Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Solvent effect on the ^{195}Pt NMR properties in pyridonate-bridged Pt^{III} dinuclear complex derivatives investigated by *ab initio* molecular dynamics and localized orbital analysis

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Contents

This document provides additional radial distribution functions of solvent and solute, CPMD structural parameters of solute, relativistic scalar corrections on the $^1J_{PtPt}$ results of NMR properties computed with CPMD configurations using nonhybrid functional, assessment of DFT functional and the evolution of average of the shielding tensor as support to discussion reported in the main text.

1 Studied Complexes

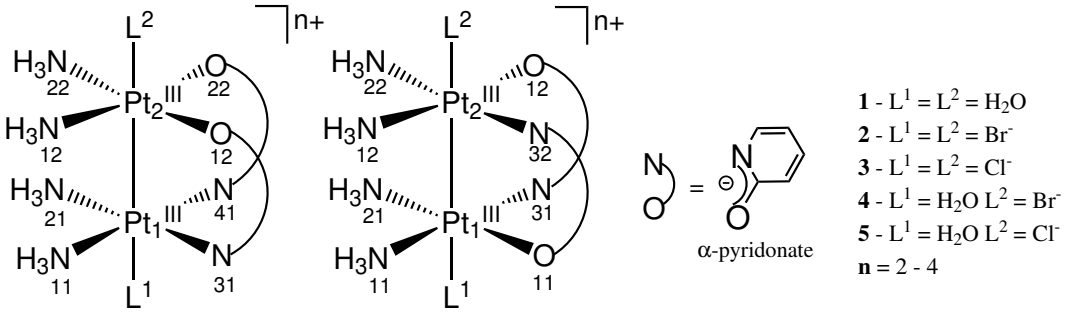

Figure S1: Head-to-Head (HH) and Head-to-Tail (HT) Pt−Pt α-pyridonate-bridge complexes labeled.

2 Solvent Structure

The oxygen-oxygen radial distribution function (RDF) shows good agreement with theoretical studies in the literature at similar levels of theory.[1,2] All oxygen atoms are included in the RDF, including oxygen atoms that are part of the pyridonate motif and aquo ligands. These oxygen atoms are responsible for additional structure visible between 2.2 and 2.5 Å and the small shelf around 3.7 Å. Also, hydrogen-hydrogen RDF of HH and HT complexes corroborates with experiment.[3–5]

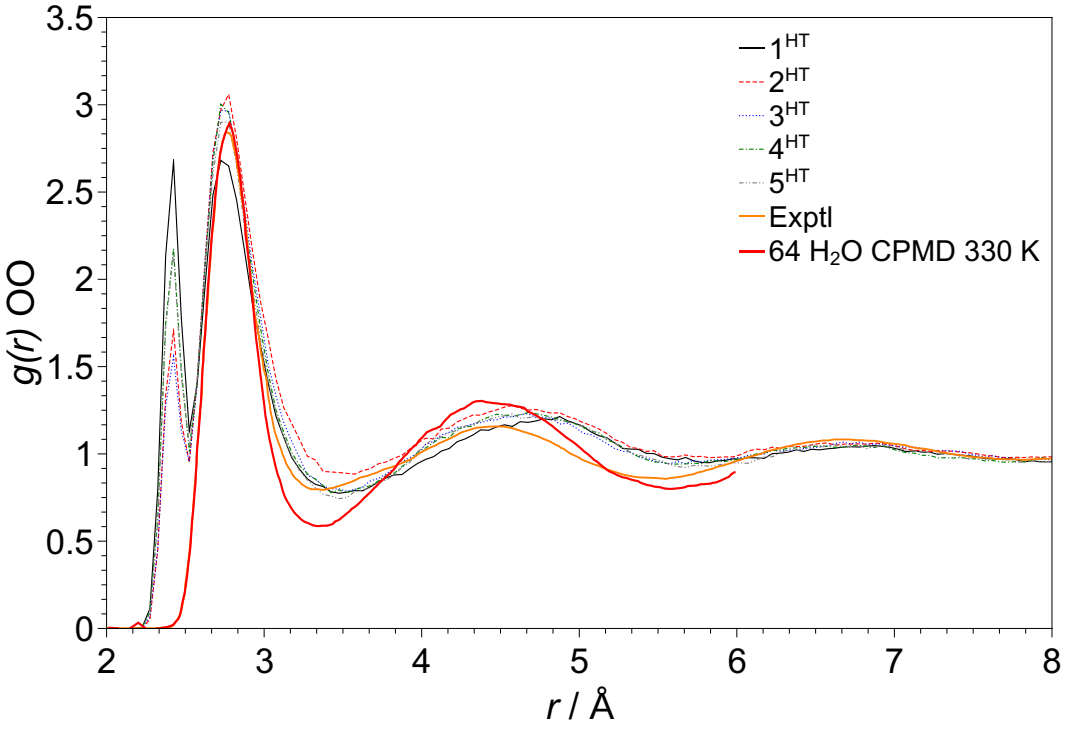

Figure S2: Oxygen-oxygen RDFs for each of the five explored HT Pt(III) complexes; *g(r)*OO denotes the RDF or pair correlation as a function of pair distance in Å. The full orange line is the experimental oxygen-oxygen RDF for heavy water from the joint X-ray diffraction and neutron scattering experiments of Soper and Benmore[6]. The full red line is the theoretical oxygen-oxygen RDF for pure water obtained by CPMD at 330 K[7]. These latter two were extracted using the engauge plot digitizer.[8].

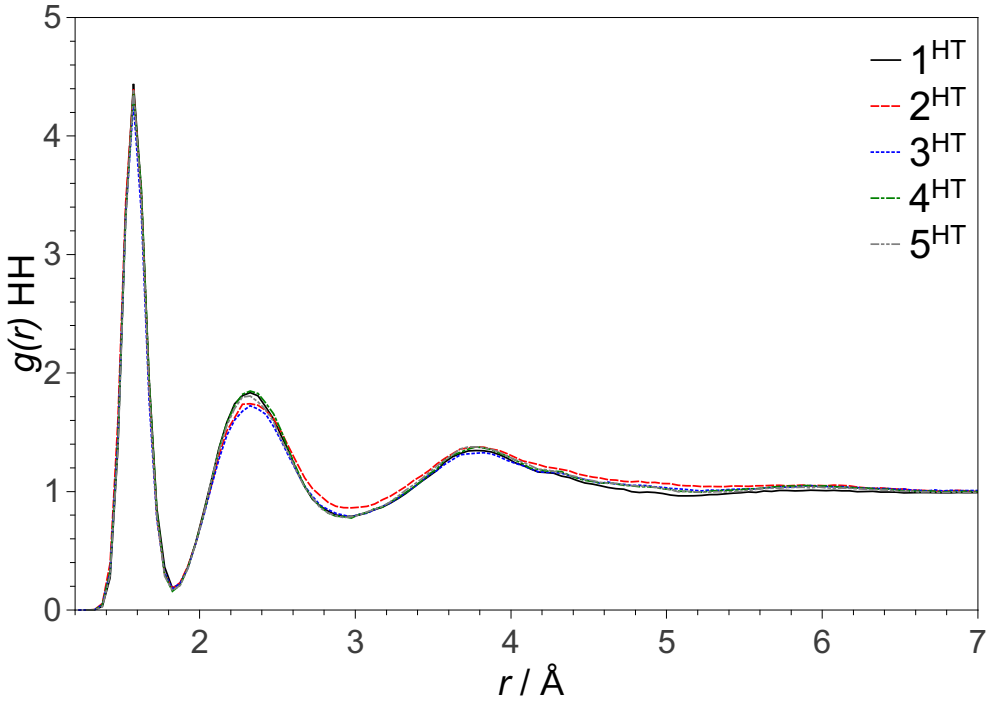

Figure S3: Hydrogen-hydrogen RDFs for 2000 configurations of the production trajectories of the five explored HT Pt(III) complexes. *g(r)* HH denotes the RDFs or pair correlations as a function of pair distance in Angstrom.

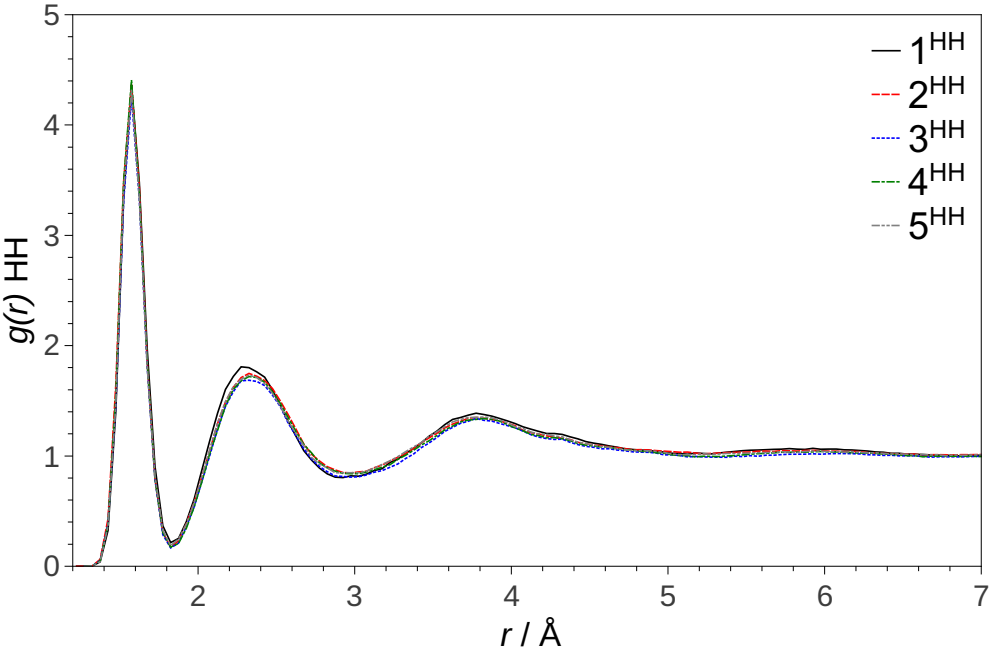

Figure S4: Hydrogen-hydrogen RDFs for 2000 configurations of the production trajectories of the five explored HH Pt(III) complexes. *g(r)* HH denotes the RDFs or pair correlations as a function of pair distance in Angstrom.

3 Dynamic properties

Table S1: Calculated average distances (in Å) between the Cl atoms of the perchlorate anions and Pt atoms of the complexes.

Complex	Distance	Mean
1^{HH}	10.6 ± 1.2	9.8 ± 0.7
1^{HT}	8.9 ± 0.7	
2^{HH}	6.9 ± 1.0	6.6 ± 0.6
2^{HT}	6.4 ± 0.8	
3^{HH}	9.2 ± 1.9	7.0 ± 1.0
3^{HT}	5.6 ± 0.7	
4^{HH}	7.7 ± 0.9	7.2 ± 0.5
4^{HT}	6.8 ± 0.6	
5^{HH}	7.8 ± 0.8	8.2 ± 0.6
5^{HT}	8.5 ± 0.9	

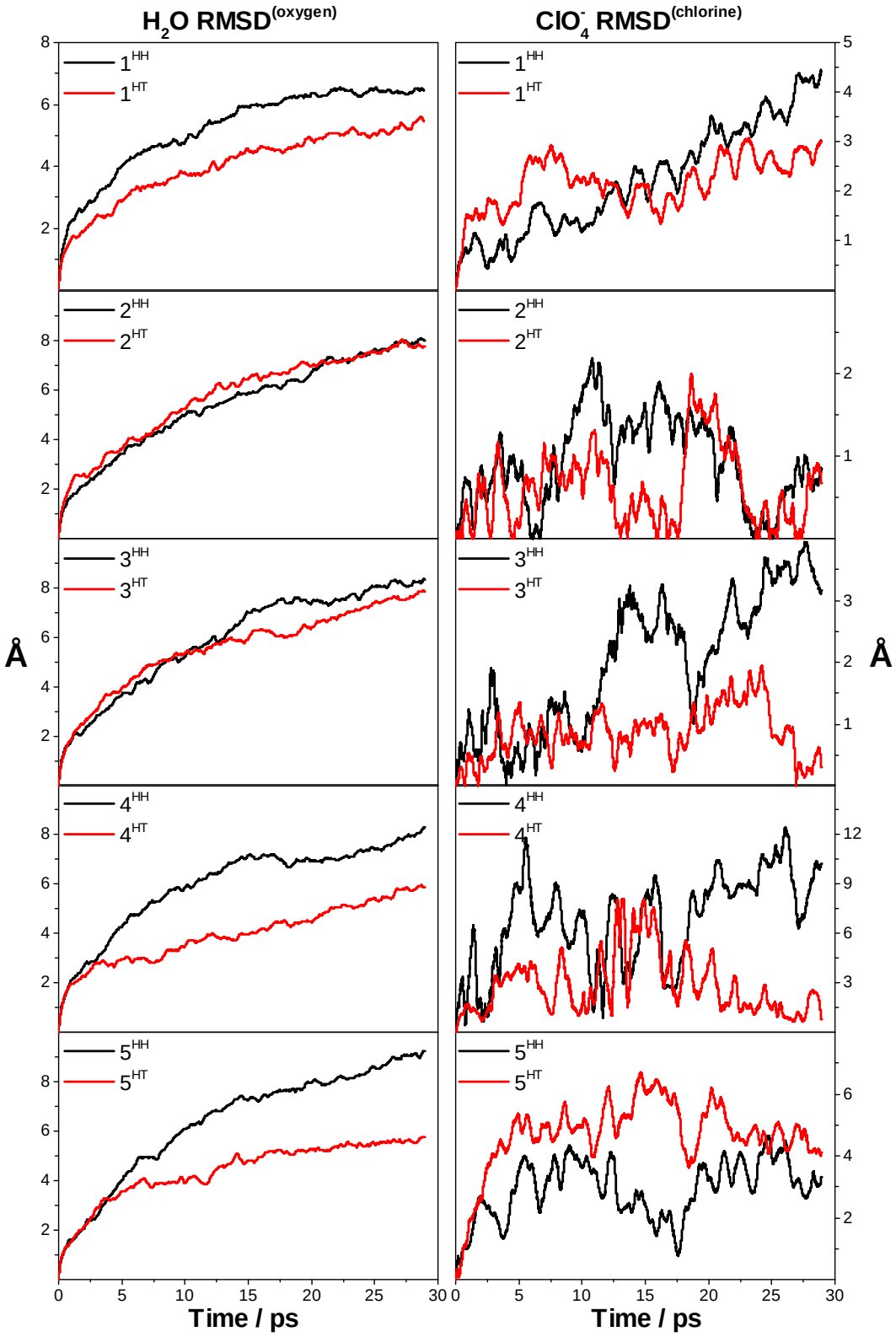

Figure S5: Root mean square deviations (RMSD) for the Cl atoms of the perchlorate anions and oxygen atoms of the water molecules obtained from production trajectory of the CPMD simulations for the HH and HT Pt^{III} complexes.

