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Electronic Supporting Information

Enzymatic reversion of Pt(II) nucleophilicity through charge dumping: The case of $Pt(CN)_4^{2-}$.

Sergi Burguera,[a] Antonio Frontera[a] and Antonio Bauzá*[a]

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Theoretical methods

*Quantum Mechanics calculations of complexes **1** to **10***

The interaction energies of all complexes included in this study were computed at the RI-MP2[1]/ def2-TZVP[2] level of theory. The calculations have been performed using the program TURBOMOLE version 7.0.[3] The binding energies were corrected by means of the Boys and Bernardi Counterpoise technique.[4] They were calculated following the supermolecule approximation ($\Delta E_{interaction} = \Delta E_{complex} - \Delta E_{monomer1} - \Delta E_{monomer2}$). In addition, the Cs and $C2_V$ symmetry point groups were imposed during the optimization of complexes **1** to **11**. The MEP (Molecular Electrostatic Potential) surfaces were computed at the RI-MP2/def2-TZVP level of theory by means of the TURBOMOLE 7.0 program and analyzed using the Multiwfn software.[5] The MEP surfaces were visualized using the Gaussview 5.0 software.[6] The calculations for the wavefunction analysis have been carried out at the RI-MP2/def2-TZVP level of theory also using Multiwfn software. The NBO analyses was performed at the HF/def2-TZVP level of theory by means of the NBO 7.0 program.[7] Lastly, the NCIplot[8] isosurfaces correspond to both favorable and unfavorable interactions, as differentiated by the sign of the second density Hessian eigenvalue and defined by the isosurface color. The color scheme is a red–yellow–green–blue scale with red for repulsive (ρ^{+}_{cut}) and blue for attractive (ρ^{-}_{cut}) NCI interaction density. Yellow and green surfaces correspond to weak repulsive and weak attractive interactions, respectively. The NCIplot isosurfaces were visualized by means of the VMD software.[9]

Quantum Mechanics calculations of the PDB structure 6IG4

A theoretical model was built containing the interacting residue (GLN), the $PtCN_4^{2-}$ molecule and the formamidinum and ammonium groups belonging to the four positively charged Arg/Lys residues (the cartesian coordinates are included below). As a starting point, the H atoms were optimized at the BP86[10]-D3[11]/def2-SVP[2] level of theory. The resulting geometry was used to compute the interaction energy between the O donor and the Pt moiety at the RI-MP2/def2-TZVP level of theory, also using the supermolecule approximation. The BSSE technique was also applied to correct the interaction energy obtained. The NBO analysis was performed at the HF/def2-TZVP level of theory by means of the NBO 7.0 program.

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Molecular Dynamics simulations

General considerations

Simulations have been performed by means of the AMBER18[12] software, using the AMBERff14SB[13] force field for the protein, the AMBER GAFF2[14] force field for the ligand and the TIP3P[15] water model for the solvent. Parametrization of the Pt(II) center was carried out using the MCPB.py script from AMBER18 suite.[16] In Figures S4 to S6 the RMSD plots of the structural parameters that characterize a square planar geometry (two C–Pt–C angles and a C–Pt–C–C dihedral angle) are also shown to validate the parametrization carried out on the $[PtCN^4]^{2-}$ moiety. As noticed in Figures S4 and S5, the two C–Pt–C angles remained very close to 120 and 90 degrees, respectively, while the C–Pt–C–C dihedral angle (Figure S6) varied between 160 and –160 degrees, as expected from a square planar geometry. The SWISS-MODEL[17] webserver was used to build a homology model to fill the missing residues in the protein structure. The total number of atoms composing the system was 48,298. The total number of solvent molecules added was 43,686, filling a rectangular box with the edges at a minimum of 10Å from the enzyme.

Preparation of the system consisted of four phases (P-1 to P-4) and Equilibration of two phases (P-5 and P-6):

Preparation phases

During the Preparation phases the NVT ensemble was used (canonical ensemble) with cutoff of 10Å for the nonbonding interactions. In phases P-1, P-2 and P-4, positional harmonic restraints of 10.0 kcal/mol/Å^2 were applied on the protein and the $Pt(CN_4)^{2-}$ coordination complex in order to let the water molecules to relax and solvate the system properly.

P-1: Water minimization using the steepest descent algorithm for 1,500 cycles. After that, 200 cycles using the conjugated gradient algorithm were carried out to reach a total number of 2,000 minimization cycles.

P-2: Water Molecular Dynamics simulation for 20ps was performed on this phase. The SHAKE algorithm[18] was used to constrain the bonds involving hydrogen atoms and an integration timestep of 0.002ps was imposed. A heat bath using the Berendsen thermostat from 200K to 300K was carried out with a heat bath coupling of 0.5ps.[19] Also, the Berendsen thermostat was used at this stage with a pressure relaxation time of 1ps.

P-3: Minimization of the whole system using the steepest descent algorithm for 1,500 cycles. After that, 200 cycles using the conjugated gradient algorithm were carried out to reach a total number of 2,000 minimization cycles.

P-4 Heating the system for 500ps to 300K. The SHAKE algorithm was used to constrain the bonds involving hydrogen atoms and an integration timestep of 0.002ps was imposed. Also, the Berendsen thermostat was used at this stage with a pressure relaxation time of 0.5ps.

Equilibration phases

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[19] H. J. C. Berendsen, J. P. M. Postma, W. F. van Gunsteren, A. DiNola, J. R. Haak, *J. Chem. Phys.* 1984, **81**, 3684-3690.

During the Equilibration phases the NPT ensemble was used (isobaric-isothermal ensemble). Also, a cutoff of 10Å for the nonbonding interactions was considered in each phase.

P-5 Equilibration of the density of the system for 500ps. The SHAKE algorithm was used to constrain the bonds involving hydrogen atoms and an integration timestep of 0.002ps was imposed. The Berendsen barostat was used with a pressure relaxation time of 1ps. Also, the Langevin thermostat was used with a collision frequency (γ) of 2 ps^{-1}.
P-6 Equilibration of the whole system for 5ns. The SHAKE algorithm was used to constrain the bonds involving hydrogen atoms and an integration timestep of 0.002ps was imposed. The Langevin thermostat was used during this phase with a temperature of 300K and a pressure relaxation time of 2ps. A random seed was used with a collision frequency of 2ps^{-1}.
Before running the production, the RMSD of the protein backbone was checked, showing fluctuations comprised between 0.5 and 1.6 Å (average of 1.2 Å).

