	59	57	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	; SI1-C29-C34-C33
1	50	59	60	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	; SI1-C29-C34-H25
1	61	62	63	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	; SI1-C35-C36-H26
1	61	62	64	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	; SI1-C35-C36-C37
1	61	70	68	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	; SI1-C35-C40-C39
1	61	70	71	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	; SI1-C35-C40-H30
2	1	38	26	3	-47.27800	-1.20353	0.06301	1.4254	-0.0668	0.175407;	C1-SI1-C22-C15
2	1	38	39	3	-47.27800	-1.20353	0.06301	1.4254	-0.0668	0.175407;	C1-SI1-C22-C23
2	1	50	51	3	-47.27800	-1.20353	0.06301	1.4254	-0.0668	0.175407;	C1-SI1-C29-C30
2	1	50	59	3	-47.27800	-1.20353	0.06301	1.4254	-0.0668	0.175407;	C1-SI1-C29-C34
2	1	61	62	3	-47.27800	-1.20353	0.06301	1.4254	-0.0668	0.175407;	C1-SI1-C35-C36
2	1	61	70	3	-47.27800	-1.20353	0.06301	1.4254	-0.0668	0.175407;	C1-SI1-C35-C40
2	3	4	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	; C1- C2- C3- H1
2	3	4	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	; C1- C2- C3- C4
2	3	12	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	; C1- C2- C7- C6
2	3	12	13	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	; C1- C2- C7- H5
2	14	15	16	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000	; C1- C8- C9-C10

2	14	15	24	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000 ; C1- C8- C9-C14
2	14	26	27	3	8.36800	0.00000	-8.36800	0.00000	0.00000	0.00000 ; C1- C8-C15-C16
2	14	26	38	3	8.36800	0.00000	-8.36800	0.00000	0.00000	0.00000 ; C1- C8-C15-C22
3	2	14	15	3	55.64720	0.00000	-55.64720	0.00000	0.00000	0.00000 ; C2- C1- C8- C9
3	2	14	26	3	55.64720	0.00000	-55.64720	0.00000	0.00000	0.00000 ; C2- C1- C8-C15
3	4	6	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C2- C3- C4- H2
3	4	6	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C2- C3- C4- C5
3	12	10	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C2- C7- C6- C5
3	12	10	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C2- C7- C6- H4
4	3	2	14	3	55.64720	0.00000	-55.64720	0.00000	0.00000	0.00000 ; C3- C2- C1- C8
4	3	12	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C3- C2- C7- C6
4	3	12	13	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C3- C2- C7- H5
4	6	8	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C3- C4- C5- H3
4	6	8	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C3- C4- C5- C6
5	4	3	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; H1- C3- C2- C7
5	4	6	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; H1- C3- C4- H2
5	4	6	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; H1- C3- C4- C5
6	4	3	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C4- C3- C2- C7
6	8	10	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C4- C5- C6- H4
6	8	10	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C4- C5- C6- C7
7	6	8	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; H2- C4- C5- H3
7	6	8	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; H2- C4- C5- C6
8	10	12	13	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C5- C6- C7- H5
9	8	10	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; H3- C5- C6- H4
9	8	10	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; H3- C5- C6- C7
11	10	12	13	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; H4- C6- C7- H5
12	3	2	14	3	55.64720	0.00000	-55.64720	0.00000	0.00000	0.00000 ; C7- C2- C1- C8
14	15	16	17	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C8- C9-C10- H6
14	15	16	18	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C8- C9-C10-C11
14	15	24	22	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C8- C9-C14-C13
14	15	24	25	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C8- C9-C14-H10
14	26	27	28	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000 ; C8-C15-C16-C17
14	26	27	36	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000 ; C8-C15-C16-C21
14	26	38	39	3	55.64720	0.00000	-55.64720	0.00000	0.00000	0.00000 ; C8-C15-C22-C23
15	14	26	27	3	8.36800	0.00000	-8.36800	0.00000	0.00000	0.00000 ; C9- C8-C15-C16
15	14	26	38	3	8.36800	0.00000	-8.36800	0.00000	0.00000	0.00000 ; C9- C8-C15-C22
15	16	18	19	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C9-C10-C11- H7
15	16	18	20	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C9-C10-C11-C12
15	24	22	20	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C9-C14-C13-C12
15	24	22	23	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C9-C14-C13- H9
16	15	14	26	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000 ; C10- C9- C8-C15
16	15	24	22	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C10- C9-C14-C13
16	15	24	25	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C10- C9-C14-H10
16	18	20	21	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C10-C11-C12- H8
16	18	20	22	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000 ; C10-C11-C12-C13