4 Solute Structure

Likewise in HH complexes, the HT isomers have the same characteristics during the simulation according to their RDFs. Figure S6 shows the *g(r)*PtO of the HT complexes **1** to **5** as an average between two Pt atoms. The first peak between 1.8 Å and 2.6 Å corresponds to the bridge ligands oxygen and the axial aquo ligands directly bonded to the Pt atoms. The integrate (Figure S7) shows 2 oxygen atoms for the complex **1**, 1.5 for complexes **4** and **5** and 1 for complexes **2** and **3**. The peak that starts at 2.9 Å and ends at 3.2 Å correponds to the bridge ligands oxygen that are not directly bonded to the Pt atoms, i.e., to the oxygen atom bonded to the opposite Pt atom. Thus, their integrate provides an average of 3 oxygen atoms for complex **1**, 2.5 for complexes **4** and **5** and 1 for complexes **2** and **3**. The third peak from 3.2 Å to 5.2 Å represents the first solvation shell, containing 13 solvent molecules for complex **1**, 11 for complexes **4** and **5**, 9 for complex **2** and 10 for complex **3**.

Figures S8 to S12 show the evolution of average of main geometrical parameters for HH complexes. The rotation around Pt−Pt bond probed by dihedral angles is not make ease because of solute takes a twisted geometry (Figures 6C and 6D in the main text) when the Pt−Pt bond is elongated due to the bridging ligands antisymmetry. The average values of geometric parameters for HH and HT complexes are given in the Tables S2 and S3, respectively.

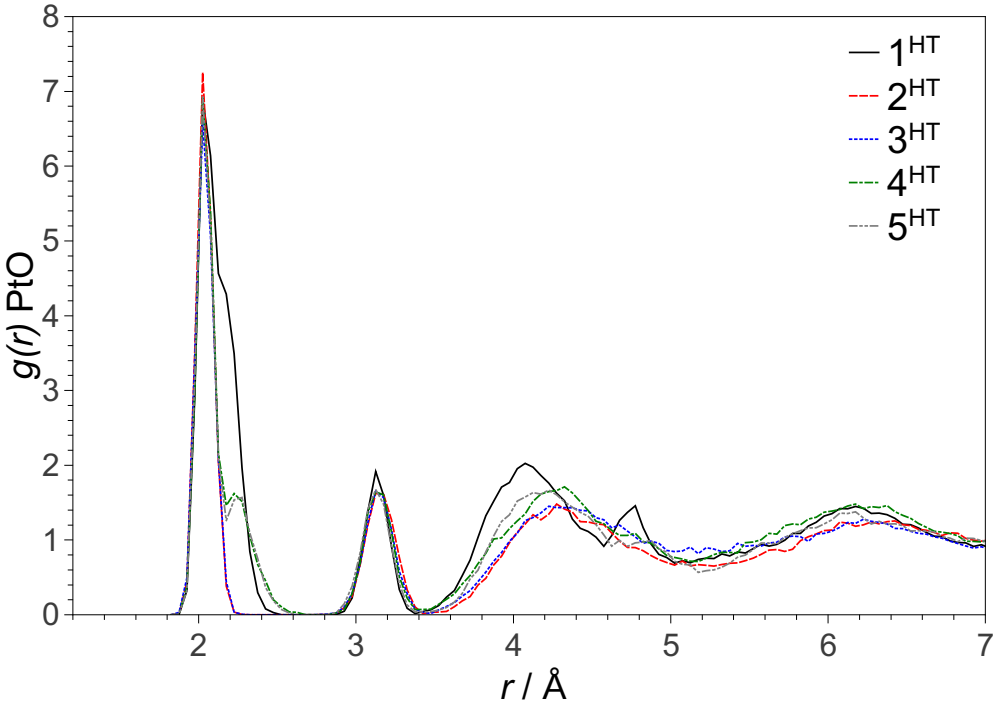

Figure S6: Platinum-oxygen RDFs for 2000 configurations of the production trajectories of the five explored HT Pt(III) complexes. *g(r)* PtO denotes the RDFs or pair correlations as a function of pair distance in Angstrom.

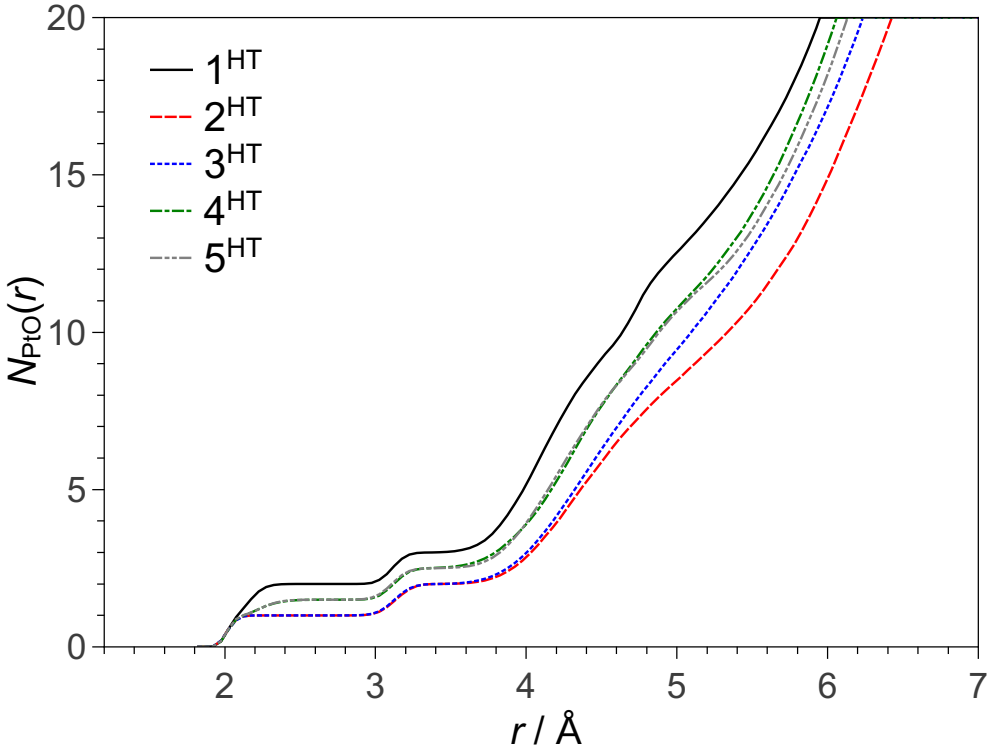

Figure S7: Platinum-oxygen RDF integrates for 2000 configurations of the production trajectories of the five explored HT Pt(III) complexes.

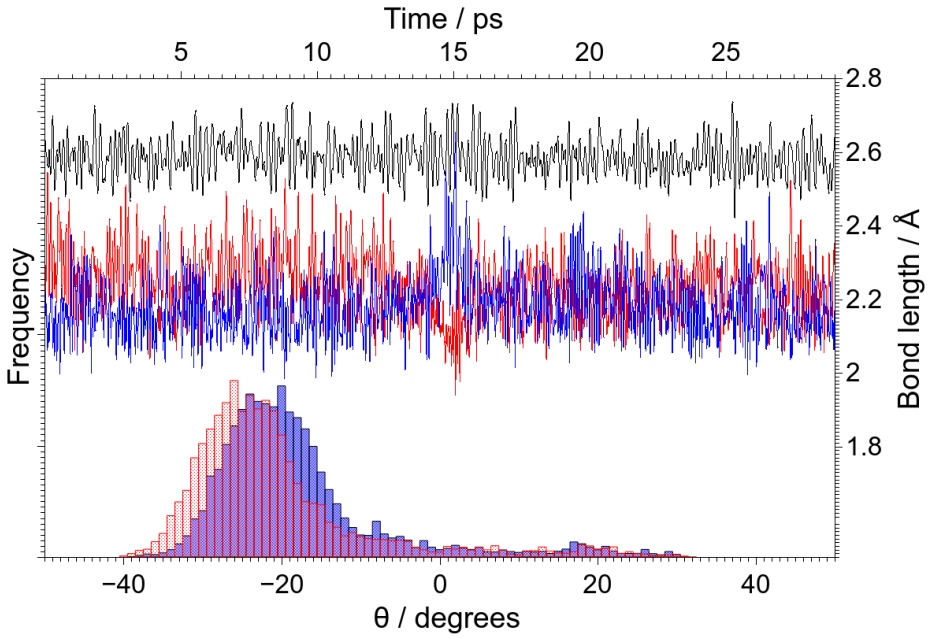

Figure S8: Geometrical data for the HH diaquo complex: Evolution of Pt−Pt (black line), Pt_1−L_1 (red line) and Pt_2−L_2 (blue line) bonds during the CPMD simulation, along with the O_{12}−Pt_2−Pt_1−N_{31} (blue histogram) and O_{22}−Pt_2−Pt_1−N_{41} (red histogram) dihedral angles distribution. Atoms are labeled in Figure S1.

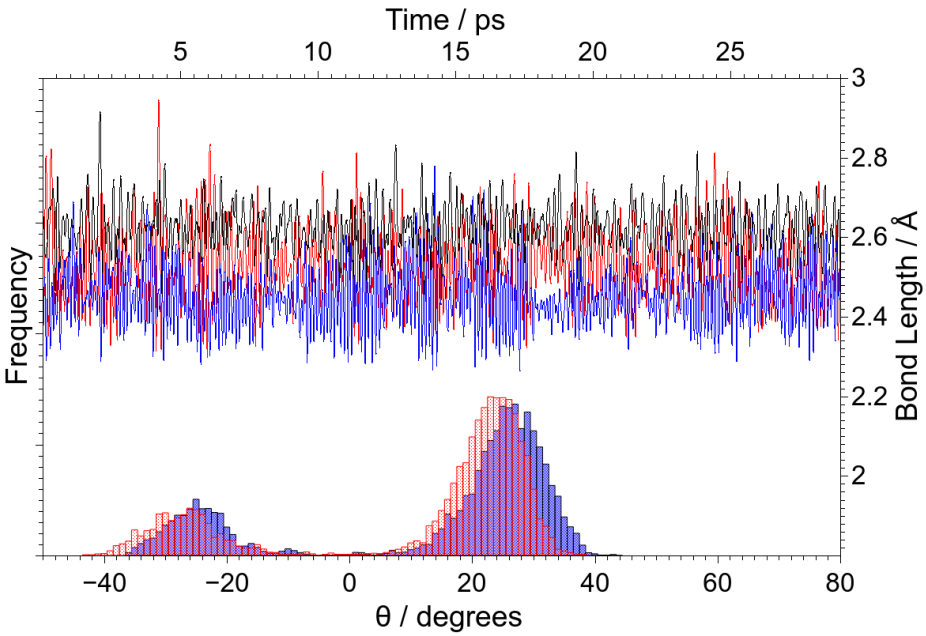

Figure S9: Geometrical data for the HH dichloro complex: Evolution of Pt−Pt (black line), Pt_1-L_1 (red line) and Pt_2-L_2 (blue line) bonds during the CPMD simulation, along with the $O_{12}-Pt_2-Pt_1-N_{31}$ (blue histogram) and $O_{22}-Pt_2-Pt_1-N_{41}$ (red histogram) dihedral angles distribution. Atoms are labeled in Figure S1.

