

Supporting Information

African Viper Poly-His Tag Peptide Fragment Efficiently Binds Metal Ions and Is Folded into an α - Helical Structure

*Joanna Watly¹, Eyal Simonovsky^{2,3}, Nuno Barbosa¹, Marta Spodzieja⁴, Robert Wieczorek¹, Sylwia
Rodziewicz-Motowidlo⁴, Yifat Miller^{2,3,*}, Henryk Kozlowski^{1,*}*

¹Faculty of Chemistry, University of Wrocław, 50-383 Wrocław, Poland

² Department of Chemistry, and ³ Ilse Katz Institute for Nanoscale Science and Technology, Ben-Gurion
University of the Negev, Beer-Sheva 84105, Israel

⁴Faculty of Chemistry, University of Gdańsk, Gdańsk, Poland

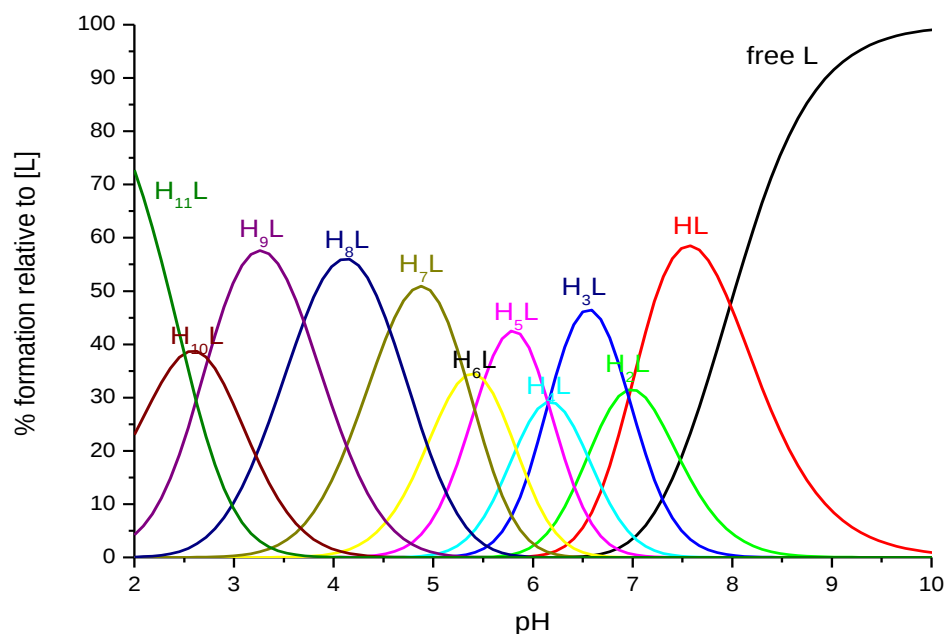


Figure S1. Representative distribution diagram for the protonation of pHG. Measurement were performed at a constant temperature of 25°C under an argon atmosphere using a Molspin pH-meter, equipped with a semi-combined electrode Mettler Toledo InLab and micrometer syringe with a volume of 0.5 cm³. The pH-metric titrations were performed in a water solution of HCl at 0.1 mol·dm⁻³ KCl. The titrant was a carbonate-free, standard solution of NaOH. $C_L = 5 \cdot 10^{-4}$ mol·dm⁻³.

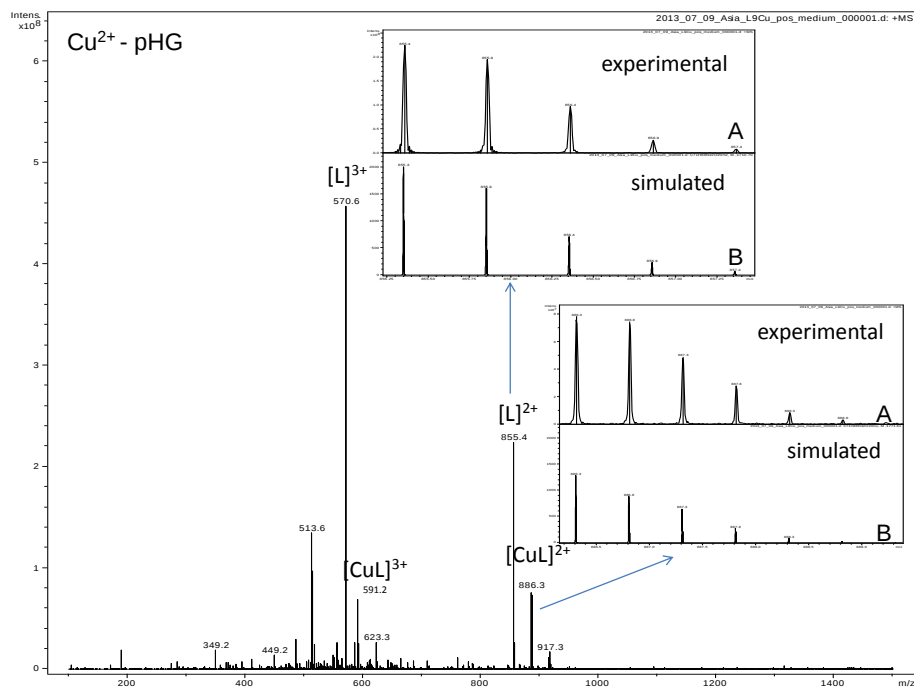


Figure S2. Experimental (A) and Simulated (B) ESI positive mass spectra (ESI-MS) for Cu^{2+} -pHG complex.

Metal/ligand in a 1:1.1 stoichiometry, where $[\text{ligand}]_{\text{tot}} = 5 \cdot 10^{-4} \text{ mol} \cdot \text{dm}^{-3}$. Measurements were prepared in 1:1 MeOH- H_2O mixture at pH 4.5.

