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Supplementary Information

The Influence of Water Molecule Coordination onto the Water/Aromatic Interaction. Strong Interactions of Water Coordinating to a Metal Ion

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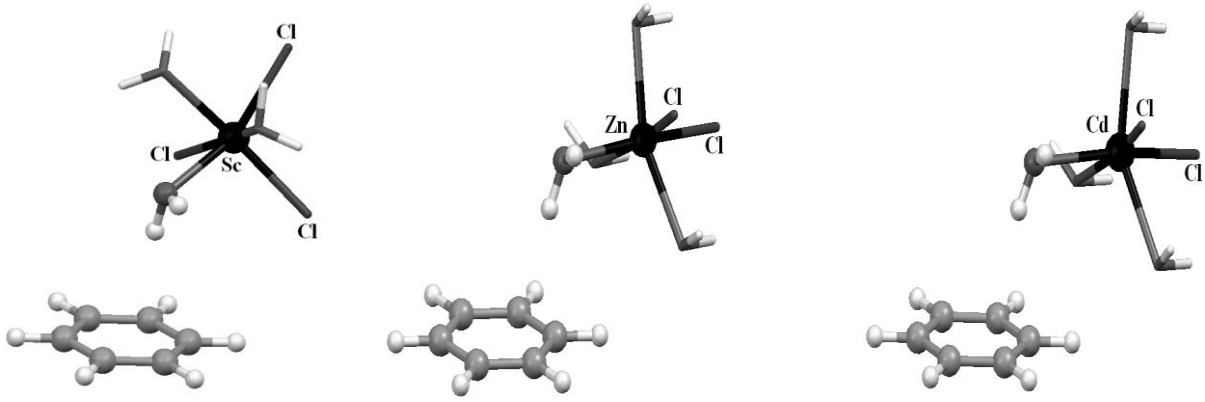
I Optimized geometries and interaction energies of aqua-complex/benzene systems

Starting with the aqua-complex/benzene geometries presented in Table 2 in main text, complete optimizations were performed, using B3LYP method with LANL2DZ basis set for metal atoms and 6-31G** basis sets for the carbon, oxygen, chlorine and hydrogen atoms. Geometries obtained by optimization are shown in Figure S1.

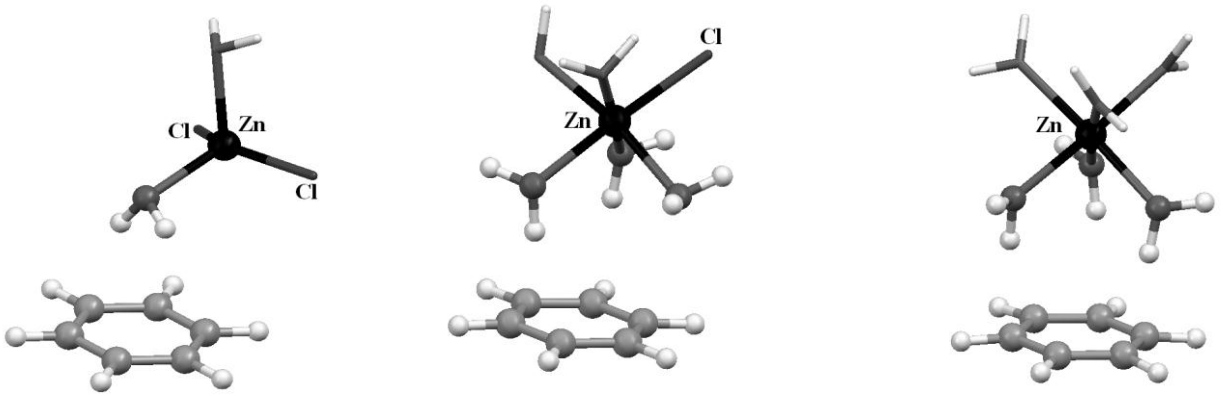
Using optimized geometries interaction energies of benzene with aqua-complex were calculated by single point calculations at MP2/def2-QZVP level. The interaction energies are shown in Table S1. The most attractive interaction was obtained for hexaaqua complex with 2+ charge (Figure S1f); the energy is -21.65 kcal/mol.



$[ScCl_3(H_2O)_3] / C_6H_6$ (a)

cis-$[ZnCl_2(H_2O)_4] / C_6H_6$ (b)

cis-$[CdCl_2(H_2O)_4] / C_6H_6$ (c)



$[ZnCl_2(H_2O)_2] / C_6H_6$ (d)

$[ZnCl(H_2O)_5]^+ / C_6H_6$ (e)

$[Zn(H_2O)_6]^{2+} / C_6H_6$ (f)

Figure S1. Optimized geometries of aqua-complex/benzene systems: $[ScCl_3(H_2O)_3]/C_6H_6$ (a), cis-$[ZnCl_2(H_2O)_4]/C_6H_6$ (b), cis-$[CdCl_2(H_2O)_4]/C_6H_6$ (c), $[ZnCl_2(H_2O)_2]/C_6H_6$ (d), $[ZnCl(H_2O)_5]^+/C_6H_6$ (e) and $[Zn(H_2O)_6]^{2+}/C_6H_6$ (f). Interaction energies are presented in Table S1.

Table S1. Interaction energies (in kcal/mol) in optimized aqua-complex/benzene geometries.