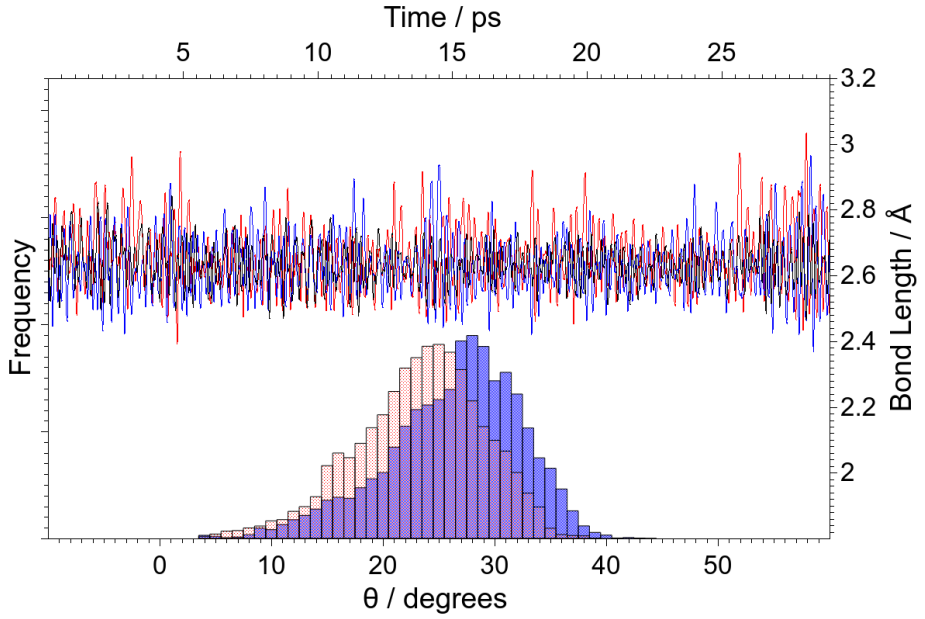

Figure S10: Geometrical data for the HH dibromo complex: Evolution of Pt−Pt (black line), Pt_1-L_1 (red line) and Pt_2-L_2 (blue line) bonds during the CPMD simulation, along with the $O_{12}-Pt_2-Pt_1-N_{31}$ (blue histogram) and $O_{22}-Pt_2-Pt_1-N_{41}$ (red histogram) dihedral angles distribution. Atoms are labeled in Figure S1.

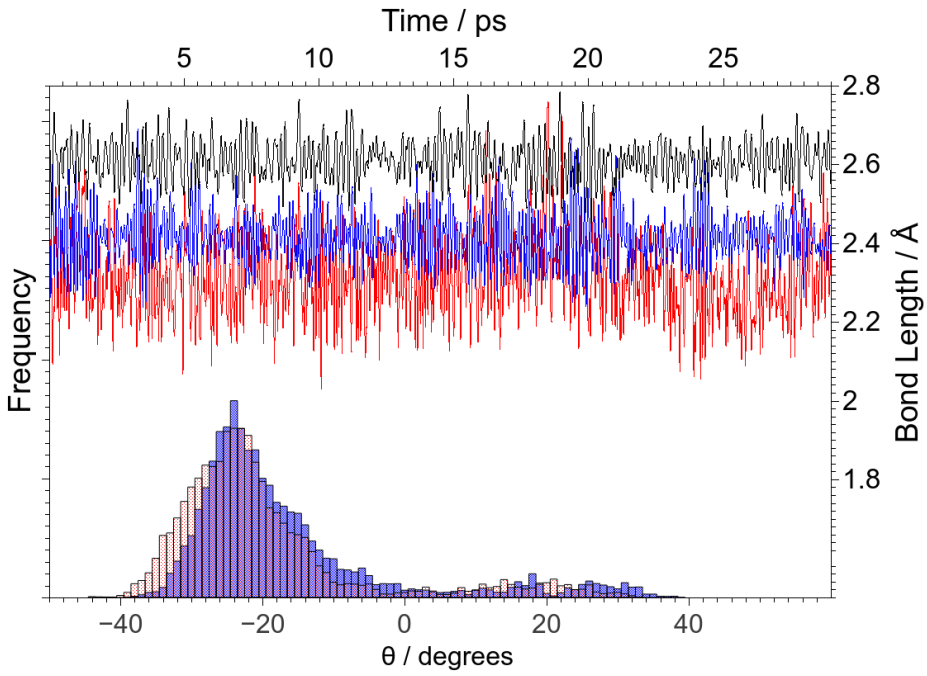

Figure S11: Geometrical data for the HH aquachloro complex: Evolution of Pt−Pt (black line), Pt_1-L_1 (red line) and Pt_2-L_2 (blue line) bonds during the CPMD simulation, along with the $O_{12}-Pt_2-Pt_1-N_{31}$ (blue histogram) and $O_{22}-Pt_2-Pt_1-N_{41}$ (red histogram) dihedral angles distribution. Atoms are labeled in Figure S1.

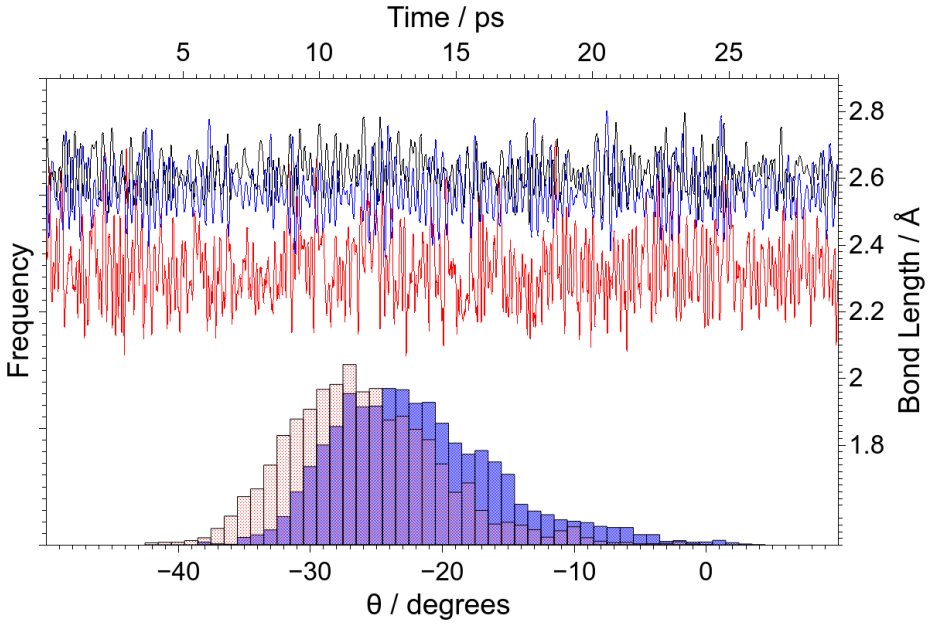

Figure S12: Geometrical data for the HH aquabromo complex: Evolution of Pt−Pt (black line), Pt_1-L_1 (red line) and Pt_2-L_2 (blue line) bonds during the CPMD simulation, along with the $O_{12}-Pt_2-Pt_1-N_{31}$ (blue histogram) and $O_{22}-Pt_2-Pt_1-N_{41}$ (red histogram) dihedral angles distribution. Atoms are labeled in Figure S1.

Table S2: Selected calculated bond lengths (R) in angstrom, angle (A), and dihedral angles (D) in degrees for complexes **1-5** Head-Head (HH).

Complex 1									
	R(Pt1-O)	R(Pt2-O)	R(Pt1-Pt2)	A(Pt1-Pt2-O)	A(Pt2-Pt1-O)	D(N12-Pt2-Pt1-N11)	D(N22-Pt2-Pt1-N21)	D(O12-Pt2-Pt1-N31)	D(O22-Pt2-Pt1-N41)
Unsolv[a]	2.192	2.122	2.540	171.68	169.27	20.45	24.97	23.07	23.94
COSMO[b]	2.358	2.159	2.631	164.82	174.92	31.59	33.56	33.02	30.28
CPMD[c]	2.244	2.180	2.594	168.37	173.05	-20.47	-20.47	-18.96	-21.90
Exptl[d]	—	2.122	2.540	171.68	—	-20.45	-24.97	-23.94	-23.07
Complex 2									
	R(Pt1-Br)	R(Pt2-Br)	R(Pt1-Pt2)	A(Pt1-Pt2-Br)	A(Pt2-Pt1-Br)	D(N12-Pt2-Pt1-N11)	D(N22-Pt2-Pt1-N21)	D(O12-Pt2-Pt1-N31)	D(O22-Pt2-Pt1-N41)
Unsolv[a]	2.613	2.542	2.663	169.36	176.30	27.93	32.94	34.30	26.67
COSMO[b]	2.628	2.574	2.606	170.86	178.09	26.02	28.13	28.98	25.45
CPMD[c]	2.655	2.631	2.635	168.60	174.30	28.10	25.89	23.30	26.55
Exptl	—	—	2.582	—	—	—	—	—	—
Complex 3									
	R(Pt1-Cl)	R(Pt2-Cl)	R(Pt1-Pt2)	A(Pt1-Pt2-Cl)	A(Pt2-Pt1-Cl)	D(N12-Pt2-Pt1-N11)	D(N22-Pt2-Pt1-N21)	D(O12-Pt2-Pt1-N31)	D(O22-Pt2-Pt1-N41)
Unsolv[a]	2.462	2.392	2.645	170.24	176.51	26.83	32.03	33.17	25.81
COSMO[b]	2.478	2.428	2.592	171.62	178.12	24.62	27.25	27.59	24.48
CPMD[c]	2.539	2.444	2.616	168.25	173.63	27.61	26.46	25.76	25.96
Exptl	—	—	2.568	—	—	—	—	—	—
Complex 4									
	R(Pt1-O)	R(Pt2-Br)	R(Pt1-Pt2)	A(Pt1-Pt2-Br)	A(Pt2-Pt1-O)	D(N12-Pt2-Pt1-N11)	D(N22-Pt2-Pt1-N21)	D(O12-Pt2-Pt1-N31)	D(O22-Pt2-Pt1-N41)
Unsolv[a]	2.573	2.539	2.690	163.31	168.96	-31.65	-24.02	-22.97	-34.23
COSMO[b]	2.416	2.485	2.604	170.92	176.28	-26.05	-26.84	-26.67	-25.59
CPMD[c]	2.320	2.565	2.613	168.48	172.24	-23.71	-25.45	-25.78	-21.52
Exptl	—	—	—	—	—	—	—	—	—
Complex 5									
	R(Pt1-O)	R(Pt2-Cl)	R(Pt1-Pt2)	A(Pt1-Pt2-Cl)	A(Pt2-Pt1-O)	D(N12-Pt2-Pt1-N11)	D(N22-Pt2-Pt1-N21)	D(O12-Pt2-Pt1-N31)	D(O22-Pt2-Pt1-N41)
Unsolv[a]	2.548	2.311	2.690	164.04	169.65	-31.65	-24.02	-22.97	-34.23
COSMO[b]	2.384	2.347	2.589	171.44	176.34	-26.02	-26.84	-27.56	-26.53
CPMD[c]	2.309	2.427	2.594	169.71	172.54	-21.36	-23.65	-22.32	-19.42
Exptl	—	—	—	—	—	—	—	—	—

[a]Using one scalar relativistically optimized geometry, no solvent. [b]Using one scalar relativistically optimized geometry with COSMO solvation. [c]Average on 64 CPMD configurations plus 64 explicit solvent molecules. [d]Data from $[Pt_2(NH_3)_4(C_5H_4NO)_2(H_2O)(NO_3)](NO_3)_3 \cdot 2\ H_2O$ X-ray data.[9] Atoms are labeled in Figure S1.

Table S3: Selected calculated bond lengths (R) in angstrom, angle (A), and dihedral angles (D) in degrees for complexes **1-5** Head-Tail (HT).

