

SUPPORTING INFORMATION

Systematic assessment of DFT methods for geometry optimization of mononuclear platinum-containing complexes

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Equations used

Root mean square deviation (calculated with Chimera)

$$RMSD = \sqrt{\frac{\sum (x_1 - x_0)^2}{n}}$$

Where:

x_0 = is the experimental value

x_1 = calculated value

n = total number of values

Percent deviation

$$\Delta = \frac{\sum_{i=1}^n (|y_i - x_i|/x_i)}{n} \times 100$$

Where:

y_i = calculated value

x_i = experimental value as reported by crystallographic data

n = number of bonds

Sample input files

Sample geometry optimization input file using B3LYP/ZORA/TZVP/D3BJ/CPCM:

```
! UKS B3LYP RIJCOSX ZORA ZORA-def2-TZVP SARC/J TightSCF SlowConv D3BJ CPCM
! NormalPrint Grid7 GridX7 NoFinalGrid
! OPT
! PAL8

%basis
  newgto Pt "SARC-ZORA-TZVP" end
  end

%method
  SpecialGridAtoms 78
  SpecialGridIntAcc 7
  end

%maxcore 1024

%scf
  maxiter 500
  end

%cpcm
  surfacetype vdw_gaussian
  end

%geom
  maxiter 200
  end

* xyzfile 0 1 CDMSOP.xyz
```

Sample geometry optimization input file using BP86/DKH2/SVP/D3BJ/CPCM:

```
! UKS BP86 DKH2 DKH-def2-SVP SARC/J TightSCF SlowConv D3BJ CPCM
! NormalPrint Grid7 NoFinalGrid
! OPT
! PAL8
```

```
%basis
  newgto Pt "SARC-DKH-TZVP" end
end
```

```
%method
  SpecialGridAtoms 78
  SpecialGridIntAcc 7
end
```

```
%rel
  Dkh1CAutoAux true
end
```

```
%maxcore 1024
```

```
%scf
  maxiter 500
end
```

```
%ccp
  surfacetype vdw_gaussian
end
```

```
%geom
  maxiter 200
end
```

```
* xyzfile 0 1 CDMSOP.xyz
```

Sample geometry optimization input file using PBE0/ZORA/TZVP/CPCM:

```
! UKS PBE0 RIJCOSX ZORA ZORA-def2-TZVP SARC/J TightSCF SlowConv CPCM  
! NormalPrint Grid7 GridX7 NoFinalGrid  
! OPT  
! PAL8
```

```
%basis  
  newgto Pt "SARC-ZORA-TZVP" end  
end
```

```
%method  
  SpecialGridAtoms 78  
  SpecialGridIntAcc 7  
end
```

```
%maxcore 1024
```

```
%scf  
  maxiter 500  
end
```

```
%cpcm  
  surfacetype vdw_gaussian  
end
```

```
%geom  
  maxiter 200  
end
```

```
* xyzfile 0 1 GUDCEN.xyz
```

Sample geometry optimization input file using PBE/ZORA/SVP/D3BJ/CPCM

```
! UKS PBE ZORA ZORA-def2-SVP SARC/J TightSCF SlowConv D3BJ CPCM  
! NormalPrint Grid7 NoFinalGrid  
! OPT  
! PAL8
```

```
%basis  
  newgto Pt "SARC-ZORA-TZVP" end  
end
```

```
%method  
  SpecialGridAtoms 78  
  SpecialGridIntAcc 7  
end
```

```
%maxcore 1024
```

```
%scf  
  maxiter 500  
end
```

```
%cpcm  
  surfacetype vdw_gaussian  
end
```

```
%geom  
  maxiter 200  
end
```

```
* xyzfile 0 1 GUDCEN.xyz
```

Sample geometry optimization input file using TPSSh/DKH2/TZVP/D3BJ/CPCM

! UKS TPSSh RIJCOSX DKH2 DKH-def2-TZVP SARC/J TightSCF SlowConv D3BJ CPCM

! NormalPrint Grid7 GridX7 NoFinalGrid

! OPT

! PAL8

%basis

newgto Pt "SARC-DKH-TZVP" end

end

%method

SpecialGridAtoms 78

SpecialGridIntAcc 7

end

%rel

Dkh1CAutoAux true

end

%maxcore 1024

%scf

maxiter 500

end

%cpcm

surfacetype vdw_gaussian

end

%geom

maxiter 200

end

* xyzfile 0 1 GUDCEN.xyz

Sample numerical frequency calculation input file using PBE0/ZORA/TZVP/CPCM:

```
! UKS PBE0 RIJCOSX ZORA ZORA-def2-TZVP SARC/J TightSCF SlowConv CPCM
! NormalPrint Grid7 GridX7 NoFinalGrid
! NumFreq
! PAL8
```

```
%basis
  newgto Pt "SARC-ZORA-TZVP" end
end
```

```
%method
  SpecialGridAtoms 78
  SpecialGridIntAcc 7
end
```

```
%maxcore 1024
```

```
%scf
  maxiter 500
end
```

```
%cpcm
  surfacetype vdw_gaussian
end
```

```
* xyzfile 0 1 GUDCEN_PBE0_ZORA_TZVP_CPCM.xyz
```


Supplementary figures

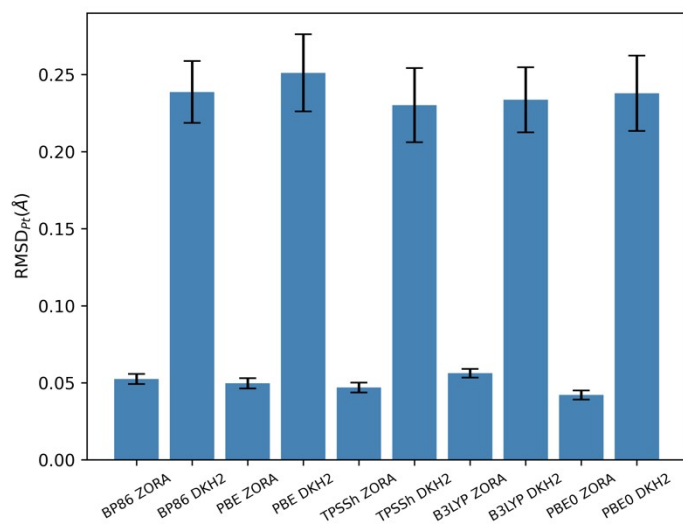


Figure S1: $RMSD_{pt}$ of the five different functionals coupled with 2 ways of accounting for relativistics

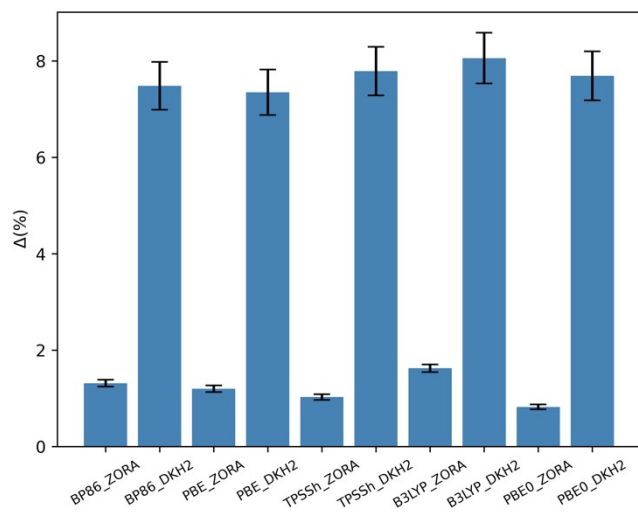


Figure S2: Δ of the five different functionals coupled with 2 ways of accounting for relativistics

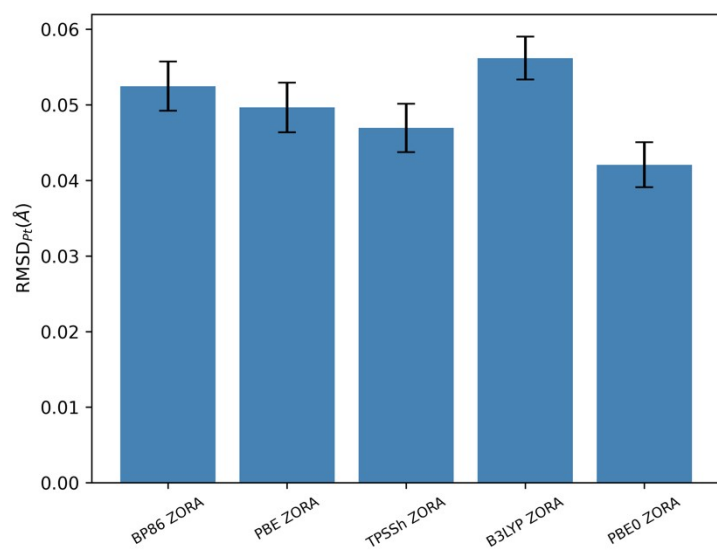


Figure S3: RMSD_{pt} of the five different functionals coupled using the ZORA approximation for relativistics

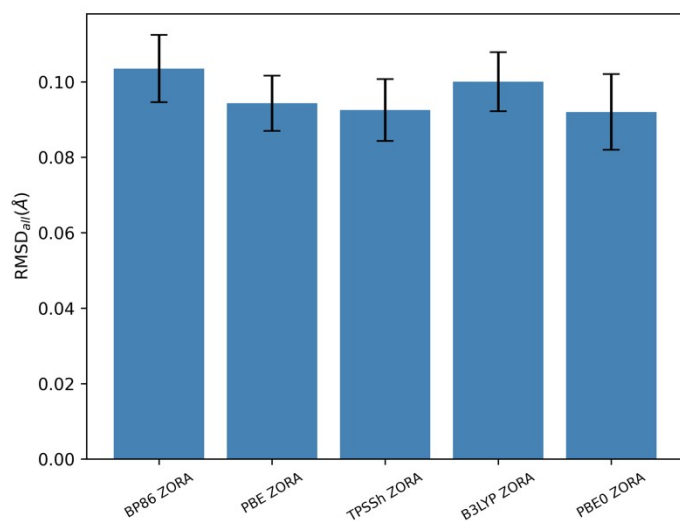


Figure S4: RMSD_{all} of the five different functionals coupled using the ZORA approximation for relativistics

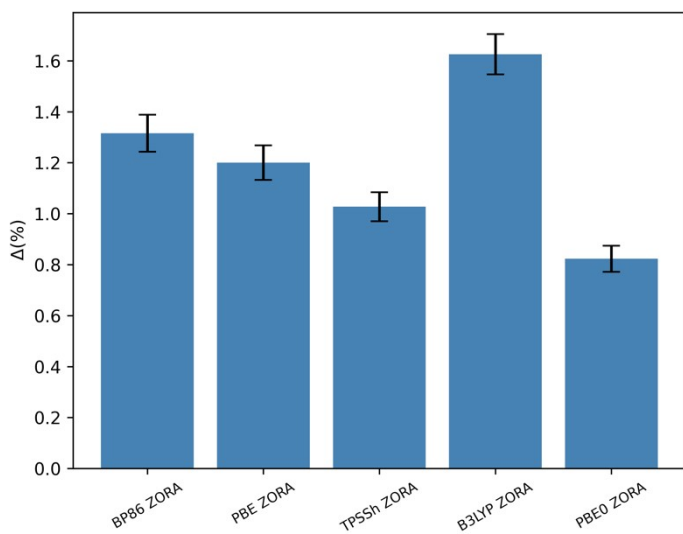


Figure S5: Mean percent deviation of the five different functionals coupled using the ZORA approximation for relativistics

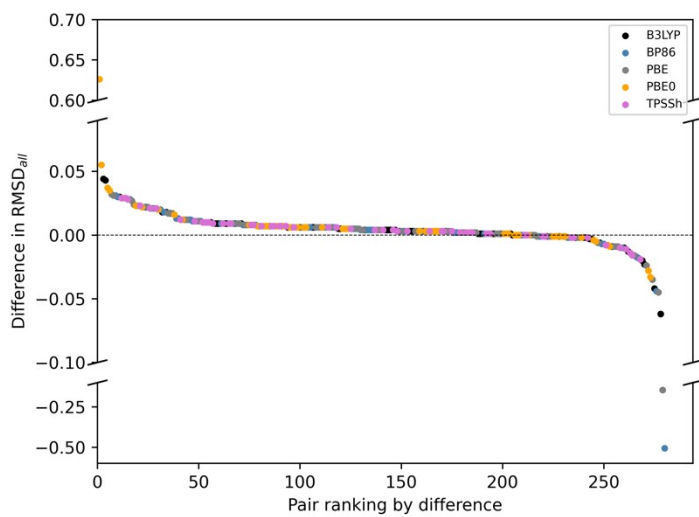


Figure S6: RMSD_{all} showing the effect of basis set using TZVP instead of SVP. The 3 outliers are caused by rotations of outlying ligand fragments, resulting in an unusually high RMSD_{all} . Those case were: (8) calculated using PBE0/ZORA/SVP/CPCM, (10) calculated using BP86/ZORA/TXVP/D3BJ/CPCM and (11) calculated using PBE/ZORA/SVP.

