Supporting Information

Elucidation of the Key Role of Pt···Pt Interactions in the Directional Self-Assembly of Platinum(II) Complexes

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1. Supplementary details of experiments

Details of the stopped-flow experiments. Kinetic experiments were performed using an Applied Photophysics SX20 stopped-flow spectrophotometer. The temperature of the solutions was maintained with a PolyScience digital temperature controller connected to a circulating water bath. PtB was dissolved in acetone-water (3:1 v/v) mixture, and it was then mixed with acetone, finally reaching a volume ratio of acetone-water of 7:1 (v/v). The total concentration of PtB is 2.25×10^{-4} M. The experiments were conducted at 298 K. The absorbance changes at 594 nm were measured as an indication of the degree of aggregation attributed to the formation of metal–metal interactions.

2. Supplementary Computational Methods

2.1. Fitting the UV curves to an isodesmic model.

The proportion of aggregates in the solution can also be modelled with isodesmic model. In this model, the fraction of aggregates (α_{agg}) can be calculated with a sigmoid equation:

$$\alpha_{agg}(T) = \frac{1}{1 + \exp\left[-0.908\Delta H \frac{T - T_m}{RT_m^2}\right]} \quad \text{(S1)}$$

Here ΔH is the enthalpy change upon addition of a monomer onto an existing aggregate, T_m is the melting temperature, which is defined as the temperature for which $\alpha_{agg}(T) = 0.5$. α_{agg} is the normalized fraction of aggregates, where $\alpha_{agg} = 1$ corresponds to the 100% fraction of aggregates. To derive $\alpha_{agg}(T)$ from experiment, we need to perform normalization on the observed absorption coefficient $A(T)$:

$$\alpha_{agg}(T) = \frac{A(T) - A_m}{A_A - A_m} \quad \text{(S2)}$$

where A_A and A_m are the maximum and minimum values of absorption coefficient. A_A corresponds to 100% of the aggregate fractions, while A_m corresponds to 0% of aggregate fractions. Finally, A_A and A_m need to be fitted together with T_m and ΔH with the experimental UV spectra data.

We have adopted a similar brute force searching in isodesmic models of experimental data, where all possible combinations of $\{A_m, A_A, T_m, \Delta H\}$ have been tested to fit with UV spectra data at all temperatures. A series of combinations of $\{A_m, A_A, T_m, \Delta H\}$ can fit well with experimental results as shown in (Fig. 1c). Among these combinations, the best fitting appears when $\Delta H = -33 \pm 3$ kJ/mol.

2.2. Fitting the UV curves to a cooperative growth model via the nucleation-elongation theory.

The proportion of aggregates in the solution can be modelled using the nucleation-elongation model. In this model, the fraction of aggregates (α_{agg}) can be calculated using elongation theory when the temperature is lower than the elongation temperature (T_e). Alternatively, when temperature is higher than the elongation temperature, nucleation-theory is used to calculate α_{agg}.

The elongation theory: In the elongation phase, the fraction of aggregates (α_{agg}) can be calculated with the Van't Hoff's theory, which finally leads to(1):

$$\alpha_{agg}(T) = 1 - e^{-\frac{H_e}{RT_e^2}(T - T_e)} \quad \text{(S3)}$$

Here, α_{agg} has the same definition as in Eq. (S1) and corresponds to the normalized fraction of aggregates. $\alpha_{agg}(T)$ can be obtained from the experimental absorption coefficient ($A(T)$) using Eq. (S2). Combing Eq. (S2) and Eq. (S3), we can then obtain the equation to fit:

$$1 - \alpha_{agg}(T) = 1 - \frac{A(T) - A_m}{A_A - A_m} = e^{-\frac{H_e}{RT^2}(T - T_e)} \quad \text{(S4)}$$

Here, H_e is the enthalpy change due to non-covalent interactions during elongation. In this equation, A_A, A_m, T_e, and H_e are fitting parameters.

With an exhaustive search for all possible combinations of $\{A_A, A_m, T_e, H_e\}$ that can fit with the UV spectra in the elongation phase, a series of combinations of $\{A_A, A_m, T_e, H_e\}$ that all fit well with experimental results can be found (Fig. 2b). We can then obtain $H_e = -15.8 \pm 2.3$ kJ/mol (Fig. 2b).

The nucleation theory: In the nucleation phase, the fraction of aggregates is calculated using nucleation theory(1):

$$\alpha_{agg}(T) = K_a^{1/3} e^{\left(\frac{2}{3K_a^{1/3}}-1\right)\frac{H_e}{RT_e^2}(T-T_e)} \quad \text{(S5)}$$

Since A_A, A_m, T_e, and H_e have already been obtained in the elongation phase, the only additional parameter in the nucleation phase, the equilibrium constant of activation K_a, can be fitted with the experimental data in the nucleation region.

The average size of the nucleus at elongation temperatures is given by(1):

$$\overline{N_n(T_e)} = K_a^{-1/3} \quad \text{(S6)}$$

Two examples of the cooperative nucleation-elongation models for bi-PtB and bi-PtT complexes are shown in Fig S1a-b and Fig. S1c-d, respectively. Both bi-PtB (Fig. S1b) and bi-PtT (Fig. S1d) clearly show non-sigmoidal curves and can be fitted to the cooperative nucleation-elongation model.(1, 2) In these nucleation-elongation models, extremely small equilibrium constants (e.g. $K_a = 1.14 \times 10^{-4}$ or 6.8×10^{-4})(1, 2) for the nucleation process were found at the elongation temperature (T_e), indicating an unfavorable nucleation process at T_e.

2.3. An extended kinetic nucleation-growth model to fit data from the stopped-flow experiments.

To fit the kinetic data obtained from the stopped-flow experiments, we developed a nucleation-growth model that considers three kinetic processes in the self-assembly of PtB: the formation of nucleus, growth of the fibril aggregates, and merging of smaller aggregates into large ones (see below for details).

(a) The formation of nucleus: Following our previous work,(3) we built a modified nucleation theory based on the classical nucleation theory (CNT). This CNT is only applicable to rigid monomer with spherical shape, and we thus introduce a pre-exponential factor A_{conf} to treat the non-spherical and flexible PtB molecule:

$$J_n(t) = A_{\text{conf}} \cdot \left[(36\pi)^{1/6}\frac{DC_e}{v^{2/3}}\right]\frac{1}{\sqrt{\theta}}(S(t)\ln S(t))e^{-4\theta^3/27\ln^2 S(t)}$$
$$C_n = J_n(t)dt \quad \text{(S7)}$$

where $J_n(t)$ is the nucleation rate, C_n is the concentration of aggregates formed at $t_n = ndt$. D is the

diffusion constant of PtB in solvent mixture, C_e is the solubility of PtB, v is the volume of PtB, $S(t)$ is the saturation ratio, and θ is related to the PtB-water interaction and can be obtained by fitting to the experimental data. A_{conf} is a pre-exponential factor that is related to the entropy change of monomer attachment to an existing aggregate.

(b) Growth of the fibril aggregates: Similar to the previous study,(3) we next consider the subsequent growth of the nucleus. For those nuclei formed at ndt, they will further grow to form aggregates with the average size $g_n(t)$ at time t ($t > ndt$):

$$f_n(t) = A_{\mathrm{conf}} \cdot 4\pi D C_e S(t) R_1$$
$$\frac{dg_n(t)}{dt} = f_n(t) - f_n^e(t) = A_{\mathrm{conf}} \cdot 4\pi D C_e (S(t) - 1) R_1 \quad \text{(S8)}$$

where R_1 is the radius of the PtB monomer. As shown in Eq. (S7), A_{conf} is a pre-exponential factor to take into account the conformational change associated with the kinetic process of a PtB monomer attaching to an existing aggregate. Therefore, we can obtain A_{conf} from the $-T\Delta S_{\mathrm{conf}}$ term of the free energy computed from the nucleation-growth theory (see SI Sec. 2.1 for details): $-T\Delta S_{\mathrm{conf}} = kT \ln A_{\mathrm{conf}}$, which can be obtained from $\Delta G_e = \Delta H_e - T\Delta S_{\mathrm{conf}}$. ΔG_e refers to the free energy change of transfer of a PtB molecule from aggregate to solution and can be computed from the solubility C_e. We obtained the solubility C_e from $C_e = \big(1 - \alpha(298\mathrm{K})\big) \times C_{total}$, where $\alpha(298\mathrm{K}) = 0.5$ (see Fig. 2). As the total concentration of PtB (C_{total}) is 2.25×10^{-4} M in our experiment, the solubility C_e can then be obtained as 1.12×10^{-4} M. $\Delta H_e = -15.8$ kJ/mol is the elongation enthalpy derived from the UV-Vis experiments (see Fig. 2 and SI Sec. 2.2 for details).

(c) Merging of small aggregates into larger ones: The original kinetic growth model (Eq. (S8)) was developed to fit the microfluidics data where the aggregation process occurs at sub-millisecond(3) timescale. However, the stopped-flow experiment in this work monitors the dynamics of the self-assembly at much longer timescales: i.e., seconds to hundreds of seconds. During this period, there is sufficient time for small aggregates (or shorter fibrils) to collide and merge into longer ones. Therefore, it is necessary to modify the original kinetic growth model to take into account this merging process.

In our growth model as shown in Eq. (S8), the elongated aggregates in the fibril shape can only grow from the two ends by addition of PtB monomers (so called "monomer-attachment sites"). However, the kinetic process of merging short fibrils into longer ones would compete with this native fibril growth, and thus occupy a fraction of available monomer-attachment sites. This is because the merging of two short fibrils will eliminate two monomer-attachment sites (the two sites where the

two ends of short fibrils meet), while the elongation of fibril by addition of PtB monomer will not change the number of the monomer-attachment sites. To consider this additional kinetic process, we introduced a quantity $\sigma_n(t)$ to describe the reduction in the fraction of available monomer-attachment sites in those aggregates that grow from nuclei formed at ndt. Correspondingly, the original growth model can be modified as below:

$$f_n(t) = A_{\text{conf}} \cdot 4\pi D C_e S(t) R_1 \sigma_n(t)$$
$$\frac{dg_n(t)}{dt} = f_n(t) - f_n^e(t) = A_{\text{conf}} \cdot 4\pi D C_e (S(t) - 1) R_1 \sigma_n(t) \quad \text{(S9)}$$

where $\sigma_n(t)$ initially equals 1 and decreases as time elapses. In general, the merging process will lead to a reduced aggregate concentration: $C_n'(t) = C_n \sigma_n(t)$ ($\sigma_n(t) \leq 1$) and produce larger-sized aggregates: $g_n'(t) = g_n(t)/\sigma_n(t)$. The time evolution of $\sigma_n(t)$ can then be described by the following equation:

$$\frac{d\sigma_n(t)}{dt} = -\gamma_n \sigma_n(t) \sum_i \sigma_i(t) C_i \quad \text{(S10)}$$

where each of the quartic term on the r.h.s. (i.e., $-\gamma_n \sigma_n(t) \sigma_i(t) C_i$) describes the kinetic process where a given fibril-shaped aggregate can merge with another one at either of its two ends. We presume that the rate constant γ_n is independent of the aggregate size: $\gamma_1 = \gamma_2 = \cdots = \gamma$. Finally, we can obtain the total number of PtB molecules that are in the aggregates:

$$I(t) = \sum_i g_i'(t) C_i'(t) = \sum_i g_i(t) C_i \quad \text{(S11)}$$

Combining Eq. (S7), (S9), (S10) and (S11), we can obtain $I(t)$ which should be proportional to the observations from the UV absorbance in the stopped-flow experiment. As shown in Fig. 3, our extended kinetic nucleation-growth model fits well to the stopped-flow experimental data, and the fitted values of the two variables are $\gamma = 3.1 \times 10^4$ $\text{M}^{-1}\text{s}^{-1}$ and $\theta = 10.3$ kJ/mol. The fitted results clearly indicate that there exists a nucleation phase at the early stage of self-assembly.

2.4. Potential functional forms in Amber force field.

We developed force field parameters for Pt(II) complexes based on the same functional form originally used in the AMBER force field.(4-6) In the AMBER force field, the potential function describing interactions among particles consists of bonded and non-bonded interactions. The functional forms are defined as:

$$E = \sum_{bonds} \frac{K_b}{2}(b - b_{eq})^2 + \sum_{angles} \frac{K_\theta}{2}(\theta - \theta_{eq})^2 + \sum_{torsions} V_n[1 + \cos(n\phi - \gamma)] + \sum_{i<j} 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{R_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{R_{ij}}\right)^{6}\right] + \sum_{i<j} \frac{q_i q_j}{4\pi\varepsilon_0 R_{ij}} \quad \text{(S12)}$$

The first three terms represent bonded interactions, describing the bond, angle, and torsion interactions, respectively. The last two terms represent non-bonded interactions, including van der Waals (vdW) and electrostatics interactions. K_b and K_θ are the force constants for the bonds and angles, respectively; b_{eq} and θ_{eq} represent the bond length and bond angle of the equilibrated conformation; b and θ represent the bond length and bond angle, respectively. ϕ and V_n represent the torsional angle and force constant, respectively; n is an integer describing the periodicity. γ is the phase angle with a value of 0° or 180°. The 12-6 Lennard-Jones (LJ) potential is used to describe the pair-wise vdW interaction. Here, ε_{ij} is the depth of the potential well, σ_{ij} is the finite distance at which the inter-particle potential is zero, and R_{ij} is the distance between the particles. Furthermore, the electrostatic potential is described by the Coulomb interactions between pairs of particles with atomic partial charges q_i and q_j, and the force field parameters were developed to reproduce the relative potential energies obtained from the QM calculation. Here, all the QM calculations were performed using the Gaussian 09 program package(7), and all the molecular mechanics calculations and MD simulations were performed with GROMACS (version 4.5.5) program.

Bonded parameters between Pt(II) and ligands. We set up the force field parameters for the aromatic ligands using the general amber force field (GAFF)(4). The central Pt(II) atom in each Pt(II) complex has coordination bonds with three nitrogen atoms on the aromatic ring and one chloride atom (PtB and PtB-b) or carbon atom (PtB-a) on the substitute. The harmonic potential was added to describe the coordination bond between the central Pt(II) atom and the ligands.

Select typical Fragment PtB-core from PtB. To get the force field parameters of Pt(II) atom in Pt(II) complexes, and to make the force field parameters transferable, the representative Pt(II) core was selected and termed PtB-core shown in Fig. 4a. Then, we chose PtB-core as the starting point for QM optimization and charge derivation. Similar to previous studies,(8) the geometric optimization of the Fragment monomer was carried out at the TPSS-D3/def2-TZVP level.(9-11)

2.5. Fitting the LJ parameters for Pt in PtB-core.

The force field parameters of Fragment were set up using the General Amber force field (GAFF), except for the Pt(II) atom. The geometric structure of a single PtB-core was first optimized at the TPSS-D3/def2-TZVP level. Then, the partial charge of each atom was fitted using the restrained

electrostatic potential (RESP) method(12, 13) to reproduce the electrostatic potential(14) of the optimized structures. The force field model for Pt(II) complexes was termed as PtFF.

To fit the LJ parameters of Pt in PtB-core, we scanned the intermolecular Pt···Pt distance vertically from 3.0 Å to 7.0 Å at a step size of 0.2 Å. The fitting procedure is as follows: (1) Optimize the geometric structure of a single PtB-core at the TPSS/def2-TZVP level; (2) Optimize the dimer of PtB-core packed in the antiparallel fashion using Gaussian 09 at the TPSS/def2-TZVP level; (3) Calculate the QM potential energy profile as a function of Pt···Pt distance ranging from 3.0 Å to 7.0 Å at a step size of 0.2 Å in the vertical direction; (4) Calculate the MM potential energy profiles of PtFF based on the geometric structures obtained from the QM scan. During the MM calculation, the LJ parameters for Pt(II) were set to zero, termed as MM_{noPt}; (5) Fit the LJ parameters of the Pt(II) atom for the PtB-core dimer in the three force field models by minimizing the relative potential energy difference between the QM and MM profile iteratively; (6) Validate the fitted LJ parameters for PtB-core using the PtFF model by scanning the Pt···Pt distance of the PtB-core dimer along the long-axis and short-axis. Here, the long axis is the direction parallel to the connection between two bzimpy moieties of the ligand, and the short axis is the direction along the middle Pt-N bond of PtB-core (see Fig. S2).

2.6.Validating force field parameters.

We first checked if the developed LJ parameters of PtB-core along the vertical direction could reproduce the QM energy profile as a function of Pt···Pt distance (ranging from 3.0 Å to 7.0 Å with the step size of 0.2 Å) along the long axis and the short axis of dimer by using PtFF (Fig. S4b). The corresponding QM and MM potential energy profiles of PtB-core along the vertical, long-axis, short-axis directions are summarized in Fig. S4b.

Second, the force field parameters were validated using two isolated Pt(II) complexes, PtB-a and PtB-b, by comparing the conformational changes between the energy minimized conformation obtained from the MM method and the optimized structure obtained from the QM method. The obtained RMSD value is summarized in Table S2. The force field parameters for PtB, PtB-a, and PtB-b were setup using GAFF, where the LJ parameters of Pt(II) were filled by our new fitted LJ parameters. In molecules PtB, PtB-a and PtB-b, the corresponding partial charge of each atom was obtained using the RESP method, which could reproduce the calculated electrostatic potential with PtB-core. The geometric structures of the PtB-a and PtB-b monomers were optimized at the TPSS/def2-TZVP level using the QM method before the electrostatic potential was calculated.

To further validate the force field parameters, MD simulations were performed for the crystal structures of PtB-a and PtB-b. For each Pt(II) complex, the supercells were constructed based on the experimental crystal structures(15, 16) using PtFF. The details of the supercells for all PtB-a and PtB-b complexes were collected and are summarized in Table S4. Then, to validate the fitted LJ parameters

of the Pt(II) atom in each system, we performed the following calculations (all the RMSD calculations were performed only for the heavy atoms of the Pt complexes): First, the supercells of each Pt(II) complex were energy minimized with the steepest descent algorithm. Second, we calculated the RMSD between the energy minimized structure of each supercell and the initial conformation of the supercell in crystal structure and summarized the results in Table S2. Third, we performed a 100 ps MD simulation with position restraints on the heavy atoms with force constants of 1000 kJ mol^{-1} $Å^{-2}$ under an isothermal (300 K) ensemble (NVT) using the Berendsen thermostat(17) with a coupling time constant of 0.1 ps. Finally, we carried out a 10 ns production MD simulation for each Pt(II) system. The temperature was slowly increased from 50 to 300 K (close to the crystallization temperature) during the initial 1 ns of the simulation, and the temperature was maintained at 300 K in the remaining 9 ns of the simulation. We carried out the production MD simulations under an isothermal (300 K), isobaric (1 bar) ensemble (NPT) using the V-rescale thermostat(18) and the Berendsen barostat(17) with a coupling time constant of 0.1 and 1.0 ps, respectively. The long-range electrostatic interactions beyond the cutoff at 12 Å were considered using the Particle Mesh Ewald (PME) method, and the LJ interactions were smoothly switched off between 10 and 11 Å. The updated frequency of the neighbor list was 10 steps, and the integration time step was 1.0 fs. The last frame of the production MD simulation was used for RMSD computation, as well as the change of unit cell size relative to the initial supercell set up from experimental crystal structures.

2.7. MD simulation and analysis of self-assembly of PtB Oligomers.

To understand the self-assembly mechanism of amphiphilic Pt(II) complexes, oligomer formation at the early stage of self-assembly in aqueous solutions for the representative Pt(II) complex, PtB, was set up using atomistic MD simulations. Here, PtB oligomers with aggregate sizes: 2, 3, 6, and 10 were considered. The initial conformations were generated by randomly placing 2, 3, 6, and 10 PtB molecules in cubic simulation boxes with an edge length of 6 nm. The total number of water molecules when the oligomer aggregate size was 2, 3, 6, and 10 were 6933, 6902, 6820, and 6700, respectively. All water molecules here were modelled by TIP3P force field. For each oligomer system, we first performed energy minimization before running a 2 ns MD simulation with position restraints (the force constants of 1000 kJ mol^{-1} $Å^{-2}$) on the heavy atoms under the NVT ensemble (300 K) using a Berendsen thermostat(17) with a coupling time constant of 0.1 ps. Then, 10 production MD trajectories, 100 ns for each trajectory, were carried out for each PtB oligomer size. The temperature was slowly increased from 50 to 300 K during the initial 2 ns of the simulation, and then the temperature was maintained at 300 K. The production MD simulations were carried out under the NPT (300 K, 1 bar) ensemble using the V-rescale thermostat(18) and Parrinello-Rahman barostat(19) with the coupling time constant of 0.1 and 1.0 ps, respectively. The long-range electrostatic interactions beyond the cutoff at 12 Å were considered using the Particle Mesh Ewald (PME) method,

and the LJ interactions were smoothly switched off between 10 and 11 Å. The updated frequency of the neighbor list was 10 steps, and the integration time step was 2.0 fs. The representative snapshots of the PtB oligomers are shown in Fig. 6a and Fig. S5.

Controlled MD simulations. To consider the influence that the Pt···Pt interactions may have on the self-assembled structure of PtB, we performed controlled MD simulations for Pt^{s}B without d^8-d^8 interactions using the same setup as the above simulations of PtB. In our force fields, the d^8-d^8 interactions between PtB molecules are mainly captured by tuning the LJ parameters of the Pt atom (see SI Sec 2.5 for details). Therefore, when designing the control system in the absence of d^8-d^8 interactions (i.e., Pt^{s}B), we take the published LJ parameters(20) for the Pt(II) atom in Pt^{s}B (σ = 0.43475 nm, ε = 1.674 kJ/mol, Table S1). In this set of parameters, the ε of the Pt atom is significantly smaller than that of PtB in our force field, rendering the long-range d^8-d^8 interactions almost negligible between two Pt^{s}B molecules (Fig. 5a). Except for LJ parameters, all other force field parameters for PtB and Pt^{s}B are the same. And then we deleted the Pt(II) atoms from the PtB system (termed Pt-free) and performed the second controlled MD simulations (shown in Fig. S6). We found that several small randomly packed oligomers formed in the aqueous solution, showing that without Pt, the non-planar ligands could only aggregate via hydrophobic interactions in aqueous solutions, and the linear packing disappears without long-range directional Pt···Pt and π-π interactions.

RMSF calculations and Angle distribution analysis. We conducted the RMSF and angle distribution analyses after the linear-assembled structure was formed in MD simulations. For the RMSF analysis, the average distance between the backbone atoms (e.g., Pt atoms) and their corresponding atoms that occurred Δt ahead, was calculated over different Δt._After projecting the two adjacent PtB molecules into the same plane, the rotational angle between the two adjacent PtBs can also be obtained, as shown in Fig. 6c. For the angle distribution analysis, each PtB molecule was treated as a PtB plane by its core molecules and the angle between each pair of neighboring PtB planes could be calculated, as shown in Fig. 6d.