17 16 15 24 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H6-C10- C9-C14
17 16 18 19 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H6-C10-C11- H7
17 16 18 20 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H6-C10-C11-C12
18 16 15 24 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C11-C10- C9-C14
18 20 22 23 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C11-C12-C13- H9
18 20 22 24 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C11-C12-C13-C14
19 18 20 21 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H7-C11-C12- H8
19 18 20 22 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H7-C11-C12-C13
20 22 24 25 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C12-C13-C14-H10
21 20 22 23 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H8-C12-C13- H9
21 20 22 24 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H8-C12-C13-C14
23 22 24 25 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H9-C13-C14-H10
24 15 14 26 3 21.33840 0.00000 -21.33840 0.00000 0.00000 0.00000 ; C14- C9- C8-C15
26 27 28 29 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C15-C16-C17-H11
26 27 28 30 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C15-C16-C17-C18
26 27 36 34 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C15-C16-C21-C20
26 27 36 37 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C15-C16-C21-H15
26 38 39 40 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; C15-C22-C23-C24
26 38 39 48 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; C15-C22-C23-C28
27 26 38 39 3 55.64720 0.00000 -55.64720 0.00000 0.00000 0.00000 ; C16-C15-C22-C23
27 28 30 31 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C16-C17-C18-H12
27 28 30 32 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C16-C17-C18-C19
27 36 34 32 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C16-C21-C20-C19
27 36 34 35 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C16-C21-C20-H14
28 27 26 38 3 21.33840 0.00000 -21.33840 0.00000 0.00000 0.00000 ; C17-C16-C15-C22
28 27 36 34 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C17-C16-C21-C20
28 27 36 37 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C17-C16-C21-H15
28 30 32 33 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C17-C18-C19-H13
28 30 32 34 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C17-C18-C19-C20
29 28 27 36 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H11-C17-C16-C21
29 28 30 31 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H11-C17-C18-H12
29 28 30 32 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H11-C17-C18-C19
30 28 27 36 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C18-C17-C16-C21
30 32 34 35 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C18-C19-C20-H14
30 32 34 36 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C18-C19-C20-C21
31 30 32 33 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H12-C18-C19-H13
31 30 32 34 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H12-C18-C19-C20
32 34 36 37 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C19-C20-C21-H15
33 32 34 35 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H13-C19-C20-H14
33 32 34 36 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H13-C19-C20-C21
35 34 36 37 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H14-C20-C21-H15
36 27 26 38 3 21.33840 0.00000 -21.33840 0.00000 0.00000 0.00000 ; C21-C16-C15-C22
38 1 2 3 3 -47.27800 -1.20353 0.06301 1.4254 -0.0668 0.175407; C22-SI1- C1- C2
38 1 2 14 3 -47.27800 -1.20353 0.06301 1.4254 -0.0668 0.175407; C22-SI1- C1- C8
38 1 50 51 3 -47.27800 -1.20353 0.06301 1.4254 -0.0668 0.175407; C22-SI1-C29-C30