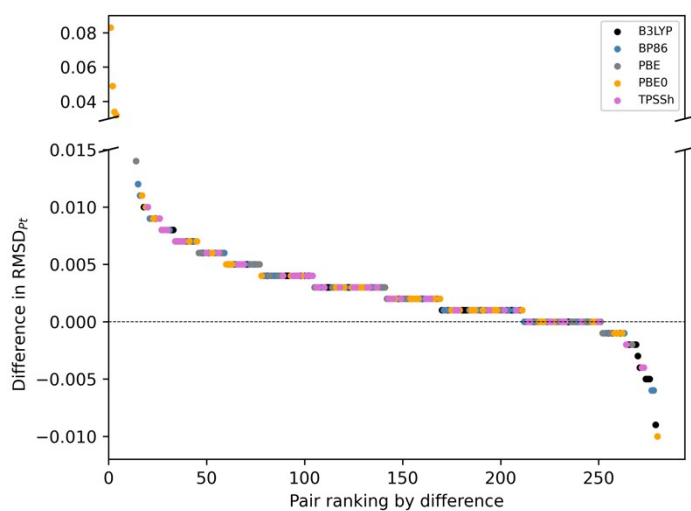


Figure S7: RMSD_{pt} showing the effect of basis set using TZVP instead of SVP.

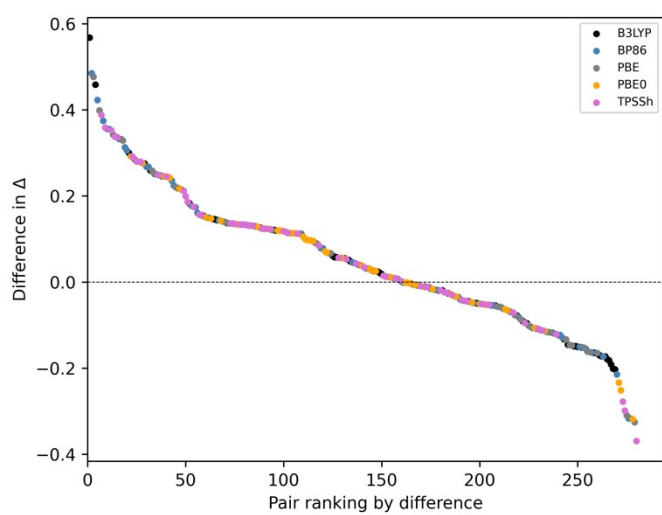


Figure S8: Δ showing the effect of basis set using TZVP instead of SVP.

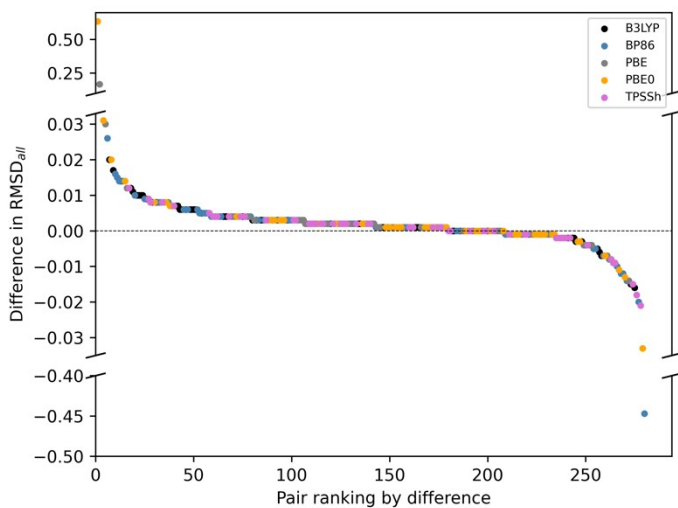


Figure S9: RMSD_{all} showing the effect of accounting for dispersion using D3BJ. The 3 outliers are caused by rotations of outlying ligand fragments, resulting in an unusually high RMSD_{all}. Those case were: (8) calculated using PBE0/ZORA/SVP/CPCM, (10) calculated using BP86/ZORA/TXVP/D3BJ/CPCM and (11) calculated using PBE/ZORA/SVP.

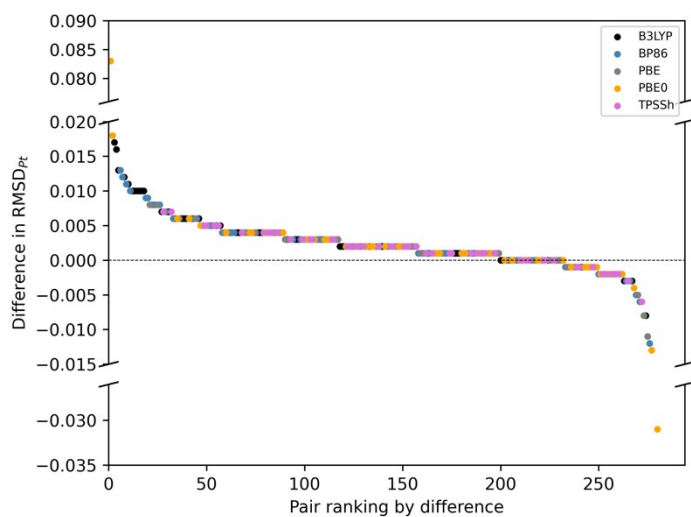


Figure S10: RMSD_{pt} showing the effect of accounting for dispersion using D3BJ

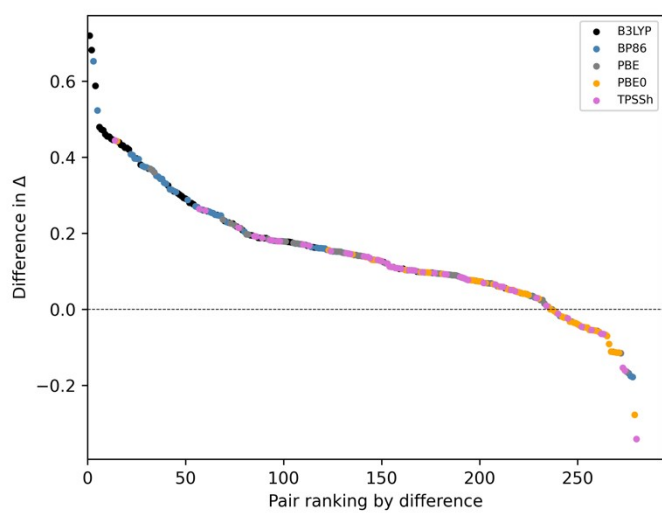


Figure S11: Δ showing the effect of accounting for dispersion using D3BJ

Supplementary tables

Table S1: Combinations of functional, basis set, relativistics, solvation and dispersion forming the 80 different methods used in this study

Functional	Pt Basis Set	Ligand Basis Set	Relativistics	Solvation	Dispersion
BP86	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---
	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---
	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ
	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ
	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---
	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---
	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ
	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ
	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---
	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---
	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ
	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ
	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---
	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---
	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ
	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ
TPSSH	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---
	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---
	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ
	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ
	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---
	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---
	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ
	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ
	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---
	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---
	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ
	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ
	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---
	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---
	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ
	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ
B3LYP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---
	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---
	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ
	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ
	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---
	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---
	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ
	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ
	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---
	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---
	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ
	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ
	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---
	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---
	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ

	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ
	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ
PBE	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---
	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---
	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ
	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ
	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---
	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---
	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ
	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ
	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---
	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---
	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ
	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ
	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---
	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---
	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ
	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ
	PBE0	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---
SARC-ZORA-TZVP		ZORA-def2-SVP	ZORA	CPCM (inf)	---
SARC-ZORA-TZVP		ZORA-def2-SVP	ZORA	---	D3BJ
SARC-ZORA-TZVP		ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ
SARC-DKH-TZVP		DKH-def2-SVP	DKH2	---	---
SARC-DKH-TZVP		DKH-def2-SVP	DKH2	CPCM (inf)	---
SARC-DKH-TZVP		DKH-def2-SVP	DKH2	---	D3BJ
SARC-DKH-TZVP		DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ
SARC-ZORA-TZVP		ZORA-def2-TZVP	ZORA	---	---
SARC-ZORA-TZVP		ZORA-def2-TZVP	ZORA	CPCM (inf)	---
SARC-ZORA-TZVP		ZORA-def2-TZVP	ZORA	---	D3BJ
SARC-ZORA-TZVP		ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ
SARC-DKH-TZVP		DKH-def2-TZVP	DKH2	---	---
SARC-DKH-TZVP		DKH-def2-TZVP	DKH2	CPCM (inf)	---
SARC-DKH-TZVP		DKH-def2-TZVP	DKH2	---	D3BJ
SARC-DKH-TZVP		DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ

Table S2: RMSD_{all}, RMSD_{pt} and Δ ranking of the different methods for the average of all 14 complexes

Name	Pt Basis Set	Ligand Basis Set	Relativistics	Solvation	Dispersion	RMSD _{all} (Å)	Variance of RMSD _{all} (Å)	RMSD _{pt} (Å)	Variance of RMSD _{pt} (Å)	Δ (%)	Variance of Δ (%)	RMSD _{all} rank	RMSD _{pt} rank	Δ rank
PBE0_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.066	0.014	0.034	0.009	0.60	0.13	1*	1*	1*
PBE0_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.067	0.013	0.034	0.007	0.64	0.13	2*	1*	2*
PBE0_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.069	0.014	0.038	0.009	0.69	0.13	3*	3*	3*
TPSSH_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.071	0.013	0.039	0.010	0.85	0.14	4*	4*	5
TPSSH_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.071	0.012	0.039	0.009	0.96	0.14	5*	5*	8
PBE_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.077	0.013	0.042	0.009	1.08	0.15	8*	6*	14
TPSSH_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.075	0.013	0.043	0.011	0.96	0.15	7*	7*	7
BP86_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.112	0.036	0.044	0.009	1.15	0.16	29	8	18
PBE_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.079	0.013	0.044	0.008	1.20	0.16	10*	9	22
PBE0_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.099	0.029	0.044	0.007	0.97	0.13	19	10	9
TPSSH_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.074	0.012	0.044	0.009	1.09	0.15	6*	11	15
PBE0_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.115	0.049	0.045	0.010	0.74	0.13	32	12	4
PBE_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.079	0.012	0.045	0.009	1.14	0.16	11*	13	17
PBE0_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.102	0.028	0.045	0.007	0.96	0.14	20	14	6
BP86_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.082	0.013	0.046	0.009	1.39	0.18	15	15	29
PBE_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.078	0.012	0.047	0.009	1.28	0.17	9*	16	27
BP86_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.082	0.012	0.047	0.009	1.21	0.17	14	17	23
PBE0_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.109	0.029	0.049	0.008	0.98	0.13	24	18	10
B3LYP_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.081	0.012	0.049	0.008	1.50	0.16	13	19	36
PBE0_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.109	0.030	0.049	0.007	1.00	0.14	23	20	11
BP86_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.083	0.012	0.050	0.009	1.47	0.19	16	21	33
B3LYP_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.080	0.012	0.051	0.008	1.49	0.17	12*	22	35
TPSSH_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.110	0.028	0.051	0.009	1.06	0.17	26	23	13
TPSSH_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.109	0.027	0.052	0.008	1.09	0.18	22	24	16
PBE_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.109	0.028	0.052	0.008	1.18	0.21	25	25	21
B3LYP_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.086	0.012	0.053	0.008	1.82	0.19	18	26	40
PBE_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.110	0.028	0.054	0.008	1.26	0.24	27	27	26
TPSSH_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.114	0.029	0.054	0.009	1.05	0.18	31	28	12
BP86_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.112	0.028	0.055	0.010	1.22	0.22	28	29	24
TPSSH_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.115	0.029	0.056	0.009	1.15	0.18	33	30	19
PBE_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.104	0.018	0.056	0.009	1.18	0.21	21	31	20