Non-covalent interactions analysis. All density functional theory (DFT) calculations were performed with the Gaussian 09 software package. The ground-state geometries of the dimer and trimer of PtB were fully optimized by DFT at the M06 level(21) in conjunction with the solvation model density (SMD) continuum method(22) using water as the solvent. Vibrational frequencies were then computed for all stationary points to verify that each was a minimum on the potential energy surface (NIMAG = 0). The Cartesian coordinates of the optimized geometries of the dimer and trimer of PtB are given in Tables S5 and S6. The Stuttgart effective core potentials (ECPs) and the associated basis set were used to describe Pt(23) with two f-type polarization functions (ζ = 0.70 and 0.14),(24) whereas the 6-31G(d,p) basis set was employed to describe all other atoms.(25-28) All DFT calculations were performed with a pruned (99,590) grid for numerical integration. Noncovalent

interaction (NCI) analysis of the dimer and trimer has been performed on the geometry optimized at the M06 level by NCIPLOT.(29)

Supplementary Figures and Tables:

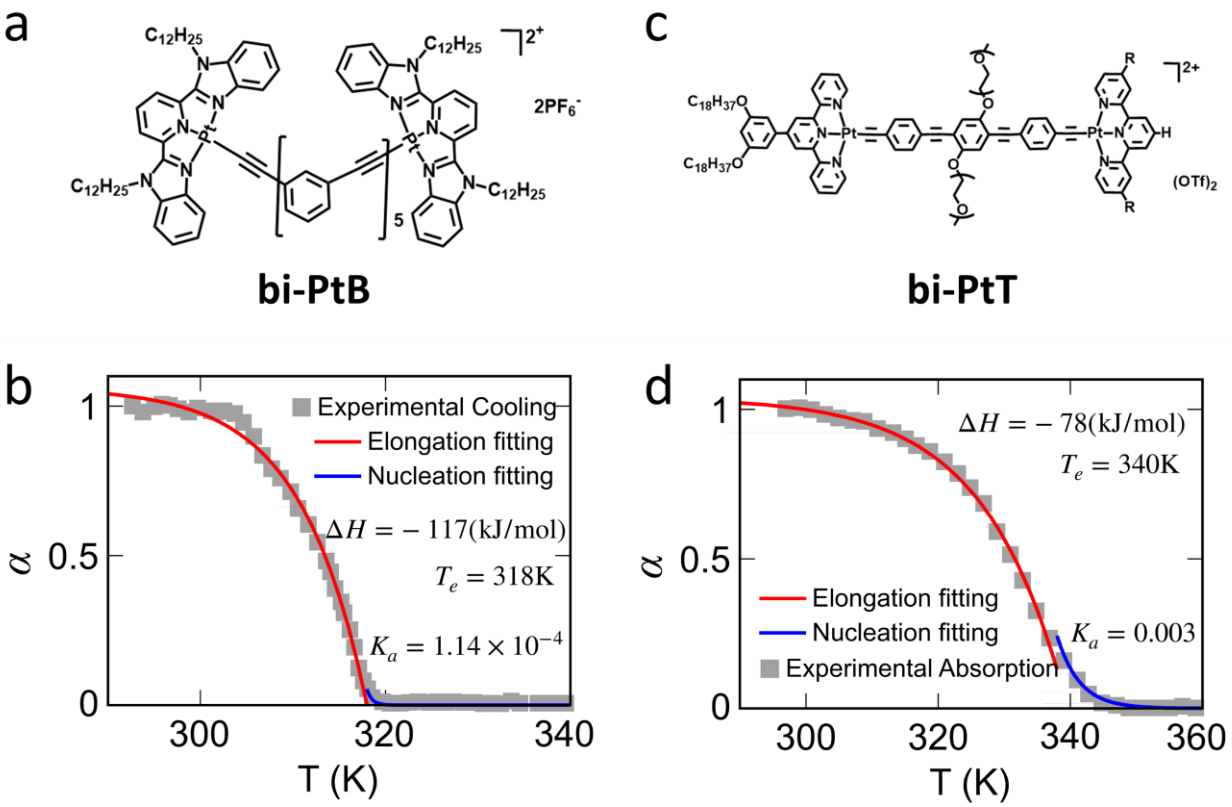


Figure S1. The chemical structure and fitted curve of bi-PtB and bi-PtT. (a) Chemical structure of bi-PtB. (b) The fraction of aggregation of bi-PtB obtained from the UV absorption data (dashed points) as a function of temperature. The fraction of aggregation was fitted to the cooperative nucleation-elongation model (red and blue curves represent elongation and nucleation, respectively).(2) (c) Chemical structure of bi-PtT. (d) Similar to (b) except the experimental data was fitted to the nucleation-elongation model for bi-PtT.(1)

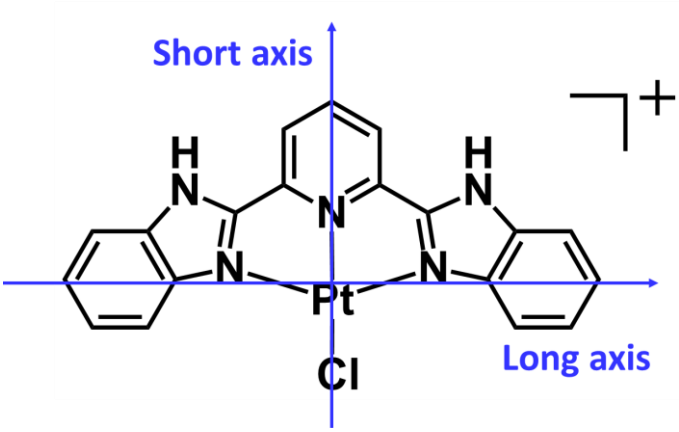


Figure S2. The definition of the long axis and short axis in the PtB-core.

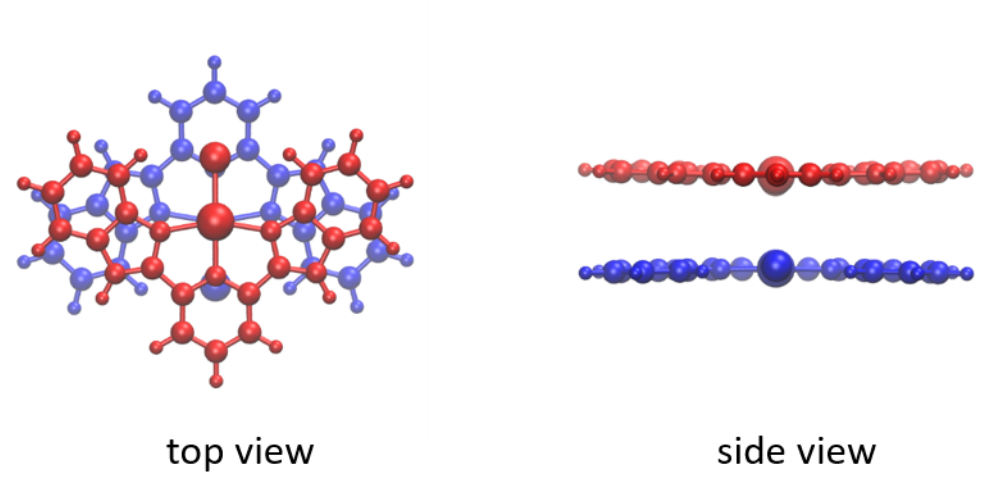


Figure S3. Dimer configurations for PtB-core at both top and side view.

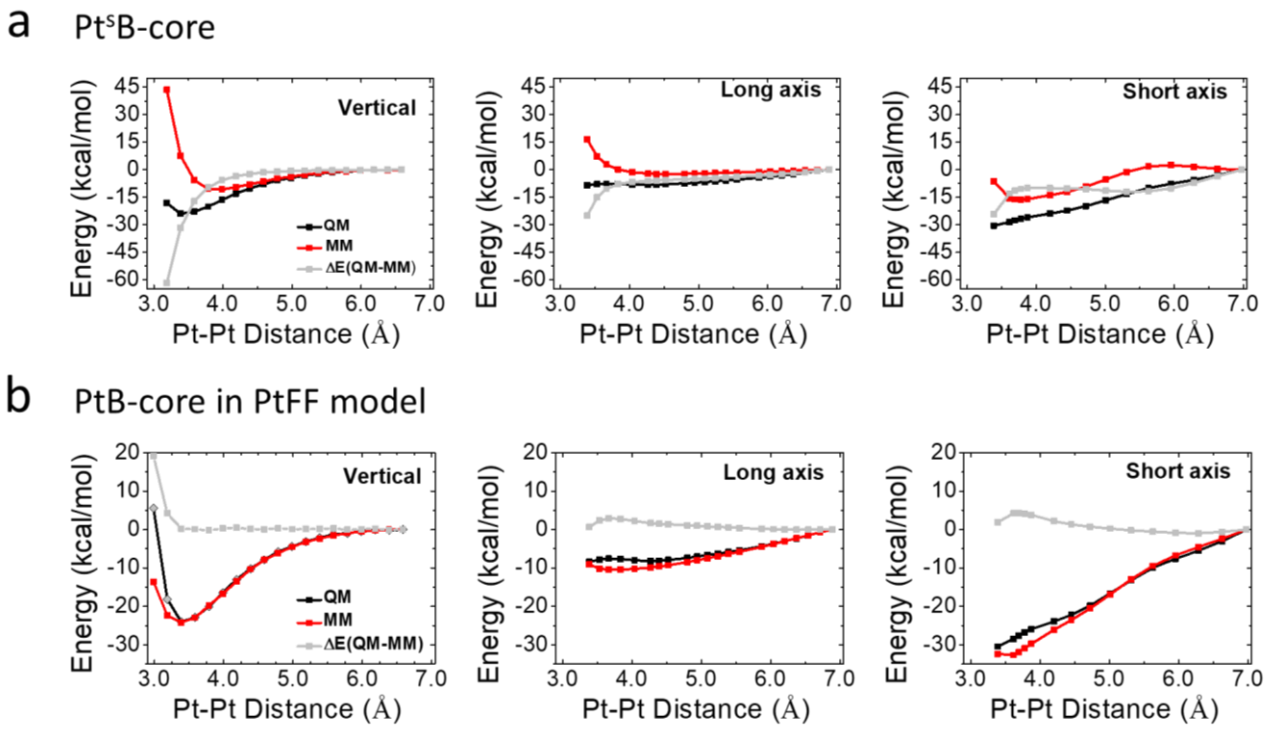


Figure S4. The potential energy profiles as a function of Pt···Pt distances in PtB-core dimers. The results obtained using QM (black curves) and MM (red curves) calculations are shown. The grey curves represent the differences between the QM and MM results: $\Delta E = E(\mathrm{QM}) - E(\mathrm{MM})$. The potential energy profiles for (a) PtˢB-core, (b) PtB-core using the PtFF model, along the vertical (left panel), long-axis (middle panel) and short-axis (right-panel), respectively.

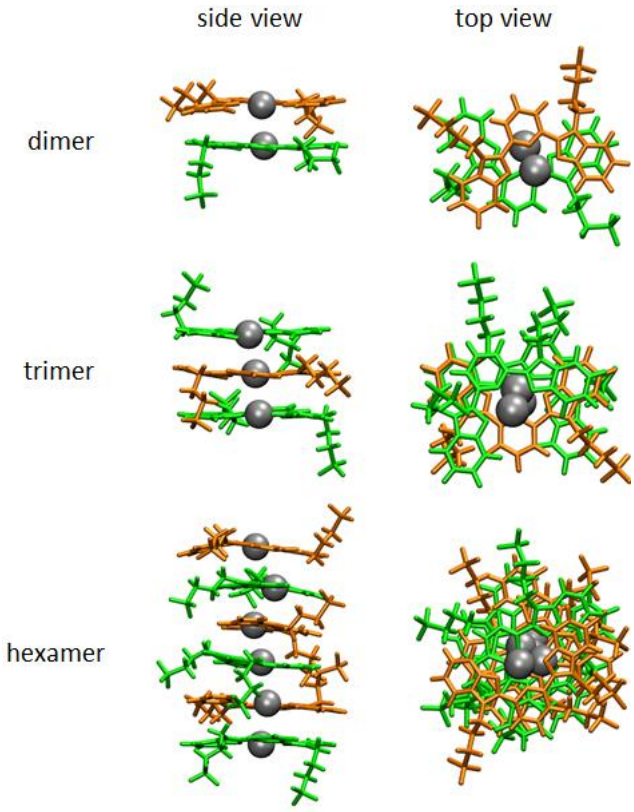


Figure S5. Snapshots of typical assembled PtB oligomers: dimer, trimer, and hexamer in both side view and top view, respectively.

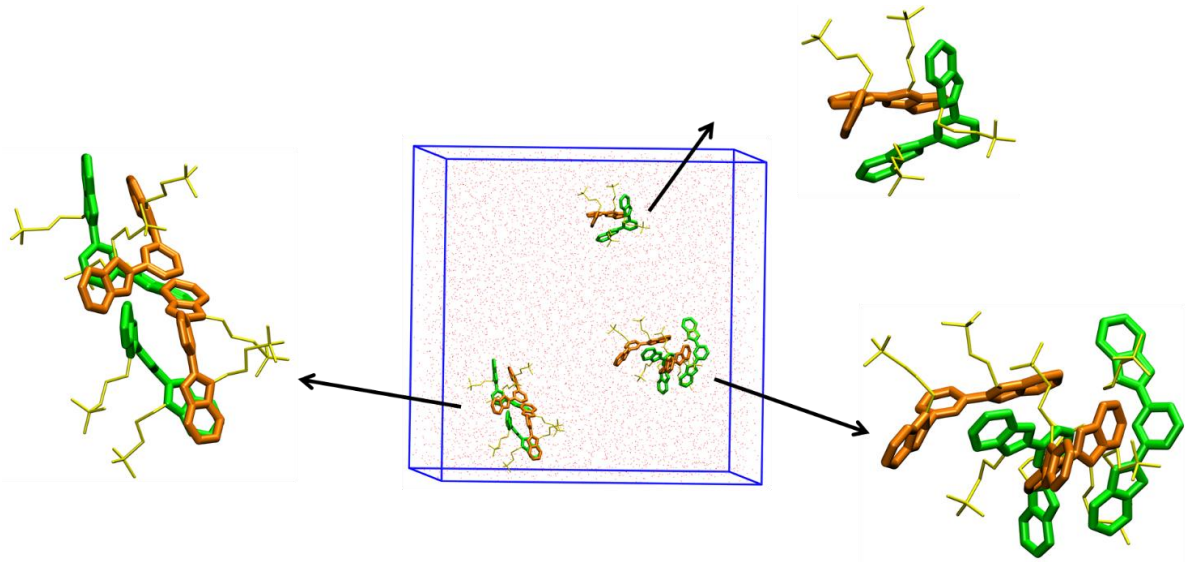


Figure S6. Representative snapshot of the assembled aggregates of Pt-free molecules. The Pt-free molecules aggregate randomly and cannot pack linearly.

Table S1. The LJ force field parameters for Pt^{s}B-core (see reference (20))and PtB-core in different force field models.

	σ (nm)	ε (kJ/mol)
Pt^{s}B-core	0.43475	1.674
PtB-core	0.33298	10.534

Table S2. RMSD comparison for PtB-a and PtB-b crystal structures to validate the LJ parameters for a Pt(II) atom.

Crystals	Initial structure	Method	Condition	RMSD (Å)
In PtFF model				
crystal PtB-a	single QM	MM optimization	vacuum	0.015
	crystal structure	MM optimization	crystal	0.049
	crystal structure	MD simulation	crystal	0.455
crystal PtB-b	single QM	MM optimization	vacuum	0.036
	crystal structure	MM optimization	crystal	0.081
	crystal structure	MD simulation	crystal	0.456

Table S3. Box vector comparison for PtB-a and PtB-b crystal structures to validate the LJ parameters of a Pt(II) atom.

Molecule	Model	*a* (Å)	*b* (Å)	*c* (Å)	Volume (Å^3)	Volume change
crystal PtB-a	experiment	22.37	27.37	14.95	8337.47	2.10%
	MD	22.21	27.18	14.84	8162.28	
crystal PtB-b	experiment	26.983	8.530	25.018	5081.20	1.86%
	MD	27.149	8.583	25.172	5175.87	
	MD	27.164	8.587	25.185	5184.35	

Table S4. The details of the PtB-a and PtB-b supercells.

systems	size	The composition in the supercells
PtB-a supercell	3×3×3	216 PtB-a, 216 $SO_3CF_3^-$ ions and 324 CH_3CN molecules
PtB-b supercell	3×4×3	288 PtB-b, 288 PF_6^- ions and 288 $(CH_3)_2NC(O)H$ molecules

Table S5. Cartesian coordinates of the optimized ground-state geometry of the dimer of **PtB** at the M06 level.

1	C	-0.754073	4.250334	-0.160389	54	N	0.064770	2.195236	-0.997432
2	C	0.560645	4.661596	0.021425	55	S	-4.805927	4.798375	3.635811
3	C	1.627475	3.833187	-0.308901	56	S	5.922925	5.711225	-3.152380
4	H	-1.569257	4.904541	0.126672	57	O	-3.553468	4.194013	4.158871
5	H	2.645351	4.179284	-0.166062	58	O	-5.960680	3.863432	3.690504
6	C	2.265471	1.491894	-1.202428	59	O	-5.106572	6.125342	4.226345
7	C	2.782254	-0.515470	-1.909022	60	O	4.577640	6.264215	-3.453254
8	C	3.976755	0.189322	-1.675849	61	O	6.476826	4.902630	-4.267845
9	C	2.800865	-1.838526	-2.361437	62	O	6.872585	6.732399	-2.645536
10	C	5.228896	-0.382747	-1.902717	63	Cl	-0.747883	-1.822721	-2.406456
11	C	4.043323	-2.406188	-2.584069	64	Cl	1.646140	-3.798627	0.504849
12	H	1.872889	-2.378619	-2.531643	65	Cl	0.624908	-4.673993	0.151825
13	C	5.236269	-1.688564	-2.363844	66	Cl	-0.710323	-4.309732	0.272606
14	H	6.151697	0.166458	-1.734642	67	H	2.681294	-4.107397	0.408637
15	H	4.103200	-3.430988	-2.941229	68	H	-1.486408	-5.002926	-0.030476
16	H	6.188439	-2.175497	-2.556991	69	C	-2.312610	-2.411602	0.992998
17	C	-2.251233	2.320776	-1.004223	70	C	-3.651490	-0.782393	1.586199
18	C	-4.346945	1.732780	-1.333329	71	C	-4.439123	-1.864475	1.156553
19	C	-3.506858	0.666351	-1.698826	72	C	-4.240330	0.405871	2.029908
20	C	-5.736415	1.642028	-1.412562	73	C	-5.831936	-1.798723	1.123631
21	C	-4.036280	-0.530573	-2.191103	74	C	-5.622759	0.465359	2.009857
22	C	-6.250858	0.449780	-1.891589	75	H	-3.629646	1.234573	2.381708
23	H	-6.382876	2.462066	-1.111067	76	C	-6.405139	-0.615533	1.556641
24	C	-5.414517	-0.614772	-2.282009	77	H	-6.437567	-2.629740	0.771778
25	H	-3.384257	-1.347531	-2.492814	78	H	-6.118299	1.370020	2.357775
26	H	-7.328332	0.330915	-1.970094	79	H	-7.487454	-0.516970	1.547508
27	H	-5.864308	-1.526140	-2.671517	80	C	2.158363	-1.425588	1.388578
28	C	1.352017	2.567786	-0.817137	81	C	3.805043	-0.040040	1.852127
29	C	-0.987109	2.987824	-0.696333	82	C	2.578216	0.604422	2.092511
30	N	1.734506	0.327235	-1.614179	83	C	5.029272	0.595528	2.059178
31	N	-2.207221	1.065552	-1.482824	84	C	2.535715	1.929636	2.536312
32	Pt	-0.304015	0.358901	-1.638066	85	C	4.975779	1.905204	2.505910
33	H	0.758835	5.646522	0.432278	86	H	5.975965	0.091123	1.883187
34	N	3.618129	1.448182	-1.223579	87	C	3.750298	2.562687	2.735486
35	N	-3.525242	2.772244	-0.930167	88	H	1.584088	2.424661	2.712701
36	C	-4.016459	4.008720	-0.316942	89	H	5.904101	2.442699	2.680382
37	H	-3.365433	4.834569	-0.619443	90	H	3.762100	3.593461	3.080182
38	H	-4.996884	4.216554	-0.757370	91	C	-1.013530	-3.045943	0.770083
39	C	4.574044	2.520274	-0.940414	92	C	1.301616	-2.538307	0.982498
40	H	4.249118	3.052546	-0.039888	93	N	-2.331476	-1.156344	1.474277
41	H	5.521580	2.036845	-0.678656	94	N	1.571818	-0.289631	1.803964
42	C	4.747380	3.442333	-2.133365	95	Pt	-0.462473	-0.393346	1.738197
43	H	5.136502	2.864170	-2.982104	96	H	0.875612	-5.658788	-0.229460
44	H	3.771334	3.849622	-2.432258	97	N	-3.568445	-2.887434	0.818282
45	C	5.690736	4.574643	-1.788348	98	N	3.506574	-1.315386	1.404771
46	H	5.308138	5.168977	-0.948318	99	C	4.509890	-2.320282	1.052438
47	H	6.685577	4.202516	-1.514442	100	H	4.165284	-2.851549	0.158432
48	C	-4.105081	3.836177	1.186792	101	H	5.410888	-1.775818	0.748960
49	H	-4.832752	3.041705	1.402529	102	C	-3.989878	-4.125696	0.159248
50	H	-3.132341	3.494816	1.570451	103	H	-3.363576	-4.949312	0.512907
51	C	-4.513041	5.107623	1.894655	104	H	-5.003619	-4.344115	0.509407
52	H	-5.443482	5.525244	1.490695	105	C	-3.946640	-3.946727	-1.345640
53	H	-3.734432	5.877958	1.828984	106	H	-4.663892	-3.162447	-1.620539

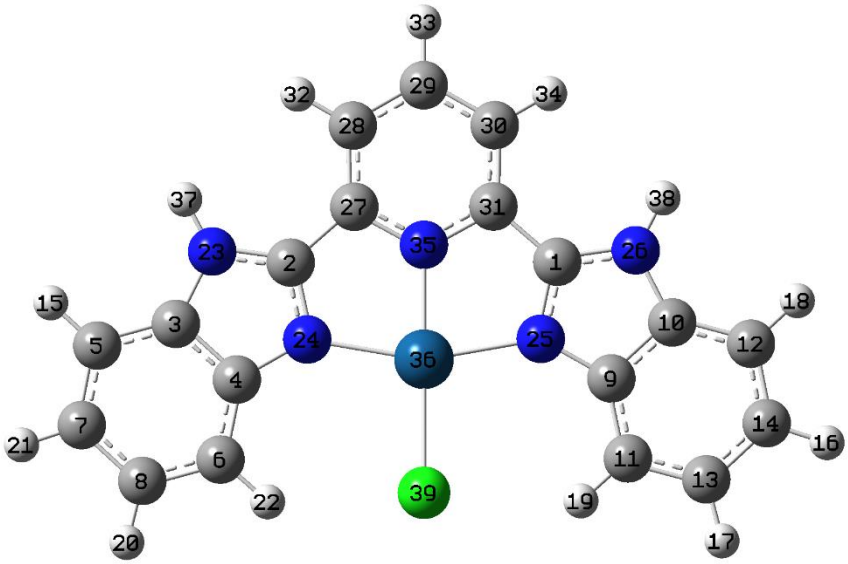
107	H	-2.948411	-3.589811	-1.640854
108	C	-4.274132	-5.219838	-2.091242
109	H	-3.528760	-6.003846	-1.906995
110	H	-5.260296	-5.614005	-1.816420
111	C	4.797513	-3.260908	2.207199
112	H	5.208651	-2.688483	3.049280
113	H	3.860964	-3.723263	2.549304
114	C	5.769057	-4.338637	1.773524
115	H	6.735449	-3.916118	1.472188
116	H	5.371513	-4.913211	0.926558
117	N	-0.004941	-2.213387	1.109027
118	S	6.101940	-5.520605	3.076924
119	S	-4.309869	-4.934329	-3.860370
120	O	4.790023	-6.130430	3.413086
121	O	6.679841	-4.738818	4.199250
122	O	7.059575	-6.488229	2.486782
123	O	-2.956064	-4.439136	-4.220529
124	O	-5.371457	-3.918049	-4.083156
125	O	-4.629489	-6.250879	-4.464120
126	Cl	-1.006926	1.763984	2.510849

Table S6. Cartesian coordinates of the optimized ground-state geometry of the trimer of **PtB** at the M06 level.