Complex 1									
	R(Pt1-O)	R(Pt2-O)	R(Pt1-Pt2)	A(Pt1-Pt2-O)	A(Pt2-Pt1-O)	D(N12-Pt2-Pt1-N11)	D(N22-Pt2-Pt1-N21)	D(N32-Pt2-Pt1-O11)	D(O12-Pt2-Pt1-N31)
Unsolv[a]	2.240	2.230	2.610	164.30	164.40	-26.70	-26.80	-24.30	-24.40
COSMO[b]	2.170	2.180	2.540	170.70	169.50	-26.70	-25.60	-23.70	-23.30
CPMD[c]	2.190	2.048	2.580	169.88	170.17	-25.13	-24.93	-21.42	-21.71
Exptl	——	——	——	——	——	——	——	——	——
Complex 2									
	R(Pt1-Br)	R(Pt2-Br)	R(Pt1-Pt2)	A(Pt1-Pt2-Br)	A(Pt2-Pt1-Br)	D(N12-Pt2-Pt1-N11)	D(N22-Pt2-Pt1-N21)	D(N32-Pt2-Pt1-O11)	D(O12-Pt2-Pt1-N31)
Unsolv[a]	2.590	2.590	2.660	175.40	175.10	21.50	21.70	18.50	18.50
COSMO[b]	2.600	2.600	2.610	173.50	173.30	25.50	25.40	24.00	24.00
CPMD[c]	2.649	2.645	2.647	172.14	171.58	23.25	23.02	21.22	21.42
Exptl[d]	2.573	2.562	2.582	171.95	171.04	30.20	29.81	26.48	25.84
Complex 3									
	R(Pt1-Cl)	R(Pt2-Cl)	R(Pt1-Pt2)	A(Pt1-Pt2-Cl)	A(Pt2-Pt1-Cl)	D(N12-Pt2-Pt1-N11)	D(N22-Pt2-Pt1-N21)	D(N32-Pt2-Pt1-O11)	D(O12-Pt2-Pt1-N31)
Unsolv[a]	2.440	2.440	2.640	175.00	174.80	25.70	25.80	29.70	29.50
COSMO[b]	2.451	2.452	2.593	174.10	174.00	24.30	24.30	22.50	22.70
CPMD[c]	2.513	2.495	2.619	172.00	171.92	23.19	22.23	21.54	21.90
Exptl[d]	2.444	2.429	2.568	173.18	174.62	28.58	30.57	25.15	25.76
Complex 4									
	R(Pt1-Br)	R(Pt2-O)	R(Pt1-Pt2)	A(Pt1-Pt2-O)	A(Pt2-Pt1-Br)	D(N12-Pt2-Pt1-N11)	D(N22-Pt2-Pt1-N21)	D(N32-Pt2-Pt1-O11)	D(O12-Pt2-Pt1-N31)
Unsolv[a]	2.480	2.640	2.690	164.83	171.09	23.90	25.80	22.23	21.99
COSMO[b]	2.515	2.321	2.590	170.56	173.11	24.95	25.95	23.54	23.57
CPMD[c]	2.600	2.280	2.604	170.85	173.40	24.96	22.71	21.40	23.61
Exptl	——	——	——	——	——	——	——	——	——
Complex 5									
	R(Pt1-Cl)	R(Pt2-O)	R(Pt1-Pt2)	A(Pt1-Pt2-O)	A(Pt2-Pt1-Cl)	D(N12-Pt2-Pt1-N11)	D(N22-Pt2-Pt1-N21)	D(N32-Pt2-Pt1-O11)	D(O12-Pt2-Pt1-N31)
Unsolv[a]	2.325	2.578	2.668	164.45	171.97	23.40	24.55	21.39	20.71
COSMO[b]	2.375	2.301	2.579	171.10	173.48	24.73	25.89	23.39	22.97
CPMD[c]	2.445	2.287	2.607	169.54	173.00	26.99	25.36	24.33	24.52
Exptl	——	——	——	——	——	——	——	——	——

[a]Using one scalar relativistically optimized geometry, no solvent. [b]Using one scalar relativistically optimized geometry with COSMO solvation. [c]Average on 64 CPMD configurations plus 64 explicit solvent molecules. [d]Data from $[X(NH_3)_2Pt(C_5H_4NO)_2Pt(NH_3)_2X](NO_3)_2 \cdot nH_2O$ ($X^- = Cl^-$, Br^-), X-Ray data.[10] Atoms are labeled in Figure S1.

5 Evolution of average

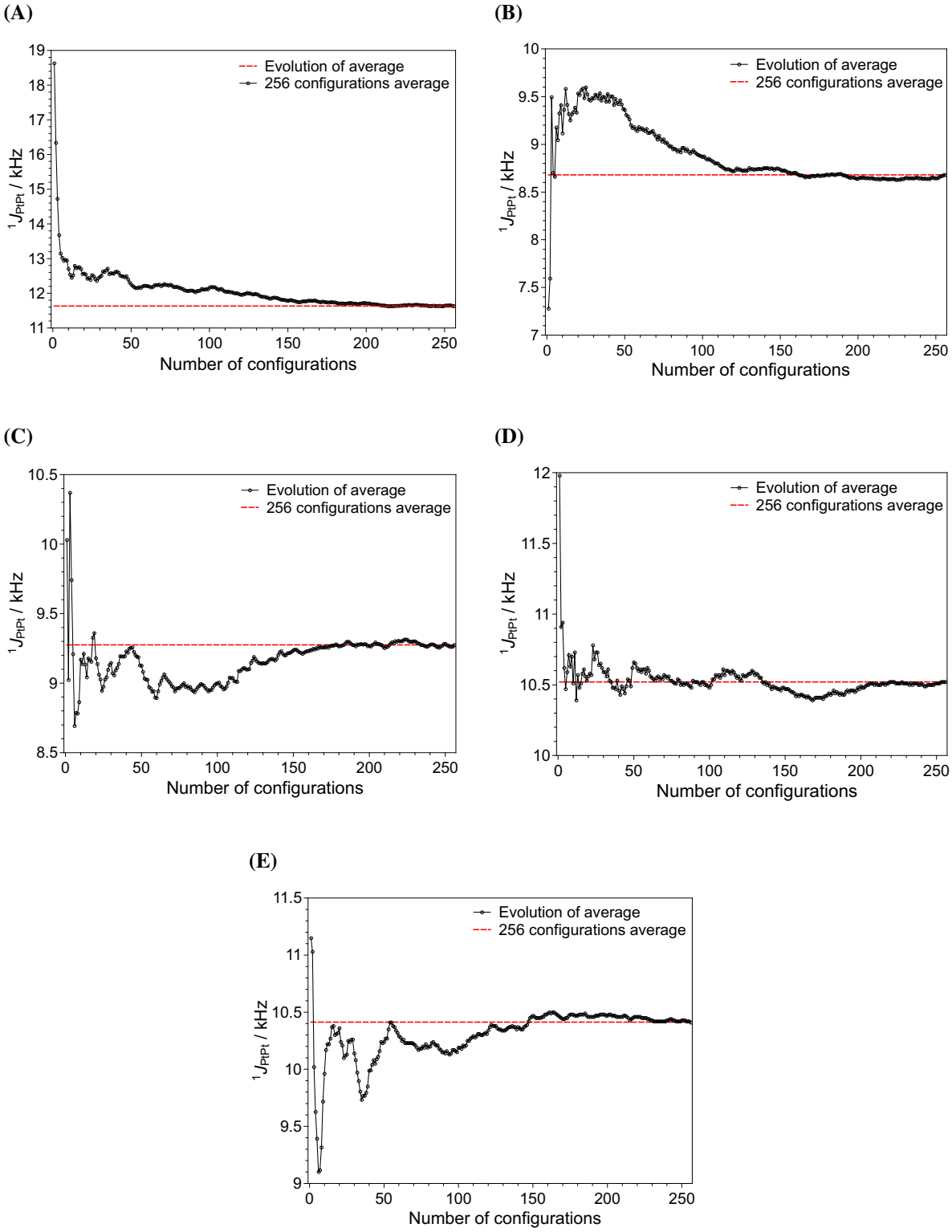

Figure S13: Evolution of the average calculated $^1J_{PtPt}$ for diaquo (**A**), dibromo (**B**), dichloro (**C**), aquabromo (**D**) and aquachloro (**E**) complexes using 256 configurations of the production trajectory.

6 Relativistic Scalar Correction on the $^1J_{PtPt}$

Table S4 shows $^1J_{PtPt}$ computed using an evenly spaced set of 64 configurations from production trajectory of the HH diaquo complex. In addition, the number of NN solvent molecules were included with increments of five, along with COSMO to treat bulk solvent effects. The bare-solute regime also was considered in order to assess only the thermal effects on the selected configurations. The values in Table S4 was used to plot the graph of the Figure 7 in the main text.

Table S4: $^1J_{PtPt}$ spin-spin coupling constant[a] dependence on solvated complexes as a functions of the number of explicit water molecules. Each data point involves a sampling of 64 CPMD configurations. The asterisk "solvent molecules" correspond to bare solute from MD-averaged data. $^1J_{PtPt}$ calculations were performed at ZORA-SR/PBE0/jcpl level of theory.

	Complex									
Solvent Count	**1**		**2**		**3**		**4**		**5**	
	HH	**HT**	**HH**	**HT**	**HH**	**HT**	**HH**	**HT**	**HH**	**HT**
$*^b$	11856	11940	4416	4638	4645	4783	5888	6083	5539	6308
0	11385	10779	6547	6878	6882	7084	8295	8204	7088	8412
5	9205	9169	6807	7157	7210	7350	8317	8034	8160	8330
10	9191	9142	6853	7218	7301	7476	8443	8063	8249	8398
15	9236	9132	6927	7238	7321	7542	8520	8093	8301	8424
20	9114	9094	6909	7240	7304	7439	8533	8074	8311	8411
25	9005	9086	6862	7211	7268	7458	8362	8047	8271	8399

[a]All values are given in Hz. [b]Average results from 256 configurations of CPMD trajectories including spin-orbit corrections, plus specified number of explicit solvent molecules and implicit solvation (COSMO) to model bulk effect.

7 PBE Functional with CPMD Configurations

Tables S5 and S6 show the $^{1}J_{PtPt}$ and the ^{195}Pt chemical shifts, respectively, computed at ZORA-SO/PBE/jcpl level of theory using CPMD configurations. The $^{1}J_{PtPt}$ average value decreases about 1 kHz for diaquo complex, and 530 Hz for dihalo and aquahalo complexes. For chemical shifts no significantly improvement was observed in comparison with the values calculated at ZORA-SO/PBE0/jcpl.

7.1 Spin-Spin Coupling Constant - $^{1}J_{PtPt}$

Table S5: Calculated $^{1}J_{PtPt}$ spin-spin coupling constants[a] for complexes 1-5 Head-to-Head (HH) with different solvation and unsolvation models. $^{1}J_{PtPt}$ calculations were performed at ZORA-SO/PBE/TZP(jcpl) level of theory. The values in square brackets are the relative error regarding the experimental data.[b]

Complex	Unsolvated[c]	COSMO[d]	CPMD-Bare[e]	CPMD[f]	Exptl[g]
1^{HH}	11920 [34]	13918 [57]	13812 [55]	10617 [19]	8886
2^{HH}	6139 [-3]	7589 [20]	5738 [-9]	8201 [30]	6306
3^{HH}	6182 [-7]	8051 [21]	6061 [-9]	8679 [31]	6636
4^{HH}	6545 [-14]	8051 [6]	7605 [4]	10002 [32]	7574
5^{HH}	6737 [-11]	10002 [29]	7663 [-1]	9879 [27]	7774

[a]All values are given in Hz. [b]All values are given in %. [c]Relativistic couplings from relativistically optimized geometry unsolvated. [d]Relativistic couplings from relativistically optimized geometry with implicit solvation. [e]Average on 64 CPMD configurations, wherein all solvent molecules were stripped. [f]Average on 256 CPMD configurations plus specified number of explicit nearest neighboring solvent molecules and implicit solvation to model bulk effect. Values in parenthesis are average on 64 CPMD configurations. [g]Measurements using an acidic D_2O solution ($DClO_4/D_2O$) to suppress deprotonation of the diaqua complexes. Data extracted of Iwatsuki and coworkers.[11]

7.2 Chemical Shift - δ^{195}Pt

Table S6: Calculated δ^{195}Pt chemical shift[a] for complexes **1** to **5** Head-to-Head (HH) with different solvation and unsolvation models at ZORA-SO/PBE/jcpl level of theory. The values in square brackets are the absolute deviation relative to experiment data.[a]

Complex	Atom	Unsolvated[b]	COSMO[c]	CPMD[d]	Exptl[e]
1	$Pt[N_4]$	-844	-844	-844	-844
	$Pt[N_2O_2]$	393	393	393	393
2	$Pt[N_4]$	-1338 [350]	-1759 [771]	-929 [59]	-988
	$Pt[N_2O_2]$	-1332 [1300]	-1008 [976]	32 [64]	-32
3	$Pt[N_4]$	-1120 [172]	-1716 [768]	-795 [153]	-948
	$Pt[N_2O_2]$	-1296 [1425]	-834 [963]	67 [62]	129
4	$Pt[N_4]$	-1346 [45]	-1193 [198]	-311 [1080]	-1391
	$Pt[N_2O_2]$	-1197 [1840]	-1475 [2118]	-465 [1108]	643
5	$Pt[N_4]$	-1229 [35]	-1426 [232]	-567 [627]	-1194
	$Pt[N_2O_2]$	-820 [1338]	-1132 [1650]	-129 [647]	518
Mean absolute deviation[a]		813	959	475	

[a] All values are given in ppm and spin-orbit corrections are included for all calculations. [b] Relativistic chemical shifts from relativistically optimized geometry unsolvated. [c] Relativistic chemical shifts from relativistically optimized geometry with implicit solvation. [d] Average on 256 CPMD configurations plus 10 explicit nearest neighboring solvent molecules and implicit solvation to model bulk effect. [e] Data extracted of Iwatsuki and coworkers.[11]

8 Assessment of DFT Functional

The level of theory for the complexes study was chosen based on molecular dynamics in solution works, as well as on NMR parameter calculations. The functional GGA of acronym PBE, presented good results with acceptable computational cost, when applied in molecular dynamics simulations.[1,12,13] The hybrid functional of acronym PBE0, on the other hand, showed good results for coupling constants calculations.[12,14] In addition, a assessment were carried out in order to check the functional and geometries effects on the $^1J_{PtPt}$ calculations. Table S7 gathers the results of $^1J_{PtPt}$ calculated with geometries of the complexes **1-5**, optimized at different level of theory with and without implicit solvation (COSMO). The values in square brackets correspond to the relative error with respect to experimental *J*-coupling and PtPt bond length data.