B3LYP_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.114	0.028	0.056	0.008	1.44	0.25	30	32	31
B3LYP_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.085	0.011	0.057	0.008	1.81	0.19	17	33	39
BP86_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.118	0.029	0.057	0.009	1.23	0.23	37	34	25
BP86_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.116	0.029	0.058	0.009	1.40	0.24	35	35	30
PBE_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.117	0.029	0.058	0.009	1.29	0.22	36	36	28
B3LYP_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.121	0.030	0.059	0.008	1.48	0.25	38	37	34
BP86_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.121	0.029	0.061	0.009	1.45	0.24	39	38	32
B3LYP_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.116	0.026	0.061	0.008	1.73	0.27	34	39	37
B3LYP_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.122	0.028	0.063	0.008	1.76	0.25	40	40	38
BP86_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.213	0.041	0.127	0.013	4.53	0.30	44	41	47
PBE0_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.242	0.056	0.127	0.013	4.42	0.38	55	42	42
PBE_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.211	0.040	0.127	0.014	4.54	0.31	41	43	48
PBE0_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.212	0.041	0.127	0.012	4.49	0.40	43	44	43
TPSSh_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.215	0.042	0.128	0.013	4.66	0.33	46	45	53
TPSSh_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.235	0.051	0.129	0.013	4.55	0.33	53	46	49
PBE0_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.225	0.053	0.129	0.014	4.42	0.37	48	47	41
BP86_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.211	0.042	0.130	0.015	4.52	0.28	42	48	46
B3LYP_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.245	0.056	0.130	0.013	4.77	0.36	58	49	57
TPSSh_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.234	0.058	0.133	0.014	4.66	0.32	52	50	54
PBE0_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.232	0.055	0.133	0.014	4.51	0.37	50	51	44
B3LYP_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.232	0.056	0.133	0.015	4.84	0.34	51	52	58
TPSSh_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.244	0.057	0.133	0.015	4.58	0.32	57	53	50
PBE_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.243	0.058	0.134	0.014	4.52	0.29	56	54	45
B3LYP_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.253	0.060	0.134	0.013	4.94	0.37	60	55	59
PBE_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.221	0.041	0.134	0.014	4.65	0.31	47	56	52
BP86_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.214	0.038	0.134	0.014	4.70	0.30	45	57	55
BP86_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.231	0.056	0.135	0.015	4.70	0.30	49	58	56
B3LYP_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.239	0.059	0.137	0.014	4.98	0.37	54	59	60
PBE_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.249	0.056	0.137	0.016	4.62	0.29	59	60	51
B3LYP_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.420	0.094	0.265	0.037	11.47	1.81	65	61	79
TPSSh_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.420	0.086	0.266	0.034	11.04	1.70	64	62	74
TPSSh_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.394	0.082	0.266	0.035	11.10	1.68	62	63	76
PBE0_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.446	0.102	0.273	0.035	11.19	1.67	70	64	77
B3LYP_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.428	0.091	0.278	0.036	11.08	1.64	67	65	75
PBE0_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.438	0.099	0.278	0.036	11.24	1.65	68	66	78
BP86_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.441	0.095	0.306	0.053	10.57	1.70	69	67	69
BP86_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.382	0.054	0.319	0.055	9.92	1.61	61	68	62

Table S3: RMSD_{all}, RMSD_{pt} and Δ ranking of the 80 different methods for complexes with platinum in oxidation state +2 (1, 3, 5, 7, 8, 10, 11, 13, 14)

Name	Pt Basis Set	Ligand Basis Set	Relativistics	Solvation	Dispersion	RMSD _{all} (Å)	Variance of RMSD _{all} (Å)	RMSD _{pt} (Å)	Variance of RMSD _{pt} (Å)	Δ (%)	Variance of Δ (%)	RMSD _{all} rank	RMSD _{pt} rank	Δ rank
PBE0_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.059	0.017	0.026	0.007	0.47	0.12	1*	1*	1*
PBE0_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.060	0.016	0.027	0.007	0.48	0.12	2*	2*	2*
TPSSH_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.063	0.016	0.029	0.007	0.70	0.10	5*	3*	5
PBE0_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.061	0.015	0.029	0.007	0.54	0.12	3*	4*	3*
TPSSH_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.062	0.014	0.030	0.007	0.81	0.10	4*	5*	6
PBE_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.069	0.015	0.030	0.007	0.85	0.10	9*	6*	8
TPSSH_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.065	0.015	0.032	0.006	0.84	0.14	7*	7*	7
PBE_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.068	0.014	0.032	0.007	0.98	0.11	8*	8*	26
BP86_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.124	0.055	0.032	0.007	0.91	0.11	31	9*	16
PBE_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.069	0.014	0.033	0.007	0.95	0.14	10*	10*	22
BP86_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.070	0.015	0.034	0.007	1.16	0.12	12*	11	32
TPSSH_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.065	0.013	0.034	0.006	0.98	0.14	6*	12	25
PBE_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.069	0.014	0.035	0.007	1.09	0.14	11*	13	30
BP86_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.073	0.015	0.036	0.007	1.00	0.14	16*	14	28
BP86_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.073	0.013	0.040	0.007	1.26	0.16	15*	15	34
PBE0_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.134	0.078	0.040	0.010	0.62	0.11	40	16	4
B3LYP_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.073	0.016	0.041	0.006	1.39	0.11	14*	17	36
B3LYP_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.072	0.014	0.042	0.006	1.40	0.14	13*	18	37
PBE0_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.114	0.041	0.044	0.010	0.94	0.15	20	19	21
PBE0_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.119	0.042	0.045	0.010	0.90	0.15	24	20	12
TPSSH_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.116	0.041	0.045	0.010	0.90	0.19	21	21	15
BP86_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.117	0.042	0.045	0.011	0.91	0.21	22	22	17
B3LYP_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.077	0.015	0.045	0.006	1.69	0.14	18	23	40
PBE_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.119	0.042	0.045	0.011	0.87	0.19	25	24	9
PBE0_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.123	0.044	0.046	0.010	0.94	0.15	30	25	20
TPSSH_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.119	0.041	0.047	0.010	0.88	0.20	26	26	11
PBE_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.120	0.043	0.047	0.010	0.88	0.20	27	27	10
PBE0_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.125	0.043	0.048	0.010	0.92	0.14	32	28	19
BP86_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.122	0.042	0.048	0.011	0.99	0.22	29	29	27
BP86_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.128	0.044	0.048	0.011	0.92	0.21	37	30	18
TPSSH_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.128	0.044	0.048	0.010	0.90	0.21	35	31	14
B3LYP_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.074	0.013	0.049	0.006	1.69	0.17	17*	32	39
PBE_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.107	0.027	0.049	0.012	0.90	0.20	19	33	13

B3LYP_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.118	0.040	0.050	0.010	1.14	0.26	23	34	31
PBE_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.126	0.043	0.050	0.011	0.97	0.19	33	35	24
TPSSH_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.126	0.042	0.050	0.010	0.96	0.20	34	36	23
BP86_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.128	0.043	0.051	0.011	1.07	0.21	36	37	29
B3LYP_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.129	0.042	0.052	0.009	1.19	0.26	38	38	33
B3LYP_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.122	0.038	0.054	0.009	1.37	0.25	28	39	35
B3LYP_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.131	0.043	0.057	0.009	1.45	0.26	39	40	38
BP86_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.232	0.050	0.131	0.016	4.77	0.37	44	41	47
TPSSH_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.233	0.054	0.131	0.015	4.98	0.42	45	42	56
PBE0_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.230	0.054	0.132	0.016	4.78	0.48	42	43	48
PBE_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.231	0.052	0.132	0.017	4.90	0.37	43	44	52
PBE_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.230	0.053	0.133	0.016	4.75	0.38	41	45	46
BP86_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.236	0.052	0.134	0.016	4.98	0.37	46	46	55
BP86_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.239	0.054	0.135	0.018	4.72	0.38	47	47	44
PBE0_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.274	0.076	0.136	0.017	4.64	0.46	49	48	41
TPSSH_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.265	0.069	0.136	0.017	4.82	0.43	48	49	50
B3LYP_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.281	0.079	0.140	0.016	5.11	0.42	50	50	57
PBE0_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.281	0.077	0.142	0.020	4.67	0.47	51	51	42
TPSSH_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.285	0.079	0.142	0.020	4.78	0.43	52	52	49
PBE0_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.295	0.083	0.144	0.018	4.74	0.46	58	53	45
PBE_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.287	0.081	0.144	0.020	4.71	0.37	53	54	43
TPSSH_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.288	0.082	0.144	0.020	4.95	0.41	54	55	54
BP86_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.294	0.083	0.144	0.019	4.94	0.36	57	56	53
B3LYP_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.296	0.085	0.145	0.016	5.33	0.45	59	57	59
B3LYP_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.289	0.079	0.146	0.019	5.20	0.38	55	58	58
PBE_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.292	0.086	0.147	0.021	4.83	0.35	56	59	51
B3LYP_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.296	0.084	0.151	0.018	5.37	0.46	60	60	60
TPSSH_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.484	0.133	0.263	0.036	11.20	1.86	75	61	73
TPSSH_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.491	0.129	0.263	0.039	11.09	1.78	76	62	72
BP86_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.366	0.065	0.264	0.039	10.17	1.55	61	63	65
TPSSH_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.453	0.122	0.264	0.038	11.33	1.75	72	64	74
B3LYP_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.500	0.145	0.267	0.041	12.08	2.16	77	65	79
B3LYP_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.478	0.147	0.267	0.040	11.56	1.81	74	66	78
PBE0_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.530	0.146	0.268	0.036	11.53	1.75	79	67	77
BP86_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.457	0.135	0.269	0.043	11.35	1.88	73	68	75
PBE_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.376	0.066	0.269	0.038	10.22	1.64	62	69	68
PBE0_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.517	0.142	0.276	0.042	11.43	1.82	78	70	76

BP86_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.392	0.079	0.276	0.045	10.20	1.53	63	71	67
BP86_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.413	0.065	0.278	0.028	9.97	1.52	66	72	62
PBE_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.398	0.072	0.279	0.038	9.76	1.55	64	73	61
TPSSh_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.437	0.073	0.281	0.030	10.18	1.54	68	74	66
PBE0_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.425	0.066	0.284	0.027	10.37	1.46	67	75	69
PBE_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.437	0.087	0.284	0.041	10.13	1.45	69	76	64
PBE0_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.450	0.080	0.288	0.029	10.48	1.45	70	77	71
B3LYP_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.451	0.084	0.299	0.040	10.38	1.45	71	78	70
B3LYP_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.560	0.128	0.300	0.023	12.52	1.14	80	79	80
PBE_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.405	0.081	0.304	0.054	10.01	1.62	65	80	63

Table S4: RMSD_{all}, RMSD_{Pt} and Δ ranking of the 80 different methods for complexes with platinum in oxidation state +4 (2, 4, 6, 9, 12)