1	C	2.130232	2.441460	-2.942008	54	N	0.471370	1.498512	-1.541502
2	C	1.195406	3.392180	-3.343021	55	S	6.689526	1.021329	-5.794034
3	C	-0.096516	3.394074	-2.832973	56	S	-2.631186	7.901560	-0.967904
4	H	3.132411	2.454563	-3.357819	57	O	5.468280	1.316730	-6.586829
5	H	-0.797683	4.160843	-3.142506	58	O	7.065731	-0.415969	-5.825958
6	C	-1.730666	2.157996	-1.250180	59	O	7.820799	1.925780	-6.115372
7	C	-3.082985	1.118504	0.124100	60	O	-1.206618	7.716973	-0.587863
8	C	-3.801377	2.155578	-0.496743	61	O	-3.549792	7.819600	0.198132
9	C	-3.694814	0.272321	1.054971	62	O	-2.860223	9.104620	-1.804660
10	C	-5.136859	2.417375	-0.186548	63	Cl	-0.650800	-1.455344	1.429234
11	C	-5.021999	0.526336	1.354167	64	C	-2.348096	-4.147126	-0.049433
12	H	-3.139946	-0.542871	1.515701	65	C	-1.151341	-4.848562	0.046890
13	C	-5.728128	1.586137	0.750041	66	C	-0.071036	-4.551716	-0.779342
14	H	-5.685729	3.232184	-0.652089	67	H	-3.176879	-4.396807	0.603747
15	H	-5.533143	-0.111780	2.074457	68	H	0.862533	-5.095998	-0.679417
16	H	-6.767750	1.750661	1.022045	69	C	0.732393	-3.030121	-2.700497
17	C	2.521508	0.426197	-1.371946	70	C	1.471739	-1.635088	-4.214394
18	C	4.070057	-0.947537	-0.622343	71	C	2.411415	-2.671603	-4.074497
19	C	2.838084	-1.269967	-0.024903	72	C	1.671291	-0.600742	-5.134083
20	C	5.244584	-1.634578	-0.313702	73	C	3.572140	-2.729399	-4.844726
21	C	2.742511	-2.287826	0.929554	74	C	2.818905	-0.663664	-5.905001
22	C	5.140163	-2.640190	0.633450	75	H	0.942639	0.200304	-5.233747
23	H	6.192065	-1.393670	-0.789949	76	C	3.753097	-1.709880	-5.763869
24	C	3.912329	-2.953494	1.251960	77	H	4.295839	-3.531987	-4.728454
25	H	1.787465	-2.525147	1.392820	78	H	3.021816	0.122740	-6.627421
26	H	6.025775	-3.209195	0.903381	79	H	4.651942	-1.698562	-6.375642
27	H	3.885452	-3.752278	1.988534	80	C	-3.559554	-2.227768	-1.291734
28	C	-0.453610	2.403295	-1.922495	81	C	-5.507980	-1.230191	-1.505206
29	C	1.743260	1.492974	-2.001211	82	C	-4.603397	-0.675634	-2.428561
30	N	-1.796957	1.153475	-0.361267	83	C	-6.833134	-0.803224	-1.420470
31	N	1.893931	-0.398372	-0.516890	84	C	-4.997510	0.347664	-3.296771
32	Pt	-0.047360	0.133865	-0.205616	85	C	-7.214765	0.204498	-2.289155
33	H	1.483969	4.150174	-4.064313	86	H	-7.529216	-1.240575	-0.709084
34	N	-2.931102	2.771628	-1.380686	87	C	-6.310347	0.774805	-3.207838
35	N	3.840305	0.130073	-1.462278	88	H	-4.290223	0.777132	-4.001906
36	C	4.908949	0.902024	-2.098935	89	H	-8.238394	0.568432	-2.260873
37	H	4.660393	1.966941	-2.010049	90	H	-6.657633	1.567263	-3.865908
38	H	5.804175	0.748156	-1.485817	91	C	-0.220667	-3.537015	-1.717019
39	C	-3.245761	3.996772	-2.114932	92	C	-2.441305	-3.117257	-0.980449
40	H	-2.745164	3.965136	-3.087788	93	N	0.426028	-1.899551	-3.358557
41	H	-4.320699	3.976499	-2.326119	94	N	-3.398344	-1.323064	-2.273660
42	C	-2.853875	5.201942	-1.281247	95	Pt	-1.498715	-1.307999	-3.007008
43	H	-3.457873	5.199549	-0.363757	96	H	-1.058362	-5.641843	0.782140
44	H	-1.801593	5.097787	-0.974250	97	N	1.911908	-3.543049	-3.119059
45	C	-3.045005	6.508016	-2.016813	98	N	-4.816558	-2.194661	-0.794870
46	H	-2.401712	6.574047	-2.903642	99	C	-5.348687	-2.916015	0.362946
47	H	-4.084279	6.651452	-2.336924	100	H	-4.555991	-2.997832	1.117548
48	C	5.179436	0.500929	-3.533391	101	H	-6.117683	-2.272767	0.805935
49	H	5.477512	-0.556139	-3.569063	102	C	2.492049	-4.860775	-2.847296
50	H	4.263887	0.598916	-4.134396	103	H	1.679007	-5.543719	-2.579090
51	C	6.277899	1.384448	-4.089295	104	H	2.890670	-5.219814	-3.803784
52	H	7.206487	1.271932	-3.515025	105	C	3.581555	-4.841048	-1.793288
53	H	5.990572	2.444415	-4.056505	106	H	4.342400	-4.093991	-2.061146

107	H	3.161103	-4.545145	-0.821582	160	N	4.874416	1.161210	2.025292
108	C	4.199890	-6.223040	-1.711695	161	N	-2.024534	1.457185	4.288986
109	H	3.460021	-6.972818	-1.403980	162	C	-2.564956	0.420377	5.173146
110	H	4.602302	-6.530166	-2.685340	163	H	-1.796107	0.128867	5.894368
111	C	-5.928753	-4.267910	-0.011244	164	H	-3.366700	0.885711	5.755625
112	H	-6.797235	-4.125684	-0.668247	165	C	5.794335	0.195761	2.628272
113	H	-5.188064	-4.852776	-0.574244	166	H	5.289668	-0.774940	2.686668
114	C	-6.330994	-5.023790	1.238830	167	H	6.619481	0.060481	1.920110
115	H	-7.076253	-4.471939	1.825369	168	C	6.300921	0.673721	3.976882
116	H	-5.463883	-5.209274	1.887490	169	H	6.880837	1.596250	3.840367
117	N	-1.383487	-2.852846	-1.776511	170	H	5.449071	0.914730	4.627937
118	S	-7.045108	-6.622999	0.869337	171	C	7.151961	-0.396434	4.627281
119	S	5.561498	-6.350462	-0.556358	172	H	6.574993	-1.315964	4.791087
120	O	-5.998798	-7.374734	0.130124	173	H	8.024859	-0.650040	4.013203
121	O	-8.250990	-6.352732	0.045298	174	C	-3.077884	-0.741846	4.345039
122	O	-7.365837	-7.217765	2.190513	175	H	-3.901514	-0.375247	3.717727
123	O	4.996957	-6.068660	0.788452	176	H	-2.280130	-1.081744	3.668356
124	O	6.561584	-5.341730	-0.991033	177	C	-3.561994	-1.895961	5.194171
125	O	6.045405	-7.746741	-0.697109	178	H	-4.285613	-1.573574	5.953132
126	Cl	-1.648323	0.536027	-4.468600	179	H	-2.734702	-2.405635	5.703170
127	C	0.575559	-0.435320	4.676359	180	N	1.414800	1.158753	3.144061
128	C	1.836740	-1.017281	4.710095	181	S	-4.401908	-3.119589	4.187112
129	C	2.889248	-0.502482	3.960650	182	S	7.776773	0.103659	6.228540
130	H	-0.234508	-0.869022	5.250883	183	O	-3.425452	-3.521352	3.136495
131	H	3.867549	-0.966379	4.015350	184	O	-5.595362	-2.429889	3.628727
132	C	3.551071	1.323570	2.254199	185	O	-4.750958	-4.229857	5.104782
133	C	4.096799	2.876142	0.810139	186	O	6.579221	0.376663	7.063628
134	C	5.254495	2.141577	1.124341	187	O	8.599938	1.315433	5.985664
135	C	4.142395	3.938037	-0.098945	188	O	8.570571	-1.053757	6.710115
136	C	6.499056	2.450463	0.574162	189	Cl	0.685138	4.512049	0.495750
137	C	5.375457	4.236585	-0.653566					
138	H	3.243565	4.500211	-0.339038					
139	C	6.534836	3.508069	-0.319284					
140	H	7.394955	1.892246	0.833433					
141	H	5.455054	5.057392	-1.361615					
142	H	7.482183	3.784727	-0.774508					
143	C	-0.812981	1.507585	3.685717					
144	C	-2.792946	2.469174	3.736217					
145	C	-1.973807	3.150768	2.819131					
146	C	-4.117693	2.841813	3.963414					
147	C	-2.450459	4.259342	2.112052					
148	C	-4.582673	3.935568	3.253754					
149	H	-4.755166	2.299647	4.656759					
150	C	-3.760636	4.636532	2.348824					
151	H	-1.809092	4.796242	1.416073					
152	H	-5.609152	4.262697	3.397129					
153	H	-4.164827	5.500640	1.824842					
154	C	2.647892	0.603641	3.152249					
155	C	0.383312	0.689488	3.880614					
156	N	3.053949	2.346824	1.537371					
157	N	-0.746727	2.527744	2.812772					
158	Pt	1.081664	2.688606	1.932557					
159	H	2.004102	-1.890649	5.332427					

Table S7. Force field parameters of PtB-core system in GROMACS format used in this work.



; PtB-core force field parameters
;PtB-core_GMX.top

```
[ defaults ]
; nbfunc        comb-rule       gen-pairs       fudgeLJ       fudgeQQ
1               2               yes             0.5           0.8333

[ atomtypes ]
; name      at.num  mass     charge ptype  sigma       epsilon
PTBc_cc     6   12.01      0.0000  A     3.39967e-01   3.59824e-01
PTBc_ca     6   12.01      0.0000  A     3.39967e-01   3.59824e-01
PTBc_ha     1   1.008      0.0000  A     2.59964e-01   6.27600e-02
PTBc_na     7   14.01      0.0000  A     3.25000e-01   7.11280e-01
PTBc_nd     7   14.01      0.0000  A     3.25000e-01   7.11280e-01
PTBc_nb     7   14.01      0.0000  A     3.25000e-01   7.11280e-01
PTBc_Pt     78  195.078    0.0000   A     3.3298e-01    1.0534e+01
PTBc_hn     1   1.008      0.0000  A     1.06908e-01   6.56888e-02
PTBc_cl     17  35.45      0.0000  A     3.47094e-01   1.10876e+00

[ moleculetype ]
; Name            nrexcl
  PTB-core        3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB     massB
; residue   1 PTP rtp PTP  q +1.0
     1     PTBc_cc     1    PTP     C1      1   0.081892     12.01   ; qtot 0.08189
     2     PTBc_cc     1    PTP     C2      2   0.081892     12.01   ; qtot 0.1638
     3     PTBc_ca     1    PTP     C3      3   0.250779     12.01   ; qtot 0.4146
     4     PTBc_ca     1    PTP     C4      4   0.148116     12.01   ; qtot 0.5627
     5     PTBc_ca     1    PTP     C5      5  -0.280998     12.01   ; qtot 0.2817
     6     PTBc_ca     1    PTP     C6      6  -0.217522     12.01   ; qtot 0.06416
     7     PTBc_ca     1    PTP     C7      7  -0.076146     12.01   ; qtot -0.01199
     8     PTBc_ca     1    PTP     C8      8  -0.106842     12.01   ; qtot -0.1188
     9     PTBc_ca     1    PTP     C9      9   0.148116     12.01   ; qtot 0.02929
    10     PTBc_ca     1    PTP    C10     10   0.250779     12.01   ; qtot 0.2801
    11     PTBc_ca     1    PTP    C11     11  -0.217522     12.01   ; qtot 0.06254
    12     PTBc_ca     1    PTP    C12     12  -0.280998     12.01   ; qtot -0.2185
    13     PTBc_ca     1    PTP    C13     13  -0.106842     12.01   ; qtot -0.3253
    14     PTBc_ca     1    PTP    C14     14  -0.076146     12.01   ; qtot -0.4014
    15     PTBc_ha     1    PTP     H1     15   0.184387     1.008   ; qtot -0.2171
    16     PTBc_ha     1    PTP     H2     16   0.151311     1.008   ; qtot -0.06574
    17     PTBc_ha     1    PTP     H3     17   0.153899     1.008   ; qtot 0.08816
    18     PTBc_ha     1    PTP     H4     18   0.184387     1.008   ; qtot 0.2725
    19     PTBc_ha     1    PTP     H5     19     0.1958     1.008   ; qtot 0.4683
    20     PTBc_ha     1    PTP     H6     20   0.153899     1.008   ; qtot 0.6222
    21     PTBc_ha     1    PTP     H7     21   0.151311     1.008   ; qtot 0.7736
    22     PTBc_ha     1    PTP     H8     22     0.1958     1.008   ; qtot 0.9694
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    23    PTBc_na     1    PTP     N1     23  -0.408906     14.01   ; qtot 0.5604
    24    PTBc_nd     1    PTP     N2     24   0.044289     14.01   ; qtot 0.6047
    25    PTBc_nd     1    PTP     N3     25   0.044289     14.01   ; qtot 0.649
    26    PTBc_na     1    PTP     N4     26  -0.408906     14.01   ; qtot 0.2401
    27    PTBc_ca     1    PTP    C15     27   0.250755     12.01   ; qtot 0.4909
    28    PTBc_ca     1    PTP    C16     28  -0.277609     12.01   ; qtot 0.2133
    29    PTBc_ca     1    PTP    C17     29   0.006689     12.01   ; qtot 0.22
    30    PTBc_ca     1    PTP    C18     30  -0.277609     12.01   ; qtot -0.05766
    31    PTBc_ca     1    PTP    C19     31   0.250755     12.01   ; qtot 0.1931
    32    PTBc_ha     1    PTP     H9     32   0.183021     1.008   ; qtot 0.3761
    33    PTBc_ha     1    PTP    H10     33   0.157288     1.008   ; qtot 0.5334
    34    PTBc_ha     1    PTP    H11     34   0.183021     1.008   ; qtot 0.7164
    35    PTBc_nb     1    PTP     N5     35   -0.04731     14.01   ; qtot 0.6691
    36    PTBc_Pt     1    PTP    PT1     36  -0.201109    195.078 ; qtot 0.468
    37    PTBc_hn     1    PTP    H12     37   0.386136     1.008   ; qtot 0.8541
    38    PTBc_hn     1    PTP    H13     38   0.386136     1.008   ; qtot 1.24
    39    PTBc_cl     1    PTP    CL1     39  -0.240282     35.45   ; qtot 1

[ bonds ]
;  ai    aj funct         c0         c1         c2         c3
    1    25    1       0.13350   413880.0
    1    26    1       0.13710   367190.0
    1    31    1       0.14340   344510.0
    2    23    1       0.13710   367190.0
    2    24    1       0.13350   413880.0
    2    27    1       0.14340   344510.0
    3     4    1       0.13870   400330.0
    3     5    1       0.13870   400330.0
    3    23    1       0.13500   393550.0
    4     6    1       0.13870   400330.0
    4    24    1       0.13360   412460.0
    5     7    1       0.13870   400330.0
    5    15    1       0.10870   288110.0
    6     8    1       0.13870   400330.0
    6    22    1       0.10870   288110.0
    7     8    1       0.13870   400330.0
    7    21    1       0.10870   288110.0
    8    20    1       0.10870   288110.0
    9    10    1       0.13870   400330.0
    9    11    1       0.13870   400330.0
    9    25    1       0.13360   412460.0
   10    12    1       0.13870   400330.0
   10    26    1       0.13500   393550.0
   11    13    1       0.13870   400330.0
   11    19    1       0.10870   288110.0
   12    14    1       0.13870   400330.0
   12    18    1       0.10870   288110.0
   13    14    1       0.13870   400330.0
   13    17    1       0.10870   288110.0
   14    16    1       0.10870   288110.0
   23    37    1       0.10110   340240.0
   24    36    1       0.20310   306270.0
   25    36    1       0.20310   306270.0
   26    38    1       0.10110   340240.0
   27    28    1       0.13870   400330.0
   27    35    1       0.13420   404260.0
   28    29    1       0.13870   400330.0
   28    32    1       0.10870   288110.0
   29    30    1       0.13870   400330.0
   29    33    1       0.10870   288110.0
   30    31    1       0.13870   400330.0
   30    34    1       0.10870   288110.0
   31    35    1       0.13420   404260.0
   35    36    1       0.19670   306270.0
   36    39    1       0.22890   131440.0

[ pairs ]
;  ai    aj funct         c0         c1         c2         c3
    1    11    1
    1    12    1
```

1	24	1
1	27	1
1	29	1
1	34	1
1	39	1
2	5	1
2	6	1
2	25	1
2	29	1
2	31	1
2	32	1
2	39	1
3	8	1
3	21	1
3	22	1
3	27	1
3	36	1
4	7	1
4	15	1
4	20	1
4	25	1
4	27	1
4	35	1
4	37	1
4	39	1
5	6	1
5	20	1
5	24	1
5	37	1
6	21	1
6	23	1
6	36	1
7	22	1
7	23	1
8	15	1
8	24	1
9	14	1
9	17	1
9	18	1
9	24	1
9	31	1
9	35	1
9	38	1
9	39	1
10	13	1
10	16	1
10	19	1
10	31	1
10	36	1
11	12	1
11	16	1
11	26	1
11	36	1
12	17	1
12	25	1
12	38	1
13	18	1
13	25	1
14	19	1
14	26	1
15	21	1
15	23	1
16	17	1
16	18	1
17	19	1
18	26	1
19	25	1
20	21	1
20	22	1
22	24	1

```
  23   28    1
  23   35    1
  23   36    1
  24   28    1
  24   31    1
  24   37    1
  25   27    1
  25   30    1
  25   38    1
  26   30    1
  26   35    1
  26   36    1
  27   30    1
  27   33    1
  27   37    1
  27   39    1
  28   31    1
  28   34    1
  28   36    1
  29   35    1
  30   32    1
  30   36    1
  31   33    1
  31   38    1
  31   39    1
  32   33    1
  32   35    1
  33   34    1
  34   35    1

[ angles ]
;  ai    aj    ak funct         c0          c1          c2          c3
  25     1    26    1        112.0200   625.7600
  25     1    31    1        123.2800   567.6900
  26     1    31    1        113.6100   570.7500
  23     2    24    1        112.0200   625.7600
  23     2    27    1        113.6100   570.7500
  24     2    27    1        123.2800   567.6900
   4     3     5    1        119.9700   562.1600
   4     3    23    1        118.3400   587.5200
   5     3    23    1        118.3400   587.5200
   3     4     6    1        119.9700   562.1600
   3     4    24    1        119.7200   586.9300
   6     4    24    1        119.7200   586.9300
   3     5     7    1        119.9700   562.1600
   3     5    15    1        120.0100   405.5100
   7     5    15    1        120.0100   405.5100
   4     6     8    1        119.9700   562.1600
   4     6    22    1        120.0100   405.5100
   8     6    22    1        120.0100   405.5100
   5     7     8    1        119.9700   562.1600
   5     7    21    1        120.0100   405.5100
   8     7    21    1        120.0100   405.5100
   6     8     7    1        119.9700   562.1600
   6     8    20    1        120.0100   405.5100
   7     8    20    1        120.0100   405.5100
  10     9    11    1        119.9700   562.1600
  10     9    25    1        119.7200   586.9300
  11     9    25    1        119.7200   586.9300
   9    10    12    1        119.9700   562.1600
   9    10    26    1        118.3400   587.5200
  12    10    26    1        118.3400   587.5200
   9    11    13    1        119.9700   562.1600
   9    11    19    1        120.0100   405.5100
  13    11    19    1        120.0100   405.5100
  10    12    14    1        119.9700   562.1600
  10    12    18    1        120.0100   405.5100
  14    12    18    1        120.0100   405.5100
  11    13    14    1        119.9700   562.1600
  11    13    17    1        120.0100   405.5100
```

14	13	17	1	120.0100	405.5100
12	14	13	1	119.9700	562.1600
12	14	16	1	120.0100	405.5100
13	14	16	1	120.0100	405.5100
2	23	3	1	113.1500	572.8700
2	23	37	1	125.6600	393.2100
3	23	37	1	125.5900	398.5700
2	24	4	1	105.4700	604.5000
2	24	36	1	111.7800	167.3600
4	24	36	1	140.9600	167.3600
1	25	9	1	105.4700	604.5000
1	25	36	1	111.7800	167.3600
9	25	36	1	140.9600	167.3600
1	26	10	1	113.1500	572.8700
1	26	38	1	125.6600	393.2100
10	26	38	1	125.5900	398.5700
2	27	28	1	120.1000	552.2000
2	27	35	1	118.4500	577.8900
28	27	35	1	122.6300	578.7300
27	28	29	1	119.9700	562.1600
27	28	32	1	120.0100	405.5100
29	28	32	1	120.0100	405.5100
28	29	30	1	119.9700	562.1600
28	29	33	1	120.0100	405.5100
30	29	33	1	119.9700	562.1600
29	30	31	1	119.9700	562.1600
29	30	34	1	120.0100	405.5100
31	30	34	1	120.0100	405.5100
1	31	30	1	120.1000	552.2000
1	31	35	1	118.4500	577.8900
30	31	35	1	122.6300	578.7300
27	35	31	1	115.8600	573.9600
27	35	36	1	118.7800	167.3600
31	35	36	1	118.7800	167.3600
24	36	25	1	160.3400	351.4600
24	36	35	1	80.1700	351.4600
24	36	39	1	99.8300	962.3200
25	36	35	1	80.1700	351.4600
25	36	39	1	99.8300	962.3200
35	36	39	1	180.0000	962.3200

[dihedrals]

; ai	aj	ak	al	funct	c0	c1	c2	c3	c4	c5
26	1	25	9	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
26	1	25	36	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
31	1	25	9	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
31	1	25	36	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
25	1	26	10	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
25	1	26	38	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
31	1	26	10	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
31	1	26	38	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
25	1	31	30	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000
25	1	31	35	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000
26	1	31	30	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000
26	1	31	35	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000
24	2	23	3	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
24	2	23	37	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
27	2	23	3	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
27	2	23	37	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
23	2	24	4	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
23	2	24	36	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
27	2	24	4	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
27	2	24	36	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
23	2	27	28	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000
23	2	27	35	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000
24	2	27	28	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000
24	2	27	35	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000
5	3	4	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
5	3	4	24	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
23	3	4	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000

23	3	4	24	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
4	3	5	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
4	3	5	15	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
23	3	5	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
23	3	5	15	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
4	3	23	2	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
4	3	23	37	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
5	3	23	2	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
5	3	23	37	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
3	4	6	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
3	4	6	22	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
24	4	6	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
24	4	6	22	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
3	4	24	2	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
3	4	24	36	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
6	4	24	2	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
6	4	24	36	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
3	5	7	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
3	5	7	21	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
15	5	7	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
15	5	7	21	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
4	6	8	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
4	6	8	20	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
22	6	8	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
22	6	8	20	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
5	7	8	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
5	7	8	20	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
21	7	8	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
21	7	8	20	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
11	9	10	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
11	9	10	26	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
25	9	10	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
25	9	10	26	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
10	9	11	13	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
10	9	11	19	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
25	9	11	13	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
25	9	11	19	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
10	9	25	1	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
10	9	25	36	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
11	9	25	36	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
9	10	12	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
9	10	12	18	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
26	10	12	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
26	10	12	18	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
9	10	26	1	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
9	10	26	38	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
12	10	26	1	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
12	10	26	38	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
9	11	13	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
9	11	13	17	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
19	11	13	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
19	11	13	17	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
10	12	14	13	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
10	12	14	16	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
18	12	14	13	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
18	12	14	16	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
11	13	14	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
11	13	14	16	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
17	13	14	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
17	13	14	16	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
2	24	36	25	3	0.69700	0.00000	-0.79600	0.00000	0.00000	0.00000
2	24	36	35	3	0.69700	0.00000	-0.79600	0.00000	0.00000	0.00000
2	24	36	39	3	0.69700	0.00000	-0.79600	0.00000	0.00000	0.00000
4	24	36	25	3	0.69700	0.00000	-0.79600	0.00000	0.00000	0.00000
4	24	36	35	3	0.69700	0.00000	-0.79600	0.00000	0.00000	0.00000
4	24	36	39	3	0.69700	0.00000	-0.79600	0.00000	0.00000	0.00000
1	25	36	24	3	0.69700	0.00000	-0.79600	0.00000	0.00000	0.00000
1	25	36	35	3	0.69700	0.00000	-0.79600	0.00000	0.00000	0.00000
1	25	36	39	3	0.69700	0.00000	-0.79600	0.00000	0.00000	0.00000
9	25	36	24	3	0.69700	0.00000	-0.79600	0.00000	0.00000	0.00000

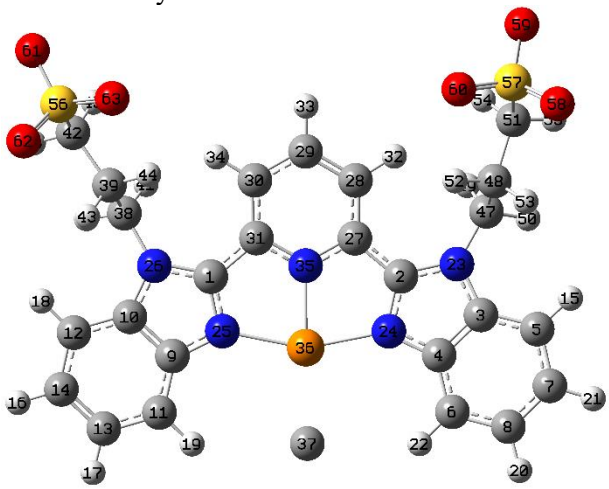
```
   9   25   36   35    3      0.69700   0.00000   -0.79600     0.00000   0.00000   0.00000
   9   25   36   39    3      0.69700   0.00000   -0.79600     0.00000   0.00000   0.00000
   2   27   28   29    3     30.33400   0.00000   -30.33400    0.00000   0.00000   0.00000
   2   27   28   32    3     30.33400   0.00000   -30.33400    0.00000   0.00000   0.00000
  35   27   28   29    3     30.33400   0.00000   -30.33400    0.00000   0.00000   0.00000
  35   27   28   32    3     30.33400   0.00000   -30.33400    0.00000   0.00000   0.00000
   2   27   35   31    3     40.16640   0.00000   -40.16640    0.00000   0.00000   0.00000
   2   27   35   36    3     40.16640   0.00000   -40.16640    0.00000   0.00000   0.00000
  28   27   35   31    3     40.16640   0.00000   -40.16640    0.00000   0.00000   0.00000
  28   27   35   36    3     40.16640   0.00000   -40.16640    0.00000   0.00000   0.00000
  27   28   29   30    3     30.33400   0.00000   -30.33400    0.00000   0.00000   0.00000
  27   28   29   33    3     30.33400   0.00000   -30.33400    0.00000   0.00000   0.00000
  32   28   29   30    3     30.33400   0.00000   -30.33400    0.00000   0.00000   0.00000
  32   28   29   33    3     30.33400   0.00000   -30.33400    0.00000   0.00000   0.00000
  28   29   30   31    3     30.33400   0.00000   -30.33400    0.00000   0.00000   0.00000
  28   29   30   34    3     30.33400   0.00000   -30.33400    0.00000   0.00000   0.00000
  33   29   30   31    3     30.33400   0.00000   -30.33400    0.00000   0.00000   0.00000
  33   29   30   34    3     30.33400   0.00000   -30.33400    0.00000   0.00000   0.00000
  29   30   31    1    3     30.33400   0.00000   -30.33400    0.00000   0.00000   0.00000
  29   30   31   35    3     30.33400   0.00000   -30.33400    0.00000   0.00000   0.00000
  34   30   31    1    3     30.33400   0.00000   -30.33400    0.00000   0.00000   0.00000
  34   30   31   35    3     30.33400   0.00000   -30.33400    0.00000   0.00000   0.00000
   1   31   35   27    3     40.16640   0.00000   -40.16640    0.00000   0.00000   0.00000
   1   31   35   36    3     40.16640   0.00000   -40.16640    0.00000   0.00000   0.00000
  30   31   35   27    3     40.16640   0.00000   -40.16640    0.00000   0.00000   0.00000
  30   31   35   36    3     40.16640   0.00000   -40.16640    0.00000   0.00000   0.00000
  27   35   36   24    3      0.69700   0.00000   -0.79600     0.00000   0.00000   0.00000
  27   35   36   25    3      0.69700   0.00000   -0.79600     0.00000   0.00000   0.00000
  27   35   36   39    3      0.69700   0.00000   -0.79600     0.00000   0.00000   0.00000
  31   35   36   24    3      0.69700   0.00000   -0.79600     0.00000   0.00000   0.00000
  31   35   36   25    3      0.69700   0.00000   -0.79600     0.00000   0.00000   0.00000
  31   35   36   39    3      0.69700   0.00000   -0.79600     0.00000   0.00000   0.00000

[ dihedrals ]
;  ai    aj    ak    al funct        c0         c1         c2         c3
    3     7     5    15    1     180.00     4.60240    2
    3     6     4    24    1     180.00     4.60240    2
    3     2    23    37    1     180.00     4.60240    2
    4     8     6    22    1     180.00     4.60240    2
    4     5     3    23    1     180.00     4.60240    2
    5     8     7    21    1     180.00     4.60240    2
    6     7     8    20    1     180.00     4.60240    2
    9    13    11    19    1     180.00     4.60240    2
    9    12    10    26    1     180.00     4.60240    2
   10    14    12    18    1     180.00     4.60240    2
   10    11     9    25    1     180.00     4.60240    2
   10     1    26    38    1     180.00     4.60240    2
   11    14    13    17    1     180.00     4.60240    2
   12    13    14    16    1     180.00     4.60240    2
   24     2    23    27    1     180.00     4.60240    2
   25     1    26    31    1     180.00     4.60240    2
   27    29    28    32    1     180.00     4.60240    2
   28    30    29    33    1     180.00     4.60240    2
   28     2    27    35    1     180.00     4.60240    2
   29    31    30    34    1     180.00     4.60240    2
   30     1    31    35    1     180.00     4.60240    2

[ system ]
; Name
PtB-core

[ molecules ]
; Compound        #mols
  PTBc              1
```

Table S8. Force field parameters of PtB system in GROMACS format used in this work.