Production phase
A production run of 100ns on the NVT ensemble was carried out followed by three replicas of 50 ns each. The SHAKE algorithm was used to constrain the bonds involving hydrogen atoms and an integration timestep of 0.002ps was imposed. The Langevin thermostat was used during this phase with a temperature of 300K and a a collision frequency (γ) of 2 ps^{-1}.
The Electrostatic Potential maps of the $[Pt(CN)_4]^{2-}$ and triphosphate molecules along with several files related to the MD simulations can be found at: https://github.com/tonibr9/PtCN4-results.git

MD replicas analysis

The RMSD distance plots corresponding to the three replicas of 50ns are shown in Figures S1-S3. Concretely, replicas 1 and 2 (Figs. S1 and S2) show a similar trend to that obtained for the 100ns simulation in the case of LYS151 (being one of the residues with the highest RMSD fluctuations) and LYS221 (exhibiting the lowest RMSD values) in both trajectories. However, in replica 1 we found that the ARG148 RMSD is lower compared to that in ARG213 during the first half of the trajectory and then reached similar RMSD values (around 7 Å) during the second half, due to the spatial rearrangements of $[Pt(CN)_4]^{2-}$. On the other hand, in replica 2 the RMSD behaviour involving these two residues is similar to that observed in replica 1 during the first half of the trajectory, however it is reverted during the second half of the simulation, exhibiting ARG148 higher RMSD values than ARG213. In the case of replica 3 (Fig. S3), we found a similar trend to that obtained for the 100ns simulation during the first 30 ns of trajectory, that is, LYS151 and ARG148 are clearly the residues with the highest RMSD values, followed by ARG213 and LYS221. However, during the last 20 ns of replica simulation, we found that the LYS151, ARG213 and ARG148 residues RMSD values became closer, comprised between 6-9 Å, while the RMSD values corresponding to LYS221 remained around 6 Å, in line with the 100 ns simulation.

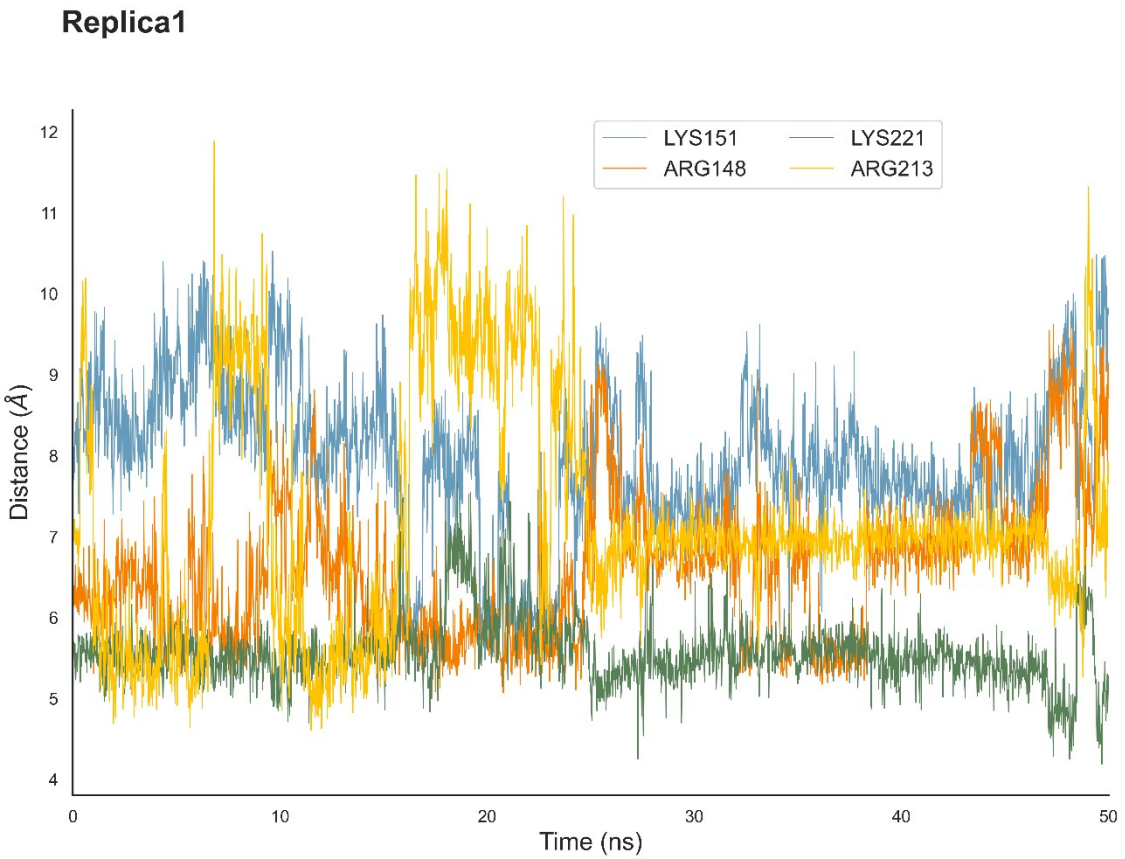

Figure S1. Distance RMSD plot of the $(CN)_4$–Pt^{-}···NH_3^+ and $(CN)_4$–Pt··· $CH_4N_2^+$ distances along the MD trajectory corresponding to the first replica. Distances Pt···ARG are measured to the central C atom from the formamidinium group. Distances Pt···LYS are measured to the N atom of the ammonium group.

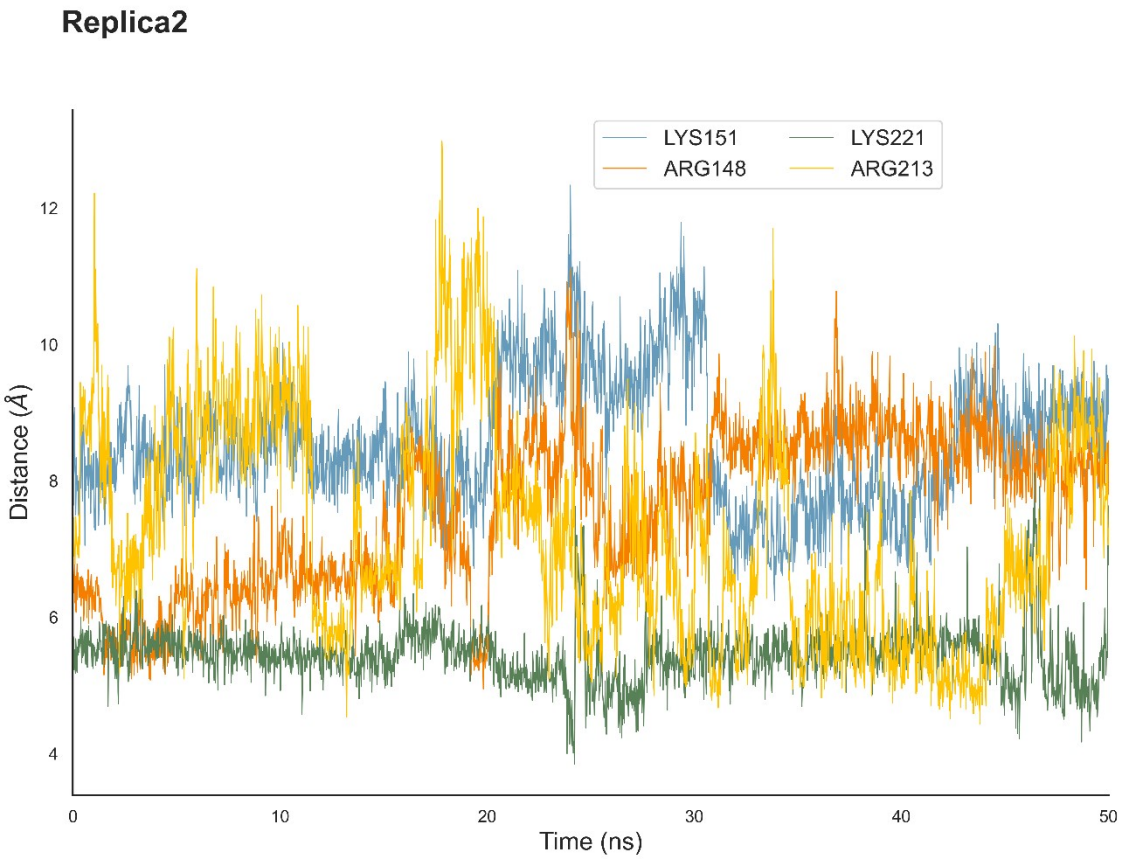

Figure S2. Distance RMSD plot of the $(CN)_4$–Pt^{-}···NH_3^+ and $(CN)_4$–Pt··· $CH_4N_2^+$ distances along the MD trajectory corresponding to the second replica. Distances Pt···ARG are measured to the central C atom from the formamidinium group. Distances Pt···LYS are measured to the N atom of the ammonium group.

