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

Computational predictions of metal-macrocycle stability constants require accurate treatments of local solvent and pH effects†

Brian M. Gentry,[a] Tae Hoon Choi,[a] William S. Belfield,[b] and John A. Keith*[a]

[a] *Department of Chemical and Petroleum Engineering, Swanson School of Engineering, University of Pittsburgh, Pittsburgh, PA, USA*

[b] *Department of Chemical Engineering, Loughborough University, Loughborough, UK*

E-mail: jakeith@pitt.edu

1 Supporting Information

Figure S1 represents the uncomplexed [2.2.2] and ion-[2.2.2] structures optimized with B3LYP-D3BJ/def2-SVP, but def2-TZVP basis set is applied for the metal ions. Figure S2 shows the three lowest energy structures of Na-, K-, and Rb-[2.2.2] complexes optimized using B3LYP-D3BJ/def2-SVP level of theory, which are used for the binding energy calculations in Scheme 3. Figure S3 represents the three lowest energy structures for the divalent cation complexes, Ca-, Sr-, Zn-, and Pb-[2.2.2] with 16 explicit water molecules optimized with the same method. Figure S4 – S7 show the optimized Cartesian coordinates for the uncomplexed [2.2.2] and ion-[2.2.2] structures. Figure S8 – S14 show the optimized Cartesian coordinates for seven metal-[2.2.2] complexes with 16 water molecules. Each metal complexes has three coordinates.

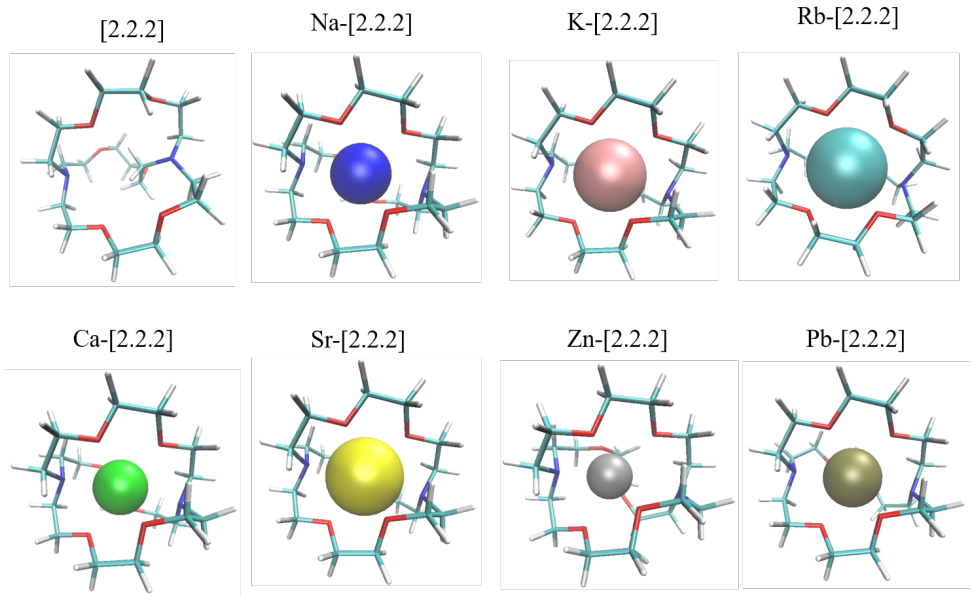


Figure S1: The optimized structures for [2.2.2] and ion-[2.2.2] complexes

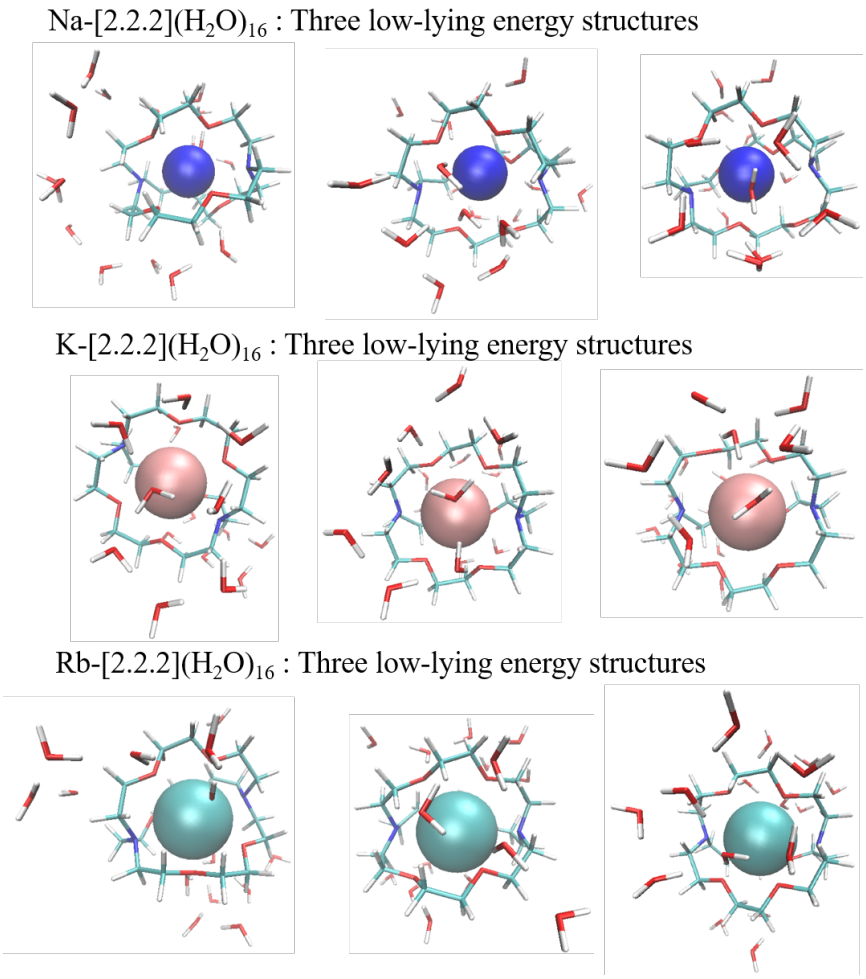
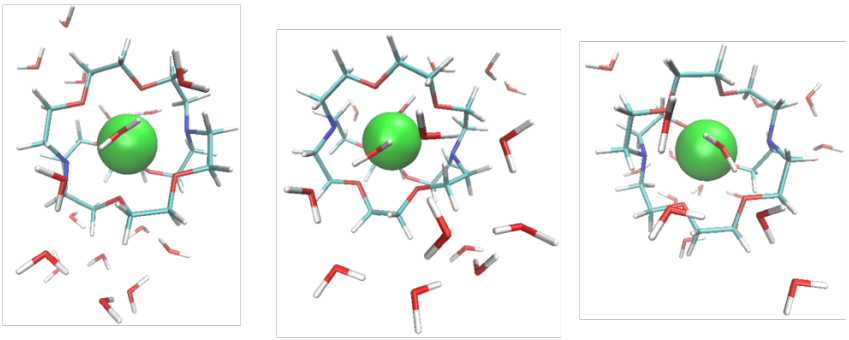
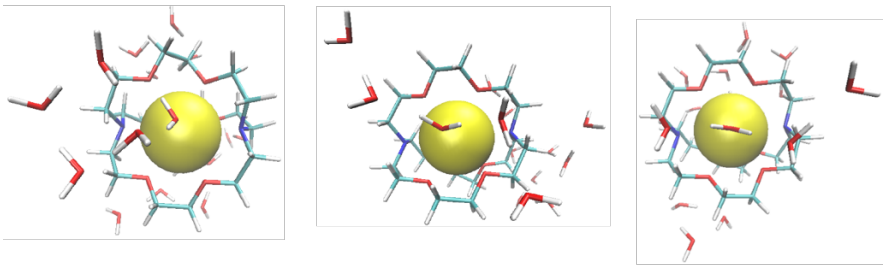


Figure S2: Three optimized structures for Na-,K-,and Rb-[2.2.2] complexes with 16 explicit water molecules

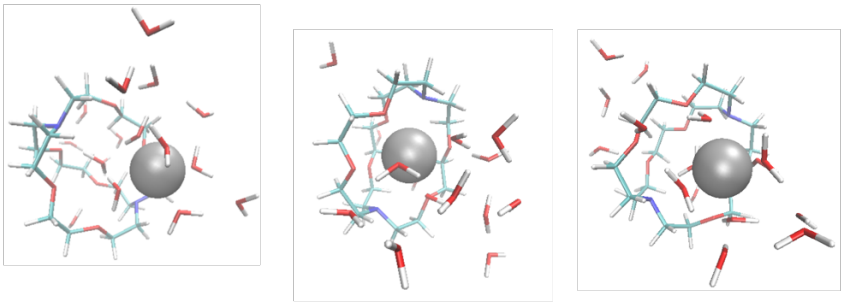
Ca-[2.2.2]$(H_2O)_{16}$: Three low-lying energy structures



Sr-[2.2.2]$(H_2O)_{16}$: Three low-lying energy structures



Zn-[2.2.2]$(H_2O)_{16}$: Three low-lying energy structures



Pb-[2.2.2]$(H_2O)_{16}$: Three low-lying energy structures

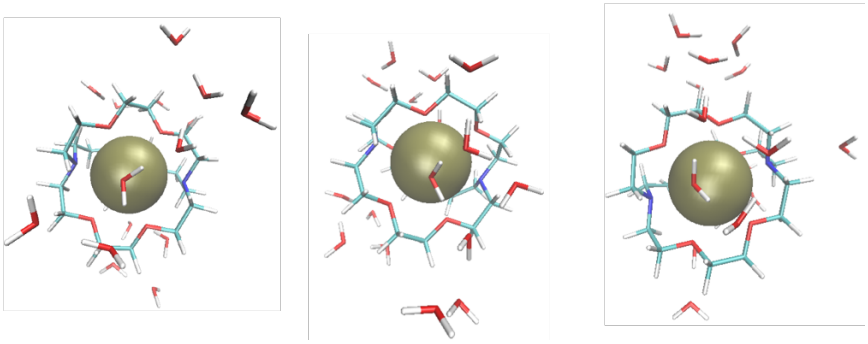


Figure S3: Three optimized structures for Ca-,Sr-,Zn-,and Pb-[2.2.2] complexes with 16 explicit water molecules

62
Coordinates from ORCA-job crypt

N	-1.54580869867551	3.24756670621938	-0.65872655266461
N	-2.38734518774433	-1.40438577489707	-2.53752424579100
C	-0.48282970498268	2.87867066413639	0.26530805079852
C	0.69384747444496	2.12745728029887	-0.34426713842822
H	-0.90348665309127	2.21861609910341	1.03667516098269
H	-0.07099519979944	3.77105910890158	0.79729536264069
O	0.29746142724775	0.85487686992758	-0.77009857862005
H	1.47619551578998	2.04919580620946	0.44308841238315
H	1.15670504376018	2.68987864276889	-1.17999746368415
C	1.36364998223661	0.03709549427105	-1.18450536961990
C	0.82965969418076	-1.28167840141523	-1.70255000651114
H	2.05137009583268	-0.15503053403389	-0.33273662853056
H	1.95534990010473	0.52652799401562	-1.98572299240463
O	0.45766300582795	-1.14924243853278	-3.05555160352234
H	-0.03110521699862	-1.57742974490423	-1.07659257353735
H	1.61799886232270	-2.05719546370265	-1.59148671723468
C	-0.29843668429536	-2.22481332450381	-3.58336422932785
C	-1.75985823886925	-1.82925752524307	-3.78219669115521
H	-0.23335396423071	-3.10632949449831	-2.91752895695686
H	0.14614618140740	-2.51626666762170	-4.55463344513292
H	-2.29754547089038	-2.69285513523017	-4.21262274493711
H	-1.82171531034210	-1.02785418842315	-4.53575383207830
C	-3.52285229369255	-2.16141277516120	-2.05862149549627
C	-3.50673202058399	-2.42182372529509	-0.54897871386213
H	-3.51782747212838	-3.15385197772614	-2.53729304869641
H	-4.49681363394766	-1.70491914437985	-2.34468264618162
O	-3.53695431472478	-1.26430383588702	0.25898781730702
H	-2.56783238841406	-2.93709312042528	-0.29087242734447
H	-4.35144765415195	-3.09503788598156	-0.28575866158235
C	-4.77890777462746	-0.62255644147144	0.37889297884250
C	-4.56689106890433	0.67700720637004	1.12433958756655
H	-5.49620620674705	-1.25764948200337	0.94102608371913
H	-5.23390131190848	-0.40258140783558	-0.60579937717498
O	-3.94854015976972	1.61546834316012	0.27776562017401
H	-3.92891817075991	0.46855710374568	2.00656381670986
H	-5.53795905619181	1.06430144296153	1.49945969809843
C	-3.44088170595604	2.73292879104723	0.95788713534240
C	-2.75727278644091	3.70503021290234	0.00884964861229
H	-2.74946466556363	2.41163867073699	1.76160156421846
H	-4.26081174002701	3.28671451134205	1.46454435078881
H	-2.56101897797060	4.63490706388279	0.59850140169685
H	-3.49054988387180	3.98211604288369	-0.76474110447797
C	-1.12134672190282	4.21600082823505	-1.66387846434507
C	-1.75024039179064	4.02302293500569	-3.03396263655675
H	-0.03505267533966	4.13769510102119	-1.80827116509842
H	-1.32112557548504	5.25858199419397	-1.32635567739147
O	-1.22895401259421	2.85366664953956	-3.61148516179636
H	-1.50923575188524	4.90521209072821	-3.66615126971253
H	-2.85407378078363	3.98307206185649	-2.94676440694921
C	-1.65522477230707	2.57236646827686	-4.92566806773276
C	-3.10007429374611	2.08600944999157	-5.04964888721311
H	-0.98474233669535	1.78119132872176	-5.29535805831953
H	-1.52412205001820	3.46474131321687	-5.57666230219138
O	-3.33847326855821	0.82985515439031	-4.47564396918483
H	-3.32860824602734	1.99744549310929	-6.12690998702929
H	-3.79893859033169	2.84485913029756	-4.64156838773172
C	-3.52249103222324	0.80297983194950	-3.05705871178231
C	-2.42685501609922	0.04474814842078	-2.31962654990309
H	-3.56453389829284	1.82339337657515	-2.64602589706811
H	-4.51136866605447	0.34545585293289	-2.86522825017848
H	-1.45437703382895	0.46864629640433	-2.59314718433966
H	-2.55001646683155	0.24821900417965	-1.24912298998833

63
Coordinates from ORCA-job na-crypt-b3lyp-opt

N	-1.40240978337929	2.89412756244158	-0.54090357514957
N	-2.29181393667308	-2.31266794332166	-2.48263600097569
C	-1.21247339636852	2.83698474493492	0.90680405038414
C	-0.04909001579517	1.96135020013914	1.33363396737692
H	-2.12467068155651	2.42293313908359	1.35879101390674
H	-1.06223066266620	3.84751094852709	1.34778396670148
O	-0.20538810614444	0.67103633155802	0.77558425546399
H	-0.02325459581759	1.90932480684335	2.43848834257396
H	0.91727848793998	2.39220381017385	1.01416401438544
C	0.98657034011134	-0.08594259126463	0.77759147082567
C	0.67595193459014	-1.49725239049450	0.35128023701793
H	1.43825532798594	-0.11633139654909	1.78737744597914
H	1.72428952814516	0.36884857951855	0.08747227921796
O	0.04432584322614	-1.48211616338093	-0.91654923991858
H	0.01344555520976	-1.98204791005704	1.09543196157095
H	1.61894635650962	-2.07401390962276	0.31511726245881
C	-0.04011740812184	-2.77379982349833	-1.49421928275658
C	-0.92308840352759	-2.75144213731548	-2.72384482194538
H	-0.41791269382430	-3.49802818596674	-0.74856774779541
H	0.96592347038881	-3.12539166728057	-1.79384965059411
H	-0.89057232828631	-3.77033626569491	-3.17364680857013
H	-0.46098318256919	-2.07137390475125	-3.45563333652769
C	-3.02024601474256	-3.07615325255268	-1.46976194740138
C	-3.01347884296322	-2.42265521317606	-0.08354542233173
H	-2.64373911002539	-4.11410153694094	-1.36822137623542
H	-4.06413154936010	-3.18017566292606	-1.80057326116994
O	-3.31809231064206	-1.04085023275438	-0.10640304066207
H	-2.02693351961476	-2.49048637459471	0.38978766559118
H	-3.72813733975446	-2.96351097361641	0.56688916100739
C	-4.61057146566598	-0.70442612439327	-0.57732721136106
C	-4.86929600319652	0.74708367773430	-0.24889719604636
H	-5.38200533175839	-1.32867430448381	-0.08834157241063
H	-4.68411313449452	-0.85337491303742	-1.66889187711335
O	-3.84898541677885	1.53442677741125	-0.82891714241676
H	-4.87064413920143	0.88751499724486	0.84954895785647
H	-5.86395943030402	1.04212167310327	-0.63698195929985
C	-3.89478944439247	2.88935467374858	-0.43519235004431
C	-2.63261507969220	3.58960273963405	-0.91065751393778
H	-4.00546548659852	2.95567618008752	0.66399456683595
H	-4.77386541750277	3.39864335927025	-0.87494104803417
H	-2.65195005346171	4.63439292202018	-0.53019375220883
H	-2.67791721341062	3.65171528932218	-2.00652962126899
C	-0.23209928017614	3.41724256043726	-1.24123302536726
C	-0.25250363019115	3.15937582513883	-2.73448146375434
H	0.66180712466449	2.92326707752930	-0.84073768287341
H	-0.09691103419728	4.50878709543624	-1.07415827178876
O	-0.34120833438039	1.76542578781942	-2.97728896918569
H	0.67462819514166	3.56560865794134	-3.18091114127820
H	-1.09248574041410	3.68889159680710	-3.21796570274075
C	-0.65357848303182	1.45141209593954	-4.32855585085002
C	-2.15822020666153	1.33270406213146	-4.52391533545576
H	-0.16362561514421	0.49305225816681	-4.55878166676713
H	-0.22896392130362	2.20403499450256	-5.01597539325404
O	-2.67386546628574	0.20712583696937	-3.83522749101857
H	-2.40954458286337	1.28304260050421	-5.59994144846687
H	-2.66463115405272	2.21727150742349	-4.10799593959967
C	-2.59053295569242	-0.99252083062501	-4.58038815624302
C	-3.04311197421939	-2.15936174079096	-3.72507132262441
H	-3.24268527214075	-0.93330447622034	-5.47248666160876
H	-1.56194115047778	-1.15096371120700	-4.95552914012642
H	-4.10030558517142	-1.99607300249453	-3.46820396099397
H	-3.00300192072035	-3.07618189578530	-4.35480756030456
Na	-1.67669435849824	0.35491416525333	-1.29049767867675

Figure S4: The optimized coordinates for uncomplexed [2.2.2] and Na-[2.2.2] complex

63
Coordinates from ORCA-job k-crypt-b3lyp-opt

N	-1.27807271717647	2.99724413064041	-0.49417483332734
N	-2.28999980960465	-2.40695747520008	-2.49795919405604
C	-0.74228327329850	2.86640588252829	0.86496128871083
C	0.44096503618951	1.92268802468621	1.01519314013108
H	-1.54185245141020	2.49274544686211	1.52119215852571
H	-0.43487955460553	3.85510202668812	1.27210867797589
O	0.05228042852875	0.58619377393783	0.75759906769829
H	0.82665171734824	2.01378643887519	2.04928514264653
H	1.27376532743889	2.20388814697341	0.34403133943313
C	1.12542967784715	-0.33384217505074	0.80719379416266
C	0.60774983944879	-1.73862489288082	0.59204700805321
H	1.63347136131599	-0.28771639495511	1.78975097617025
H	1.87312735222069	-0.08834812408550	0.02731798364434
O	0.01248346266481	-1.82544804364118	-0.68897663273686
H	-0.13043612035061	-1.99713165615264	1.37625845068877
H	1.45698459386295	-2.44289507707735	0.68146746800460
C	-0.29068629016851	-3.13680562064530	-1.11889883119519
C	-0.99573777943617	-3.09032032089111	-2.46421726271664
H	-0.90258403307872	-3.66308477878220	-0.36246711649224
H	0.63933096662301	-3.72501223051974	-1.23911001708200
H	-1.08958931617273	-4.13887460588682	-2.82625443527433
H	-0.32032308580973	-2.57712607604400	-3.16655750685864
C	-3.32219199575427	-3.02145397117282	-1.65554984072597
C	-3.47005554538876	-2.42172357039768	-0.25254428425109
H	-3.15990284576778	-4.11318003062561	-1.53546015872719
H	-4.28888810049135	-2.92416836142315	-2.17160060575530
O	-3.68885732611932	-1.02553656912227	-0.21827921515218
H	-2.55992051612426	-2.57797072073814	0.34184571118972
H	-4.29439482492599	-2.95372144732763	0.26215058311487
C	-4.89286366686266	-0.53654297643509	-0.77214671284844
C	-5.05406465274109	0.89603024393421	-0.30889344615260
H	-5.76048397350758	-1.12660088657406	-0.41805925674297
H	-4.87371020518037	-0.58103800037719	-1.87775555280927
O	-3.94231224237509	1.66352294051081	-0.73743162651526
H	-5.11106735252876	0.90397190139935	0.79576487163032
H	-5.99710218530808	1.31835777843003	-0.70681840692836
C	-3.75485302844263	2.83907506844852	0.02592587720142
C	-2.58848426785896	3.65574396423350	-0.50520511067579
H	-3.61131864620952	2.56616382583677	1.09019905882507
H	-4.65808605326517	3.47868510405782	-0.02544017327632
H	-2.55959321540429	4.60781598509097	0.06821353652162
H	-2.83027683564915	3.92865183091131	-1.54187007969980
C	-0.34484792220906	3.69254833027067	-1.38363469499601
C	-0.59504223436737	3.46097389649760	-2.86272597467272
H	0.67525390874907	3.34362655207524	-1.17149362041073
H	-0.35289727650195	4.78869611371173	-1.19636971475726
O	-0.34408965466574	2.10441430666094	-3.18734172889592
H	0.08043004129215	4.11853476581670	-3.44180569500128
H	-1.62717802441191	3.74470132019974	-3.14101722303746
C	-0.67151484923755	1.76074303454725	-4.52548408090912
C	-2.13386971236813	1.35064576736205	-4.66923953432945
H	-0.00830746450255	0.92889449210140	-4.81077752137394
H	-0.45181383533418	2.59887407453530	-5.21258663079958
O	-2.44438558746811	0.16384607593598	-3.96041007989218
H	-2.39077123920204	1.24101879176572	-5.74051215691190
H	-2.78937709554102	2.13044460122411	-4.25141123398142
C	-2.08389489124951	-1.04398430602188	-4.60504998749631
C	-2.73398445650854	-2.21201461707734	-3.88376421751334
H	-2.45022699107774	-1.03741047254718	-5.64976592839440
H	-0.98349624807432	-1.15716330873106	-4.64663782423937
H	-3.81674590060382	-2.02105691118649	-3.87630522716336
H	-2.57167165916368	-3.12479968504679	-4.49745417864148
K	-1.61818476002579	0.28996866986777	-1.37268858091119

63
Coordinates from ORCA-job rb-crypt-b3lyp-opt

N	-1.39902047500562	3.13931098164078	-0.51959184499594
N	-2.38167218510751	-2.40224266835054	-2.65613521806431
C	-0.62498723030771	3.05667366208822	0.72120203570606
C	0.55584277850822	2.10124335735006	0.65715470361517
H	-1.28295132147467	2.70442002589475	1.52728571259415
H	-0.24723751140966	4.05362306153440	1.03712860891214
O	0.09370621418079	0.77061117813471	0.51733131662425
H	1.14146622353361	2.20310690368284	1.59129696541242
H	1.23641439241349	2.35247503648135	-0.17892559075564
C	1.12821736961134	-0.19497493037025	0.55698373962178
C	0.53748988609392	-1.58531596442552	0.51502479310827
H	1.71584933451929	-0.08865641125470	1.48917799166038
H	1.82105388363137	-0.05475329573073	-0.29630657330706
O	-0.04272653341717	-1.82595498982702	-0.75374231452416
H	-0.22552585823957	-1.68987941810888	1.31258229505397
H	1.33889117009299	-2.32077835931637	0.72173523918437
C	-0.69307228729712	-3.08031537418160	-0.84403590715797
C	-1.28815750419432	-3.28713248428669	-2.23405979408936
H	-1.45126282204688	-3.16057789314144	-0.04684629082260
H	0.03678743447619	-3.89588523875047	-0.66945420740342
H	-1.60048675730112	-4.35162722067927	-2.31192031562065
H	-0.45505216370344	-3.15653451775038	-2.94192394669164
C	-3.71479231124680	-2.82054433599176	-2.20516478575648
C	-3.99749694243634	-2.70725193550291	-0.70689903557000
H	-3.93127315133485	-3.87234041323476	-2.50171243867838
H	-4.44910931909345	-2.19347270718853	-2.73352402246405
O	-3.84383419514597	-1.39435161306671	-0.18890239603031
H	-3.33701535467026	-3.36336281496105	-0.12422927530236
H	-5.02585066082380	-3.07053480533056	-0.52761940515214
C	-5.03749130117238	-0.63295826609956	-0.10748599072102
C	-4.77218809418473	0.66197579278796	0.62563726020778
H	-5.80680561936906	-1.19549539437633	0.45400905419685
H	-5.44638321437336	-0.41466037900589	-1.11315205461331
O	-3.99746620279066	1.54252933085694	-0.16951026069797
H	-4.24307729830670	0.43745190664532	1.57291173006886
H	-5.74019912014695	1.13215665876959	0.88627012340930
C	-3.69136242794364	2.75320640526779	0.50349202913200
C	-2.76216295925391	3.64049862461347	-0.31390768031336
H	-3.25399159438384	2.52370891115706	1.49322290491782
H	-4.62236165942206	3.32020084883296	0.69765758554467
H	-2.74869196238685	4.63684115835313	0.18120463236311
H	-3.22616896208213	3.79052257837902	-1.30121581151837
C	-0.69909951699451	3.91338309355911	-1.54885662580199
C	-0.93532904038842	3.44918362914226	-2.97824247295684
H	0.38427975108768	3.84695585933921	-1.37269048239574
H	-0.96296901181171	4.99065349070408	-1.48179336878102
O	-0.29377246605308	2.19814495371779	-3.18436906616043
H	-0.51002789569294	4.20450629162252	-3.66624537709826
H	-2.01980576085562	3.38862305446822	-3.19736551228523
C	-0.19307214986047	1.77909696690587	-4.53438100931587
C	-1.49928971689563	1.23583346531797	-5.10586464075904
H	0.58665614634539	1.00125203020422	-4.55423758017678
H	0.15763760132877	2.61047209316153	-5.17689382437220
O	-2.02667451378224	0.13906238958784	-4.38056066531263
H	-1.33859693627185	0.95987269084999	-6.16635942477886
H	-2.28073081289535	2.01256977242093	-5.08478583535567
C	-1.42665062688050	-1.12601378218668	-4.61926808635132
C	-2.35935786795221	-2.22124556878975	-4.11764298045723
H	-1.26861208696697	-1.26250484743968	-5.70565026123977
H	-0.43440291476229	-1.19543070061598	-4.13191161023258
H	-3.36963056272922	-1.95038061776579	-4.45658968177962
H	-2.09665577950166	-3.16807522509974	-4.63353377281299
Rb	-1.82916952545576	0.31653596935760	-1.50744128265885