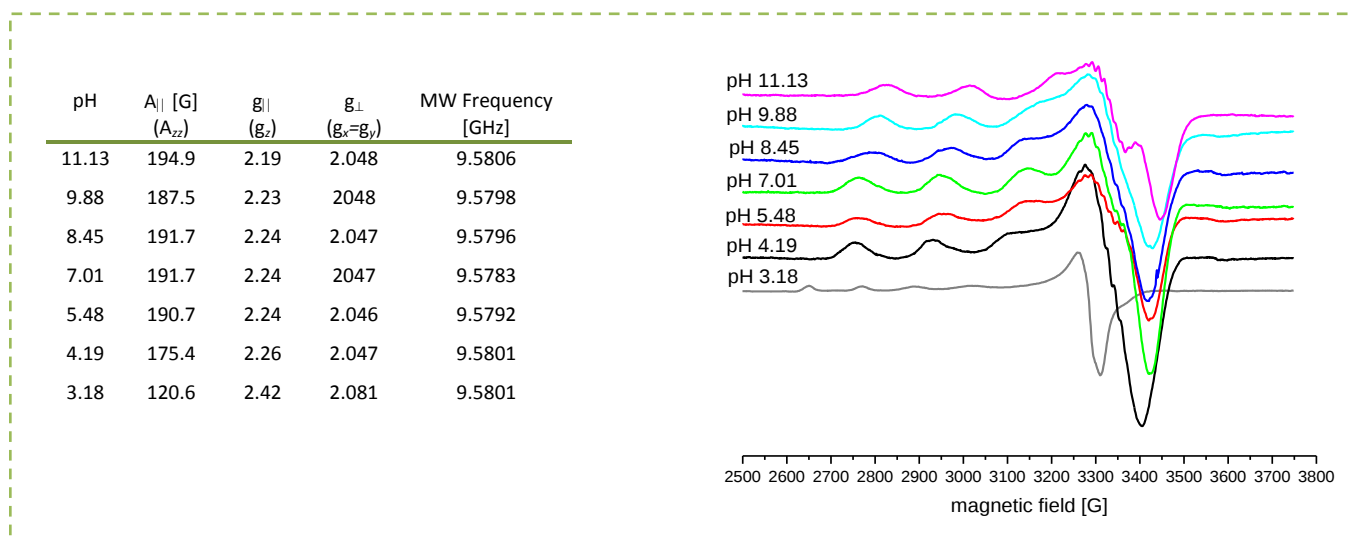


Figure S3. X-band EPR spectra of frozen solution (77 K), at different pH values, for the system Cu^{2+} - pHG. pHG in water solution of HCl at $I=0.1 \text{ mol}\cdot\text{dm}^{-3}$ (KCl). $C_M^\circ = 1\cdot 10^{-3} \text{ mol}\cdot\text{dm}^{-3}$; M/L molar ratio 1:1.1. Ethylene glycol (30%) was used as a cryoprotectant.

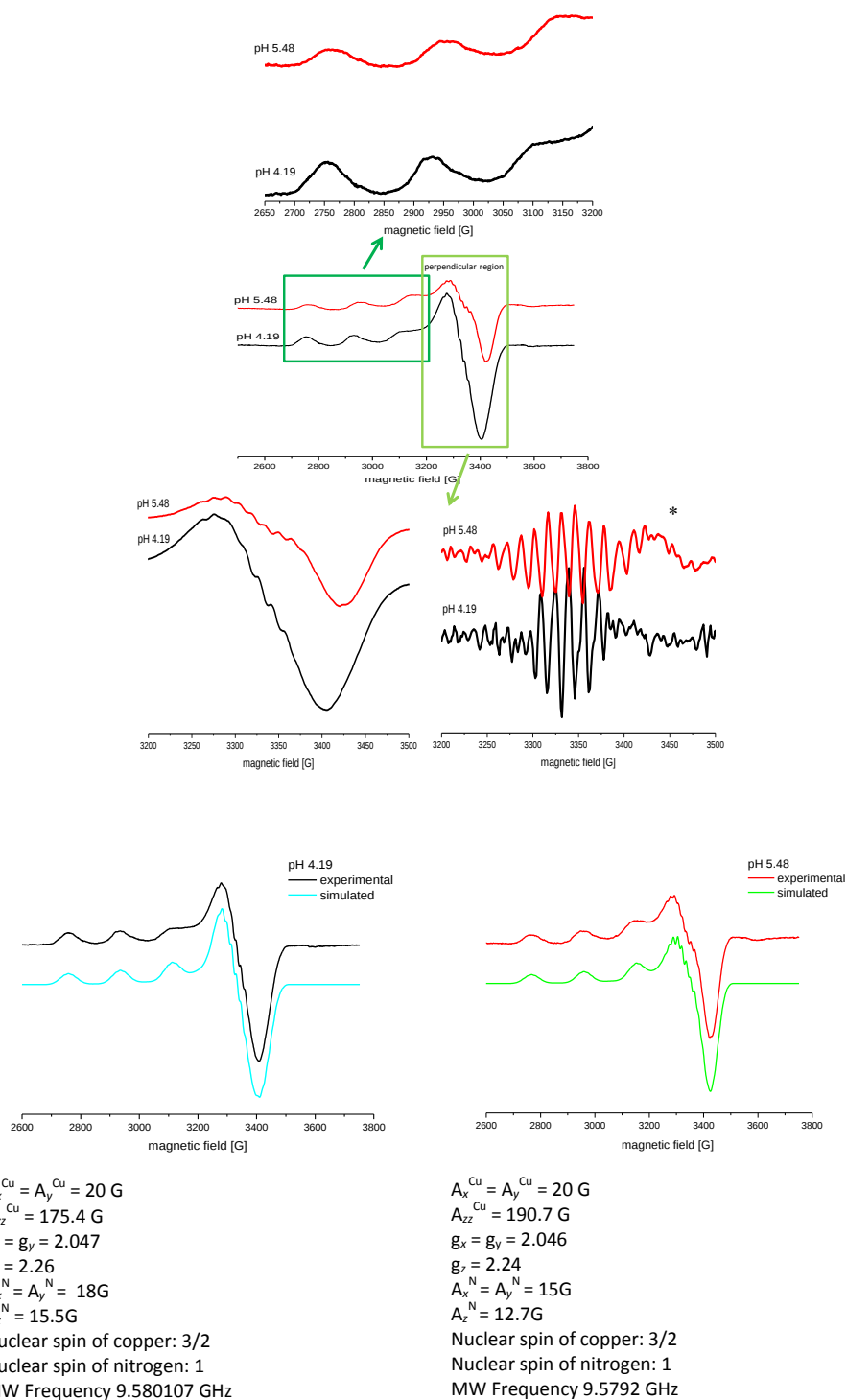


Figure S4. Comparison of the experimental X-band EPR spectra for the systems Cu^{2+} - pHG at pH 4.19 and 5.48 and the second derivative X-band EPR spectra for the same system (with star *). The X-band EPR spectra of frozen solution at MW Frequency 9.58 [GHz].