; PtB force field parameters
;PtB_GMX.top

```
[ defaults ]
; nbfunc        comb-rule       gen-pairs       fudgeLJ         fudgeQQ
1               2               yes             0.5             0.8333

[ atomtypes ]
; name      at.num  mass    charge ptype  sigma       epsilon
PTB_cc      6    12.01      0.0000   A     3.39967e-01    3.59824e-01
PTB_ca      6    12.01      0.0000   A     3.39967e-01    3.59824e-01
PTB_ha      1    1.008      0.0000   A     2.59964e-01    6.27600e-02
PTB_na      7    14.01      0.0000   A     3.25000e-01    7.11280e-01
PTB_nd      7    14.01      0.0000   A     3.25000e-01    7.11280e-01
PTB_nb      7    14.01      0.0000   A     3.25000e-01    7.11280e-01
PTB_Pt     78  195.078      0.0000   A      3.3298e-01     1.0534e+01
PTB_cl     17   35.45      0.0000   A     3.47094e-01    1.10876e+00
PTB_c3      6    12.01      0.0000   A     3.39967e-01    4.57730e-01
PTB_h1      1    1.008      0.0000   A     2.47135e-01    6.56888e-02
PTB_hc      1    1.008      0.0000   A     2.64953e-01    6.56888e-02
PTB_s6     16   32.06      0.0000   A     3.56359e-01    1.04600e+00
PTB_ o      8   16.00      0.0000   A     2.95992e-01    8.78640e-01


[ moleculetype ]
; Name            nrexcl
PtB               3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB     massB
; residue   1 PTB rtp PTB  q -1.0
     1     PTB_cc      1    PTB     C1      1     0.081892     12.01  ; qtot 0.08189
     2     PTB_cc      1    PTB     C2      2     0.081892     12.01  ; qtot 0.1638
     3     PTB_ca      1    PTB     C3      3     0.250779     12.01  ; qtot 0.4146
     4     PTB_ca      1    PTB     C4      4     0.148116     12.01  ; qtot 0.5627
     5     PTB_ca      1    PTB     C5      5    -0.280998     12.01  ; qtot 0.2817
     6     PTB_ca      1    PTB     C6      6    -0.217522     12.01  ; qtot 0.06416
     7     PTB_ca      1    PTB     C7      7    -0.076146     12.01  ; qtot -0.01199
     8     PTB_ca      1    PTB     C8      8    -0.106842     12.01  ; qtot -0.1188
     9     PTB_ca      1    PTB     C9      9     0.148116     12.01   ; qtot 0.02929
    10     PTB_ca      1    PTB    C10     10     0.250779     12.01   ; qtot 0.2801
    11     PTB_ca      1    PTB    C11     11    -0.217522     12.01   ; qtot 0.06254
    12     PTB_ca      1    PTB    C12     12    -0.280998     12.01   ; qtot -0.2185
    13     PTB_ca      1    PTB    C13     13    -0.106842     12.01   ; qtot -0.3253
    14     PTB_ca      1    PTB    C14     14    -0.076146     12.01   ; qtot -0.4014
    15     PTB_ha      1    PTB     H1     15     0.184387     1.008   ; qtot -0.2171
    16     PTB_ha      1    PTB     H2     16     0.151311     1.008   ; qtot -0.06574
    17     PTB_ha      1    PTB     H3     17     0.153899     1.008   ; qtot 0.08816
    18     PTB_ha      1    PTB     H4     18     0.184387     1.008   ; qtot 0.2725
    19     PTB_ha      1    PTB     H5     19     0.1958       1.008   ; qtot 0.4683
```

```
    20    PTB_ha     1    PTB     H6    20     0.153899     1.008    ; qtot 0.6222
    21    PTB_ha     1    PTB     H7    21     0.151311     1.008    ; qtot 0.7736
    22    PTB_ha     1    PTB     H8    22     0.1958       1.008    ; qtot 0.9694
    23    PTB_na     1    PTB     N1    23    -0.408906     14.01    ; qtot 0.5604
    24    PTB_nd     1    PTB     N2    24     0.044289     14.01    ; qtot 0.6047
    25    PTB_nd     1    PTB     N3    25     0.044289     14.01    ; qtot 0.649
    26    PTB_na     1    PTB     N4    26    -0.408906     14.01    ; qtot 0.2401
    27    PTB_ca     1    PTB    C15    27     0.250755     12.01    ; qtot 0.4909
    28    PTB_ca     1    PTB    C16    28    -0.277609     12.01    ; qtot 0.2133
    29    PTB_ca     1    PTB    C17    29     0.006689     12.01    ; qtot 0.22
    30    PTB_ca     1    PTB    C18    30    -0.277609     12.01    ; qtot -0.05766
    31    PTB_ca     1    PTB    C19    31     0.250755     12.01    ; qtot 0.1931
    32    PTB_ha     1    PTB     H9    32     0.183021     1.008    ; qtot 0.3761
    33    PTB_ha     1    PTB    H10    33     0.157288     1.008    ; qtot 0.5334
    34    PTB_ha     1    PTB    H11    34     0.183021     1.008    ; qtot 0.7164
    35    PTB_nb     1    PTB     N5    35    -0.04731      14.01    ; qtot 0.6691
    36    PTB_Pt     1    PTB    PT1    36    -0.201109     195.0    ; qtot 0.468
    37    PTB_cl     1    PTB    CL1    37    -0.240282     35.45    ; qtot 0.2277
    38    PTB_c3     1    PTB    C20    38    -0.668119     12.01    ; qtot -0.4404
    39    PTB_c3     1    PTB    C21    39     0.050403     12.01    ; qtot -0.39
    40    PTB_h1     1    PTB    H12    40     0.412608     1.008    ; qtot 0.02262
    41    PTB_h1     1    PTB    H13    41     0.412608     1.008    ; qtot 0.4352
    42    PTB_c3     1    PTB    C22    42     0.466356     12.01    ; qtot 0.9016
    43    PTB_hc     1    PTB    H14    43    -0.017213     1.008    ; qtot 0.8844
    44    PTB_hc     1    PTB    H15    44    -0.017213     1.008    ; qtot 0.8672
    45    PTB_h1     1    PTB    H16    45    -0.175945     1.008    ; qtot 0.6912
    46    PTB_h1     1    PTB    H17    46    -0.175945     1.008    ; qtot 0.5153
    47    PTB_c3     1    PTB    C23    47    -0.668119     12.01    ; qtot -0.1529
    48    PTB_c3     1    PTB    C24    48     0.050403     12.01    ; qtot -0.1024
    49    PTB_h1     1    PTB    H18    49     0.412608     1.008    ; qtot 0.3102
    50    PTB_h1     1    PTB    H19    50     0.412608     1.008    ; qtot 0.7228
    51    PTB_c3     1    PTB    C25    51     0.466356     12.01    ; qtot 1.189
    52    PTB_hc     1    PTB    H20    52    -0.017213     1.008    ; qtot 1.172
    53    PTB_hc     1    PTB    H21    53    -0.017213     1.008    ; qtot 1.155
    54    PTB_h1     1    PTB    H22    54    -0.175945     1.008    ; qtot 0.9788
    55    PTB_h1     1    PTB    H23    55    -0.175945     1.008    ; qtot 0.8028
    56    PTB_s6     1    PTB     S1    56     1.1828       32.06    ; qtot 1.986
    57    PTB_s6     1    PTB     S2    57     1.1828       32.06    ; qtot 3.168
    58    PTB_ o     1    PTB     O1    58    -0.694737     16.00    ; qtot 2.474
    59    PTB_ o     1    PTB     O2    59    -0.694737     16.00    ; qtot 1.779
    60    PTB_ o     1    PTB     O3    60    -0.694737     16.00    ; qtot 1.084
    61    PTB_ o     1    PTB     O4    61    -0.694737     16.00    ; qtot 0.3895
    62    PTB_ o     1    PTB     O5    62    -0.694737     16.00    ; qtot -0.3053
    63    PTB_ o     1    PTB     O6    63    -0.694737     16.00    ; qtot -1

[ bonds ]
;  ai    aj funct          c0          c1          c2          c3
    1    25    1        0.13350   413880.0
    1    26    1        0.13710   367190.0
    1    31    1        0.14340   344510.0
    2    23    1        0.13710   367190.0
    2    24    1        0.13350   413880.0
    2    27    1        0.14340   344510.0
    3     4    1        0.13870   400330.0
    3     5    1        0.13870   400330.0
    3    23    1        0.13500   393550.0
    4     6    1        0.13870   400330.0
    4    24    1        0.13360   412460.0
    5     7    1        0.13870   400330.0
    5    15    1        0.10870   288110.0
    6     8    1        0.13870   400330.0
    6    22    1        0.10870   288110.0
    7     8    1        0.13870   400330.0
    7    21    1        0.10870   288110.0
    8    20    1        0.10870   288110.0
    9    10    1        0.13870   400330.0
    9    11    1        0.13870   400330.0
    9    25    1        0.13360   412460.0
   10    12    1        0.13870   400330.0
   10    26    1        0.13500   393550.0
```

```
  11   13    1        0.13870   400330.0
  11   19    1        0.10870   288110.0
  12   14    1        0.13870   400330.0
  12   18    1        0.10870   288110.0
  13   14    1        0.13870   400330.0
  13   17    1        0.10870   288110.0
  14   16    1        0.10870   288110.0
  23   47    1        0.14560   280080.0
  24   36    1        0.20310   306270.0
  25   36    1        0.20310   306270.0
  26   38    1        0.14560   280080.0
  27   28    1        0.13870   400330.0
  27   35    1        0.13420   404260.0
  28   29    1        0.13870   400330.0
  28   32    1        0.10870   288110.0
  29   30    1        0.13870   400330.0
  29   33    1        0.10870   288110.0
  30   31    1        0.13870   400330.0
  30   34    1        0.10870   288110.0
  31   35    1        0.13420   404260.0
  35   36    1        0.19670   306270.0
  36   37    1        0.22890   131440.0
  38   39    1        0.15350   253630.0
  38   40    1        0.10930   281080.0
  38   41    1        0.10930   281080.0
  39   42    1        0.15350   253630.0
  39   43    1        0.10920   282250.0
  39   44    1        0.10920   282250.0
  42   45    1        0.10930   281080.0
  42   46    1        0.10930   281080.0
  42   56    1        0.17740   212550.0
  47   48    1        0.15350   253630.0
  47   49    1        0.10930   281080.0
  47   50    1        0.10930   281080.0
  48   51    1        0.15350   253630.0
  48   52    1        0.10920   282250.0
  48   53    1        0.10920   282250.0
  51   54    1        0.10930   281080.0
  51   55    1        0.10930   281080.0
  51   57    1        0.17740   212550.0
  56   61    1        0.14360   452790.0
  56   62    1        0.14360   452790.0
  56   63    1        0.14360   452790.0
  57   58    1        0.14360   452790.0
  57   59    1        0.14360   452790.0
  57   60    1        0.14360   452790.0

[ pairs ]
;  ai    aj funct          c0          c1          c2          c3
    1    11    1
    1    12    1
    1    24    1
    1    27    1
    1    29    1
    1    34    1
    1    37    1
    1    39    1
    1    40    1
    1    41    1
    2     5    1
    2     6    1
    2    25    1
    2    29    1
    2    31    1
    2    32    1
    2    37    1
    2    48    1
    2    49    1
    2    50    1
    3     8    1
```

3	21	1
3	22	1
3	27	1
3	36	1
3	48	1
3	49	1
3	50	1
4	7	1
4	15	1
4	20	1
4	25	1
4	27	1
4	35	1
4	37	1
4	47	1
5	6	1
5	20	1
5	24	1
5	47	1
6	21	1
6	23	1
6	36	1
7	22	1
7	23	1
8	15	1
8	24	1
9	14	1
9	17	1
9	18	1
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49 51 1
49 52 1
49 53 1
50 51 1
50 52 1
50 53 1
52 54 1
52 55 1
52 57 1
53 54 1
53 55 1
53 57 1

```
  54   58    1
  54   59    1
  54   60    1
  55   58    1
  55   59    1
  55   60    1

[ angles ]
;  ai    aj    ak funct         c0         c1         c2         c3
  25     1    26     1     112.0200   625.7600
  25     1    31     1     123.0200   568.3500
  26     1    31     1     123.4500   560.9100
  23     2    24     1     112.0200   625.7600
  23     2    27     1     123.4500   560.9100
  24     2    27     1     123.0200   568.3500
   4     3     5     1     119.9700   562.1600
   4     3    23     1     118.3400   587.5200
   5     3    23     1     119.9700   562.1600
   3     4     6     1     119.9700   562.1600
   3     4    24     1     119.7200   586.9300
   6     4    24     1     119.7200   586.9300
   3     5     7     1     119.9700   562.1600
   3     5    15     1     120.0100   405.5100
   7     5    15     1     120.0100   405.5100
   4     6     8     1     119.9700   562.1600
   4     6    22     1     120.0100   405.5100
   8     6    22     1     120.0100   405.5100
   5     7     8     1     119.9700   562.1600
   5     7    21     1     120.0100   405.5100
   8     7    21     1     120.0100   405.5100
   6     8     7     1     119.9700   562.1600
   6     8    20     1     120.0100   405.5100
   7     8    20     1     120.0100   405.5100
  10     9    11     1     119.9700   562.1600
  10     9    25     1     119.7200   586.9300
  11     9    25     1     119.7200   586.9300
   9    10    12     1     119.9700   562.1600
   9    10    26     1     118.3400   587.5200
  12    10    26     1     118.3400   587.5200
   9    11    13     1     119.9700   562.1600
   9    11    19     1     120.0100   405.5100
  13    11    19     1     120.0100   405.5100
  10    12    14     1     119.9700   562.1600
  10    12    18     1     120.0100   405.5100
  14    12    18     1     120.0100   405.5100
  11    13    14     1     119.9700   562.1600
  11    13    17     1     120.0100   405.5100
  14    13    17     1     120.0100   405.5100
  12    14    13     1     119.9700   562.1600
  12    14    16     1     120.0100   405.5100
  13    14    16     1     120.0100   405.5100
   2    23     3     1     113.1500   572.8700
   2    23    47     1     125.0900   523.5000
   3    23    47     1     124.3600   528.4400
   2    24     4     1     104.9400   606.0900
   2    24    36     1     104.9400   606.0900
   4    24    36     1     140.9600   167.3600
   1    25     9     1     104.9400   606.0900
   1    25    36     1     111.7800   167.3600
   9    25    36     1     140.9600   167.3600
   1    26    10     1     113.1500   572.8700
   1    26    38     1     125.0900   523.5000
  10    26    38     1     124.3600   528.4400
   2    27    28     1     120.1000   552.2000
   2    27    35     1     118.0200   578.9800
  28    27    35     1     122.6300   578.7300
  27    28    29     1     119.9700   562.1600
  27    28    32     1     120.0100   405.5100
  29    28    32     1     120.0100   405.5100
  28    29    30     1     119.9700   562.1600
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  28   29   33    1      120.0100   405.5100
  30   29   33    1      120.0100   405.5100
  29   30   31    1      119.9700   562.1600
  29   30   34    1      120.0100   405.5100
  31   30   34    1      120.0100   405.5100
   1   31   30    1      120.1000   552.2000
   1   31   35    1      118.0200   578.9800
  30   31   35    1      122.6300   578.7300
  27   35   31    1      115.8600   573.9600
  27   35   36    1      118.7800   167.3600
  31   35   36    1      118.7800   167.3600
  24   36   25    1      160.3400   351.4600
  24   36   35    1       80.1700   351.4600
  24   36   37    1       99.8300   962.3200
  25   36   35    1       80.1700   351.4600
  25   36   37    1       99.8300   962.3200
  35   36   37    1      180.0000   962.3200
  26   38   39    1      112.8100   550.0300
  26   38   40    1      109.4500   417.5600
  26   38   41    1      109.4500   417.5600
  39   38   40    1      110.0700   387.9400
  39   38   41    1      110.0700   387.9400
  40   38   41    1      109.5500   327.8600
  38   39   42    1      110.6300   528.9400
  38   39   43    1      110.0500   388.0200
  38   39   44    1      110.0500   388.0200
  42   39   43    1      110.0500   388.0200
  42   39   44    1      110.0500   388.0200
  43   39   44    1      108.3500   329.9500
  39   42   45    1      110.0700   387.9400
  39   42   46    1      110.0700   387.9400
  39   42   56    1      110.0000   527.0200
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  45   42   56    1      108.1100   367.0200
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  23   47   48    1      112.8100   550.0300
  23   47   49    1      109.4500   417.5600
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  48   47   49    1      110.0700   387.9400
  48   47   50    1      110.0700   387.9400
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  47   48   51    1      110.6300   528.9400
  47   48   52    1      110.0500   388.0200
  47   48   53    1      110.0500   388.0200
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  52   48   53    1      108.3500   329.9500
  48   51   54    1      110.0700   387.9400
  48   51   55    1      110.0700   387.9400
  48   51   57    1      110.0000   527.0200
  54   51   55    1      109.5500   327.8600
  54   51   57    1      108.1100   367.0200
  55   51   57    1      108.1100   367.0200
  42   56   61    1      108.3200   557.2300
  42   56   62    1      108.3200   557.2300
  42   56   63    1      108.3200   557.2300
  61   56   62    1      119.7300   624.0900
  61   56   63    1      119.7300   624.0900
  62   56   63    1      119.7300   624.0900
  51   57   58    1      108.3200   557.2300
  51   57   59    1      108.3200   557.2300
  51   57   60    1      108.3200   557.2300
  58   57   59    1      119.7300   624.0900
  58   57   60    1      119.7300   624.0900
  59   57   60    1      119.7300   624.0900

[ dihedrals ]
;  ai    aj    ak    al   funct          c0          c1          c2          c3          c4          c5
  26     1    25     9     3     39.74800     0.00000   -39.74800     0.00000     0.00000     0.00000
  26     1    25    36     3     39.74800     0.00000   -39.74800     0.00000     0.00000     0.00000
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25	1	26	38	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
31	1	26	10	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
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25	1	31	30	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000
25	1	31	35	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000
26	1	31	30	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000
26	1	31	35	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000
24	2	23	3	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
24	2	23	47	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
27	2	23	3	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
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23	2	24	4	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
23	2	24	36	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
27	2	24	4	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
27	2	24	36	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
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23	2	27	35	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000
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23	3	4	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
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3	4	24	36	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
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38	39	42	46	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
38	39	42	56	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
43	39	42	45	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
43	39	42	46	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
43	39	42	56	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
44	39	42	45	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
44	39	42	46	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
44	39	42	56	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
39	42	56	61	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
39	42	56	62	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
39	42	56	63	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
45	42	56	61	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
45	42	56	62	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
45	42	56	63	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
46	42	56	61	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
46	42	56	62	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
46	42	56	63	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
23	47	48	51	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
23	47	48	52	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
23	47	48	53	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
49	47	48	51	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
49	47	48	52	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
49	47	48	53	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
50	47	48	51	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
50	47	48	52	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
50	47	48	53	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
47	48	51	54	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
47	48	51	55	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
47	48	51	57	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
52	48	51	54	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
52	48	51	55	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
52	48	51	57	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
53	48	51	54	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
53	48	51	55	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
53	48	51	57	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
48	51	57	58	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
48	51	57	59	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
48	51	57	60	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
54	51	57	58	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
54	51	57	59	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
54	51	57	60	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
55	51	57	58	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
55	51	57	59	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
55	51	57	60	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000

[dihedrals]

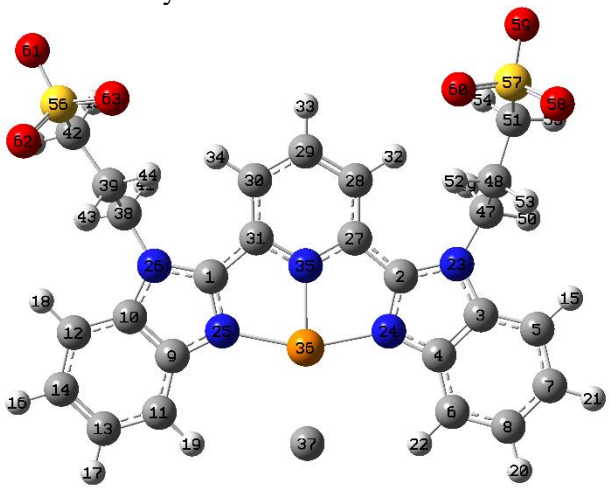
; ai	aj	ak	al	funct	c0	c1	c2	c3
1	26	10	38	1	180.00	4.60240	2	
2	23	3	47	1	180.00	4.60240	2	
3	7	5	15	1	180.00	4.60240	2	
3	6	4	24	1	180.00	4.60240	2	
4	8	6	22	1	180.00	4.60240	2	
4	5	3	23	1	180.00	4.60240	2	
5	8	7	21	1	180.00	4.60240	2	
6	7	8	20	1	180.00	4.60240	2	
9	13	11	19	1	180.00	4.60240	2	
9	12	10	26	1	180.00	4.60240	2	
10	14	12	18	1	180.00	4.60240	2	
10	11	9	25	1	180.00	4.60240	2	
11	14	13	17	1	180.00	4.60240	2	

```
   12    13    14    16     1    180.00     4.60240     2
   24     2    23    27     1    180.00     4.60240     2
   25     1    26    31     1    180.00     4.60240     2
   27    29    28    32     1    180.00     4.60240     2
   28    30    29    33     1    180.00     4.60240     2
   28     2    27    35     1    180.00     4.60240     2
   29    31    30    34     1    180.00     4.60240     2
   30     1    31    35     1    180.00     4.60240     2

[ system ]
; Name
  PTB

[ molecules ]
; Compound        #mols
   PtB              1
```

Table S9. Force field parameters of Pt^{s}B system in GROMACS format used in this work.



; Pt^{s}B force field parameters
;PtsB_GMX.top

```
[ defaults ]
; nbfunc        comb-rule       gen-pairs       fudgeLJ         fudgeQQ
1               2               yes             0.5             0.8333

[ atomtypes ]
; name      at.num  mass    charge ptype  sigma       epsilon
PTsB_cc     6    12.01      0.0000   A    3.39967e-01  3.59824e-01
PTsB_ca     6    12.01      0.0000   A    3.39967e-01  3.59824e-01
PTsB_ha     1    1.008      0.0000   A    2.59964e-01  6.27600e-02
PTsB_na     7    14.01      0.0000   A    3.25000e-01  7.11280e-01
PTsB_nd     7    14.01      0.0000   A    3.25000e-01  7.11280e-01
PTsB_nb     7    14.01      0.0000   A    3.25000e-01  7.11280e-01
PTsB_Pt     78   195.078    0.0000   A    4.34750e-01  1.6736        ; the only different parameters corresponding to PtB
PTsB_cl     17   35.45      0.0000   A    3.47094e-01  1.10876e+00
PTsB_c3     6    12.01      0.0000   A    3.39967e-01  4.57730e-01
PTsB_h1     1    1.008      0.0000   A    2.47135e-01  6.56888e-02
PTsB_hc     1    1.008      0.0000   A    2.64953e-01  6.56888e-02
PTsB_s6     16   32.06      0.0000   A    3.56359e-01  1.04600e+00
PTsB_ o     8    16.00      0.0000   A    2.95992e-01  8.78640e-01