38 1 50 59 3 -47.27800 -1.20353 0.06301 1.4254 -0.0668 0.175407; C22-SI1-C29-C34
38 1 61 62 3 -47.27800 -1.20353 0.06301 1.4254 -0.0668 0.175407; C22-SI1-C35-C36
38 1 61 70 3 -47.27800 -1.20353 0.06301 1.4254 -0.0668 0.175407; C22-SI1-C35-C40
38 39 40 41 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C22-C23-C24-H16
38 39 40 42 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C22-C23-C24-C25
38 39 48 46 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C22-C23-C28-C27
38 39 48 49 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C22-C23-C28-H20
39 40 42 43 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C23-C24-C25-H17
39 40 42 44 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C23-C24-C25-C26
39 48 46 44 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C23-C28-C27-C26
39 48 46 47 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C23-C28-C27-H19
40 39 48 46 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C24-C23-C28-C27
40 39 48 49 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C24-C23-C28-H20
40 42 44 45 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C24-C25-C26-H18
40 42 44 46 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C24-C25-C26-C27
41 40 39 48 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H16-C24-C23-C28
41 40 42 43 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H16-C24-C25-H17
41 40 42 44 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H16-C24-C25-C26
42 40 39 48 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C25-C24-C23-C28
42 44 46 47 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C25-C26-C27-H19
42 44 46 48 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C25-C26-C27-C28
43 42 44 45 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H17-C25-C26-H18
43 42 44 46 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H17-C25-C26-C27
44 46 48 49 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C26-C27-C28-H20
45 44 46 47 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H18-C26-C27-H19
45 44 46 48 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H18-C26-C27-C28
47 46 48 49 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H19-C27-C28-H20
50 1 2 3 3 -47.27800 -1.20353 0.06301 1.4254 -0.06680 0.175407 ; C29-SI1- C1- C2
50 1 2 14 3 -47.27800 -1.20353 0.06301 1.4254 -0.06680 0.175407 ; C29-SI1- C1- C8
50 1 38 26 3 -47.27800 -1.20353 0.06301 1.4254 -0.06680 0.175407 ; C29-SI1-C22-C15
50 1 38 39 3 -47.27800 -1.20353 0.06301 1.4254 -0.06680 0.175407 ; C29-SI1-C22-C23
50 1 61 62 3 -47.27800 -1.20353 0.06301 1.4254 -0.06680 0.175407 ; C29-SI1-C35-C36
50 1 61 70 3 -47.27800 -1.20353 0.06301 1.4254 -0.06680 0.175407 ; C29-SI1-C35-C40
50 51 53 54 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C29-C30-C31-H22
50 51 53 55 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C29-C30-C31-C32
50 59 57 55 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C29-C34-C33-C32
50 59 57 58 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C29-C34-C33-H24
51 50 59 57 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C30-C29-C34-C33
51 50 59 60 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C30-C29-C34-H25
51 53 55 56 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C30-C31-C32-H23
51 53 55 57 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C30-C31-C32-C33
52 51 50 59 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H21-C30-C29-C34
52 51 53 54 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H21-C30-C31-H22
52 51 53 55 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H21-C30-C31-C32
53 51 50 59 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C31-C30-C29-C34

53 55 57 58 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C31-C32-C33-H24
53 55 57 59 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C31-C32-C33-C34
54 53 55 56 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H22-C31-C32-H23
54 53 55 57 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H22-C31-C32-C33
55 57 59 60 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C32-C33-C34-H25
56 55 57 58 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H23-C32-C33-H24
56 55 57 59 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H23-C32-C33-C34
58 57 59 60 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H24-C33-C34-H25
61 1 2 3 3 -47.27800 -1.20353 0.06301 1.4254 -0.06680 0.175407; C35-SI1- C1- C2
61 1 2 14 3 -47.27800 -1.20353 0.06301 1.4254 -0.06680 0.175407; C35-SI1- C1- C8
61 1 38 26 3 -47.27800 -1.20353 0.06301 1.4254 -0.06680 0.175407; C35-SI1-C22-C15
61 1 38 39 3 -47.27800 -1.20353 0.06301 1.4254 -0.06680 0.175407; C35-SI1-C22-C23
61 1 50 51 3 -47.27800 -1.20353 0.06301 1.4254 -0.06680 0.175407; C35-SI1-C29-C30
61 1 50 59 3 -47.27800 -1.20353 0.06301 1.4254 -0.06680 0.175407; C35-SI1-C29-C34
61 62 64 65 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C35-C36-C37-H27
61 62 64 66 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C35-C36-C37-C38
61 70 68 66 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C35-C40-C39-C38
61 70 68 69 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C35-C40-C39-H29
62 61 70 68 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C36-C35-C40-C39
62 61 70 71 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C36-C35-C40-H30
62 64 66 67 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C36-C37-C38-H28
62 64 66 68 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C36-C37-C38-C39
63 62 61 70 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H26-C36-C35-C40
63 62 64 65 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H26-C36-C37-H27
63 62 64 66 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H26-C36-C37-C38
64 62 61 70 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C37-C36-C35-C40
64 66 68 69 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C37-C38-C39-H29
64 66 68 70 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C37-C38-C39-C40
65 64 66 67 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H27-C37-C38-H28
65 64 66 68 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H27-C37-C38-C39
66 68 70 71 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; C38-C39-C40-H30
67 66 68 69 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H28-C38-C39-H29
67 66 68 70 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H28-C38-C39-C40
69 68 70 71 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ; H29-C39-C40-H30