Figure S5: The optimized coordinates for K-[2.2.2] and Rb-[2.2.2] complexes

63
Coordinates from ORCA-job ca-crypt-b3lyp-opt

N	-1.50664681018969	2.82483493881902	-0.66601626799272
N	-2.24110173063412	-2.24115552189784	-2.37574946018248
C	-1.54100990839953	2.80190127110850	0.80586604892490
C	-0.42801776858428	1.95253831096427	1.39280770624460
H	-2.50557509812861	2.38278913331545	1.12148044056096
H	-1.47509528754777	3.81936679740616	1.23965706858808
O	-0.37081027415535	0.71269076265755	0.67946654399236
H	-0.62487656073800	1.76272034577828	2.46139336788810
H	0.54906479770543	2.45798694642217	1.32131559071305
C	0.88209046873266	0.03884143968838	0.80789102029094
C	0.69351814520626	-1.39429026878940	0.38632444387529
H	1.23396092958138	0.06023259495006	1.85263208105357
H	1.63404720140879	0.54591596059353	0.17648827790212
O	0.01315225265870	-1.42112385766748	-0.87137690778376
H	0.09407096361192	-1.94617659140115	1.13294976382886
H	1.67644187337528	-1.88730676938279	0.30368853687161
C	0.02034182742008	-2.72386344244930	-1.46677754360586
C	-0.88476082902799	-2.72393553002367	-2.67737024016184
H	-0.30356296714504	-3.46641933733954	-0.71743352045386
H	1.04587519209269	-2.99228403846325	-1.77389145737854
H	-0.89581456423875	-3.74647753520106	-3.10616340682923
H	-0.44059021521309	-2.06768192234677	-3.44102411176788
C	-2.94820609194155	-3.06104481517373	-1.36800751827577
C	-2.97687100138829	-2.39487802788674	0.00691612461025
H	-2.50694781643901	-4.06877907609027	-1.27158862233279
H	-3.97872023465171	-3.22943563385831	-1.71089640127123
O	-3.31368813428153	-1.00777065396249	-0.08367855980603
H	-1.99562202104614	-2.42163882926312	0.49487690356156
H	-3.69054154606491	-2.91485457156101	0.66770156187488
C	-4.66473924020845	-0.72976036127969	-0.46290206499921
C	-4.90274094049644	0.74929809320593	-0.29589182876111
H	-5.36583145062269	-1.29191168260683	0.17532857976056
H	-4.84179576358149	-1.02768581223389	-1.51033382642987
O	-3.86331036518516	1.45794797587425	-0.97371225870845
H	-4.88769936409660	1.02730192637181	0.77317877713351
H	-5.88859072625390	1.01614495436794	-0.71482815975273
C	-3.98696925195554	2.87625447204947	-0.84568115952468
C	-2.66965798455390	3.52194487310983	-1.23743397992140
H	-4.26733317073204	3.11855011492432	0.19316947014952
H	-4.79525238806802	3.24918741085101	-1.49689201303316
H	-2.69945952433189	4.58948054297102	-0.94144324966957
H	-2.57744823946733	3.50046676329271	-2.33221367107200
C	-0.23678957001488	3.36746601664123	-1.17767280894672
C	-0.04946410118731	3.10932745910022	-2.65677746339439
H	0.58921726645486	2.88010405856396	-0.64488234821849
H	-0.14416580102788	4.45483197540345	-0.98586105376204
O	-0.25189810200431	1.71355143776905	-2.90667338277813
H	0.96969097761727	3.40349858768975	-2.95963670160924
H	-0.75296271801171	3.70013806291848	-3.26755894779025
C	-0.39762048799120	1.40112841220011	-4.30034924149805
C	-1.87600801707972	1.26526464217574	-4.59765024658086
H	0.12631527624216	0.45046690589266	-4.48455471844125
H	0.08054065171725	2.16898534200485	-4.92808696828103
O	-2.39904896286303	0.19775589066154	-3.79434861457179
H	-2.06657288413209	1.07602327311303	-5.66599780898106
H	-2.41883463812598	2.18276496897994	-4.32006836304391
C	-2.54837416788050	-1.02318409198414	-4.52830864971487
C	-3.05005587061635	-2.10228828318512	-3.59817356672521
H	-3.27813439296776	-0.87970100594014	-5.34251851231847
H	-1.58627653575628	-1.29674525251342	-4.99667680901982
H	-4.07506993869637	-1.84464354797977	-3.29500316034274
H	-3.10866557291753	-3.05170618787368	-4.16704175921678
Ca	-1.70560179318302	0.30822798651897	-1.37685395287540

63
Coordinates from ORCA-job sr-crypt-b3lyp-opt

N	-1.33563174205924	2.87031320400371	-0.52266005640283
N	-2.36577767879445	-2.28455772838780	-2.44182332669538
C	-1.09319520508168	2.77664968344385	0.92953065540299
C	0.08594773228683	1.89068526148197	1.29148780380686
H	-1.99398127112249	2.35940761275238	1.40329733856929
H	-0.92626576909855	3.77470697346267	1.38178381266114
O	-0.07509922934933	0.61384709931805	0.66725101274011
H	0.13109330899348	1.77262200184349	2.38767875497149
H	1.04514547469221	2.33139482142050	0.97242121728007
C	1.11649396816667	-0.17495501461405	0.66889429247686
C	0.76227409169015	-1.59731029750360	0.31575395714509
H	1.58631941942645	-0.16437629116106	1.66693117616156
H	1.83629297335516	0.24621419050834	-0.05732058681483
O	0.01371052192922	-1.61005174705718	-0.90447386536930
H	0.16014698370572	-2.06193498773838	1.11813932304575
H	1.69029306755059	-2.18234573096480	0.19800612333411
C	-0.16772571709355	-2.93236907415903	-1.42419119262265
C	-1.03991117343439	-2.88658992341554	-2.66021455580735
H	-0.60226991904241	-3.57772757497416	-0.64020221497095
H	0.81170830042540	-3.36240135305536	-1.69749877007779
H	-1.12293472391412	-3.91870732879771	-3.05822412221407
H	-0.51201489240825	-2.29901757472033	-3.42712513401440
C	-3.21328147909962	-3.04260413041673	-1.49236248462124
C	-3.29055875767936	-2.40903525681094	-0.10363506478997
H	-2.87112457773334	-4.08788612812134	-1.38389457401161
H	-4.22890437821453	-3.11082621720023	-1.90794132149264
O	-3.56170450386393	-1.00629897958250	-0.14800993866811
H	-2.33576510128649	-2.49534468822799	0.43402233839544
H	-4.05523362978181	-2.92590759136066	0.50109509163123
C	-4.86658007484837	-0.59595100806424	-0.55463268539007
C	-5.00406104998706	0.86973998227894	-0.20545195300036
H	-5.63973143572280	-1.17531897926452	-0.02302513327812
H	-5.00386480130154	-0.75283167830689	-1.63988604303695
O	-3.88801861866051	1.58239668384991	-0.74892294316829
H	-5.01477505292877	0.99840885568650	0.89151061597255
H	-5.94834502397226	1.26801642520472	-0.61593878794176
C	-3.84500753694857	2.94739967956316	-0.32389824547632
C	-2.57466282042591	3.60861066984368	-0.83054984034389
H	-3.91677714271346	2.98409278704622	0.77761468411530
H	-4.71397134109915	3.49664348957225	-0.72607807723666
H	-2.54327197402231	4.63832825561373	-0.42230677938980
H	-2.64930068812559	3.70561488245129	-1.92327308985037
C	-0.17838962881989	3.45653229918502	-1.22526675713634
C	-0.20047826980308	3.24318119099951	-2.72435865084376
H	0.73622067998172	2.98856994065814	-0.84067968652076
H	-0.08916441684138	4.54234862908081	-1.02194918873833
O	-0.28529297553068	1.84068658433847	-2.99990782237888
H	0.72754395732518	3.65302087714508	-3.15805705824528
H	-1.04264907692957	3.77112349413289	-3.20371932021586
C	-0.48306087991898	1.53915803748202	-4.38879420363040
C	-1.96300604910802	1.32919370536042	-4.64528580537791
H	0.08750577631512	0.62338882499445	-4.60908622750373
H	-0.07576305132596	2.34122199579707	-5.02482433404197
O	-2.42958712774423	0.21489967887755	-3.87178211126167
H	-2.16984922942087	1.16920526608608	-5.71585906424257
C	-2.54340678349833	2.20844945448157	-4.32296558233721
C	-2.48233154401190	-1.01336242400074	-4.60484317190678
C	-3.07183743188821	-2.09238360558121	-3.72381145366578
H	-3.12915070953477	-0.88813388642290	-5.48927720527581
H	-1.47568793399684	-1.27746788141073	-4.97545160022416
H	-4.10982507103378	-1.80860659850260	-3.49688865423756
H	-3.11326321648897	-3.03214853691486	-4.31002961034798
Sr	-1.69763555013453	0.29382967877365	-1.35863481109139

Figure S6: The optimized coordinates for Ca-[2.2.2] and Sr-[2.2.2] complexes

63
Coordinates from ORCA-job zn-crypt-b3lyp-opt

N	-1.65474898203347	2.77463475992493	-0.77555423708877
N	-2.17644411342960	-2.27530990160253	-2.63241292802845
C	-1.80106102247032	2.81041922132999	0.69378531991761
C	-0.76108358745160	1.92680145147557	1.37040831980449
H	-2.80265837466527	2.44800441439864	0.95016025991625
H	-1.71652451278714	3.83885696262493	1.09115123353495
O	-0.60981740588150	0.71724382429718	0.61485265325243
H	-1.07803046301723	1.68258026659836	2.39701174317775
H	0.21352245065620	2.43417865979651	1.43443337660482
C	0.71873348146084	0.17935090782515	0.65466163346684
C	0.68222404673277	-1.22986576554697	0.13591501044769
H	1.08858499842172	0.16969696264913	1.69227189203607
H	1.38237745354239	0.81325181597175	0.04291301363263
O	0.01371099947096	-1.25974301747230	-1.12069192888802
H	0.15405140498102	-1.88656932168307	0.85215891468642
H	1.71626648967426	-1.60407278979885	0.03991454529080
C	0.10463719972205	-2.56427035181077	-1.71032653052073
C	-0.81316769485225	-2.69709626428233	-2.90819589416620
H	-0.14468100998007	-3.31932520811783	-0.94505496171966
H	1.14718512445682	-2.75465698160721	-2.02049778745185
H	-0.74581964928693	-3.75318300228577	-3.24813111054002
H	-0.42271924796305	-2.08715287961642	-3.73480020161868
C	-2.87196142246300	-2.98730103304496	-1.57159555423206
C	-2.73115388439812	-2.30963951067893	-0.20722141471245
H	-2.52109220956155	-4.03305859881404	-1.46749268960375
H	-3.93862195534453	-3.06400417307534	-1.83298261882575
O	-3.08403661091842	-0.91386656338838	-0.25747992107418
H	-1.70675592758159	-2.34071853620074	0.16724380132120
H	-3.37111209201226	-2.80908635833873	0.53684136483754
C	-4.50221224354430	-0.71352084928489	-0.25112255717797
C	-4.78435377960759	0.75902625322527	-0.13611486090583
H	-4.94789210724238	-1.24585939965843	0.60399536089038
H	-4.94538777946480	-1.12028295352083	-1.17402002320084
O	-3.95759603919093	1.41141044364526	-1.08751521784517
H	-4.54943806696072	1.12831416888584	0.87955708707267
H	-5.85198351443794	0.95337866293621	-0.33923190347672
C	-4.11297171815100	2.82707900979623	-1.12612598425708
C	-2.76958684229575	3.44023643334251	-1.47989416272607
H	-4.46979358522348	3.18535052656494	-0.14630945581789
H	-4.87085505570674	3.11143808293655	-1.87432095672435
H	-2.79496779347544	4.52240437314253	-1.25287648029154
H	-2.59141431817015	3.33388031756698	-2.55904995424981
C	-0.35999658641247	3.35352594437137	-1.19847926096889
C	0.04533905518569	2.85429625101840	-2.56743048857827
H	0.41306128986629	3.05270898657369	-0.48237942378517
H	-0.39631988608376	4.45750304122001	-1.18719424967902
O	0.01733112433646	1.42883390951071	-2.50903359359323
H	1.06205559731092	3.20027179145084	-2.81781082836758
H	-0.63311363789358	3.22191318339748	-3.35451192747601
C	0.04804142257204	0.78211899741473	-3.77662841293973
C	-1.35130664418117	0.75473080408905	-4.36915355265279
H	0.41557040158139	-0.23142419285741	-3.58074684543398
H	0.75227780494970	1.28459976374621	-4.45888257658051
O	-2.27277169329294	0.40865418713359	-3.32233085620206
H	-1.39415186776803	0.01648894876067	-5.18408311549998
H	-1.65359332268379	1.72952958806176	-4.78628749233513
C	-3.38316144602405	-0.42052098680119	-3.71566102327074
C	-2.95293836471207	-1.88518976184777	-3.80036729164039
H	-4.14571222149044	-0.25803512174734	-2.94673288010820
H	-3.78745209785142	-0.05250520153329	-4.67226416439881
H	-3.85198122602045	-2.51121926489203	-3.93761668529724
H	-2.35048019669317	-2.04287593903394	-4.70865052060739
Zn	-1.71850914424506	0.54676999285931	-1.26490000533160

63
Coordinates from ORCA-job pb-crypt-b3lyp-opt

N	-1.67273092306110	3.07342275844668	-0.66271637268033
N	-2.25309354346677	-2.36440523850601	-2.51417549848038
C	-1.26978344187015	3.01490700842537	0.75098110896479
C	0.02554190181851	2.26169997910775	0.98110524079444
H	-2.05817208479297	2.50600442997318	1.32442301383950
H	-1.16337133203401	4.03071520272266	1.18016965613519
O	-0.14529363339762	0.90720633723324	0.55674665533728
H	0.27040253837329	2.28452531433774	2.05727734154279
H	0.87383961838262	2.71800797477893	0.44222957743721
C	0.99912601005320	0.07370411402740	0.74177714073926
C	0.58292958072777	-1.36267984025410	0.53752047263605
H	1.39833124621714	0.19504437767731	1.76343351697884
H	1.78870117056225	0.35932354693451	0.02375191356750
O	-0.03178070914941	-1.48146981269193	-0.74861874992321
H	-0.12883478314374	-1.67967433911587	1.32117906274414
H	1.47460252345423	-2.00875026916150	0.59810024853027
C	-0.08801804221235	-2.81292513485376	-1.26835060233107
C	-0.85040217288370	-2.82716641708203	-2.57570178328167
H	-0.53398420470417	-3.48862268946163	-0.51848186358219
H	0.93688857301563	-3.17418766045323	-1.46285756654721
H	-0.79896634375063	-3.86228566185707	-2.96977842319087
H	-0.32432558566878	-2.18254329633208	-3.29426216928120
C	-3.10017250451072	-3.14283754417712	-1.59385292741624
C	-3.17535916883202	-2.57645217654512	-0.17645397630704
H	-2.77069742486698	-4.19763480186843	-1.52162665958138
H	-4.11704161031984	-3.17614295763695	-2.00951087040345
O	-3.50460598228935	-1.18807893518614	-0.14105874786556
H	-2.21844194165303	-2.65437211695012	0.35193357649161
H	-3.91880226191632	-3.15085450499541	0.40300035042165
C	-4.83409167407606	-0.84818104586848	-0.53034755067670
C	-5.08829973312167	0.57787840310723	-0.10665696774238
H	-5.56137097752702	-1.51199155465198	-0.03335191490583
H	-4.96381526691311	-0.95899787540466	-1.62331433793929
O	-4.08751132700628	1.41711840379230	-0.68527742471097
H	-5.04076750029174	0.65832380845610	0.99406575052549
H	-6.08998650690808	0.89813705488584	-0.44466403004854
C	-4.14896060398640	2.76506315273761	-0.21731804490471
C	-3.04587005727776	3.59414955580858	-0.84168788864545
H	-4.10337018226779	2.76769660160275	0.88641159018230
H	-5.11747261036072	3.21121421661565	-0.50527723490232
H	-3.13774434204753	4.61969841343282	-0.43233246377659
H	-3.22883118541582	3.66238287141185	-1.92389818926374
C	-0.72365065943754	3.86001666031523	-1.48989234779285
C	0.16538292525466	3.01337395377077	-2.38675604188708
H	-0.09036511928339	4.50689023342384	-0.85775040051574
H	-1.29950477140710	4.53382977346160	-2.14023360807841
O	-0.68421910871055	2.17002733858262	-3.15859724113661
H	0.88570125161508	2.39787311197017	-1.81501605367083
H	0.74875271836115	3.68002264629238	-3.04506952176513
C	-0.12739978575306	1.62328803095796	-4.35167034048344
C	-1.22487856613717	0.83469976792536	-5.02481204495015
H	0.73457471473641	0.97254551967487	-4.11331277443897
H	0.22196178214322	2.43021870652828	-5.01953576835064
O	-1.62997483927295	-0.19432650163099	-4.12280410749797
H	-0.85575663842137	0.39200139193081	-5.96592973297215
H	-2.07482363567155	1.50120228904653	-5.25541280052893
C	-2.86598474745654	-0.84644013697646	-4.41227220619346
C	-2.79795090561954	-2.27356580425391	-3.89090970213159
H	-3.69484707811808	-0.28308026625107	-3.93855786018303
H	-3.05736729320982	-0.85926346107155	-5.49815352309728
H	-3.81145694420157	-2.69815522724021	-3.92774213870392
H	-2.18777293021781	-2.88146874369108	-4.57959631954495
Pb	-1.78528687007351	0.36349406477287	-1.46139042455693