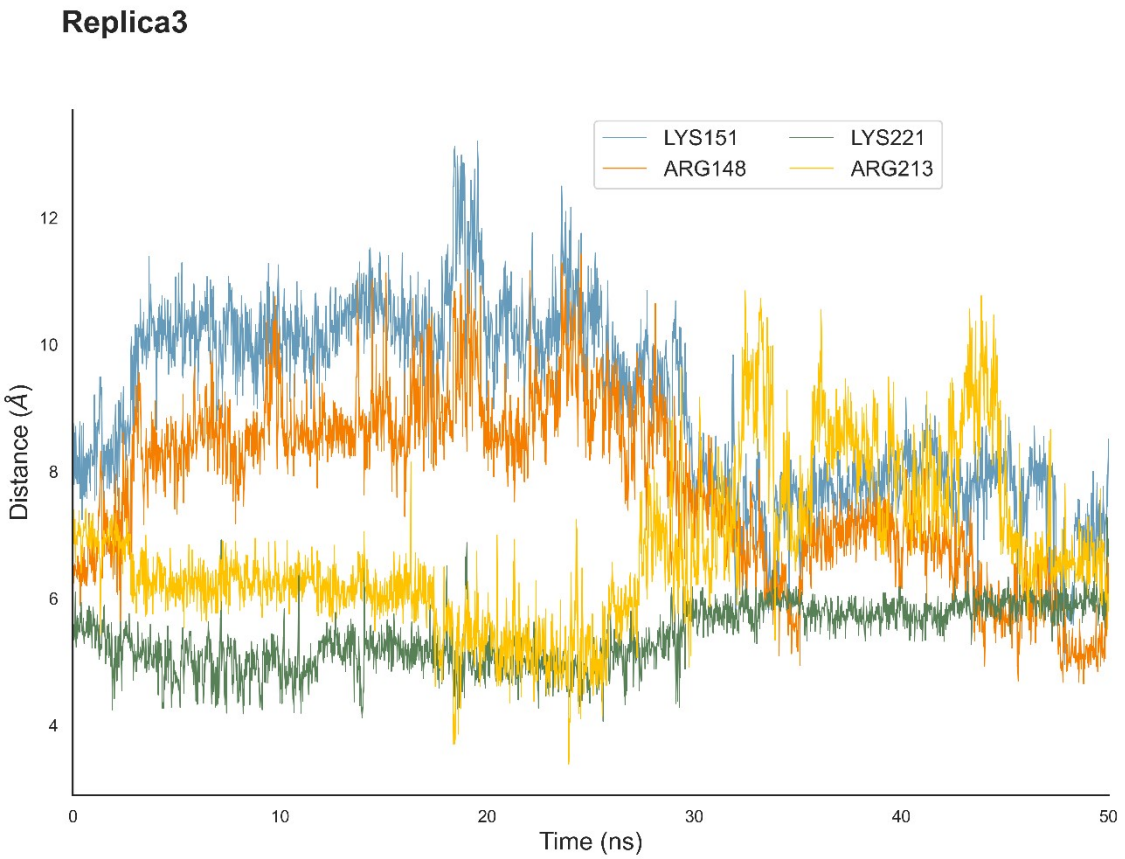

Figure S3. Distance RMSD plot of the $(CN)_4$–Pt^{-}···NH_3^+ and $(CN)_4$–Pt··· $CH_4N_2^+$ distances along the MD trajectory corresponding to the third replica. Distances Pt···ARG are measured to the central C atom from the formamidinium group. Distances Pt···LYS are measured to the N atom of the ammonium group.

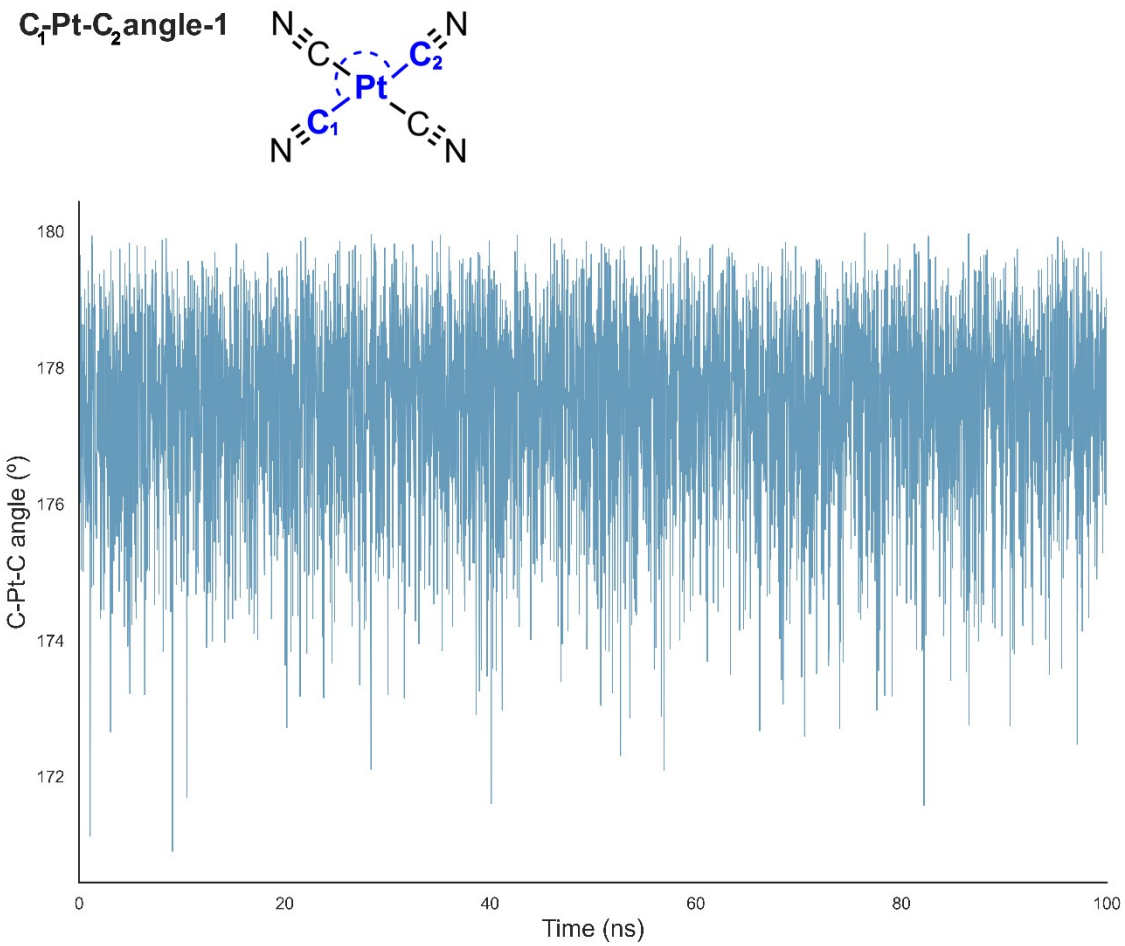

Figure S4. Angle RMSD plot of the C_1–Pt–C_2 angle along the 100ns MD trajectory.