[dihedrals] ; impropers

; treated as propers in GROMACS to use correct AMBER analytical function

; i j k l func phase kd pn

1 3 2 14 1 180.00 4.60240 2 ; SI1- C2- C1- C8
1 39 38 26 1 180.00 4.60240 2 ; SI1-C23-C22-C15
1 51 50 59 1 180.00 4.60240 2 ; SI1-C30-C29-C34
1 62 61 70 1 180.00 4.60240 2 ; SI1-C36-C35-C40
3 6 4 5 1 180.00 4.60240 2 ; C2- C4- C3- H1
3 10 12 13 1 180.00 4.60240 2 ; C2- C6- C7- H5
4 8 6 7 1 180.00 4.60240 2 ; C3- C5- C4- H2

4	12	3	2	1	180.00	4.60240	2 ; C3- C7- C2- C1
6	10	8	9	1	180.00	4.60240	2 ; C4- C6- C5- H3
8	12	10	11	1	180.00	4.60240	2 ; C5- C7- C6- H4
15	2	14	26	1	180.00	4.60240	2 ; C9- C1- C8-C15
15	18	16	17	1	180.00	4.60240	2 ; C9-C11-C10- H6
15	22	24	25	1	180.00	4.60240	2 ; C9-C13-C14-H10
16	20	18	19	1	180.00	4.60240	2 ; C10-C12-C11- H7
16	24	15	14	1	180.00	4.60240	2 ; C10-C14- C9- C8
18	22	20	21	1	180.00	4.60240	2 ; C11-C13-C12- H8
20	24	22	23	1	180.00	4.60240	2 ; C12-C14-C13- H9
27	30	28	29	1	180.00	4.60240	2 ; C16-C18-C17-H11
27	34	36	37	1	180.00	4.60240	2 ; C16-C20-C21-H15
27	38	26	14	1	180.00	4.60240	2 ; C16-C22-C15- C8
28	32	30	31	1	180.00	4.60240	2 ; C17-C19-C18-H12
28	36	27	26	1	180.00	4.60240	2 ; C17-C21-C16-C15
30	34	32	33	1	180.00	4.60240	2 ; C18-C20-C19-H13
32	36	34	35	1	180.00	4.60240	2 ; C19-C21-C20-H14
39	42	40	41	1	180.00	4.60240	2 ; C23-C25-C24-H16
39	46	48	49	1	180.00	4.60240	2 ; C23-C27-C28-H20
40	44	42	43	1	180.00	4.60240	2 ; C24-C26-C25-H17
40	48	39	38	1	180.00	4.60240	2 ; C24-C28-C23-C22
42	46	44	45	1	180.00	4.60240	2 ; C25-C27-C26-H18
44	48	46	47	1	180.00	4.60240	2 ; C26-C28-C27-H19
50	53	51	52	1	180.00	4.60240	2 ; C29-C31-C30-H21
50	57	59	60	1	180.00	4.60240	2 ; C29-C33-C34-H25
51	55	53	54	1	180.00	4.60240	2 ; C30-C32-C31-H22
53	57	55	56	1	180.00	4.60240	2 ; C31-C33-C32-H23
55	59	57	58	1	180.00	4.60240	2 ; C32-C34-C33-H24
61	64	62	63	1	180.00	4.60240	2 ; C35-C37-C36-H26
61	68	70	71	1	180.00	4.60240	2 ; C35-C39-C40-H30
62	66	64	65	1	180.00	4.60240	2 ; C36-C38-C37-H27
64	68	66	67	1	180.00	4.60240	2 ; C37-C39-C38-H28
66	70	68	69	1	180.00	4.60240	2 ; C38-C40-C39-H29

Supplementary References

(1) Hess, B.; Kutzner, C.; van der Spoel, D.; Lindahl, E. *Journal of Chemical Theory and Computation* **2008**, *4*, 435.

(2) Wang, J.; Wolf, R. M.; Caldwell, J. W.; Kollman, P. A.; Case, D. A. *J. Comput. Chem.* **2004**, *25*, 1157.