The diaquo complex (**1**) was the one that present the worst results and a dramatic dependence of the functional and geometry. The three level of theory overestimate the $^1J_{PtPt}$ values even upon solvation, being the PBE level in unsolvated model with the lowest error (34%). For dihalo complexes, the $^1J_{PtPt}$ is overestimate in the three levels of the unsolvated model. For dibromo complex (**2**), the PBE0/PBE and PBE present almost the same results, with lowest error (3%), while for dichloro complex (**3**) the level of theory that yield the better result is the PBE without solvation and, the PBE0/PBE and PBE0 levels are very similar. In the COSMO model the better result is obtained with the PBE level of theory for both complexes, even though the values are overestimate by 20% and 21%, respectively. The aquahalo complexes (**4** and **5**) in unsolvated model have the majority results underestimate with the three levels. However, the PBE0 level proves to be the better for both complexes, with errors of -3% and 1% for complex **4** and **5**, respectively. In the COSMO model, the PBE0/PBE level overestimates the results, but is the better for complex **5**, and the PBE is the better for complex **4**, overestimating the $^1J_{PtPt}$ by 6%.

The Pt−Pt bond lengths show poor agreement with the three level of theory analyzed, overestimating the experimental values by ∼200 pm. However, these results are not surprising, since the experimental data were obtained by X-ray diffraction in solid state (see footnote of Table S7), i.e., the lengths of the experimental chemical bonds tend to be shorter in the crystalline structure. Thus, Pt−Pt bonds show to be longer in unsolvated calculations when compared to those obtained using COSMO, which suggest that the inclusion of the solvent effect may compress the complex structures.

In general, in unsolvated model, the three levels underestimated the $^1J_{PtPt}$ values of the complexes containing halides and overestimated the results for diaquo complex. Despite this, the $^1J_{PtPt}$ calculations at PBE level show the better results for diaquo and dihalo complexes. For aquahalo complexes, the better results are obtained with the PBE0 level. On the other hand, in the COSMO model, all $^1J_{PtPt}$ values are overestimated. However, for dihalo complexes, the three levels present very similar errors, as well as the PBE and PBE0/PBE have almost equal errors for aquahalo complexes.

Therefore, in order to better assess the accuracy of one functional for the five complexes, the mean relative error (MRE) of unsolvated and COSMO models were calculated. Thus, the PBE0/PBE level has the lowest MRE for unsolvated calculations, 1%, while the PBE and PBE0 levels show MREs of 8% and

20%. For COSMO model, the PBE level has the lowest MRE, 27% and, for PBE0/PBE and PBE0 levels, the MREs are 32% and 47%. Despite PBE present a MRE somewhat lower than PBE0/PBE, the PBE0 hybrid functional has 25% of exact exchange which reduces the self-interaction error.[15,16] In this sense, the PBE0/PBE is the best choice to avoid minimum approaches and provide more reliable calculated results in solvated model. These results indicate that the geometry is better described with GGA functional and the hybrid functional is the better choice for properties calculations.

Table S7: $^1J_{PtPt}$(Hz) and Pt−Pt bond lengths (Å) calculated using static geometries of the Head-to-Head complexes **1-5** with different level of theory with and without implicit solvation via COSMO. Value in square brackets are the relative error (%) regarding the experimental data (Exptl).

Complex	**Level of Theory***	**Unsolv.**	R(Pt-Pt)	**COSMO**	R(Pt-Pt)	**Exptl**	
						$^1J_{PtPt}$	**R[PtPt)**
	PBE	11920 [34]	2.684	13918 [57]	2.581		
1	PBE0/PBE	13841 [56]	2.684	15439 [74]	2.581	8886	2.540[a]
	PBE0	19971 [125]	2.540	18843 [112]	2.631		
	PBE	6139 [-3]	2.717	7589 [20]	2.648		
2	PBE0/PBE	6113 [-3]	2.717	7881 [25]	2.648	6306	2.582[a]
	PBE0	5578 [-12]	2.663	7921 [26]	2.606		
	PBE	6182 [-7]	2.671	8051 [21]	2.631		
3	PBE0/PBE	5854 [-12]	2.671	8397 [27]	2.631	6636	2.568[a]
	PBE0	5922 [-11]	2.645	8285 [25]	2.592		
	PBE	6545 [-14]	2.746	8051 [6]	2.626		
4	PBE0/PBE	6034 [-20]	2.746	8087 [7]	2.626	7574	2.561[b]
	PBE0	7358 [-3]	2.690	9694 [28]	2.604		
	PBE	6737 [-11]	2.728	10002 [29]	2.624		
5	PBE0/PBE	6333 [-16]	2.728	10017 [29]	2.624	7774	2.554[b]
	PBE0	7649 [1]	2.690	10752 [42]	2.589		
	PBE	8	6	27	2		
MRE**	PBE0/PBE	1	6	32	2	—	—
	PBE0	20	3	47	2		

*PBE = Geometry optimized at ZORA-SR/PBE/TZP and $^1J_{PtPt}$ calculated at ZORA-SO/PBE/jcpl; PBE0/PBE = $^1J_{PtPt}$ calculated at ZORA-SO/PBE0/jcpl using optimized geometries at ZORA-SR/PBE/TZP; PBE0 = Geometry optimized at ZORA-SR/PBE0/TZP and $^1J_{PtPt}$ calculated at ZORA-SO/PBE0/jcpl. **Mean Relative Error in %. [a]Bond lengths from X-Ray diffraction[9] of $[Pt_2(NH_3)_4(C_5H_4NO)_2(H_2O)(NO_3)](NO_3)_3 \cdot 2\,H_2O$; [b]Average values between the diaquo and the respective aquahalo complex. Data estimated for use as a reference only, since the aquahalo complexes do not have experimental data.

In the same way, for chemical shifts the PBE0/PBE level present the lowest MRE for the two platinum atoms in both models evaluated. However, in the unsolvated model the shifts values are overestimate (23% for Pt[N_4] and 174% for Pt[N_2O_2]), while in the COSMO model the shifts values are underestimate

with a smaller MRE (-23% for Pt[N_4] and -18% for Pt[N_2O_2]). The PBE and PBE0 levels yield larger MREs with greater difference between the two platinum atoms. These results are give in Table S8.

Table S8: Calculated ^{195}Pt chemical shift[a] for complexes **1** to **5** Head-to-Head (HH) with different level of theory with and without implicit solvation via COSMO. The values in square brackets are the relative error regarding the experimental data.[b]

Complex	Level of Theory*	Unsolv.		COSMO		Exptl	
		Pt[PtN_4]	**Pt[PtN_2O_2]**	**Pt[PtN_4]**	**Pt[PtN_2O_2]**	**Pt[PtN_4]**	**Pt[PtN_2O_2]**
1	PBE	-844	393	-844	393	-844	393
	PBE0/PBE	-844	393	-844	393		
	PBE0	-844	393	-844	393		
2	PBE	-1540 [56]	-553 [1630]	-1003 [1]	-101 [214]	-988	-32
	PBE0/PBE	-1521 [54]	-508 [1487]	-925 [10]	-115 [259]		
	PBE0	-891 [-10]	-1164 [3538]	-1767 [79]	-1085 [3291]		
3	PBE	-1722 [82]	-509 [-494]	-959 [1]	95 [-26]	-948	129
	PBE0/PBE	-1748 [84]	-444 [-444]	-890 [10]	82 [-37]		
	PBE0	-654 [-31]	-1123 [-971]	-1730 [82]	-909 [-805]		
4	PBE	-926 [-33]	-833 [-230]	-517 [-63]	-444 [-169]	-1391	643
	PBE0/PBE	-964 [-31]	-684 [-206]	-456 [-52]	-456 [-171]		
	PBE0	-1322 [-5]	-518 [-181]	-1294 [-7]	-1446 [-325]		
5	PBE	-1008 [-16]	-351 [-168]	-543 [-54]	-180 [-135]	-1194	518
	PBE0/PBE	-1027 [-14]	-215 [-141]	-550 [-60]	-109 [-121]		
	PBE0	-527 [-56]	-855 [-265]	-1476 [24]	-1121 [-316]		
MRE**	PBE	22	184	-29	-29	—	—
	PBE0/PBE	23	174	-23	-18		
	PBE0	-26	530	44	461		

*PBE = Geometry optimized at ZORA-SR/PBE/TZP and δ^{195}Pt calculated at ZORA-SO/PBE/jcpl; PBE0/PBE = δ^{195}Pt calculated at ZORA-SO/PBE0/jcpl using optimized geometries at ZORA-SR/PBE/TZP; PBE0 = Geometry optimized at ZORA-SR/PBE0/TZP and δ^{195}Pt calculated at ZORA-SO/PBE0/jcpl; δ^{195}Pt calculated as $\delta_{calc} = \sigma_{ref} - \sigma_{probe} + \delta_{ref}^{exptl}$ where the complex $\mathbf{1}^{\mathbf{HH}}$ is used as internal reference. **Mean Relative Error in %. [a]All values are given in ppm and spin-orbit corrections are included for all calculations. [b]All values are given in %. [c]Data extracted of Iwatsuki and coworkers.[11]

9 *J*-coupling analysis

9.1 Natural Localized Molecular Orbitals

Figure S14 shows the natural localized molecular orbitals of the $L_1-Pt[N_4]$ and $L_2-Pt[N_2O_2]$ bonds, which contribute to spin-spin Pt−Pt coupling constant.

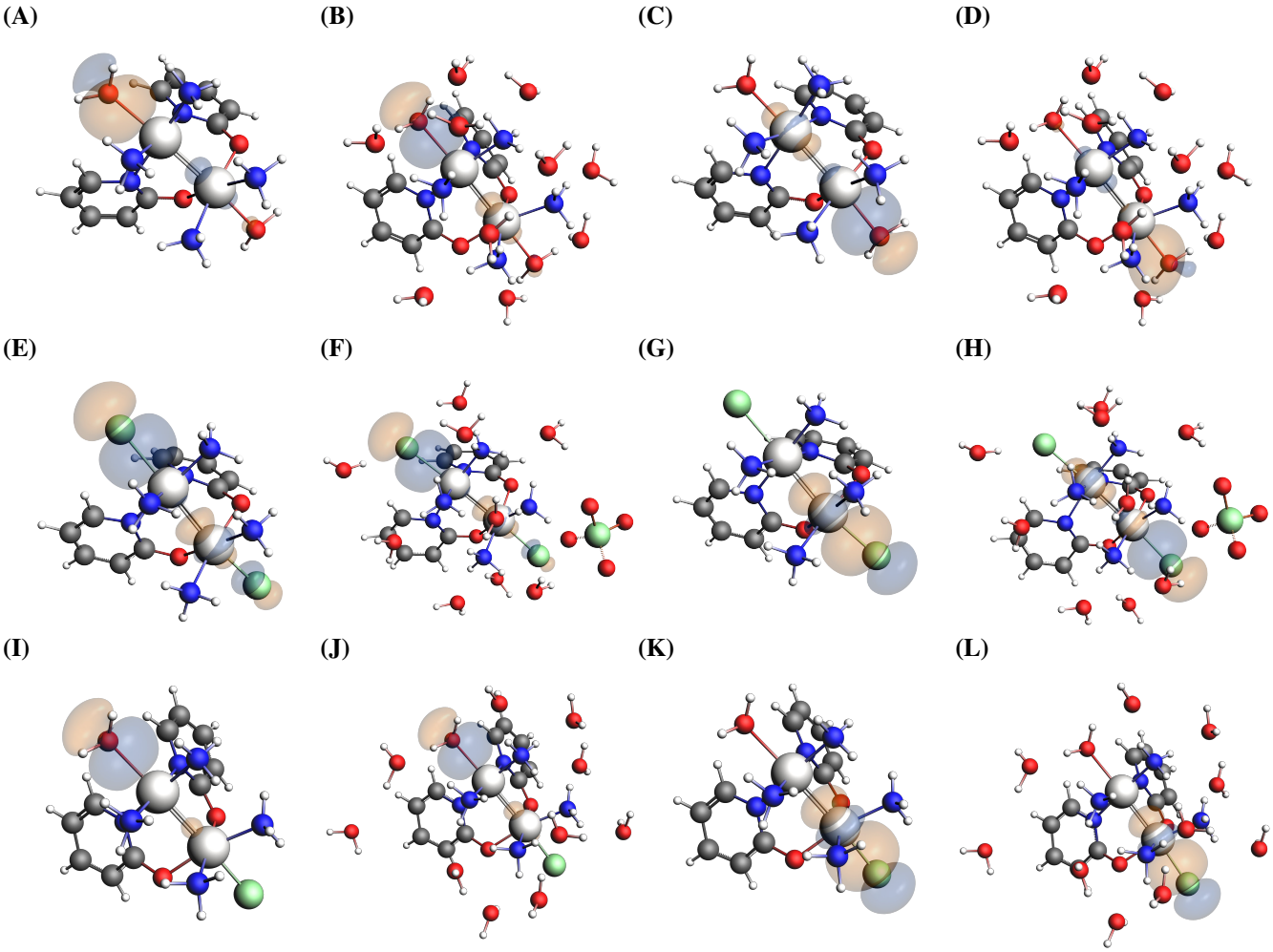

Figure S14: Snapshots from the production trajectory of HH diaquo (A to D), dichloro (E to H) and aquachloro (I to L) complexes showing the $L_1-Pt[N_4]$ and $L_2-Pt[N_2O_2]$ bonding NLMOs in the CPMD-Bare and CPMD models. Such snapshots were chosen because they represent more faithfully the average value obtained in each evaluated solvation model. Isosurface values: 0.03 au.