Model systems	**ΔE**
Neutral octahedral complexes	
$[ScCl_3(H_2O)_3]$ /C_6H_6	-9.24
cis-$[ZnCl_2(H_2O)_4]$ /C_6H_6	-6.96
cis-$[CdCl_2(H_2O)_4]$ /C_6H_6	-7.02
Neutral tetrahedral complex	
$[ZnCl_2(H_2O)_2]$ /C_6H_6	-9.44
Charged octahedral complexes	
$[ZnCl(H_2O)_5]^+$/C_6H_6	-10.74
$[Zn(H_2O)_6]^{2+}$/C_6H_6	-21.65

1. The coordinates of optimized $[ScCl_3(H_2O)_3]$ / C_6H_6 system

21	-0.1857472148	-0.1661031282	0.0485562144
8	1.8356348355	0.9673676608	0.1388465683
1	2.0633946878	0.8905297041	1.0804497226
1	2.5059971245	0.4631591209	-0.3458101959
17	-0.1719827659	0.3669151935	2.355755661
8	0.3493252595	-0.0309563055	-2.1696312413
1	0.4255560799	-0.9429381578	-2.4914040306
1	-0.3641649217	0.3924757033	-2.6687748846
8	-0.689165381	1.9443980805	-0.5292809957
1	-0.0222027028	2.5802078752	-0.2332587958
1	-1.5461253127	2.2585665765	-0.1793127367
17	1.0844505445	-2.1564778354	-0.1434106179
17	-2.4002622233	-0.6962544203	-0.5119428228
6	-2.4293183733	5.4975133755	0.4639335604
6	-3.3217953285	4.8739643876	-0.4116647593
6	-3.7766656118	3.5799778629	-0.1409107872
6	-3.3385612077	2.9089321319	1.0078263703
6	-2.4408368527	3.5348597199	1.8835415519
6	-1.9873843289	4.8282983073	1.6092788592
1	-2.0790686097	6.5044656129	0.2548135312
1	-3.665091346	5.3952359499	-1.3006611109
1	-4.4729643895	3.0928959059	-0.8173545395

1 -3.6924480364 1.904387111 1.2202347401
1 -2.093018392, 3.0055373022 2.7650589354
1 -1.2953065331 5.3155912655 2.2903468035

2. The coordinates of optimized cis-[$ZnCl_2(H_2O)_4$] / C_6H_6 system

30 -0.0579876925 -0.0596700853 -0.253286672
8 2.1030245249 -0.0129402285 -0.2523937486
1 2.2778280533 0.0359065959 0.7034041614
1 2.5072135476 0.7733137319 -0.6607194693
17 0.1928570286 -0.1386304567 2.1586388734
8 0.269609956 -0.0577215392 -2.4447327214
1 0.6457894075 -0.8983120728 -2.7413440165
1 -0.6836932254 -0.0860426776 -2.6645425196
8 -0.4536515723 2.095047506 0.0330722659
1 -0.4737656112 2.070981546 1.0068329457
1 -1.3868704574 2.0841926138 -0.2482977835
8 -0.3493411828 -2.2377759318 -0.1629790517
1 -1.3125376362 -2.2253457699 -0.312021919
1 -0.2368073209 -2.3563159253 0.7963924567
17 -2.4089997802 -0.072611156 -1.0735673126
6 5.3542192985 2.6135876028 -1.9068002497
6 5.0761303122 3.3377548422 -0.7440579446
6 3.7528540781 3.5848237811 -0.3732213932
6 2.7020086055 3.1107196176 -1.1667992991
6 2.9816922834 2.3850284955 -2.3326606575
6 4.3088937565 2.1357881061 -2.6993960743
1 6.3842696663 2.4216700604 -2.1932828067
1 5.8905410678 3.708163769 -0.1280356198
1 3.5374503255 4.1498765169 0.5291670184
1 1.670825388 3.3014617273 -0.8832615373
1 2.1651845537 2.0149341714 -2.9464960703
1 4.5253116256 1.5741221592 -3.603711855

3. The coordinates of optimized cis-[$CdCl_2(H_2O)_4$] / C_6H_6 system

48 0.113199 -0.047198 -0.323172
8 2.446061 -0.171320 -0.187538
1 2.512829 -0.104424 0.781585
1 2.921168 0.592963 -0.557098
17 0.382419 -0.032924 2.235822
8 0.529823 -0.057879 -2.679557
1 0.836576 -0.892474 -3.058928
1 -0.428387 0.000076 -2.874044

8	-0.256355	2.294546	0.052882
1	-0.293568	2.210923	1.022310
1	-1.180351	2.321936	-0.249634
8	-0.549925	-2.309150	-0.003016
1	-1.487317	-2.185455	-0.231815
1	-0.513447	-2.321194	0.968477
17	-2.256602	0.123663	-1.383806
6	5.709051	2.421143	-1.619429
6	5.408138	3.163507	-0.474322
6	4.079982	3.463231	-0.163252
6	3.047676	3.025027	-0.999661
6	3.349822	2.282346	-2.149206
6	4.681442	1.979122	-2.455396
1	6.742398	2.187183	-1.858904
1	6.208224	3.506256	0.175571
1	3.846962	4.040221	0.727066
1	2.013341	3.256193	-0.760926
1	2.548074	1.940851	-2.798398
1	4.915488	1.403456	-3.346452