Figure S7: The optimized coordinates for Zn-[2.2.2] and Pb-[2.2.2] complexes

```
111
Coordinates 1 from ORCA-job na-crypt222-b3lyp-opt
 Na  0.41151927812690    0.11661606951608   -0.01743035275647
 N   2.89133236385600    1.65988575193515   -0.71830313492082
 N  -1.71565210694259   -1.38736419893350    0.97999217096604
 C   2.75161390947788    3.10271494063035   -0.56313510000488
 C   2.18442403935412    3.50187376578026    0.78711420557299
 H   2.05015648430432    3.46991259996552   -1.32287130745071
 H   3.71349065535326    3.63889676413824   -0.72712910168924
 O   0.86546553209755    3.01014845275375    0.89562585562333
 H   2.19793732070139    4.60820340067576    0.87259976386441
 H   2.79564116028270    3.11062184638318    1.62061276066481
 C   0.28050703893318    3.27261036872553    2.15107282301224
 C  -1.05349546498058    2.57803260260799    2.24585922889236
 H   0.13025899012781    4.36236307277112    2.30213450772903
 H   0.93478999248488    2.90898446689402    2.96003373468864
 O  -0.88545489249621    1.18412829036097    2.06973339080328
 H  -1.76859001962790    2.97093676599273    1.49701069072368
 H  -1.47273952715255    2.78776356307816    3.24747538276797
 C  -1.91750633116433    0.44097110611124    2.69904016271409
 C  -1.76509374177896   -1.03346755887089    2.39681493026729
 H  -2.90351946636105    0.82812195375681    2.39437270863716
 H  -1.84838493284171    0.55946434108956    3.79377868117643
 H  -2.60529778363010   -1.54651307184591    2.90986715983807
 H  -0.84156124969217   -1.37248726198169    2.88164999358577
 C  -2.93789806791896   -1.02190906117760    0.25450528389696
 C  -2.94864799522228    0.38471005575450   -0.30787449446249
 H  -3.84320500728555   -1.13480751434141    0.88049419800109
 H  -3.05258844612905   -1.70234546076156   -0.60103238245251
 O  -1.83556828234557    0.54104702392344   -1.18552928453397
 H  -2.90856885581964    1.16661444643161    0.46237624618844
 H  -3.88533671368526    0.51918630749193   -0.86773914259028
 C  -1.78454221721312    1.80812770457235   -1.82317189692602
 C  -0.65102944059017    1.78572621451647   -2.81756946159268
 H  -1.62006828160988    2.59756495793068   -1.06784060780473
 H  -2.73695536130882    2.01235983061077   -2.33860353358885
 O   0.54093485101405    1.48373915316491   -2.13335260441227
 H  -0.58577988862241    2.77592206594075   -3.31163565773532
 H  -0.85066010327858    1.02300112984839   -3.59480258752395
 C   1.70416141416395    1.62273764557585   -2.91558715914970
 C   2.93221541074220    1.21835685492813   -2.10608026918473
 H   1.78329534198213    2.66937867226006   -3.27122946259552
 H   1.65071909587514    0.98022286160448   -3.81458839283421
 H   3.82772912911867    1.61558304530016   -2.63904085759290
 H   3.00660768427357    0.12343308207276   -2.10338118553189
 C   3.99965073652327    1.10601022529913    0.04394315025979
 C   3.79781266994417   -0.33858856534745    0.46781516718880
 H   4.13779228517674    1.70772749218613    0.95372779343377
 H   4.95821690175874    1.16947578617763   -0.51890844291901
 O   2.71246945096667   -0.40435451815562    1.40698273633867
 H   4.71902944758326   -0.69947328365874    0.96396069721506
 H   3.59678673434894   -1.00535451055192   -0.38388085598889
 C   2.64420087834643   -1.61909845472531    2.15245799886489
 C   2.21578996664586   -2.80402051617454    1.30604574550311
 H   1.91031296901835   -1.44086313344131    2.95403730370379
 H   3.62785408493687   -1.82729085588852    2.61989313257879
 O   0.92525210847692   -2.57351115941784    0.77905495171072
 H   2.24546740032915   -3.71587781315013    1.93148121879626
 H   2.90624219087250   -2.95707688834077    0.46098546409198
 C  -0.12539729897747   -3.29249901322738    1.38039144841851
 C  -1.44828598909024   -2.81504517774105    0.80991747065873
 H  -0.03035450822447   -4.37562613763050    1.15730403336001
 H  -0.09512900805623   -3.18521614974832    2.48115758149803
 H  -1.45536168126846   -3.03106604660747   -0.26887921272192
 H  -2.24587194378973   -3.43786431068521    1.27733197688961
 O  -4.91283434253587    3.08067912085327   -0.91632610772939
 H  -5.44925933893039    3.88140507572074   -0.98468349989536
 H  -4.89794389034841    2.86371838350383    0.05066506295118
 O  -2.65960057059434   -0.86403740786555    5.77935743100947
 H  -1.74846649604171   -1.18665236579736    5.57347901915079
 H  -2.53430961022464    0.01328592366798    6.16308694694574
 O  -5.02991321768433    1.30184282545466   -2.93040108415049
 H  -4.91007988788244    1.87538772586918   -3.69822839299137
 H  -5.07252914978865    1.91753314820559   -2.15430309660145
 O   1.16760938789566   -4.11414984936157   -4.55915188054616
 H   2.05599301179506   -4.15449431973078   -4.93949297562995
 H   0.90314565565997   -3.16566001401648   -4.64042247890240
 O   1.41776480568447   -4.13270584148981   -1.92430175420613
 H   1.26819927996061   -4.22526680035084   -2.90904405960471
 H   0.99058908578139   -4.89253431541143   -1.51009854501152
 O  -0.06799558272248   -1.49455125448095    5.19473801912849
 H   0.21737501679979   -0.54323256253271    5.19068999962145
 H   0.44536972238844   -1.92110537560902    5.89369386897830
 O  -4.79087533142617   -1.34977293056691    4.19868743767968
 H  -4.84879739764273   -2.31322145091355    4.24055075172613
 H  -4.01724829586775   -1.12407295678779    4.77526705704645
 O  -5.59610575249657   -0.09480791651560    1.97320380103557
 H  -5.30424535450411   -0.55015600036010    2.80759977688482
 H  -6.47733763623426   -0.44061663658633    1.78079471330807
 O  -4.82702380519376    2.43444777750544    1.71588646891592
 H  -5.19209013850182    1.51775528628042    1.84107586657783
 H  -5.19688601752193    2.96459113356400    2.43313503381744
 O   0.46436429973627   -1.47908843524397   -4.39925145517795
 H  -0.46212422528434   -1.50519086073308   -3.99269547143433
 H   0.40050444895689   -0.91583268461526   -5.18154341926547
 O  -4.39371908783215   -1.35306082481291   -2.96004579858940
 H  -5.15320769013059   -1.85887383945514   -3.27280454169320
 H  -4.66991130307795   -0.40562937877110   -2.97976691254078
 O   3.97720640847550   -3.11145991727664   -1.58371939643533
 H   4.56371990243032   -3.84838549891714   -1.36861054506346
 H   3.10044342317245   -3.53746805875339   -1.69987721645387
 O   2.62662264193697    1.34305862475255    3.39575133684894
 H   2.60613816048021    0.78785348464042    2.57362163860092
 H   3.48568250452459    1.15776316459130    3.79944072277653
 O  -1.73609050246904   -1.52842334283664   -3.04861445123744
 H  -1.65912323147705   -0.85891893798824   -2.33753744173399
 H  -2.70824745660131   -1.58104376765042   -3.20517467724081
 O   0.47246989619346    1.12059097396927    5.00838319012778
 H   1.24279475580973    1.20787083851726    4.38920522840184
 H   0.68513231708635    1.70403718508507    5.74908409668025
 O   1.16857585488439   -1.34849852177262   -1.63150934814994
 H   1.11421486409805   -2.30743730298316   -1.45761685958144
 H   1.07391095917083   -1.26392631834642   -2.59623331950780
```

```
111
Coordinates 2 from ORCA-job na-crypt222-b3lyp-opt
 Na -0.24587098727236    0.26665783942399   -0.06777774817313
 N  -1.36939710408310    0.45165910869126    2.58900267735185
 N   1.29627787535607   -1.04908506640073   -2.60894226588423
 C  -1.18764700885172    1.84178535692597    3.00889787941283
 C  -0.72115754357397    2.77317880683810    1.90254199225515
 H  -0.45507817054254    1.87975126528665    3.82768509689239
 H  -2.12266669374067    2.26128481084340    3.43415628035364
 O   0.47948305971420    2.24110493862276    1.32194718134936
 H  -0.50575184109942    3.76487505496836    2.34297195874998
 H  -1.47819317252089    2.91161445196891    1.11789472032244
 C   1.14727361852151    3.17577022861628    0.47629775204338
 C   2.26634993728240    2.48110781349782   -0.25503345084611
 H   1.57915303114584    3.98572204706115    1.09411966850491
 H   0.42302310593074    3.62589838485468   -0.22182888034802
 O   1.73266810942114    1.54355462982859   -1.19057192835048
 H   2.94490875193156    1.95555455968200    0.43913182936163
 H   2.86417825508607    3.23987604111451   -0.79303249896310
 C   2.78012917543471    0.83147748793454   -1.87064125050002
 C   2.20861598737885    0.01319993707553   -3.01239482114936
 H   3.31644411803954    0.22780320212598   -1.12946280606550
 H   3.49775348320542    1.56716492109895   -2.27813066211034
 H   3.06733052654444   -0.39159978799354   -3.59243583862271
 H   1.69108719569858    0.70013023283403   -3.69840282565959
 C   1.96341383871946   -2.32549846846632   -2.36507293896770
 C   2.93127283477082   -2.33535953626057   -1.19341863623346
 H   2.52854606681732   -2.66754564438404   -3.26315196105776
 H   1.18409223004035   -3.07605530755825   -2.17694397980328
 O   2.29221463626650   -1.78835787682653   -0.05008555541565
 H   3.85529833685615   -1.76458640076053   -1.39745206796640
 H   3.21902318509681   -3.38369391491628   -1.00024952516694
 C   2.96463234464066   -2.06301471871728    1.17194436958754
 C   2.49834010078692   -1.10976771894070    2.24028892431234
 H   4.04567328664632   -1.89954704032787    1.04003184525103
 H   2.77156950934700   -3.11399057255553    1.45815114289006
 O   1.12055699933368   -1.31300740273687    2.52238906701781
 H   2.65682531463545   -0.07560142246552    1.89995733664406
 H   3.11322675603673   -1.26102648975021    3.14681991900832
 C   0.64944103886012   -0.58415135783457    3.64439306042593
 C  -0.86381876938688   -0.49000615633046    3.58623761702544
 H   1.11740250906143    0.41134325665685    3.65894750459482
 H   0.95188913362751   -1.10231164677050    4.57642729587422
 H  -1.23797333301885   -0.24005932475432    4.60394798432226
 H  -1.25458484818078   -1.48872361298397    3.34455892536766
 C  -2.75285518040926    0.12257854928062    2.24115542493059
 C  -3.35048631207906    0.95964754006990    1.12843637924354
 H  -3.42381031223185    0.24174451830033    3.12350971365843
 H  -2.78935131736903   -0.93557696841465    1.94165447339311
 O  -2.51459978633167    0.93160337977317   -0.02037580978253
 H  -3.52512463289134    2.00928623269795    1.41845734049987
 H  -4.33327037747635    0.51797340395592    0.88108562906035
 C  -3.22076733218049    1.23260699823556   -1.21319716738465
 C  -2.23920337649722    1.30276087582578   -2.35500214987535
 H  -3.72337300877814    2.20843981364735   -1.11345351313239
 H  -3.96516661890470    0.43769427969115   -1.40076701758070
 O  -1.42948266234727    0.13420578820708   -2.35069977332728
 H  -1.59060737009658    2.19326143505543   -2.28108164636167
 H  -2.81112346619601    1.37863118987716   -3.29912071168844
 C  -0.78764718190679   -0.07786812962445   -3.59992344308885
 C   0.17779887236563   -1.24118641369653   -3.52639158043614
 H  -1.54836905026211   -0.31266492100409   -4.36761714267552
 H  -0.28361774493053    0.85419584288061   -3.91178066984986
 H  -0.38423785641593   -2.13133248192686   -3.21679904949668
 H   0.52659951731934   -1.44693918199418   -4.56495644453330
 O   0.91024909005064    2.31888866827546    5.77305510727304
 H   1.23878478367614    1.68831497118908    6.43023809435365
 H   0.60368175555694    3.07872110812086    6.28872876896394
 O   4.80727295325643    0.36285661601537    0.59339336832304
 H   4.87178923808881    0.64035932725400    1.53457577820685
 H   5.17916124598169    1.10232389740944    0.08210881193029
 O  -3.08226720800268   -2.11819711776654   -1.38183365738473
 H  -3.02406816609572   -2.51842377638135   -0.48651747885697
 H  -2.36605451646944   -1.46008074191140   -1.40802824673542
 O  -0.36151267247278   -3.64421791758354    2.14366141170705
 H   0.17638848318978   -4.22615091632866    1.54454778424404
 H   0.26547449880629   -2.95434372256914    2.44258616669659
 O   1.09462757155641   -4.87393290680522    0.24665431339510
 H   0.47631351013902   -4.83750860208195   -0.53123001469376
 H   1.40127721973464   -5.78872698611725    0.29580753191099
 O  -3.25354822249699    4.11706606781837    0.19239324145557
 H  -4.01585076030695    4.64743619305632   -0.07044267389892
 H  -2.55872580137581    4.33714144815550   -0.46580167171091
 O   5.72147262202055    2.40029757582092   -1.19012005082072
 H   6.21295987195918    3.16168992350930   -0.84965194862507
 H   6.35717719200481    1.94241539705509   -1.75924402136872
 O   0.61739207538787    3.39671172237689   -2.89095587003041
 H   0.92896901674183    2.60948713247486   -2.39832366537971
 H   0.69309396545931    3.18951228912670   -3.84500553362178
 O   4.68341788580226    1.12637933440932    3.25141133373906
 H   3.85378316497928    1.65799458042917    3.32715684640495
 H   5.36738361274770    1.67258812541708    3.66000572490067
 O  -0.70955427974009   -4.29199091017371   -1.58444319697589
 H  -1.25500476657673   -4.25234189465048   -2.40336338284728
 H  -0.81697844009291   -3.41013870183366   -1.17258859926780
 O  -2.39925276273051   -3.52863744899829   -3.55358175202999
 H  -3.09847500305887   -4.07892406370412   -3.92871010392984
 H  -2.81496858128190   -3.04553170335222   -2.79201395818296
 O   0.81838530424603    2.74913557280292   -5.56905734518405
 H   0.01740261640924    2.91107466222552   -6.08862542946047
 H   1.53134092166677    3.15623385377758   -6.08172757655773
 O  -2.90547572617170   -3.08953221077856    1.24974996471679
 H  -3.58859823263036   -3.64359492113347    1.64874998738320
 H  -2.05369528667257   -3.40723462007726    1.62993659031006
 O  -1.19896588937578    4.72716489502102   -1.51877391281465
 H  -0.70956840941933    5.51663353852993   -1.25372930866796
 H  -0.57843963088532    4.23793360539051   -2.11998747029243
 O   2.36206369365460    2.53690345829288    3.38231687948735
 H   1.69559813205500    2.28258936877256    2.71281207696024
 H   1.88708244704491    2.53319590589843    4.23796252580120
 O  -0.36735933445281   -1.99186172837657   -0.08846351365265
 H  -0.53317690624594   -2.46176858164004    0.75233220251356
 H   0.61974004199527   -1.99749842541450   -0.13380935689419
```

```
111
Coordinates 3 from ORCA-job na-crypt222-b3lyp-opt
 Na -0.09903781511696   -0.15329013329384    0.08759153039972
 N   0.96457559287036   -0.15494586370736   -2.54661666529112
 N  -1.05452656977378   -0.84277487363821    2.90304146558232
 C   1.46582474578609    1.19356513604179   -2.80613351123114
 C   1.78060897768859    2.00200624680011   -1.56125744195121
 H   0.70020955825918    1.75089731943376   -3.36415713359492
 H   2.36797898685482    1.17849115862022   -3.45548215288093
 O   0.62341797362559    2.08022188428886   -0.73767419311087
 H   2.09991968085878    3.01457182443315   -1.86969252513038
 H   2.60885210360615    1.57412625161549   -0.97876558498895
 C   0.70054337774038    3.15623292107371    0.17769453967207
 C  -0.39283878282556    3.03078154202294    1.20075969367788
 H   0.55771626970992    4.11251865325463   -0.34952590550877
 H   1.68906694698193    3.17851790445547    0.66879905874884
 O  -0.17817858631592    1.85194524182828    1.98430414357463
 H  -1.37937703567336    2.96697077721699    0.71921935977564
 H  -0.37159782035964    3.92680880317753    1.84418056824170
 C  -1.19066585693419    1.68292729134553    2.97833633452506
 C  -0.99821701934755    0.36508948815167    3.71593627139093
 H  -2.17116618017640    1.79634218294604    2.50123345862255
 H  -1.10601696890082    2.50283811215748    3.72030771427224
 H  -1.74129482101559    0.33673990092329    4.54632816349859
 H  -0.00883803209614    0.41180190071655    4.19228817275921
 C  -2.41334728593010   -1.27775909568202    2.58823845267120
 C  -3.26705011651043   -0.35070108761742    1.74405632763141
 H  -2.98937131381956   -1.48124579665216    3.52185081876155
 H  -2.32798512275764   -2.22918055809840    2.05514800397179
 O  -2.58827400232411    0.03744245051651    0.56554362518122
 H  -3.61373216433435    0.54300544977191    2.29118384366785
 H  -4.17764179186257   -0.92126432588602    1.47678665927833
 C  -3.47530940932752    0.57238708291628   -0.40418376280450
 C  -2.70549298786356    1.02422438166872   -1.61739293677138
 H  -4.00903461462877    1.43952145656792    0.01791342984807
 H  -4.20916802797072   -0.20481922392060   -0.69345941166004
 O  -1.95651282347065   -0.06761076585419   -2.12766172402871
 H  -2.02557085375372    1.85504957886034   -1.36925768349467
 H  -3.42905900949724    1.39635316157745   -2.36675038946161
 C  -1.36514293707883    0.16999903292371   -3.39646841561547
 C  -0.05317992994738   -0.57893141893674   -3.50966186952226
 H  -1.22117860340074    1.25466075485479   -3.53856938367772
 H  -2.04626001643034   -0.17845420193844   -4.19601028588650
 H   0.30998272741307   -0.47184926854257   -4.55762130340419
 H  -0.24450271660228   -1.64977580978126   -3.34865184553302
 C   2.01098384583997   -1.16942664239713   -2.48132831235610
 C   3.05671404071906   -0.96466992092797   -1.40613337709494
 H   2.56403292752802   -1.24459932913057   -3.44702559697849
 H   1.51886101992440   -2.14242302770592   -2.32615626937147
 O   2.44463558149825   -0.89092428761638   -0.12144201371859
 H   3.67204355893240   -0.06418389664069   -1.57316301639282
 H   3.74073112255115   -1.83350372699785   -1.43690735474930
 C   3.41773467454009   -0.99881786542153    0.91364263045091
 C   2.77961662034337   -0.87751601429845    2.27410413100859
 H   4.16913533618636   -0.19698248997014    0.80150627646714
 H   3.92516637659356   -1.97676587009598    0.82249900378130
 O   1.77816514852816   -1.86471966137598    2.43390487256029
 H   2.34999978908523    0.12594323257310    2.42308123351916
 H   3.58253991489491   -1.00668310060234    3.02733144994762
 C   1.12918645967534   -1.85009780278748    3.69486783789133
 C  -0.37200297393708   -1.98000529603353    3.53549578709544
 H   1.49091204511290   -2.69766532278518    4.30564404945335
 H   1.40151877636824   -0.93259567495345    4.24379685133003
 H  -0.57639609283412   -2.87162145128453    2.92411686056664
 H  -0.79830021033017   -2.19001415995971    4.54386340666127
 O  -3.40047726250177   -3.32336453687971    0.13275352088038
 H  -2.90342645461673   -3.97226300698943    0.70934894575700
 H  -4.24262191952592   -3.17027191144559    0.57925136752757
 O  -1.01388163654712    5.93026441884848   -0.58026752070730
 H  -0.52742706908028    6.25078301330725   -1.35111523433049
 H  -0.38992515963193    6.05624504643825    0.17589096261059
 O   3.51605878792554    5.85456082025317    0.86414063730815
 H   4.15176769794369    6.47900153223644    1.24162236806622
 H   3.69422600927900    4.96205403600012    1.32470463117542
 O  -2.95739095875850   -2.64218544272564   -2.51745109779635
 H  -3.27161143156732   -2.99851783473503   -1.66156409086345
 H  -2.67444659982620   -1.73074771763120   -2.29777359194290
 O  -1.77568544793685   -4.76333830304633    1.62174190528087
 H  -1.15298599397980   -5.00869150013646    0.87185140206454
 H  -2.00711091697876   -5.60011562958915    2.04637811736606
 O  -0.65915080908192   -4.00065739353057   -2.76901451959819
 H  -1.52837079440923   -3.50978835424216   -2.71506560459155
 H  -0.69040669945165   -4.47316620743824   -3.61166875316998
 O   0.85049536093674    6.10329640843978    1.41016397087409
 H   1.81086779642517    6.10329792693291    1.17253288558392
 H   0.75988179867824    6.73637882640365    2.13458538042700
 O  -3.83626860509201    3.14145630084116    1.55921441608992
 H  -3.61797993075359    3.57699242687013    0.70285549795368
 H  -4.76946950960199    3.34264851219671    1.70473755657194
 O   2.12665861685069    2.23562814807720    3.30196570660128
 H   1.88537421442633    2.64708272927328    4.14219009403472
 H   1.27826630587289    2.08822122039675    2.81366048291017
 O  -0.18412323279579   -5.20522472046504   -0.39177856032314
 H  -0.39175767469169   -4.92636719542048   -1.31716113372484
 H   0.69978817717114   -4.81198142209630   -0.19785606591197
 O   4.84542125103811    2.03187935343951   -0.31409833392180
 H   4.72440881826837    2.86952037438346   -0.83080211727714
 H   5.80219840486104    1.89866030533358   -0.26511017275751
 O   1.89037684229814   -3.63971888985866    0.29267195249077
 H   1.83465972021114   -3.36078676708554    1.22744411338927
 H   1.78425765521157   -2.77316048269083   -0.13643751069085
 O  -3.06888880143681    4.15416974473590   -0.88131012177643
 H  -2.32058176929495    4.79107468361690   -0.76481231275381
 H  -3.74487832608120    4.66290006445850   -1.34980610800285
 O   3.97665731563710    3.53380900143025    1.81612090881796
 H   4.29585871934053    2.88866345839940    1.14527569060768
 H   3.32693345309560    3.05646070705933    2.38335284753595
 O  -0.76569351078886   -2.26126680229997   -0.15681756681820
 H  -0.45658745987513   -3.18058018864376   -0.17567570024167
 H  -1.73544918867257   -2.33209770886965   -0.13225388285087
 O   4.28706176873807    4.42525083553954   -1.38116698949064
 H   4.00870673822463    5.05566418821050   -0.67171762627467
 H   4.72726602397626    4.95716477448715   -2.05117670638412
```