(3) Chen, J.; Law, C. C. W.; Lam, J. W. Y.; Dong, Y.; Lo, S. M. F.; Williams, I. D.; Zhu, D.; Tang, B. Z. *Chem. Mater.* **2003**, *15*, 1535.

(4) Zhang, T.; Jiang, Y.; Niu, Y.; Wang, D.; Peng, Q.; Shuai, Z. *J. Phys. Chem. A* **2014**, *118*, 9094.

(5) Xie, Y.; Zhang, T.; Li, Z.; Peng, Q.; Yi, Y.; Shuai, Z. *Chem. Asian J.* **2015**, *10*, 2154.

(6) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, *98*, 11623.

(7) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M. L., X.; ; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J., J. A.; ; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian, Inc.* Wallingford CT, **2009**.

(8) Ryckaert, J.-P.; Bellemans, A. *Faraday Discuss. Chem. Soc.* **1978**, *66*, 95.

(9) Zhang, T.; Ma, H.; Niu, Y.; Li, W.; Wang, D.; Peng, Q.; Shuai, Z.; Liang, W. *J. Phys. Chem. C* **2015**, *119*, 5040.

(10) Bayly, C. I.; Cieplak, P.; Cornell, W.; Kollman, P. A. *J. Phys. Chem.* **1993**, *97*, 10269.

(11) Cornell, W. D.; Cieplak, P.; Bayly, C. I.; Kollmann, P. A. *J. Am. Chem. Soc.* **1993**, *115*, 9620.

(12) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 1372.

(13) Jorgensen, W. L.; Chandrasekhar, J.; Madura, J. D.; Impey, R. W.; Klein, M. L. *J. Chem. Phys.* **1983**, *79*, 926.

(14) Bussi, G.; Donadio, D.; Parrinello, M. *J. Chem. Phys.* **2007**, *126*, 014101.

(15) Berendsen, H. J. C.; Postma, J. P. M.; van Gunsteren, W. F.; DiNola, A.; Haak, J. R. *J. Chem. Phys.* **1984**, *81*, 3684.

(16) Berendsen, H.; Postma, J.; van Gunsteren, W.; Hermans, J. In *Intermolecular Forces*; Reidel: Dordrecht: 1981, p 331.

(17) Darden, T.; York, D.; Pedersen, L. *J. Chem. Phys.* **1993**, *98*, 10089.

(18) Essmann, U.; Perera, L.; Berkowitz, M. L.; Darden, T.; Lee, H.; Pedersen, L. G. *J. Chem. Phys.* **1995**, *103*, 8577.

(19) Hess, B.; Bekker, H.; Berendsen, H. J. C.; Fraaije, J. G. E. M. *J. Comput. Chem.* **1997**, *18*, 1463.

(20) Rudnick, J.; Gaspari, G. *J. Phys. A: Math. Gen.* **1986**, *19*, L191.

(21) Zifferer, G. *J. Chem. Phys.* **1995**, *102*, 3720.

(22) Noguchi, H.; Yoshikawa, K. *J. Chem. Phys.* **1998**, *109*, 5070.

(23) Lin, C.-M.; Chen, Y.-Z.; Sheng, Y.-J.; Tsao, H.-K. *React. Funct. Polym.* **2009**, *69*, 539.

(24) Zhang, J.; Lu, Z.-Y.; Sun, Z.-Y. *Soft Matter* **2011**, *7*, 9944.

(25) Weigend, F.; Häser, M.; Patzelt, H.; Ahlrichs, R. *Chem. Phys. Lett.* **1998**, *294*, 143.

(26) Aaqvist, J.; Warshel, A. *Chem. Rev.* **1993**, *93*, 2523.

(27) Lin, H.; Truhlar, D. G. *Theor. Chem. Acc.* **2007**, *117*, 185.

(28) Kwon, O.; Coropceanu, V.; Gruhn, N. E.; Durivage, J. C.; Laquindanum, J. G.; Katz, H. E.; Cornil, J.; Bredas, J. L. *J. Chem. Phys.* **2004**, *120*, 8186.

(29) Sánchez-Carrera, R. S.; Coropceanu, V.; da Silva Filho, D. A.; Friedlein, R.; Osikowicz, W.; Murdey, R.; Suess, C.; Salaneck, W. R.; Brédas, J.-L. *J. Phys. Chem. B* **2006**, *110*, 18904.