Name	Pt Basis Set	Ligand Basis Set	Relativistics	Solvation	Dispersion	RMSD _{all} (Å)	Variance of RMSD _{all} (Å)	RMSD _{Pt} (Å)	Variance of RMSD _{Pt} (Å)	Δ (%)	Variance of Δ (%)	RMSD _{all} rank	RMSD _{Pt} rank	Δ rank
PBE0_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.071	0.018	0.044	0.008	1.04	0.25	1*	1*	5*
PBE0_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.072	0.017	0.045	0.007	1.08	0.27	2*	2*	6*
PBE0_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.074	0.021	0.045	0.015	0.93	0.29	3*	3*	2*
PBE0_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.080	0.025	0.051	0.021	0.87	0.29	4*	4*	1*
PBE0_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.082	0.019	0.052	0.012	1.11	0.28	5*	5*	8*
PBE0_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.083	0.025	0.053	0.021	0.97	0.28	7*	6	4*
PBE0_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.083	0.026	0.054	0.021	0.94	0.28	6*	7	3*
PBE0_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.083	0.021	0.054	0.015	1.08	0.25	8*	8	7*
TPSSh_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.086	0.023	0.057	0.020	1.13	0.30	9*	9	9*
TPSSh_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.089	0.022	0.058	0.019	1.23	0.31	10*	10	11*
TPSSh_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.090	0.017	0.060	0.012	1.48	0.30	11	11	16
TPSSh_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.091	0.022	0.060	0.020	1.28	0.32	12	12	12*
TPSSh_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.091	0.026	0.062	0.023	1.18	0.31	14	13	10*
PBE_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.091	0.021	0.063	0.018	1.47	0.32	13	14	15
BP86_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.093	0.020	0.064	0.019	1.53	0.33	16	15	19
TPSSh_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.092	0.021	0.064	0.017	1.33	0.29	15	16	13
PBE_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.101	0.022	0.064	0.018	1.61	0.36	28	17	22
B3LYP_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.094	0.020	0.065	0.017	1.68	0.41	21	18	23
TPSSh_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.096	0.021	0.065	0.016	1.37	0.30	22	19	14
PBE_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.094	0.021	0.065	0.019	1.49	0.34	18	20	17
PBE_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.094	0.016	0.066	0.012	1.73	0.36	17	21	26
B3LYP_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.094	0.019	0.066	0.017	1.68	0.40	20	22	24
PBE_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.094	0.014	0.066	0.010	1.90	0.36	19	23	32
BP86_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.096	0.020	0.067	0.019	1.57	0.35	24	24	20
PBE_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.097	0.020	0.067	0.018	1.61	0.36	25	25	21
BP86_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.102	0.021	0.067	0.018	1.82	0.38	35	26	28
TPSSh_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.097	0.021	0.068	0.017	1.50	0.30	26	27	18
B3LYP_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.096	0.015	0.068	0.011	2.02	0.46	23	28	34
B3LYP_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.102	0.018	0.068	0.016	2.02	0.46	34	29	36
BP86_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.103	0.020	0.070	0.018	1.86	0.38	36	30	31
PBE_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.100	0.018	0.071	0.015	1.70	0.37	27	31	25
B3LYP_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.102	0.019	0.071	0.017	2.02	0.44	32	32	35
PBE_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.101	0.017	0.072	0.014	1.86	0.37	30	33	30

B3LYP_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.101	0.017	0.073	0.015	1.99	0.44	29	34	33
BP86_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.102	0.019	0.073	0.016	1.82	0.39	33	35	27
BP86_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.103	0.019	0.074	0.018	1.83	0.38	38	36	29
B3LYP_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.101	0.014	0.074	0.012	2.37	0.46	31	37	40
B3LYP_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.103	0.014	0.074	0.013	2.32	0.47	37	38	39
BP86_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.105	0.017	0.075	0.015	2.12	0.38	39	39	37
BP86_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.108	0.019	0.079	0.017	2.13	0.39	40	40	38
B3LYP_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.124	0.018	0.107	0.016	4.16	0.49	41	41	52
PBE0_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.126	0.017	0.108	0.015	3.99	0.55	43	42	41
PBE0_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.128	0.017	0.110	0.015	4.08	0.52	44	43	44
B3LYP_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.131	0.023	0.111	0.017	4.22	0.48	46	44	59
TPSSH_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.130	0.017	0.112	0.015	4.12	0.39	45	45	50
B3LYP_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.171	0.059	0.113	0.020	4.12	0.53	47	46	49
PBE0_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.175	0.058	0.114	0.019	4.00	0.62	54	47	42
BP86_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.125	0.017	0.116	0.021	4.25	0.45	42	48	60
B3LYP_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.174	0.057	0.117	0.021	4.18	0.54	51	49	56
PBE_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.174	0.059	0.117	0.024	4.16	0.42	50	50	53
TPSSH_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.173	0.059	0.117	0.117	4.17	0.44	49	51	55
TPSSH_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.183	0.062	0.118	0.020	4.08	0.50	57	52	45
PBE_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.174	0.060	0.119	0.021	4.10	0.47	53	53	46
BP86_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.177	0.061	0.119	0.022	4.11	0.47	55	54	48
TPSSH_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.182	0.060	0.119	0.020	4.11	0.47	56	55	47
PBE_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.174	0.060	0.120	0.024	4.21	0.43	52	56	58
BP86_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.172	0.057	0.120	0.023	4.19	0.44	48	57	57
PBE0_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.184	0.056	0.122	0.021	4.02	0.62	58	58	43
BP86_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.186	0.055	0.133	0.026	4.16	0.49	59	59	54
PBE_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.198	0.060	0.133	0.025	4.15	0.47	60	60	51
B3LYP_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.284	0.060	0.264	0.069	10.37	3.31	61	61	68
TPSSH_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.297	0.060	0.267	0.072	10.55	3.32	63	62	71
TPSSH_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.292	0.061	0.272	0.068	10.44	3.26	62	63	70
PBE0_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.301	0.063	0.281	0.074	11.02	3.19	64	64	75
PBE0_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.302	0.061	0.281	0.072	10.72	3.21	65	65	73
B3LYP_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.339	0.066	0.300	0.065	10.38	3.23	66	66	69
BP86_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.403	0.107	0.370	0.112	9.46	3.33	68	67	62
PBE_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.394	0.095	0.377	0.104	9.27	3.27	67	68	61
BP86_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.405	0.109	0.409	0.121	9.85	3.33	69	69	64
PBE_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.515	0.185	0.481	0.188	9.99	3.33	70	70	65

B3LYP_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.552	0.171	0.516	0.180	9.61	3.26	71	71	63
BP86_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.630	0.178	0.545	0.182	10.14	3.38	73	72	67
BP86_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.685	0.203	0.570	0.195	11.89	3.65	77	73	80
PBE_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.630	0.239	0.600	0.258	11.21	3.53	72	74	76
TPSSh_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.632	0.261	0.602	0.276	10.09	3.30	74	75	66
B3LYP_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.643	0.299	0.604	0.300	11.63	3.69	75	76	78
PBE0_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.739	0.277	0.629	0.263	10.81	3.43	80	77	74
TPSSh_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.691	0.287	0.630	0.278	11.83	3.55	78	78	79
PBE_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.685	0.242	0.641	0.265	10.61	3.35	76	79	72
PBE0_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.735	0.341	0.698	0.334	11.25	3.40	79	80	77

Table S5: RMSD_{all}, RMSD_{pt} and Δ ranking of the 80 different methods for platinum complexes with no overall charge (2, 3, 4, 5, 6, 9)

Name	Pt Basis Set	Ligand Basis Set	Relativistics	Solvation	Dispersion	RMSD _{all} (Å)	Variance of RMSD _{all} (Å)	RMSD _{pt} (Å)	Variance of RMSD _{pt} (Å)	Δ (%)	Variance of Δ (%)	RMSD _{all} rank	RMSD _{pt} rank	Δ rank
PBE0_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.081	0.015	0.043	0.011	0.76	0.24	1*	1*	2*
PBE0_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.084	0.018	0.045	0.015	0.73	0.22	2*	2*	1*
TPSSh_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.088	0.018	0.047	0.015	0.88	0.21	6*	3*	7*
TPSSh_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.084	0.018	0.047	0.014	1.02	0.21	3*	4*	21
PBE0_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.086	0.018	0.047	0.014	0.77	0.22	4*	5*	3*
PBE_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.092	0.017	0.049	0.015	1.05	0.19	12*	6*	22
PBE_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.090	0.017	0.050	0.014	1.13	0.20	7*	7*	28
PBE_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.090	0.016	0.050	0.015	1.20	0.20	8*	8*	31
BP86_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.152	0.060	0.050	0.015	1.12	0.19	37	9*	26
BP86_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.093	0.017	0.052	0.015	1.41	0.21	14*	10*	34
TPSSh_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.088	0.017	0.052	0.014	1.13	0.21	5*	11*	29
TPSSh_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.090	0.019	0.052	0.017	0.99	0.22	9*	12*	16*
PBE0_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.133	0.043	0.052	0.010	1.06	0.20	20	13*	24
PBE_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.092	0.017	0.053	0.015	1.25	0.20	11*	14*	32
BP86_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.094	0.018	0.053	0.014	1.14	0.20	15*	15*	30
PBE0_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.136	0.042	0.055	0.011	1.01	0.22	21	16	19
B3LYP_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.094	0.017	0.056	0.013	1.57	0.21	16*	17	38
BP86_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.095	0.017	0.057	0.015	1.43	0.21	17*	18	35
B3LYP_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.091	0.017	0.057	0.013	1.54	0.21	10*	19	37
PBE_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.139	0.042	0.058	0.014	0.89	0.25	22	20	9*
PBE_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.139	0.045	0.059	0.013	0.91	0.27	23	21	12*
TPSSh_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.143	0.045	0.059	0.014	0.88	0.25	26	22	8*
PBE0_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.159	0.080	0.060	0.014	0.86	0.21	40	23	5*
B3LYP_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.142	0.045	0.060	0.013	1.10	0.33	24	24	25
PBE0_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.146	0.044	0.060	0.013	1.00	0.19	30	25	18*
PBE0_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.145	0.046	0.060	0.011	0.99	0.20	29	26	17*
B3LYP_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.097	0.017	0.060	0.012	1.91	0.22	18	27	40
TPSSh_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.146	0.045	0.061	0.014	0.91	0.23	31	28	13*
BP86_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.144	0.047	0.061	0.016	0.94	0.27	27	29	14*
BP86_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.152	0.045	0.062	0.016	0.89	0.24	35	30	10*
B3LYP_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.093	0.016	0.062	0.013	1.87	0.24	13*	31	39
BP86_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.145	0.043	0.062	0.015	1.02	0.29	28	32	20
TPSSh_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.152	0.047	0.064	0.015	0.85	0.23	34	33	4*

B3LYP_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.150	0.044	0.064	0.014	1.12	0.29	32	34	27
TPSSh_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.152	0.046	0.064	0.014	0.90	0.23	36	35	11*
PBE_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.129	0.027	0.064	0.016	0.88	0.23	19	36	6*
PBE_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.150	0.045	0.065	0.015	0.98	0.23	33	37	15*
B3LYP_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.142	0.042	0.065	0.013	1.39	0.34	25	38	33
BP86_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.154	0.046	0.067	0.016	1.06	0.25	39	39	23
B3LYP_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.153	0.045	0.068	0.013	1.44	0.31	38	40	36
BP86_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.249	0.055	0.139	0.017	4.80	0.40	42	41	51
PBE_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.248	0.056	0.139	0.018	4.73	0.43	41	42	49
TPSSh_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.255	0.055	0.140	0.016	4.91	0.46	43	43	54
PBE0_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.256	0.054	0.142	0.015	4.67	0.51	44	44	46
PBE0_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.297	0.083	0.142	0.017	4.51	0.53	49	45	42
TPSSh_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.292	0.075	0.144	0.018	4.68	0.48	48	46	47
BP86_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.260	0.056	0.145	0.020	4.70	0.42	46	47	48
PBE0_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.310	0.085	0.149	0.020	4.47	0.54	50	48	41
TPSSh_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.314	0.088	0.149	0.020	4.65	0.47	54	49	44
PBE_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.259	0.052	0.150	0.017	4.88	0.41	45	50	53
BP86_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.263	0.054	0.150	0.017	5.04	0.42	47	51	56
B3LYP_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.310	0.083	0.150	0.017	5.21	0.49	51	52	57
PBE_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.314	0.088	0.153	0.021	4.65	0.41	53	53	45
PBE0_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.322	0.090	0.153	0.019	4.62	0.49	58	54	43
TPSSh_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.315	0.085	0.155	0.021	4.83	0.48	55	55	52
B3LYP_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.314	0.083	0.156	0.019	5.24	0.42	52	56	58
BP86_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.317	0.085	0.156	0.020	4.93	0.40	56	57	55
PBE_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.318	0.087	0.156	0.021	4.77	0.42	57	58	50
B3LYP_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.324	0.089	0.156	0.016	5.48	0.49	59	59	60
B3LYP_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.329	0.087	0.164	0.019	5.46	0.51	60	60	59
TPSSh_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.511	0.143	0.258	0.024	10.56	1.59	74	61	73
TPSSh_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.471	0.131	0.258	0.022	10.55	1.57	72	62	72
BP86_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.375	0.065	0.260	0.027	9.29	1.15	61	63	65
TPSSh_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.520	0.140	0.261	0.024	10.63	1.52	76	64	75
PBE_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.377	0.065	0.262	0.027	9.24	1.19	62	65	64
B3LYP_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.542	0.146	0.262	0.024	10.71	1.51	79	66	78
TPSSh_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.423	0.088	0.262	0.028	9.38	1.15	67	67	66
BP86_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.402	0.075	0.262	0.025	9.15	1.11	63	68	62
B3LYP_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.529	0.149	0.263	0.031	11.62	2.16	77	69	80
PBE0_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.552	0.152	0.264	0.023	10.57	1.53	80	70	74