Figure S8: Three optimized coordinates for Na-[2.2.2] complexes with 16 explicit water molecules

```
111
Coordinates 1  from ORCA-job k-crypt222-b3lyp-opt
  K   -0.04517241331054    0.41250011880781   -0.18866831432601
  N   -0.47031514884616   -1.05124053457118    2.39036697948254
  N    0.55769575697107    1.90801874675460   -2.77086468333490
  C    0.77321210484930   -1.31889307286987    3.10695563968527
  C    1.93079363789463   -0.39119960926569    2.77947541270058
  H    1.11830475960252   -2.32379649520736    2.84294776591791
  H    0.62487620489903   -1.33028599307089    4.20721074201045
  O    2.16759498087047   -0.42387912997948    1.38897490327424
  H    2.81729743216018   -0.77188476093621    3.32504038532591
  H    1.76074318530836    0.65035388973878    3.10202257628193
  C    3.45054986554106    0.04335172962661    1.02995290682983
  C    3.61292683735204   -0.06740812207618   -0.46203918228143
  H    4.22064955697577   -0.58153130613856    1.50765109527528
  H    3.59389737888901    1.09548967467850    1.34525583142163
  O    2.78725239417311    0.90018076541150   -1.10469914229556
  H    3.33134914387624   -1.08531833329488   -0.78075640314354
  H    4.67509465392512    0.10219318116158   -0.72289236181931
  C    2.78676653047962    0.77050061916550   -2.51819138098198
  C    1.97122997342586    1.89574165967180   -3.13614881490509
  H    2.39245347626173   -0.22312317304539   -2.77873330733217
  H    3.82556527292727    0.83829757497838   -2.89971075219082
  H    2.10898161508975    1.86133421271861   -4.23879257884386
  H    2.42682219330398    2.83996042991969   -2.80297378320574
  C   -0.30170787562518    1.14791957129995   -3.67509887872489
  C    0.05110998103061   -0.32065724735320   -3.85234573253013
  H   -0.31199925795352    1.59797368980633   -4.69569762184064
  H   -1.32650736184726    1.22002674194812   -3.28629146529207
  O    0.18810565442749   -0.97122442674845   -2.60728576294180
  H    0.97696655005329   -0.44610306760244   -4.44870112223659
  H   -0.76300707042671   -0.78448270698698   -4.43942564866547
  C   -0.08186296995892   -2.36274610391743   -2.66161093590980
  C    0.17118776287694   -2.99131764768844   -1.31186169796051
  H    0.57993971213949   -2.85693541366859   -3.40076149376008
  H   -1.13238682056958   -2.51558005995997   -2.95686030900969
  O   -0.58664812368328   -2.35120486976082   -0.30543405065302
  H    1.24501727515936   -2.95522200259785   -1.04892368035100
  H   -0.12032837940614   -4.05920735490808   -1.39010511114380
  C   -0.55704299287310   -3.08255745497840    0.91026075442475
  C   -1.18061573267250   -2.28181611175716    2.03287599552159
  H    0.47919483368757   -3.36697527800913    1.15563477671536
  H   -1.14411283987234   -4.01140324041484    0.78914644590394
  H   -1.27252301560482   -2.96070057119437    2.90648780990604
  H   -2.19654989375186   -2.01016200327557    1.72438491676979
  C   -1.37645567426867   -0.13167044509614    3.06163208539305
  C   -0.82366757365065    1.24965432209233    3.36127850439147
  H   -1.74735883022251   -0.54848437629600    4.02987447635801
  H   -2.25797993004481   -0.00039735716347    2.41728812286803
  O   -0.29475777007760    1.83690378349012    2.18800385373011
  H   -0.04634816367901    1.21935926737466    4.15052376161264
  H   -1.66026722518231    1.85856889200567    3.74512086717933
  C   -0.25062172256927    3.24640174510343    2.24153529160688
  C    0.49426969236301    3.79616733764673    1.04836684451040
  H    0.28179547177583    3.59187350306923    3.15066095358543
  H   -1.28121214301296    3.64156206743660    2.28553122304948
  O   -0.09416277053242    3.34073717550677   -0.16966336617969
  H    1.55734079323797    3.50757201304808    1.06606255225327
  H    0.44289800309379    4.90150649867804    1.09834951489765
  C    0.49757193851650    3.95335498267969   -1.31991045268078
  C    0.03429190766939    3.26548472428663   -2.59058441575029
  H    0.18789848098866    5.01567981377617   -1.36174095466915
  H    1.59351384069127    3.92995251901319   -1.20659479304914
  H   -1.06351123954551    3.21138528181712   -2.58042041365102
  H    0.30972965137759    3.92418896889027   -3.44502643748673
  O    4.23199039562298   -3.18039323905160    4.27722551452340
  H    4.67686372570670   -2.82056459228388    3.45457692339971
  H    4.84254219024554   -3.85469155201967    4.60761228833950
  O    1.97877363839752   -3.07677973623312    5.84528400557190
  H    2.81021676475630   -2.96793098470202    5.33112924493443
  H    1.84016822153066   -2.23917007851689    6.30460018862000
  O    5.25944225102251   -2.63352364876556    1.94724221438920
  H    5.88913117161443   -2.00787735387289    1.53969291828792
  H    4.63437066665153   -2.87362357024657    1.22175299587125
  O    3.53933599553190    3.35067796518063   -0.01831133845363
  H    4.45059647894524    3.50455898775109   -0.29867710743117
  H    3.28755836563200    2.50315170287594   -0.44184369651503
  O   -3.13750934073280   -1.93696446097672   -2.09240549510949
  H   -3.94413665430214   -2.02810701053795   -2.61723786173904
  H   -3.21317853976664   -2.64543597190746   -1.39675518888623
  O   -4.52891688221977   -2.32162744647530    1.89539624022327
  H   -4.50136374183432   -1.34977464769996    1.73669137696929
  H   -4.11221286198168   -2.44782859591941    2.75792289433093
  O    0.31614545420463   -4.40666818254509    4.19498075495103
  H    0.15227627848498   -5.26661397832850    4.60560967054850
  H    0.81740958386187   -3.89367731700935    4.87820493278403
  O   -4.53041690167196    0.32611583428721    1.20605233165425
  H   -4.21486319748729    1.20150545905240    1.59644512462234
  H   -5.41620303882395    0.51086755791245    0.86355149974181
  O   -3.57378635765618   -3.77057486006500   -0.16258186016242
  H   -4.13316947382836   -4.54884529498656   -0.28022742667264
  H   -3.94817447486373   -3.28530685516770    0.61540511435976
  O    3.33235342942778   -3.33011738584122    0.13675078440427
  H    2.82747987300165   -3.65932931914027    0.93064853662716
  H    3.54811647104703   -4.14038957261518   -0.34621245397969
  O   -3.59644762813555    2.62460672108100    1.95580948074586
  H   -4.07091302405006    3.24472168283375    2.52567851701390
  H   -3.29422023452422    3.17561924275266    1.15917406955591
  O   -3.23987185129057    2.66585768191117   -2.29759184934671
  H   -3.87339205848070    2.55090410006655   -3.01656145041943
  H   -3.12478835250862    1.77719740626621   -1.86089142528968
  O   -2.74589588462738    0.44198801689754   -0.93846890314687
  H   -3.35975602958331    0.38132473930689   -0.17387510101039
  H   -2.84539876105465   -0.43810861994046   -1.39170228351890
  O    6.81216039805727   -0.85718755353655    0.47370268044475
  H    7.42900689803008   -0.24847054911044    0.90607814328025
  H    7.34513535255485   -1.30699515378413   -0.19813563260819
  O   -2.74791394961233    4.05285211237561   -0.04044761937621
  H   -1.79937985804214    3.80677344352139   -0.11043102220964
  H   -3.11570757969913    3.73497196745169   -0.89548765214539
  O    2.41233193050632   -4.29744529249033    2.43003988011604
  H    1.57771794888433   -4.43762303534147    2.93582524213744
  H    3.04472762838209   -3.98783599418243    3.11070385983632
```

```
111
Coordinates 2  from ORCA-job k-crypt222-b3lyp-opt
  K   -0.31020719519563   -0.07217364260825   -0.50053656237962
  N    2.65554021940610    0.22331651287518   -0.68419266815573
  N   -3.28989800773059   -0.57007091797305   -0.31481898720572
  C    3.35999996416052   -0.63113554873476    0.27382929525946
  C    2.54702640510183   -1.79061143315518    0.84214350662722
  H    3.67358948989940   -0.01927913462382    1.12988603460771
  H    4.29110044640636   -1.04483952319605   -0.16553833075852
  O    1.31067609435502   -1.30189159065062    1.34135692953592
  H    3.13207435613207   -2.23930306040995    1.66208772328176
  H    2.35634428522680   -2.57361043626635    0.08960282697175
  C    0.73803680016870   -2.11086882182982    2.34838335637669
  C   -0.58733779556117   -1.55630650704332    2.78508502494056
  H    1.38040068418437   -2.13310573405689    3.23869343281299
  H    0.63899232465322   -3.14850288107422    1.99494974111514
  O   -1.57071381374554   -1.69957191510127    1.76402207005277
  H   -0.48109177842240   -0.49324632277166    3.04379308676469
  H   -0.92183300878693   -2.07351944494877    3.70035007830796
  C   -2.79862006946318   -1.04843831365102    2.09584162575921
  C   -3.76258746524909   -1.17721405863484    0.92761608902544
  H   -2.58095203983702   -0.00300831337270    2.34874175707198
  H   -3.23672592720939   -1.52146179065665    2.99451509629326
  H   -4.74190108004209   -0.75845661384390    1.24077910076616
  H   -3.93859464640381   -2.24980984489656    0.75591708872811
  C   -3.71123734957899    0.81905882717274   -0.48828136962928
  C   -3.29805604607145    1.77825516259491    0.61709504119968
  H   -4.81836961935136    0.90203446786222   -0.58547255428392
  H   -3.28508381829968    1.18632743553886   -1.43017456690860
  O   -1.90573352746511    1.68354048045355    0.86637098030278
  H   -3.85307698935481    1.59528079892678    1.55670835339964
  H   -3.55232780560082    2.78851461154646    0.25648194767120
  C   -1.35260620312543    2.81496098462857    1.50632743903656
  C    0.08689529715033    2.51818194850029    1.85938193489451
  H   -1.89848239194072    3.03732978531734    2.43967580198594
  H   -1.41306551806032    3.69575162253123    0.83984583484326
  O    0.80608637008200    2.19858438869722    0.67788151763689
  H    0.15178010953872    1.67491737402764    2.56869149048618
  H    0.52916138274765    3.40766936885170    2.34834179368645
  C    2.21908099172409    2.13400072572365    0.85589134145128
  C    2.85157001813702    1.64656939627241   -0.43763098377648
  H    2.44521173499364    1.46697106633433    1.70382412378801
  H    2.60066710316586    3.14487757399549    1.09313669938053
  H    3.92930050119596    1.92540425708670   -0.43430138169552
  H    2.39553152354570    2.21035062939292   -1.26669919740376
  C    2.89513416764874   -0.11603487340233   -2.07968073791329
  C    2.55896145476454   -1.55437247441824   -2.43327789623555
  H    3.95939443576883    0.05254658980444   -2.37312311515574
  H    2.29630862819592    0.55586372814531   -2.71342339492361
  O    1.24074301972694   -1.84902123159630   -2.00710743108967
  H    3.26860265687546   -2.25710107697438   -1.95467158233526
  H    2.64071803005545   -1.66839701229040   -3.52759234001021
  C    0.77792130652128   -3.11486735792339   -2.41407248936416
  C   -0.52741850793818   -3.42773872946942   -1.71125474898087
  H    1.50409197742488   -3.90777544719382   -2.14250112750415
  H    0.65103836619641   -3.13656056369273   -3.51476122266402
  O   -1.43287211844983   -2.34815558709761   -1.88614763598189
  H   -0.35592416363592   -3.60727197407985   -0.63549237585433
  H   -0.94392488445442   -4.35705952468123   -2.14233555525534
  C   -2.79262225789106   -2.65733492645151   -1.60189182324681
  C   -3.58956991739821   -1.36737867486743   -1.50250860950863
  H   -3.20853247513410   -3.28198686258617   -2.41566174783704
  H   -2.84664115521083   -3.24677084266307   -0.67210417080360
  H   -3.35574281876245   -0.75838280489932   -2.39085448219775
  H   -4.67049422793325   -1.62250760698906   -1.57582792247065
  O   -2.40615558369104    1.50512372526142    4.28084454506117
  H   -2.48801760616461    0.63746021870527    4.74559672417134
  H   -2.78347835187354    2.14456062217512    4.89994370459988
  O    3.45555914883115   -2.50930323845411    4.00704533320925
  H    4.37379229807372   -2.77498730361541    4.14417929996654
  H    2.95022791829314   -3.35841954040576    3.92863731370673
  O   -1.87972684592384   -4.35099021959352    1.37675385762049
  H   -1.78302192845518   -3.37092717645192    1.49501970702793
  H   -2.55956171324060   -4.62383092865060    2.00755136078066
  O    2.29560280915415    2.09874772582839   -4.90735945683483
  H    3.25081033513472    2.00818058305015   -4.80003788445118
  H    1.94102828140063    1.17301632140876   -5.02053329607027
  O    0.18070629970929    0.63061151816668    5.17091127815562
  H    0.98530320963443    0.47745128572286    4.62604720036978
  H   -0.42402055447667    1.21451159506049    4.67889607175035
  O    0.64018975146064   -5.33553105277361    1.43247943494089
  H    0.70388982428921   -6.13225455280226    0.89048262957540
  H   -0.31591660250693   -5.08383041929648    1.43447099212018
  O    0.80587508140862    4.49565048617430   -0.84722126777766
  H    0.93334677755194    4.27927851998631   -1.79640163014885
  H    0.68026055597484    3.62623287937489   -0.41639951849436
  O   -1.52633506969368    5.76314087280044   -0.80616075709637
  H   -1.65865219237333    6.24236975979843    0.02143549398391
  H   -0.60350598405474    5.38544881016392   -0.76518820211583
  O   -2.88969684192664    3.72422788839513   -1.86003134051430
  H   -3.42667142223373    4.09790351330297   -2.57132717433698
  H   -2.45310340977030    4.50705442159649   -1.42715008692338
  O   -1.03716798382877    1.81824644678898   -2.48586559578263
  H   -0.35473612824178    2.41277135148420   -2.87365788344115
  H   -1.75741206067539    2.45496312988164   -2.24878607442305
  O    1.33852325049990   -0.36773078928831   -5.07848045904914
  H    0.42282246028502   -0.42227202393920   -4.66844583271900
  H    1.23897354793170   -0.72474255084433   -5.97118005227166
  O    2.10246881409478   -4.85001238064803    3.72988603054077
  H    1.63176327559964   -5.08183124033498    2.89541676991756
  H    1.54763034526964   -5.20815004075994    4.43466386179548
  O    0.78281981581464    3.65045850648841   -3.46539339272850
  H    0.36674950789987    4.26863226711484   -4.08265569969601
  H    1.42931162357252    3.11517695577302   -4.01607703054623
  O    2.58183844026168    0.12670012900916    3.81973388494965
  H    3.23551346778582    0.63361281237636    4.32043696399722
  H    2.89325195151196   -0.80834498625132    3.89163320494052
  O   -1.98865409827381   -0.88072551073421    5.53686858985350
  H   -1.06739890025195   -0.51063694153770    5.53196423118636
  H   -2.21635614274779   -0.98674588691427    6.47066862516441
  O   -1.04008959844370   -0.42971666413070   -3.96700947274470
  H   -1.15909089991546    0.42226734584418   -3.47755290976134
  H   -1.15822439452962   -1.13398055981355   -3.30096324398976
```

```
111
Coordinates 3  from ORCA-job k-crypt222-b3lyp-opt
  K    0.68743910082481   -0.20562229357065    0.41506089445893
  N    0.51641075712251   -1.31520809446457   -2.37061380088799
  N    0.68198395483958    1.12970376642078    3.05556289185224
  C    1.28984645478250   -0.52717983042061   -3.33047134357135
  C    2.48180694623768    0.20995236537066   -2.75234548055470
  H    0.63558010221590    0.22729468817780   -3.78869705711453
  H    1.66234915520376   -1.14462602028917   -4.17227397397217
  O    2.06788976980292    1.20443479305763   -1.81199366114945
  H    3.03265217271997    0.69919952284105   -3.56867323233904
  H    3.18337484517957   -0.46184027009645   -2.24305643316481
  C    3.21107914655720    1.79502139953133   -1.18329279910795
  C    2.79629921705618    2.83761398234421   -0.18207645624790
  H    3.85058551344398    2.25950412377077   -1.94826879676950
  H    3.80243321555173    1.00383796825172   -0.69387160589291
  O    2.24912004218139    2.20804462884451    0.95322862359153
  H    2.06541067399545    3.53394738167559   -0.62348359388939
  H    3.69229385894583    3.42991970953447    0.09757353811863
  C    1.58585485541091    3.11012981028499    1.82035748757383
  C    1.35091611276087    2.42303254240771    3.15719562372252
  H    0.65825004210370    3.46111754547465    1.34299745884250
  H    2.21912639440279    4.00281871150367    1.99632005833461
  H    0.79227633555380    3.11789327626905    3.81818715216128
  H    2.33370192041232    2.28377401674988    3.63110049200849
  C   -0.76089991310345    1.19600087428856    3.23698507453492
  C   -1.48297255608096    2.05991933930569    2.22023799623107
  H   -1.03551821142403    1.58712704195436    4.24412460213005
  H   -1.16338232226885    0.17748437563846    3.16426663249282
  O   -1.16960740983856    1.63600823302247    0.90774635198404
  H   -1.22903746552447    3.13099115947304    2.33686414277013
  H   -2.56686492676902    1.95033356806336    2.40634465121805
  C   -1.89841865793994    2.32565882438206   -0.08867832249350
  C   -1.52546183764443    1.79640384337861   -1.45168489096848
  H   -1.65697015356061    3.40316418179351   -0.07321886712129
  H   -2.98589448642113    2.19367658356473    0.08045790625491
  O   -1.83287103905430    0.40951411928986   -1.53206118159360
  H   -0.45232969824129    1.95302005027222   -1.64537549533389
  H   -2.08857387393574    2.36532805542331   -2.21345198938799
  C   -1.69961014845644   -0.18222421241122   -2.82188191945169
  C   -0.88790332140007   -1.46529084951398   -2.76404705256195
  H   -1.26796462532160    0.55233492445378   -3.52094675273349
  H   -2.70394981064400   -0.43970682317367   -3.20479341950504
  H   -0.97755099863937   -1.95415816582744   -3.76271367298167
  H   -1.37631258116610   -2.14862040486151   -2.04952794259041
  C    1.06244641178216   -2.65361818001896   -2.12527750401654
  C    2.47002309420160   -2.74252338511160   -1.55328960187226
  H    1.06759941721404   -3.25448835530285   -3.06392922509219
  H    0.39459057818161   -3.16440477465724   -1.41868857147118
  O    2.60182200329720   -1.92590664954544   -0.40859807114952
  H    3.24413029934411   -2.47447897168377   -2.29811862789542
  H    2.64063791211131   -3.80290588597076   -1.28505013743272
  C    3.66900864829159   -2.28343697754303    0.44332454000501
  C    3.81073577060868   -1.25677654381314    1.54670428813236
  H    4.62064017696373   -2.31660488531711   -0.12116073346103
  H    3.47839242816255   -3.28535434957592    0.87553808838798
  O    2.57991839267529   -1.09017017540631    2.21549145022941
  H    4.15179215701011   -0.29017436467235    1.12685564761826
  H    4.59567901819623   -1.61234817845391    2.24356281053385
  C    2.67673204466920   -0.34030768162723    3.41176574851462
  C    1.29091322079328    0.08340504940812    3.87244516499690
  H    3.15182997431266   -0.95393898377555    4.20294192576348
  H    3.32437703132270    0.53987807195301    3.24709023635348
  H    0.63941793654887   -0.80282454224517    3.82313488824225
  H    1.36043353653256    0.38170955960077    4.94296345238238
  O    1.15969345583253    3.53576246569350   -3.00122123153835
  H    0.56255660706957    3.33651387593421   -3.76583698945294
  H    1.33764329078102    2.65012972456886   -2.61142902638124
  O   -3.89155453452433   -0.16852250064678    3.00055725355560
  H   -4.78517805844382    0.19284709146040    3.07482457730707
  H   -3.69655780467048   -0.20093197420132    2.02766330177430
  O    5.85654165351413    2.02878817370482   -3.38667507876937
  H    6.58066077350012    2.66133252306758   -3.49245383050368
  H    5.03075764357044    2.52402141718792   -3.66793015803780
  O   -3.26293253819947   -2.73830936275386    3.17172953218499
  H   -3.38460880789858   -3.17653411033819    4.02499750655925
  H   -3.59951425351259   -1.80722537538357    3.28438497445020
  O    5.76516043752087   -0.23656499153224   -1.73660169038228
  H    6.67191640527691   -0.52176285793462   -1.55856275165968
  H    5.85763494365139    0.66416986010759   -2.11796297841687
  O    3.03119530879951   -0.21761589144256   -6.02829942393776
  H    3.84933903888136   -0.34021534092619   -5.46643036818716
  H    3.06586840875160   -0.90774319416466   -6.70318098614340
  O    5.21471189087887   -0.40972757041998   -4.52082097171062
  H    5.59051549662696    0.48866350203616   -4.41049684187030
  H    5.26989683440388   -0.73890702418326   -3.60219757110149
  O   -0.22340176640815    2.58448753985505   -5.07812764524282
  H    0.55691635324120    2.41798473424614   -5.66127833499508
  H   -0.88139052948962    3.02564750427099   -5.63200983378194
  O   -0.01633008450148    4.76225491337315   -0.81128193674816
  H    0.44476876007345    5.59993096092698   -0.67456839180513
  H    0.35707279147846    4.42002254827501   -1.65401110712337
  O    3.66107216153007    3.24144712735117   -4.20129694328360
  H    2.88067121475175    3.54483828807816   -3.68642977520654
  H    3.24617246529253    2.90602773602360   -5.02575688223384
  O   -2.78724684632745   -4.18519677202412   -0.69134421145047
  H   -3.16943012754518   -4.81819069974383   -1.31235259158895
  H   -3.55708470513136   -3.83093381444610   -0.15536290384713
  O   -3.11832611495638   -0.81270008678238    0.52106936186172
  H   -2.30769083112209   -1.24108376643628    0.90002610572666
  H   -2.77653363490851   -0.31376940128855   -0.25498182290822
  O   -0.98892275847819   -1.92568824489301    1.84485876279323
  H   -0.69810629932840   -2.75461051775731    1.37864905195396
  H   -1.64338079102525   -2.26028055613129    2.49525262846981
  O    2.16428633912376    2.21994030834952   -6.31316393577594
  H    2.48601745221962    1.26813665771273   -6.30120786323069
  H    2.39751161447359    2.57399117384207   -7.18290062992492
  O   -0.42685143460364   -4.13060178522182    0.44850531040617
  H   -0.22711934292191   -4.94398942589581    0.92943084174310
  H   -1.31478969569552   -4.27453083922250    0.01437943321908
  O   -4.69971233382637   -3.07141033938447    0.74448949234652
  H   -4.35232626174834   -3.17622843158472    1.65313627058747
  H   -4.36129838806704   -2.18112148975323    0.50940269663570
```

Figure S9: Three optimized coordinates for K-[2.2.2] complexes with 16 explicit water molecules

```
111
Coordinates 1 from ORCA-job rb-crypt222-b3lyp-opt
  Rb  -0.03667768276628   0.12978837007053   -0.23223914009113
  N   1.05881302425399   -2.21165960001761   1.28058136317990
  N   -1.39003969481819   2.54765239211539   -1.53398706756327
  C   2.47458772256862   -1.89233658593157   1.46385030425375
  C   2.78527026860498   -0.44735678199224   1.84059763237457
  H   3.00146781906747   -2.10904192257391   0.52379772271403
  H   2.93105368290708   -2.54144634829669   2.24397118753160
  O   2.71158636692594   0.40741139720846   0.70200612590735
  H   3.80851509722573   -0.40438575086170   2.25990569303012
  H   2.09021468212776   -0.07238855551106   2.61125666251700
  C   2.93824296839170   1.78167502109611   1.00605999630301
  C   2.74104606159463   2.63247284305558   -0.22945339232311
  H   3.97374722040369   1.92034723836805   1.37399093180845
  H   2.22398660980424   2.08597377075454   1.78634944135027
  O   1.41819145712081   2.46128077096690   -0.71036501046517
  H   3.47478559345186   2.37130121236098   -1.01194850919872
  H   2.91359275957104   3.68744609853081   0.06505266574919
  C   1.00018007426077   3.42976470562326   -1.65007114885117
  C   -0.27162855370579   3.00129738248726   -2.36774834705723
  H   1.75980996140775   3.56668549257578   -2.44160793315832
  H   0.87498088733201   4.40607100492013   -1.14006437137315
  H   -0.01998266676490   2.17389693258524   -3.04603936559133
  H   -0.55766634017909   3.85237882367696   -3.02030135620707
  C   -2.53341326613625   2.14323704162680   -2.35643260622135
  C   -3.07005587926395   0.74287764588253   -2.07439696037190
  H   -2.24933980925515   2.21388510277520   -3.41638133530716
  H   -3.38571080012856   2.83777631976622   -2.23102964575258
  O   -2.04347394126587   -0.23103978638171   -2.26821114410241
  H   -3.90388603043863   0.54707798098498   -2.77511635703435
  H   -3.46411313710393   0.65568380121674   -1.05310849365243
  C   -2.50919212979704   -1.57512452886514   -2.33684641094143
  C   -1.33107612141040   -2.52725488466181   -2.32391777750514
  H   -3.09647528584268   -1.71931304915345   -3.26291571884430
  H   -3.16411235386992   -1.78931495212459   -1.47234509570277
  O   -0.77968636286590   -2.58100106944247   -1.02606855763661
  H   -0.57953584207795   -2.18848011104683   -3.06349828275108
  H   -1.68214602131723   -3.52859250651576   -2.64412441986863
  C   0.47075831222956   -3.26316418856038   -0.94364329393777
  C   0.85612287238969   -3.45813959331142   0.51547748610905
  H   1.24002333151017   -2.68954135941403   -1.48907630769828
  H   0.38143334515903   -4.26092797697561   -1.41536653072239
  H   1.77496663681768   -4.07622176902166   0.53393566721294
  H   0.07880221674880   -4.06796776981054   1.00020502628105
  C   0.33587662115870   -2.24459693012389   2.55651818374172
  C   -1.17618270501029   -2.15272739123290   2.42863231569549
  H   0.65332330360720   -1.39824344998911   3.18212638875310
  H   0.56322302966541   -3.16298558621725   3.12982184901637
  O   -1.55011307538216   -0.77762891194643   2.24618512362621
  H   -1.63646504190189   -2.52824423885166   3.35839343360399
  H   -1.55557880417514   -2.76201296253630   1.59652590358166
  C   -2.89811050160431   -0.57859842620621   1.87842819214131
  C   -3.21764883937206   0.90288937916879   1.87477875475128
  H   -3.58367449711246   -1.08915393436459   2.58141658250715
  H   -3.07854321866213   -1.00311284526756   0.87254430579169
  O   -2.31836810007144   1.57633451095450   1.00583182144051
  H   -3.13195269986291   1.31894869165465   2.89841530327661
  H   -4.25551376702817   1.03929768877363   1.52278539896952
  C   -2.77256839464361   2.83764274275271   0.51646449380408
  C   -1.73420893130158   3.42664831354006   -0.42905044474239
  H   -3.74470351822921   2.69275630133746   0.01877410929581
  H   -2.92804409459992   3.54000116024845   1.35816608793651
  H   -2.13990752370273   4.40511855744213   -0.77976553231173
  H   -0.82217706482477   3.64004919274948   0.14718861756375
  O   -0.24612732313579   2.57442976070909   5.13309933933184
  H   0.54144379744175   2.95668597494268   5.54878936483878
  H   -0.99535887651510   2.98650510674850   5.58822960777473
  O   -0.95913280947408   0.11759722370749   -4.74727335980164
  H   -1.40781458259657   0.09202973882177   -3.88130603523879
  H   -1.10410519874979   1.03126751015909   -5.09835167292715
  O   -0.68164423850112   -2.63593191624466   6.04310314432690
  H   -1.53631743945660   -2.69937597452161   6.49075751470252
  H   -0.67946815745428   -1.73186353169973   5.64559726467642
  O   -1.20757207351738   2.71077950703173   -5.47697056993606
  H   -0.27154231366433   3.03987405616886   -5.43149598459306
  H   -1.49948642946413   2.89447078846540   -6.37981926786110
  O   -0.16514636994403   -4.89226957706977   4.66726703948430
  H   0.75490618283625   -5.11086594192486   4.86140104296499
  H   -0.34189023752481   -4.05991346442153   5.17413228165203
  O   1.30388471343380   3.56620465448781   -5.22217396282985
  H   1.61948016594053   4.41374536493480   -5.56041032228064
  H   2.12214677551776   3.04559685587343   -5.00347269309378
  O   3.29951316714170   1.98261629578047   -4.49634898450489
  H   3.91808433635999   2.05449731278782   -3.73368858993523
  H   2.60272964516789   1.33366296508586   -4.21127098988186
  O   -1.37031809732013   -5.11876985969160   2.20650798561629
  H   -1.65463829171230   -6.03446031012157   2.09431713911918
  H   -0.93442909829598   -5.10264636474680   3.08954095199819
  O   3.79054119531066   -0.62025303814107   -5.42080353402901
  H   2.86146745158243   -0.65637918848788   -5.09825190232915
  H   3.89682674446328   0.34768731707062   -5.51635437561152
  O   -0.90166238171178   -0.18720045122589   4.87506073755601
  H   -0.48581883797555   0.67399985757622   5.05094794941069
  H   -1.09212647586119   -0.19175485910892   3.91445282572061
  O   -5.68643574061926   1.58774155659739   -0.71852299341526
  H   -6.11846807316858   0.85950660784780   -1.18603056673359
  H   -6.36993343698034   2.27140602108926   -0.67044108273942
  O   1.55355897262576   0.07265336587897   -3.99497594369527
  H   1.69971765773501   -0.27226324286940   -3.08485737492045
  H   0.58821481645068   0.04588270921078   -4.26251973496209
  O   4.94045377424552   -0.86997008098440   -3.11896327472330
  H   5.60656254744467   -1.57095070975237   -3.11191541412905
  H   4.55836702550690   -0.84256505534212   -4.06316864000886
  O   0.08881614949888   1.86997240368404   2.37380233385866
  H   -0.78180664750261   1.79818978090784   1.93806675577925
  H   -0.09869093948165   2.21585083729669   3.26208418018001
  O   5.09076303722575   1.72769668649331   -2.40051849047976
  H   5.94514905386204   2.12233581233869   -2.62282279812737
  H   5.18759855565706   0.76582221370339   -2.60841997803153
  O   2.58628582255854   -0.82006059779563   -1.70921991340306
  H   3.45985276120073   -0.96686808383908   -2.13867599910416
  H   2.77594049160620   -0.30201015747543   -0.89802722449903
```

```
111
Coordinates 2 from ORCA-job rb-crypt222-b3lyp-opt
  Rb  0.26343970715885   -0.29252189521471   -0.07710375148822
  N   1.90726040982527   2.19417539464366   0.33389832493742
  N   -1.56008853943729   -2.74570216563178   -0.48832868914833
  C   2.88860372814901   2.05704901032498   -0.74594044902290
  C   2.31376310198356   2.04151695479901   -2.15450849604305
  H   3.42719961940704   1.11211097127331   -0.59100420704081
  H   3.63999483288380   2.88006760363161   -0.70811954765621
  O   1.28862510245788   1.06174923359576   -2.25178158858586
  H   3.14398055501710   1.79212331864334   -2.84383419276864
  H   1.90603772003027   3.02199441826256   -2.45366163923901
  C   0.75322125551225   0.91393824968756   -3.54994915375186
  C   -0.61651259778843   0.28222655443205   -3.45819950471415
  H   1.42761058159216   0.29506968757105   -4.17229594024207
  H   0.61942167892703   1.89255510926751   -4.03531737638740
  O   -0.52795712962964   -0.99441931636905   -2.82343735569840
  H   -1.03933613110229   0.17822187886881   -4.47351141414004
  H   -1.29271000469640   0.93157364408142   -2.87873516104328
  C   -1.75608212100696   -1.71393604048692   -2.78794770737351
  C   -1.60694334367680   -2.96864616786848   -1.94273794162377
  H   -2.03590770494086   -2.01353291759566   -3.81674787832493
  H   -2.55075150338967   -1.04858767372416   -2.41042447368336
  H   -0.68170801615863   -3.47761874013053   -2.24811290396675
  H   -2.43329124591474   -3.66102113225347   -2.21165865283640
  C   -0.89870604517153   -3.87922196712715   0.16599668346913
  C   -0.45424916503657   -3.66520379454694   1.60419587878501
  H   -0.01041783469101   -4.14859033414786   -0.42606596121682
  H   -1.56216435742263   -4.77347326021913   0.16801948037079
  O   0.66863489635482   -2.78307150472777   1.65742895334605
  H   -0.16449223041250   -4.64512016031304   2.03115756332421
  H   -1.26029770008281   -3.26496679330273   2.24035403941803
  C   0.97386748497257   -2.30919661528451   2.97000992110919
  C   2.17326702236859   -1.38635208305624   2.91971795966046
  H   1.21775144978935   -3.16391818672523   3.63111522615188
  H   0.09734923289645   -1.78771011510378   3.39085899703550
  O   1.81733577382670   -0.12261110256621   2.37824890659338
  H   2.96623051458323   -1.84432392292803   2.30445381416928
  H   2.57027088015421   -1.25358537383157   3.94430401748163
  C   2.96995035980931   0.66412537007315   2.01955611752352
  C   2.54173165906303   2.07214228237373   1.63716607474607
  H   3.48962385129891   0.15352500679960   1.19327582052793
  H   3.64010633823287   0.71994838618239   2.89425430862275
  H   3.44242801772489   2.72615879168158   1.71001389392683
  H   1.84459149205637   2.42319713563800   2.41254813503517
  C   1.07268609340193   3.38975887417414   0.22535200602995
  C   -0.24210533383099   3.30621307244503   0.97493420764824
  H   0.83797738363441   3.57112441404023   -0.83026590056247
  H   1.61154856041236   4.29417567179159   0.58935463209729
  O   -1.07799452955037   2.30158753333541   0.39915412901993
  H   -0.73823429307013   4.28467114133520   0.87782943409216
  H   -0.10270439593254   3.08775952654344   2.04882577915497
  C   -2.40620669361318   2.30342769218940   0.88533438267569
  C   -2.74822577928012   0.97943342974147   1.52972957716054
  H   -3.09619457819892   2.52294711478903   0.05289573527890
  H   -2.54638715935476   3.07944849894933   1.65525510920766
  O   -2.68878865995324   -0.07694450942925   0.56915966890790
  H   -3.76591991531762   1.02962402630011   1.96440538585707
  H   -2.04367071757380   0.76581892681227   2.34479486817424
  C   -2.94926275140958   -1.35522204283877   1.13564960959830
  C   -2.88341063460825   -2.44502312815522   0.07257533002479
  H   -2.24804612554089   -1.52161761171051   1.97007141465586
  H   -3.96649438445050   -1.35960453658566   1.57580436103120
  H   -3.33146998004280   -3.35806992770259   0.52007296964969
  H   -3.56960948363508   -2.14696835649516   -0.73349019610496
  O   0.66471809251434   -5.70280848237836   -3.78016134143382
  H   0.80730607447753   -6.64178895674707   -3.95378300132931
  H   1.13160784101635   -5.50415857305280   -2.93198690055775
  O   -3.89411343952763   0.73938999670667   -1.72635436017727
  H   -4.65132183248441   0.12849018027085   -1.81881439056856
  H   -3.43941572653287   0.43158424955326   -0.90974676701792
  O   -3.39511708558565   3.17738570825582   -2.57792641539730
  H   -3.60138876060986   2.24627625553569   -2.27493956816338
  H   -4.25057981297326   3.62434040086554   -2.63757254000917
  O   0.84032924023479   1.15505148074700   4.61092309550196
  H   1.05232056346236   0.75502331425890   3.73832800295817
  H   1.72195009485433   1.28365582852970   5.01609019740178
  O   -1.39484230222435   3.14512345348072   -4.42769320852378
  H   -1.64465817830202   3.61936880262237   -5.23186063212300
  H   -2.18291598633207   3.19170367699834   -3.84362217415693
  O   -1.61815601855573   4.91495055975348   -1.24317608401040
  H   -2.18299398051186   4.22151549538555   -1.64413601458018
  H   -2.05216339161078   5.74535645487611   -1.48264587351312
  O   3.01979752172156   -3.78897538426020   0.66176722119477
  H   2.15770051801907   -3.50105463617096   1.04602956156062
  H   3.49301931258996   -4.26801185842070   1.35474602406352
  O   1.89892671582907   -2.25225130551637   -3.05677106564448
  H   1.94439310052192   -2.68407851066272   -3.95241734945259
  H   1.01222812938283   -1.83044779262066   -3.02864609456128
  O   3.01738826512189   -1.25958501139866   -0.72505728784412
  H   2.81312136175982   -1.48284311053142   -1.65725961943711
  H   3.27990189115480   -2.10732037829613   -0.32793461170941
  O   0.56200354860779   4.64901751102200   -3.02843102427847
  H   -0.05809662754825   4.88234260730978   -2.31198801889714
  H   -0.01810843566784   4.11936683702184   -3.61034628139963
  O   1.77799233554498   -4.56716448758298   -1.66919675501196
  H   2.36782662606554   -4.51840936956451   -0.89472931411186
  H   1.86399708155669   -3.69032263584011   -2.12244449728630
  O   -1.49039831546263   -0.44361181818928   4.38217170499588
  H   -0.64354778866988   -0.19587061588579   4.79442609359443
  H   -1.90595587173584   0.43808387086796   4.32177723433931
  O   -1.56769973432902   2.39593333029101   4.13660136254050
  H   -1.87439894232030   2.98176452296116   4.84156806374687
  H   -0.64177690194975   2.16886853273458   4.37934323700074
  O   1.65615638674134   -3.69381890560590   -5.28577722419441
  H   1.25551755041828   -4.49040142794930   -4.85099758095495
  H   2.44471108655230   -4.02611974959259   -5.73539986304077
  O   3.55517267181585   1.27912298259388   5.25502621199252
  H   3.99687831011206   2.13513679094488   5.15413856710206
  H   3.95382056883990   0.88973477703821   6.04715827941024
  O   -5.76076044208477   -1.31236444659049   -1.58770418070745
  H   -6.05394183580049   -1.82071742040178   -2.35779071884459
  H   -6.54560169569894   -1.24013029156940   -1.02537673230027
```

```
111
Coordinates 3 from ORCA-job rb-crypt222-b3lyp-opt
  Rb  0.15367193205196   0.13700876496462   0.30672178703677
  N   -2.78972926458550   0.81691574873927   -0.12159983319933
  N   3.01830484969586   -0.83299065485543   1.01435696659483
  C   -2.91180638225646   0.68193320079317   -1.56856318584505
  C   -2.49936041415313   -0.66792500604991   -2.15533751586832
  H   -2.30931251805741   1.46966969473103   -2.03890911502741
  H   -3.96446681454882   0.85995480993744   -1.89775903507585
  O   -1.16526473458286   -1.00537420578919   -1.82131570901905
  H   -2.61223179134675   -0.58805772147266   -3.25539041574933
  H   -3.16890858863649   -1.48810293413958   -1.84801132487642
  C   -0.52762925285856   -1.92286006361176   -2.69894974107736
  C   0.58844174945332   -2.66012404670862   -1.99064756923714
  H   -0.13567842377209   -1.38531621117612   -3.58105614725486
  H   -1.23713532251950   -2.69458090116256   -3.04002065433557
  O   1.56773083645355   -1.76706210651795   -1.46326744213312
  H   1.05446213898213   -3.34782931999004   -2.72026848334689
  H   0.19262455285373   -3.27638938438284   -1.16994090775110
  C   2.69617211054088   -2.43665229540699   -0.90841085968664
  C   3.58917318350334   -1.43087742438039   -0.20106738660176
  H   3.27866898398291   -2.91063663542126   -1.72321369342888
  H   2.36703655379511   -3.25170483428550   -0.24437480490557
  H   3.80601229859330   -0.62042136266573   -0.91074331438472
  H   4.55516296606186   -1.93935002524915   0.01497745327813
  C   3.75373179222532   0.37793589645154   1.39520945809758
  C   2.96273321356399   1.51256264452191   2.03623178910481
  H   4.21133278750248   0.79913335713862   0.48753983477140
  H   4.59167494570337   0.12955767423472   2.08221250326633
  O   2.07326760670317   2.09907242348067   1.10629455356559
  H   3.70075039915573   2.26673471659441   2.37704296891330
  H   2.40807017466551   1.18923394904754   2.93461098382358
  C   1.47565676570635   3.28788799014610   1.59869053011923
  C   0.30958608199588   3.72393947258408   0.74402985545934
  H   2.22346739604054   4.10696323697894   1.60785035413287
  H   1.11313941093999   3.13357802785233   2.63105307422499
  O   -0.75098167752737   2.79241347119768   0.85210762950894
  H   0.60673936283497   3.85484835907935   -0.31069351741346
  H   -0.02130334096879   4.71652783680087   1.11275187029808
  C   -1.88252240818846   3.16467399065353   0.08685812073903
  C   -3.02731038667786   2.18995300533014   0.31656374023972
  H   -1.61057912338583   3.23535090270038   -0.98051206602479
  H   -2.23089277367143   4.16989453526856   0.40135154208681
  H   -3.93200810240603   2.61285891996223   -0.17637973772814
  H   -3.23339213228538   2.18123012805800   1.39591569641454
  C   -3.60698435608592   -0.15189608309897   0.59643004884314
  C   -3.29027869604744   -0.30704421690697   2.07420416985888
  H   -3.45859605644830   -1.13833176051514   0.14504742278486
  H   -4.69458716415264   0.08369553666597   0.51263795774583
  O   -1.91631708444877   -0.57936022897530   2.26074516640197
  H   -3.90262243470682   -1.14873876476486   2.44722960030658
  H   -3.56958215191013   0.58902581867381   2.66220011120326
  C   -1.59056957214562   -0.97065689197022   3.57715356583442
  C   -0.12290201058736   -0.73256761642231   3.83319676882420
  H   -1.85237228812633   -2.03631570163502   3.73082686903092
  H   -2.14078785364951   -0.37021603814374   4.32268183508302
  O   0.67712592008302   -1.38674584472696   2.85652436629810
  H   0.11869716410251   -1.10292713369935   4.84276027693673
  H   0.08892354589672   0.34917534445985   3.81101061835049
  C   2.04045985156643   -1.51933629026182   3.25999918171462
  C   2.93418927144465   -1.83482329643699   2.07721885130822
  H   2.35328476702390   -0.60487878479626   3.78832077101011
  H   2.12125640785901   -2.35916122081696   3.97438548737760
  H   3.94591474278942   -2.05480662752064   2.49061770146160
  H   2.57896919306117   -2.77785228934557   1.64230036051106
  O   0.38304166695949   1.82622561345598   -2.17153517915664
  H   0.41342196485169   2.80709904106656   -2.29370680985549
  H   -0.21483270765920   1.51937581458258   -2.88352878729600
  O   -0.08820406070752   -5.54574869122527   -0.16694554900778
  H   -0.31035283986292   -4.76590507183465   0.38410499736469
  H   0.87332163639846   -5.65298849244228   0.00442377055575
  O   1.07765658493340   -4.80943406517856   3.13456193569041
  H   0.70648667697726   -5.57805575648350   3.58875800546721
  H   0.31393811072645   -4.39767498624608   2.66177204715758
  O   -0.63189355226250   -3.45224538758037   1.54174480194777
  H   -0.23494026514118   -2.61978988643320   1.87410759436112
  H   -1.60806082316223   -3.31180939307827   1.41570502122274
  O   -1.13842765961986   -5.25802932101004   -2.55456378212891
  H   -1.24038973853219   -6.12541516708389   -2.96820890835168
  H   -0.67760359475151   -5.42928210256556   -1.67999013418566
  O   -0.80019276295683   0.93235274807720   6.21054449194977
  H   -1.24316383657111   1.10328163621263   7.05215222516879
  H   -0.79939992475109   1.79161212994105   5.72856883859232
  O   0.20370385773942   4.51985700005938   -2.65028897164251
  H   0.83570299795948   4.83737996151599   -3.30941138544431
  H   -0.64659980082281   4.41189643613326   -3.14549765235996
  O   -3.23180554434804   -3.36967577811611   0.96699775241397
  H   -3.74488566741475   -4.06435947709976   1.40040192082316
  H   -3.26119366238533   -3.59058481446732   -0.00241496275111
  O   2.42777113262399   -5.32503598065710   0.84631593230828
  H   2.05346682269237   -5.20909163000640   1.75645427236485
  H   3.20843447428876   -5.88529467440792   0.94602593969258
  O   -2.01506728924691   3.70965426876054   -3.93850696413574
  H   -2.53132733632726   4.13895844242161   -4.63282786547562
  H   -1.68123720305982   2.86806026167515   -4.32392073357203
  O   -1.03291508507118   1.23990732921999   -4.54334140691771
  H   -0.20887669845353   0.79781731467677   -4.91288396518841
  H   -1.71020284834968   0.55048732880900   -4.58091896753817
  O   0.06704838279960   3.02091329259728   4.75675968853929
  H   0.93223846809432   2.62657958917184   5.00927193619190
  H   0.14670410408094   3.97273118763780   4.90190749567035
  O   -3.22081607368331   -3.89936904217699   -1.67303441556772
  H   -4.00931423970947   -4.12389999021307   -2.18388771037851
  H   -2.48345107819357   -4.46312540302891   -2.04570146513433
  O   1.88185789530249   1.18904549964074   5.63068988654347
  H   1.03651132583669   0.88415675679660   6.03516896632004
  H   2.50590137966153   1.26845723620067   6.36496566357368
  O   1.11146150672087   -0.13219145487349   -5.15848017799327
  H   1.65663905632056   -0.07186830673474   -5.95421384995250
  H   1.72940205698259   0.04599927546231   -4.38265663865566
  O   2.46603982129060   0.34533480879381   -2.95606202768357
  H   2.18711332494257   -0.45293300727479   -2.45840457058432
  H   1.84497120876576   1.02980937356540   -2.60289968555275
```