[ moleculetype ]
; Name            nrexcl
PtsB              3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB      massB
     1    PTsB_cc     1    PTsB     C1      1     0.081892    12.01  ; qtot 0.08189
     2    PTsB_cc     1    PTsB     C2      2     0.081892    12.01  ; qtot 0.1638
     3    PTsB_ca     1    PTsB     C3      3     0.250779    12.01  ; qtot 0.4146
     4    PTsB_ca     1    PTsB     C4      4     0.148116    12.01  ; qtot 0.5627
     5    PTsB_ca     1    PTsB     C5      5    -0.280998    12.01  ; qtot 0.2817
     6    PTsB_ca     1    PTsB     C6      6    -0.217522    12.01  ; qtot 0.06416
     7    PTsB_ca     1    PTsB     C7      7    -0.076146    12.01  ; qtot -0.01199
     8    PTsB_ca     1    PTsB     C8      8    -0.106842    12.01  ; qtot -0.1188
     9    PTsB_ca     1    PTsB     C9      9     0.148116    12.01   ; qtot 0.02929
    10    PTsB_ca     1    PTsB    C10     10     0.250779    12.01   ; qtot 0.2801
    11    PTsB_ca     1    PTsB    C11     11    -0.217522    12.01   ; qtot 0.06254
    12    PTsB_ca     1    PTsB    C12     12    -0.280998    12.01   ; qtot -0.2185
    13    PTsB_ca     1    PTsB    C13     13    -0.106842    12.01   ; qtot -0.3253
    14    PTsB_ca     1    PTsB    C14     14    -0.076146    12.01   ; qtot -0.4014
    15    PTsB_ha     1    PTsB     H1     15     0.184387    1.008   ; qtot -0.2171
    16    PTsB_ha     1    PTsB     H2     16     0.151311    1.008   ; qtot -0.06574
    17    PTsB_ha     1    PTsB     H3     17     0.153899    1.008   ; qtot 0.08816
    18    PTsB_ha     1    PTsB     H4     18     0.184387    1.008   ; qtot 0.2725
    19    PTsB_ha     1    PTsB     H5     19     0.1958      1.008   ; qtot 0.4683
    20    PTsB_ha     1    PTsB     H6     20     0.153899    1.008   ; qtot 0.6222
```

```
    21    PTsB_ha     1    PTsB     H7    21     0.151311     1.008   ; qtot 0.7736
    22    PTsB_ha     1    PTsB     H8    22     0.1958       1.008   ; qtot 0.9694
    23    PTsB_na     1    PTsB     N1    23    -0.408906    14.01    ; qtot 0.5604
    24    PTsB_nd     1    PTsB     N2    24     0.044289    14.01    ; qtot 0.6047
    25    PTsB_nd     1    PTsB     N3    25     0.044289    14.01    ; qtot 0.649
    26    PTsB_na     1    PTsB     N4    26    -0.408906    14.01    ; qtot 0.2401
    27    PTsB_ca     1    PTsB    C15    27     0.250755    12.01    ; qtot 0.4909
    28    PTsB_ca     1    PTsB    C16    28    -0.277609    12.01    ; qtot 0.2133
    29    PTsB_ca     1    PTsB    C17    29     0.006689    12.01    ; qtot 0.22
    30    PTsB_ca     1    PTsB    C18    30    -0.277609    12.01    ; qtot -0.05766
    31    PTsB_ca     1    PTsB    C19    31     0.250755    12.01    ; qtot 0.1931
    32    PTsB_ha     1    PTsB     H9    32     0.183021     1.008   ; qtot 0.3761
    33    PTsB_ha     1    PTsB    H10    33     0.157288     1.008   ; qtot 0.5334
    34    PTsB_ha     1    PTsB    H11    34     0.183021     1.008   ; qtot 0.7164
    35    PTsB_nb     1    PTsB     N5    35    -0.04731     14.01    ; qtot 0.6691
    36    PTsB_Pt     1    PTsB    PT1    36    -0.201109   195.0     ; qtot 0.468
    37    PTsB_cl     1    PTsB    CL1    37    -0.240282    35.45    ; qtot 0.2277
    38    PTsB_c3     1    PTsB    C20    38    -0.668119    12.01    ; qtot -0.4404
    39    PTsB_c3     1    PTsB    C21    39     0.050403    12.01    ; qtot -0.39
    40    PTsB_h1     1    PTsB    H12    40     0.412608     1.008   ; qtot 0.02262
    41    PTsB_h1     1    PTsB    H13    41     0.412608     1.008   ; qtot 0.4352
    42    PTsB_c3     1    PTsB    C22    42     0.466356    12.01    ; qtot 0.9016
    43    PTsB_hc     1    PTsB    H14    43    -0.017213     1.008   ; qtot 0.8844
    44    PTsB_hc     1    PTsB    H15    44    -0.017213     1.008   ; qtot 0.8672
    45    PTsB_h1     1    PTsB    H16    45    -0.175945     1.008   ; qtot 0.6912
    46    PTsB_h1     1    PTsB    H17    46    -0.175945     1.008   ; qtot 0.5153
    47    PTsB_c3     1    PTsB    C23    47    -0.668119    12.01    ; qtot -0.1529
    48    PTsB_c3     1    PTsB    C24    48     0.050403    12.01    ; qtot -0.1024
    49    PTsB_h1     1    PTsB    H18    49     0.412608     1.008   ; qtot 0.3102
    50    PTsB_h1     1    PTsB    H19    50     0.412608     1.008   ; qtot 0.7228
    51    PTsB_c3     1    PTsB    C25    51     0.466356    12.01    ; qtot 1.189
    52    PTsB_hc     1    PTsB    H20    52    -0.017213     1.008   ; qtot 1.172
    53    PTsB_hc     1    PTsB    H21    53    -0.017213     1.008   ; qtot 1.155
    54    PTsB_h1     1    PTsB    H22    54    -0.175945     1.008   ; qtot 0.9788
    55    PTsB_h1     1    PTsB    H23    55    -0.175945     1.008   ; qtot 0.8028
    56    PTsB_s6     1    PTsB     S1    56     1.1828      32.06    ; qtot 1.986
    57    PTsB_s6     1    PTsB     S2    57     1.1828      32.06    ; qtot 3.168
    58    PTsB_ o     1    PTsB     O1    58    -0.694737    16.00    ; qtot 2.474
    59    PTsB_ o     1    PTsB     O2    59    -0.694737    16.00    ; qtot 1.779
    60    PTsB_ o     1    PTsB     O3    60    -0.694737    16.00    ; qtot 1.084
    61    PTsB_ o     1    PTsB     O4    61    -0.694737    16.00    ; qtot 0.3895
    62    PTsB_ o     1    PTsB     O5    62    -0.694737    16.00    ; qtot -0.3053
    63    PTsB_ o     1    PTsB     O6    63    -0.694737    16.00    ; qtot -1

[ bonds ]
;  ai    aj funct          c0          c1          c2          c3
    1    25    1        0.13350   413880.0
    1    26    1        0.13710   367190.0
    1    31    1        0.14340   344510.0
    2    23    1        0.13710   367190.0
    2    24    1        0.13350   413880.0
    2    27    1        0.14340   344510.0
    3     4    1        0.13870   400330.0
    3     5    1        0.13870   400330.0
    3    23    1        0.13500   393550.0
    4     6    1        0.13870   400330.0
    4    24    1        0.13360   412460.0
    5     7    1        0.13870   400330.0
    5    15    1        0.10870   288110.0
    6     8    1        0.13870   400330.0
    6    22    1        0.10870   288110.0
    7     8    1        0.13870   400330.0
    7    21    1        0.10870   288110.0
    8    20    1        0.10870   288110.0
    9    10    1        0.13870   400330.0
    9    11    1        0.13870   400330.0
    9    25    1        0.13360   412460.0
   10    12    1        0.13870   400330.0
   10    26    1        0.13500   393550.0
   11    13    1        0.13870   400330.0
```

```
  11   19    1          0.10870   288110.0
  12   14    1          0.13870   400330.0
  12   18    1          0.10870   288110.0
  13   14    1          0.13870   400330.0
  13   17    1          0.10870   288110.0
  14   16    1          0.10870   288110.0
  23   47    1          0.14560   280080.0
  24   36    1          0.20310   306270.0
  25   36    1          0.20310   306270.0
  26   38    1          0.14560   280080.0
  27   28    1          0.13870   400330.0
  27   35    1          0.13420   404260.0
  28   29    1          0.13870   400330.0
  28   32    1          0.10870   288110.0
  29   30    1          0.13870   400330.0
  29   33    1          0.10870   288110.0
  30   31    1          0.13870   400330.0
  30   34    1          0.10870   288110.0
  31   35    1          0.13420   404260.0
  35   36    1          0.19670   306270.0
  36   37    1          0.22890   131440.0
  38   39    1          0.15350   253630.0
  38   40    1          0.10930   281080.0
  38   41    1          0.10930   281080.0
  39   42    1          0.15350   253630.0
  39   43    1          0.10920   282250.0
  39   44    1          0.10920   282250.0
  42   45    1          0.10930   281080.0
  42   46    1          0.10930   281080.0
  42   56    1          0.17740   212550.0
  47   48    1          0.15350   253630.0
  47   49    1          0.10930   281080.0
  47   50    1          0.10930   281080.0
  48   51    1          0.15350   253630.0
  48   52    1          0.10920   282250.0
  48   53    1          0.10920   282250.0
  51   54    1          0.10930   281080.0
  51   55    1          0.10930   281080.0
  51   57    1          0.17740   212550.0
  56   61    1          0.14360   452790.0
  56   62    1          0.14360   452790.0
  56   63    1          0.14360   452790.0
  57   58    1          0.14360   452790.0
  57   59    1          0.14360   452790.0
  57   60    1          0.14360   452790.0

[ pairs ]
;  ai    aj funct          c0          c1          c2          c3
    1    11    1
    1    12    1
    1    24    1
    1    27    1
    1    29    1
    1    34    1
    1    37    1
    1    39    1
    1    40    1
    1    41    1
    2     5    1
    2     6    1
    2    25    1
    2    29    1
    2    31    1
    2    32    1
    2    37    1
    2    48    1
    2    49    1
    2    50    1
    3     8    1
    3    21    1
```

3	22	1
3	27	1
3	36	1
3	48	1
3	49	1
3	50	1
4	7	1
4	15	1
4	20	1
4	25	1
4	27	1
4	35	1
4	37	1
4	47	1
5	6	1
5	20	1
5	24	1
5	47	1
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49 53 1
50 51 1
50 52 1
50 53 1
52 54 1
52 55 1
52 57 1
53 54 1
53 55 1
53 57 1
54 58 1

```
  54   59    1
  54   60    1
  55   58    1
  55   59    1
  55   60    1

[ angles ]
;  ai    aj    ak funct       c0         c1         c2         c3
  25     1    26    1     112.0200   625.7600
  25     1    31    1     123.0200   568.3500
  26     1    31    1     123.4500   560.9100
  23     2    24    1     112.0200   625.7600
  23     2    27    1     123.4500   560.9100
  24     2    27    1     123.0200   568.3500
   4     3     5    1     119.9700   562.1600
   4     3    23    1     118.3400   587.5200
   5     3    23    1     119.9700   562.1600
   3     4     6    1     119.9700   562.1600
   3     4    24    1     119.7200   586.9300
   6     4    24    1     119.7200   586.9300
   3     5     7    1     119.9700   562.1600
   3     5    15    1     120.0100   405.5100
   7     5    15    1     120.0100   405.5100
   4     6     8    1     119.9700   562.1600
   4     6    22    1     120.0100   405.5100
   8     6    22    1     120.0100   405.5100
   5     7     8    1     119.9700   562.1600
   5     7    21    1     120.0100   405.5100
   8     7    21    1     120.0100   405.5100
   6     8     7    1     119.9700   562.1600
   6     8    20    1     120.0100   405.5100
   7     8    20    1     120.0100   405.5100
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  10     9    25    1     119.7200   586.9300
  11     9    25    1     119.7200   586.9300
   9    10    12    1     119.9700   562.1600
   9    10    26    1     118.3400   587.5200
  12    10    26    1     118.3400   587.5200
   9    11    13    1     119.9700   562.1600
   9    11    19    1     120.0100   405.5100
  13    11    19    1     120.0100   405.5100
  10    12    14    1     119.9700   562.1600
  10    12    18    1     120.0100   405.5100
  14    12    18    1     120.0100   405.5100
  11    13    14    1     119.9700   562.1600
  11    13    17    1     120.0100   405.5100
  14    13    17    1     120.0100   405.5100
  12    14    13    1     119.9700   562.1600
  12    14    16    1     120.0100   405.5100
  13    14    16    1     120.0100   405.5100
   2    23     3    1     113.1500   572.8700
   2    23    47    1     125.0900   523.5000
   3    23    47    1     124.3600   528.4400
   2    24     4    1     104.9400   606.0900
   2    24    36    1     104.9400   606.0900
   4    24    36    1     140.9600   167.3600
   1    25     9    1     104.9400   606.0900
   1    25    36    1     111.7800   167.3600
   9    25    36    1     140.9600   167.3600
   1    26    10    1     113.1500   572.8700
   1    26    38    1     125.0900   523.5000
  10    26    38    1     124.3600   528.4400
   2    27    28    1     120.1000   552.2000
   2    27    35    1     118.0200   578.9800
  28    27    35    1     122.6300   578.7300
  27    28    29    1     119.9700   562.1600
  27    28    32    1     120.0100   405.5100
  29    28    32    1     120.0100   405.5100
  28    29    30    1     119.9700   562.1600
  28    29    33    1     120.0100   405.5100
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  30   29   33    1      120.0100   405.5100
  29   30   31    1      119.9700   562.1600
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   1   31   30    1      120.1000   552.2000
   1   31   35    1      118.0200   578.9800
  30   31   35    1      122.6300   578.7300
  27   35   31    1      115.8600   573.9600
  27   35   36    1      118.7800   167.3600
  31   35   36    1      118.7800   167.3600
  24   36   25    1      160.3400   351.4600
  24   36   35    1       80.1700   351.4600
  24   36   37    1       99.8300   962.3200
  25   36   35    1       80.1700   351.4600
  25   36   37    1       99.8300   962.3200
  35   36   37    1      180.0000   962.3200
  26   38   39    1      112.8100   550.0300
  26   38   40    1      109.4500   417.5600
  26   38   41    1      109.4500   417.5600
  39   38   40    1      110.0700   387.9400
  39   38   41    1      110.0700   387.9400
  40   38   41    1      109.5500   327.8600
  38   39   42    1      110.6300   528.9400
  38   39   43    1      110.0500   388.0200
  38   39   44    1      110.0500   388.0200
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  43   39   44    1      108.3500   329.9500
  39   42   45    1      110.0700   387.9400
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  45   42   46    1      109.5500   327.8600
  45   42   56    1      108.1100   367.0200
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  23   47   48    1      112.8100   550.0300
  23   47   49    1      109.4500   417.5600
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  48   47   49    1      110.0700   387.9400
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  47   48   51    1      110.6300   528.9400
  47   48   52    1      110.0500   388.0200
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  48   51   54    1      110.0700   387.9400
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  48   51   57    1      110.0000   527.0200
  54   51   55    1      109.5500   327.8600
  54   51   57    1      108.1100   367.0200
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  42   56   61    1      108.3200   557.2300
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  61   56   63    1      119.7300   624.0900
  62   56   63    1      119.7300   624.0900
  51   57   58    1      108.3200   557.2300
  51   57   59    1      108.3200   557.2300
  51   57   60    1      108.3200   557.2300
  58   57   59    1      119.7300   624.0900
  58   57   60    1      119.7300   624.0900
  59   57   60    1      119.7300   624.0900

[ dihedrals ]
;  ai    aj    ak    al   funct          c0          c1          c2          c3          c4          c5
  26    1    25     9    3    39.74800    0.00000   -39.74800    0.00000    0.00000    0.00000
  26    1    25    36    3    39.74800    0.00000   -39.74800    0.00000    0.00000    0.00000
  31    1    25     9    3    39.74800    0.00000   -39.74800    0.00000    0.00000    0.00000
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25	1	26	38	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
31	1	26	10	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
31	1	26	38	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
25	1	31	30	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000
25	1	31	35	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000
26	1	31	30	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000
26	1	31	35	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000
24	2	23	3	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
24	2	23	47	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
27	2	23	3	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
27	2	23	47	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
23	2	24	4	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
23	2	24	36	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
27	2	24	4	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
27	2	24	36	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
23	2	27	28	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000
23	2	27	35	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000
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5	3	4	24	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
23	3	4	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
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4	3	23	2	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
4	3	23	47	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
5	3	23	2	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
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3	4	6	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
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3	4	24	36	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
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9	10	26	38	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
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41	38	39	42	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
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38	39	42	46	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
38	39	42	56	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
43	39	42	45	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
43	39	42	46	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
43	39	42	56	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
44	39	42	45	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
44	39	42	46	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
44	39	42	56	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
39	42	56	61	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
39	42	56	62	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
39	42	56	63	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
45	42	56	61	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
45	42	56	62	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
45	42	56	63	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
46	42	56	61	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
46	42	56	62	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
46	42	56	63	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
23	47	48	51	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
23	47	48	52	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
23	47	48	53	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
49	47	48	51	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
49	47	48	52	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
49	47	48	53	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
50	47	48	51	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
50	47	48	52	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
50	47	48	53	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
47	48	51	54	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
47	48	51	55	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
47	48	51	57	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
52	48	51	54	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
52	48	51	55	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
52	48	51	57	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
53	48	51	54	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
53	48	51	55	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
53	48	51	57	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
48	51	57	58	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
48	51	57	59	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
48	51	57	60	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
54	51	57	58	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
54	51	57	59	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
54	51	57	60	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
55	51	57	58	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
55	51	57	59	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
55	51	57	60	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000

[dihedrals]

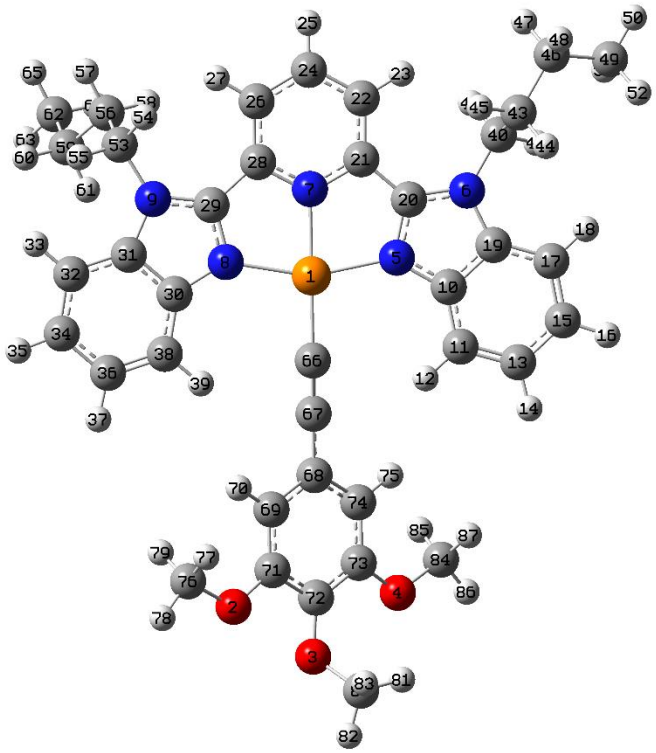
; ai	aj	ak	al	funct	c0	c1	c2	c3
1	26	10	38	1	180.00	4.60240	2	
2	23	3	47	1	180.00	4.60240	2	
3	7	5	15	1	180.00	4.60240	2	
3	6	4	24	1	180.00	4.60240	2	
4	8	6	22	1	180.00	4.60240	2	
4	5	3	23	1	180.00	4.60240	2	
5	8	7	21	1	180.00	4.60240	2	
6	7	8	20	1	180.00	4.60240	2	
9	13	11	19	1	180.00	4.60240	2	
9	12	10	26	1	180.00	4.60240	2	
10	14	12	18	1	180.00	4.60240	2	
10	11	9	25	1	180.00	4.60240	2	
11	14	13	17	1	180.00	4.60240	2	
12	13	14	16	1	180.00	4.60240	2	

```
   24     2   23   27    1    180.00      4.60240      2
   25     1   26   31    1    180.00      4.60240      2
   27    29   28   32    1    180.00      4.60240      2
   28    30   29   33    1    180.00      4.60240      2
   28     2   27   35    1    180.00      4.60240      2
   29    31   30   34    1    180.00      4.60240      2
   30     1   31   35    1    180.00      4.60240      2

[ system ]
; Name
  PTsB

[ molecules ]
; Compound        #mols
   PtsB              1
```

Table S10. Force field parameters of PtB-a system in GROMACS format used in this work.