9.2 Canonical Molecular Orbitals

Figures S15-S17 show the main canonical molecular orbitals which contribute to spin-spin Pt−Pt coupling constant.

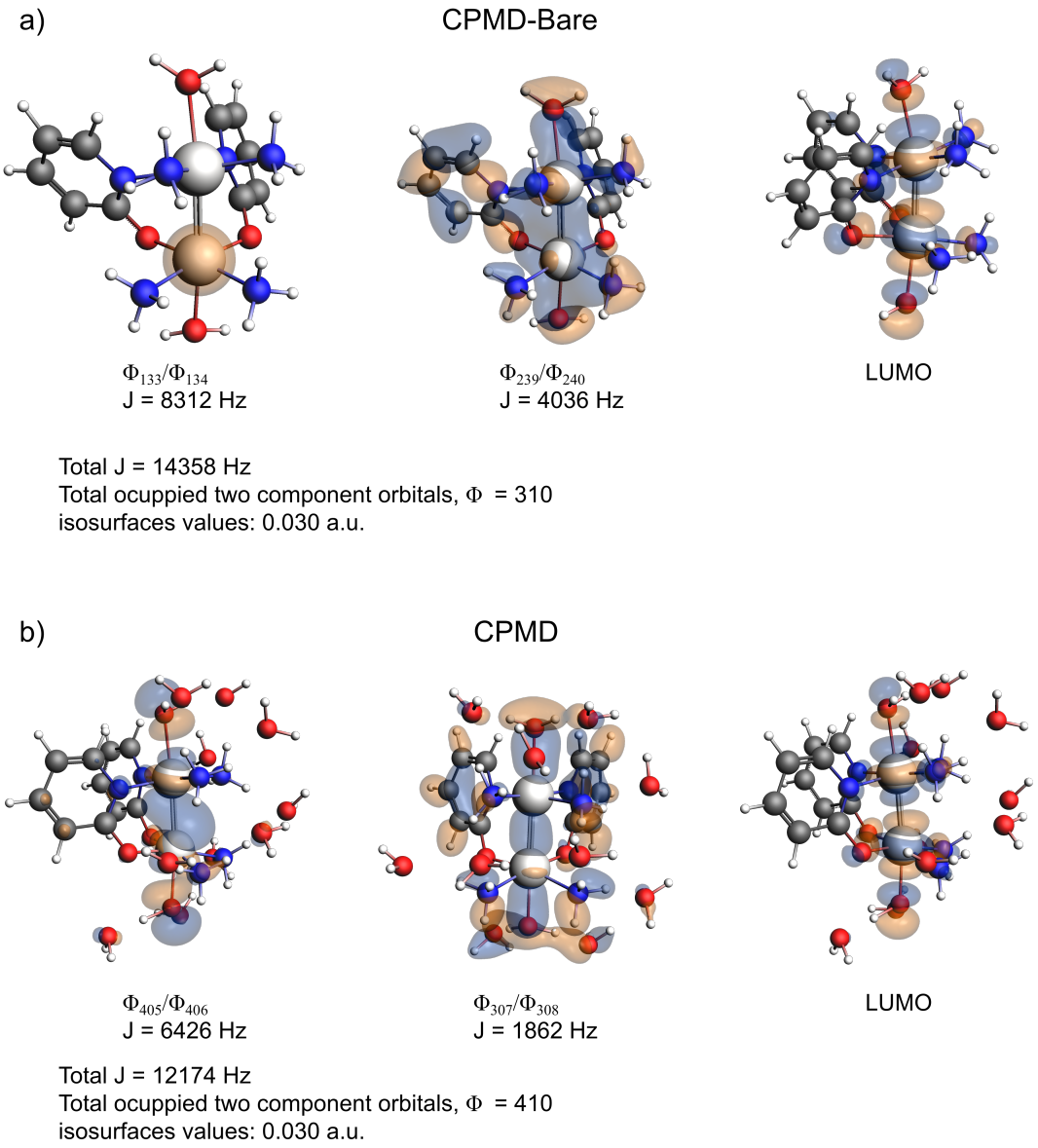

Figure S15: Plots of scalar ZORA canonical molecular orbitals (CMOs) with the main contributions to reduced spin-spin coupling for diaquo complex ($\mathbf{1}^{\mathbf{HH}}$) in the CPMD-Bare model (a) and CPMD model (b). Listed contributions are for spin-orbit ZORA CMOs.

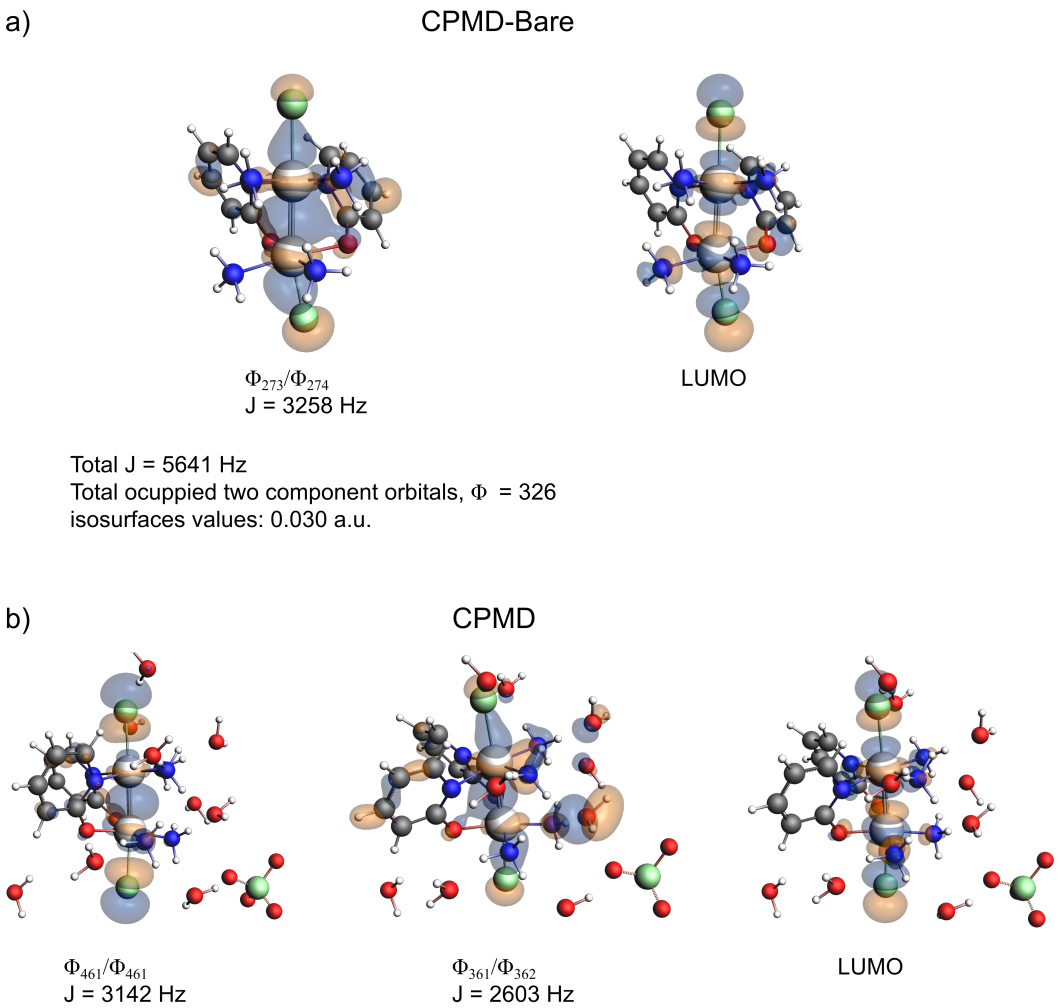

Figure S16: Plots of scalar ZORA canonical molecular orbitals (CMOs) with the main contributions to reduced spin-spin coupling for dihalo complex ($\mathbf{3^{HH}}$) in the CPMD-Bare model (a) and CPMD model (b). Listed contributions are for spin-orbit ZORA CMOs.

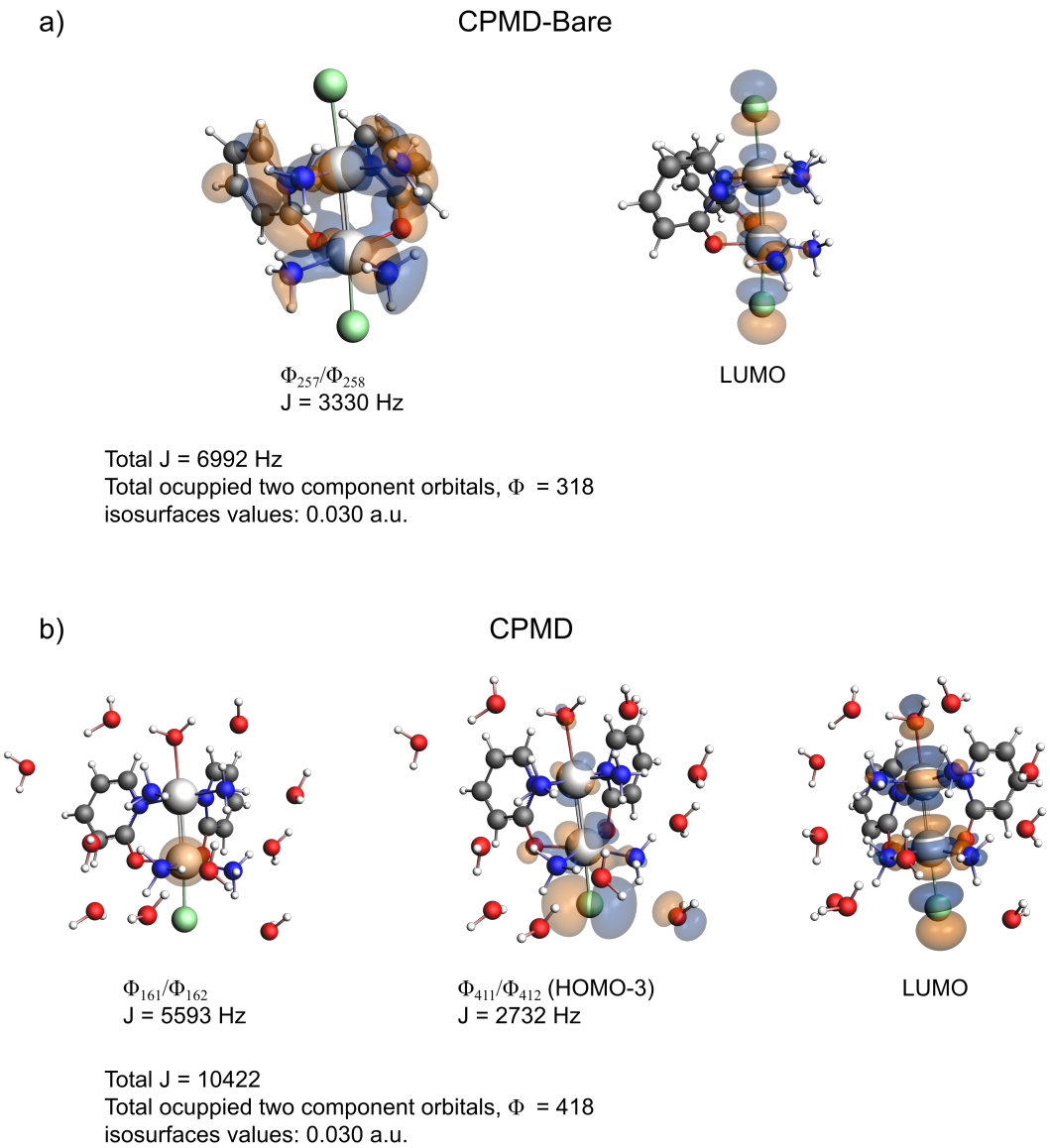

Figure S17: Plots of scalar ZORA canonical molecular orbitals (CMOs) with the main contributions to reduced spin-spin coupling for aquahalo complex ($\mathbf{5^{HH}}$) in the CPMD-Bare model (a) and CPMD model (b). Listed contributions are for spin-orbit ZORA CMOs.