Figure S10: Three optimized coordinates for Rb-[2.2.2] complexes with 16 explicit water molecules

```
111
Coordinates 1 from ORCA-job ca-crypt222-b3lyp-opt
  Ca  -0.42528143406374      0.23262602319667     -0.35867097663057
  N   -2.99855477963597      1.46733345507927     -0.39258645818917
  N   2.33632835597584     -0.58970039761743     -0.36284157509070
  C   -2.83040382926837      2.90731570302100     -0.14051491980405
  C   -1.58024245985330      3.23613368581179      0.67014349989551
  H   -3.72034775330674      3.34050075971901      0.35891318801406
  H   -2.74436859361013      3.40904014947686     -1.11371910885621
  O   -0.41757245966097      2.70783191031379      0.04999456147438
  H   -1.60539221670221      2.81894041200864      1.68064601525206
  H   -1.48452029075638      4.33062596046612      0.77108036299992
  C   0.15265485314950      3.56953910132440     -0.93536322739445
  C   1.40548680504484      2.91040532780479     -1.43902962155778
  H   0.41162566811967      4.53459520976010     -0.46960830415205
  H   -0.55165007387755      3.70980049745374     -1.77132919887786
  O   1.07516437551688      1.57466925233388     -1.81300210061866
  H   2.19257818600475      2.90229834453932     -0.66405192410350
  H   1.77575464524343      3.45262597535323     -2.32449165253742
  C   2.17717970359489      0.87303350318046     -2.39101368630082
  C   3.06735263416430      0.27499708842159     -1.30725612171110
  H   2.75754908762157      1.56248594230787     -3.02485568712714
  H   1.74045743505234      0.11783254709534     -3.04910678958615
  H   3.54319856586364      1.08745105812873     -0.74163871372403
  H   3.89645888535692     -0.27888817999431     -1.79211972576192
  C   2.80556148877557     -0.42537118005657      1.02121426583722
  C   2.15315971224945      0.77126554879715      1.68723524729498
  H   3.90669322991820     -0.31431201442346      1.07510007385077
  H   2.55453207359451     -1.32529356309898      1.59511217474129
  O   0.73969498956579      0.61757568867130      1.76523649073317
  H   2.32235493038171      1.68637416302230      1.10829382269842
  H   2.57133043031434      0.92989864557412      2.69325503953602
  C   0.21633943586416     -0.00694425782378      2.93469986462926
  C   -1.18032927240429      0.52078648368798      3.15678817714872
  H   0.83538860189703      0.22403472940030      3.81281860844130
  H   0.20408977844397     -1.09761167000595      2.80775418601657
  O   -1.90863016276910      0.38676974947930      1.94588798654748
  H   -1.13214157848661      1.58381505607817      3.45330760137909
  H   -1.66830917136944     -0.05361856803155      3.96731335521073
  C   -3.23832111906683      0.85573948173045      2.01218120467394
  C   -3.82857229746980      0.80279220220230      0.61856992072773
  H   -3.26533759488698      1.87828223533359      2.43440258977263
  H   -3.84289196541176      0.22288416300146      2.68904962911063
  H   -4.84795072522870      1.24152970496811      0.65280414882364
  H   -3.93229121776000     -0.25468581957831      0.34045017000740
  C   -3.53393883908555      1.23883515066809     -1.74227564116205
  C   -3.42199817403067     -0.19867214273386     -2.19096392760143
  H   -2.95431383296996      1.85142839531886     -2.44687508028379
  H   -4.59990128069645      1.54329923662364     -1.81628691033670
  O   -2.04985772152899     -0.58273080217680     -2.15951738750201
  H   -3.79945711705960     -0.26694489091679     -3.22667918235314
  H   -4.01076714123403     -0.89916368304042     -1.57270064317535
  C   -1.80663721718293     -1.84190061499408     -2.77824985366723
  C   -0.37090447753910     -1.89258706611684     -3.23835600312540
  H   -2.47454921334719     -1.97121395588027     -3.64825877611043
  H   -2.01024837435979     -2.65336476027053     -2.05670663573022
  O   0.44115666078530     -1.61703505674896     -2.11369161887952
  H   -0.17718480820080     -1.15313468317216     -4.03501568688997
  H   -0.15243522779265     -2.89778395093288     -3.64204359097313
  C   1.71320794331508     -2.24622924975319     -2.10581689053676
  C   2.35816599754959     -2.00074704484507     -0.75709189782291
  H   1.59916838969511     -3.33586753486988     -2.25738990398383
  H   2.32600800296207     -1.87775587103738     -2.94523824990214
  H   1.82340270182874     -2.57189727114744      0.01272503315954
  H   3.39624830979237     -2.39538742832494     -0.80084904587638
  O   -0.83294550325824     -1.91510706713803      0.56627241444126
  H   -0.25352838526935     -2.42575445249889      1.17751346725348
  H   -1.75293241709792     -2.21899117459297      0.69084387360340
  O   0.92214826024586     -3.19336953651512      2.23760879480376
  H   1.57260548686494     -2.83787234823563      2.89830007113655
  H   1.16996114261653     -4.11819177396952      2.10724942565100
  O   2.11706875830897     -0.09542886922204      5.59848069051107
  H   1.52302623925279     -0.25009168954649      6.34533559448180
  H   2.21763955052451      0.88150289226098      5.53328718025024
  O   2.19192372378132      2.62653978493689      5.24175927292858
  H   2.41716245044962      3.19466479510483      5.99309246723323
  H   1.34171570636924      2.99296081979843      4.86259404460175
  O   2.79224607197730     -2.11028192785692      3.87702967583217
  H   3.47795449244379     -2.64090533292316      4.30496616962645
  H   2.57474512446629     -1.39462886685090      4.52085146783084
  O   0.92516113022170      2.81851246374049     -4.61163452866840
  H   1.20874716855965      3.40600649967963     -5.32500111917271
  H   0.97070247043135      1.91196039146105     -5.00217405954773
  O   3.59670417736009      3.53382906890988      3.02622240876768
  H   3.20504800471975      3.10246453666672      3.81842483403946
  H   4.56841756912856      3.61632095042951      3.20098058283757
  O   6.24046656171255      3.34942964182176      2.87870397930211
  H   6.92475947015841      2.90426553545724      3.39648808629102
  H   6.15019113362384      2.84554198392379      2.04965419709168
  O   0.98073605552866      0.29663970241526     -5.63874466279205
  H   1.64890683904258     -0.40918876759466     -5.49539547261629
  H   0.37499583050516     -0.11763700173691     -6.27375962386574
  O   4.59916450844456      2.62234676576325      0.61308819190876
  H   4.07349996915672      2.88882391526870      1.39972694925741
  H   4.75037757354323      3.44867102811544      0.13242410703833
  O   -3.58919739017458     -2.61277919135919      0.46723212085040
  H   -4.12874658530558     -2.76234149935307      1.25790362490096
  H   -3.81186262806030     -3.35152177533476     -0.11879130312221
  O   2.22948564264281     -2.11617390177082     -5.43473794634951
  H   3.08275415722714     -2.40422869742265     -5.78940618744103
  H   1.57020980679935     -2.35925539176310     -6.11558016984506
  O   0.09653413033594      3.60906763690028      3.93502941360470
  H   0.50028974129036      4.09315927324773      3.16277032013272
  H   -0.54247819437583      4.22046940161954      4.32671414196665
  O   0.20177429144049     -1.97960289282330     -7.32111659182833
  H   0.50865083897161     -1.86563314493340     -8.23426831866053
  H   -0.60434987945807     -2.51153874075049     -7.39980296579907
  O   1.47870745414340      4.81416931905845      1.96200963723996
  H   2.34832663531023      4.47337521185256      2.29368881055578
  H   1.55083282217775      5.77794697742564      2.01510843470844
  O   -1.63682166385727      3.03376966700087     -3.60801489814275
  H   -0.72945368895140      2.95326776138796     -3.98969312388972
  H   -2.03531411099369      3.76926713618333     -4.09300397897808
```

```
111
Coordinates 2 from ORCA-job ca-crypt222-b3lyp-opt
  Ca  -0.36960333791993     -0.00013528813287     -0.70333938360707
  N   -0.95389420178795     -0.17977075377811     -3.40539192428215
  N   0.54211720858350      0.80832857620481      2.12415785057663
  C   -0.10013205162760     -1.22826045602462     -3.99373971340408
  C   1.28725273370315     -1.37159777303759     -3.38376980681860
  H   0.00014329937599     -1.10428746735245     -5.09126653129722
  H   -0.59928423050592     -2.18979544116890     -3.81507798908593
  O   1.15103533878029     -1.46606936385792     -1.97883547609805
  H   1.97534453383169     -0.55142134240124     -3.64015254615313
  H   1.72479220845326     -2.30540162707130     -3.77867327064757
  C   2.25143879792389     -2.04393232267812     -1.28522334835282
  C   1.75858531834711     -2.50268812694366      0.06826561852344
  H   3.05740757944156     -1.29653241610532     -1.17680791221530
  H   2.62321181322001     -2.92557005982076     -1.83286413342431
  O   1.15947243092189     -1.39830666009343      0.71512640571513
  H   2.60836187266278     -2.88058095985664      0.66410328106872
  H   1.02495532837087     -3.31268567442042     -0.04790205366400
  C   0.57428507023829     -1.65940254464875      1.98636332003493
  C   0.83832002973024     -0.43652708100884      2.85038198855542
  H   1.02928386047305     -2.55095923970121      2.43649125386284
  H   -0.50371164220661     -1.84432994863863      1.86327275183290
  H   1.89551464265306     -0.45025874619817      3.15028896443986
  H   0.24791252475478     -0.51101525516597      3.77880941919993
  C   1.70158592618510      1.68758256930817      2.01516586313016
  C   2.81030610915715      1.13198230639922      1.13135001365672
  H   2.12999701627360      1.92415347100862      3.01470069826590
  H   1.35837453949108      2.64432078360933      1.59277495639026
  O   2.44028477581918      1.07774694854532     -0.23648034044494
  H   3.07946153633347      0.11191349746187      1.43459522691099
  H   3.70859639734466      1.76543054064271      1.24903585971351
  C   2.66268529074069      2.29217762254916     -0.92954790131642
  C   2.42578736178068      2.06237798884549     -2.39722954048110
  H   3.70435827860530      2.63832502602654     -0.78549493613238
  H   1.98141889841697      3.08591318060926     -0.58185821700435
  O   1.10372189263907      1.59966212550738     -2.57438352812781
  H   3.14670482515463      1.32393507734197     -2.80018488396092
  H   2.57679923499830      3.01731191805826     -2.93271772109828
  C   0.65513230439500      1.67965238355352     -3.91247232423693
  C   -0.75934574478150      1.15553773924833     -3.98678599434777
  H   1.32886178134889      1.11283067741534     -4.58047914021244
  H   0.66053616523628      2.72861278512827     -4.25875005124800
  H   -1.07468172544450      1.17165612414688     -5.05255123569615
  H   -1.41025412091527      1.85289899404670     -3.44114713623558
  C   -2.36772344480557     -0.55834415143992     -3.55425009928958
  C   -3.30733899868309      0.21027148519109     -2.65248940196830
  H   -2.46246571667688     -1.62257917740459     -3.29824565819544
  H   -2.70234230493679     -0.42975107698011     -4.60529617691998
  O   -2.92881216298113     -0.03467479097726     -1.31478135958029
  H   -4.33572815313714     -0.15658081222597     -2.83068023612912
  H   -3.30798278336207      1.29720408410127     -2.85823350100087
  C   -3.88540046041692      0.38178797126835     -0.35849609266753
  C   -3.45319254381174     -0.13946225105100      0.99079354454747
  H   -4.88138538914180     -0.02968967574675     -0.61147793269296
  H   -3.94564673345307      1.48384178624999     -0.32211705480435
  O   -2.12216380516365      0.29096559306248      1.23987362120466
  H   -3.50057347694752     -1.24131203001784      1.03505997591216
  H   -4.13663767954911      0.26976431827669      1.75415102922787
  C   -1.88637526164527      0.69838971676561      2.58607344881308
  C   -0.61817478015895      1.51877131737642      2.64396098128402
  H   -2.70763648185123      1.34374383252650      2.93211642195446
  H   -1.84442646790597     -0.19408306835961      3.23319796881642
  H   -0.76296043879316      2.42296071862361      2.03709913486568
  H   -0.47559573272720      1.85195501738804      3.69563628833617
  O   -0.73699860915978     -5.48840424149381      2.18165542795106
  H   0.10595696175004     -5.59484407620826      1.68966029005837
  H   -1.34519895642416     -4.94534638580721      1.64061850592634
  O   -0.46605366455753     -4.18759440529467     -2.46472225954249
  H   0.33858283817339     -4.65691906355991     -2.12907891903465
  H   -1.09050187242963     -4.88635007520160     -2.70287950360117
  O   -1.17231179769978     -2.28811947865748     -0.65336250015597
  H   -0.92411105755083     -2.96381957256922     -1.32944897607815
  H   -1.80569646295648     -2.72524942128147     -0.05151102671260
  O   1.75647343373276     -5.29879217197311     -1.41300907271302
  H   2.26075470515188     -6.00208151264099     -1.84231010459712
  H   1.84652208536017     -5.44846037115706     -0.44235789605217
  O   -2.93233794112768      3.69824303283000      3.51015381109769
  H   -3.80105044767969      3.67949839063737      3.93480382752785
  H   -2.40460433303546      4.33494700199431      4.04828749019088
  O   -0.97795133663666      2.28775640611720     -0.72722610741892
  H   -0.47845306183824      3.03685149893997     -1.12051279409493
  H   -1.67079482419563      2.67667030810272     -0.14376513363844
  O   0.47919022443036      5.12835740226429     -4.44465256598748
  H   1.24931016934553      5.52633756618815     -4.87701153654418
  H   -0.27809402136539      5.41474904002283     -4.97599681628982
  O   3.99331036170046     -1.86265174528029      3.11687801864055
  H   4.42948643819960     -1.50301230312993      3.90434851316354
  H   4.72312067951699     -2.08150800778891      2.51821580850555
  O   -2.94285642161633      3.38568621673293      0.83381497454506
  H   -2.92137165038716      3.55942883908910      1.80919674422633
  H   -3.41454606675167      4.13600227531541      0.44922741876250
  O   -1.57810919214855      5.45663158394122      5.08798113514549
  H   -1.69483718278193      6.41590788652516      5.03445787835998
  H   -1.38980020165686      5.27977279949962      6.02049962475084
  O   -2.18218310300975     -2.62932097981026      3.68818631057683
  H   -2.85788901686579     -2.62187858920050      4.38040049388809
  H   -1.42347129741509     -3.14981981869746      4.06330873647206
  O   1.85735006195497     -5.65861219287847      1.31230571008951
  H   2.16946838881357     -5.04230171498056      2.04425903755810
  H   2.16366175082586     -6.53531189547859      1.58980720383567
  O   0.36338926048726      4.48884069663119     -1.72335156021803
  H   0.36166197966130      5.32005839303136     -1.23111199658121
  H   0.38971619906136      4.74869764251587     -2.67012133619795
  O   2.45521066097154     -4.19203077531548      3.38887701646848
  H   2.95229415677471     -3.35003027099870      3.41575217414264
  H   1.62293741970970     -4.08414290223913      3.90016140366673
  O   -0.14083785036389     -4.27757582187283      4.35915563032646
  H   -0.26145862364425     -4.86183104253551      5.12274058436377
  H   -0.39422058234628     -4.83176358339153      3.54322749188012
  O   -2.62435191750179     -3.65421255640584      1.25098587694736
  H   -2.57094090911548     -3.25955432694971      2.16552485233688
  H   -3.50794242740752     -4.04189827175923      1.17628678005562
```

```
111
Coordinates 3 from ORCA-job ca-crypt222-b3lyp-opt
  Ca  0.25490639709226      0.12542637038348      0.01172446337873
  N   1.43695676013959      1.24529101927623     -2.28950926980204
  N   -0.96799261946520     -1.41584549178381      2.01500181493765
  C   2.03408724136571      0.19118555747916     -3.13888307022248
  C   2.13419250401167     -1.14954490285499     -2.41533284129871
  H   3.04350250139480      0.46636009694034     -3.48784044836935
  H   1.41572077887541      0.07517110539446     -4.04123376657537
  O   0.91430864296887     -1.48963061526137     -1.76491076908133
  H   2.89554691371056     -1.13370518467880     -1.63042816684120
  H   2.40796384434366     -1.93908932032068     -3.13652090571652
  C   -0.15461137211563     -1.84441520052269     -2.63785406717305
  C   -1.27736191083844     -2.34684172974117     -1.77599005608048
  H   0.15869225001274     -2.62205537003802     -3.35416349197999
  H   -0.49843435357855     -0.97519321118413     -3.21924117319352
  O   -1.57937244721252     -1.30519195932533     -0.83907054432702
  H   -0.99665495626218     -3.26798659489564     -1.23816287692964
  H   -2.15935462284189     -2.55205314740657     -2.40161079192015
  C   -2.59601275815234     -1.64446198563890      0.10350560438349
  C   -1.99074177693328     -2.25431328380163      1.35957568515583
  H   -3.29900872822429     -2.35498227956983     -0.35643139606387
  H   -3.16172142440495     -0.72638363055749      0.28227440619831
  H   -1.51805435797959     -3.19578688728006      1.06220911390553
  H   -2.80073430893118     -2.52640467983862      2.06360701552560
  C   0.07320573814828     -2.24912272965591      2.64812562329431
  C   1.10983942563257     -2.72231691210300      1.64371633236142
  H   -0.36460392437444     -3.13363809726911      3.14677805423583
  H   0.56973054378006     -1.64602887135423      3.42275927764745
  O   1.78990135618413     -1.63088431610890      1.02087986855503
  H   0.64172666698595     -3.30788330834764      0.84056042267341
  H   1.84207493385962     -3.37693186449738      2.14938813442111
  C   2.83052999504806     -1.03647796490375      1.78326916546239
  C   3.64440949812285     -0.16727065157883      0.84803144098850
  H   3.48387626697317     -1.81407740645481      2.21827621635760
  H   2.40766835915696     -0.43465732622846      2.60350482374620
  O   2.75986810871274      0.63954658644329      0.08652684778123
  H   4.24929949061593     -0.79036142490299      0.16306914067520
  H   4.32965701080835      0.46967405545423      1.43501910501715
  C   3.44411484008549      1.47519757932119     -0.84050267802048
  C   2.41460002918009      2.16813276305749     -1.70612396135825
  H   4.13631606640151      0.85883111985016     -1.43751382578418
  H   4.02798614532520      2.23170114195735     -0.28876771354215
  H   2.94968766363731      2.74896631016633     -2.48811666065448
  H   1.87426807762308      2.89429727639575     -1.08044188682706
  C   0.38733410709787      1.96069981393408     -3.01944119789564
  C   -0.42049386963847      2.89513177941455     -2.15066884511994
  H   -0.29634751383373      1.21713376030432     -3.44591572448538
  H   0.79839420815502      2.54689728422920     -3.86839432363560
  O   -0.90701721443061      2.17462655438126     -1.01941994218834
  H   -1.27930016328561      3.26479468899207     -2.73292739858914
  H   0.16705653827872      3.76499765746447     -1.80618645303839
  C   -1.73360784409321      2.98808486270856     -0.19615449072778
  C   -2.63525368899231      2.10778429999136      0.62926871628164
  H   -2.36605606983452      3.63487957752132     -0.82762266258610
  H   -1.09325143465624      3.62477539940374      0.44384646505838
  O   -1.82065443591565      1.17372975059721      1.32449749946253
  H   -3.35054486181114      1.57017395011563     -0.01656497328982
  H   -3.19332513996402      2.73335981589872      1.34687041135542
  C   -2.47390677267794      0.52925041089875      2.40437742588943
  C   -1.53837270001589     -0.50119113641960      3.00330211272311
  H   -2.73963555127731      1.27046592848816      3.17606812831334
  H   -3.41695841372094      0.07145115085028      2.05914107768754
  H   -0.70435038041396      0.02293334561578      3.49029025571616
  H   -2.09577233965780     -1.05132678987226      3.79185813599150
  O   -0.74312304810987      3.24186602913560      3.44617252712890
  H   -0.47929801916428      3.25379653801512      4.37828215871524
  H   -1.71001015883652      3.43712854793433      3.45325391900932
  O   -0.99239038946873     -2.70257889502834     -5.81027727399669
  H   -0.90913950363857     -3.48114112720909     -6.37585443647269
  H   -1.89760428005331     -2.73166644109293     -5.43137983133843
  O   -3.42172470437209      2.10558582492316     -3.05704905041921
  H   -3.95068760817779      1.51177051893172     -2.46640544801360
  H   -4.07756344491526      2.62025119590413     -3.54789881843290
  O   -3.45627027775191      3.72644524491448      3.50760317714914
  H   -3.79281438161386      4.61265308379412      3.30502886962811
  H   -3.99214473624244      3.42401817074030      4.25639304467631
  O   -2.40357591866314      0.02577902614155     -4.49883160116034
  H   -1.60062120271940      0.18412729591200     -5.04725266677539
  H   -2.69405178324282      0.85958389531185     -4.06131322966866
  O   -0.08377357297238     -0.15912211176274     -5.84487714617085
  H   0.09579583879186      0.18491448047120     -6.73032686957092
  H   -0.29896389186462     -1.11772465321950     -5.96193212364949
  O   -3.54599943867539     -2.26680790805574     -4.66740302099170
  H   -3.17738265237648     -1.32432545889006     -4.61194333444535
  H   -4.17264002939164     -2.25200907140955     -5.40574468050633
  O   0.85210032179437      1.32642416657834      1.99604561040267
  H   1.72717658185637      1.77687546628255      2.09142845596659
  H   0.18776084107620      1.89779307517837      2.42303183435611
  O   3.12269403218340      2.80065214825338      2.17162798343587
  H   3.62377633748696      2.95622439237229      2.98400278250847
  H   2.57020816937098      3.60787256640372      2.04425839474429
  O   1.11457291310996      4.56864621171377      1.86204859969306
  H   0.39547379304354      4.25470017922743      2.45170171496995
  H   1.07020683117877      5.53435399215797      1.86305496781944
  O   -4.79284890722371     -2.22101292255835     -2.22645779568440
  H   -5.60128564735745     -2.75087188483089     -2.23794646540122
  H   -4.38594781939250     -2.33571525294997     -3.12267007475326
  O   -0.72897354168642     -5.07713646419273      0.11991152904936
  H   0.01037224925719     -5.63608503669843     -0.15110355360079
  H   -0.88503423840627     -5.30245625744507      1.06446134398745
  O   -4.01469274861367     -4.69910276343715      2.63318973342559
  H   -4.62386275588993     -4.80252802774760      3.37952293783289
  H   -4.44693566318414     -5.16036290190995      1.89896072055122
  O   -4.76724178556033      0.38454787118275     -1.44036203847770
  H   -4.79306105563064     -0.56078293979244     -1.74281009552816
  H   -5.66328802559237      0.57810188052884     -1.13263733700848
  O   5.26115036477342     -0.59832000160003     -2.74145105755559
  H   5.91484217165491     -0.04789687804096     -3.19586135714343
  H   5.64220128157237     -1.48706570699209     -2.78010246045599
  O   -1.32101484932602     -5.31304005358611      2.79941427634688
  H   -1.15726268489944     -6.09578924376249      3.34280312195961
  H   -2.29101791033126     -5.15846653832908      2.83731765200160
```