Table S1. Conformational energies and populations obtained from the GBMV and Monte-Carlo calculations.

Model	Conformational energy [kcal/mol]*	Standard Deviation [kcal/mol]	Populations [%]
M1	-1004.69 (0.89)	19.92	9.5361
M2	-970.22 (0.68)	15.26	2.422
M3	-985.79(0.69)	15.33	5.1488
M4	-999.38 (0.87)	19.54	8.2467
M5	-1011.10 (1.27)	28.33	10.0925
M6	-995.56 (0.87)	19.44	7.6204
M7	-1012.93 (0.97)	21.78	10.8783
M8	-999.62 (0.89)	19.98	8.4538
M9	-994.82 (0.79)	17.62	7.3627
M10	-1009.33 (0.83)	18.56	10.51
M11	-1017.02 (1.15)	25.67	11.6147
M12	-998.36 (1.22)	27.20	8.114

* Standard error of the averaged conformational energy values in parenthesis.

Figure YS1

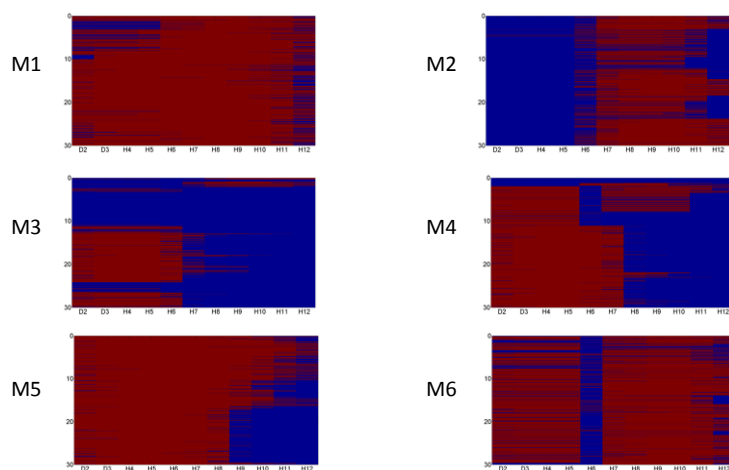


Figure S5. DSSP calculations for each residue along the pHG peptide along the time of the simulations for models M1-M6.

Figure YS2

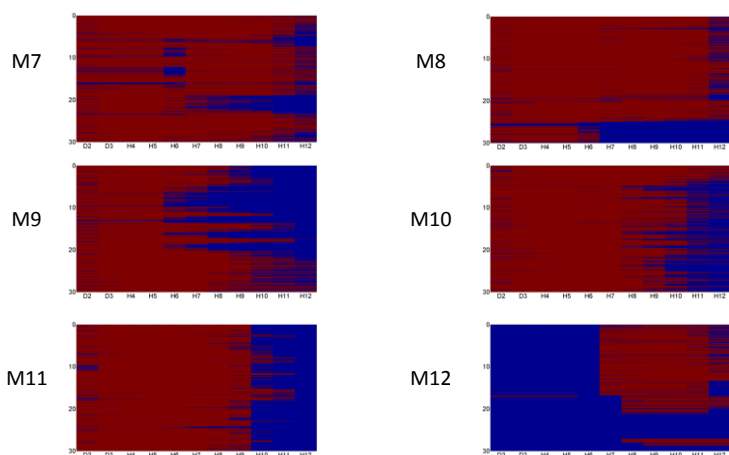
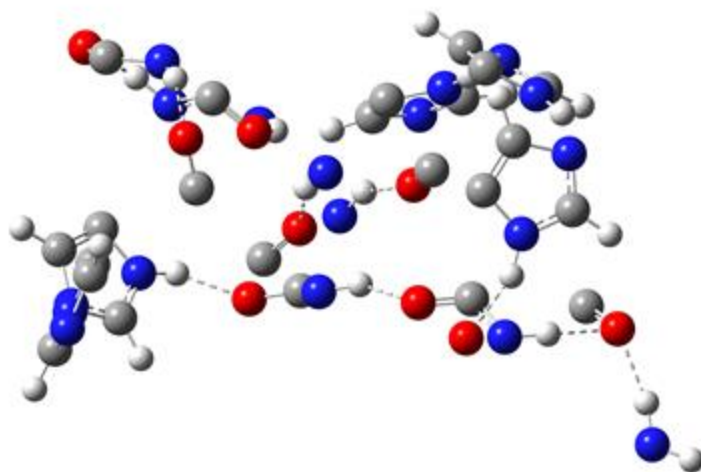
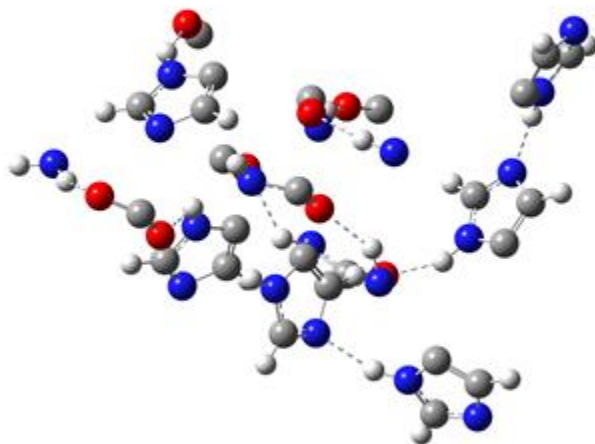


Figure S6. DSSP calculations for each residue along the pHG peptide along the time of the simulations for models M7-M12.