;PtB-a force field parameters
;PtB-a_GMX.top

```
[ defaults ]
; nbfunc        comb-rule       gen-pairs       fudgeLJ         fudgeQQ
1               2               yes             0.5             0.8333

[ atomtypes ]
; name      at.num  mass     charge ptype  sigma       epsilon
PTC_Pt     78    195.078   0.0000  A     3.3298e-01     1.0534e+01
PTC_os      8    16.00     0.0000  A     3.00001e-01    7.11280e-01
PTC_nc      7    14.01     0.0000  A     3.25000e-01    7.11280e-01
PTC_na      7    14.01     0.0000  A     3.25000e-01    7.11280e-01
PTC_nb      7    14.01     0.0000  A     3.25000e-01    7.11280e-01
PTC_ca      6    12.01     0.0000  A     3.39967e-01    3.59824e-01
PTC_ha      1    1.008     0.0000  A     2.59964e-01    6.27600e-02
PTC_cd      6    12.01     0.0000  A     3.39967e-01    3.59824e-01
PTC_c3      6    12.01     0.0000  A     3.39967e-01    4.57730e-01
PTC_h1      1    1.008     0.0000  A     2.47135e-01    6.56888e-02
PTC_hc      1    1.008     0.0000  A     2.64953e-01    6.56888e-02
PTC_c1      6    12.01     0.0000  A     3.39967e-01    8.78640e-01
PTC_cg      6    12.01     0.0000  A     3.39967e-01    8.78640e-01

[ moleculetype ]
; Name            nrexcl
PtB-a             3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB     massB
; residue   1 PTC rtp PTC  q +1.0
     1     PTC_Pt     1    PTC    PT1     1    -0.201109    195.078; qtot -0.2011
     2     PTC_os     1    PTC     O1     2    -0.2164       16.00   ; qtot -0.4175
     3     PTC_os     1    PTC     O2     3    -0.249979     16.00   ; qtot -0.6675
     4     PTC_os     1    PTC     O3     4    -0.2164       16.00   ; qtot -0.8839
     5     PTC_nc     1    PTC     N1     5     0.044289     14.01   ; qtot -0.8396
     6     PTC_na     1    PTC     N2     6    -0.408905     14.01   ; qtot -1.249
     7     PTC_nb     1    PTC     N3     7    -0.04731      14.01   ; qtot -1.296
     8     PTC_nc     1    PTC     N4     8     0.044289     14.01   ; qtot -1.252
     9     PTC_na     1    PTC     N5     9    -0.408905     14.01   ; qtot -1.66
    10     PTC_ca     1    PTC     C1    10     0.148116     12.01   ; qtot -1.512
```

```
11   PTC_ca   1   PTC    C2   11    -0.217522    12.01   ; qtot -1.73
12   PTC_ha   1   PTC    H1   12     0.1958      1.008   ; qtot -1.534
13   PTC_ca   1   PTC    C3   13    -0.106842    12.01   ; qtot -1.641
14   PTC_ha   1   PTC    H2   14     0.153899    1.008   ; qtot -1.487
15   PTC_ca   1   PTC    C4   15    -0.076146    12.01   ; qtot -1.563
16   PTC_ha   1   PTC    H3   16     0.151311    1.008   ; qtot -1.412
17   PTC_ca   1   PTC    C5   17    -0.280998    12.01   ; qtot -1.693
18   PTC_ha   1   PTC    H4   18     0.184387    1.008   ; qtot -1.508
19   PTC_ca   1   PTC    C6   19     0.250779    12.01   ; qtot -1.258
20   PTC_cd   1   PTC    C7   20     0.081892    12.01   ; qtot -1.176
21   PTC_ca   1   PTC    C8   21     0.250755    12.01   ; qtot -0.925
22   PTC_ca   1   PTC    C9   22    -0.277609    12.01   ; qtot -1.203
23   PTC_ha   1   PTC    H5   23     0.183021    1.008   ; qtot -1.02
24   PTC_ca   1   PTC   C10   24     0.006689    12.01   ; qtot -1.013
25   PTC_ha   1   PTC    H6   25     0.157288    1.008   ; qtot -0.8556
26   PTC_ca   1   PTC   C11   26    -0.277609    12.01   ; qtot -1.133
27   PTC_ha   1   PTC    H7   27     0.183021    1.008   ; qtot -0.9502
28   PTC_ca   1   PTC   C12   28     0.250755    12.01   ; qtot -0.6994
29   PTC_cd   1   PTC   C13   29     0.081892    12.01   ; qtot -0.6176
30   PTC_ca   1   PTC   C14   30     0.148116    12.01   ; qtot -0.4694
31   PTC_ca   1   PTC   C15   31     0.250779    12.01   ; qtot -0.2187
32   PTC_ca   1   PTC   C16   32    -0.280998    12.01   ; qtot -0.4997
33   PTC_ha   1   PTC    H8   33     0.184387    1.008   ; qtot -0.3153
34   PTC_ca   1   PTC   C17   34    -0.076146    12.01   ; qtot -0.3914
35   PTC_ha   1   PTC    H9   35     0.151311    1.008   ; qtot -0.2401
36   PTC_ca   1   PTC   C18   36    -0.106842    12.01   ; qtot -0.3469
37   PTC_ha   1   PTC   H10   37     0.153899    1.008   ; qtot -0.193
38   PTC_ca   1   PTC   C19   38    -0.217522    12.01   ; qtot -0.4106
39   PTC_ha   1   PTC   H11   39     0.1958      1.008   ; qtot -0.2148
40   PTC_c3   1   PTC   C20   40     0.374263    12.01   ; qtot 0.1595
41   PTC_h1   1   PTC   H12   41    -0.010174    1.008   ; qtot 0.1493
42   PTC_h1   1   PTC   H13   42    -0.010174    1.008   ; qtot 0.1391
43   PTC_c3   1   PTC   C21   43    -0.248219    12.01   ; qtot -0.1091
44   PTC_hc   1   PTC   H14   44     0.057939    1.008   ; qtot -0.05113
45   PTC_hc   1   PTC   H15   45     0.057939    1.008   ; qtot 0.006807
46   PTC_c3   1   PTC   C22   46     0.247039    12.01   ; qtot 0.2538
47   PTC_hc   1   PTC   H16   47    -0.038393    1.008   ; qtot 0.2155
48   PTC_hc   1   PTC   H17   48    -0.038393    1.008   ; qtot 0.1771
49   PTC_c3   1   PTC   C23   49    -0.169898    12.01   ; qtot 0.007162
50   PTC_hc   1   PTC   H18   50     0.042932    1.008   ; qtot 0.05009
51   PTC_hc   1   PTC   H19   51     0.042932    1.008   ; qtot 0.09303
52   PTC_hc   1   PTC   H20   52     0.042932    1.008   ; qtot 0.136
53   PTC_c3   1   PTC   C24   53     0.374263    12.01   ; qtot 0.5102
54   PTC_h1   1   PTC   H21   54    -0.010174    1.008   ; qtot 0.5
55   PTC_h1   1   PTC   H22   55    -0.010174    1.008   ; qtot 0.4899
56   PTC_c3   1   PTC   C25   56    -0.248219    12.01   ; qtot 0.2417
57   PTC_hc   1   PTC   H23   57     0.057939    1.008   ; qtot 0.2996
58   PTC_hc   1   PTC   H24   58     0.057939    1.008   ; qtot 0.3575
59   PTC_c3   1   PTC   C26   59     0.247039    12.01   ; qtot 0.6046
60   PTC_hc   1   PTC   H25   60    -0.038393    1.008   ; qtot 0.5662
61   PTC_hc   1   PTC   H26   61    -0.038393    1.008   ; qtot 0.5278
62   PTC_c3   1   PTC   C27   62    -0.169898    12.01   ; qtot 0.3579
63   PTC_hc   1   PTC   H27   63     0.042932    1.008   ; qtot 0.4008
64   PTC_hc   1   PTC   H28   64     0.042932    1.008   ; qtot 0.4438
65   PTC_hc   1   PTC   H29   65     0.042932    1.008   ; qtot 0.4867
66   PTC_c1   1   PTC   C28   66    -0.269551    12.01   ; qtot 0.2171
67   PTC_cg   1   PTC   C29   67    -0.004993    12.01   ; qtot 0.2121
68   PTC_ca   1   PTC   C30   68     0.055008    12.01   ; qtot 0.2671
69   PTC_ca   1   PTC   C31   69    -0.30574     12.01   ; qtot -0.03859
70   PTC_ha   1   PTC   H30   70     0.126839    1.008   ; qtot 0.08825
71   PTC_ca   1   PTC   C32   71     0.325435    12.01   ; qtot 0.4137
72   PTC_ca   1   PTC   C33   72    -0.047993    12.01   ; qtot 0.3657
73   PTC_ca   1   PTC   C34   73     0.325435    12.01   ; qtot 0.6911
74   PTC_ca   1   PTC   C35   74    -0.30574     12.01   ; qtot 0.3854
75   PTC_ha   1   PTC   H31   75     0.126839    1.008   ; qtot 0.5122
76   PTC_c3   1   PTC   C36   76    -0.021785    12.01   ; qtot 0.4904
77   PTC_h1   1   PTC   H32   77     0.057304    1.008   ; qtot 0.5477
78   PTC_h1   1   PTC   H33   78     0.057304    1.008   ; qtot 0.605
79   PTC_h1   1   PTC   H34   79     0.057304    1.008   ; qtot 0.6623
80   PTC_c3   1   PTC   C37   80    -0.049849    12.01   ; qtot 0.6125
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    81    PTC_h1     1   PTC    H35    81   0.079124     1.008   ; qtot 0.6916
    82    PTC_h1     1   PTC    H36    82   0.079124     1.008   ; qtot 0.7707
    83    PTC_h1     1   PTC    H37    83   0.079124     1.008   ; qtot 0.8499
    84    PTC_c3     1   PTC    C38    84  -0.021785     12.01   ; qtot 0.8281
    85    PTC_h1     1   PTC    H38    85   0.057304     1.008   ; qtot 0.8854
    86    PTC_h1     1   PTC    H39    86   0.057304     1.008   ; qtot 0.9427
    87    PTC_h1     1   PTC    H40    87   0.057304     1.008   ; qtot 1

[ bonds ]
;  ai    aj funct         c0         c1         c2         c3
    1     5    1       0.20101   306270.0
    1     7    1       0.19961   306270.0
    1     8    1       0.20101   306270.0
    1    66    1       0.19492   306270.0
    2    71    1       0.13730   311620.0
    2    76    1       0.14390   252300.0
    3    72    1       0.13730   311620.0
    3    80    1       0.14390   252300.0
    4    73    1       0.13730   311620.0
    4    84    1       0.14390   252300.0
    5    10    1       0.13360   412460.0
    5    20    1       0.13350   413880.0
    6    19    1       0.13500   393550.0
    6    20    1       0.13710   367190.0
    6    40    1       0.14560   280080.0
    7    21    1       0.13420   404260.0
    7    28    1       0.13420   404260.0
    8    29    1       0.13350   413880.0
    8    30    1       0.13360   412460.0
    9    29    1       0.13710   367190.0
    9    31    1       0.13500   393550.0
    9    53    1       0.14560   280080.0
   10    11    1       0.13870   400330.0
   10    19    1       0.13870   400330.0
   11    12    1       0.10870   288110.0
   11    13    1       0.13870   400330.0
   13    14    1       0.10870   288110.0
   13    15    1       0.13870   400330.0
   15    16    1       0.10870   288110.0
   15    17    1       0.13870   400330.0
   17    18    1       0.10870   288110.0
   17    19    1       0.13870   400330.0
   20    21    1       0.14340   344510.0
   21    22    1       0.13870   400330.0
   22    23    1       0.10870   288110.0
   22    24    1       0.13870   400330.0
   24    25    1       0.10870   288110.0
   24    26    1       0.13870   400330.0
   26    27    1       0.10870   288110.0
   26    28    1       0.13870   400330.0
   28    29    1       0.14340   344510.0
   30    31    1       0.13870   400330.0
   30    38    1       0.13870   400330.0
   31    32    1       0.13870   400330.0
   32    33    1       0.10870   288110.0
   32    34    1       0.13870   400330.0
   34    35    1       0.10870   288110.0
   34    36    1       0.13870   400330.0
   36    37    1       0.10870   288110.0
   36    38    1       0.13870   400330.0
   38    39    1       0.10870   288110.0
   40    41    1       0.10930   281080.0
   40    42    1       0.10930   281080.0
   40    43    1       0.15350   253630.0
   43    44    1       0.10920   282250.0
   43    45    1       0.10920   282250.0
   43    46    1       0.15350   253630.0
   46    47    1       0.10920   282250.0
   46    48    1       0.10920   282250.0
   46    49    1       0.15350   253630.0
```

```
  49   50    1       0.10920   282250.0
  49   51    1       0.10920   282250.0
  49   52    1       0.10920   282250.0
  53   54    1       0.10930   281080.0
  53   55    1       0.10930   281080.0
  53   56    1       0.15350   253630.0
  56   57    1       0.10920   282250.0
  56   58    1       0.10920   282250.0
  56   59    1       0.15350   253630.0
  59   60    1       0.10920   282250.0
  59   61    1       0.10920   282250.0
  59   62    1       0.15350   253630.0
  62   63    1       0.10920   282250.0
  62   64    1       0.10920   282250.0
  62   65    1       0.10920   282250.0
  66   67    1       0.12220   707770.0
  67   68    1       0.14380   340240.0
  68   69    1       0.13870   400330.0
  68   74    1       0.13870   400330.0
  69   70    1       0.10870   288110.0
  69   71    1       0.13870   400330.0
  71   72    1       0.13870   400330.0
  72   73    1       0.13870   400330.0
  73   74    1       0.13870   400330.0
  74   75    1       0.10870   288110.0
  76   77    1       0.10930   281080.0
  76   78    1       0.10930   281080.0
  76   79    1       0.10930   281080.0
  80   81    1       0.10930   281080.0
  80   82    1       0.10930   281080.0
  80   83    1       0.10930   281080.0
  84   85    1       0.10930   281080.0
  84   86    1       0.10930   281080.0
  84   87    1       0.10930   281080.0

[ pairs ]
;  ai    aj funct          c0          c1          c2          c3
    1     6    1
    1     9    1
    1    11    1
    1    19    1
    1    22    1
    1    26    1
    1    31    1
    1    38    1
    1    68    1
    2     3    1
    2    68    1
    2    70    1
    2    73    1
    3     4    1
    3    69    1
    3    74    1
    4    68    1
    4    71    1
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  74   84    1

[ angles ]
;  ai    aj    ak funct       c0              c1        c2       c3
    5     1     7    1     79.5643   351.4600
    5     1     8    1    159.385    351.4600
    5     1    66    1     99.8300   962.3200
    7     1     8    1     79.5643   351.4600
    7     1    66    1    180.0000   962.3200
    8     1    66    1     99.8300   962.3200
   71     2    76    1    124.3600   528.4400
   72     3    80    1    117.9700   521.0800
   73     4    84    1    117.9700   521.0800
    1     5    10    1    140.6420   167.3600
    1     5    20    1    113.4881   167.3600
   10     5    20    1    104.9400   606.0900
   19     6    20    1    113.1500   572.8700
   19     6    40    1    124.3600   528.4400
   20     6    40    1    125.0900   523.5000
    1     7    21    1    120.4944   167.3600
    1     7    28    1    120.4944   167.3600
   21     7    28    1    115.8600   573.9600
    1     8    29    1    113.4881   167.3600
    1     8    30    1    140.6420   167.3600
   29     8    30    1    104.9400   606.0900
   29     9    31    1    113.1500   572.8700
   29     9    53    1    125.0900   523.5000
   31     9    53    1    124.3600   528.4400
    5    10    11    1    119.7200   586.9300
    5    10    19    1    119.7200   586.9300
   11    10    19    1    119.9700   562.1600
   10    11    12    1    120.0100   405.5100
   10    11    13    1    119.9700   562.1600
   12    11    13    1    120.0100   405.5100
   11    13    14    1    120.0100   405.5100
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11	13	15	1	119.9700	562.1600
14	13	15	1	120.0100	405.5100
13	15	16	1	120.0100	405.5100
13	15	17	1	119.9700	562.1600
16	15	17	1	120.0100	405.5100
15	17	18	1	120.0100	405.5100
15	17	19	1	119.9700	562.1600
18	17	19	1	120.0100	405.5100
6	19	10	1	118.3400	587.5200
6	19	17	1	118.3400	587.5200
10	19	17	1	119.9700	562.1600
5	20	6	1	112.0200	625.7600
5	20	21	1	123.0200	568.3500
6	20	21	1	123.4500	560.9100
7	21	20	1	122.6300	578.7300
7	21	22	1	122.6300	578.7300
20	21	22	1	120.1000	552.2000
21	22	23	1	120.0100	405.5100
21	22	24	1	119.9700	562.1600
23	22	24	1	120.0100	405.5100
22	24	25	1	120.0100	405.5100
22	24	26	1	119.9700	562.1600
25	24	26	1	120.0100	405.5100
24	26	27	1	120.0100	405.5100
24	26	28	1	119.9700	562.1600
27	26	28	1	120.0100	405.5100
7	28	26	1	122.6300	578.7300
7	28	29	1	118.0200	578.9800
26	28	29	1	120.1000	552.2000
8	29	9	1	112.0200	625.7600
8	29	28	1	123.0200	568.3500
9	29	28	1	123.4500	560.9100
8	30	31	1	119.7200	586.9300
8	30	38	1	119.7200	586.9300
31	30	38	1	119.9700	562.1600
9	31	30	1	118.3400	587.5200
9	31	32	1	118.3400	587.5200
30	31	32	1	119.9700	562.1600
31	32	33	1	120.0100	405.5100
31	32	34	1	119.9700	562.1600
33	32	34	1	120.0100	405.5100
32	34	35	1	120.0100	405.5100
32	34	36	1	119.9700	562.1600
35	34	36	1	120.0100	405.5100
34	36	37	1	120.0100	405.5100
34	36	38	1	119.9700	562.1600
37	36	38	1	120.0100	405.5100
30	38	36	1	119.9700	562.1600
30	38	39	1	120.0100	405.5100
36	38	39	1	120.0100	405.5100
6	40	41	1	109.4500	417.5600
6	40	42	1	109.4500	417.5600
6	40	43	1	112.8100	550.0300
41	40	42	1	109.5500	327.8600
41	40	43	1	110.0700	387.9400
42	40	43	1	110.0700	387.9400
40	43	44	1	110.0500	388.0200
40	43	45	1	110.0500	388.0200
40	43	46	1	110.6300	528.9400
44	43	45	1	108.3500	329.9500
44	43	46	1	110.0500	388.0200
45	43	46	1	110.0500	388.0200
43	46	47	1	110.0500	388.0200
43	46	48	1	110.0500	388.0200
43	46	49	1	110.6300	528.9400
47	46	48	1	108.3500	329.9500
47	46	49	1	110.0500	388.0200
48	46	49	1	110.0500	388.0200
46	49	50	1	110.0500	388.0200
46	49	51	1	110.0500	388.0200

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   9   53   54    1     109.4500   417.5600
   9   53   55    1     109.4500   417.5600
   9   53   56    1     112.8100   550.0300
  54   53   55    1     109.5500   327.8600
  54   53   56    1     110.0700   387.9400
  55   53   56    1     110.0700   387.9400
  53   56   57    1     110.0500   388.0200
  53   56   58    1     110.0500   388.0200
  53   56   59    1     110.6300   528.9400
  57   56   58    1     108.3500   329.9500
  57   56   59    1     110.0500   388.0200
  58   56   59    1     110.0500   388.0200
  56   59   60    1     110.0500   388.0200
  56   59   61    1     110.0500   388.0200
  56   59   62    1     110.6300   528.9400
  60   59   61    1     108.3500   329.9500
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  67   68   69    1     120.0500   551.4500
  67   68   74    1     120.0500   551.4500
  69   68   74    1     119.9700   562.1600
  68   69   70    1     120.0100   405.5100
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  70   69   71    1     120.0100   405.5100
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   4   73   74    1     119.2000   584.0000
  72   73   74    1     119.9700   562.1600
  68   74   73    1     119.9700   562.1600
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   3   80   82    1     108.8200   425.4300
   3   80   83    1     108.8200   425.4300
  81   80   82    1     109.5500   327.8600
  81   80   83    1     109.5500   327.8600
  82   80   83    1     109.5500   327.8600
   4   84   85    1     108.8200   425.4300
   4   84   86    1     108.8200   425.4300
   4   84   87    1     108.8200   425.4300
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  85   84   87    1     109.5500   327.8600
  86   84   87    1     109.5500   327.8600

[ dihedrals ]
;   ai     aj    ak    al funct          c0          c1          c2          c3          c4          c5
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8	1	5	20	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
66	1	5	10	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
66	1	5	20	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
5	1	7	21	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
5	1	7	28	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
8	1	7	21	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
8	1	7	28	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
66	1	7	21	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
66	1	7	28	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
5	1	8	29	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
5	1	8	30	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
7	1	8	29	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
7	1	8	30	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
66	1	8	29	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
66	1	8	30	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
5	1	66	67	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
7	1	66	67	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
8	1	66	67	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
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76	2	71	72	3	7.53120	0.00000	-7.53120	0.00000	0.00000	0.00000
71	2	76	77	3	1.60387	4.81160	0.00000	-6.41547	0.00000	0.00000
71	2	76	78	3	1.60387	4.81160	0.00000	-6.41547	0.00000	0.00000
71	2	76	79	3	1.60387	4.81160	0.00000	-6.41547	0.00000	0.00000
80	3	72	71	3	7.53120	0.00000	-7.53120	0.00000	0.00000	0.00000
80	3	72	73	3	7.53120	0.00000	-7.53120	0.00000	0.00000	0.00000
72	3	80	81	3	1.60387	4.81160	0.00000	-6.41547	0.00000	0.00000
72	3	80	82	3	1.60387	4.81160	0.00000	-6.41547	0.00000	0.00000
72	3	80	83	3	1.60387	4.81160	0.00000	-6.41547	0.00000	0.00000
84	4	73	72	3	7.53120	0.00000	-7.53120	0.00000	0.00000	0.00000
84	4	73	74	3	7.53120	0.00000	-7.53120	0.00000	0.00000	0.00000
73	4	84	85	3	1.60387	4.81160	0.00000	-6.41547	0.00000	0.00000
73	4	84	86	3	1.60387	4.81160	0.00000	-6.41547	0.00000	0.00000
73	4	84	87	3	1.60387	4.81160	0.00000	-6.41547	0.00000	0.00000
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1	5	10	19	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
20	5	10	11	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
20	5	10	19	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
1	5	20	6	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
1	5	20	21	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
10	5	20	6	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
10	5	20	21	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
20	6	19	10	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
20	6	19	17	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
40	6	19	10	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
40	6	19	17	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
19	6	20	5	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
19	6	20	21	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
40	6	20	5	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
40	6	20	21	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
19	6	40	41	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
19	6	40	42	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
19	6	40	43	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
20	6	40	41	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
20	6	40	42	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
20	6	40	43	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1	7	21	20	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
1	7	21	22	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
28	7	21	20	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
28	7	21	22	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
1	7	28	26	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
1	7	28	29	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
21	7	28	26	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
21	7	28	29	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
1	8	29	9	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
1	8	29	28	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
30	8	29	9	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
30	8	29	28	3	39.74800	0.00000	-39.74800	0.00000	0.00000	0.00000
1	8	30	31	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000

1	8	30	38	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
29	8	30	31	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
29	8	30	38	3	40.16640	0.00000	-40.16640	0.00000	0.00000	0.00000
31	9	29	8	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
31	9	29	28	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
53	9	29	8	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
53	9	29	28	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000
29	9	31	30	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
29	9	31	32	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
53	9	31	30	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
53	9	31	32	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
29	9	53	54	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
29	9	53	55	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
29	9	53	56	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
31	9	53	54	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
31	9	53	55	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
31	9	53	56	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
5	10	11	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
5	10	11	13	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
19	10	11	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
19	10	11	13	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
5	10	19	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
5	10	19	17	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
11	10	19	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
11	10	19	17	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
10	11	13	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
10	11	13	15	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
12	11	13	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
12	11	13	15	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
11	13	15	16	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
11	13	15	17	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
14	13	15	16	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
14	13	15	17	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
13	15	17	18	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
13	15	17	19	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
16	15	17	18	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
16	15	17	19	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
15	17	19	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
15	17	19	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
18	17	19	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
18	17	19	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
5	20	21	7	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000
5	20	21	22	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000
6	20	21	7	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000
6	20	21	22	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000
7	21	22	23	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
7	21	22	24	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
20	21	22	23	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
20	21	22	24	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
21	22	24	25	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
21	22	24	26	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
23	22	24	25	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
23	22	24	26	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
22	24	26	27	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
22	24	26	28	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
25	24	26	27	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
25	24	26	28	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
24	26	28	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
24	26	28	29	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
27	26	28	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
27	26	28	29	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
7	28	29	8	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000
7	28	29	9	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000
26	28	29	8	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000
26	28	29	9	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000
8	30	31	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
8	30	31	32	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
38	30	31	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
38	30	31	32	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
8	30	38	36	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000

8	30	38	39	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
31	30	38	36	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
31	30	38	39	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
9	31	32	33	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
9	31	32	34	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
30	31	32	33	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
30	31	32	34	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
31	32	34	35	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
31	32	34	36	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
33	32	34	35	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
33	32	34	36	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
32	34	36	37	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
32	34	36	38	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
35	34	36	37	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
35	34	36	38	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
34	36	38	30	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
34	36	38	39	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
37	36	38	30	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
37	36	38	39	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
6	40	43	44	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
6	40	43	45	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
6	40	43	46	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
41	40	43	44	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
41	40	43	45	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
41	40	43	46	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
42	40	43	44	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
42	40	43	45	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
42	40	43	46	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
40	43	46	47	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
40	43	46	48	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
40	43	46	49	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000
44	43	46	47	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000
44	43	46	48	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000
44	43	46	49	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000
45	43	46	47	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000
45	43	46	48	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000
45	43	46	49	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000
43	46	49	50	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000
43	46	49	51	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000
43	46	49	52	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000
47	46	49	50	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000
47	46	49	51	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000
47	46	49	52	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000
48	46	49	50	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000
48	46	49	51	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000
48	46	49	52	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000
9	53	56	57	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
9	53	56	58	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
9	53	56	59	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
54	53	56	57	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
54	53	56	58	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
54	53	56	59	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
55	53	56	57	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
55	53	56	58	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
55	53	56	59	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
53	56	59	60	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000
53	56	59	61	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000
53	56	59	62	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000
57	56	59	60	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000
57	56	59	61	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000
57	56	59	62	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000
58	56	59	60	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000
58	56	59	61	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000
58	56	59	62	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000
56	59	62	63	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000
56	59	62	64	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000
56	59	62	65	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000
60	59	62	63	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000
60	59	62	64	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000
60	59	62	65	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000

61	59	62	63	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000
61	59	62	64	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000
61	59	62	65	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000
1	66	67	68	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
66	67	68	69	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
66	67	68	74	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
67	68	69	70	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
67	68	69	71	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
74	68	69	70	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
74	68	69	71	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
67	68	74	73	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
67	68	74	75	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
69	68	74	73	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
69	68	74	75	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
68	69	71	2	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
68	69	71	72	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
70	69	71	2	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
70	69	71	72	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
2	71	72	3	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
2	71	72	73	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
69	71	72	3	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
69	71	72	73	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
3	72	73	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
3	72	73	74	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
71	72	73	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
71	72	73	74	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
4	73	74	68	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
4	73	74	75	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
72	73	74	68	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
72	73	74	75	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000

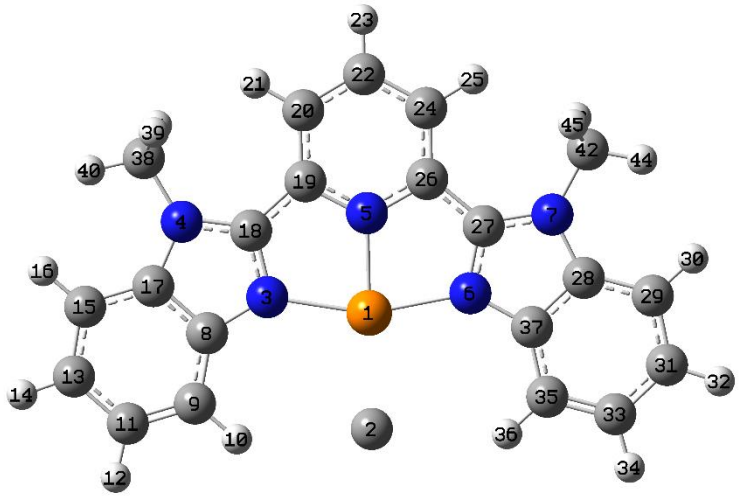
[dihedrals]

; ai	aj	ak	al	funct	c0	c1	c2	c3
2	71	72	69	1	180.00	4.60240	2	
3	72	73	71	1	180.00	4.60240	2	
4	73	74	72	1	180.00	4.60240	2	
5	10	19	11	1	180.00	4.60240	2	
5	20	6	21	1	180.00	4.60240	2	
6	19	17	10	1	180.00	4.60240	2	
7	21	20	22	1	180.00	4.60240	2	
7	28	29	26	1	180.00	4.60240	2	
8	29	9	28	1	180.00	4.60240	2	
8	30	38	31	1	180.00	4.60240	2	
9	31	32	30	1	180.00	4.60240	2	
10	13	11	12	1	180.00	4.60240	2	
11	15	13	14	1	180.00	4.60240	2	
13	17	15	16	1	180.00	4.60240	2	
15	19	17	18	1	180.00	4.60240	2	
20	6	19	40	1	180.00	4.60240	2	
21	24	22	23	1	180.00	4.60240	2	
22	26	24	25	1	180.00	4.60240	2	
24	28	26	27	1	180.00	4.60240	2	
29	9	31	53	1	180.00	4.60240	2	
30	36	38	39	1	180.00	4.60240	2	
31	34	32	33	1	180.00	4.60240	2	
32	36	34	35	1	180.00	4.60240	2	
34	38	36	37	1	180.00	4.60240	2	
67	68	74	69	1	180.00	4.60240	2	
68	71	69	70	1	180.00	4.60240	2	
68	73	74	75	1	180.00	4.60240	2	

[system]
; Name
PtB-a

[molecules]
; Compound #mols
PtB-a 1

Table S11. Force field parameters of PtB-b system in GROMACS format used in this work.



;PtB-b force field parameters

;PtB-b_GMX.top

```
[ defaults ]
; nbfunc        comb-rule       gen-pairs       fudgeLJ         fudgeQQ
1               2               yes             0.5             0.8333