10 Evolution of Average of the Shielding Tensor

Figures S18–S21 show the evolution of average of shielding tensor. Likewise for $^{1}J_{\mathrm{PtPt}}$ the statistic stabilizes the reported averages for 256 configurations. Around 150 configurations are enough to achieve the average values and therefore, the configuration sampling are representative for complete simulations.

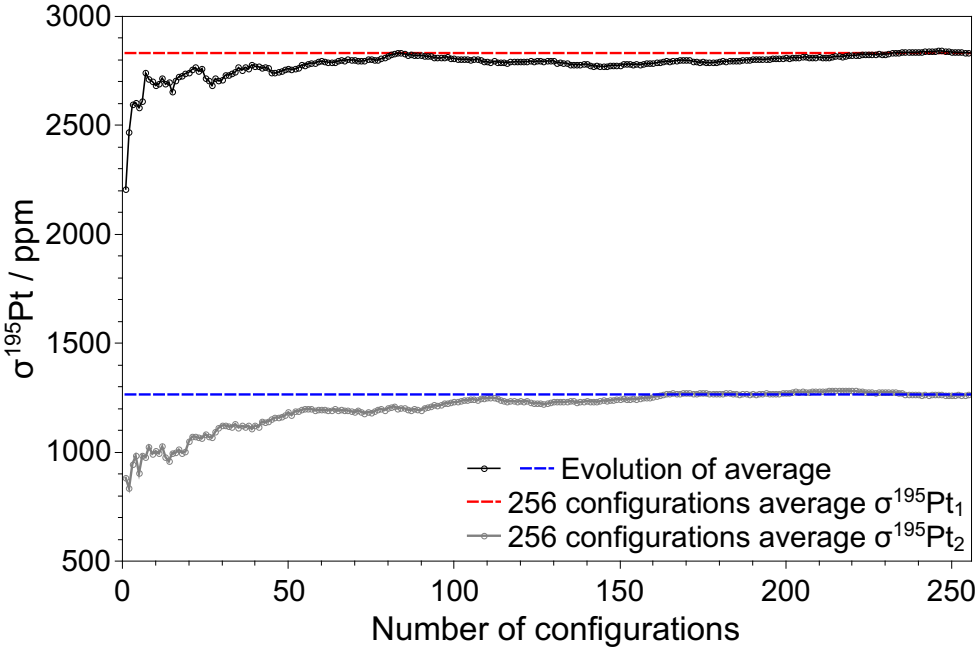

Figure S18: Evolution of average of the shielding tensor values for diaquo complex, using 256 configurations of production trajectory.

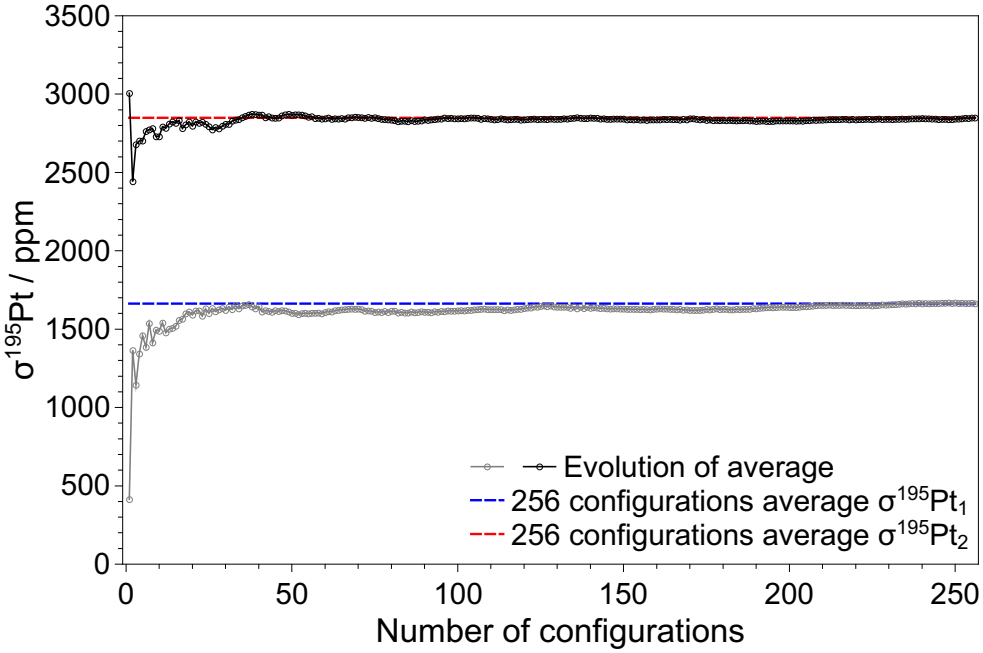

Figure S19: Evolution of average of the shielding tensor values for dibromo complex, using 256 configurations of production trajectory.

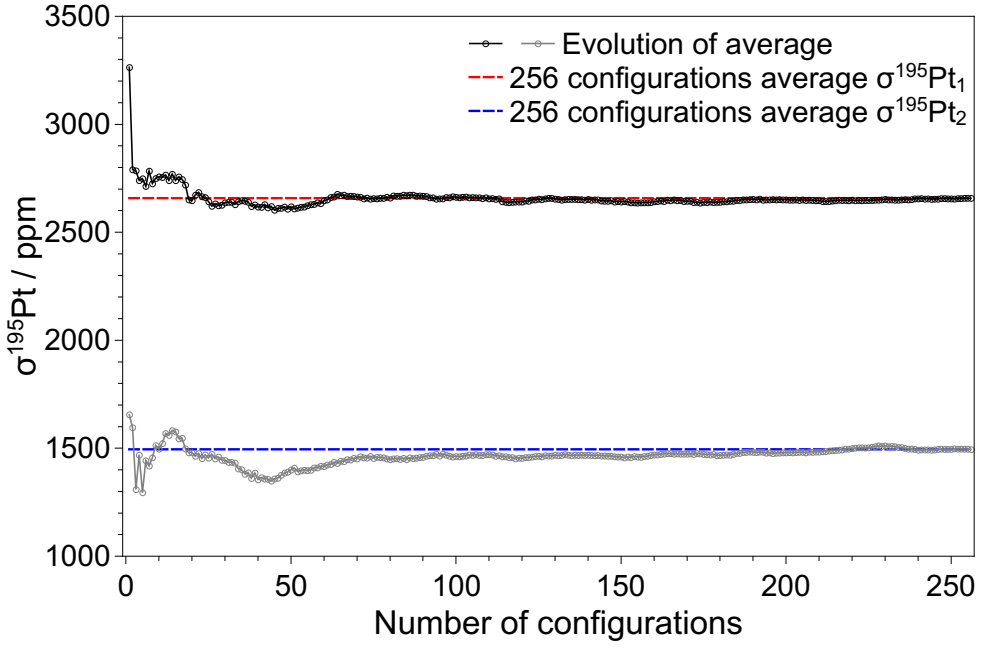

Figure S20: Evolution of average of the shielding tensor values for dichloro complex, using 256 configurations of production trajectory..

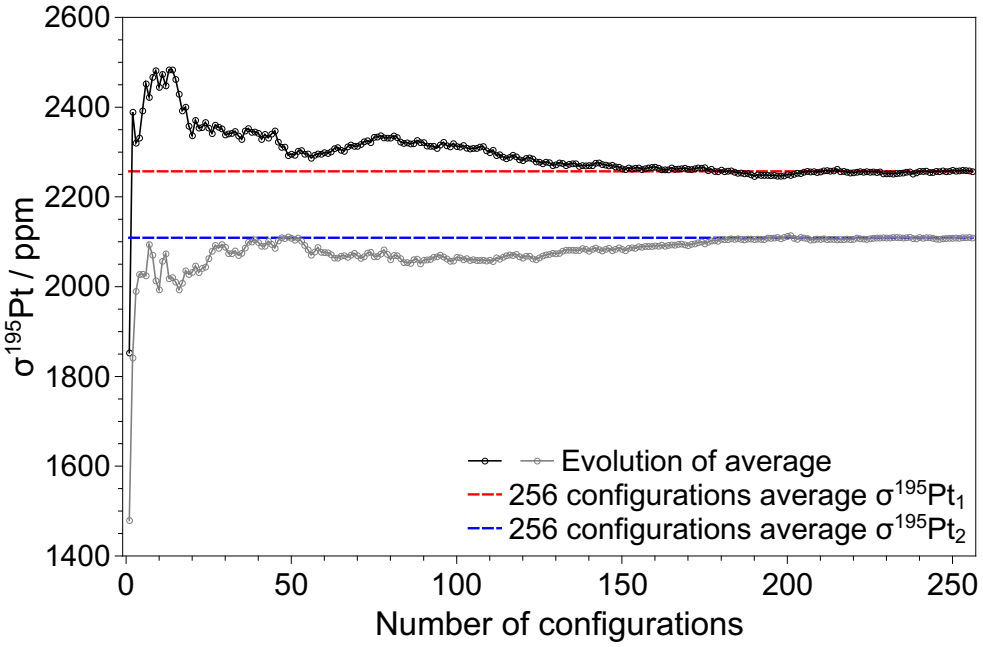

Figure S21: Evolution of average of the shielding tensor values for aquabromo complex, using 256 configurations of production trajectory..

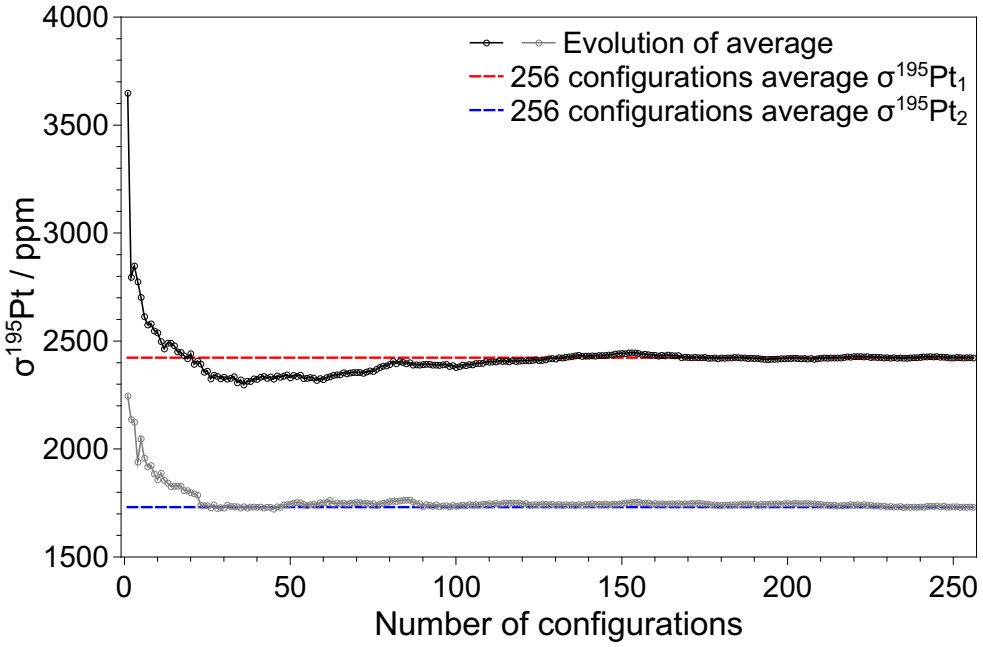

Figure S22: Evolution of average of the shielding tensor values for aquachloro complex, using 256 configurations of production trajectory..

11 Isotropic shielding of ^{195}Pt

The chemical shifts were calculated from isotropic shielding values and experimental shifts (Table S9) using: $\delta_{calc} = \sigma_{ref} - \sigma_{probe} + \delta_{ref}^{exptl}$. Here, $\mathbf{1}^{HH}$ was used as a secondary reference 'ref' in the calculations, and the experimental chemical shift of $\mathbf{1}^{HH}$ with respect to aqueous H_2PtCl_6 was added to convert the calculated shifts to the standard reference.

Table S9: Calculated isotropic shielding[a] of ^{195}Pt of the Head-to-Head (HH) and Head-to-Tail (HT) complexes at ZORA-SO/PBE0/jcpl level of theory with different approaches.