4. The coordinates of optimized [$ZnCl_2(H_2O)_2$] / C_6H_6 system

30	-0.9221674282	0.1564276472	0.3585148035
17	0.034901879	1.1776186447	2.1320698871
8	-0.4121688648	1.4799203398	-1.1973194775
1	-0.0420937437	2.2912732157	-0.8167102972
1	-1.1787996525	1.7721581005	-1.7226557303
8	0.3521235221	-1.5640469408	0.2437811671
1	-0.2043402845	-2.3549751885	0.180849533
1	0.8618537939	-1.6314407169	1.0650709434
17	-2.8653768574	-0.8415156774	-0.1952597501
6	-1.4593694972	4.7727349937	-1.8309222349
6	-1.8081182395	4.646975426	-0.4824555363
6	-2.792563721	3.731949584	-0.0945685221
6	-3.4283622073	2.9394095683	-1.0546359016
6	-3.0793379241	3.0643295299	-2.4057192902
6	-2.0959709911	3.9823927508	-2.7939768601
1	-0.6988080022	5.4876706132	-2.1317572527
1	-1.3158502794	5.2611861661	0.2659643323
1	-3.055880156	3.6305562396	0.9537803721
1	-4.1775854397	2.2141646991	-0.753882979
1	-3.5790426958	2.4529257513	-3.1517280685
1	-1.8299722107	4.0828182537	-3.8424101379

5. The coordinates of optimized $[ZnCl(H_2O)_5]^+ / C_6H_6$ system

30	0.2713237447	0.0493243615	-0.0428204309
8	2.1883024849	1.1324632089	-0.0508730529
1	2.4495919374	1.2045517697	0.8808609809
1	2.9730148119	0.8752696189	-0.5689173377
17	0.0947061752	0.4418354053	2.2443763827
8	0.4999531091	-0.3808284876	-2.1134329129
1	1.3575556664	-0.7051893073	-2.446876876
1	0.2256708541	0.3391997156	-2.6985841328
8	-0.3460015686	2.0384722412	-0.7760258586
1	0.4582428019	2.5540727685	-0.6024451281
1	-1.0428939103	2.4627617479	-0.2537770513
8	1.0302344563	-1.947984877	0.3817809115
1	0.452647071	-2.6827639187	0.1291220244
1	1.0489529568	-1.9434147731	1.3548286474
8	-1.7684975498	-0.705166074	-0.0276625935
1	-2.1312834087	-0.5437123897	0.8578385816
1	-2.4946010126	-0.6689065999	-0.6639511527
6	4.7378017128	-0.9576274823	-1.1136442621
6	4.8130523989	0.2722091147	-1.7836583152
6	4.163582697	0.4340328468	-3.0147217033
6	3.4584990852	-0.6353588874	-3.5810206751
6	3.3944155342	-1.8653682269	-2.9116993589
6	4.0258248815	-2.021691511	-1.6720256607
1	5.2587288278	-1.0886942125	-0.1693478089
1	5.4067486729	1.0835168242	-1.3713556214
1	4.2392308785	1.3780554184	-3.5465118042
1	3.0028056493	-0.5256276038	-4.561624877
1	2.8823498198	-2.7076269744	-3.3692366427
1	3.9841974623	-2.9760331209	-1.1572908784

6 .The coordinates of optimized $[Zn(H_2O)_6]^{2+} / C_6H_6$ system

30	0.1946230266	0.3276813405	0.0196494016
8	2.1432467044	1.1374996695	-0.2451142055
1	2.8232129697	1.0381800198	0.4504144819
1	2.6092038084	1.1139042737	-1.0932878381
8	0.2872725932	0.7452400584	2.1023215238
1	0.0400494311	1.6031355737	2.4765366019
1	1.0227786959	0.4034272844	2.6482856632
8	0.0395956389	-0.2375352604	-2.03023524
1	0.3741709528	-1.075143808	-2.3813616346
1	-0.263817472	0.2936339199	-2.7799800201
8	-0.5344683205	2.2752982699	-0.4458373642

1	0.0416152341	3.0395607344	-0.5900658217
1	-1.4491238556	2.5906101388	-0.462084534
8	1.0293465006	-1.6000252181	0.3568496696
1	0.4930698516	-2.3676308243	0.6024733196
1	1.8855520818	-1.6984689394	0.8182754542
8	-1.7954297656	-0.350895985	0.3647000934
1	-2.1986506639	-0.4085866086	1.2427029488
1	-2.4140268512	-0.7430796583	-0.2676418311
6	4.4815354366	-0.6605548846	1.4922162668
6	3.8096974607	-1.7682953835	2.0350076444
6	3.0014070969	-1.6079445759	3.1680395638
6	2.8590804243	-0.3415154206	3.7588572237
6	3.5304346838	0.761679033	3.2155008556
6	4.3414756112	0.6037627782	2.0795127944
1	5.1534594125	-0.797217571	0.6493323267
1	3.983864491	-2.7601513759	1.6249440942
1	2.5274647183	-2.4724680424	3.6247287371
1	2.2956635241	-0.2364003167	4.6828477956
1	3.4689136702	1.7303344648	3.703894246
1	4.922401597	1.4449333391	1.7091003257

II The coordinates of water/benzene and aqua-complex/benzene systems from Table 2.