[ atomtypes ]
; name      at.num  mass     charge ptype  sigma       epsilon
PTI_Pt      78    195.078    0.0000  A     3.3298e-01    1.0534e+01
PTI_cl      17    35.450     0.0000  A     3.47094e-01   1.10876e+00
PTI_nc       7    14.01      0.0000  A     3.25000e-01   7.11280e-01
PTI_na       7    14.01      0.0000  A     3.25000e-01   7.11280e-01
PTI_nb       7    14.01      0.0000  A     3.25000e-01   7.11280e-01
PTI_ca       6    12.01      0.0000  A     3.39967e-01   3.59824e-01
PTI_ha       1     1.008     0.0000  A     2.59964e-01   6.27600e-02
PTI_cd       6    12.01      0.0000  A     3.39967e-01   3.59824e-01
PTI_c3       6    12.01      0.0000  A     3.39967e-01   4.57730e-01
PTI_h1       1     1.008     0.0000  A     2.47135e-01   6.56888e-02

[ moleculetype ]
; Name            nrexcl
PtB-b             3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB     massB
; residue   1 PTI rtp PTI  q +1.0
     1     PTI_Pt      1    PTI    PT1      1    -0.201109   195.078   ; qtot -0.2011
     2     PTI_cl      1    PTI    CL1      2    -0.240282    35.45    ; qtot -0.4414
     3     PTI_nc      1    PTI     N1      3     0.044289    14.01    ; qtot -0.3971
     4     PTI_na      1    PTI     N2      4    -0.408906    14.01    ; qtot -0.806
     5     PTI_nb      1    PTI     N3      5    -0.04731     14.01    ; qtot -0.8533
     6     PTI_nc      1    PTI     N4      6     0.044289    14.01    ; qtot -0.809
     7     PTI_na      1    PTI     N5      7    -0.408906    14.01    ; qtot -1.218
     8     PTI_ca      1    PTI     C1      8     0.148116    12.01    ; qtot -1.07
     9     PTI_ca      1    PTI     C2      9    -0.217522    12.01    ; qtot -1.287
    10     PTI_ha      1    PTI     H1     10     0.1958       1.008    ; qtot -1.092
    11     PTI_ca      1    PTI     C3     11    -0.106842    12.01    ; qtot -1.198
    12     PTI_ha      1    PTI     H2     12     0.153899    1.008    ; qtot -1.044
    13     PTI_ca      1    PTI     C4     13    -0.076146    12.01    ; qtot -1.121
    14     PTI_ha      1    PTI     H3     14     0.151311    1.008    ; qtot -0.9693
    15     PTI_ca      1    PTI     C5     15    -0.280998    12.01    ; qtot -1.25
    16     PTI_ha      1    PTI     H4     16     0.184387    1.008    ; qtot -1.066
    17     PTI_ca      1    PTI     C6     17     0.250779    12.01    ; qtot -0.8152
    18     PTI_cd      1    PTI     C7     18     0.081892    12.01    ; qtot -0.7333
    19     PTI_ca      1    PTI     C8     19     0.250755    12.01    ; qtot -0.4825
    20     PTI_ca      1    PTI     C9     20    -0.277609    12.01    ; qtot -0.7601
    21     PTI_ha      1    PTI     H5     21     0.183021    1.008    ; qtot -0.5771
```

```
    22    PTI_ca     1    PTI    C10    22     0.006689     12.01   ; qtot -0.5704
    23    PTI_ha     1    PTI     H6    23     0.157288     1.008   ; qtot -0.4131
    24    PTI_ca     1    PTI    C11    24    -0.277609     12.01   ; qtot -0.6907
    25    PTI_ha     1    PTI     H7    25     0.183021     1.008   ; qtot -0.5077
    26    PTI_ca     1    PTI    C12    26     0.250755     12.01   ; qtot -0.2569
    27    PTI_cd     1    PTI    C13    27     0.081892     12.01   ; qtot -0.1751
    28    PTI_ca     1    PTI    C14    28     0.250779     12.01   ; qtot 0.07572
    29    PTI_ca     1    PTI    C15    29    -0.280998     12.01   ; qtot -0.2053
    30    PTI_ha     1    PTI     H8    30     0.184387     1.008   ; qtot -0.02089
    31    PTI_ca     1    PTI    C16    31    -0.076146     12.01   ; qtot -0.09703
    32    PTI_ha     1    PTI     H9    32     0.151311     1.008   ; qtot 0.05428
    33    PTI_ca     1    PTI    C17    33    -0.106842     12.01   ; qtot -0.05256
    34    PTI_ha     1    PTI    H10    34     0.153899     1.008   ; qtot 0.1013
    35    PTI_ca     1    PTI    C18    35    -0.217522     12.01   ; qtot -0.1162
    36    PTI_ha     1    PTI    H11    36     0.1958       1.008   ; qtot 0.07961
    37    PTI_ca     1    PTI    C19    37     0.148116     12.01   ; qtot 0.2277
    38    PTI_c3     1    PTI    C20    38     0.507137     12.01   ; qtot 0.7349
    39    PTI_h1     1    PTI    H12    39    -0.040334     1.008   ; qtot 0.6945
    40    PTI_h1     1    PTI    H13    40    -0.040334     1.008   ; qtot 0.6542
    41    PTI_h1     1    PTI    H14    41    -0.040334     1.008   ; qtot 0.6139
    42    PTI_c3     1    PTI    C21    42     0.507137     12.01   ; qtot 1.121
    43    PTI_h1     1    PTI    H15    43    -0.040334     1.008   ; qtot 1.081
    44    PTI_h1     1    PTI    H16    44    -0.040334     1.008   ; qtot 1.04
    45    PTI_h1     1    PTI    H17    45    -0.040334     1.008   ; qtot 1

[ bonds ]
;  ai    aj funct          c0          c1          c2          c3
    1     2     1          0.22925   131440.0
    1     3     1          0.20087   306270.0
    1     5     1          0.19043   306270.0
    1     6     1          0.20087   306270.0
    3     8     1          0.13360   412460.0
    3    18     1          0.13350   413880.0
    4    17     1          0.13500   393550.0
    4    18     1          0.13710   367190.0
    4    38     1          0.14560   280080.0
    5    19     1          0.13420   404260.0
    5    26     1          0.13420   404260.0
    6    27     1          0.13350   413880.0
    6    37     1          0.13360   412460.0
    7    27     1          0.13710   367190.0
    7    28     1          0.13500   393550.0
    7    42     1          0.14560   280080.0
    8     9     1          0.13870   400330.0
    8    17     1          0.13870   400330.0
    9    10     1          0.10870   288110.0
    9    11     1          0.13870   400330.0
   11    12     1          0.10870   288110.0
   11    13     1          0.13870   400330.0
   13    14     1          0.10870   288110.0
   13    15     1          0.13870   400330.0
   15    16     1          0.10870   288110.0
   15    17     1          0.13870   400330.0
   18    19     1          0.14340   344510.0
   19    20     1          0.13870   400330.0
   20    21     1          0.10870   288110.0
   20    22     1          0.13870   400330.0
   22    23     1          0.10870   288110.0
   22    24     1          0.13870   400330.0
   24    25     1          0.10870   288110.0
   24    26     1          0.13870   400330.0
   26    27     1          0.14340   344510.0
   28    29     1          0.13870   400330.0
   28    37     1          0.13870   400330.0
   29    30     1          0.10870   288110.0
   29    31     1          0.13870   400330.0
   31    32     1          0.10870   288110.0
   31    33     1          0.13870   400330.0
   33    34     1          0.10870   288110.0
   33    35     1          0.13870   400330.0
```

```
   35   36    1          0.10870   288110.0
   35   37    1          0.13870   400330.0
   38   39    1          0.10930   281080.0
   38   40    1          0.10930   281080.0
   38   41    1          0.10930   281080.0
   42   43    1          0.10930   281080.0
   42   44    1          0.10930   281080.0
   42   45    1          0.10930   281080.0

[ pairs ]
;  ai    aj funct          c0          c1          c2          c3
    1     4    1
    1     7    1
    1     9    1
    1    17    1
    1    20    1
    1    24    1
    1    28    1
    1    35    1
    2     8    1
    2    18    1
    2    19    1
    2    26    1
    2    27    1
    2    37    1
    3    10    1
    3    11    1
    3    15    1
    3    20    1
    3    26    1
    3    27    1
    3    37    1
    3    38    1
    4     5    1
    4     9    1
    4    13    1
    4    16    1
    4    20    1
    5     7    1
    5     8    1
    5    21    1
    5    22    1
    5    25    1
    5    37    1
    6     8    1
    6    18    1
    6    19    1
    6    24    1
    6    29    1
    6    33    1
    6    36    1
    6    42    1
    7    24    1
    7    30    1
    7    31    1
    7    35    1
    8    12    1
    8    13    1
    8    16    1
    8    19    1
    8    38    1
    9    14    1
    9    15    1
    9    18    1
   10    12    1
   10    13    1
   10    17    1
   11    16    1
   11    17    1
   12    14    1
```

```
  12   15    1
  14   16    1
  14   17    1
  15   18    1
  15   38    1
  17   19    1
  17   39    1
  17   40    1
  17   41    1
  18   21    1
  18   22    1
  18   26    1
  18   39    1
  18   40    1
  18   41    1
  19   23    1
  19   24    1
  19   27    1
  19   38    1
  20   25    1
  20   26    1
  21   23    1
  21   24    1
  22   27    1
  23   25    1
  23   26    1
  25   27    1
  26   28    1
  26   37    1
  26   42    1
  27   29    1
  27   35    1
  27   43    1
  27   44    1
  27   45    1
  28   32    1
  28   33    1
  28   36    1
  28   43    1
  28   44    1
  28   45    1
  29   34    1
  29   35    1
  29   42    1
  30   32    1
  30   33    1
  30   37    1
  31   36    1
  31   37    1
  32   34    1
  32   35    1
  34   36    1
  34   37    1
  37   42    1

[ angles ]
;  ai    aj    ak funct         c0          c1          c2          c3
    2     1     3     1       99.2792    962.3200
    2     1     5     1      180.000     962.3200
    2     1     6     1       99.2792    962.3200
    3     1     5     1       80.7208    351.4600
    3     1     6     1      161.4417    351.4600
    5     1     6     1       80.7208    351.4600
    1     3     8     1      141.3038    167.3600
    1     3    18     1      112.8504    167.3600
    8     3    18     1      104.2400    608.1000
   17     4    18     1      113.1500    572.8700
   17     4    38     1      124.3600    528.4400
   18     4    38     1      125.0900    523.5000
    1     5    19     1      121.2232    167.3600
```

1	5	26	1	121.2232	167.3600
19	5	26	1	115.8600	573.9600
1	6	27	1	112.8504	167.3600
1	6	37	1	141.3038	167.3600
27	6	37	1	104.2400	608.1000
27	7	28	1	113.1500	572.8700
27	7	42	1	125.0900	523.5000
28	7	42	1	124.3600	528.4400
3	8	9	1	119.7200	586.9300
3	8	17	1	119.7200	586.9300
9	8	17	1	119.9700	562.1600
8	9	10	1	120.0100	405.5100
8	9	11	1	119.9700	562.1600
10	9	11	1	120.0100	405.5100
9	11	12	1	120.0100	405.5100
9	11	13	1	119.9700	562.1600
12	11	13	1	120.0100	405.5100
11	13	14	1	120.0100	405.5100
11	13	15	1	119.9700	562.1600
14	13	15	1	120.0100	405.5100
13	15	16	1	120.0100	405.5100
13	15	17	1	119.9700	562.1600
16	15	17	1	120.0100	405.5100
4	17	8	1	118.3400	587.5200
4	17	15	1	118.3400	587.5200
8	17	15	1	119.9700	562.1600
3	18	4	1	112.0200	625.7600
3	18	19	1	115.0500	587.6800
4	18	19	1	123.4500	560.9100
5	19	18	1	117.5000	580.2400
5	19	20	1	122.6300	578.7300
18	19	20	1	120.1000	552.2000
19	20	21	1	120.0100	405.5100
19	20	22	1	119.9700	562.1600
21	20	22	1	120.0100	405.5100
20	22	23	1	120.0100	405.5100
20	22	24	1	119.9700	562.1600
23	22	24	1	120.0100	405.5100
22	24	25	1	120.0100	405.5100
22	24	26	1	119.9700	562.1600
25	24	26	1	120.0100	405.5100
5	26	24	1	122.6300	578.7300
5	26	27	1	117.5000	580.2400
24	26	27	1	120.1000	552.2000
6	27	7	1	112.0200	625.7600
6	27	26	1	115.0500	587.6800
7	27	26	1	123.4500	560.9100
7	28	29	1	118.3400	587.5200
7	28	37	1	118.3400	587.5200
29	28	37	1	119.9700	562.1600
28	29	30	1	120.0100	405.5100
28	29	31	1	119.9700	562.1600
30	29	31	1	120.0100	405.5100
29	31	32	1	120.0100	405.5100
29	31	33	1	119.9700	562.1600
32	31	33	1	120.0100	405.5100
31	33	34	1	120.0100	405.5100
31	33	35	1	119.9700	562.1600
34	33	35	1	120.0100	405.5100
33	35	36	1	120.0100	405.5100
33	35	37	1	119.9700	562.1600
36	35	37	1	120.0100	405.5100
6	37	28	1	119.7200	586.9300
6	37	35	1	119.7200	586.9300
28	37	35	1	119.9700	562.1600
4	38	39	1	109.4500	417.5600
4	38	40	1	109.4500	417.5600
4	38	41	1	109.4500	417.5600
39	38	40	1	109.5500	327.8600
39	38	41	1	109.5500	327.8600

```
  40   38   41    1      109.5500  327.8600
   7   42   43    1      109.4500  417.5600
   7   42   44    1      109.4500  417.5600
   7   42   45    1      109.4500  417.5600
  43   42   44    1      109.5500  327.8600
  43   42   45    1      109.5500  327.8600
  44   42   45    1      109.5500  327.8600

[ dihedrals ]
; ai   aj   ak   al funct       c0        c1        c2        c3        c4        c5
   2    1    3    8    3     0.69700   0.00000  -0.79600   0.00000   0.00000   0.00000
   2    1    3   18    3     0.69700   0.00000  -0.79600   0.00000   0.00000   0.00000
   5    1    3    8    3     0.69700   0.00000  -0.79600   0.00000   0.00000   0.00000
   5    1    3   18    3     0.69700   0.00000  -0.79600   0.00000   0.00000   0.00000
   6    1    3    8    3     0.69700   0.00000  -0.79600   0.00000   0.00000   0.00000
   6    1    3   18    3     0.69700   0.00000  -0.79600   0.00000   0.00000   0.00000
   2    1    5   19    3     0.69700   0.00000  -0.79600   0.00000   0.00000   0.00000
   2    1    5   26    3     0.69700   0.00000  -0.79600   0.00000   0.00000   0.00000
   3    1    5   19    3     0.69700   0.00000  -0.79600   0.00000   0.00000   0.00000
   3    1    5   26    3     0.69700   0.00000  -0.79600   0.00000   0.00000   0.00000
   6    1    5   19    3     0.69700   0.00000  -0.79600   0.00000   0.00000   0.00000
   6    1    5   26    3     0.69700   0.00000  -0.79600   0.00000   0.00000   0.00000
   2    1    6   27    3     0.69700   0.00000  -0.79600   0.00000   0.00000   0.00000
   2    1    6   37    3     0.69700   0.00000  -0.79600   0.00000   0.00000   0.00000
   3    1    6   27    3     0.69700   0.00000  -0.79600   0.00000   0.00000   0.00000
   3    1    6   37    3     0.69700   0.00000  -0.79600   0.00000   0.00000   0.00000
   5    1    6   27    3     0.69700   0.00000  -0.79600   0.00000   0.00000   0.00000
   5    1    6   37    3     0.69700   0.00000  -0.79600   0.00000   0.00000   0.00000
   1    3    8    9    3    39.74800   0.00000 -39.74800   0.00000   0.00000   0.00000
   1    3    8   17    3    39.74800   0.00000 -39.74800   0.00000   0.00000   0.00000
  18    3    8    9    3    40.16640   0.00000 -40.16640   0.00000   0.00000   0.00000
  18    3    8   17    3    40.16640   0.00000 -40.16640   0.00000   0.00000   0.00000
   1    3   18    4    3    39.74800   0.00000 -39.74800   0.00000   0.00000   0.00000
   1    3   18   19    3    39.74800   0.00000 -39.74800   0.00000   0.00000   0.00000
   8    3   18    4    3    39.74800   0.00000 -39.74800   0.00000   0.00000   0.00000
   8    3   18   19    3    39.74800   0.00000 -39.74800   0.00000   0.00000   0.00000
  18    4   17    8    3     2.51040   0.00000  -2.51040   0.00000   0.00000   0.00000
  18    4   17   15    3     2.51040   0.00000  -2.51040   0.00000   0.00000   0.00000
  38    4   17    8    3     2.51040   0.00000  -2.51040   0.00000   0.00000   0.00000
  38    4   17   15    3     2.51040   0.00000  -2.51040   0.00000   0.00000   0.00000
  17    4   18    3    3    14.22560   0.00000 -14.22560   0.00000   0.00000   0.00000
  17    4   18   19    3    14.22560   0.00000 -14.22560   0.00000   0.00000   0.00000
  38    4   18    3    3    14.22560   0.00000 -14.22560   0.00000   0.00000   0.00000
  38    4   18   19    3    14.22560   0.00000 -14.22560   0.00000   0.00000   0.00000
  17    4   38   39    3     0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
  17    4   38   40    3     0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
  17    4   38   41    3     0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
  18    4   38   39    3     0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
  18    4   38   40    3     0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
  18    4   38   41    3     0.00000   0.00000   0.00000   0.00000   0.00000   0.00000
   1    5   19   18    3    39.74800   0.00000 -39.74800   0.00000   0.00000   0.00000
   1    5   19   20    3    39.74800   0.00000 -39.74800   0.00000   0.00000   0.00000
  26    5   19   18    3    40.16640   0.00000 -40.16640   0.00000   0.00000   0.00000
  26    5   19   20    3    40.16640   0.00000 -40.16640   0.00000   0.00000   0.00000
   1    5   26   24    3    39.74800   0.00000 -39.74800   0.00000   0.00000   0.00000
   1    5   26   27    3    39.74800   0.00000 -39.74800   0.00000   0.00000   0.00000
  19    5   26   24    3    40.16640   0.00000 -40.16640   0.00000   0.00000   0.00000
  19    5   26   27    3    40.16640   0.00000 -40.16640   0.00000   0.00000   0.00000
   1    6   27    7    3    39.74800   0.00000 -39.74800   0.00000   0.00000   0.00000
   1    6   27   26    3    39.74800   0.00000 -39.74800   0.00000   0.00000   0.00000
  37    6   27    7    3    39.74800   0.00000 -39.74800   0.00000   0.00000   0.00000
  37    6   27   26    3    39.74800   0.00000 -39.74800   0.00000   0.00000   0.00000
   1    6   37   28    3    39.74800   0.00000 -39.74800   0.00000   0.00000   0.00000
   1    6   37   35    3    39.74800   0.00000 -39.74800   0.00000   0.00000   0.00000
  27    6   37   28    3    40.16640   0.00000 -40.16640   0.00000   0.00000   0.00000
  27    6   37   35    3    40.16640   0.00000 -40.16640   0.00000   0.00000   0.00000
  28    7   27    6    3    14.22560   0.00000 -14.22560   0.00000   0.00000   0.00000
  28    7   27   26    3    14.22560   0.00000 -14.22560   0.00000   0.00000   0.00000
  42    7   27    6    3    14.22560   0.00000 -14.22560   0.00000   0.00000   0.00000
  42    7   27   26    3    14.22560   0.00000 -14.22560   0.00000   0.00000   0.00000
```

27	7	28	29	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
27	7	28	37	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
42	7	28	29	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
42	7	28	37	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
27	7	42	43	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
27	7	42	44	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
27	7	42	45	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
28	7	42	43	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
28	7	42	44	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
28	7	42	45	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
3	8	9	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
3	8	9	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
17	8	9	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
17	8	9	11	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
3	8	17	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
3	8	17	15	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
9	8	17	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
9	8	17	15	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
8	9	11	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
8	9	11	13	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
10	9	11	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
10	9	11	13	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
9	11	13	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
9	11	13	15	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
12	11	13	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
12	11	13	15	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
11	13	15	16	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
11	13	15	17	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
14	13	15	16	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
14	13	15	17	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
13	15	17	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
13	15	17	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
16	15	17	4	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
16	15	17	8	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
3	18	19	5	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000
3	18	19	20	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000
4	18	19	5	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000
4	18	19	20	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000
5	19	20	21	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
5	19	20	22	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
18	19	20	21	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
18	19	20	22	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
19	20	22	23	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
19	20	22	24	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
21	20	22	23	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
21	20	22	24	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
20	22	24	25	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
20	22	24	26	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
23	22	24	25	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
23	22	24	26	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
22	24	26	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
22	24	26	27	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
25	24	26	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
25	24	26	27	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
5	26	27	6	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000
5	26	27	7	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000
24	26	27	6	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000
24	26	27	7	3	21.33840	0.00000	-21.33840	0.00000	0.00000	0.00000
7	28	29	30	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
7	28	29	31	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
37	28	29	30	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
37	28	29	31	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
7	28	37	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
7	28	37	35	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
29	28	37	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
29	28	37	35	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
28	29	31	32	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
28	29	31	33	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
30	29	31	32	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
30	29	31	33	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000

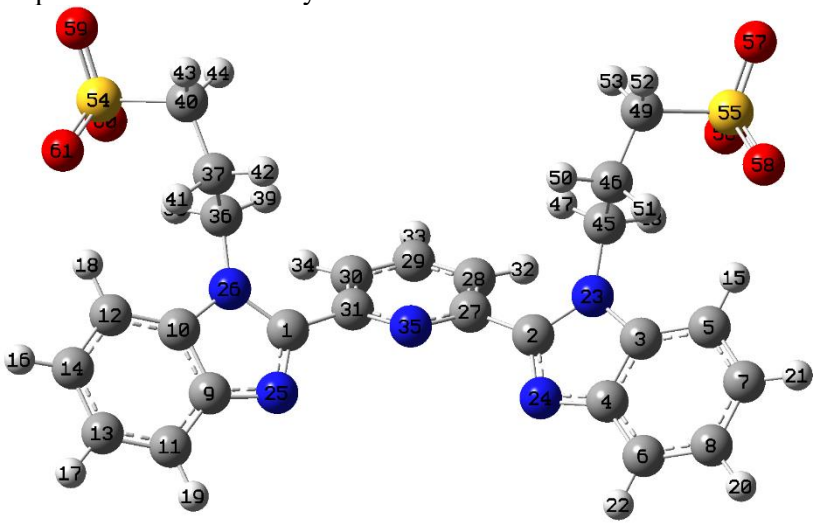
```
   29   31   33   34    3       30.33400     0.00000    -30.33400     0.00000     0.00000     0.00000
   29   31   33   35    3       30.33400     0.00000    -30.33400     0.00000     0.00000     0.00000
   32   31   33   34    3       30.33400     0.00000    -30.33400     0.00000     0.00000     0.00000
   32   31   33   35    3       30.33400     0.00000    -30.33400     0.00000     0.00000     0.00000
   31   33   35   36    3       30.33400     0.00000    -30.33400     0.00000     0.00000     0.00000
   31   33   35   37    3       30.33400     0.00000    -30.33400     0.00000     0.00000     0.00000
   34   33   35   36    3       30.33400     0.00000    -30.33400     0.00000     0.00000     0.00000
   34   33   35   37    3       30.33400     0.00000    -30.33400     0.00000     0.00000     0.00000
   33   35   37    6    3       30.33400     0.00000    -30.33400     0.00000     0.00000     0.00000
   33   35   37   28    3       30.33400     0.00000    -30.33400     0.00000     0.00000     0.00000
   36   35   37    6    3       30.33400     0.00000    -30.33400     0.00000     0.00000     0.00000
   36   35   37   28    3       30.33400     0.00000    -30.33400     0.00000     0.00000     0.00000

[ dihedrals ]
;  ai    aj    ak    al funct         c0         c1         c2         c3
    3     8    17     9     1       180.00     4.60240    2
    3    18     4    19     1       180.00     4.60240    2
    4    17    15     8     1       180.00     4.60240    2
    5    19    18    20     1       180.00     4.60240    2
    5    26    27    24     1       180.00     4.60240    2
    6    27     7    26     1       180.00     4.60240    2
    6    37    35    28     1       180.00     4.60240    2
    7    28    37    29     1       180.00     4.60240    2
    8    11     9    10     1       180.00     4.60240    2
    9    13    11    12     1       180.00     4.60240    2
   11    15    13    14     1       180.00     4.60240    2
   13    17    15    16     1       180.00     4.60240    2
   18     4    17    38     1       180.00     4.60240    2
   19    22    20    21     1       180.00     4.60240    2
   20    24    22    23     1       180.00     4.60240    2
   22    26    24    25     1       180.00     4.60240    2
   27     7    28    42     1       180.00     4.60240    2
   28    31    29    30     1       180.00     4.60240    2
   29    33    31    32     1       180.00     4.60240    2
   31    35    33    34     1       180.00     4.60240    2
   33    37    35    36     1       180.00     4.60240    2

[ system ]
; Name
PtB-b

[ molecules ]
; Compound        #mols
   PtB-b             1
```

Table S12. Force field parameters of Pt-free system in GROMACS format used in this work.



Pt-free force field parameters
;Pt-free_GMX.top

```
[ defaults ]
; nbfunc        comb-rule       gen-pairs       fudgeLJ       fudgeQQ
      1               2             yes           0.5          0.8333