Figure S11: Three optimized coordinates for Ca-[2.2.2] complexes with 16 explicit water molecules

```
111
Coordinates 1 from ORCA-job sr-crypt222-b3lyp-opt
 Sr  0.06407934261372    0.29350756773926    0.11540106293607
 N  -2.01267480440141    2.15048208743447    0.86787171845327
 N   1.99679036059538   -1.91714819843429   -0.04151259418303
 C  -2.82345122710905    2.48325782749230   -0.31126301445833
 C  -3.17096755600831    1.33547985119116   -1.24459559970085
 H  -2.24637048313177    3.20581265917658   -0.90723378368536
 H  -3.76534761902196    2.99285151206340   -0.01691668303525
 O  -1.98486859205716    0.70211674860016   -1.68686385798212
 H  -3.70877439764739    1.75441075689902   -2.11402026407441
 H  -3.83417320239587    0.58945582056407   -0.77874577549342
 C  -2.24886542637675   -0.35267735560821   -2.60197687892594
 C  -0.95313637456503   -0.96158050422583   -3.06919534510917
 H  -2.79258018651107    0.04571512242656   -3.47676837151313
 H  -2.88350733038275   -1.12299201961380   -2.12822818748203
 O  -0.22562220355330   -1.44615608394874   -1.94587134051531
 H  -0.34771591609404   -0.21367006620981   -3.60713710621880
 H  -1.18135671875296   -1.80195897712659   -3.74488445029776
 C   0.97125242351127   -2.11968871881868   -2.32157223915157
 C   1.54613920949044   -2.82361983475837   -1.10810144020023
 H   1.67489413917689   -1.39718222418196   -2.77668184884167
 H   0.73309125786314   -2.88295685258273   -3.08232676676512
 H   2.36968280033929   -3.49018089908016   -1.43962236251331
 H   0.74556389984392   -3.46454225914031   -0.72494858274027
 C   3.31289394227648   -1.35261381424732   -0.37132103186391
 C   3.70166476622197   -0.13317760785975    0.43372328078502
 H   3.31117189222930   -1.05997900411331   -1.43129358021751
 H   4.10810669606555   -2.11863492227929   -0.23914572201193
 O   2.73044692970038    0.88654498709664    0.22360645067782
 H   4.67915395567616    0.21396906803070    0.05570531681621
 H   3.80151591556374   -0.33890606752567    1.51356955337772
 C   3.14437179676860    2.14163541987360    0.73463229786533
 C   2.14088959087771    3.19756899917465    0.34311608388832
 H   4.12978836694006    2.41249873896359    0.31186809403091
 H   3.24495929472159    2.08426558021532    1.83505302485907
 O   0.87239143970624    2.82381431704664    0.85836266849060
 H   2.08704147038549    3.30021190529904   -0.75405360945917
 H   2.45447287869766    4.16521004007748    0.77843966882303
 C  -0.13355517812951    3.79674417472360    0.64153627859487
 C  -1.37571872039655    3.37143411067711    1.39684764087037
 H  -0.31443521565911    3.91332465788938   -0.44340299606266
 H   0.20189682336097    4.77656283876498    1.02986350257282
 H  -2.09369568265216    4.21613854367369    1.42478845867513
 H  -1.07137568320429    3.17456847549087    2.43482843466654
 C  -2.74273114122270    1.48623929008776    1.96060462418783
 C  -3.29746102594087    0.10338689910855    1.64386944644317
 H  -3.58006896573272    2.11457152240577    2.33176955825032
 H  -2.02018298468500    1.37000410008584    2.77850137118967
 O  -2.34298966224085   -0.62322158846681    0.89411550901264
 H  -4.24890766760561    0.14952982959423    1.08480079033225
 H  -3.51438670279936   -0.39993505786341    2.60406491553985
 C  -2.51405440611215   -2.03446020563227    0.83932152552621
 C  -1.61712991843077   -2.70255086150506    1.85726679998202
 H  -2.21138181944418   -2.35487042849968   -0.16679774489168
 H  -3.56519861364803   -2.32386796771268    0.99175833819783
 O  -0.28795431663563   -2.23675388646547    1.63382713307779
 H  -1.67724403598712   -3.79428876824146    1.72428256683085
 H  -1.92180993046364   -2.45679573371292    2.89173362923572
 C   0.74471379471245   -3.21376778733923    1.71316782296580
 C   2.04997620515636   -2.58122150659744    1.26999230896974
 H   0.86419355436639   -3.55858993592373    2.75183161620909
 H   0.46454068890041   -4.07514649101559    1.08602675828023
 H   2.35340265217922   -1.83640843100465    2.01753335563894
 H   2.82983777230063   -3.37087094111840    1.30000485005137
 O  -3.20610554804842    2.25536421413966   -4.59850071309698
 H  -3.66521787535867    3.09433706317397   -4.45270154596240
 H  -3.36388150228857    2.04770605726762   -5.55149541711847
 O  -3.38048760730239    1.79394956240343   -7.26107615577272
 H  -3.85725198168306    1.09022322575654   -7.72418799479597
 H  -3.30553040494055    2.51011344645614   -7.90789712404140
 O  -3.71417009119227   -4.66498923708333   -0.25364941717150
 H  -4.01850615482158   -4.16416128270847   -1.05634481179499
 H  -4.32990311364681   -5.40146595433402   -0.14137016129482
 O  -0.53287342489400    2.29899436598760   -4.24418459270461
 H  -0.20093306652696    1.77021290908212   -4.98358776739604
 H  -1.52156299146482    2.32202283103017   -4.35234552547942
 O   0.21027591128117    0.21793253684233    2.67305778850332
 H   0.73219065766764    0.43931398071101    3.47317987138193
 H   0.06919684612696   -0.74848589061639    2.70866165293599
 O   0.76106870639482    1.49387584511670   -1.90308521120216
 H   0.12791648067414    1.72851287289026   -2.60962678641769
 H   1.63770557226080    1.44517978582869   -2.37630917622854
 O   5.35001764244609    1.07007888224260   -2.26212884209580
 H   5.79335168075272    0.34163726977067   -2.72266406461568
 H   6.03005067728091    1.75698061988482   -2.19501716643717
 O   2.85938164686951    1.52456600032699   -3.47346101914360
 H   2.67587781322115    2.46851551690384   -3.67787613915750
 H   3.75287673783490    1.48330320608541   -3.07877781445952
 O   1.64884168839398    3.95793944859425   -3.71361378383130
 H   0.77894449963472    3.58181902193449   -3.96371653393300
 H   1.79475571917971    4.70412927000337   -4.31012221565596
 O  -1.14355416903127   -4.87610488091373   -0.84897620538757
 H  -2.09612338424199   -4.90359706759266   -0.55073791073543
 H  -0.78952077215059   -5.75873073969944   -0.67022781669914
 O   1.70651933860385    0.24984946335088    4.95874874002404
 H   1.71610424748580    0.85405144748583    5.71422115023331
 H   2.64844466133405    0.16121490183558    4.62897098394210
 O   3.62288814242851   -2.92780769183615    4.00633773663324
 H   4.12577572993259   -3.55134978271467    4.54762249206171
 H   2.71433263037464   -2.89103364164472    4.39638573550492
 O   1.10562110241926   -2.38235544915314    4.83293153563577
 H   0.65640026310145   -2.78692537955134    5.58792515924231
 H   1.22432033286196   -1.42917010617554    5.06334518653770
 O   4.00627572212582   -0.32267430348228    3.84801548194434
 H   4.88777562409197   -0.01090351166742    4.09338310935905
 H   4.02557009449769   -1.31828913624830    3.91799284956941
 O  -1.68160530130405   -4.09604915630145   -3.39272952132345
 H  -1.36311964856671   -4.43279391039835   -2.51580885093044
 H  -1.55364519905242   -4.82635312756269   -4.01384134362039
 O  -4.05488911620335   -3.25731862811346   -2.48072167550852
 H  -3.25335422380562   -3.56880918903705   -2.97454286816752
 H  -4.78547474399521   -3.26835412928317   -3.11365858024017
```

```
111
Coordinates 2 from ORCA-job sr-crypt222-b3lyp-opt
 Sr -0.93439715117342   -0.60981657236369    0.43945046440131
 N   0.57860304150772    0.46515556376605   -1.78765530663820
 N  -2.01799922515913   -1.74852430612271    2.96100369915804
 C  -0.25542442486937    1.48158864391068   -2.44631654306369
 C  -1.08489751292077    2.37713567459553   -1.54244005425596
 H  -0.96244917655771    0.94888238635528   -3.09808352128818
 H   0.36058280565558    2.13412289891426   -3.09700183566587
 O  -1.94894335153032    1.59506465940490   -0.72534748866449
 H  -1.70029915862440    3.02421522365436   -2.19306498554179
 H  -0.46970834944506    3.03661115149952   -0.91228249847826
 C  -2.80826973004581    2.40768035866690    0.05514020665118
 C  -3.75473704830380    1.54897291181715    0.85478374995242
 H  -3.39910500153837    3.06880537441164   -0.60515463674619
 H  -2.20731839201387    3.04756524539048    0.73184455750173
 O  -3.00919325924345    0.72295481873492    1.73148659124559
 H  -4.36136995906197    0.92135337342666    0.18011823348961
 H  -4.42582191657637    2.21127876677840    1.43457651314389
 C  -3.83143226584657   -0.09973874130314    2.54871982960761
 C  -2.96458212714264   -0.80874057572137    3.57077259139688
 H  -4.39274748034372   -0.80893691524770    1.91165859755498
 H  -4.56977378838477    0.52533317142492    3.08499725050050
 H  -3.62225897366529   -1.31756944584624    4.30562869425327
 H  -2.41141365907079   -0.03609658648345    4.11830741825675
 C  -2.69116442792679   -3.01153319915795    2.65086858404098
 C  -1.90490934083587   -3.92858702520514    1.73903791273065
 H  -3.63649540151552   -2.78749309131558    2.13794899781220
 H  -2.93896016114452   -3.56648955343460    3.58224495498170
 O  -1.66884085734639   -3.25406787570982    0.51324966786097
 H  -2.50946347095582   -4.83155721500445    1.55114913778305
 H  -0.94629231218437   -4.25720261871436    2.18202903668652
 C  -1.20637345689271   -4.11372252875386   -0.51304095043012
 C  -1.25519856538911   -3.38732934986812   -1.83581865673853
 H  -1.84992613112499   -5.00945568504878   -0.56963748461229
 H  -0.17281096293509   -4.44504377710851   -0.29493720223545
 O  -0.48043597516044   -2.21358805424570   -1.73732597323547
 H  -2.29732550396221   -3.13544787565837   -2.10670939615278
 H  -0.84352940333045   -4.05571690925505   -2.61563751466813
 C  -0.20186122739598   -1.58355130377576   -2.98193409997178
 C   0.91967656810615   -0.59923956172651   -2.75059779424856
 H  -1.12201395360416   -1.11743818110391   -3.37494593366426
 H   0.14100204632029   -2.34006685634095   -3.71184946016193
 H   1.24639694116665   -0.16479494307379   -3.71584198506534
 H   1.75803657287262   -1.17440267152454   -2.33973359034019
 C   1.84283469154071    0.98239582743483   -1.23715171393155
 C   1.70678911725572    1.97947316503614   -0.11139303822772
 H   2.45314184382311    1.46768483762437   -2.02252362646607
 H   2.41271812834189    0.11945051550676   -0.87242453867239
 O   0.77532263329537    1.48282647839509    0.84408860489462
 H   1.38918173131368    2.96356130892231   -0.47643820185520
 H   2.70013614721895    2.10684593366906    0.34763656972662
 C   0.68620363479831    2.20928320945395    2.06057668542764
 C   0.87314211319807    1.25043371306437    3.21706858975239
 H  -0.30993091542979    2.68256883976969    2.12029408026340
 H   1.44612177620288    3.00760995150824    2.09768496717786
 O  -0.02219240827487    0.16510238682836    3.04647446177903
 H   0.66876079618869    1.77585354020576    4.17034725882335
 H   1.91164545490735    0.86913701048542    3.23590816823405
 C  -0.07255545610892   -0.71032280397111    4.15427097710114
 C  -0.81294678190070   -1.98007766228676    3.76468949120174
 H   0.94734135114460   -0.99166630009765    4.47973440612062
 H  -0.54814831762988   -0.19801115154379    5.01177961771373
 H  -0.13026445152716   -2.59915134382385    3.16635012895778
 H  -1.04028712372363   -2.54404199443928    4.69571649920717
 O   2.11671063124561    1.92979217557994   -5.02374848744919
 H   2.83741439977100    1.44134690127497   -5.44914710842505
 H   1.60183159300142    2.28952256392369   -5.76139745682891
 O  -4.91364386402221   -3.04962541109589    0.08381285153716
 H  -4.77659695893434   -4.01912738469462    0.15709502842899
 H  -5.86108367784363   -2.90778629339191    0.21153140700744
 O  -3.31077776076121   -0.17338667833455   -3.31813375192998
 H  -3.59191836005573    0.76887083015615   -3.29607096815900
 H  -3.85188725005541   -0.58532556390740   -4.00559933826109
 O   1.43299214986243    5.01067684456406   -1.49489283954936
 H   1.89727867083246    5.08196321069165   -0.62086653178861
 H   1.24860350404879    5.91864461732929   -1.76972378492924
 O   3.77889136571529   -0.26606878172238    1.70005395686625
 H   4.27896905879872   -0.56806434114609    2.47175240942650
 H   4.17592262571054    0.62263610330627    1.46571604771159
 O  -4.09140865065591    2.50802972222724   -3.22961771644061
 H  -4.98237268270488    2.72568856113998   -2.91767061160086
 H  -3.97055216221342    3.05641444906850   -4.01882492915814
 O   5.07516590087594    1.81921048186544    0.77857331097787
 H   5.20324571690286    2.74871172662562    1.04824214898087
 H   5.12699887588377    1.88342480100161   -0.19788270041935
 O   1.30596319994635   -1.72867245722398    0.96352391208021
 H   1.79137210607986   -2.18907746065013    0.23163247386258
 H   1.98550839549713   -1.13989994795553    1.34465393784982
 O  -3.19834784461600   -1.03472677169739   -0.71693435515663
 H  -3.32346391796046   -0.78818648899357   -1.65918443669843
 H  -3.77283401110556   -1.80410077595018   -0.51904614888219
 O  -4.42729194329747   -5.77526859772915    0.35439282651080
 H  -4.56871639862219   -6.38248468936442   -0.38724944119359
 H  -4.78456240441307   -6.24412243352988    1.12375815412765
 O   2.72992743364231    4.96340370495635    0.88665488732163
 H   2.58561786189586    5.69363944182147    1.50443225349749
 H   3.71118993890853    4.92069457446173    0.76184173136655
 O   2.81697312746772   -2.70024297983075   -1.05499099250531
 H   3.62384924233759   -2.12440671448208   -1.06162228380992
 H   3.14375507519374   -3.60980684027978   -1.07131085165202
 O   3.18556464662963    3.65627918233932   -3.07690292322167
 H   2.49027177616259    4.15093317653862   -2.58109613079705
 H   2.75192055097915    3.11629499645814   -3.76539713912653
 O   4.75946625217846   -0.89411453706557   -0.77250383556717
 H   5.71074046082790   -1.06302508914612   -0.80541667969235
 H   4.54087303531770   -0.76252512549724    0.17868742680547
 O   5.35867133520367    4.61202968914239    0.45300335660255
 H   6.12296039107849    5.18378170092778    0.60708898899338
 H   5.46373990436587    4.20923621086622   -0.45051855153657
 O   5.29903732548959    3.06072837652986   -1.69856208542331
 H   6.02422628595797    2.95641376235831   -2.33105878261817
 H   4.48123621241118    3.25415329315444   -2.25942541150493
```

```
111
Coordinates 3 from ORCA-job sr-crypt222-b3lyp-opt
 Sr  0.05489682137062   -0.11866433770025    0.12144571186994
 N  -0.10729294270398    0.97664815339460   -2.63572860634254
 N   0.36455900401150   -1.34909257886630    2.71440466580160
 C  -0.15696290288939    2.41931504922066   -2.38508464816354
 C   1.04403663845962    3.00134421378809   -1.66793133338422
 H  -1.03166814009717    2.62317916679441   -1.75775070291738
 H  -0.29960964933159    2.98548447805003   -3.33191918368697
 O   1.34867257040677    2.19164250646935   -0.54469578061216
 H   0.76691659901355    4.01400807053084   -1.33062666835584
 H   1.92576730888263    3.08925959883907   -2.32941386641243
 C   2.35224529902744    2.72203854139508    0.31916738018603
 C   1.93608225656081    2.52748626364555    1.75551809997686
 H   2.48476651758941    3.80098248313472    0.13308010549281
 H   3.31363338766062    2.21466983025682    0.12782585165747
 O   1.69859340636733    1.14741145365258    1.96812899561044
 H   1.01517785157157    3.10280293977474    1.96250606505178
 H   2.74500801719992    2.87592991818133    2.41933840303689
 C   1.39239544755035    0.84096360928953    3.32410627900197
 C   1.39417432742417   -0.66250450318946    3.50449309369684
 H   0.42311288690177    1.29388580708420    3.59397236118989
 H   2.16730195005883    1.27455223901938    3.97958444275315
 H   1.28279127501262   -0.89208495498884    4.58459866434009
 H   2.38908612375330   -1.00736239965643    3.20887082346158
 C  -0.91974758531568   -1.30962139102538    3.41925649154202
 C  -2.09285647599514   -1.81559408470519    2.60532829094097
 H  -1.12091073898900   -0.26912303125241    3.70839537388993
 H  -0.87191435490259   -1.90654136007054    4.35565567158737
 O  -2.16326395266377   -1.08296141993711    1.39271949289541
 H  -3.01595901573650   -1.64430437006845    3.19322948578711
 H  -2.02971310810827   -2.89523750930452    2.38267300770524
 C  -3.31253778553423   -1.38438071756963    0.61613615377756
 C  -3.53686177768639   -0.27845235601997   -0.38192210791603
 H  -4.20229450709612   -1.45632585774778    1.26935885397504
 H  -3.18943289686658   -2.35138934495372    0.10098616092741
 O  -2.37028161460520   -0.11556301551177   -1.16811071904232
 H  -3.77510487153238    0.66909144919348    0.13892020090998
 H  -4.38660748915124   -0.56423754623314   -1.02512816981674
 C  -2.59051080448800    0.63924853826994   -2.34499893876935
 C  -1.37536774518538    0.53602845748204   -3.24005334664819
 H  -2.85262624393170    1.68414439289675   -2.08566503678559
 H  -3.43828833183110    0.20895939519904   -2.90669472073521
 H  -1.59198560111379    1.10885414579327   -4.16678210090462
 H  -1.26812323805240   -0.50941734564753   -3.54044199082231
 C   0.99952017259900    0.56261275340604   -3.50731540665895
 C   2.33983949974613    0.33866015672932   -2.82945680776640
 H   1.15397413297957    1.28711580611832   -4.33421034413179
 H   0.70219301717980   -0.38412444915935   -3.98077869318705
 O   2.22807129001478   -0.69751131866740   -1.85497734014777
 H   2.73170660602713    1.24004251955676   -2.33983958890769
 H   3.07399287358055    0.03665221277430   -3.59922793209543
 C   3.42487947726598   -0.84208582982553   -1.08541375701546
 C   3.28799349494849   -2.03465495684821   -0.17733875555232
 H   3.60247521126029    0.06615277433482   -0.48818710583432
 H   4.29100228973721   -0.98925638058733   -1.75623462622364
 O   2.17092374792364   -1.84705136272835    0.66040721414269
 H   4.21358835316469   -2.12126292662855    0.42249352735808
 H   3.17420970598255   -2.96988215211119   -0.75946713492478
 C   2.07255918682279   -2.84549187007787    1.66824129401527
 C   0.73090916630681   -2.72619724035618    2.36581835812422
 H   2.12459265403212   -3.84767146183308    1.21267182307465
 H   2.92040255592146   -2.72802766314120    2.36641942319648
 H  -0.04167027001549   -3.12619956068622    1.69796520379999
 H   0.75471164729446   -3.38153880922774    3.26330488663116
 O   5.32198636534762    0.84643353650376    0.99650945334236
 H   6.20815046886046    0.98485417609946    0.63318062935365
 H   5.22233905301064    1.52230329844000    1.70905427960906
 O   0.52887196715398   -5.46592133813657   -2.28488340465226
 H   0.99900019505269   -4.64513890247403   -2.59066215883266
 H   0.76791930627597   -6.16581082649298   -2.90916420449025
 O  -4.15029967314374   -2.99187291012872   -2.30625673853306
 H  -4.94098023397596   -3.54604795253909   -2.37063770317171
 H  -3.40709296955018   -3.61471685925463   -2.10337734295061
 O  -1.84979070911982    1.99939501610439    3.84270932054415
 H  -1.50003539295621    2.69729453410699    4.41592899712333
 H  -2.72997612250547    1.80616423690040    4.19759603606146
 O   1.38919428263082   -3.09518666989745   -3.05988145542354
 H   0.74272828821975   -2.83133115607925   -3.77009306686995
 H   1.84147960759680   -2.28313648613368   -2.75707482248752
 O  -3.03895802161090   -1.91835174639560   -4.47538589775772
 H  -3.52232371516245   -2.32047158390152   -3.70360855523669
 H  -3.64937806350684   -1.98225239605837   -5.22268981812424
 O  -0.32433121596031   -2.33344809113027   -1.01166945835444
 H   0.33063021120626   -2.63689450895726   -1.67247178094665
 H  -1.09534831759550   -2.91828859556559   -1.18084636795037
 O   4.72076277679100    2.07160431561234    3.33234719735573
 H   4.66076206828906    1.13374152958293    3.62329774970102
 H   5.29490850592004    2.51638628665416    3.97134316834911
 O   0.76964283112319   -5.56991542682143    0.41037805974689
 H   0.77732535361379   -5.62172783329467   -0.57734512702165
 H   1.21682812438909   -6.36945811743720    0.72091374785516
 O  -1.44606580504217    4.34075862828277   -0.10854786063662
 H  -2.17297652809242    4.56584268419382   -0.73538553415361
 H  -1.26387188068391    5.15904157084016    0.37165027896465
 O  -1.20741625426002    1.88414459333612    1.10319230116141
 H  -1.31741124564235    2.77607614640952    0.70269896863722
 H  -1.53630017493671    1.94067048297741    2.02021464052679
 O  -0.45173214859655   -2.45415548913651   -4.83825911648187
 H  -0.29755979217502   -2.29637896086720   -5.77911067694633
 H  -1.43138662809205   -2.33666727023386   -4.69881501512153
 O  -1.79136732225548   -4.96093330647683    0.95399891732723
 H  -0.84259736055236   -5.24773947985235    0.89338505619269
 H  -2.25806754902693   -5.68043027989302    1.40116440270482
 O   4.63960304951682   -0.67155592521746    3.20844264041081
 H   5.33867540314891   -1.22357330622490    3.58671939436384
 H   4.96405765252409   -0.40495596917796    2.31783834905619
 O  -2.00671354685218   -4.38937465825324   -1.63164592891743
 H  -1.27000387206641   -4.88188224629124   -2.05208056947594
 H  -2.03980903438374   -4.71009673545035   -0.69109926530169
 O  -3.45126048155483    4.86726853469143   -1.89700387198374
 H  -4.36272323798134    5.03904422470066   -1.61939443152260
 H  -3.32525894117637    5.40833841438847   -2.68979985868955
```