1. The coordinates of H_2O / C_6H_6 system, with r=0.0 Å and R=2.3 Å

8	-0.186925	-1.878217	-0.133582
1	0.300096	-2.263623	0.604882
1	0.329691	-2.130366	-0.908574
6	2.405888	-3.696377	1.473728
6	2.582515	-2.423479	2.021580
6	1.637672	-1.909440	2.913007
6	0.516201	-2.668299	3.256583
6	0.339574	-3.941198	2.708731
6	1.284418	-4.455237	1.817304
1	3.141068	-4.096349	0.780112
1	3.455127	-1.833013	1.754245
1	1.775104	-0.919003	3.339289
1	-0.218979	-2.268328	3.950199
1	-0.533038	-4.531663	2.976066
1	1.146985	-5.445674	1.391022

2. The coordinates of H_2O / C_6H_6 system, with r=0.6 Å and R=2.4 Å

8	-0.186925	-1.878217	-0.133582
1	0.300096	-2.263623	0.604882
1	0.329691	-2.130366	-0.908574
6	0.160872	-2.487466	3.715975
6	-0.015755	-3.760365	3.168123
6	0.929089	-4.274404	2.276695
6	2.050560	-3.515544	1.933120
6	2.227187	-2.242646	2.480972
6	1.282343	-1.728607	3.372399
1	-0.574308	-2.087495	4.409591
1	-0.888367	-4.350830	3.435458
1	0.791656	-5.264841	1.850414
1	2.785739	-3.915516	1.239504
1	3.099799	-1.652180	2.213637
1	1.419775	-0.738170	3.798680

3. The coordinates of $[ScCl_3(H_2O)_3]$ / C_6H_6 system, with r=0.0 Å and R=2.9 Å

21	-0.078925	-0.077714	0.079922
8	2.171682	0.312678	-0.055828
1	2.551836	0.005408	0.782244
1	2.580316	-0.209194	-0.761536
17	0.314909	0.313209	2.369099
8	0.311972	0.053190	-2.171851
1	0.010347	-0.789829	-2.545763
1	-0.217830	0.751608	-2.582865
8	0.055831	2.173135	-0.310809
1	0.756509	2.582043	0.217631
1	-0.785407	2.550634	-0.008842
17	0.310738	-2.367803	-0.312471
17	-2.367980	0.316634	-0.312932
6	2.547164	5.051480	1.245283
6	3.492337	4.226903	0.630198
6	3.800181	2.982382	1.185184
6	3.162851	2.562438	2.355256
6	2.217678	3.387015	2.970341
6	1.909834	4.631536	2.415355
1	2.307632	6.019836	0.813451
1	3.988241	4.553659	-0.280230
1	4.535616	2.340782	0.706589
1	3.402383	1.594082	2.787088
1	1.721774	3.060259	3.880769
1	1.174399	5.273136	2.893950

4. The coordinates of $[ScCl_3(H_2O)_3]$ / C_6H_6 system, with r=0.6 Å and R=2.5 Å

21	-0.078925	-0.077714	0.079922
8	2.171682	0.312678	-0.055828
1	2.551836	0.005408	0.782244
1	2.580316	-0.209194	-0.761536
17	0.314909	0.313209	2.369099
8	0.311972	0.053190	-2.171851
1	0.010347	-0.789829	-2.545763
1	-0.217830	0.751608	-2.582865
8	0.055831	2.173135	-0.310809
1	0.756509	2.582043	0.217631
1	-0.785407	2.550634	-0.008842
17	0.310738	-2.367803	-0.312471
17	-2.367980	0.316634	-0.312932
6	-0.794551	2.115464	-5.418029
6	-1.962730	1.475653	-4.996592
6	-2.517873	1.783763	-3.752208
6	-1.904837	2.731683	-2.929259
6	-0.736658	3.371493	-3.350696
6	-0.181515	3.063384	-4.595081
1	-0.362596	1.875725	-6.386280
1	-2.439731	0.738081	-5.636925
1	-3.426829	1.285929	-3.424289
1	-2.336792	2.971422	-1.961009
1	-0.259657	4.109066	-2.710363
1	0.727441	3.561217	-4.922999

5. The coordinates of cis-$[ZnCl_2(H_2O)_4]$ / C_6H_6 system, with r=0.0 Å and R=2.3 Å

30	0.230000	0.007000	-0.226000
8	2.422000	-0.041000	-0.419000
1	2.608000	-0.050000	0.540000
1	2.776000	0.791000	-0.763000
17	0.803000	-0.117000	2.141000
8	0.386000	-0.066000	-2.421000
1	0.679000	-0.934000	-2.734000
1	-0.574000	-0.016000	-2.592000
8	0.202000	2.188000	0.071000
1	0.253000	2.179000	1.043000
1	-0.734000	2.357000	-0.139000

8	-0.181000	-2.150000	-0.082000
1	-1.152000	-2.093000	-0.121000
1	0.035000	-2.281000	0.858000
17	-2.139000	0.228000	-0.770000
6	4.908634	2.250461	-1.510216
6	4.369956	2.930591	-0.415292
6	3.075326	3.450963	-0.484251
6	2.319375	3.291206	-1.648134
6	2.858052	2.611077	-2.743058
6	4.152682	2.090704	-2.674099
1	5.915980	1.845562	-1.456560
1	4.958159	3.054897	0.490321
1	2.656183	3.980169	0.367705
1	1.312028	3.696106	-1.701790
1	2.269849	2.486770	-3.648671
1	4.571825	1.561499	-3.526055