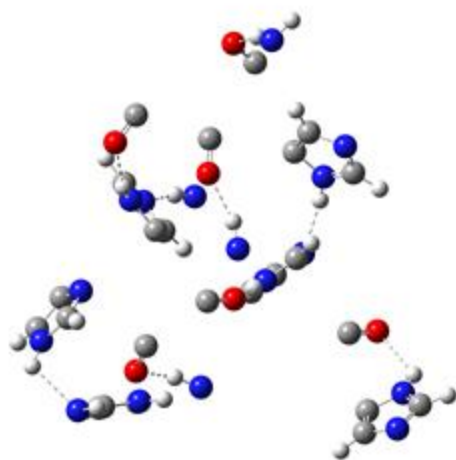
Cu^{2+} - pHG complex A



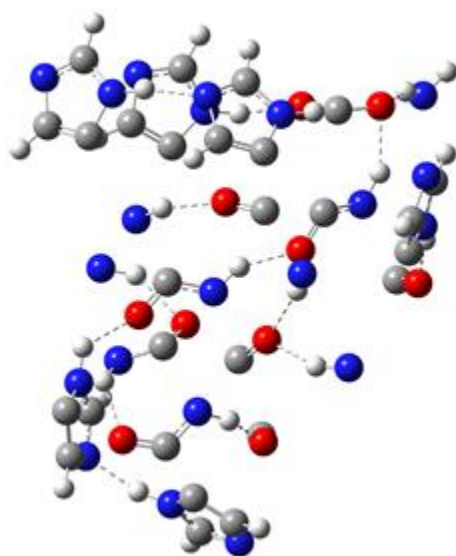
Cu^{2+} - pHG complex B



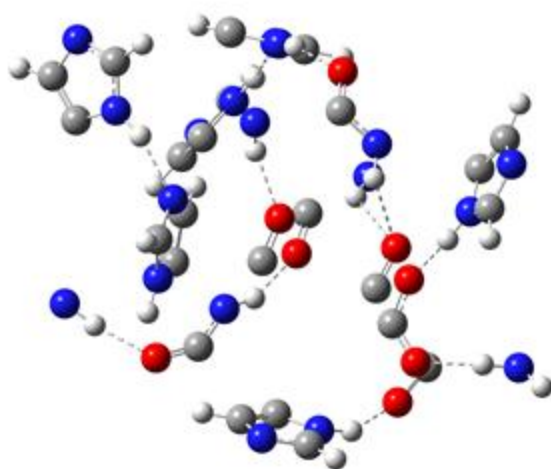
Cu^{2+} - pHG complex C



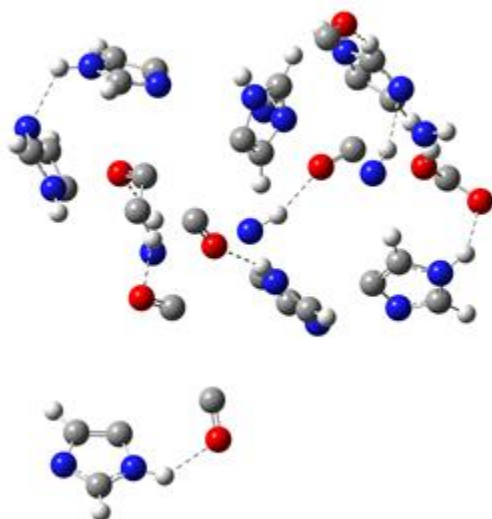
Ni^{2+} - pHG complex A



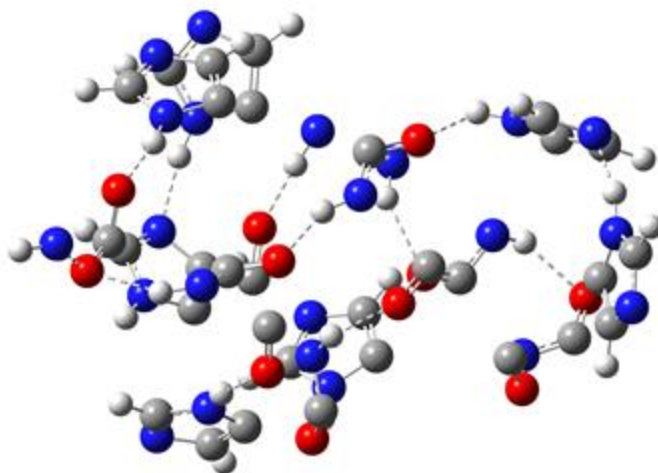
Ni^{2+} - pHG complex B



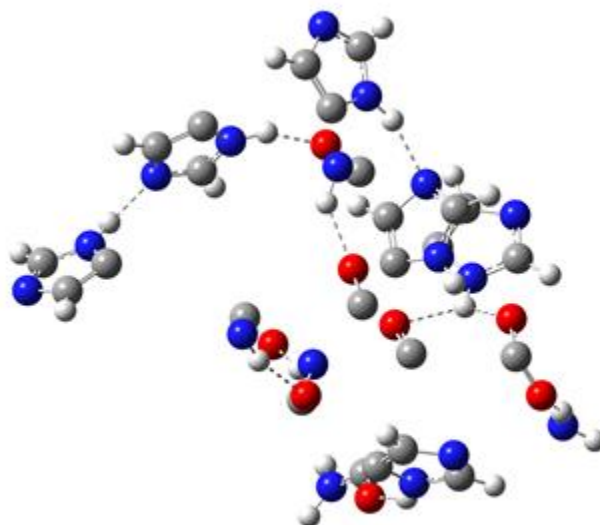
Ni^{2+} - pHG complex C



Zn^{2+} - pHG complex A



Zn^{2+} - pHG complex B



Zn²⁺ - pHG complex C

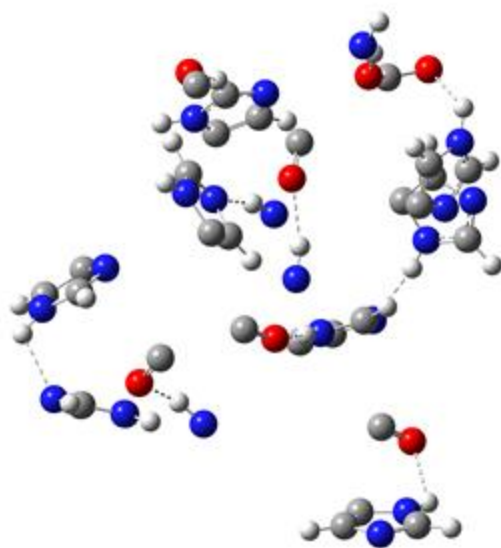


Figure S7. Hydrogen bonds in complexes A, B and C.