Figure S12: Three optimized coordinates for Sr-[2.2.2] complexes with 16 explicit water molecules

```
111
Coordinates 1 from ORCA-job zn-crypt222-b3lyp-opt
 Zn  -1.41099965042525   2.08983471132627   0.15224644127381
 N   0.60619278643465   5.50548013518810   1.70644435386000
 N   -0.57342634006909   5.14197396556557   -4.02090339983851
 C   1.09672939311328   6.83508323830833   2.06819828140858
 C   0.62840525160432   7.97408937678743   1.17622821969006
 H   2.19533921405105   6.82765706489817   2.01677261349342
 H   0.83551057544090   7.08971187186332   3.11901129781747
 O   1.08246511275884   7.74986739693463   -0.15160109346572
 H   1.07771539146469   8.91241497042715   1.56342662074494
 H   -0.46186686851197   8.12081374136554   1.16878541883154
 C   0.83749134077943   8.86162135378844   -1.00916037881199
 C   1.32767346339680   8.55581157835394   -2.39856018365062
 H   1.38269470122633   9.74801770126358   -0.63239671371692
 H   -0.23185070056276   9.11108825128834   -0.99966899214050
 O   0.50610839188226   7.58411043153851   -3.00626253739095
 H   2.37182433898500   8.19207559666337   -2.33625813273288
 H   1.31290060915225   9.49640499319874   -2.97909857821310
 C   1.11214114005152   6.97499919042880   -4.12768750056979
 C   0.05494802334066   6.17120368076974   -4.86489281786942
 H   1.94389540930102   6.33138793225215   -3.79043210015469
 H   1.52357413208696   7.73843657582352   -4.81798194537169
 H   0.50094157942665   5.72465788993680   -5.77275208950753
 H   -0.71580083982337   6.87255322189903   -5.21705902277834
 C   -0.06842377765662   3.78701622422308   -4.26565052986719
 C   1.44116657367086   3.61707180612630   -4.14274825099903
 H   -0.35484926759400   3.43340873516389   -5.28174003617410
 H   -0.55813310946998   3.11591696873992   -3.54316248232943
 O   1.89023158718748   4.05377340505386   -2.87996245649734
 H   1.97588459501579   4.15796366846391   -4.94818454786190
 H   1.66149607251430   2.54241040282864   -4.29078450926766
 C   3.07968178526449   3.44664442426437   -2.42577064091280
 C   3.51291249182150   4.04253437670263   -1.10363491360882
 H   3.90903588325721   3.61007245245326   -3.14336206001589
 H   2.93284234456325   2.35079650642052   -2.33267000549683
 O   2.54143463279395   3.79690434104053   -0.08627174725351
 H   3.67340437813524   5.12739483965777   -1.20058681923310
 H   4.47764264503787   3.57989845007795   -0.81963504447862
 C   2.83385036935204   4.38861042954198   1.17631249498448
 C   1.58126418831327   4.45941103136955   2.04110965663233
 H   3.27842633961634   5.38200057376390   1.01355907666839
 H   3.58713798897277   3.77223395956852   1.70420917927104
 H   1.91561881004479   4.55264693914962   3.09898588086332
 H   1.06428247097056   3.48847750549215   1.97665620249540
 C   -0.67587909238552   5.17950669636816   2.33144374581852
 C   -1.87370585458276   6.05232646468957   1.99051099026974
 H   -0.59070567999603   5.19543781323696   3.44350332262711
 H   -0.93427829342665   4.14940367803284   2.05504388636834
 O   -2.04554676562545   6.13659242085634   0.60117385164686
 H   -1.78489648456186   7.06497717717538   2.42936775757561
 H   -2.75567792598758   5.57983684320588   2.47092830833613
 C   -3.19918248363731   6.84570648224449   0.19622765644413
 C   -3.04827537046526   7.25668250555271   -1.24739452442953
 H   -3.31266110563154   7.77588378277478   0.77848091169148
 H   -4.10228923708439   6.21888945667535   0.34744312188233
 O   -3.07682664781085   6.11601129275668   -2.10832514971771
 H   -2.09007656274122   7.77641878471091   -1.37396416667429
 H   -3.85384919384415   7.96284537895909   -1.51945096638378
 C   -2.67802294632300   6.40316686144115   -3.45242214878435
 C   -2.04068498860508   5.16686977162811   -4.09289478915875
 H   -3.56237897992434   6.72663215018789   -4.03261149403331
 H   -1.96878961116321   7.24547383483645   -3.43629426646618
 H   -2.42313550566843   4.27707644307381   -3.56929904976301
 H   -2.37689761561213   5.08287136395844   -5.14841520538158
 O   -2.99592881855723   1.00746155013356   -3.20998448101965
 H   -3.88691222569340   1.40446847634239   -3.30362444243394
 H   -2.87716960536030   0.42464703757640   -3.97266310260863
 O   -2.18214873947410   10.12694291639824   -2.56032087485493
 H   -1.38316308205636   10.70324014226938   -2.57107620819680
 H   -2.87964926082305   10.67176655236367   -2.95034032779100
 O   -2.21019860544060   0.29326955617437   3.47328621110424
 H   -2.80528175281658   -0.47403181333660   3.46482068319854
 H   -2.02071031258364   0.46242545674805   4.41005780387542
 O   0.01799754372960   11.65547922919839   -2.10453364160792
 H   -0.01064471458392   11.92491466000842   -1.16360926739327
 H   0.40782212769012   12.39620011769513   -2.58717621994798
 O   -5.53991797801178   2.24064165629205   -3.31821223315661
 H   -6.25016757433255   1.71881146667688   -2.91014337082946
 H   -5.89648538722324   2.51009259392137   -4.18047507734195
 O   3.83216552504042   7.12389143994501   -0.28188355285419
 H   2.88198540937065   7.36018272917546   -0.24457685533532
 H   4.30688350784657   7.93766359392960   -0.06934465423819
 O   0.28577637926032   2.70764177724569   -0.64881443229371
 H   1.20138720436333   2.81869782260499   -0.29129434707109
 H   0.15357784844151   3.65216218195673   -1.01189081263997
 O   -0.42483850080185   0.55383967275997   1.36983770593753
 H   -0.88028770347839   0.32742725912669   2.20922136659375
 H   0.52756850096516   0.52053865139725   1.53337360703565
 O   -0.18549374336951   12.05476755549772   0.68612501065614
 H   0.60170857360799   11.91707900476028   1.23348113207359
 H   -0.63086371662094   12.82304804389115   1.07613489248780
 O   -0.25355208228257   5.11503412167729   -1.29751082113925
 H   -0.17288748612842   5.38573877776858   -2.24999549698155
 H   0.11802111850487   5.80715487649323   -0.71963870745635
 O   -4.84324884285932   4.19155143165928   -1.41280494292713
 H   -5.13724354877376   3.63988906593009   -2.16452531779700
 H   -4.39568860368526   4.99782103160679   -1.77806082277329
 O   -2.28072391671562   3.50667255402315   -0.99598768358478
 H   -1.75949356708821   4.35737949974200   -1.03408189613322
 H   -3.23640078707347   3.71846671665759   -1.07749950329978
 O   -2.54904928138805   2.45378129059900   1.78625536119852
 H   -3.46773948038463   2.81106869406496   1.58128117266020
 H   -2.63442955787662   1.73261991726597   2.44061789575734
 O   -4.93165577833704   3.27723624619592   1.15464895776646
 H   -5.46820376701114   3.83783901889549   1.73147946748864
 H   -5.01854471332286   3.66098408495786   0.25093644020166
 O   -2.12891474170594   9.83552685748093   0.22044967557163
 H   -1.53234250243320   10.54987713221609   0.49534859622033
 H   -2.26599584306767   9.99417567151381   -0.73851109246196
 O   -2.23748132202239   0.47694984425112   -0.77629122438416
 H   -1.68092036436070   -0.31343406332139   -0.74338333064790
 H   -2.53126894291491   0.61530678723298   -1.72621923832019
```

```
111
Coordinates 2 from ORCA-job zn-crypt222-b3lyp-opt
 Zn  1.11827672249500   4.03112082698318   -0.90497576998282
 N   2.08083664578932   6.67503461140495   1.82950210699530
 N   -2.06791939105783   4.53929281411319   -2.31855030576785
 C   1.81262388040141   8.09100764565672   2.14480136399226
 C   0.35855494257918   8.51222191536291   2.03031365199762
 H   2.38363777358029   8.72732015330345   1.45365435460328
 H   2.17958424826099   8.34024061415975   3.16035465214217
 O   -0.03682081159662   8.39226992054519   0.67730320426194
 H   0.27643049419164   9.56937835137186   2.35796803825244
 H   -0.31913221988889   7.93148149027637   2.67554650325933
 C   -1.36072445559958   8.82449580765178   0.44208532085629
 C   -1.67417286997173   8.65590107880184   -1.02099285770347
 H   -1.48515801618157   9.89264410546483   0.71225121253056
 H   -2.08233429949981   8.25711336500437   1.05207182229111
 O   -1.75829371838581   7.27558350008937   -1.34022653749795
 H   -0.88604957572928   9.14420499495184   -1.62646610824529
 H   -2.63722868840596   9.15150509896709   -1.24569616025560
 C   -1.91867152735347   7.01470128196222   -2.72959716631616
 C   -2.69460336310992   5.72108351257675   -2.91122753427454
 H   -0.93693052323107   6.98405421585257   -3.22756136641521
 H   -2.49530488300115   7.83154677658568   -3.20160306934745
 H   -2.86886004843191   5.57277764981570   -3.99556220027826
 H   -3.69003984629901   5.87108169194910   -2.46433272573440
 C   -1.38316785325513   3.70404549349259   -3.29576776316182
 C   -0.14832705569375   4.34210927331752   -3.90997565961107
 H   -2.04414736368913   3.42576457387089   -4.14855077318956
 H   -1.08640378660573   2.77944260593778   -2.79445302930852
 O   0.74349947212494   4.84823736933523   -2.90641687173341
 H   -0.41224505712847   5.18377371106797   -4.56771779613896
 H   0.37426655843540   3.58264592162758   -4.52030111415953
 C   1.88621735602063   5.51750554949620   -3.45237260792542
 C   2.35992140739855   6.58128522310711   -2.49313743930043
 H   1.59466204325371   6.02319897095830   -4.38601760513655
 H   2.67732587154972   4.77725780829517   -3.65770974279088
 O   2.73820966757473   6.01769451253554   -1.25109395093682
 H   1.55442638494844   7.32295314552917   -2.33369162488884
 H   3.21842582927431   7.10689446205649   -2.95535506134425
 C   3.26917439819315   7.00227897177305   -0.36675211642197
 C   3.33157007931137   6.50208868526417   1.06773328533342
 H   2.65107505784233   7.91470659418277   -0.42970498511501
 H   4.28780894310115   7.26785584822222   -0.70662668747082
 H   4.17281670242969   7.01746206468947   1.57486782415194
 H   3.58629507795920   5.43237825086713   1.04055249476790
 C   2.11198425079435   5.84771412941815   3.04443006498592
 C   0.74903597292053   5.58399780375972   3.66931739344549
 H   2.75981396181228   6.30276877077573   3.82334389178470
 H   2.55678970545318   4.88121399575625   2.77521794313144
 O   -0.09787395233636   5.02420805479358   2.67599264510038
 H   0.28937609380773   6.50414036724535   4.06777943804171
 H   0.87627741345238   4.87723756730968   4.51071761062904
 C   -1.43704512578504   4.75710062825395   3.06898794020810
 C   -2.40942506878979   5.07929276063277   1.95855830700783
 H   -1.71531418520416   5.42163162397550   3.90061905083626
 H   -1.52807303349946   3.70604066642379   3.40316269313958
 O   -2.32648811528906   4.17604178228359   0.85780427060007
 H   -2.21887309604502   6.10061791407492   1.60041990004515
 H   -3.43056654199479   5.05359893623232   2.38414112836793
 C   -3.31673855540789   4.44540470460348   -0.13990848601398
 C   -2.97489854691377   3.77595624617103   -1.46633634707521
 H   -4.29345885107021   4.06982898775295   0.22165202999862
 H   -3.39929150869929   5.53685387244066   -0.26480808459726
 H   -2.51058054114195   2.80421480298885   -1.24871320900574
 H   -3.93212118639605   3.55331574995343   -1.98670803323530
 O   -1.48565571680134   1.71747742372547   1.06191224370107
 H   -2.22506659697385   1.09380148564548   1.03172781403893
 H   -1.88232625449151   2.63852499247521   1.06644856499632
 O   0.77407647862496   1.86898424235442   5.17004511529650
 H   1.60614933233945   1.82061040717967   5.66420665018863
 H   0.12326396661730   1.44819734471457   5.75128216727837
 O   0.82484463715792   1.37489560904995   2.47180467485498
 H   -0.10822762725023   1.45180998696062   2.17313867265941
 H   0.82472774096421   1.48234552013056   3.45202942408240
 O   1.49015906739723   3.57946049088324   1.09087461508082
 H   0.83623926698405   4.09948469350021   1.62289035650791
 H   1.44111664385238   2.68219231496121   1.50212008600911
 O   -4.37153523336474   11.05316579725399   1.09876380417772
 H   -4.32666555830807   11.75880297023836   1.76002278704356
 H   -4.85752538194789   11.44176432431071   0.35694117223034
 O   -4.40560415536172   8.39516847623952   1.79795295988525
 H   -5.31826989911159   8.14316037032593   1.99199362001739
 H   -4.44553688154962   9.34827127642662   1.55689030032058
 O   1.11774799279876   -0.09827736477331   -1.72642135097450
 H   1.14825156233379   -0.40847268199161   -0.76339820316855
 H   0.68298691161178   -0.79086275849676   -2.24272769556882
 O   3.55987969672396   0.67428773008633   -0.85386716355894
 H   2.98530333175062   0.21361524013938   -1.49933970611366
 H   4.49210376125057   0.56200679014107   -1.12863548009886
 O   1.64256430878077   -0.58647932589970   0.74087986577845
 H   1.33094368451236   -0.00751697633999   1.47206245391880
 H   2.54615833995869   -0.26719631385859   0.55854375420560
 O   2.81412263940306   3.16140452666673   -1.61958817467632
 H   3.01329154514795   2.25377906311130   -1.27406760891342
 H   3.69014647044120   3.61456720686641   -1.54397295285319
 O   0.11825832591496   5.60326139551652   -0.14015730021416
 H   0.60033188624963   6.14019209980024   0.53210600327693
 H   [illegible]
 O   -0.00976397195626   7.30693006933004   -5.49797144655461
 H   0.09186971718183   8.26797929921946   -5.54860034026012
 H   -0.06594694662267   7.03106429931612   -6.42452657471640
 O   -2.49047730245633   7.67064657120217   3.60446105738186
 H   -3.21790676593117   7.95934081258524   3.00484736068745
 H   -2.53384624382213   8.28132536858681   4.35182654718549
 O   6.33031396951470   0.91118978559554   -1.34628135316962
 H   6.81366391382803   0.53145448957634   -2.09686178326276
 H   6.84363394612794   0.65081699405079   -0.56468195412446
 O   5.41886460933587   3.66872040959680   -1.34670480800269
 H   6.01091710354730   4.23685601182153   -1.85704331734344
 H   5.83007725693117   2.78215498606278   -1.36557862247559
 O   0.06505165451846   2.25294891412587   -1.09751103886038
 H   -0.47728806063227   1.97521691013793   -0.32258518863716
 H   0.46700443806433   1.41972433795582   -1.46456951838399
```

```
111
Coordinates 3 from ORCA-job zn-crypt222-b3lyp-opt
 Zn  3.26522322527075   2.58169862725654   0.21121242415554
 N   5.91795233411399   4.00723112563624   3.27992228055952
 N   -0.01856955479172   4.83878372534508   2.37003349350631
 C   6.36557557755511   4.76666887172338   4.47322108786999
 C   5.32294349473238   5.18406043690857   5.49169506211938
 H   6.85948336658865   5.68766209890425   4.13787270339996
 H   7.14120602594908   4.19039808020096   5.01133476507281
 O   4.47734796831463   6.18835951752734   4.93476274870912
 H   5.86547759343196   5.60611102844691   6.36225289134409
 H   4.70117801246568   4.35881347643705   5.86975631171567
 C   3.51507052586328   6.67698406458256   5.86176244069617
 C   2.37867762576292   7.34143038101176   5.12580446910056
 H   3.98828152513808   7.40608596570959   6.54785944745560
 H   3.12770161375770   5.84242008359944   6.46812610633541
 O   1.55090118004784   6.34888301975325   4.53157233649168
 H   2.76471840806520   8.03127228949285   4.35495871728514
 H   1.79012439522773   7.94554359680961   5.84404905537400
 C   0.46576391036834   6.91487802582271   3.80284223634777
 C   -0.50367341713957   5.84446314073064   3.31977623279437
 H   0.86797431897253   7.54999431562368   3.00305781809563
 H   -0.10985158955567   7.58916125651143   4.46929985254794
 H   -1.39092868975406   6.37425160695449   2.90903969460655
 H   -0.86232003969699   5.31923453602416   4.21630134067078
 C   -0.11117910979087   5.27162717143692   0.97542258287171
 C   0.78264993655304   6.44036769099934   0.60297953554100
 H   -1.15029541412797   5.55987058414216   0.69727376231086
 H   0.16022799185257   4.41451660232152   0.34058599042939
 O   2.13964496360979   6.10544302439946   0.90470279909571
 H   0.51005021886135   7.36540560376762   1.13156236398278
 H   0.67297638305649   6.64652681655128   -0.47783900845781
 C   3.04582257012025   7.21430519861586   0.87833867734491
 C   4.28369610927730   6.92968099998710   1.68534803520154
 H   2.55219689349118   8.08190619257540   1.33361135115728
 H   3.30009510053469   7.48826701310912   -0.16086521388198
 O   5.17002817966366   6.03026471579953   1.01293872169532
 H   4.01045175208608   6.51475260800619   2.66725975982608
 H   4.78405552196762   7.89159023176774   1.85737881527918
 C   6.45734592551927   5.86158488710223   1.61796947385907
 C   6.69659674038737   4.43439161689896   2.09555855996004
 H   6.58470845268884   6.60854512132943   2.41613406788792
 H   7.21861528942427   6.08559053945751   0.85069080404863
 H   7.78508447347093   4.33000951256663   2.28989326811830
 H   6.44696513620468   3.7556332625936   1.26896454545674
 C   6.12319383042289   2.55644827173545   3.48298568502493
 C   5.12062391150599   1.84887597305657   4.38996832706940
 H   7.13939788359032   2.38319540599592   3.89143720820818
 H   6.10197722713115   2.06192115324627   2.50054799032968
 O   4.03254427968259   1.34105311760060   3.61332110379840
 H   4.73141609229939   2.50777788459413   5.17844387957161
 H   5.62092713255800   1.00003084913231   4.89143790474142
 C   2.88903569072932   0.92425578279582   4.35928888853145
 C   1.85466538260290   2.01661143000075   4.55660101652012
 H   3.21383621689765   0.55341683724326   5.34384470495253
 H   2.43335335296261   0.08343816101009   3.81244610735648
 O   0.96462243570904   2.09892197184184   3.44953488971094
 H   2.35382233993156   2.98409041571120   4.70601862426881
 H   1.28005543265035   1.78750622604508   5.46805454038857
 C   -0.28039172387574   2.75130476845742   3.73974629765158
 C   -0.74978637498717   3.57549240430835   2.55408723550623
 H   -1.03678578141957   1.98026176627781   3.97230088942237
 H   -0.16004322134422   3.37793917700244   4.63562163199073
 H   -0.63585368310154   2.97148816335431   1.64374195373537
 H   -1.83964092739937   3.75279031561979   2.67692982042186
 O   5.24630072333979   2.82255042910356   -0.44408401184425
 H   5.61651421004344   2.02330539518096   -0.87415039880187
 H   5.41146226539632   3.61930897379365   -1.00193837793581
 O   3.56399081182117   -0.89338137487670   -2.02391850280509
 H   4.49066197220817   -0.65304140231313   -1.77235515516594
 H   3.60531777515393   -1.44617037542099   -2.81798580095775
 O   4.28653478426824   9.92698094808850   3.12749988910820
 H   5.04092583503450   9.43394842114904   3.51070992193301
 H   4.49445048682353   10.10699506988577   2.18821138342297
 O   4.09671202664140   0.72977231830017   1.08915910085590
 H   4.14953138754426   0.92106760216519   2.07243303646173
 H   3.39665136591412   0.03421350807128   0.97272309796917
 O   3.19009482085696   3.14282463824338   6.93134409117924
 H   2.31690367931352   3.59315106164329   6.89276921111896
 H   3.40291962354335   3.08303024413733   7.87260456163383
 O   6.19055028366038   8.21281515146746   4.16224680114084
 H   5.57601341768944   7.52694668875226   4.50728524259948
 H   6.73337215735278   8.49788337058833   4.91047191707188
 O   3.75956551286237   10.18119498080887   0.44397355894194
 H   2.88382531269566   10.26810321894018   0.87573094831340
 H   3.87946509370754   10.99609920065059   -0.06279317262157
 O   2.62163801719955   1.58277711910534   -1.59879456922494
 H   2.89651857461880   0.73175565337628   -2.00816492620815
 H   2.26642045504241   2.17615840417901   -2.27324845790954
 O   1.76612938360997   9.83279981523812   2.39854876164809
 H   2.61616239503389   9.88349197870864   2.90751439931539
 H   1.19085204603313   10.51493160189347   2.77034104734923
 O   3.38304123011400   3.70532315776856   1.99267793362849
 H   4.19939186574485   3.95315010335434   2.50516802417746
 H   2.72478454003514   4.41770993534106   2.10171824037688
 O   2.71483191496937   4.27356250434598   -0.90398727015001
 H   3.49882016267721   4.66385856558806   -1.35287106705052
 H   2.47638538228447   4.96555078188347   -0.23141749891254
 O   2.12956172451737   -0.87550393838930   0.31718907877548
 H   1.80036222506298   -1.71377431428006   0.67165169742430
 H   2.49976628253210   -1.07601696771904   -0.57489736718798
 O   0.85115141572879   4.52793705687489   6.46024311131425
 H   0.28965500420028   4.99149436870486   7.09751075746080
 H   1.05452336153434   5.18172576879545   5.74991095490259
 O   5.17068246301827   5.27335539708482   -1.47581552539870
 H   5.20291366820854   5.73394103022431   -0.59001277264978
 H   5.58229727338043   5.84968607437099   -2.13457489245536
 O   1.43273098960122   1.91085899623703   0.88707780228594
 H   1.32266908657029   1.94803188019679   1.87874413028084
 H   1.31006906973610   0.98340588785251   0.61100109288197
 O   5.75925723719673   0.20205916316032   -0.91513393027037
 H   5.35120718762832   0.25167352657153   -0.01226932224034
 H   6.63444975476613   -0.20203033129594   -0.82082788096318
```