6. The coordinates of cis-[$ZnCl_2(H_2O)_4$] / C_6H_6 system, with r=0.6 Å and R=2.2 Å

30	0.230000	0.007000	-0.226000
8	2.422000	-0.041000	-0.419000
1	2.608000	-0.050000	0.540000
1	2.776000	0.791000	-0.763000
17	0.803000	-0.117000	2.141000
8	0.386000	-0.066000	-2.421000
1	0.679000	-0.934000	-2.734000
1	-0.574000	-0.016000	-2.592000
8	0.202000	2.188000	0.071000
1	0.253000	2.179000	1.043000
1	-0.734000	2.357000	-0.139000
8	-0.181000	-2.150000	-0.082000
1	-1.152000	-2.093000	-0.121000
1	0.035000	-2.281000	0.858000
17	-2.139000	0.228000	-0.770000
6	5.428181	1.940898	-1.445087
6	4.672229	1.781141	-2.608970
6	3.377599	2.301513	-2.677929
6	2.838921	2.981643	-1.583005
6	3.594873	3.141400	-0.419122
6	4.889503	2.621027	-0.350163
1	6.435527	1.535999	-1.391431
1	5.091372	1.251935	-3.460926
1	2.789396	2.177207	-3.583541
1	1.831575	3.386542	-1.636661
1	3.175730	3.670605	0.432835
1	5.477706	2.745334	0.555450

7. The coordinates of cis-[$CdCl_2(H_2O)_4$] / C_6H_6 system, with r=0.0 Å and R=2.3 Å

48	0.280048	-0.002515	-0.281720
8	2.648013	-0.054534	-0.386562
1	2.731095	-0.076217	0.588068
1	3.090375	0.752882	-0.681366
17	0.965336	-0.116765	2.208727
8	0.392699	-0.062103	-2.649408
1	0.645859	-0.896789	-3.065994
1	-0.578958	0.010001	-2.738273
8	0.060987	2.326832	0.163404
1	0.122180	2.280294	1.132547
1	-0.887236	2.403991	-0.038923
8	-0.297615	-2.283495	0.078378
1	-1.262658	-2.187585	0.011798
1	-0.099458	-2.317193	1.030026
17	-2.196668	0.223197	-0.984702
6	5.383058	2.048395	-1.236336
6	4.822069	2.747089	-0.164549
6	3.581738	3.372913	-0.311283
6	2.902395	3.300043	-1.529804
6	3.463384	2.601349	-2.601591
6	4.703716	1.975525	-2.454857
1	6.348155	1.561444	-1.122163
1	5.350663	2.803788	0.783577
1	3.145234	3.916564	0.522670
1	1.937298	3.786994	-1.643977
1	2.934791	2.544649	-3.549717
1	5.140220	1.431874	-3.288810

8. The coordinates of cis-[$CdCl_2(H_2O)_4$] / C_6H_6 system, with r=0.6 Å and R=2.3 Å

48	0.280048	-0.002515	-0.281720
8	2.648013	-0.054534	-0.386562
1	2.731095	-0.076217	0.588068
1	3.090375	0.752882	-0.681366
17	0.965336	-0.116765	2.208727
8	0.392699	-0.062103	-2.649408
1	0.645859	-0.896789	-3.065994
1	-0.578958	0.010001	-2.738273
8	0.060987	2.326832	0.163404
1	0.122180	2.280294	1.132547
1	-0.887236	2.403991	-0.038923
8	-0.297615	-2.283495	0.078378

1	-1.262658	-2.187585	0.011798
1	-0.099458	-2.317193	1.030026
17	-2.196668	0.223197	-0.984702
6	5.915771	1.779609	-1.173315
6	5.236428	1.706739	-2.391836
6	3.996097	2.332563	-2.538570
6	3.435107	3.031257	-1.466783
6	4.114450	3.104126	-0.248262
6	5.354781	2.478302	-0.101528
1	6.880868	1.292657	-1.059142
1	5.672932	1.163088	-3.225789
1	3.467503	2.275863	-3.486696
1	2.470010	3.518208	-1.580956
1	3.677946	3.647777	0.585691
1	5.883375	2.535002	0.846598

9. The coordinates of $[ZnCl_2(H_2O)_2]$ / C_6H_6 system, with r=0.0 Å and R=2.8 Å

30	-0.590764	-0.000876	0.700991
17	0.694525	-0.002304	2.545387
8	0.152825	1.740551	-0.280062
1	0.686674	2.283291	0.318539
1	-0.563941	2.294534	-0.622205
8	0.155502	-1.738535	-0.284847
1	-0.561460	-2.292286	-0.627006
1	0.690525	-2.282023	0.312019
17	-2.723888	-0.002352	-0.002817
6	-1.697925	4.804950	-2.105880
6	-2.200147	4.954762	-0.810914
6	-3.138633	4.045856	-0.316198
6	-3.574896	2.987139	-1.116448
6	-3.072674	2.837327	-2.411415
6	-2.134189	3.746233	-2.906131
1	-0.967693	5.512166	-2.490817
1	-1.860692	5.778545	-0.188242
1	-3.529410	4.162423	0.691411
1	-4.305128	2.279923	-0.731512
1	-3.412129	2.013544	-3.034086
1	-1.743412	3.629665	-3.913739