[ atomtypes ]
;name   bond_type     mass     charge   ptype   sigma         epsilon       Amb
 cc       cc          0.00000  0.00000   A     3.39967e-01   3.59824e-01 ; 1.91  0.0860
 ca       ca          0.00000  0.00000   A     3.39967e-01   3.59824e-01 ; 1.91  0.0860
 ha       ha          0.00000  0.00000   A     2.59964e-01   6.27600e-02 ; 1.46  0.0150
 na       na          0.00000  0.00000   A     3.25000e-01   7.11280e-01 ; 1.82  0.1700
 nd       nd          0.00000  0.00000   A     3.25000e-01   7.11280e-01 ; 1.82  0.1700
 nb       nb          0.00000  0.00000   A     3.25000e-01   7.11280e-01 ; 1.82  0.1700
 c3       c3          0.00000  0.00000   A     3.39967e-01   4.57730e-01 ; 1.91  0.1094
 h1       h1          0.00000  0.00000   A     2.47135e-01   6.56888e-02 ; 1.39  0.0157
 hc       hc          0.00000  0.00000   A     2.64953e-01   6.56888e-02 ; 1.49  0.0157
 s6       s6          0.00000  0.00000   A     3.56359e-01   1.04600e+00 ; 2.00  0.2500
  o        o          0.00000  0.00000   A     2.95992e-01   8.78640e-01 ; 1.66  0.2100

[ moleculetype ]
;name            nrexcl
 PtF              3

[ atoms ]
;   nr  type  resi  res  atom  cgnr     charge       mass       ; qtot   bond_type
     1    cc     1   PtF    C1     1     0.283166     12.01000 ; qtot 0.283
     2    cc     1   PtF    C2     2     0.283166     12.01000 ; qtot 0.566
     3    ca     1   PtF    C3     3     0.010862     12.01000 ; qtot 0.577
     4    ca     1   PtF    C4     4     0.474664     12.01000 ; qtot 1.052
     5    ca     1   PtF    C5     5    -0.166976     12.01000 ; qtot 0.885
     6    ca     1   PtF    C6     6    -0.329791     12.01000 ; qtot 0.555
     7    ca     1   PtF    C7     7    -0.181568     12.01000 ; qtot 0.374
     8    ca     1   PtF    C8     8    -0.147237     12.01000 ; qtot 0.226
     9    ca     1   PtF    C9     9     0.474664     12.01000 ; qtot 0.701
    10    ca     1   PtF   C10    10     0.010862     12.01000 ; qtot 0.712
    11    ca     1   PtF   C11    11    -0.329791     12.01000 ; qtot 0.382
    12    ca     1   PtF   C12    12    -0.166976     12.01000 ; qtot 0.215
    13    ca     1   PtF   C13    13    -0.147237     12.01000 ; qtot 0.068
    14    ca     1   PtF   C14    14    -0.181568     12.01000 ; qtot -0.114
    15    ha     1   PtF    H1    15     0.194165      1.00800 ; qtot 0.080
    16    ha     1   PtF    H2    16     0.116815      1.00800 ; qtot 0.197
    17    ha     1   PtF    H3    17     0.099511      1.00800 ; qtot 0.297
    18    ha     1   PtF    H4    18     0.194165      1.00800 ; qtot 0.491
    19    ha     1   PtF    H5    19     0.151666      1.00800 ; qtot 0.643
    20    ha     1   PtF    H6    20     0.099511      1.00800 ; qtot 0.742
    21    ha     1   PtF    H7    21     0.116815      1.00800 ; qtot 0.859
    22    ha     1   PtF    H8    22     0.151666      1.00800 ; qtot 1.011
```

```
    23   na    1   PtF    N1   23    -0.170932    14.01000 ; qtot 0.840
    24   nd    1   PtF    N2   24    -0.639284    14.01000 ; qtot 0.200
    25   nd    1   PtF    N3   25    -0.639284    14.01000 ; qtot -0.439
    26   na    1   PtF    N4   26    -0.170932    14.01000 ; qtot -0.610
    27   ca    1   PtF   C15   27     0.469989    12.01000 ; qtot -0.140
    28   ca    1   PtF   C16   28    -0.378064    12.01000 ; qtot -0.518
    29   ca    1   PtF   C17   29     0.085623    12.01000 ; qtot -0.432
    30   ca    1   PtF   C18   30    -0.378064    12.01000 ; qtot -0.810
    31   ca    1   PtF   C19   31     0.469989    12.01000 ; qtot -0.340
    32   ha    1   PtF    H9   32     0.141193     1.00800 ; qtot -0.199
    33   ha    1   PtF   H10   33     0.085033     1.00800 ; qtot -0.114
    34   ha    1   PtF   H11   34     0.141193     1.00800 ; qtot 0.027
    35   nb    1   PtF    N5   35    -0.544791    14.01000 ; qtot -0.518
    36   c3    1   PtF   C20   36     0.026149    12.01000 ; qtot -0.492
    37   c3    1   PtF   C21   37    -0.041801    12.01000 ; qtot -0.533
    38   h1    1   PtF   H12   38     0.058539     1.00800 ; qtot -0.475
    39   h1    1   PtF   H13   39     0.058539     1.00800 ; qtot -0.416
    40   c3    1   PtF   C22   40    -0.100808    12.01000 ; qtot -0.517
    41   hc    1   PtF   H14   41     0.037303     1.00800 ; qtot -0.480
    42   hc    1   PtF   H15   42     0.037303     1.00800 ; qtot -0.443
    43   h1    1   PtF   H16   43     0.015993     1.00800 ; qtot -0.427
    44   h1    1   PtF   H17   44     0.015993     1.00800 ; qtot -0.411
    45   c3    1   PtF   C23   45     0.026149    12.01000 ; qtot -0.384
    46   c3    1   PtF   C24   46    -0.041801    12.01000 ; qtot -0.426
    47   h1    1   PtF   H18   47     0.058539     1.00800 ; qtot -0.368
    48   h1    1   PtF   H19   48     0.058539     1.00800 ; qtot -0.309
    49   c3    1   PtF   C25   49    -0.100808    12.01000 ; qtot -0.410
    50   hc    1   PtF   H20   50     0.037303     1.00800 ; qtot -0.373
    51   hc    1   PtF   H21   51     0.037303     1.00800 ; qtot -0.335
    52   h1    1   PtF   H22   52     0.015993     1.00800 ; qtot -0.319
    53   h1    1   PtF   H23   53     0.015993     1.00800 ; qtot -0.303
    54   s6    1   PtF    S1   54     1.060675    32.06000 ; qtot 0.757
    55   s6    1   PtF    S2   55     1.060675    32.06000 ; qtot 1.818
    56    o    1   PtF    O1   56    -0.636333    16.00000 ; qtot 1.182
    57    o    1   PtF    O2   57    -0.636333    16.00000 ; qtot 0.545
    58    o    1   PtF    O3   58    -0.636333    16.00000 ; qtot -0.091
    59    o    1   PtF    O4   59    -0.636333    16.00000 ; qtot -0.727
    60    o    1   PtF    O5   60    -0.636333    16.00000 ; qtot -1.364
    61    o    1   PtF    O6   61    -0.636333    16.00000 ; qtot -2.000
[ bonds ]
;   ai    aj funct   r             k
     1    25   1    1.3172e-01   4.3965e+05
     1    26   1    1.3802e-01   3.5631e+05
     1    31   1    1.4555e-01   3.2225e+05
     2    23   1    1.3802e-01   3.5631e+05
     2    24   1    1.3172e-01   4.3965e+05
     2    27   1    1.4555e-01   3.2225e+05
     3     4   1    1.3984e-01   3.8585e+05
     3     5   1    1.3984e-01   3.8585e+05
     3    23   1    1.3840e-01   3.5187e+05
     4     6   1    1.3984e-01   3.8585e+05
     4    24   1    1.3517e-01   3.9137e+05
     5     7   1    1.3984e-01   3.8585e+05
     5    15   1    1.0860e-01   2.8937e+05
     6     8   1    1.3984e-01   3.8585e+05
     6    22   1    1.0860e-01   2.8937e+05
     7     8   1    1.3984e-01   3.8585e+05
     7    21   1    1.0860e-01   2.8937e+05
     8    20   1    1.0860e-01   2.8937e+05
     9    10   1    1.3984e-01   3.8585e+05
     9    11   1    1.3984e-01   3.8585e+05
     9    25   1    1.3517e-01   3.9137e+05
    10    12   1    1.3984e-01   3.8585e+05
    10    26   1    1.3840e-01   3.5187e+05
    11    13   1    1.3984e-01   3.8585e+05
    11    19   1    1.0860e-01   2.8937e+05
    12    14   1    1.3984e-01   3.8585e+05
    12    18   1    1.0860e-01   2.8937e+05
    13    14   1    1.3984e-01   3.8585e+05
    13    17   1    1.0860e-01   2.8937e+05
    14    16   1    1.0860e-01   2.8937e+05
    23    45   1    1.4629e-01   2.7422e+05
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    26    36   1    1.4629e-01    2.7422e+05
    27    28   1    1.3984e-01    3.8585e+05
    27    35   1    1.3390e-01    4.0836e+05
    28    29   1    1.3984e-01    3.8585e+05
    28    32   1    1.0860e-01    2.8937e+05
    29    30   1    1.3984e-01    3.8585e+05
    29    33   1    1.0860e-01    2.8937e+05
    30    31   1    1.3984e-01    3.8585e+05
    30    34   1    1.0860e-01    2.8937e+05
    31    35   1    1.3390e-01    4.0836e+05
    36    37   1    1.5375e-01    2.5179e+05
    36    38   1    1.0969e-01    2.7665e+05
    36    39   1    1.0969e-01    2.7665e+05
    37    40   1    1.5375e-01    2.5179e+05
    37    41   1    1.0969e-01    2.7665e+05
    37    42   1    1.0969e-01    2.7665e+05
    40    43   1    1.0969e-01    2.7665e+05
    40    44   1    1.0969e-01    2.7665e+05
    40    54   1    1.8075e-01    1.9539e+05
    45    46   1    1.5375e-01    2.5179e+05
    45    47   1    1.0969e-01    2.7665e+05
    45    48   1    1.0969e-01    2.7665e+05
    46    49   1    1.5375e-01    2.5179e+05
    46    50   1    1.0969e-01    2.7665e+05
    46    51   1    1.0969e-01    2.7665e+05
    49    52   1    1.0969e-01    2.7665e+05
    49    53   1    1.0969e-01    2.7665e+05
    49    55   1    1.8075e-01    1.9539e+05
    54    59   1    1.4533e-01    4.2903e+05
    54    60   1    1.4533e-01    4.2903e+05
    54    61   1    1.4533e-01    4.2903e+05
    55    56   1    1.4533e-01    4.2903e+05
    55    57   1    1.4533e-01    4.2903e+05
    55    58   1    1.4533e-01    4.2903e+05

[ pairs ]
;   ai    aj    funct
     1    11     1
     1    12     1
     1    27     1
     1    29     1
     1    34     1
     1    37     1
     1    38     1
     1    39     1
     2     5     1
     2     6     1
     2    29     1
     2    31     1
     2    32     1
     2    46     1
     2    47     1
     2    48     1
     3     8     1
     3    21     1
     3    22     1
     3    27     1
     3    46     1
     3    47     1
     3    48     1
     4     7     1
     4    15     1
     4    20     1
     4    27     1
     4    45     1
     5     6     1
     5    20     1
     5    24     1
     5    45     1
     6    21     1
     6    23     1
     7    22     1
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7	23	1
8	15	1
8	24	1
9	14	1
9	17	1
9	18	1
9	36	1
10	13	1
10	16	1
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27	33	1
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34	35	1
36	43	1
36	44	1
36	54	1
37	59	1
37	60	1
37	61	1
38	40	1
38	41	1

```
    38    42     1
    39    40     1
    39    41     1
    39    42     1
    41    43     1
    41    44     1
    41    54     1
    42    43     1
    42    44     1
    42    54     1
    43    59     1
    43    60     1
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    44    59     1
    44    60     1
    44    61     1
    45    52     1
    45    53     1
    45    55     1
    46    56     1
    46    57     1
    46    58     1
    47    49     1
    47    50     1
    47    51     1
    48    49     1
    48    50     1
    48    51     1
    50    52     1
    50    53     1
    50    55     1
    51    52     1
    51    53     1
    51    55     1
    52    56     1
    52    57     1
    52    58     1
    53    56     1
    53    57     1
    53    58     1

[ angles ]
;   ai    aj    ak    funct   theta         cth
     1    25     9     1   1.0488e+02   6.0651e+02
     1    26    10     1   1.1315e+02   5.6400e+02
     1    26    36     1   1.2646e+02   5.1781e+02
     1    31    30     1   1.2079e+02   5.4409e+02
     1    31    35     1   1.1775e+02   5.7505e+02
     2    23     3     1   1.1315e+02   5.6400e+02
     2    23    45     1   1.2646e+02   5.1781e+02
     2    24     4     1   1.0488e+02   6.0651e+02
     2    27    28     1   1.2079e+02   5.4409e+02
     2    27    35     1   1.1775e+02   5.7505e+02
     3     4     6     1   1.2002e+02   5.5748e+02
     3     4    24     1   1.1972e+02   5.8124e+02
     3     5     7     1   1.2002e+02   5.5748e+02
     3     5    15     1   1.1988e+02   4.0317e+02
     3    23    45     1   1.2436e+02   5.2149e+02
     4     3     5     1   1.2002e+02   5.5748e+02
     4     3    23     1   1.1834e+02   5.7806e+02
     4     6     8     1   1.2002e+02   5.5748e+02
     4     6    22     1   1.1988e+02   4.0317e+02
     5     3    23     1   1.1834e+02   5.7806e+02
     5     7     8     1   1.2002e+02   5.5748e+02
     5     7    21     1   1.1988e+02   4.0317e+02
     6     4    24     1   1.1972e+02   5.8124e+02
     6     8     7     1   1.2002e+02   5.5748e+02
     6     8    20     1   1.1988e+02   4.0317e+02
     7     5    15     1   1.1988e+02   4.0317e+02
     7     8    20     1   1.1988e+02   4.0317e+02
     8     6    22     1   1.1988e+02   4.0317e+02
     8     7    21     1   1.1988e+02   4.0317e+02
```

9	10	12	1	1.2002e+02	5.5748e+02
9	10	26	1	1.1834e+02	5.7806e+02
9	11	13	1	1.2002e+02	5.5748e+02
9	11	19	1	1.1988e+02	4.0317e+02
10	9	11	1	1.2002e+02	5.5748e+02
10	9	25	1	1.1972e+02	5.8124e+02
10	12	14	1	1.2002e+02	5.5748e+02
10	12	18	1	1.1988e+02	4.0317e+02
10	26	36	1	1.2436e+02	5.2149e+02
11	9	25	1	1.1972e+02	5.8124e+02
11	13	14	1	1.2002e+02	5.5748e+02
11	13	17	1	1.1988e+02	4.0317e+02
12	10	26	1	1.1834e+02	5.7806e+02
12	14	13	1	1.2002e+02	5.5748e+02
12	14	16	1	1.1988e+02	4.0317e+02
13	11	19	1	1.1988e+02	4.0317e+02
13	14	16	1	1.1988e+02	4.0317e+02
14	12	18	1	1.1988e+02	4.0317e+02
14	13	17	1	1.1988e+02	4.0317e+02
23	2	24	1	1.1222e+02	6.2676e+02
23	2	27	1	1.2345e+02	5.5463e+02
23	45	46	1	1.1288e+02	5.4827e+02
23	45	47	1	1.0878e+02	4.1698e+02
23	45	48	1	1.0878e+02	4.1698e+02
24	2	27	1	1.2324e+02	5.6568e+02
25	1	26	1	1.1222e+02	6.2676e+02
25	1	31	1	1.2324e+02	5.6568e+02
26	1	31	1	1.2345e+02	5.5463e+02
26	36	37	1	1.1288e+02	5.4827e+02
26	36	38	1	1.0878e+02	4.1698e+02
26	36	39	1	1.0878e+02	4.1698e+02
27	28	29	1	1.2002e+02	5.5748e+02
27	28	32	1	1.1988e+02	4.0317e+02
27	35	31	1	1.1722e+02	5.7195e+02
28	27	35	1	1.2294e+02	5.7597e+02
28	29	30	1	1.2002e+02	5.5748e+02
28	29	33	1	1.1988e+02	4.0317e+02
29	28	32	1	1.1988e+02	4.0317e+02
29	30	31	1	1.2002e+02	5.5748e+02
29	30	34	1	1.1988e+02	4.0317e+02
30	29	33	1	1.1988e+02	4.0317e+02
30	31	35	1	1.2294e+02	5.7597e+02
31	30	34	1	1.1988e+02	4.0317e+02
36	37	40	1	1.1151e+02	5.2601e+02
36	37	41	1	1.0980e+02	3.8777e+02
36	37	42	1	1.0980e+02	3.8777e+02
37	36	38	1	1.0956e+02	3.8819e+02
37	36	39	1	1.0956e+02	3.8819e+02
37	40	43	1	1.0956e+02	3.8819e+02
37	40	44	1	1.0956e+02	3.8819e+02
37	40	54	1	1.1022e+02	5.1940e+02
38	36	39	1	1.0846e+02	3.2836e+02
40	37	41	1	1.0980e+02	3.8777e+02
40	37	42	1	1.0980e+02	3.8777e+02
40	54	59	1	1.0861e+02	5.4702e+02
40	54	60	1	1.0861e+02	5.4702e+02
40	54	61	1	1.0861e+02	5.4702e+02
41	37	42	1	1.0758e+02	3.2970e+02
43	40	44	1	1.0846e+02	3.2836e+02
43	40	54	1	1.0715e+02	3.6141e+02
44	40	54	1	1.0715e+02	3.6141e+02
45	46	49	1	1.1151e+02	5.2601e+02
45	46	50	1	1.0980e+02	3.8777e+02
45	46	51	1	1.0980e+02	3.8777e+02
46	45	47	1	1.0956e+02	3.8819e+02
46	45	48	1	1.0956e+02	3.8819e+02
46	49	52	1	1.0956e+02	3.8819e+02
46	49	53	1	1.0956e+02	3.8819e+02
46	49	55	1	1.1022e+02	5.1940e+02
47	45	48	1	1.0846e+02	3.2836e+02
49	46	50	1	1.0980e+02	3.8777e+02
49	46	51	1	1.0980e+02	3.8777e+02

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   49    55    57     1   1.0861e+02   5.4702e+02
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   50    46    51     1   1.0758e+02   3.2970e+02
   52    49    53     1   1.0846e+02   3.2836e+02
   52    49    55     1   1.0715e+02   3.6141e+02
   53    49    55     1   1.0715e+02   3.6141e+02
   56    55    57     1   1.2005e+02   6.1580e+02
   56    55    58     1   1.2005e+02   6.1580e+02
   57    55    58     1   1.2005e+02   6.1580e+02
   59    54    60     1   1.2005e+02   6.1580e+02
   59    54    61     1   1.2005e+02   6.1580e+02
   60    54    61     1   1.2005e+02   6.1580e+02

[ 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    25     9    10     3   40.16640  0.00000  -40.16640  0.00000  0.00000  0.00000
     1    25     9    11     3   40.16640  0.00000  -40.16640  0.00000  0.00000  0.00000
     1    26    10     9     3    2.51040  0.00000   -2.51040  0.00000  0.00000  0.00000
     1    26    10    12     3    2.51040  0.00000   -2.51040  0.00000  0.00000  0.00000
     1    26    36    37     3    0.00000  0.00000    0.00000  0.00000  0.00000  0.00000
     1    26    36    38     3    0.00000  0.00000    0.00000  0.00000  0.00000  0.00000
     1    26    36    39     3    0.00000  0.00000    0.00000  0.00000  0.00000  0.00000
     1    31    30    29     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     1    31    30    34     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     1    31    35    27     3   40.16640  0.00000  -40.16640  0.00000  0.00000  0.00000
     2    23     3     4     3    2.51040  0.00000   -2.51040  0.00000  0.00000  0.00000
     2    23     3     5     3    2.51040  0.00000   -2.51040  0.00000  0.00000  0.00000
     2    23    45    46     3    0.00000  0.00000    0.00000  0.00000  0.00000  0.00000
     2    23    45    47     3    0.00000  0.00000    0.00000  0.00000  0.00000  0.00000
     2    23    45    48     3    0.00000  0.00000    0.00000  0.00000  0.00000  0.00000
     2    24     4     3     3   40.16640  0.00000  -40.16640  0.00000  0.00000  0.00000
     2    24     4     6     3   40.16640  0.00000  -40.16640  0.00000  0.00000  0.00000
     2    27    28    29     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     2    27    28    32     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     2    27    35    31     3   40.16640  0.00000  -40.16640  0.00000  0.00000  0.00000
     3     4     6     8     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     3     4     6    22     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     3     5     7     8     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     3     5     7    21     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     3    23     2    24     3   14.22560  0.00000  -14.22560  0.00000  0.00000  0.00000
     3    23     2    27     3   14.22560  0.00000  -14.22560  0.00000  0.00000  0.00000
     3    23    45    46     3    0.00000  0.00000    0.00000  0.00000  0.00000  0.00000
     3    23    45    47     3    0.00000  0.00000    0.00000  0.00000  0.00000  0.00000
     3    23    45    48     3    0.00000  0.00000    0.00000  0.00000  0.00000  0.00000
     4     3     5     7     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     4     3     5    15     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     4     3    23    45     3    2.51040  0.00000   -2.51040  0.00000  0.00000  0.00000
     4     6     8     7     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     4     6     8    20     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     4    24     2    23     3   39.74800  0.00000  -39.74800  0.00000  0.00000  0.00000
     4    24     2    27     3   39.74800  0.00000  -39.74800  0.00000  0.00000  0.00000
     5     3     4     6     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     5     3     4    24     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     5     3    23    45     3    2.51040  0.00000   -2.51040  0.00000  0.00000  0.00000
     5     7     8     6     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     5     7     8    20     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     6     4     3    23     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     6     8     7    21     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     7     5     3    23     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     7     8     6    22     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     8     6     4    24     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     8     7     5    15     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     9    10    12    14     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     9    10    12    18     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     9    10    26    36     3    2.51040  0.00000   -2.51040  0.00000  0.00000  0.00000
     9    11    13    14     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
     9    11    13    17     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
    10     9    11    13     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
    10     9    11    19     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
    10    12    14    13     3   30.33400  0.00000  -30.33400  0.00000  0.00000  0.00000
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10	26	36	37	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
10	26	36	38	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
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11	13	14	12	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
11	13	14	16	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
12	10	9	25	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
12	10	26	36	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000
12	14	13	17	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
13	11	9	25	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
13	14	12	18	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
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20	8	7	21	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000
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26	1	31	30	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000
26	1	31	35	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000
26	36	37	40	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
26	36	37	41	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
26	36	37	42	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
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36	37	40	44	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
36	37	40	54	3	0.65084	1.95253	0.00000	-2.60338	0.00000	0.00000
37	40	54	59	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
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37	40	54	61	3	0.60436	1.81307	0.00000	-2.41742	0.00000	0.00000
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   43    40    54    59     3   0.60436   1.81307   0.00000  -2.41742   0.00000   0.00000
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   45    46    49    52     3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000
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   46    49    55    56     3   0.60436   1.81307   0.00000  -2.41742   0.00000   0.00000
   46    49    55    57     3   0.60436   1.81307   0.00000  -2.41742   0.00000   0.00000
   46    49    55    58     3   0.60436   1.81307   0.00000  -2.41742   0.00000   0.00000
   47    45    46    49     3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000
   47    45    46    50     3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000
   47    45    46    51     3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000
   48    45    46    49     3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000
   48    45    46    50     3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000
   48    45    46    51     3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000
   50    46    49    52     3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000
   50    46    49    53     3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000
   50    46    49    55     3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000
   51    46    49    52     3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000
   51    46    49    53     3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000
   51    46    49    55     3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000
   52    49    55    56     3   0.60436   1.81307   0.00000  -2.41742   0.00000   0.00000
   52    49    55    57     3   0.60436   1.81307   0.00000  -2.41742   0.00000   0.00000
   52    49    55    58     3   0.60436   1.81307   0.00000  -2.41742   0.00000   0.00000
   53    49    55    56     3   0.60436   1.81307   0.00000  -2.41742   0.00000   0.00000
   53    49    55    57     3   0.60436   1.81307   0.00000  -2.41742   0.00000   0.00000
   53    49    55    58     3   0.60436   1.81307   0.00000  -2.41742   0.00000   0.00000

[ dihedrals ] ; impropers
; treated as propers in GROMACS to use correct AMBER analytical function
;    i     j     k     l  func  phase     kd      pn
     1    26    10    36     1  180.00   4.60240   2
     3     6     4    24     1  180.00   4.60240   2
     3     7     5    15     1  180.00   4.60240   2
     4     5     3    23     1  180.00   4.60240   2
     4     8     6    22     1  180.00   4.60240   2
     5     8     7    21     1  180.00   4.60240   2
     6     7     8    20     1  180.00   4.60240   2
     9    12    10    26     1  180.00   4.60240   2
     9    13    11    19     1  180.00   4.60240   2
    10    11     9    25     1  180.00   4.60240   2
    10    14    12    18     1  180.00   4.60240   2
    11    14    13    17     1  180.00   4.60240   2
    12    13    14    16     1  180.00   4.60240   2
    25     1    26    31     1  180.00   4.60240   2
    27    23     2    24     1  180.00   4.60240   2
    27    29    28    32     1  180.00   4.60240   2
    28     2    27    35     1  180.00   4.60240   2
    28    30    29    33     1  180.00   4.60240   2
    29    31    30    34     1  180.00   4.60240   2
    30     1    31    35     1  180.00   4.60240   2
    45     3    23     2     1  180.00   4.60240   2

[ system ]
 PtF

[ molecules ]
; Compound        nmols
 PtF             1
```

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