Figure S13: Three optimized coordinates for Zn-[2.2.2] complexes with 16 explicit water molecules

```
111
Coordinates 1 from ORCA-job pb-crypt222
 Pb 0.19667997987371    0.17029075003338    0.21205248240810
 N  -0.54000831428057   2.95617938230323    -0.02073942354675
 N  1.17226239031567    -2.50370319222985   0.36090061690586
 C  -1.88305215376582   3.08169514607413    0.56784323994454
 C  -1.96817110924010   2.64849182650477    2.02327450461935
 H  -2.59475513500835   2.46741886948808    -0.01737027260011
 H  -2.24946841707100   4.13860973668962    0.50330182343262
 O  -1.47148410992518   1.31936534024231    2.13296995586697
 H  -3.03952598254723   2.68217120265991    2.33426925928238
 H  -1.41033858090830   3.32767476726573    2.70688469232897
 C  -1.32251666195876   0.84613587783113    3.46699430919127
 C  -1.18160953056316   -0.65786244114267   3.46044841578265
 H  -2.22260360260421   1.10396332752143    4.07422111119843
 H  -0.43694323497741   1.31251399774046    3.95383438576578
 O  -0.04432374285720   -1.04186733582659   2.69227412704295
 H  -2.09381733313192   -1.12652136492233   3.02817803751988
 H  -1.04443570160124   -1.00112877513239   4.51054809318347
 C  0.04512629435284    -2.46697857309625   2.61034655923541
 C  1.25861446368769    -2.86560536762878   1.79236836396576
 H  -0.90709641567689   -2.86098653424277   2.18777049200435
 H  0.16872907960107    -2.88116485204059   3.63668980953732
 H  1.41591584990373    -3.96616018871735   1.91147097193395
 H  2.12148841279525    -2.35498459576567   2.26438152450837
 C  0.28890153750631    -3.42821386821823   -0.36665945188757
 C  -0.08707826226256   -2.99471986673823   -1.77790998602282
 H  -0.64452611460858   -3.54141152016031   0.21913267109346
 H  0.75425169219292    -4.44458041672596   -0.43471002111572
 O  -0.87139429881300   -1.80262593265161   -1.69748600339033
 H  -0.68542495303719   -3.81018214796436   -2.24846046613779
 H  0.80097354806159    -2.81691901033210   -2.42489946202903
 C  -1.33685922203987   -1.29253641338772   -2.95133199282174
 C  -2.03344434485822   0.03006698549655    -2.70930415112260
 H  -2.06073385634463   -2.00675165719875   -3.40797121082187
 H  -0.47791017412169   -1.13093813066419   -3.63677106156554
 O  -1.11713207266764   0.93579009425845    -2.09809032372270
 H  -2.94522462680239   -0.06635972935468   -2.08124738537598
 H  -2.35201072352704   0.42239714900659    -3.70259340231914
 C  -1.48550469380551   2.30734063525460    -2.27052570496465
 C  -0.54968640624971   3.20056247418664    -1.47716256100894
 H  -2.54857995709162   2.44123367351774    -1.97355461959510
 H  -1.38846717451969   2.58175647435463    -3.34802028188137
 H  -0.84356393590689   4.25776861524120    -1.70436544325875
 H  0.49359452047557    3.06277126613240    -1.83044967169601
 C  0.46064211987115    3.83386269121995    0.61266292665050
 C  1.19256044409206    3.25126982270946    1.81395809019218
 H  0.01098918872456    4.81597383779181    0.90171922851111
 H  1.24393683301156    4.03615752227130    -0.14145746964983
 O  1.82282798189990    2.04511893947313    1.39336905264909
 H  0.54238091054409    3.06357804188072    2.69492306578787
 H  1.97820514811012    3.98470979631982    2.10453813267186
 C  2.75910168709461    1.50389641541786    2.32176981875356
 C  3.65712793135367    0.54595010553832    1.57839449775519
 H  2.22619114573621    0.94944208370102    3.12575024377641
 H  3.38770133342259    2.31047333917489    2.75978291207865
 O  2.81914572661641    -0.38230707516344   0.90980148989488
 H  4.29485222024071    0.02286910102374    2.32392449052715
 H  4.28612843152418    1.09489522558145    0.83813561644213
 C  3.48523767770128    -1.55029103033109   0.46725175513835
 C  2.49136984924084    -2.42325494445629   -0.28997236045404
 H  4.32648549229631    -1.29147946421237   -0.21894782973937
 H  3.91789867349172    -2.07544981789644   1.34963313525773
 H  2.34299333669529    -1.98695803065668   -1.29555159868605
 H  2.94585148355512    -3.43953361555203   -0.41364979109331
 O  2.92615684771742    2.73514633776057    -1.37099620130638
 H  3.53357819821327    3.28400494174976    -1.91425623423931
 H  3.19316513337549    3.00685295710608    -0.44438665130283
 O  1.21779040863185    0.00700586524300    -4.37101819433858
 H  1.79731938174672    -0.80211835204198   -4.38191186868956
 H  1.52752500889101    0.55792206935246    -5.11299336172201
 O  2.59294596417709    -2.31597424838905   -4.05152715124900
 H  2.64510981874293    -3.01927503986615   -4.72759236402637
 H  3.49365824317698    -2.26726312446649   -3.67813528518957
 O  -4.42248629122535   1.72572829470466    -0.99851460820195
 H  -4.58469150987874   0.96560744035381    -0.38557183792358
 H  -4.98230443011056   1.50166129051027    -1.77155686718087
 O  1.85612806663852    0.33661473479336    -1.74430836395213
 H  2.35927014882848    1.19812054887331    -1.61408195951152
 H  1.48242507050121    0.40088311629695    -2.66556594432839
 O  -4.74247069528187   -0.66570781565213   0.32667157761076
 H  -4.93002602907868   -1.16237318526457   -0.53387957171713
 H  -5.42489548730513   -0.94035829764592   0.96691530971197
 O  -2.10302263586356   -1.25349563667662   0.55895117002404
 H  -3.05636396554938   -0.97141722243817   0.58528559191476
 H  -1.96844863814234   -1.64003421086954   -0.33823748628370
 O  1.37556575823491    1.82557808909327    5.49122105532760
 H  2.02636540337430    2.05229783041290    4.80114179647963
 H  0.68513221942728    2.53845061717660    5.41552059636015
 O  -0.45320507317115   3.84274945297606    5.09412493796035
 H  -1.31486786363033   3.74134882067074    5.54321450793903
 H  -0.14856688248938   4.72965867268421    5.36949762033303
 O  -6.19314441087477   0.63671474745774    -3.08965073053854
 H  -7.11213751351819   0.87982986145545    -2.85993538068829
 H  -6.07920233124272   0.95192474944965    -4.00798734348475
 O  3.32526325896578    -1.46385849138493   3.85057500440831
 H  2.55390532673635    -1.28677849074764   4.46423765690633
 H  3.83324204341708    -2.15408654967500   4.31466144904311
 O  3.98873605707664    4.10864590898613    0.68394918578465
 H  4.70966233233352    3.78628436651711    1.28352213889175
 H  4.44406433507216    4.57524008266098    -0.05404879653530
 O  5.75977768438289    3.12483221650030    2.55320075034901
 H  6.55763932714882    2.59751081124319    2.35775981040531
 H  6.05205120396467    3.75024758210069    3.24415891244529
 O  -4.99942124246901   -1.63477711551491   -2.10800188700950
 H  -5.46060270694224   -2.46177853199828   -2.34234942719949
 H  -5.50141690740973   -0.91152350715690   -2.57046564850264
 O  1.22196542603720    -0.87930894276221   5.50404483063938
 H  1.34544110798330    -1.15469500807895   6.43198994985328
 H  1.21151356359066    0.12079573512417    5.54951927872944
 O  4.72927568572378    4.87592367540574    -1.94173505083938
 H  5.62759494489190    4.89941485005257    -2.32503711826672
 H  4.31253210396565    5.69890948242100    -2.26498575322091
```

```
111
Coordinates 2 from ORCA-job pb-crypt222
 Pb -0.01363963226087   0.17316448506623    0.02497211996622
 N  -2.04316705686590   2.16838845463857    0.62781153624805
 N  1.75463468629830    -2.03631474769979   -0.30493537709518
 C  -2.47236112875990   2.75547120740514    -0.65240140388083
 C  -3.06392569755616   1.75644026660828    -1.63411050480332
 H  -1.59400957526456   3.23453639350443    -1.12991750174712
 H  -3.23202128328161   3.56203880347760    -0.48521062364871
 O  -2.14212757374142   0.69491941032456    -1.81991875288668
 H  -3.26232040049936   2.27453902626365    -2.60207029608655
 H  -4.04662860327552   1.36614606461993    -1.28289909819457
 C  -2.64117158127830   -0.39443103967132   -2.60184258761128
 C  -1.46639682243221   -1.20808021276070   -3.08614464105319
 H  -3.18133887784803   -0.00827627792163   -3.49403755419175
 H  -3.33092325748126   -1.03097918873584   -1.99908318073779
 O  -0.72601007689018   -1.70741675280230   -1.97576303688101
 H  -0.80734215459029   -0.56941941931907   -3.72006507977304
 H  -1.83612854375522   -2.06262725737547   -3.69644197236775
 C  0.43453991340248    -2.41872350294601   -2.41441740148007
 C  1.13751341877840    -3.01894102979734   -1.21265016336983
 H  1.08588300572253    -1.72781349416116   -2.99818376518938
 H  0.11520476366933    -3.25006951640915   -3.08126428722520
 H  1.90347584143437    -3.74866198101833   -1.57902677259715
 H  0.37600114181926    -3.60486636177000   -0.66611276437349
 C  2.96242513744406    -1.45730630402931   -0.91744847679105
 C  3.61213143598746    -0.34753679883967   -0.10830677150591
 H  2.67264748667711    -1.03844826463843   -1.90091355937425
 H  3.73249320485988    -2.24933326568190   -1.09951283549038
 O  2.66420977405329    0.70413472144007    0.05499462294369
 H  4.49151789768604    0.02797537936974    -0.68235203825464
 H  3.98536181428551    -0.69547617374992   0.88168746193724
 C  3.15090870577046    1.83152104874052    0.77871416772848
 C  2.20534049944417    2.98298213876236    0.52451086962696
 H  4.15621376749730    2.12434467647861    0.40185994928456
 H  3.21495630452264    1.58797050474330    1.86406468069158
 O  0.89854946925243    2.60296381534366    0.94463652839212
 H  2.20229626566307    3.22173888576519    -0.55908396974144
 H  2.54888377794558    3.87725705841258    1.09451889463557
 C  -0.04011529896463   3.67792921799501    0.91212769013808
 C  -1.36529900117126   3.18185264491299    1.46235512655338
 H  -0.11286913847947   4.08426310242202    -0.12227595435263
 H  0.31835476496146    4.50289425804280    1.57188364492109
 H  -2.02623708530756   4.06844871849626    1.63116721770777
 H  -1.16369762851001   2.71792515882579    2.44824373856830
 C  -3.15384103250124   1.55691598015285    1.38501515363732
 C  -3.46034168218104   0.09731182956356    1.07200888009862
 H  -4.09250445085040   2.15300574989073    1.26881286588469
 H  -2.88487822402584   1.59396199207749    2.45871801734710
 O  -2.33861510309430   -0.69277852448638   1.43512447723697
 H  -3.72309336397197   -0.07996998225616   0.00794758470861
 H  -4.34717034309934   -0.20209944631449   1.67964145247248
 C  -2.53828493669476   -2.09496896157379   1.24548938142904
 C  -1.49826084137727   -2.83219927507496   2.06030943992526
 H  -2.44218308752381   -2.35105840943085   0.16708529342991
 H  -3.55223912192153   -2.40361758035794   1.58099785354862
 O  -0.21345634056720   -2.32215473209966   1.69998017511595
 H  -1.57437102479012   -3.91328881823711   1.82271332623042
 H  -1.66469953794102   -2.68930635650945   3.15217363719904
 C  0.85662927458594    -3.26345444264980   1.69733699011634
 C  2.05006687151242    -2.60521863587132   1.02348871655514
 H  1.15685195963210    -3.54070840509767   2.72947427136728
 H  0.52985849705973    -4.18743127000557   1.17012954056441
 H  2.40799693190499    -1.78317825222502   1.67321735134381
 H  2.87795556301972    -3.35515966772505   0.98043208681252
 O  -2.89388325733395   1.55596268203465    -5.27844982458791
 H  -3.63210182063986   2.10816549069495    -5.59937356720783
 H  -2.27993693591341   1.46791632848604    -6.05102910121026
 O  -0.57363894177620   1.63789246291787    -6.79523277290423
 H  -0.12135625893872   0.83010537045160    -7.10984493046801
 H  -0.45233134936665   2.27714249540408    -7.52563775934026
 O  -3.55583714307530   -4.87606379738159   0.47829407163127
 H  -3.92805046633856   -4.31026033386157   -0.27404594011967
 H  -4.21609146222910   -5.57366970910931   0.64482150045127
 O  -0.67598033653588   2.37699146632970    -4.05537252338404
 H  -0.21770689607069   2.25130118131691    -4.91856221487560
 H  -1.62496060152288   2.17404136884154    -4.30970852529016
 O  0.36144259382519    0.21559057738629    2.57788292246823
 H  1.22778376865826    0.40255767171511    3.02140292181440
 H  0.20367306747852    -0.75020415868795   2.70627494450322
 O  0.85409524195533    0.93059688424384    -2.24669837770741
 H  0.13758832279155    1.31374409299156    -2.81669350477222
 H  1.61053165354019    1.59132120608407    -2.37089083700961
 O  4.90291761969893    3.51258700724019    -1.59778438690889
 H  5.64031714927811    3.12962781109629    -2.11171119522304
 H  5.14029136059893    4.45753927136966    -1.52456151358986
 O  2.50120465420961    2.90727407225054    -2.87248880941353
 H  1.83511365309978    3.62276779174232    -2.68842963351642
 H  3.33452355424818    3.16887499174825    -2.40379853620860
 O  0.21102274092666    4.31113989235468    -2.43564604240879
 H  -0.21595945195917   3.68647236195297    -3.09467355216541
 H  -0.01089102134024   5.20641541994993    -2.75326004121365
 O  -1.18804100380976   -5.30823285079513   -0.55636107363720
 H  -2.08783528780180   -5.25599499168592   -0.08324713108470
 H  -0.88224130841386   -6.22635451289944   -0.43220233550476
 O  2.68201984718304    0.35180131985959    4.04580512429770
 H  3.00277126650180    1.10199080598132    4.57996989337326
 H  3.50719318878785    -0.14117367774149   3.68469084794786
 O  3.35083192167258    -3.30897898380555   3.93356768530395
 H  3.69968550722774    -3.98726705909094   4.54025432800828
 H  2.56567830909181    -2.88109930648055   4.40061561249316
 O  1.32847958503146    -1.84509789401773   4.78232254674447
 H  0.87688985347657    -1.86011626331220   5.64622498019121
 H  1.77677847543646    -0.95249676038192   4.72396118404088
 O  4.52833767121771    -1.15902932651852   3.06322788478603
 H  5.47088152239210    -1.09371998916628   3.30441665671741
 H  4.21076859758711    -2.06635121168554   3.40422416942690
 O  -2.06971569195460   -4.43138571948164   -2.90884346372360
 H  -1.64286372537135   -4.84007261838514   -2.08760481753114
 H  -2.23291621158128   -5.18201261508773   -3.51042958622846
 O  -4.10710401914577   -3.34314959997479   -1.60310613117815
 H  -3.39587787583903   -3.72835797199338   -2.21227799717401
 H  -4.93873272509370   -3.39145731700090   -2.11024552227458
```

```
111
Coordinates 3 from ORCA-job pb-crypt222
 Pb -0.49359315145752   -0.70909266549450   0.05887388723232
 N  0.71842614413183    -0.09353330255689   -2.47553153118912
 N  -1.63809644125541   -1.20256470362545   2.79065439228995
 C  -0.30798406343912   0.62241353457547    -3.26489040896281
 C  -0.85497343637622   1.90306816364097    -2.65667789640083
 H  -1.16953948261559   -0.06200153973465   -3.38761498551465
 H  0.09405897299304    0.85956219627016    -4.27823284591937
 O  -1.23594469995041   1.65244294949922    -1.31121056552189
 H  -1.75004700377735   2.18945524386981    -3.25450800002704
 H  -0.13144787357383   2.74985876962642    -2.71258709264413
 C  -2.02782169885498   2.66872212343563    -0.69799545795455
 C  -3.03589310831666   2.00156401250073    0.21203200490409
 H  -2.59854690475408   3.23228895294540    -1.46868484180843
 H  -1.37966059909745   3.38094972035197    -0.13550954571155
 O  -2.35442781328111   1.25151957951624    1.20579900377035
 H  -3.69018799805658   1.33109045049164    -0.39274855626930
 H  -3.67869499477541   2.78240873542305    0.68664899017013
 C  -3.25041161152223   0.56221547089790    2.07688264799634
 C  -2.44939603669627   -0.05179536860342   3.21281398784120
 H  -3.82230256178361   -0.20593554934647   1.50306489337939
 H  -3.98852344119824   1.28251479881221    2.50430819807479
 H  -3.14441250613399   -0.32770638111267   4.04370986760587
 H  -1.78596325767762   0.74361918672236    3.59957461683847
 C  -2.47080453223941   -2.41029485798681   2.73030340485245
 C  -1.81374688052850   -3.58306575468863   2.02929156078725
 H  -3.39879823248309   -2.17163730416573   2.17360773043431
 H  -2.76866536055932   -2.73809045901718   3.75951584794906
 O  -1.58772142840654   -3.23499137814704   0.66995353590370
 H  -2.50313089182168   -4.45674273002220   2.07703777862221
 H  -0.85762557729657   -3.88843098704158   2.51332742242202
 C  -1.05745577915271   -4.31996870782221   -0.08704077752225
 C  -1.03014529042611   -3.91743746233784   -1.53897082414234
 H  -1.71193806898327   -5.21347330417338   0.03250287567050
 H  -0.02902288464443   -4.57438823673694   0.25431853869612
 O  -0.15365465009195   -2.81081117322769   -1.69535642463572
 H  -2.05277133323089   -3.63648542383731   -1.88256567071063
 H  -0.66696234147812   -4.77686968055731   -2.14898319619317
 C  -0.02809714034984   -2.41975052589643   -3.05759416197039
 C  1.04969139714378    -1.36553156642905   -3.16345442937393
 H  -1.01661359661555   -2.07513315456018   -3.44236746631042
 H  0.27801665222553    -3.29883644099750   -3.67156189039890
 H  1.28055211174429    -1.16739324222998   -4.23731142043058
 H  1.96435238774134    -1.77211247337077   -2.68965714644670
 C  1.96400544802087    0.67761745756206    -2.29859316077448
 C  1.93789549912003    1.72188124226821    -1.20295681221765
 H  2.26103494496625    1.17100622710020    -3.25592255862891
 H  2.75929453958572    -0.05126292905830   -2.04479160865024
 O  1.70769243113421    1.09808919844296    0.05796599811834
 H  1.18688830067186    2.51844749991946    -1.36869596871115
 H  2.92430198527676    2.23921660175921    -1.19290796821629
 C  1.52372759057996    2.06946510873288    1.08447966419588
 C  1.58439703917735    1.39904712625605    2.43242635907259
 H  0.55143212638272    2.59204858869983    0.94943178225334
 H  2.33291083548670    2.82737768026374    1.03843379661997
 O  0.59256225057542    0.39077913962287    2.47560994967043
 H  1.41477269018262    2.17988513919323    3.20890948198560
 H  2.59147745697698    0.94781449184253    2.58992706328159
 C  0.45305736620971    -0.21059905391616   3.74909882820626
 C  -0.44732676010847   -1.43010161351780   3.62209809125560
 H  1.44248580875242    -0.54319891226886   4.14273002741883
 H  0.05761299152486    0.53800784828196    4.47846239997161
 H  0.14469784731641    -2.23064314895883   3.13895856949903
 H  -0.71868908809108   -1.77386632230128   4.65309977979203
 O  1.85448969595881    0.46381567363437    -5.83745854952318
 H  2.79458651175420    0.26931638970332    -6.01221943407689
 H  1.42992461458681    0.27462405916792    -6.69588777902563
 O  -4.62080408958072   -2.31013319614896   0.21817524359742
 H  -4.53641194312162   -3.30438663626278   0.23453246844926
 H  -5.55492214735003   -2.14144338046171   -0.00481834583192
 O  -3.76251103468883   0.52259069342205    -3.05754207400276
 H  -4.14470170948763   1.43965207043220    -3.00279630849075
 H  -4.21808008678377   0.09788899010603    -3.80655825803586
 O  0.28772184758466    5.10604632100834    0.77988784894190
 H  0.77746747696729    4.98942979425179    1.65709653945896
 H  -0.24555842686331   5.91471561175065    0.89087779468007
 O  3.89263928964603    -0.81761497758676   1.02947733617883
 H  4.55090292243896    -1.17325822962953   1.65745859972100
 H  4.10575767706790    0.18026266294488    0.99468186128649
 O  -4.64613954189546   3.09974261099503    -2.89490035498219
 H  -5.53767904829737   3.31468438335647    -2.55856403667265
 H  -4.55251134211869   3.65180616350445    -3.69539573178180
 O  4.73295535569212    1.66472319422873    1.02424079248110
 H  4.61859629993293    2.26145592447005    1.80499101125174
 H  4.58733330454954    2.30857645993554    0.28866136687463
 O  1.39443606562076    -2.09809071443517   1.02940547179245
 H  1.70639267190717    -2.89446120480552   0.49179269464155
 H  2.20424436811503    -1.53365229646388   1.13523549127996
 O  -2.65849759436848   -1.16216825059813   -1.24842026277000
 H  -3.08507906530468   -0.49070737799976   -1.84697098278914
 H  -3.39620633063324   -1.59443344293000   -0.73144146481091
 O  -4.38744794376648   -5.03122184308306   0.31537281489166
 H  -4.50865579874392   -5.56895375628455   -0.49092020398301
 H  -4.89546826980603   -5.50966347739114   0.99929359724623
 O  1.66460893748811    4.64756296316157    2.98663224797630
 H  1.56195693408758    5.08817906906320    3.84935395511879
 H  2.64625815831815    4.47568100634573    2.87633307564206
 O  2.36642812349980    -4.09883314282532   -0.44087720928551
 H  2.97994264403277    -3.47134564856402   -0.92609843473601
 H  2.96820852461792    -4.67324209346018   0.06938589422347
 O  2.02289425564494    4.96975359119959    -1.18908393440358
 H  1.33058349119659    5.07362816170286    -0.44958795314529
 H  2.02110229235932    5.82212745366424    -1.66285035460167
 O  3.86122282181019    -2.06371283325118   -1.34921374397006
 H  4.74240556513068    -2.08192430502566   -1.76646882605878
 H  3.97737590125195    -1.56576400259457   -0.48275933954383
 O  4.23425829952923    4.04768753298403    2.41197683084211
 H  4.96951938805484    4.49929573390450    2.86892417806750
 H  4.32373795900733    4.28947834424644    1.43264630353213
 O  4.28205107092754    4.14866934693894    -0.21662803880519
 H  4.99878694775183    4.52051772397761    -0.76490020187780
 H  3.40457865945976    4.50446799491805    -0.62500135849519
```

Figure S14: Three optimized coordinates for Pb-[2.2.2] complexes with 16 explicit water molecules

Figure S15 shows the partial charges used in OPLS force field for the molecular dynamics simulations, which are taken from [1].

Atoms	Partial Charge	Atoms	Partial Charge	Atoms	Partial Charge
NT	-0.171	HC	0.128	CT	-0.198
NT	-0.171	CT	-0.198	CT	0.244
CT	-0.198	CT	0.244	HC	0.128
CT	0.244	HC	0.128	HC	0.128
HC	0.128	HC	0.128	OS	-0.405
HC	0.128	OS	-0.405	HC	-0.021
OS	-0.405	HC	-0.021	HC	-0.021
HC	-0.021	HC	-0.021	CT	0.244
HC	-0.021	CT	0.244	CT	0.244
CT	0.244	CT	0.244	HC	-0.021
CT	0.244	HC	-0.021	HC	-0.021
HC	-0.021	HC	-0.021	OS	-0.405
HC	-0.021	OS	-0.405	HC	-0.021
OS	-0.405	HC	-0.021	HC	-0.021
HC	-0.021	HC	-0.021	CT	0.244
HC	-0.021	CT	0.244	CT	-0.198
CT	0.244	CT	-0.198	HC	-0.021
CT	-0.198	HC	-0.021	HC	-0.021
HC	-0.021	HC	-0.021	HC	0.128
HC	-0.021	HC	0.128	HC	0.128
HC	0.128	HC	0.128		

Figure S15: Partial charges for [2.2.2] atoms used in OPLS force field.

References

(1) Wipff, G.; Auffinger, P. *J. Am. Chem. Soc.* **1991**, *113*, 5976–5988.