10. The coordinates of $[ZnCl_2(H_2O)_2]$ / C_6H_6 system, with r=0.6 Å and R=2.4 Å

30	-0.590764	-0.000876	0.700991
17	0.694525	-0.002304	2.545387

8	0.152825	1.740551	-0.280062
1	0.686674	2.283291	0.318539
1	-0.563941	2.294534	-0.622205
8	0.155502	-1.738535	-0.284847
1	-0.561460	-2.292286	-0.627006
1	0.690525	-2.282023	0.312019
17	-2.723888	-0.002352	-0.002817
6	-0.998756	4.966497	-2.177051
6	-1.435020	3.907779	-2.977301
6	-2.373505	2.998874	-2.482585
6	-2.875727	3.148685	-1.187619
6	-2.439464	4.207402	-0.387368
6	-1.500978	5.116308	-0.882084
1	-0.268524	5.673712	-2.561987
1	-1.044243	3.791212	-3.984910
1	-2.712960	2.175090	-3.105257
1	-3.605959	2.441469	-0.802682
1	-2.830240	4.323970	0.620240
1	-1.161523	5.940092	-0.259412

11. The coordinates of $[ZnCl(H_2O)_5]^+ / C_6H_6$ system, with r=0.0 Å and R=2.2 Å

30	-0.071412	-0.055372	-0.109202
8	2.142075	0.360232	-0.047661
1	2.277727	0.227417	0.908773
1	2.876403	-0.076488	-0.501754
17	0.122404	-0.203672	2.200840
8	-0.207172	-0.006966	-2.243103
1	0.173488	-0.651812	-2.853826
1	-0.132693	0.868364	-2.648433
8	0.035351	2.109240	-0.445644
1	0.968219	2.313786	-0.270109
1	-0.479711	2.685983	0.137587
8	0.172933	-2.208727	-0.298427
1	-0.590157	-2.743691	-0.561748
1	0.375609	-2.475178	0.615154
8	-2.214985	-0.154115	0.044908
1	-2.501341	-0.130244	0.970941
1	-2.946738	0.141244	-0.512296
6	5.445834	-0.192000	-0.924048
6	4.878033	0.135819	-2.157639
6	3.978703	-0.741862	-2.767959
6	3.647174	-1.947362	-2.144687
6	4.214974	-2.275181	-0.911096
6	5.114304	-1.397499	-0.300777

1	6.145599	0.490921	-0.449161
1	5.135995	1.073814	-2.642604
1	3.536900	-0.486788	-3.727811
1	2.947409	-2.630283	-2.619575
1	3.957012	-3.213175	-0.426132
1	5.556107	-1.652574	0.659075

12. The coordinates of $[ZnCl(H_2O)_5]^+$ / C_6H_6 system, with r=0.6 Å and R=2.2 Å

30	-0.071412	-0.055372	-0.109202
8	2.142075	0.360232	-0.047661
1	2.277727	0.227417	0.908773
1	2.876403	-0.076488	-0.501754
17	0.122404	-0.203672	2.200840
8	-0.207172	-0.006966	-2.243103
1	0.173488	-0.651812	-2.853826
1	-0.132693	0.868364	-2.648433
8	0.035351	2.109240	-0.445644
1	0.968219	2.313786	-0.270109
1	-0.479711	2.685983	0.137587
8	0.172933	-2.208727	-0.298427
1	-0.590157	-2.743691	-0.561748
1	0.375609	-2.475178	0.615154
8	-2.214985	-0.154115	0.044908
1	-2.501341	-0.130244	0.970941
1	-2.946738	0.141244	-0.512296
6	5.832088	0.184957	-0.661921
6	5.500559	-1.020543	-0.038650
6	4.601229	-1.898224	-0.648969
6	4.033428	-1.570405	-1.882560
6	4.364958	-0.364906	-2.505832
6	5.264288	0.512776	-1.895512
1	6.531853	0.867878	-0.187034
1	5.942362	-1.275617	0.921202
1	4.343267	-2.836219	-0.164004
1	3.333663	-2.253326	-2.357447
1	3.923155	-0.109831	-3.465684
1	5.522250	1.450770	-2.380477

13. The coordinates of $[Zn(H_2O)_6]^{2+}$ / C_6H_6 system, with r=0.0 Å and R=2.1 Å

30	0.000000	0.000000	0.000000
8	2.131219	0.000000	0.000000
1	2.705854	-0.000354	0.779276

1	2.705854	0.000354	-0.779276
8	0.000000	0.000000	2.131219
1	-0.000354	0.779276	2.705854
1	0.000354	-0.779276	2.705854
8	0.000000	0.000000	-2.131219
1	-0.000354	-0.779276	-2.705854
1	0.000354	0.779276	-2.705854
8	0.000000	2.131219	0.000000
1	0.779276	2.705854	-0.000354
1	-0.779276	2.705854	0.000354
8	0.000000	-2.131219	0.000000
1	-0.779276	-2.705854	-0.000354
1	0.779276	-2.705854	0.000354
8	-2.131219	0.000000	0.000000
1	-2.705854	0.000354	0.779276
1	-2.705854	-0.000354	-0.779276
6	5.076265	-0.000859	1.640408
6	4.514047	-1.210913	2.054277
6	3.389610	-1.211347	2.883283
6	2.827392	-0.001727	3.298420
6	3.389610	1.208327	2.884550
6	4.514047	1.208761	2.055544
1	5.951184	-0.000521	0.995361
1	4.951506	-2.152114	1.731261
1	2.952150	-2.152886	3.205314
1	1.952472	-0.002065	3.943466
1	2.952150	2.149528	3.207566
1	4.951506	2.150300	1.733514