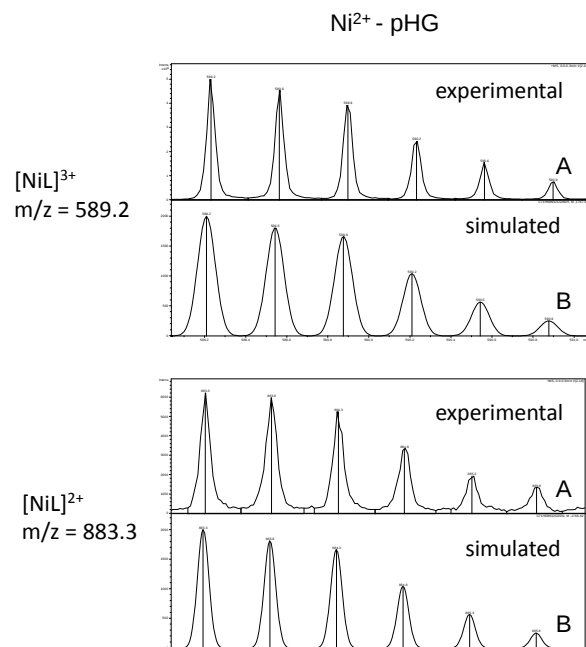


Figure S8. Experimental (A) and Simulated (B) ESI positive mass spectra (ESI-MS) for Ni^{2+} - pHG complex at pH 4.5 in methanol/water solution. Metal/ligand in a 1:1.1 stoichiometry, where $[\text{ligand}]_{\text{tot}} = 5 \cdot 10^{-4} \text{ mol} \cdot \text{dm}^{-3}$. Measurements were prepared in 1:1 MeOH- H_2O mixture at pH 4.5.

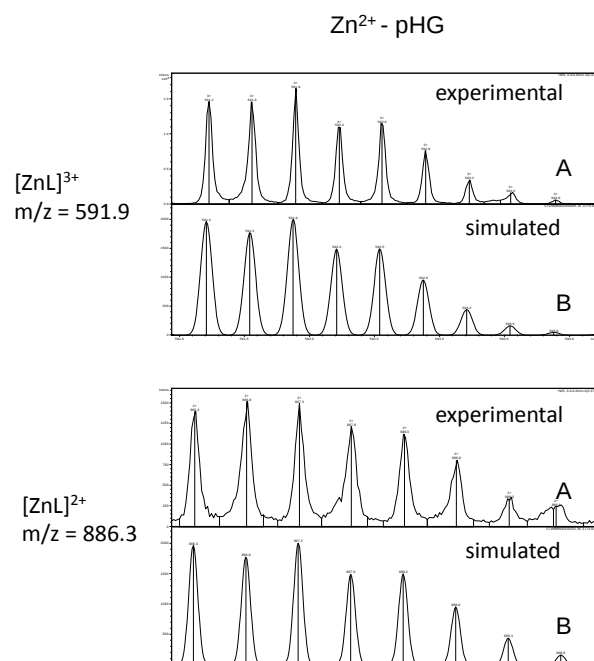


Figure S9. Experimental (A) and Simulated (B) ESI positive mass spectra (ESI-MS) for Zn^{2+} - pHG complex at pH 4.5 in methanol/water solution. Metal/ligand in a 1:1.1 stoichiometry, where $[\text{ligand}]_{\text{tot}} = 5 \cdot 10^{-4} \text{ mol} \cdot \text{dm}^{-3}$. Measurements were prepared in 1:1 MeOH- H_2O mixture at pH 4.5.

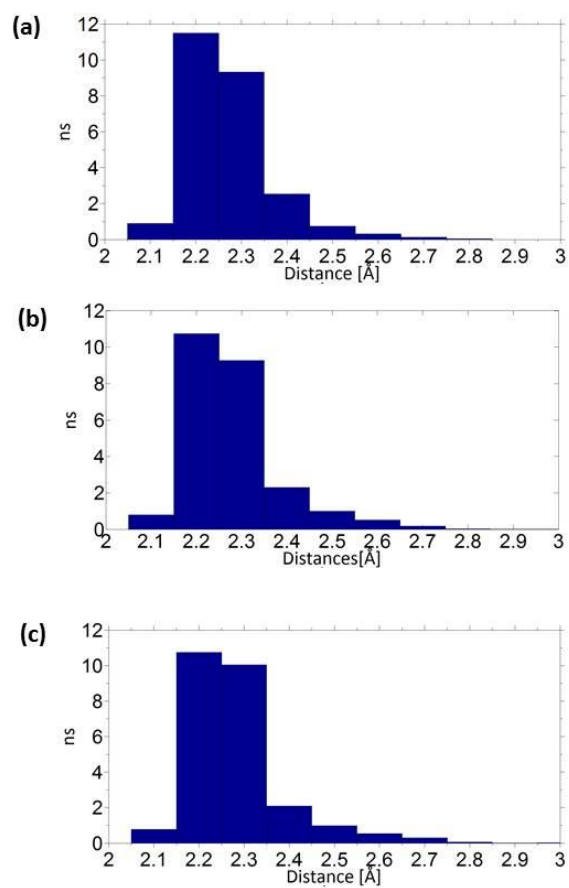


Figure S10. The distance distribution between Cu^{2+} and imidazole groups in the M12 model: (a) Cu^{2+} -His 5, (b) Cu^{2+} -His7 and (c) Cu^{2+} -His8.