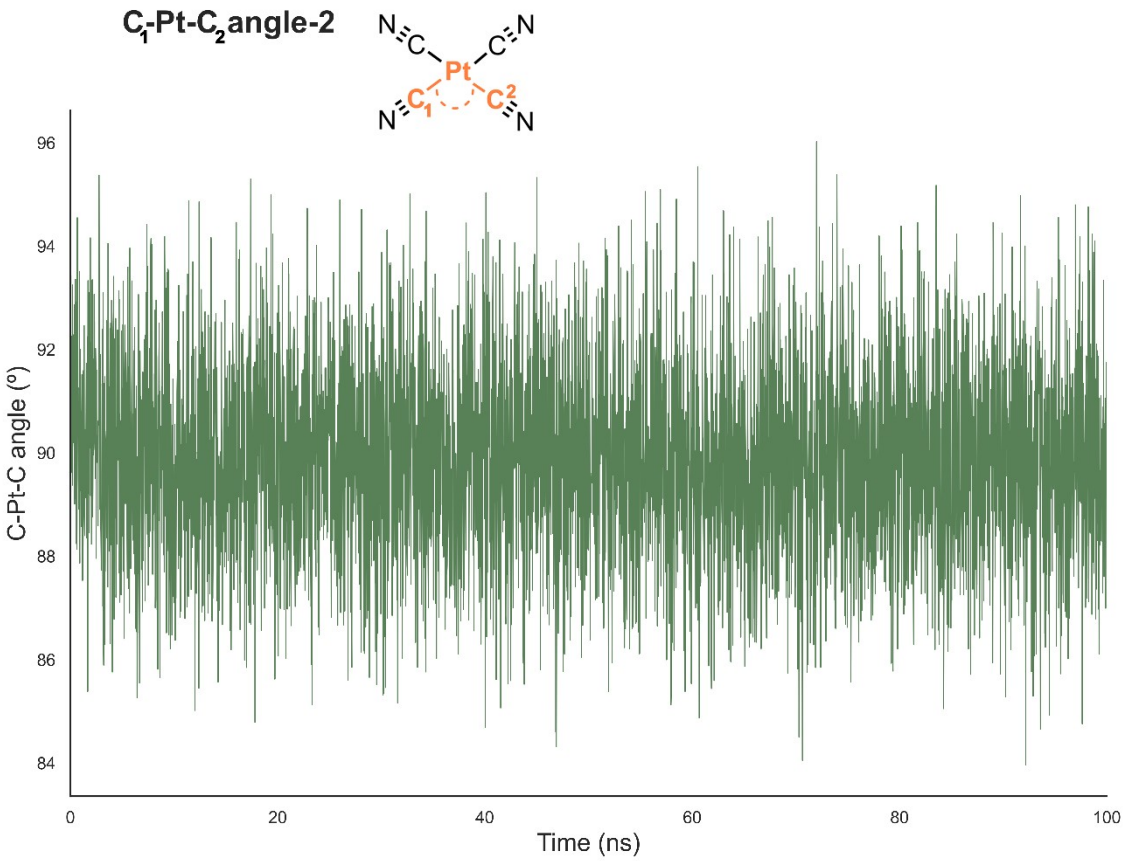

Figure S5. Angle RMSD plot of the C_1–Pt–C_2 angle along the 100ns MD trajectory.

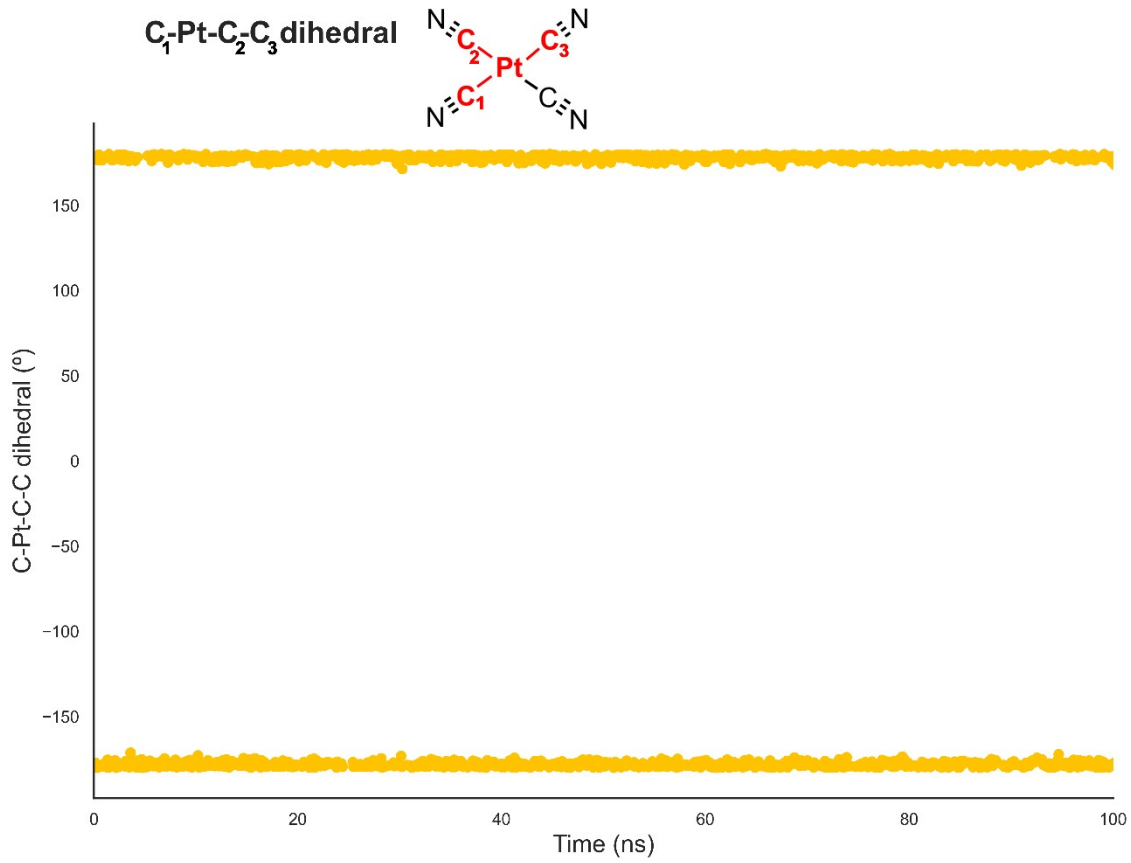

Figure S6. Dihedral angle RMSD plot of the C_1–Pt–C_2–C_3 dihedral angle along the 100ns MD trajectory.