BP86_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.481	0.150	0.265	0.032	10.70	1.60	73	71	76
PBE0_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.414	0.081	0.269	0.027	9.60	1.14	66	72	69
PBE0_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.446	0.088	0.274	0.028	9.63	1.17	70	73	70
PBE_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.403	0.079	0.274	0.031	9.10	1.14	64	74	61
PBE0_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.533	0.154	0.275	0.030	10.71	1.58	78	75	77
BP86_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.410	0.081	0.280	0.039	9.53	1.14	65	76	68
B3LYP_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.518	0.148	0.281	0.025	10.86	1.74	75	77	79
PBE_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.446	0.097	0.284	0.039	9.42	1.14	71	78	67
B3LYP_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.444	0.089	0.294	0.041	9.63	1.20	69	79	71
PBE_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.426	0.081	0.314	0.045	9.20	1.15	68	80	63

Table S6: RMSD_{all}, RMSD_{pt} and Δ ranking of the 80 different methods for platinum complexes with an overall charge (2, 3, 4, 5, 6, 9)

Name	Pt Basis Set	Ligand Basis Set	Relativistics	Solvation	Dispersion	RMSD _{all} (Å)	Variance of RMSD _{all} (Å)	RMSD _{pt} (Å)	Variance of RMSD _{pt} (Å)	Δ (%)	Variance of Δ (%)	RMSD _{all} rank	RMSD _{pt} rank	Δ rank
PBE0_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.044	0.019	0.020	0.006	0.44	0.08	1*	1*	1*
PBE0_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.045	0.019	0.021	0.006	0.50	0.07	2*	2*	2*
PBE0_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.046	0.018	0.023	0.006	0.56	0.07	3*	3*	3
PBE0_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.048	0.017	0.024	0.005	0.61	0.08	4*	4*	4
TPSSH_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.051	0.016	0.027	0.005	0.80	0.15	5*	5	5
TPSSH_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.053	0.016	0.029	0.004	0.89	0.17	6*	6	7
TPSSH_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.055	0.016	0.031	0.004	0.93	0.16	9*	7	9
PBE0_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.055	0.017	0.031	0.005	0.87	0.12	7*	8	6
PBE0_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.055	0.016	0.032	0.005	0.92	0.14	8*	9	8
TPSSH_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.057	0.015	0.032	0.004	1.03	0.20	10*	10	12
PBE_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.057	0.015	0.033	0.006	1.09	0.26	11*	11	13
PBE0_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.057	0.017	0.034	0.006	0.95	0.15	12*	12	10
BP86_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.058	0.015	0.035	0.006	1.16	0.27	14*	13	14
PBE0_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.058	0.016	0.035	0.005	0.99	0.18	13*	14	11
PBE_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.064	0.018	0.035	0.006	1.21	0.28	19	15	16
PBE_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.062	0.014	0.038	0.005	1.19	0.28	15*	16	15
PBE_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.063	0.014	0.038	0.006	1.31	0.29	17*	17	19
BP86_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.066	0.017	0.038	0.006	1.39	0.30	23	18	21
B3LYP_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.062	0.014	0.039	0.004	1.40	0.27	16*	19	23
TPSSH_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.063	0.015	0.040	0.004	1.25	0.22	18*	20	17
BP86_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.064	0.013	0.040	0.006	1.29	0.29	20	21	18
TPSSH_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.065	0.015	0.041	0.004	1.39	0.23	21	22	22
TPSSH_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.067	0.016	0.042	0.005	1.34	0.25	24	23	20
B3LYP_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.065	0.012	0.042	0.004	1.46	0.30	22	24	24
TPSSH_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.069	0.015	0.044	0.004	1.48	0.24	26	25	25
B3LYP_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.070	0.016	0.044	0.005	1.67	0.28	28	26	30
BP86_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.069	0.014	0.044	0.006	1.50	0.33	27	27	26
PBE_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.068	0.014	0.045	0.006	1.58	0.29	25	28	27
BP86_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.071	0.014	0.047	0.006	1.63	0.31	29	29	29
PBE_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.072	0.014	0.047	0.006	1.70	0.30	30	30	32
PBE_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.072	0.014	0.048	0.006	1.60	0.32	31	31	28
B3LYP_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.073	0.013	0.048	0.005	1.72	0.32	32	32	33
PBE_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.074	0.014	0.049	0.006	1.75	0.33	34	33	34

BP86_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.074	0.014	0.049	0.006	1.68	0.34	36	34	31
BP86_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.074	0.014	0.051	0.006	1.88	0.32	35	35	35
B3LYP_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.074	0.012	0.052	0.005	1.89	0.35	33	36	37
B3LYP_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.076	0.013	0.053	0.005	1.89	0.36	37	37	36
BP86_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.077	0.013	0.053	0.006	1.94	0.35	38	38	38
B3LYP_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.078	0.012	0.056	0.005	2.18	0.35	39	39	39
B3LYP_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.080	0.011	0.057	0.006	2.21	0.38	40	40	40
B3LYP_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.115	0.016	0.100	0.012	4.27	0.43	42	41	46
B3LYP_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.118	0.019	0.101	0.012	4.31	0.42	43	42	50
PBE0_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.120	0.016	0.104	0.012	4.37	0.47	46	43	55
PBE0_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.120	0.016	0.104	0.013	4.35	0.50	45	44	53
B3LYP_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.153	0.050	0.104	0.017	4.19	0.44	47	45	41
TPSSH_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.119	0.015	0.104	0.011	4.40	0.40	44	46	59
BP86_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.114	0.014	0.105	0.016	4.36	0.39	41	47	54
B3LYP_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.154	0.051	0.106	0.016	4.23	0.42	49	48	43
TPSSH_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.161	0.053	0.109	0.017	4.33	0.45	58	49	52
PBE0_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.161	0.052	0.109	0.017	4.31	0.56	57	50	49
PBE0_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.158	0.050	0.109	0.018	4.28	0.59	54	51	47
BP86_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.160	0.051	0.109	0.020	4.21	0.42	55	52	42
TPSSH_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.158	0.052	0.110	0.017	4.47	0.41	53	53	60
PBE_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.164	0.054	0.110	0.019	4.30	0.44	59	54	48
TPSSH_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.161	0.052	0.110	0.017	4.37	0.43	56	55	56
BP86_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.157	0.053	0.111	0.020	4.33	0.39	52	56	51
PBE_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.155	0.050	0.111	0.020	4.39	0.39	51	57	58
BP86_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.154	0.048	0.111	0.021	4.25	0.41	48	58	44
PBE_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.165	0.053	0.112	0.019	4.27	0.42	60	59	45
PBE_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.155	0.049	0.112	0.020	4.37	0.40	50	60	57
B3LYP_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.291	0.060	0.268	0.072	11.47	3.30	61	61	70
B3LYP_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.308	0.067	0.271	0.080	11.31	3.31	66	62	67
TPSSH_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.299	0.064	0.273	0.074	11.71	3.28	63	63	73
TPSSH_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.296	0.063	0.277	0.076	11.45	3.29	62	64	69
PBE0_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.307	0.063	0.281	0.077	11.92	3.22	65	65	75
PBE0_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.307	0.062	0.282	0.074	11.91	3.15	64	66	74
PBE_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.369	0.097	0.346	0.100	10.55	3.33	67	67	62
BP86_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.390	0.094	0.355	0.107	10.48	3.26	68	68	61
BP86_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.396	0.094	0.384	0.110	10.93	3.39	69	69	63
PBE_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.475	0.152	0.441	0.158	11.25	3.17	70	70	66

B3LYP_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.539	0.146	0.479	0.157	11.01	3.11	71	71	64
BP86_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.601	0.184	0.517	0.174	12.25	3.55	74	72	78
BP86_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.611	0.149	0.532	0.159	11.16	3.38	75	73	65
TPSSH_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.587	0.238	0.555	0.239	11.31	3.19	72	74	68
PBE_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.596	0.214	0.560	0.221	12.06	3.39	73	75	77
PBE_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.625	0.212	0.567	0.225	11.60	3.11	76	76	71
TPSSH_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.641	0.239	0.594	0.249	12.52	3.46	77	77	79
PBE0_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.713	0.222	0.595	0.216	11.63	3.07	80	78	72
B3LYP_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.660	0.231	0.604	0.231	14.34	2.69	78	79	80
PBE0_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.687	0.277	0.611	0.270	11.94	3.07	79	80	76

Table S7: RMSD_{all}, RMSD_{Pt} and Δ ranking of the 80 different methods for complexes where platinum is only bonded to light atoms (C, N, O) (5, 6, 12, 13)

Name	Pt Basis Set	Ligand Basis Set	Relativistics	Solvation	Dispersion	RMSD _{all} (Å)	Variance of RMSD _{all} (Å)	RMSD _{Pt} (Å)	Variance of RMSD _{Pt} (Å)	Δ (%)	Variance of Δ (%)	RMSD _{all} rank	RMSD _{Pt} rank	Δ rank
PBE0_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.056	0.018	0.035	0.011	0.83	0.38	1*	1*	8*
PBE0_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.059	0.018	0.037	0.012	0.82	0.38	2*	2*	4*
PBE0_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.067	0.024	0.043	0.020	0.78	0.42	3*	3*	1*
PBE_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.075	0.022	0.047	0.019	1.24	0.42	8	4	32
PBE_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.074	0.023	0.048	0.021	1.10	0.40	7*	5	25*
PBE0_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.071	0.020	0.048	0.017	0.90	0.39	4*	6	15*
TPSSh_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.075	0.023	0.048	0.020	1.08	0.40	9	7	24*
PBE0_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.073	0.031	0.051	0.027	0.80	0.41	6*	8	2*
PBE0_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.072	0.022	0.051	0.019	0.88	0.37	5*	9	11*
TPSSh_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.077	0.029	0.052	0.027	0.88	0.43	13	10	10*
TPSSh_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.078	0.027	0.052	0.024	0.93	0.40	14	11	18*
PBE_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.080	0.030	0.053	0.028	1.02	0.46	16	12	20*
PBE_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.081	0.031	0.053	0.027	0.93	0.40	19	13	17*
PBE_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.083	0.027	0.053	0.028	0.84	0.40	25	14	9*
PBE_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.083	0.027	0.053	0.025	1.04	0.41	24	15	21*
BP86_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.085	0.029	0.053	0.028	0.89	0.42	30	16	12*
BP86_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.080	0.030	0.053	0.028	0.92	0.43	17	17	16*
TPSSh_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.077	0.030	0.053	0.029	0.81	0.41	12	18	3*
BP86_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.087	0.026	0.054	0.027	1.11	0.42	38	19	26*
PBE0_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.077	0.028	0.054	0.026	0.82	0.41	11	20	5*
PBE_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.086	0.025	0.055	0.025	1.16	0.40	36	21	28*
B3LYP_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.076	0.023	0.055	0.019	1.54	0.52	10	22	38
PBE_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.086	0.028	0.055	0.028	0.90	0.41	35	23	14*
PBE0_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.078	0.030	0.056	0.028	0.83	0.39	15	24	7*
BP86_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.083	0.029	0.056	0.028	1.13	0.49	21	25	27*
TPSSh_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.084	0.029	0.056	0.026	0.89	0.45	28	26	13*
BP86_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.083	0.028	0.056	0.027	1.17	0.44	23	27	30*
TPSSh_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.084	0.026	0.057	0.025	0.99	0.42	26	28	19*
B3LYP_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.080	0.027	0.057	0.025	1.23	0.53	18	29	31
BP86_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.085	0.028	0.057	0.026	1.41	0.44	29	30	35
B3LYP_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.086	0.026	0.058	0.025	1.16	0.50	32	31	29*
B3LYP_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.083	0.027	0.059	0.024	1.49	0.56	22	32	37
BP86_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.093	0.028	0.059	0.027	1.36	0.47	42	33	33