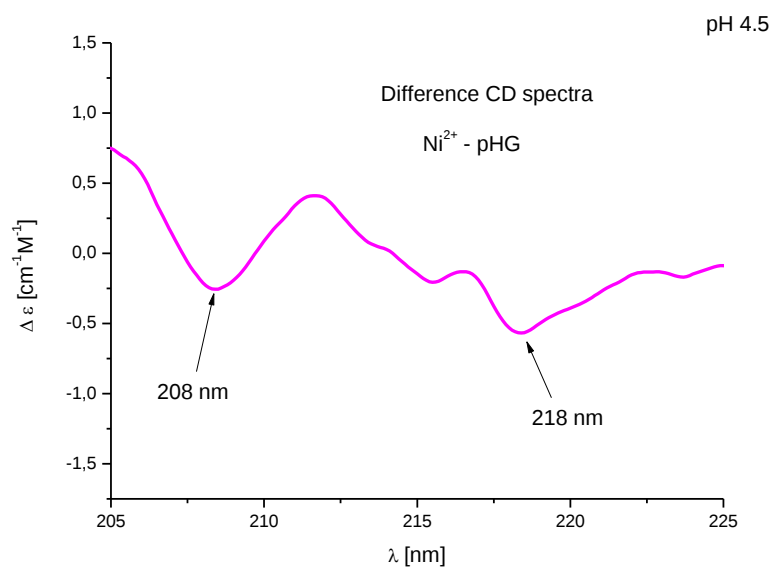


Figure S11. Difference CD spectra, at pH 4.5 for the Ni^{2+} -pHG system. $C_M^\circ = 4 \cdot 10^{-4} \text{ mol} \cdot \text{dm}^{-3}$; M/L molar ratio 1:1.1. Path length 0.01cm.

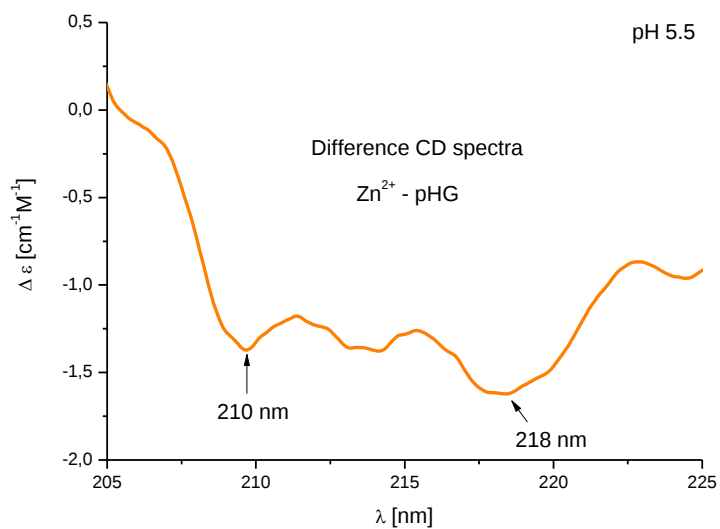


Figure S12. Difference CD spectra, at pH 5.5 for the Zn^{2+} -pHG system. $C_M^\circ = 4 \cdot 10^{-4} \text{ mol} \cdot \text{dm}^{-3}$; M/L molar ratio 1:1.1. Path length 0.01cm.

H	7.97781100	-2.37038400	-1.78964700
C	8.34510600	-2.96806700	-0.95063500
H	8.26398700	-4.02551700	-1.20570700
C	7.58413000	-2.59067200	0.28394600
O	7.65329300	-1.44547100	0.77530200
H	9.39697300	-2.71466700	-0.81425200
N	6.78054400	-3.55525400	0.81300800
H	6.70497600	-4.46937500	0.39033400
C	5.94847500	-3.30377700	1.97004100
H	6.36068900	-3.78260800	2.86659800
H	5.93924900	-2.22640800	2.15225400
C	4.56193700	-3.85495400	1.74542400
O	4.39143300	-4.95330100	1.16117900
N	3.55905000	-3.09829400	2.23175900
H	3.76049900	-2.12934100	2.48882000
C	2.16476400	-3.53380600	2.27151300
H	2.15507200	-4.59610300	2.54285300
C	1.51596200	-3.38887900	0.89315200
O	0.69734000	-2.47234200	0.62467600
C	1.40806000	-2.72643500	3.31360300
H	2.03337100	-2.65048100	4.21072500
H	1.25434400	-1.70465600	2.93398100
C	0.11141000	-3.36633500	3.65411200
N	-0.65169100	-2.92686000	4.72160400
H	-0.49616200	-2.04499200	5.20200200
C	-0.57310500	-4.43880400	3.13112500
H	-0.32989100	-5.06504700	2.28645400
C	-1.75404300	-3.74011100	4.80324600
H	-2.52844600	-3.61436600	5.54077000
N	-1.74023800	-4.66172400	3.85305700
N	1.90888700	-4.29911700	-0.01771400
H	2.63064100	-4.96994600	0.24752900
C	1.38183900	-4.27862500	-1.37681400
H	1.10413600	-3.23251900	-1.56443700
C	0.07599100	-5.07954300	-1.47931000
O	-0.01198800	-6.09211700	-2.18792600
C	2.40871500	-4.74524100	-2.41708100
H	3.26358900	-5.22116600	-1.92673800
H	1.92734500	-5.51700200	-3.02799300
C	2.90168300	-3.61636000	-3.24502600
N	2.05212500	-2.70977600	-3.85227100
H	1.02994800	-2.67379300	-3.83382000
C	4.16951100	-3.15809400	-3.51622100
H	5.11186700	-3.58942500	-3.22008100
C	2.80881000	-1.74416200	-4.43942600
H	2.38055500	-0.93928900	-5.01210000
N	4.10749100	-1.97855700	-4.25251200
N	-0.96351800	-4.53296100	-0.79149200