Cartesian coordinates of complexes 1 to 10

1.

Pt	0.0000000	0.0000000	-0.2340171
C	0.0000000	-1.9473825	-0.2349589
C	1.9529320	0.0000000	-0.2336498
C	0.0000000	1.9473825	-0.2349589
C	-1.9529320	0.0000000	-0.2336498
N	0.0000000	-3.1216530	-0.2347706
N	3.1307342	0.0000000	-0.2327533
N	0.0000000	3.1216530	-0.2347706
N	-3.1307342	0.0000000	-0.2327533
C	6.3996948	0.0000000	-0.2328778
N	5.7707316	1.1469028	-0.2326955
H	4.7457891	1.1375976	-0.2333557
H	6.2929211	2.0079840	-0.2330010
N	5.7707316	-1.1469028	-0.2326955
H	6.2929211	-2.0079840	-0.2330010
H	4.7457891	-1.1375976	-0.2333557
H	7.4835628	-0.0000000	-0.2328193
C	-6.3996948	0.0000000	-0.2328778
N	-5.7707316	-1.1469028	-0.2326955
H	-4.7457891	-1.1375976	-0.2333557
H	-6.2929211	-2.0079840	-0.2330010
N	-5.7707316	1.1469028	-0.2326955
H	-6.2929211	2.0079840	-0.2330010

H	-4.7457891	1.1375976	-0.2333557
H	-7.4835628	0.0000000	-0.2328193
H	0.0000000	-4.5971047	-0.2353301
H	0.0000000	4.5971047	-0.2353301
N	0.0000000	-5.7296556	-0.2332421
N	0.0000000	5.7296556	-0.2332421
H	-0.8267724	-6.0838003	-0.7113026
H	0.8267724	-6.0838003	-0.7113026
H	-0.8267724	6.0838003	-0.7113026
H	0.8267724	6.0838003	-0.7113026
H	0.0000000	-6.0805267	0.7231678
H	0.0000000	6.0805267	0.7231678
C	0.0000000	0.0000000	3.5164100
O	0.0000000	0.0000000	4.6534947

2.

Pt	-0.0000000	0.0000000	-0.2874152
C	0.0000000	-1.9463514	-0.2896690
C	1.9516739	0.0000000	-0.2886997
C	0.0000000	1.9463514	-0.2896690
C	-1.9516739	0.0000000	-0.2886997
N	0.0000000	-3.1202210	-0.2863858
N	3.1296873	0.0000000	-0.2779985
N	0.0000000	3.1202210	-0.2863858
N	-3.1296873	0.0000000	-0.2779985
C	6.3890031	0.0000000	-0.5025643
N	5.7615479	1.1469577	-0.4596374
H	4.7389974	1.1377165	-0.3903673
H	6.2821493	2.0082522	-0.4962892
N	5.7615479	-1.1469577	-0.4596374
H	6.2821493	-2.0082522	-0.4962892
H	4.7389974	-1.1377165	-0.3903673
H	7.4704662	0.0000000	-0.5760864
C	-6.3890031	0.0000000	-0.5025643
N	-5.7615479	-1.1469577	-0.4596374
H	-4.7389974	-1.1377165	-0.3903673
H	-6.2821493	-2.0082522	-0.4962892
N	-5.7615479	1.1469577	-0.4596374
H	-6.2821493	2.0082522	-0.4962892
H	-4.7389974	1.1377165	-0.3903673
H	-7.4704662	0.0000000	-0.5760864
H	0.0000000	-4.5879079	-0.2574811
H	0.0000000	4.5879079	-0.2574811
N	0.0000000	-5.7225506	-0.2303470
N	0.0000000	5.7225506	-0.2303470
H	-0.8266882	-6.0874280	-0.7002065
H	0.8266882	-6.0874280	-0.7002065
H	-0.8266882	6.0874280	-0.7002065
H	0.8266882	6.0874280	-0.7002065
H	0.0000000	-6.0513552	0.7338670
H	0.0000000	6.0513552	0.7338670
C	-0.6066075	0.0000000	3.1044877
H	-1.6710468	0.0000000	3.1075856
C	0.6066075	0.0000000	3.1044877
H	1.6710468	0.0000000	3.1075856

3.

Pt	-0.0000000	0.0000000	-0.7633840
C	0.0000000	-1.9443131	-0.7709405
C	1.9505752	0.0000000	-0.7617847
C	0.0000000	1.9443131	-0.7709405

C	-1.9505752	-0.0000000	-0.7617847
N	-0.0000000	-3.1185962	-0.7805327
N	3.1287698	0.0000000	-0.7571612
N	-0.0000000	3.1185962	-0.7805327
N	-3.1287698	0.0000000	-0.7571612
C	6.3815486	0.0000000	-0.9731027
N	5.7539241	1.1468466	-0.9286447
H	4.7310531	1.1360160	-0.8571603
H	6.2744607	2.0080996	-0.9659538
N	5.7539241	-1.1468466	-0.9286447
H	6.2744607	-2.0080996	-0.9659538
H	4.7310531	-1.1360160	-0.8571603
H	7.4627875	0.0000000	-1.0498321
C	-6.3815486	0.0000000	-0.9731027
N	-5.7539241	-1.1468466	-0.9286447
H	-4.7310531	-1.1360160	-0.8571603
H	-6.2744607	-2.0080996	-0.9659538
N	-5.7539241	1.1468466	-0.9286447
H	-6.2744607	2.0080996	-0.9659538
H	-4.7310531	1.1360160	-0.8571603
H	-7.4627875	-0.0000000	-1.0498321
H	-0.0000000	-4.5761327	-0.8739033
H	-0.0000000	4.5761327	-0.8739033
N	0.0000000	-5.7117754	-0.9598077
N	0.0000000	5.7117754	-0.9598077
H	-0.8263378	-6.0271908	-1.4647512
H	0.8263378	-6.0271908	-1.4647512
H	-0.8263378	6.0271908	-1.4647512
H	0.8263378	6.0271908	-1.4647512
H	0.0000000	-6.1384900	-0.0348595
H	0.0000000	6.1384900	-0.0348595
C	1.2072752	0.6967947	2.6243815
C	-0.0000000	1.3929785	2.6271208
C	-1.2072752	0.6967947	2.6243815
C	-1.2072752	-0.6967947	2.6243815
C	-0.0000000	-1.3929785	2.6271208
C	1.2072752	-0.6967947	2.6243815
H	2.1469534	1.2381401	2.6312728
H	-0.0000000	2.4773218	2.6382070
H	-2.1469534	1.2381401	2.6312728
H	-2.1469534	-1.2381401	2.6312728
H	-0.0000000	-2.4773218	2.6382070
H	2.1469534	-1.2381401	2.6312728

4.