14. The coordinates of $[Zn(H_2O)_6]^{2+}$ / C_6H_6 system, with r=0.6 Å and R=2.1 Å

30	0.000000	0.000000	0.000000
8	2.131219	0.000000	0.000000
1	2.705854	-0.000354	0.779276
1	2.705854	0.000354	-0.779276
8	0.000000	0.000000	2.131219
1	-0.000354	0.779276	2.705854
1	0.000354	-0.779276	2.705854
8	0.000000	0.000000	-2.131219
1	-0.000354	-0.779276	-2.705854
1	0.000354	0.779276	-2.705854
8	0.000000	2.131219	0.000000
1	0.779276	2.705854	-0.000354
1	-0.779276	2.705854	0.000354
8	0.000000	-2.131219	0.000000

1	-0.779276	-2.705854	-0.000354
1	0.779276	-2.705854	0.000354
8	-2.131219	0.000000	0.000000
1	-2.705854	0.000354	0.779276
1	-2.705854	-0.000354	-0.779276
6	5.559201	-0.000672	1.284356
6	4.996983	1.208948	1.699493
6	3.872546	1.208514	2.528499
6	3.310328	-0.001541	2.942369
6	3.872546	-1.211161	2.527232
6	4.996983	-1.210727	1.698226
1	6.434121	-0.000335	0.639310
1	5.434443	2.150486	1.377463
1	3.435086	2.149714	2.851515
1	2.435408	-0.001878	3.587415
1	3.435086	-2.152699	2.849262
1	5.434443	-2.151927	1.375210

III The coordinates of water/benzene and aqua-complex/benzene systems at R distance of 3.0 Å, given in Table 3.

1. The coordinates of H_2O / C_6H_6 system, with r=0.0 Å and R= 3.0 Å

8	-0.186925	-1.878217	-0.133582
1	0.300096	-2.263623	0.604882
1	0.329691	-2.130366	-0.908574
6	2.759205	-3.975974	2.009445
6	2.935832	-2.703076	2.557297
6	1.990988	-2.189037	3.448724
6	0.869517	-2.947897	3.792300
6	0.692890	-4.220795	3.244448
6	1.637734	-4.734834	2.353021
1	3.494384	-4.375946	1.315829
1	3.808444	-2.112611	2.289962
1	2.128421	-1.198600	3.875006
1	0.134338	-2.547925	4.485916
1	-0.179722	-4.811260	3.511783
1	1.500301	-5.725271	1.926739

2. The coordinates of $[ScCl_3(H_2O)_3]$ / C_6H_6 system, with r=0.0 Å and R= 3.0 Å

21	-0.078925	-0.077714	0.079922
8	2.171682	0.312678	-0.055828
1	2.551836	0.005408	0.782244
1	2.580316	-0.209194	-0.761536
17	0.314909	0.313209	2.369099
8	0.311972	0.053190	-2.171851
1	0.010347	-0.789829	-2.545763
1	-0.217830	0.751608	-2.582865
8	0.055831	2.173135	-0.310809
1	0.756509	2.582043	0.217631
1	-0.785407	2.550634	-0.008842
17	0.310738	-2.367803	-0.312471
17	-2.367980	0.316634	-0.312932
6	2.619531	5.093719	1.299861
6	3.564705	4.269142	0.684776
6	3.872548	3.024622	1.239762
6	3.235219	2.604678	2.409834
6	2.290046	3.429255	3.024919
6	1.982202	4.673775	2.469933
1	2.380000	6.062076	0.868029
1	4.060608	4.595899	-0.225652
1	4.607984	2.383022	0.761167
1	3.474751	1.636322	2.841666
1	1.794142	3.102498	3.935347
1	1.246766	5.315375	2.948528

3. The coordinates of cis-$[ZnCl_2(H_2O)_4]$ / C_6H_6 system, with r=0.0 Å and R= 3.0 Å

30	0.230000	0.007000	-0.226000
8	2.422000	-0.041000	-0.419000
1	2.608000	-0.050000	0.540000
1	2.776000	0.791000	-0.763000
17	0.803000	-0.117000	2.141000
8	0.386000	-0.066000	-2.421000
1	0.679000	-0.934000	-2.734000
1	-0.574000	-0.016000	-2.592000
8	0.202000	2.188000	0.071000
1	0.253000	2.179000	1.043000
1	-0.734000	2.357000	-0.139000
8	-0.181000	-2.150000	-0.082000
1	-1.152000	-2.093000	-0.121000
1	0.035000	-2.281000	0.858000
17	-2.139000	0.228000	-0.770000

6	5.164038	2.852936	-1.758800
6	4.625360	3.533065	-0.663876
6	3.330730	4.053437	-0.732834
6	2.574778	3.893680	-1.896717
6	3.113456	3.213551	-2.991641
6	4.408086	2.693179	-2.922683
1	6.171384	2.448036	-1.705143
1	5.213563	3.657371	0.241737
1	2.911587	4.582643	0.119122
1	1.567432	4.298580	-1.950374
1	2.525253	3.089245	-3.897254
1	4.827229	2.163973	-3.774639