Complex	Atom	Unsolvated	COSMO	CPMD
		σ_{probe}[ppm]	σ_{probe} [ppm]	σ_{probe} [ppm]
$\mathbf{1}^{HH}$	Pt[N_4]	2167	2313	2832
	Pt[N_2O_2]	1476	815	1265
$\mathbf{2}^{HH}$	Pt[N_4]	2214	3236	2849
	Pt[N_2O_2]	3033	2292	1663
$\mathbf{3}^{HH}$	Pt[N_4]	1977	3199	2658
	Pt[N_2O_2]	2992	2116	1495
$\mathbf{4}^{HH}$	Pt[N_4]	2645	2763	2257
	Pt[N_2O_2]	2387	2654	2109
$\mathbf{5}^{HH}$	Pt[N_4]	1849	2945	2423
	Pt[N_2O_2]	2724	2328	1731
$\mathbf{1}^{HT}$	Pt	3078	2543	2068
$\mathbf{2}^{HT}$	Pt	2683	2752	2259
$\mathbf{3}^{HT}$	Pt	2501	2657	2117
$\mathbf{4}^{HT}$	Pt[H_2O]	2195	2166	1746
	Pt[Br]	2902	3158	2663
$\mathbf{5}^{HT}$	Pt[H_2O]	2259	2290	1768
	Pt[Cl]	2418	2921	2466

[a]Isotropic shielding of the $\mathbf{1}^{HH}$ used as a secondary reference (σ_{ref}) at the different approaches: Unsolvated: Pt[N_4] = 2167 ppm; Pt[N_2O_2] = 1476 ppm; COSMO: Pt[N_4] = 2313 ppm; Pt[N_2O_2] = 815 ppm; CPMD: Pt[N_4] = 2832 ppm; Pt[N_2O_2] = 1265 ppm. [b]Experimental chemical shifts of the $\mathbf{1}^{HH}$ complex relative to aqueous H_2PtCl_6 used as reference: Pt[N_4] = -844 ppm; Pt[N_2O_2] = 393 ppm. For $\mathbf{1}^{HT}$, $\mathbf{2}^{HT}$ and $\mathbf{3}^{HT}$ complexes, the average of σ_{ref} and δ_{ref}^{exptl} reference values was used to calculate the chemical shifts of the complexes.

12 Coordinates of atomic positions of the last one snapshot from CPMD equilibration trajectory

The atomic positions, in Å, equilibrated in the NVT ensamble at 350 K by 3 ps with CPMD are listed.

12.1 Diaquo complex 1^{HH}

246
Last snapshot from equilibration trajectory
Pt 7.416243 7.837546 6.744898
Pt 9.991084 7.664002 6.808564
C 8.720590 7.985087 9.487734
C 8.732982 8.004483 10.933730
C 7.528220 7.830688 11.591734
C 6.313718 7.539681 11.012206
C 6.364395 7.543036 9.634056
C 9.082666 10.374116 6.518701
C 9.364464 11.790863 6.553878
C 8.382539 12.592138 7.068001
C 7.214750 12.034020 7.605829
C 6.924247 10.706018 7.470372
N 7.543583 7.777291 8.897840
N 7.891023 9.863346 7.018816
N 6.974784 5.800530 6.876545
N 7.363903 7.782065 4.753348
N 10.193554 5.770405 7.489888
N 10.533774 7.264457 4.910362
O 9.827131 8.249997 8.778152
O 9.988013 9.594435 6.090142
O -1.838995 9.688653 6.240414
O 9.447195 4.579360 12.448998
O 7.234532 3.726859 11.317471
O 3.199499 2.958117 11.106586
O 1.719200 15.186716 2.018480
O 1.651633 9.186220 14.715131
O 6.241594 1.722814 4.990422
O 1.163940 16.579988 12.535599
O -1.169257 1.351499 2.692675
O 12.493128 6.115824 8.807031
O 5.355547 9.734104 4.205635
O 2.392403 7.228189 11.997996
O 15.031374 5.462778 5.277826
O 12.519841 3.037435 16.619684
O 7.447033 4.492947 -1.075085
O 3.696583 10.069986 6.540642
O 7.960763 2.038370 7.826227

O 3.212549 10.925767 9.096502
O 8.041756 3.898780 5.227252
O 15.086579 13.417016 6.012648
O 1.297399 7.513321 1.470690
O 12.800258 8.767670 3.795028
O 13.628018 16.435852 11.743775
O 10.380743 0.740399 10.920355
O 12.775311 11.210485 14.977163
O 8.312840 4.592134 8.907869
O 6.453018 10.157986 17.216330
O 5.714833 12.383378 0.821802
O -0.590881 2.434495 4.807003
O 12.723207 12.749840 7.306658
O 14.411790 3.770227 -2.944111
O 8.848629 -4.121305 3.185004
O -1.273202 6.390440 17.034863
O 11.899765 13.129700 4.810756
O 4.946959 7.611486 6.665421
O 9.735877 3.757033 3.057169
O 12.204666 12.708261 1.829272
O 14.738486 4.541509 8.751467
O 11.651767 15.293764 2.829267
O 11.542896 4.575829 4.717971
O 11.063106 10.042036 2.299232
O 3.254498 0.448166 19.795486
O 0.939087 10.557617 5.550981
O -0.732662 4.280372 -0.399223
O 10.139323 0.398653 8.376111
O 8.994332 7.813737 2.528340
O 3.855935 11.856627 -1.418863
O 7.372816 -0.708715 1.458757
O -3.238851 7.829838 6.976183
O 0.642464 0.811296 6.301368
O 4.887060 6.260001 4.345127
O 9.426848 1.394437 1.711022
O 5.558589 -0.996895 3.494903
O 4.012750 9.830935 11.583346
O 4.413882 18.535904 13.539574
O 12.044869 2.780818 10.141953
O 2.300756 15.087179 14.516660
O 1.298429 4.800865 11.526186
O 4.393382 16.395313 -0.026742
O 8.955591 5.413612 0.955640
O 12.731292 5.490075 11.317244
O 18.138668 8.992578 3.459342
O 10.940511 8.412195 13.200101
O 11.289680 6.183901 13.776487

O 10.380218 7.727716 15.463306
O 12.673030 7.994465 14.839665
O 4.945965 7.508434 16.459837
O 6.274244 7.574879 14.422169
O 4.299347 8.704224 14.475157
O 4.379208 6.198724 14.409087
O 3.225558 3.330082 5.691165
O 3.845734 4.885432 7.462431
O 2.969371 2.696218 7.999592
O 1.546917 4.409269 7.094594
O 16.215542 11.927423 15.542344
O 16.804161 11.717032 17.931284
O 14.864496 10.624887 17.081594
O 14.901291 13.076918 17.224731
H 9.644542 8.059125 11.582295
H 7.521140 8.023702 12.663399
H 5.425298 7.478822 11.632925
H 5.438306 7.382355 9.031484
H 10.307469 12.155897 6.170608
H 8.601943 13.623712 7.232963
H 6.487551 12.698366 8.049532
H 6.079221 10.155908 7.908015
H 7.373108 5.502193 7.761494
H 7.477292 5.115448 6.146631
H 5.993616 5.581248 6.948618
H 7.135278 6.838217 4.385935
H 8.203633 8.085565 4.232994
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H 9.381397 5.446787 7.941740
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H 8.295563 -4.505309 2.448757
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12.2 Diaquo complex 1^{HT}

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Last snapshot from equilibration trajectory
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Pt 9.27511050 7.19645812 7.67581646
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C 9.40218654 11.86565968 8.67355539
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12.3 Dibromo complex 2^{HH}

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Last snapshot from equilibration trajectory
Pt 6.752236 8.191100 5.588234
Pt 9.265512 8.276096 5.782055
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C 7.981750 4.847795 7.877200
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C 7.715948 9.672093 7.949843
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O 10.490314 1.067526 6.120594
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H 18.061563 7.819531 16.545553
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12.4 Dibromo complex 2^{HT}

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Last snapshot from equilibration trajectory
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Br 4.01145231 8.61687551 6.53926975
Cl 3.93088130 1.46622003 2.31923830
Cl 8.40019659 4.97827760 2.23979356

12.5 Dichloro complex 3^{HH}

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Last snapshot from equilibration trajectory
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Pt 9.097945 7.943642 6.957417
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C 6.271353 4.784726 7.459255
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C 5.151687 6.386884 5.607520
C 7.193613 8.982003 8.816739
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12.6 Dichloro complex 3^{HT}

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Last snapshot from equilibration trajectory
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H 12.27492037 5.88330338 12.18115932
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Cl 4.53177061 8.25257272 4.81171634
Cl 3.50583243 3.84297730 4.16235646
Cl 11.49134752 6.79909998 2.54103770

12.7 Aquabromo complex 4^{HH}

242
Last snapshot from equilibration trajectory
Pt 6.879545 7.067048 5.408997
Pt 9.273239 7.519839 6.361329
C 7.505095 5.660323 7.990326
C 7.267428 4.684796 9.032274
C 6.178752 3.826342 8.914199
C 5.358647 3.914922 7.762199
C 5.641345 4.798493 6.749343
C 7.214974 9.192614 7.535758
C 6.797464 9.935707 8.663071
C 5.454557 9.878069 9.049102
C 4.490196 9.166479 8.314343
C 5.050847 8.360132 7.297905
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N 6.323900 8.415789 6.936104

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12.8 Aquabromo complex 4^{HT}

242
Last snapshot from equilibration trajectory
Pt 9.02787592 6.89533964 7.61313445

Pt 6.85293655 7.71461094 6.29338305
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C 8.01460038 9.54023495 8.41277857
C 7.80343959 10.71777271 9.21632245
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C 8.95030296 11.16263120 9.85674266
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O 7.06501237 9.33473151 7.51059168
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O 3.27912227 8.20402872 13.91825541
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H 10.62949628 2.33817391 4.23930325
H 8.73176080 1.46592172 11.93112854
H 8.90090789 -0.05516157 11.96098720
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H 4.33369532 1.78377231 14.15455053
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H 0.72576386 9.64055780 -1.07579553
H 1.48981768 7.18045086 13.70778855
H 1.75938156 5.84811765 12.84039016
H 11.90402617 10.17952546 7.88099935
H 11.56735689 10.38811338 6.32507810
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H 3.34787631 2.42083294 8.30583110
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H 8.69245146 10.59218314 14.61481882
H 9.91156204 10.00246316 13.81313840

H 10.45843391 8.89089165 1.92396870
H 11.85874953 8.66179359 2.41388089
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Cl 6.48134198 11.23569316 2.18003525
Cl 5.60134545 4.84274870 2.06588515
Cl 13.52966927 13.18130266 1.68755337

12.9 Aquachloro complex 5^{HH}

242
Last snapshot from equilibration trajectory
Pt 6.076719 8.732503 6.435009
Pt 8.377820 7.853343 6.227111
C 6.388353 5.898290 6.896638
C 5.928210 4.516874 7.136252
C 4.585726 4.266947 6.975611
C 3.690487 5.363962 6.884923
C 4.152726 6.638248 6.670006
C 7.684081 8.370248 9.038250
C 7.946801 8.099410 10.409630
C 6.873164 8.110424 11.310225
C 5.615192 8.385674 10.753349
C 5.369273 8.496236 9.441363
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O 10.711649 3.560519 8.738718
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O -3.398941 2.408902 16.934715
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O 13.369510 15.702959 5.925705
O 9.925276 2.108316 11.318075
O 16.200270 14.107694 9.938745
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O 12.369447 6.622004 8.853674
O 13.739036 9.173356 2.885680
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O 3.714928 9.203776 -1.311079
O 5.830285 10.150253 -0.808767
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H 7.847673 11.795334 -1.827985
H 8.941561 12.824039 -2.138926
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H 6.526836 10.572160 10.795126
H 7.554843 11.781885 10.889200
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H 2.715140 1.334107 7.013020
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H 8.993302 -0.762289 6.328047
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H 16.673925 9.657088 6.619117
H 8.069070 9.770559 1.839762
H 7.759498 8.270600 1.328449
H 10.320545 4.068886 9.455056
H 10.723997 4.185343 8.024482
H 3.415897 1.237096 12.204767
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H 2.347949 7.609810 19.960014
H 2.310666 8.158830 18.561604
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H 8.863661 0.915919 14.348695
H 7.527169 0.128021 14.890662
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Cl 4.377726 10.347083 -0.669434
Cl 3.824547 3.256542 0.991000
Cl 11.574164 6.495109 2.342716

12.10 Aquachloro complex 5^{HT}

242
Last snapshot from equilibration trajectory
Pt 6.11927309 7.90864281 6.69108507
Pt 8.73331572 7.04093902 6.62143325
C 7.13587652 6.08384139 8.93053973
C 6.89304858 5.25572417 10.06963615
C 5.60767528 4.91509225 10.37490581
C 4.49090874 5.35304872 9.62055048
C 4.79269598 6.10265049 8.51495141
C 8.05862012 9.59955393 8.21631329
C 8.28200203 10.62338322 9.20547178
C 10.38112197 9.30163103 8.01706391
C 9.54522683 10.93315146 9.56826565
C 10.63988940 10.24850328 8.96826830
N 6.06459436 6.49162293 8.20276144
N 4.90229622 6.70178032 5.48267224
N 6.22900606 9.27241183 5.19694887
N 7.97728292 5.39223964 5.63710188
N 9.15571634 7.90633945 4.83654522
N 9.13243332 8.93789113 7.65868433
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O 3.80743017 8.68274628 6.97049027
O 6.83956095 9.23691375 8.01805310
O 1.08219874 3.93168039 1.65886983

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O 8.46101324 6.91862168 13.72188618
O 6.02750725 2.61739569 1.30885338
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O 5.86051907 13.03075034 8.07702116
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O 11.22235825 14.72224224 14.22794854
O 10.56382766 5.01432677 12.60450465
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O 2.41550657 14.79308888 4.22308985
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