C	0.00000000	0.00000000	4.54631680
O	0.00000000	0.00000000	3.40863610
Pt	0.00000000	0.00000000	-0.20987980
C	0.00000000	-1.94653860	-0.20962190
C	1.95199230	0.00000000	-0.20830810
C	0.00000000	1.94653860	-0.20962190
C	-1.95199230	0.00000000	-0.20830810
N	0.00000000	-3.12042800	-0.20918120
N	3.12949660	0.00000000	-0.20696260
N	0.00000000	3.12042800	-0.20918120
N	-3.12949660	0.00000000	-0.20696260
C	6.39576370	0.00000000	-0.23489450
N	5.76687060	1.14691960	-0.23026200
H	4.74213620	1.13759470	-0.22208320
H	6.28858820	2.00824540	-0.23462500
N	5.76687060	-1.14691960	-0.23026200

H	6.28858820	-2.00824540	-0.23462500
H	4.74213620	-1.13759470	-0.22208320
H	7.47965130	0.00000000	-0.24288380
C	-6.39576370	0.00000000	-0.23489450
N	-5.76687060	-1.14691960	-0.23026200
H	-4.74213620	-1.13759470	-0.22208320
H	-6.28858820	-2.00824540	-0.23462500
N	-5.76687060	1.14691960	-0.23026200
H	-6.28858820	2.00824540	-0.23462500
H	-4.74213620	1.13759470	-0.22208320
H	-7.47965130	0.00000000	-0.24288380
H	0.00000000	-4.60022710	-0.22563930
H	0.00000000	4.60022710	-0.22563930
N	0.00000000	-5.72995020	-0.23727640
N	0.00000000	5.72995020	-0.23727640
H	-0.82697560	-6.07812990	-0.71948980
H	0.82697560	-6.07812990	-0.71948980
H	-0.82697560	6.07812990	-0.71948980
H	0.82697560	6.07812990	-0.71948980
H	0.00000000	-6.09173870	0.71515150
H	0.00000000	6.09173870	0.71515150

5.

Pt	-0.1359646	-0.6317336	0.0000000
C	-0.1395306	-0.6411170	-1.9448733
C	-2.0882329	-0.6672063	0.0000000
C	-0.1395306	-0.6411170	1.9448733
C	1.8133444	-0.6023738	0.0000000
N	-0.1433468	-0.6425372	-3.1192138
N	-3.2656300	-0.6856772	0.0000000
N	-0.1433468	-0.6425372	3.1192138
N	2.9915307	-0.5769556	0.0000000
C	-6.5274617	-0.6032035	0.0000000
N	-5.8982360	-0.6193761	1.1465951
H	-4.8732757	-0.6448954	1.1351604
H	-6.4193919	-0.6053842	2.0080760
N	-5.8982360	-0.6193761	-1.1465951
H	-6.4193919	-0.6053842	-2.0080760
H	-4.8732757	-0.6448954	-1.1351604
H	-7.6110660	-0.5755083	0.0000000
C	6.2322921	-0.9546343	0.0000000
N	5.6080330	-0.8785190	-1.1470049
H	4.5905690	-0.7539900	-1.1371734
H	6.1260830	-0.9416956	-2.0083137
N	5.6080330	-0.8785190	1.1470049
H	6.1260830	-0.9416956	2.0083137
H	4.5905690	-0.7539900	1.1371734
H	7.3082434	-1.0858525	0.0000000
H	-0.1832887	-0.7071987	-4.5844864
H	-0.1832887	-0.7071987	4.5844864
N	-0.2147912	-0.7651040	-5.7181667
N	-0.2147912	-0.7651040	5.7181667
H	0.5984379	-1.2691028	-6.0675434
H	-1.0542929	-1.2543207	-6.0236898
H	0.5984379	-1.2691028	6.0675434
H	-1.0542929	-1.2543207	6.0236898
H	-0.2171459	0.1705595	-6.1209840
H	-0.2171459	0.1705595	6.1209840
C	0.5941699	2.8152652	1.1617242
H	-0.0196829	2.5435245	2.0188472
H	1.5333369	2.2487541	1.1970038

H	0.8260610	3.8857720	1.2071681
C	0.5941699	2.8152652	-1.1617242
H	1.5333369	2.2487541	-1.1970038
H	-0.0196829	2.5435245	-2.0188472
H	0.8260610	3.8857720	-1.2071681
O	-0.1444717	2.5018755	0.0000000

6.

Pt	0.4085548	0.2878973	0.0000000
C	0.8893590	-1.5928361	0.0000000
C	0.4591998	0.3006619	1.9505004
C	-0.0056003	2.1920891	0.0000000
C	0.4591998	0.3006619	-1.9505004
N	1.1553737	-2.7380974	0.0000000
N	0.4848585	0.3052901	3.1288676
N	-0.2818097	3.3332627	0.0000000
N	0.4848585	0.3052901	-3.1288676
C	0.9910624	0.5922359	6.3357344
N	0.5668844	1.6381912	5.6741098
H	0.4064777	1.5413812	4.6665163
H	0.4028967	2.5074291	6.1552413
N	1.2163610	-0.5595612	5.7586363
H	1.5429775	-1.3410911	6.3033055
H	1.0488707	-0.6343722	4.7491164
H	1.1624605	0.6847279	7.4020571
C	0.9910624	0.5922359	-6.3357344
N	1.2163610	-0.5595612	-5.7586363
H	1.0488707	-0.6343722	-4.7491164
H	1.5429775	-1.3410911	-6.3033055
N	0.5668844	1.6381912	-5.6741098
H	0.4028967	2.5074291	-6.1552413
H	0.4064777	1.5413812	-4.6665163
H	1.1624605	0.6847279	-7.4020571
H	1.6107608	-4.1367709	0.0000000
H	-0.7681985	4.7006620	0.0000000
N	1.9732847	-5.2117383	0.0000000
N	-1.1738500	5.7695601	0.0000000
H	2.5402922	-5.3927157	-0.8266229
H	2.5402922	-5.3927157	0.8266229
H	-0.8538285	6.2712589	-0.8263629
H	-0.8538285	6.2712589	0.8263629
H	1.1822486	-5.8537215	0.0000000
H	-2.1924625	5.7573210	0.0000000
C	-2.5303082	-1.5741611	-1.3665391
H	-2.4849861	-0.9946765	-2.2887328
H	-1.6338155	-2.1929642	-1.2954638
H	-3.4210831	-2.2031554	-1.3827014
C	-2.5303082	-1.5741611	1.3665391
H	-1.6338155	-2.1929642	1.2954638
H	-2.4849861	-0.9946765	2.2887328
H	-3.4210831	-2.2031554	1.3827014
S	-2.5943006	-0.4045856	0.0000000

7.