TPSSh_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.086	0.025	0.059	0.025	1.06	0.41	34	34	23*
BP86_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.089	0.029	0.059	0.029	1.06	0.46	40	35	22*
TPSSh_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.087	0.032	0.060	0.032	0.83	0.45	37	36	6*
B3LYP_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.086	0.022	0.060	0.019	1.72	0.55	33	37	39
B3LYP_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.082	0.024	0.061	0.019	1.81	0.58	20	38	40
B3LYP_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.084	0.024	0.061	0.022	1.47	0.52	27	39	36
B3LYP_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.089	0.026	0.062	0.025	1.40	0.53	39	40	34
PBE0_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.086	0.011	0.078	0.009	2.64	0.68	31	41	41
PBE0_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.090	0.009	0.081	0.009	2.94	0.74	41	42	43
PBE_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.097	0.010	0.084	0.009	3.35	0.59	44	43	47
BP86_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.099	0.011	0.086	0.010	3.46	0.61	48	44	48
PBE0_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.095	0.011	0.086	0.011	3.07	0.73	43	45	44
TPSSh_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.098	0.014	0.087	0.012	3.17	0.63	47	46	45
PBE0_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.098	0.017	0.087	0.015	2.77	0.69	46	47	42
PBE_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.100	0.010	0.088	0.009	3.65	0.63	50	48	51
TPSSh_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.100	0.013	0.089	0.011	3.28	0.63	49	49	46
TPSSh_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.098	0.011	0.090	0.010	3.49	0.69	45	50	49
BP86_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.103	0.011	0.091	0.012	3.76	0.64	52	51	55
PBE_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.105	0.010	0.093	0.011	3.80	0.62	55	52	56
B3LYP_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.100	0.010	0.093	0.011	3.66	0.79	51	53	53
TPSSh_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.105	0.013	0.095	0.012	3.66	0.71	54	54	52
BP86_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.110	0.013	0.098	0.012	4.00	0.67	57	55	58
B3LYP_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.104	0.010	0.098	0.011	4.14	0.71	53	56	64
B3LYP_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.107	0.012	0.099	0.013	3.88	0.81	56	57	57
PBE_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.121	0.025	0.105	0.023	3.53	0.58	60	58	50
B3LYP_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.113	0.011	0.105	0.012	4.21	0.86	58	59	68
BP86_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.121	0.024	0.106	0.023	3.71	0.62	59	60	54
BP86_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.148	0.037	0.121	0.058	4.25	2.58	61	61	70
B3LYP_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.154	0.039	0.123	0.059	4.21	2.67	63	62	67
BP86_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.151	0.039	0.125	0.059	4.13	2.55	62	63	62
PBE_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.155	0.039	0.125	0.059	4.29	2.52	64	64	72
TPSSh_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.159	0.038	0.130	0.060	4.42	2.58	65	65	74
TPSSh_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.162	0.040	0.130	0.059	4.27	2.49	66	66	71
PBE0_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.169	0.040	0.135	0.057	4.55	2.50	68	67	76
PBE0_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.168	0.039	0.137	0.059	4.62	2.52	67	68	77
PBE_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.179	0.043	0.143	0.054	4.16	2.49	69	69	66
PBE_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.179	0.042	0.150	0.063	4.37	2.58	70	70	73

BP86_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.191	0.041	0.151	0.054	4.01	2.52	72	71	59
TP5Sh_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.193	0.041	0.152	0.055	4.15	2.46	73	72	65
B3LYP_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.188	0.049	0.156	0.066	4.09	2.46	71	73	61
PBE0_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.219	0.031	0.170	0.046	4.78	2.46	75	74	78
PBE_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.217	0.028	0.176	0.043	4.23	2.48	74	75	69
PBE0_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.231	0.024	0.176	0.044	4.80	2.49	76	76	79
TP5Sh_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.244	0.026	0.186	0.038	4.53	2.55	78	77	75
BP86_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.247	0.020	0.189	0.035	4.14	2.48	79	78	63
B3LYP_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.243	0.014	0.190	0.039	4.07	2.50	77	79	60
B3LYP_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.299	0.077	0.232	0.056	7.20	2.61	80	80	80

Table S8: RMSD_{all}, RMSD_{Pt} and Δ ranking of the 80 different methods for complexes where platinum is not bonded to any light atoms (2, 3, 4, 8, 10, 11)

Name	Pt Basis Set	Ligand Basis Set	Relativistics	Solvation	Dispersion	RMSD _{all} (Å)	Variance of RMSD _{all} (Å)	RMSD _{Pt} (Å)	Variance of RMSD _{Pt} (Å)	Δ (%)	Variance of Δ (%)	RMSD _{all} rank	RMSD _{Pt} rank	Δ rank
PBE0_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.060	0.023	0.018	0.002	0.43	0.05	1*	1*	1*
PBE0_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.064	0.023	0.021	0.003	0.49	0.06	3*	2	2
PBE0_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.061	0.023	0.022	0.002	0.53	0.06	2*	3	3
TPSSH_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.072	0.021	0.027	0.002	0.87	0.10	7*	4	5
TPSSH_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.069	0.019	0.029	0.002	1.05	0.09	4*	5	10
TPSSH_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.070	0.020	0.030	0.002	1.06	0.11	5*	6	11
PBE_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.080	0.019	0.033	0.003	1.22	0.18	11*	7	15
PBE0_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.128	0.060	0.033	0.004	0.91	0.11	20	8	7
TPSSH_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.070	0.018	0.034	0.001	1.29	0.07	6*	9	17
PBE0_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.142	0.060	0.035	0.004	0.92	0.14	24	10	8
PBE_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.078	0.017	0.035	0.003	1.40	0.17	9*	11	22
PBE0_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.140	0.062	0.037	0.005	0.91	0.13	21	12	6
BP86_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.164	0.077	0.037	0.004	1.30	0.19	38	13	18
PBE0_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.145	0.062	0.038	0.003	0.98	0.17	26	14	9
PBE0_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.168	0.115	0.038	0.013	0.71	0.04	40	15	4
PBE_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.078	0.019	0.039	0.003	1.41	0.16	10*	16	23
BP86_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.084	0.017	0.039	0.003	1.64	0.17	14	17	31
TPSSH_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.142	0.060	0.040	0.002	1.11	0.26	23	18	12
PBE_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.078	0.018	0.041	0.003	1.61	0.15	8*	19	30
BP86_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.083	0.019	0.041	0.003	1.49	0.18	13*	20	26
TPSSH_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.147	0.062	0.042	0.002	1.15	0.29	28	21	14
B3LYP_ZORA_TZVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	D3BJ	0.086	0.019	0.043	0.002	1.72	0.12	17	22	32
TPSSH_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.145	0.061	0.043	0.002	1.15	0.30	27	23	13
PBE_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.141	0.061	0.044	0.003	1.28	0.40	22	24	16
BP86_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.145	0.060	0.045	0.004	1.35	0.41	25	25	21
B3LYP_ZORA_SVP_D3BJ_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	D3BJ	0.083	0.018	0.045	0.002	1.84	0.13	12*	26	35
TPSSH_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.153	0.062	0.046	0.001	1.31	0.29	31	27	19
PBE_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.148	0.059	0.047	0.003	1.34	0.44	29	28	20
BP86_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.156	0.061	0.048	0.004	1.46	0.40	34	29	25
BP86_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.085	0.015	0.048	0.002	1.86	0.15	15	30	36
PBE_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.124	0.038	0.048	0.004	1.42	0.40	19	31	24

B3LYP_ZORA_TZVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	CPCM (inf)	---	0.092	0.018	0.049	0.002	2.14	0.10	18	32	38
PBE_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.155	0.061	0.050	0.003	1.53	0.39	33	33	28
BP86_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.148	0.056	0.050	0.004	1.51	0.44	30	34	27
B3LYP_ZORA_TZVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	D3BJ	0.154	0.058	0.051	0.004	1.57	0.45	32	35	29
B3LYP_ZORA_SVP_D3BJ	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	D3BJ	0.160	0.060	0.052	0.004	1.78	0.39	37	36	34
BP86_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.157	0.059	0.055	0.003	1.78	0.41	35	37	33
B3LYP_ZORA_SVP_CPCM	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	CPCM (inf)	---	0.086	0.014	0.055	0.002	2.25	0.10	16	38	40
B3LYP_ZORA_TZVP	SARC-ZORA-TZVP	ZORA-def2-TZVP	ZORA	---	---	0.157	0.055	0.059	0.004	1.97	0.41	36	39	37
B3LYP_ZORA_SVP	SARC-ZORA-TZVP	ZORA-def2-SVP	ZORA	---	---	0.167	0.061	0.061	0.003	2.20	0.36	39	40	39
BP86_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.265	0.072	0.114	0.010	4.59	0.30	42	41	41
BP86_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.265	0.072	0.114	0.008	4.77	0.28	44	42	46
BP86_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.263	0.077	0.116	0.009	4.87	0.35	41	43	48
PBE_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.266	0.070	0.118	0.009	4.86	0.27	45	44	47
PBE_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.265	0.070	0.118	0.009	4.94	0.29	43	45	52
TPSSH_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.278	0.073	0.118	0.008	5.17	0.29	47	46	59
B3LYP_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.343	0.108	0.120	0.014	4.88	0.34	51	47	50
B3LYP_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.336	0.113	0.121	0.016	4.75	0.35	49	48	45
PBE0_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.277	0.070	0.122	0.007	5.24	0.25	46	49	60
BP86_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.347	0.117	0.122	0.018	4.70	0.32	55	50	43
B3LYP_DKH2_TZVP_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	---	0.360	0.121	0.123	0.016	5.02	0.42	59	51	54
B3LYP_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.343	0.117	0.124	0.019	4.88	0.43	52	52	49
PBE_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.348	0.111	0.124	0.017	4.67	0.29	57	53	42
TPSSH_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.326	0.092	0.125	0.013	5.04	0.25	48	54	56
TPSSH_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.348	0.112	0.126	0.016	4.88	0.26	56	55	51
PBE_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.344	0.118	0.126	0.018	4.72	0.31	53	56	44
PBE0_DKH2_TZVP_D3BJ	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	D3BJ	0.345	0.110	0.129	0.014	5.03	0.26	54	57	55
PBE0_DKH2_TZVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	CPCM (inf)	D3BJ	0.337	0.103	0.129	0.012	5.15	0.24	50	58	58
TPSSH_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.355	0.110	0.130	0.017	4.97	0.28	58	59	53
PBE0_DKH2_TZVP	SARC-DKH-TZVP	DKH-def2-TZVP	DKH2	---	---	0.363	0.111	0.131	0.016	5.08	0.25	60	60	57
TPSSH_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.636	0.147	0.350	0.035	15.32	1.57	63	61	75
TPSSH_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.682	0.146	0.351	0.034	15.13	1.68	66	62	74
PBE0_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.744	0.165	0.358	0.035	15.35	1.71	72	63	77
B3LYP_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.687	0.163	0.358	0.037	16.08	2.30	67	64	80
B3LYP_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.672	0.171	0.359	0.035	15.34	1.74	65	65	76
PBE0_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.707	0.167	0.371	0.039	15.50	1.80	69	66	78
BP86_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.572	0.036	0.420	0.059	12.79	1.98	61	67	63
BP86_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.725	0.159	0.436	0.063	14.33	2.03	71	68	71

PBE_DKH2_SVP	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	---	0.633	0.061	0.490	0.065	12.43	2.06	62	69	62
BP86_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.695	0.110	0.509	0.136	12.16	1.87	68	70	61
PBE_DKH2_SVP_D3BJ	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	---	D3BJ	0.667	0.103	0.510	0.135	13.12	1.85	64	71	66
BP86_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.714	0.123	0.543	0.146	14.09	1.77	70	72	70
B3LYP_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.754	0.119	0.550	0.139	12.88	1.68	73	73	64
PBE0_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.789	0.163	0.587	0.206	13.07	1.77	75	74	65
TPSSH_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.941	0.204	0.610	0.232	14.77	1.60	79	75	73
B3LYP_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.983	0.215	0.612	0.238	15.59	1.71	80	76	79
TPSSH_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.852	0.214	0.626	0.235	14.41	1.99	77	77	72
PBE_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.844	0.182	0.626	0.207	13.52	1.69	76	78	67
PBE_DKH2_SVP_D3BJ_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	D3BJ	0.783	0.174	0.626	0.203	13.72	2.05	74	79	68
PBE0_DKH2_SVP_CPCM	SARC-DKH-TZVP	DKH-def2-SVP	DKH2	CPCM (inf)	---	0.901	0.237	0.679	0.270	13.89	1.69	78	80	69

Table S9: xyz coordinates of tetrakis(triphenylphosphine)platinum(0) as calculated by PBEO / ZORA / TZVP / CPCM