H	-0.80419100	-3.65950500	-0.29287900
C	-2.34026700	-4.83014200	-1.20414100
H	-2.33367900	-5.83160800	-1.63642300
C	-2.60366600	-3.86190400	-2.35811600
O	-2.57264700	-4.22735100	-3.54366800
C	-3.34342200	-4.75025800	-0.06246000
H	-2.99275200	-5.39530600	0.75480900
H	-3.38144700	-3.73263300	0.35621700
C	-4.68938200	-5.15594800	-0.55987600
N	-5.86938100	-4.81371300	0.07533000
H	-5.95220200	-4.23469500	0.91820400
C	-5.06617800	-5.90132600	-1.65582500
H	-4.44744500	-6.34226600	-2.41970300
C	-6.89332200	-5.35304200	-0.65286600
H	-7.92845600	-5.21100400	-0.39828400
N	-6.44730100	-6.02243100	-1.70584700
N	-2.70711600	-2.55297500	-1.98478600
H	-2.87349900	-2.27239800	-1.02250900
C	-2.67322100	-1.49240800	-2.97659400
H	-2.78480900	-1.98881500	-3.94653300
C	-1.24474300	-0.94915700	-2.95425300
O	-0.34833300	-1.49507100	-3.64768200
C	-3.75764300	-0.43248200	-2.79088100
H	-3.50628300	0.19340900	-1.92965100
H	-3.72850700	0.22992800	-3.66772800
C	-5.12956200	-0.97992200	-2.58502300
N	-6.16637600	-0.14280900	-2.18981500
H	-6.14721000	0.86709900	-2.00610000
C	-5.68655300	-2.23617900	-2.67376100
H	-5.22162700	-3.17179600	-2.93824800
C	-7.28581400	-0.91891300	-2.06220700
H	-8.24130000	-0.51251600	-1.77771400
N	-7.03651200	-2.18766300	-2.34627600
N	-0.93960400	0.09860100	-2.14029400
H	-1.62857500	0.56280700	-1.54643900
C	0.37962300	0.68832500	-2.16971200
H	0.88888000	0.21942100	-3.01940600
C	1.20355500	0.41429100	-0.90910500
O	0.78598700	0.68107300	0.23765600
C	0.29346900	2.21763600	-2.41026500
H	-0.31721300	2.37464300	-3.30586600
H	-0.24168400	2.67976800	-1.57608000
C	1.65689100	2.77101600	-2.54770300
N	2.47700600	2.48705800	-3.63603300
H	2.16789400	2.07008300	-4.50017200
C	2.47288600	3.37966700	-1.63755600
H	2.20446200	3.76971100	-0.66795100
C	3.74016000	2.90341900	-3.36067700

H	4.57842800	2.80457400	-4.02529700
N	3.77491200	3.43647300	-2.14279400
N	2.46673900	-0.03859100	-1.13815200
H	2.71844400	-0.24299700	-2.10023400
C	3.35161600	-0.62009600	-0.12941100
H	2.82715900	-1.47303800	0.31356600
C	3.73710400	0.22208800	1.07541600
O	4.14250000	-0.38075100	2.09886000
C	4.62974600	-1.15632300	-0.80954000
H	5.23884200	-1.60697400	-0.02363600
H	4.33470100	-1.96366700	-1.48685500
C	5.43971700	-0.12475300	-1.51761700
N	5.57815200	-0.03845800	-2.89741700
H	5.16621500	-0.70298900	-3.58164600
C	6.19043600	0.90616100	-1.01081500
H	6.40486400	1.10876200	0.02477000
C	6.39484800	1.02281500	-3.16047200
H	6.70370100	1.29425800	-4.15592800
N	6.77269800	1.63847300	-2.04077300
N	3.66069500	1.56853000	1.05485000
H	3.36259100	2.03304500	0.20781100
C	3.91747600	2.32973600	2.27575800
H	4.58001100	1.70044700	2.88165400
C	2.66409100	2.52547500	3.13543000
O	2.70605400	3.31664100	4.09572400
C	4.60578900	3.68055400	2.04119800
H	4.08465600	4.24487800	1.25808500
H	4.47485100	4.24257700	2.96958700
C	6.04334900	3.57494600	1.68510700
N	6.46997500	3.65852100	0.35778900
C	7.13982700	3.34267000	2.46831900
H	7.23723600	3.21507000	3.53133200
C	7.78733600	3.47265800	0.33970300
H	8.39157600	3.40975700	-0.54720000
N	1.58149600	1.78270200	2.81743600
H	1.54590600	1.26088600	1.94375700
C	0.33655000	1.93526200	3.56818300
H	0.59979800	2.23212900	4.58578300
C	-0.39254700	0.59676900	3.69260200
O	-0.47062900	0.01050700	4.79506600
C	-0.50323900	3.02986600	2.89362500
H	0.05531600	3.96945400	2.98377100
H	-0.56123400	2.81713900	1.81400400
C	-1.88117800	3.19213400	3.42773100
N	-2.77492800	4.04386000	2.79952400
H	-2.52105400	4.63419100	2.00496900
C	-2.59195600	2.61416300	4.45618100
H	-2.24969000	1.91605200	5.20247200

C	-3.97121000	3.95588100	3.46038200
H	-4.84186500	4.52269100	3.17434000
N	-3.90421300	3.08543900	4.46098500
N	-0.97923200	0.16346300	2.55429500
H	-0.64181400	0.54006100	1.66873900
C	-2.09343900	-0.78111300	2.42774500
H	-1.74033400	-1.78491300	2.16199100
C	-2.92630800	-0.27153500	1.25687600
O	-3.13722600	-0.96073100	0.24053400
C	-3.02546000	-0.86621700	3.66131300
H	-2.50706800	-1.34513100	4.48411500
H	-3.27934100	0.14104900	4.00405100
C	-4.26126700	-1.59939700	3.27147100
N	-5.45564500	-0.93241600	3.02340400
H	-5.62849100	0.03854000	3.23639800
C	-4.47538300	-2.88847200	2.85225100
H	-3.79385700	-3.72598300	2.88243900
C	-6.32992000	-1.82213800	2.46618800
H	-7.33283500	-1.56749100	2.17211300
N	-5.76479200	-3.01456200	2.34799400
N	-3.42930800	0.97549800	1.41448300
H	-3.17820100	1.51435600	2.23908700
C	-4.18501300	1.64893300	0.36946900
H	-4.37094500	0.89271000	-0.39980200
C	-3.24340900	2.65113400	-0.29176400
O	-2.14700000	2.22621400	-0.75284200
C	-5.55042000	2.13716300	0.85445600
H	-6.16465100	1.24560000	1.01590600
H	-5.46996100	2.68640100	1.79406600
C	-6.20473300	3.02051900	-0.20839200
O	-6.38670200	2.51699300	-1.35643300
O	-6.36387800	4.25580000	0.10942200
N	-3.58883700	3.93959200	-0.40326600
H	-4.48864100	4.27384600	-0.03941100
C	-2.84152800	4.84984200	-1.24611900
H	-2.55045200	4.31420900	-2.16156800
C	-1.57844000	5.32436300	-0.55359900
O	-1.44500600	5.34356400	0.68502800
C	-3.75214000	6.03087700	-1.60653700
H	-4.15705800	6.44326400	-0.67267400
H	-3.17731600	6.83408600	-2.07818500
C	-4.89504100	5.60511000	-2.53773900
H	-4.52350200	5.52101500	-3.56209400
H	-5.31534300	4.63924600	-2.24270900
C	-5.96647500	6.67243200	-2.51549400
O	-5.87046100	7.69679600	-3.22103700
N	-6.95818100	6.44597100	-1.62954800
H	-7.68263100	7.13965500	-1.53725600