4. The coordinates of cis-[$CdCl_2(H_2O)_4$] / C_6H_6 system, with r=0.0 Å and R= 3.0 Å

48	0.280048	-0.002515	-0.281720
8	2.648013	-0.054534	-0.386562
1	2.731095	-0.076217	0.588068
1	3.090375	0.752882	-0.681366
17	0.965336	-0.116765	2.208727
8	0.392699	-0.062103	-2.649408
1	0.645859	-0.896789	-3.065994
1	-0.578958	0.010001	-2.738273
8	0.060987	2.326832	0.163404
1	0.122180	2.280294	1.132547
1	-0.887236	2.403991	-0.038923
8	-0.297615	-2.283495	0.078378
1	-1.262658	-2.187585	0.011798
1	-0.099458	-2.317193	1.030026
17	-2.196668	0.223197	-0.984702
6	5.703321	2.633068	-1.449852
6	5.142332	3.331762	-0.378065
6	3.902001	3.957586	-0.524799
6	3.222658	3.884716	-1.743320
6	3.783648	3.186022	-2.815106
6	5.023979	2.560198	-2.668372
1	6.668418	2.146117	-1.335678
1	5.670926	3.388461	0.570061
1	3.465497	4.501237	0.309154
1	2.257561	4.371667	-1.857493
1	3.255054	3.129322	-3.763233
1	5.460483	2.016547	-3.502325

5. The coordinates of $[ZnCl_2(H_2O)_2]$ / C_6H_6 system, with r=0.0 Å and R= 3.0 Å

30	-0.590764	-0.000876	0.700991
17	0.694525	-0.002304	2.545387
8	0.152825	1.740551	-0.280062
1	0.686674	2.283291	0.318539
1	-0.563941	2.294534	-0.622205
8	0.155502	-1.738535	-0.284847
1	-0.561460	-2.292286	-0.627006
1	0.690525	-2.282023	0.312019
17	-2.723888	-0.002352	-0.002817
6	-1.845974	4.919360	-2.176533
6	-2.348196	5.069172	-0.881567
6	-3.286681	4.160266	-0.386851
6	-3.722945	3.101549	-1.187101
6	-3.220723	2.951738	-2.482068
6	-2.282237	3.860643	-2.976784
1	-1.115742	5.626576	-2.561470
1	-2.008741	5.892956	-0.258895
1	-3.677458	4.276834	0.620758
1	-4.453177	2.394333	-0.802165
1	-3.560178	2.127954	-3.104739
1	-1.891460	3.744076	-3.984392

6. The coordinates of $[ZnCl(H_2O)_5]^+$ / C_6H_6 system, with r=0.0 Å and R= 3.0 Å

30	-0.071412	-0.055372	-0.109202
8	2.142075	0.360232	-0.047661
1	2.277727	0.227417	0.908773
1	2.876403	-0.076488	-0.501754
17	0.122404	-0.203672	2.200840
8	-0.207172	-0.006966	-2.243103
1	0.173488	-0.651812	-2.853826
1	-0.132693	0.868364	-2.648433
8	0.035351	2.109240	-0.445644
1	0.968219	2.313786	-0.270109
1	-0.479711	2.685983	0.137587
8	0.172933	-2.208727	-0.298427
1	-0.590157	-2.743691	-0.561748
1	0.375609	-2.475178	0.615154
8	-2.214985	-0.154115	0.044908
1	-2.501341	-0.130244	0.970941
1	-2.946738	0.141244	-0.512296
6	6.053012	-0.553089	-1.299479
6	5.485212	-0.225270	-2.533070

6	4.585882	-1.102952	-3.143390
6	4.254352	-2.308452	-2.520118
6	4.822153	-2.636270	-1.286527
6	5.721483	-1.758589	-0.676208
1	6.752777	0.129831	-0.824592
1	5.743174	0.712724	-3.018035
1	4.144079	-0.847877	-4.103242
1	3.554587	-2.991372	-2.995006
1	4.564191	-3.574265	-0.801562
1	6.163286	-2.013663	0.283644

7. The coordinates of $[Zn(H_2O)_6]^{2+}$ / C_6H_6 system, with r=0.0 Å and R= 3.0 Å

30	0.000000	0.000000	0.000000
8	2.131219	0.000000	0.000000
1	2.705854	-0.000354	0.779276
1	2.705854	0.000354	-0.779276
8	0.000000	0.000000	2.131219
1	-0.000354	0.779276	2.705854
1	0.000354	-0.779276	2.705854
8	0.000000	0.000000	-2.131219
1	-0.000354	-0.779276	-2.705854
1	0.000354	0.779276	-2.705854
8	0.000000	2.131219	0.000000
1	0.779276	2.705854	-0.000354
1	-0.779276	2.705854	0.000354
8	0.000000	-2.131219	0.000000
1	-0.779276	-2.705854	-0.000354
1	0.779276	-2.705854	0.000354
8	-2.131219	0.000000	0.000000
1	-2.705854	0.000354	0.779276
1	-2.705854	-0.000354	-0.779276
6	5.610342	-0.001238	2.364812
6	5.048124	-1.211293	2.778682
6	3.923687	-1.211727	3.607688
6	3.361469	-0.002106	4.022824
6	3.923687	1.207948	3.608955
6	5.048124	1.208382	2.779949
1	6.485261	-0.000900	1.719766
1	5.485583	-2.152493	2.455666
1	3.486227	-2.153265	3.929718
1	2.486549	-0.002444	4.667870
1	3.486227	2.149149	3.931971
1	5.485583	2.149920	2.457918