Pt	0.011787155	0.006499722	-0.033693495
P	1.272977904	-1.871264692	0.731415949
P	1.500645433	1.872053086	-0.249796191
P	-1.488808662	0.54743056	1.740220186
P	-1.03541824	-0.304471173	-2.141699253
C	2.902448218	-2.265628057	-0.05703262
C	2.999855671	-2.172284596	-1.443706911
C	4.014879534	-2.733921279	0.643938116
C	4.161997106	-2.526236336	-2.113399643
C	5.186093452	-3.074325767	-0.019608121
C	5.265959769	-2.972006622	-1.400946487
H	2.146793694	-1.825683434	-2.013080432
H	3.975989694	-2.844912449	1.719635058
H	4.204401747	-2.445507321	-3.194161935
H	6.037869295	-3.429230892	0.550427522
H	6.180515811	-3.240052514	-1.918167559
C	0.486656516	-3.543877779	0.620047533
C	-0.893375547	-3.640240126	0.771589636
C	1.215527006	-4.717512029	0.428144266
C	-1.534837035	-4.870037211	0.740458418
C	0.575865569	-5.948869997	0.381814009
C	-0.801023192	-6.030655685	0.539268517
H	-1.469140847	-2.734973186	0.920378229
H	2.291270189	-4.679758317	0.307330795
H	-2.610981325	-4.918278265	0.867217245
H	1.159546711	-6.849128493	0.222499088
H	-1.29865428	-6.993403507	0.50240652
C	1.762775804	-1.916424771	2.510204429
C	2.764211676	-1.057429832	2.968739652
C	1.154855673	-2.768343032	3.430670302
C	3.157939713	-1.065519986	4.297188669
C	1.535144108	-2.763065307	4.767190004
C	2.542250413	-1.917443191	5.205476182
H	3.249839868	-0.376990482	2.279832594
H	0.37662887	-3.449749029	3.111416634
H	3.945371149	-0.395642674	4.624182581
H	1.042504483	-3.43223443	5.464373467
H	2.846253735	-1.920251633	6.246362459
C	2.354602045	2.197795936	-1.862146306
C	2.843996295	1.107062357	-2.575327183
C	2.625574316	3.474736271	-2.354754891
C	3.625951158	1.274216779	-3.708405189
C	3.389868409	3.647390708	-3.501421676
C	3.90695376	2.549556865	-4.174815652
H	2.616548894	0.109553833	-2.226126327
H	2.24701844	4.351637686	-1.846113071
H	4.006529819	0.403448365	-4.231530699
H	3.585559308	4.650587147	-3.864900444
H	4.512984322	2.688147086	-5.063378978
C	0.849195635	3.560726948	0.112875525
C	1.656286813	4.634463273	0.498613971
C	-0.506687399	3.796147155	-0.075284544
C	1.115112679	5.896592194	0.690996092
C	-1.053068076	5.060173235	0.1018481
C	-0.242356922	6.115524079	0.489912555
H	2.719129584	4.490958478	0.650170271
H	-1.142357103	2.965947172	-0.35081725

H	1.759143582	6.714772389	0.994601989
H	-2.115862202	5.213620279	-0.051315827
H	-0.663325435	7.10365628	0.639753855
C	2.998871194	1.867396419	0.833814149
C	2.909740623	2.342445901	2.143113327
C	4.221888138	1.351180322	0.405721782
C	4.009495093	2.325238942	2.987096392
C	5.321052973	1.320915119	1.254231864
C	5.223005145	1.814523852	2.547096784
H	1.971839908	2.738189196	2.51157692
H	4.33150715	0.972006966	-0.602656203
H	3.913198368	2.708957156	3.997059798
H	6.260745749	0.915033619	0.895266109
H	6.083432018	1.799510227	3.206760124
C	-0.770595141	1.6076301	3.06922647
C	-1.152598147	2.938002927	3.249666236
C	0.233334649	1.100686201	3.895426322
C	-0.576055865	3.719528332	4.241836776
C	0.78794237	1.869520418	4.907779581
C	0.384024177	3.184304441	5.088641808
H	-1.907446744	3.379265172	2.612889545
H	0.607088709	0.096879976	3.740962524
H	-0.88908751	4.751877435	4.35570608
H	1.55420787	1.440153458	5.543767626
H	0.822728519	3.790439193	5.873490729
C	-3.073113033	1.458777949	1.440390106
C	-3.446575623	1.839713294	0.162858145
C	-3.944088992	1.741423334	2.497469119
C	-4.645824212	2.50370558	-0.072783767
C	-5.137863626	2.405134398	2.273469476
C	-5.492448186	2.791982056	0.984336867
H	-2.794636706	1.589069099	-0.662111621
H	-3.686834549	1.439429241	3.506691673
H	-4.914821099	2.787205751	-1.084302514
H	-5.7983375	2.619998205	3.106523462
H	-6.429078876	3.309897333	0.809608946
C	-2.283771624	-0.817917474	2.720599793
C	-3.341467091	-1.488318286	2.098887366
C	-1.935498111	-1.212410423	4.008926841
C	-4.018451612	-2.516565281	2.732197631
C	-2.611079556	-2.24748815	4.647368241
C	-3.65232419	-2.906538954	4.014798706
H	-3.655378972	-1.18848394	1.106148672
H	-1.143321435	-0.711083721	4.546047515
H	-4.838277356	-3.011633734	2.222714506
H	-2.318300117	-2.530204552	5.652929226
H	-4.179493666	-3.710444607	4.516311212
C	-0.756423401	1.042973634	-3.369723944
C	0.111112868	0.885535658	-4.449633644
C	-1.370752088	2.286392102	-3.207358011
C	0.324396326	1.915714117	-5.355023633
C	-1.162803009	3.317656188	-4.110345819
C	-0.318197541	3.134075601	-5.196312744
H	0.62777655	-0.05406626	-4.598107436
H	-2.041100229	2.462157599	-2.37629203
H	1.002325951	1.761548467	-6.187287173
H	-1.667220286	4.266498916	-3.963622498
H	-0.156867541	3.936658441	-5.907367995
C	-0.742110949	-1.793953083	-3.216395102
C	-0.102241807	-2.913178633	-2.708354032
C	-1.273645812	-1.868390642	-4.508163257
C	0.033439394	-4.074458457	-3.462765696

C	-1.136392172	-3.01732945	-5.268034951
C	-0.477915675	-4.127615301	-4.748092528
H	0.277062465	-2.889150238	-1.697641406
H	-1.806550196	-1.022459014	-4.926550142
H	0.539242095	-4.934581566	-3.037491323
H	-1.551299185	-3.05089955	-6.26967414
H	-0.3739672	-5.028199994	-5.343197748
C	-2.881292496	-0.511072689	-2.224331437
C	-3.740050349	0.19280336	-3.064820127
C	-3.416568955	-1.541042679	-1.451333229
C	-5.096542374	-0.108149018	-3.108516198
C	-4.76586408	-1.852440153	-1.501367874
C	-5.616748747	-1.128494979	-2.327308155
H	-3.361594994	0.980599072	-3.703138947
H	-2.759339268	-2.118946911	-0.811232067
H	-5.746545164	0.459200444	-3.766055874
H	-5.153979746	-2.661847209	-0.892162417
H	-6.674704493	-1.363034823	-2.364847034

Table S10: xyz coordinates of tetrakis(triphenylphosphine)platinum(0) as calculated by PBE0 / ZORA / TZVP / D3BJ / CPCM

Pt	0.017044347	-0.012718859	-0.018591223
P	1.234281252	-1.855512616	0.745432302
P	1.463999109	1.820626909	-0.242261268
P	-1.43958281	0.561404369	1.720973936
P	-0.989028223	-0.304774424	-2.09666551
C	2.82765103	-2.252860942	-0.084488722
C	2.866321288	-2.176665372	-1.474646259
C	3.971744768	-2.685529237	0.58391743
C	4.00955511	-2.513193245	-2.182118392
C	5.125757638	-3.00385999	-0.118845427
C	5.150307442	-2.919080437	-1.503677812
H	1.984139551	-1.848785609	-2.009817767
H	3.97060127	-2.779547033	1.661924869
H	4.010704271	-2.444950106	-3.264423598
H	6.008393358	-3.326690668	0.422150051
H	6.052381075	-3.169026798	-2.050610492
C	0.418723167	-3.504024129	0.658614566
C	-0.948625523	-3.575157984	0.911206449
C	1.103806638	-4.678071341	0.353594439
C	-1.621769011	-4.785279264	0.860529625
C	0.429214462	-5.889669798	0.286371981
C	-0.934459649	-5.948007496	0.538276823
H	-1.487557126	-2.667356295	1.150416547
H	2.167726175	-4.651710912	0.152251182
H	-2.686381542	-4.815224428	1.064412345
H	0.974119921	-6.792344881	0.032785816
H	-1.459216202	-6.895002958	0.481284955
C	1.75311209	-1.883586006	2.506011374
C	2.756741143	-1.013587374	2.936501162
C	1.147957544	-2.713796437	3.446617084
C	3.150727663	-0.984891353	4.263234927
C	1.524308016	-2.665890155	4.782714685
C	2.529604172	-1.80567804	5.196199708
H	3.235459267	-0.350998563	2.227562804
H	0.368583814	-3.400718785	3.144558871
H	3.935396858	-0.303614818	4.570781861
H	1.027914421	-3.310493391	5.499786677
H	2.827628611	-1.772455014	6.238050634
C	2.308215686	2.134638788	-1.846813813
C	2.87790904	1.048151971	-2.504314328
C	2.475824495	3.401734818	-2.39970294
C	3.641094212	1.216815725	-3.64765615
C	3.218511499	3.572756968	-3.559971838
C	3.817184631	2.48580142	-4.180016439
H	2.723361846	0.055896132	-2.104778543
H	2.027202765	4.267581778	-1.930261083
H	4.085683526	0.352320162	-4.128851204
H	3.330074837	4.566653233	-3.979582092
H	4.403229481	2.625666659	-5.0814466
C	0.768286703	3.484441803	0.094079114
C	1.527641265	4.580857806	0.504906315
C	-0.587771282	3.667829204	-0.136173749
C	0.93097838	5.81688035	0.699735417
C	-1.188583257	4.90515941	0.040328201
C	-0.42969218	5.983602903	0.468537589
H	2.591255545	4.472662323	0.678488439
H	-1.174375743	2.813207061	-0.439363765
H	1.532453449	6.656472429	1.030205133
H	-2.252055689	5.017989633	-0.140536161
H	-0.892981306	6.951473027	0.624292637

C	2.94048176	1.83279943	0.852165739
C	2.833654838	2.332758872	2.14986299
C	4.155439361	1.273684992	0.457176481
C	3.913785093	2.298196299	3.016850439
C	5.233407715	1.226010855	1.329970876
C	5.120680829	1.744902933	2.61212039
H	1.897145988	2.755289937	2.489488874
H	4.271267763	0.867033339	-0.53910866
H	3.804411569	2.695537531	4.019752791
H	6.166327447	0.781251564	1.001345169
H	5.963768344	1.711467685	3.292774204
C	-0.675673795	1.594414527	3.033183181
C	-0.958654593	2.955859956	3.150773521
C	0.290246352	1.051961894	3.880695483
C	-0.323466835	3.736075511	4.105958784
C	0.896106085	1.820455637	4.861849686
C	0.591724619	3.16824857	4.981469615
H	-1.674424765	3.42117019	2.487651305
H	0.609228482	0.027370126	3.75639287
H	-0.553689794	4.79410056	4.16732487
H	1.634215662	1.36492235	5.51194059
H	1.077529092	3.775575544	5.736751166
C	-2.979719822	1.516834167	1.397225636
C	-3.382156173	1.763876545	0.097046261
C	-3.808894733	1.927795688	2.44313306
C	-4.572723753	2.423797359	-0.178268645
C	-4.993845015	2.592994291	2.17996995
C	-5.378955186	2.845657979	0.866297108
H	-2.754897409	1.406138304	-0.705960197
H	-3.527032081	1.723330265	3.46999278
H	-4.865936753	2.600347031	-1.207138296
H	-5.62554344	2.912496679	3.001399772
H	-6.309388562	3.36407927	0.663531435
C	-2.274673169	-0.787294675	2.671333809
C	-3.422699528	-1.337944636	2.092566998
C	-1.824491927	-1.336860968	3.867556046
C	-4.077264204	-2.41191805	2.66951043
C	-2.4813347	-2.413926847	4.450780737
C	-3.604056597	-2.963397167	3.853886694
H	-3.814584141	-0.91578181	1.176617389
H	-0.959734604	-0.934302412	4.371105563
H	-4.962263889	-2.817431829	2.191282398
H	-2.103359	-2.822387587	5.381743234
H	-4.110997141	-3.806987609	4.308287858
C	-0.750985207	1.086541147	-3.264945193
C	0.235205908	1.038218993	-4.248801395
C	-1.481025925	2.26748285	-3.12786205
C	0.462674308	2.119335572	-5.08555125
C	-1.253825095	3.352160436	-3.96035137
C	-0.283682713	3.279998133	-4.94945483
H	0.835275024	0.145685045	-4.367619435
H	-2.254020039	2.351085929	-2.375765919
H	1.237234985	2.054942891	-5.840421872
H	-1.841499669	4.254640479	-3.833803595
H	-0.104175202	4.126184841	-5.60297084
C	-0.644218074	-1.75695671	-3.189819096
C	-0.184472448	-2.932405521	-2.615477241
C	-0.987342214	-1.769381987	-4.54353534
C	-0.0387034	-4.092699929	-3.365091804
C	-0.833830745	-2.919627447	-5.299738014
C	-0.35499828	-4.086986955	-4.713957665
H	0.046513326	-2.945150491	-1.560730805