Pt	-0.6867312	0.0402126	0.0000000
C	-0.7486135	0.0408712	-1.9421676
C	-0.7899929	1.9855017	0.0000000
C	-0.7486135	0.0408712	1.9421676
C	-0.6674226	-1.9114486	0.0000000
N	-0.7767524	0.0413276	-3.1168531
N	-0.8381784	3.1632958	0.0000000

N	-0.7767524	0.0413276	3.1168531
N	-0.6314672	-3.0899128	0.0000000
C	-1.1152303	6.4081396	0.0000000
N	-1.0659046	5.7802607	1.1465020
H	-0.9827562	4.7579143	1.1334961
H	-1.1068245	6.2995845	2.0082681
N	-1.0659046	5.7802607	-1.1465020
H	-1.1068245	6.2995845	-2.0082681
H	-0.9827562	4.7579143	-1.1334961
H	-1.1999111	7.4888332	0.0000000
C	-1.0906137	-6.3129962	0.0000000
N	-0.9976439	-5.6906060	-1.1467576
H	-0.8450274	-4.6764666	-1.1352535
H	-1.0738149	-6.2066902	-2.0080650
N	-0.9976439	-5.6906060	1.1467576
H	-1.0738149	-6.2066902	2.0080650
H	-0.8450274	-4.6764666	1.1352535
H	-1.2512251	-7.3849382	0.0000000
H	-0.9224232	0.0306552	-4.5583278
H	-0.9224232	0.0306552	4.5583278
N	-1.0471044	0.0197598	-5.6961265
N	-1.0471044	0.0197598	5.6961265
H	-1.5562396	-0.8126301	-5.9876592
H	-1.5674832	0.8396463	-6.0027602
H	-1.5562396	-0.8126301	5.9876592
H	-1.5674832	0.8396463	6.0027602
H	-0.1368720	0.0220067	-6.1531690
H	-0.1368720	0.0220067	6.1531690
N	2.1088587	-0.0742101	0.0000000
C	2.6272348	1.2833285	0.0000000
H	2.2675104	1.8117341	-0.8845952
H	2.2675104	1.8117341	0.8845952
H	3.7292360	1.3077401	0.0000000
C	2.5371529	-0.7862608	-1.1919455
H	2.1004613	-1.7870339	-1.1944766
H	2.1910777	-0.2544881	-2.0800009
H	3.6339789	-0.8813575	-1.2452492
C	2.5371529	-0.7862608	1.1919455
H	2.1910777	-0.2544881	2.0800009
H	2.1004613	-1.7870339	1.1944766
H	3.6339789	-0.8813575	1.2452492

8.

Pt	0.0000000	0.0000000	-0.3187233
C	-0.0000000	-1.9452256	-0.3253577
C	1.9513788	0.0000000	-0.3258935
C	-0.0000000	1.9452256	-0.3253577
C	-1.9513788	0.0000000	-0.3258935
N	-0.0000000	-3.1189700	-0.3356007
N	3.1289900	0.0000000	-0.3371650
N	0.0000000	3.1189700	-0.3356007
N	-3.1289900	-0.0000000	-0.3371650
C	6.3829757	0.0000000	-0.3936881
N	5.7535115	1.1465421	-0.3779771
H	4.7281225	1.1338016	-0.3555349
H	6.2740944	2.0083368	-0.3920181
N	5.7535115	-1.1465421	-0.3779771
H	6.2740944	-2.0083368	-0.3920181
H	4.7281225	-1.1338016	-0.3555349
H	7.4665853	0.0000000	-0.4208577
C	-6.3829757	0.0000000	-0.3936881

N	-5.7535115	-1.1465421	-0.3779771
H	-4.7281225	-1.1338016	-0.3555349
H	-6.2740944	-2.0083368	-0.3920181
N	-5.7535115	1.1465421	-0.3779771
H	-6.2740944	2.0083368	-0.3920181
H	-4.7281225	1.1338016	-0.3555349
H	-7.4665853	0.0000000	-0.4208577
H	0.0000000	-4.5693393	-0.3709378
H	0.0000000	4.5693393	-0.3709378
N	0.0000000	-5.7124595	-0.3985528
N	0.0000000	5.7124595	-0.3985528
H	-0.8263700	-6.0548941	-0.8852770
H	0.8263700	-6.0548941	-0.8852770
H	-0.8263700	6.0548941	-0.8852770
H	0.8263700	6.0548941	-0.8852770
H	-0.0000000	-6.0874822	0.5484019
H	0.0000000	6.0874822	0.5484019
C	0.0000000	0.0000000	4.3930470
H	0.0000000	0.0000000	5.4617145
N	-0.0000000	0.0000000	3.2264923

9.

Pt	0.5166605	-0.0002053	-0.0000087
C	0.5687588	0.0001090	1.9420237
C	0.5579008	1.9507058	-0.0000172
C	0.5686885	0.0000101	-1.9420584
C	0.5581893	-1.9512006	0.0000534
N	0.5925512	0.0005654	3.1168165
N	0.5814499	3.1286855	-0.0000474
N	0.5925755	0.0004384	-3.1168461
N	0.5819061	-3.1291825	-0.0000000
C	0.7010511	6.3749216	0.0000011
N	0.6748813	5.7452459	-1.1462432
H	0.6341798	4.7198924	-1.1313343
H	0.6965090	6.2651657	-2.0081845
N	0.6754654	5.7452251	1.1462439
H	0.6969283	6.2651604	2.0081841
H	0.6348185	4.7198720	1.1313453
H	0.7449968	7.4580612	-0.0000078
C	0.7011699	-6.3749998	-0.0000224
N	0.6760984	-5.7456242	1.1464140
H	0.6349715	-4.7203009	1.1321820
H	0.6953049	-6.2661606	2.0080709
N	0.6763595	-5.7455933	-1.1464421
H	0.6955092	-6.2661082	-2.0081203
H	0.6352371	-4.7202737	-1.1321779
H	0.7444553	-7.4580937	-0.0000244
H	0.7881315	-0.0002720	4.5474615
H	0.7880948	-0.0003065	-4.5469460
N	0.9618653	-0.0002790	5.6814862
N	0.9618594	-0.0002689	-5.6814190
H	1.4894896	-0.8263393	5.9577400
H	1.4892098	0.8261316	5.9572186
H	1.4893830	-0.8263153	-5.9579141
H	1.4892728	0.8260690	-5.9573145
H	0.0728899	-0.0002686	6.1784729
H	0.0729338	-0.0001369	-6.1785322
C	-3.0025335	0.0001381	1.1454522
C	-4.3934284	0.0007174	1.1955619
C	-5.1053465	0.0008600	-0.0000115
C	-4.3934232	0.0007565	-1.1955863

C	-3.0025238	0.0002110	-1.1454558
N	-2.3091441	-0.0003778	0.0000011
H	-6.1890424	0.0006670	-0.0000030
H	-2.4106557	0.0002527	2.0568388
H	-4.9050344	0.0004522	2.1506205
H	-4.9050230	0.0005378	-2.1506487
H	-2.4106204	0.0002845	-2.0568227

10.