H	-1.384784749	-0.877640967	-5.01286313
H	0.324388753	-4.996488655	-2.888265811
H	-1.097308291	-2.908453497	-6.351722484
H	-0.238216279	-4.986256893	-5.308318182
C	-2.814626714	-0.579981544	-2.169699615
C	-3.677095583	0.001126105	-3.095027377
C	-3.326142038	-1.524430772	-1.284077851
C	-5.025829626	-0.329879301	-3.104988588
C	-4.66704143	-1.871173271	-1.303778281
C	-5.527199266	-1.26362632	-2.209467025
H	-3.304829278	0.717751673	-3.815836841
H	-2.655748366	-1.989268984	-0.570326758
H	-5.68664731	0.144384301	-3.822401642
H	-5.042730551	-2.608816525	-0.602768904
H	-6.580620716	-1.519605807	-2.219395483

Table S11: Pt EXAFS fitting results for tetrakis(triphenylphosphine)platinum(0)

R-factor	ΔE_0 (eV)	P			C_{short}			C_{long}		
		N	R (Å)	$\sigma^2 \times 10^{-3}$ (Å ²)	N	R (Å)	$\sigma^2 \times 10^{-3}$ (Å ²)	N	R (Å)	$\sigma^2 \times 10^{-3}$ (Å ²)
0.4141646	4.167	1	2.32862	1.39						
0.2108676	2.81	2	2.32458	5.06						
0.1107222	1.822	3	2.32144	7.73						
0.0643505	1.102	4	2.31873	9.98						
0.0493163	0.346	5	2.31651	11.99						
0.1001759	1.648	3	2.32033	7.73	1	3.62009	1.43			
0.0955696	1.706	3	2.32065	7.73	2	3.63705	5.91			
0.0921992	1.75	3	2.32089	7.73	3	3.6493	9.1			
0.0896898	1.794	3	2.32112	7.73	4	3.65826	11.64			
0.0877173	1.829	3	2.32131	7.73	5	3.66499	13.79			
0.086138	1.857	3	2.32146	7.73	6	3.6703	15.68			
0.0550806	0.894	4	2.31792	9.99	1	3.60975	1.08			
0.0510066	0.921	4	2.31806	9.99	2	3.62693	5.71			
0.0483061	0.97	4	2.31833	9.99	3	3.63966	9.03			
0.0463496	1.015	4	2.31858	9.99	4	3.64885	11.66			
0.0448698	1.052	4	2.31878	9.99	5	3.65571	13.87			
0.0437284	1.082	4	2.31895	9.99	6	3.66108	15.81			
0.0408819	0.242	5	2.31577	12	1	3.60182	0.79			
0.037536	0.272	5	2.31592	12	2	3.61873	5.51			
0.0353969	0.325	5	2.31622	12	3	3.63166	8.94			
0.0339141	0.373	5	2.31649	12	4	3.64108	11.65			
0.0328475	0.413	5	2.31672	12	5	3.64808	13.92			
0.0320746	0.446	5	2.3169	12	6	3.65354	15.9			
0.0892758	2.012	3	2.3223	7.76	3	3.64103	4.36	1	3.82493	-0.92
0.0873354	2.075	3	2.32264	7.75	3	3.62319	3.65	2	3.80469	2.76
0.0857712	2.114	3	2.32286	7.75	3	3.61131	3.77	3	3.79222	5.61
0.0845369	2.144	3	2.32301	7.75	3	3.60331	4.16	4	3.78435	8.12
0.0835588	2.169	3	2.32314	7.75	3	3.59784	4.64	5	3.77922	10.42
0.0827798	2.188	3	2.32324	7.75	3	3.59409	5.16	6	3.77583	12.57
0.0869483	2.025	3	2.32234	7.75	4	3.64996	6.82	1	3.83918	-0.89
0.0855266	2.09	3	2.32271	7.75	4	3.63415	5.81	2	3.82244	2.62
0.0843262	2.128	3	2.32291	7.75	4	3.62218	5.63	3	3.81045	5.27
0.0833629	2.155	3	2.32306	7.75	4	3.61332	5.83	4	3.80203	7.62
0.0826037	2.177	3	2.32317	7.75	4	3.60679	6.21	5	3.79609	9.82
0.081989	2.194	3	2.32326	7.75	4	3.60197	6.68	6	3.79185	11.91
0.0851096	2.03	3	2.32235	7.75	5	3.65608	8.97	1	3.84901	-0.79

0.0840561	2.096	3	2.32272	7.75	5	3.64218	7.79	2	3.83545	2.65
0.0831524	2.134	3	2.32293	7.75	5	3.63085	7.41	3	3.82466	5.18
0.082411	2.159	3	2.32306	7.75	5	3.62186	7.45	4	3.81639	7.42
0.0818147	2.178	3	2.32316	7.75	5	3.61483	7.71	5	3.81014	9.53
0.0813344	2.193	3	2.32324	7.75	5	3.60941	8.11	6	3.80542	11.56
0.0844879	1.888	3	2.32162	7.72	6	3.6715	15.63	1	4.4883	-0.34
0.0828682	2.096	3	2.32271	7.75	6	3.64829	9.62	2	3.8454	2.76
0.0822035	2.134	3	2.32292	7.75	6	3.63781	9.11	3	3.83601	5.23
0.0816389	2.158	3	2.32305	7.75	6	3.62907	9.02	4	3.82828	7.4
0.081182	2.176	3	2.32314	7.75	6	3.62195	9.19	5	3.8221	9.44
0.0808088	2.189	3	2.32321	7.75	6	3.61625	9.53	6	3.81721	11.44
0.0456522	1.237	4	2.31983	10.01	3	3.63369	4.07	1	3.81796	-1.3
0.0442901	1.301	4	2.32019	10.01	3	3.61616	3.38	2	3.79857	2.45
0.0432594	1.346	4	2.32043	10.01	3	3.60437	3.51	3	3.78629	5.39
0.0424853	1.38	4	2.32061	10.01	3	3.59642	3.93	4	3.7784	7.98
0.0419117	1.406	4	2.32075	10.01	3	3.591	4.45	5	3.77318	10.37
0.0414843	1.426	4	2.32086	10.01	3	3.58731	5	6	3.76962	12.62
0.0439113	1.253	4	2.31989	10.01	4	3.64213	6.6	1	3.83158	-1.2
0.0430049	1.321	4	2.32028	10.01	4	3.62676	5.58	2	3.81581	2.35
0.0422762	1.362	4	2.32051	10.01	4	3.61492	5.43	3	3.80408	5.07
0.0417307	1.392	4	2.32067	10.01	4	3.6061	5.65	4	3.79569	7.5
0.0413337	1.415	4	2.32079	10.01	4	3.59958	6.06	5	3.78969	9.78
0.0410458	1.433	4	2.32089	10.01	4	3.59481	6.57	6	3.78534	11.95
0.0425961	1.261	4	2.31992	10.01	5	3.64792	8.79	1	3.84103	-1.06
0.0420072	1.33	4	2.32031	10.01	5	3.63448	7.61	2	3.82841	2.42
0.04153	1.371	4	2.32054	10.01	5	3.62332	7.25	3	3.81796	5.01
0.0411683	1.398	4	2.31069	10.01	5	3.61438	7.3	4	3.80977	7.32
0.0409074	1.419	4	2.3208	10.01	5	3.60737	7.6	5	3.80348	9.5
0.0407232	1.435	4	2.32089	10.01	5	3.60197	8.04	6	3.79867	11.62
0.0416145	1.264	4	2.31992	10.01	6	3.65225	10.76	1	3.8481	-0.9
0.0412529	1.332	4	2.32031	10.01	6	3.64032	9.48	2	3.83806	2.56
0.0409702	1.373	4	2.32054	10.01	6	3.63004	8.99	3	3.82903	5.09
0.0407564	1.4	4	2.32069	10.01	6	3.62138	8.91	4	3.82143	7.31
0.0406032	1.419	4	2.32079	10.01	6	3.61427	9.11	5	3.81522	9.43
0.0404964	1.433	4	2.32087	10.01	6	3.60858	9.5	6	3.81023	11.52
0.0408926	1.264	4	2.31991	10.01	7	3.65569	12.56	1	3.85367	-0.74
0.0406984	1.33	4	2.32029	10.01	7	3.64493	11.23	2	3.84574	2.75
0.0405615	1.371	4	2.32052	10.01	7	3.63549	10.64	3	3.83807	5.25
0.040463	1.398	4	2.32067	10.01	7	3.6273	10.48	4	3.83124	7.44
0.0404932	1.417	4	2.32077	10.01	7	3.62034	10.61	5	3.82536	9.53
0.0403447	1.429	4	2.32084	10.01	7	3.61462	10.95	6	3.82042	11.61
0.0329218	0.6	5	2.31782	12.02	3	3.6281	3.89	1	3.81303	-1.53
0.0320227	0.667	5	2.3182	12.02	3	3.61074	3.21	2	3.79404	2.29

0.0313871	0.711	5	2.31844	12.02	3	3.59893	3.37	3	3.78172	5.31
0.0309752	0.746	5	2.31863	12.02	3	3.59101	3.81	4	3.77377	7.98
0.0307219	0.772	5	2.31878	12.02	3	3.58563	4.36	5	3.76844	10.45
0.0305766	0.792	5	2.31888	12.02	3	3.58202	4.94	6	3.76474	12.79
0.0316568	0.618	5	2.3179	12.02	4	3.63614	6.46	1	3.82626	-1.4
0.0311468	0.686	5	2.31829	12.02	4	3.621	5.45	2	3.81094	2.22
0.0307871	0.729	5	2.31853	12.02	4	3.6092	5.31	3	3.79928	5
0.0305704	0.759	5	2.3187	12.02	4	3.60039	5.55	4	3.79085	7.5
0.0304653	0.783	5	2.31883	12.02	4	3.5939	5.99	5	3.78478	9.84
0.0304363	0.801	5	2.31893	12.02	4	3.58918	6.53	6	3.78033	12.1
0.0307789	0.628	5	2.31794	12.02	5	3.64163	8.69	1	3.83544	-1.24
0.0305415	0.697	5	2.31833	12.02	5	3.62846	7.51	2	3.82331	2.3
0.0303965	0.739	5	2.31857	12.02	5	3.61738	7.15	3	3.81298	4.94
0.0303332	0.767	5	2.31873	12.02	5	3.60845	7.23	4	3.80477	7.31
0.0303379	0.788	5	2.31885	12.02	5	3.60145	7.55	5	3.79842	9.56
0.0303893	0.804	5	2.31893	12.02	5	3.59609	8.03	6	3.79354	11.76
0.0301978	0.633	5	2.31795	12.02	6	3.64573	10.68	1	3.84229	-1.07
0.0301524	0.701	5	2.31834	12.02	6	3.63408	9.4	2	3.83275	2.45
0.0301682	0.743	5	2.31858	12.02	6	3.62391	8.91	3	3.8239	5.02
0.0302241	0.771	5	2.31874	12.02	6	3.61528	8.86	4	3.81631	7.31
0.0303115	0.79	5	2.31884	12.02	6	3.60818	9.09	5	3.81006	9.5
0.0304175	0.804	5	2.31892	12.02	6	3.60251	9.5	6	3.805	11.66