Pt	1.3684129	-0.0001010	0.0000000
C	1.3907053	0.0001215	1.9428337
C	1.3748933	1.9503708	0.0000000
C	1.3907053	0.0001215	-1.9428337
C	1.3750109	-1.9506475	0.0000000
N	1.4203033	0.0005144	3.1161817
N	1.3840466	3.1279848	0.0000000
N	1.4203033	0.0005144	-3.1161817
N	1.3836547	-3.1282684	0.0000000
C	1.4046661	6.3743111	0.0000000
N	1.3964903	5.7444317	-1.1463890
H	1.3856449	4.7183642	-1.1317911
H	1.4033827	6.2648782	-2.0082258
N	1.3964903	5.7444317	1.1463890
H	1.4033827	6.2648782	2.0082258
H	1.3856449	4.7183642	1.1317911
H	1.4183815	7.4580866	0.0000000
C	1.4033864	-6.3746298	0.0000000
N	1.3956363	-5.7447024	1.1463663
H	1.3845641	-4.7186368	1.1316979
H	1.4020970	-6.2651032	2.0082356
N	1.3956363	-5.7447024	-1.1463663
H	1.4020970	-6.2651032	-2.0082356
H	1.3845641	-4.7186368	-1.1316979
H	1.4163228	-7.4584263	0.0000000
H	1.5558187	-0.0003495	4.5363706
H	1.5558187	-0.0003495	-4.5363706
N	1.6810246	-0.0003608	5.6860369
N	1.6810246	-0.0003608	-5.6860369
H	2.1954607	-0.8262988	5.9858802
H	2.1960248	0.8254170	5.9853413
H	2.1954607	-0.8262988	-5.9858802
H	2.1960248	0.8254170	-5.9853413
H	0.7714832	0.0001473	6.1437112
H	0.7714832	0.0001473	-6.1437112
C	-3.6508342	-0.0002713	1.1792113
C	-5.0309429	0.0007002	1.1897003
C	-5.7541789	0.0017852	0.0000000
C	-5.0309429	0.0007002	-1.1897003
C	-3.6508342	-0.0002713	-1.1792113
N	-2.9455453	-0.0006837	0.0000000
H	-6.8358211	0.0039865	0.0000000
H	-3.0198304	-0.0000998	2.0565486
H	-5.5337010	0.0001758	2.1492318
H	-5.5337010	0.0001758	-2.1492318
H	-3.0198304	-0.0000998	-2.0565486
O	-1.6798844	-0.0016237	0.0000000

Cartesian coordinates of the 6IG4 PDB model for QM calculations

Theoretical model including the amide moiety

O	-13.6815220	1.5706667	2.3720000
C	-14.5695220	2.2056667	1.8020000
C	-15.9055220	1.5836667	1.5520000
N	-14.3965220	3.4436667	1.3510000
H	-13.5470965	3.9386968	1.6406477
H	-15.1539708	4.0016063	0.9595672
H	-16.2586358	1.1260297	2.4968865
H	-16.6841332	2.2680628	1.1560622
H	-15.7868504	0.7474391	0.8336140
C	-5.4685220	6.0216667	2.7150000
N	-6.7425220	5.6306667	2.1360000
C	-7.5305220	4.6876667	2.6310000
N	-7.1635220	4.0326667	3.7200000
N	-8.6755220	4.3956667	2.0190000
C	-6.2355220	1.1496667	2.0900000
N	-5.4795220	1.0196667	3.3590000
C	-12.5945220	1.6556667	9.9480000
N	-13.3585220	2.9046667	10.0630000
C	-12.8195220	4.1056667	10.3040000
N	-13.5895220	5.1826667	10.3870000
N	-11.5095220	4.2406667	10.4780000
C	-18.9295220	2.8756667	6.0830000
N	-17.9865220	3.9036667	5.5790000
C	-14.4345220	4.4006667	5.6220000
N	-15.3745220	5.0496667	5.8940000
C	-13.8495220	1.9576667	6.3960000
Pt	-12.8775220	3.2656667	5.2890000
N	-14.5215220	1.1826667	7.0440000
C	-11.1465220	2.2886667	5.2400000
N	-10.0425220	1.7756667	5.2070000
C	-12.0495220	4.6786667	4.2060000
N	-11.5375220	5.5496667	3.5480000
H	-10.8760574	3.4693073	10.2699190
H	-11.1084016	5.0808524	10.8928855
H	-13.2025704	6.1192162	10.2715791
H	-14.6047874	5.1009371	10.3339021
H	-14.2289748	2.8995849	9.5161171
H	-11.8342485	1.7152003	9.1386851
H	-13.2992175	0.8618307	9.6434279
H	-17.6507141	3.6725538	4.6250655
H	-18.4274634	4.8371044	5.4922443
H	-17.0419717	4.1221811	6.0722301
H	-19.3092803	3.1810566	7.0742050
H	-19.7716293	2.7710747	5.3755979
H	-8.9431147	4.9199248	1.1819204
H	-9.5061968	4.1397494	2.5942848
H	-6.6320067	4.5641943	4.4179993
H	-7.9083782	3.4549339	4.1625313
H	-7.1270149	6.2296902	1.4013328
H	-4.8227393	5.1371752	2.8896654
H	-5.5954422	6.5796869	3.6685613
H	-5.5620568	1.8938700	3.9170009
H	-5.8528145	0.2525260	3.9546632
H	-4.4694797	0.8270195	3.2145399
H	-5.8187249	1.9894826	1.5068300
H	-7.2986595	1.3388757	2.3275928
H	-18.3899472	1.9155989	6.1781217
H	-6.1453968	0.2115200	1.5131200

H	-4.9373829	6.6844390	2.0087276
H	-12.1270346	1.3917657	10.9174440

Theoretical model without the amide moiety

C	-5.46852200	6.02166670	2.71500000
N	-6.74252200	5.63066670	2.13600000
C	-7.53052200	4.68766670	2.63100000
N	-7.16352200	4.03266670	3.72000000
N	-8.67552200	4.39566670	2.01900000
C	-6.23552200	1.14966670	2.09000000
N	-5.47952200	1.01966670	3.35900000
C	-12.59452200	1.65566670	9.94800000
N	-13.35852200	2.90466670	10.06300000
C	-12.81952200	4.10566670	10.30400000
N	-13.58952200	5.18266670	10.38700000
N	-11.50952200	4.24066670	10.47800000
C	-18.92952200	2.87566670	6.08300000
N	-17.98652200	3.90366670	5.57900000
C	-14.43452200	4.40066670	5.62200000
N	-15.37452200	5.04966670	5.89400000
C	-13.84952200	1.95766670	6.39600000
Pt	-12.87752200	3.26566670	5.28900000
N	-14.52152200	1.18266670	7.04400000
C	-11.14652200	2.28866670	5.24000000
N	-10.04252200	1.77566670	5.20700000
C	-12.04952200	4.67866670	4.20600000
N	-11.53752200	5.54966670	3.54800000
H	-10.87605740	3.46930730	10.26991900
H	-11.10840160	5.08085240	10.89288550
H	-13.20257040	6.11921620	10.27157910
H	-14.60478740	5.10093710	10.33390210
H	-14.22897480	2.89958490	9.51611710
H	-11.83424850	1.71520030	9.13868510
H	-13.29921750	0.86183070	9.64342790
H	-17.65071410	3.67255380	4.62506550
H	-18.42746340	4.83710440	5.49224430
H	-17.04197170	4.12218110	6.07223010
H	-19.30928030	3.18105660	7.07420500
H	-19.77162930	2.77107470	5.37559790
H	-8.94311470	4.91992480	1.18192040
H	-9.50619680	4.13974940	2.59428480
H	-6.63200670	4.56419430	4.41799930
H	-7.90837820	3.45493390	4.16253130
H	-7.12701490	6.22969020	1.40133280
H	-4.82273930	5.13717520	2.88966540
H	-5.59544220	6.57968690	3.66856130
H	-5.56205680	1.89387000	3.91700090
H	-5.85281450	0.25252600	3.95466320
H	-4.46947970	0.82701950	3.21453990
H	-5.81872490	1.98948260	1.50683000
H	-7.29865950	1.33887570	2.32759280
H	-18.38994720	1.91559890	6.17812170
H	-6.14539680	0.21152000	1.51312000
H	-4.93738290	6.68443900	2.00872760
H	-12.12703460	1.39176570	10.91744400