H	-6.96249900	5.61209800	-1.03385300
N	-0.59802300	5.76587900	-1.37899700
H	-0.71518400	5.79783700	-2.37823400
H	0.21552800	6.20250600	-0.97529800
Cu	5.25739000	3.57379100	-1.04308800
H	9.17608300	3.09546800	1.87593600
N	8.22454600	3.28076300	1.60668900

Structure S1. The Cu²⁺-pHG complex A. Coordinates in Å.

H	-5.83708900	-0.66029700	2.32449500
C	-6.27986400	-0.32844700	3.26505200
H	-7.33177800	-0.60813900	3.27492700
C	-6.17241500	1.15509600	3.38538100
O	-7.09570600	1.94100700	3.10794500
H	-5.75493300	-0.84869800	4.06878300
N	-4.96846400	1.63775700	3.85449100
H	-4.24470600	0.97504500	4.11918700
C	-4.91333100	3.01088300	4.30557000
H	-5.85699900	3.28596300	4.78349000
H	-4.11843500	3.10931400	5.05239000
C	-4.66883500	4.07622200	3.25813700
O	-4.96980500	5.26161900	3.49694700
N	-4.01932600	3.68770100	2.12990800
H	-3.91025600	2.69811700	1.92757300
C	-3.56309200	4.63059200	1.12405800
H	-4.41845500	5.14920500	0.66586800
C	-2.84558700	3.82716300	0.05036100
O	-2.67561300	2.59006900	0.18621700
C	-2.65894900	5.72108000	1.77747900
H	-3.30043200	6.22741000	2.50243200
H	-1.87759000	5.20517500	2.34262200
C	-2.06313300	6.68090200	0.81532800
N	-0.70892900	6.69674500	0.51392500
H	-0.00553300	6.12670600	0.99005000
C	-2.63195300	7.60343300	-0.03462800
H	-3.66528200	7.90195300	-0.10049200
C	-0.51887200	7.61153700	-0.48737300
H	0.44218500	7.81145200	-0.92563400
N	-1.66075900	8.17817500	-0.85022200
N	-2.38815800	4.47457300	-1.05104900
H	-2.47025800	5.48511100	-1.12105100
C	-1.62363300	3.74281000	-2.05208800
H	-1.79101000	2.68568200	-1.83135200
C	-0.13683200	4.04128500	-1.92660100
O	0.34890000	5.11109600	-2.34111100
C	-2.06534600	4.01584700	-3.50414700

H	-3.13400800	4.24715700	-3.50734200
H	-1.53202400	4.89177100	-3.88471900
C	-1.85647400	2.78062900	-4.30870900
N	-0.64570900	2.11020100	-4.42823800
H	0.29275900	2.43652000	-4.18761600
C	-2.79250100	1.91515400	-4.80886300
H	-3.85744800	2.06311500	-4.88923300
C	-0.89173600	0.88295000	-4.97139300
H	-0.11044800	0.16726000	-5.17858800
N	-2.19392700	0.72231700	-5.20400200
N	0.61956000	3.04643600	-1.39367100
H	0.21382600	2.20857600	-0.97517500
C	2.06776200	3.09191000	-1.51079800
H	2.26481400	4.01593100	-2.06842400
C	2.42704400	1.99021700	-2.50534500
O	2.03535600	2.16024500	-3.68757700
C	2.78339400	3.19352300	-0.15980200
H	2.29411000	3.99813100	0.40403800
H	2.63714300	2.28515700	0.42893400
C	4.22822700	3.45569200	-0.35222800
N	4.70140500	4.58290900	-1.02154100
H	4.13974400	5.37305000	-1.29849200
C	5.32411900	2.67894800	-0.12422800
H	5.38100400	1.73431100	0.40837200
C	6.03986000	4.45460900	-1.20812700
H	6.65434700	5.17630100	-1.71489700
N	6.45166800	3.30207500	-0.68765100
N	3.05787100	0.84629000	-2.15550400
H	3.26620000	0.59758800	-1.19219200
C	3.20510300	-0.17062900	-3.19649200
H	3.43098200	0.35594400	-4.12611900
C	1.90880400	-0.93392700	-3.44899000
O	1.72272500	-1.51649900	-4.53594400
C	4.29326400	-1.23442000	-2.92680200
H	3.89588100	-1.96979500	-2.22087400
H	4.44951900	-1.74973700	-3.87814900
C	5.58239200	-0.72440500	-2.39054000
N	5.90515700	-0.88919600	-1.05360300
H	5.28007900	-1.16675000	-0.29986900
C	6.64970400	-0.06156100	-2.94099100
H	6.80927500	0.24266900	-3.96022200
C	7.11589700	-0.35969900	-0.81448000
H	7.58867800	-0.40169200	0.15132900
N	7.62298900	0.17161400	-1.95420300
N	1.05106600	-1.02948400	-2.40201400
H	1.30538200	-0.61933000	-1.50579700
C	0.00164300	-2.04227900	-2.39000600
H	-0.36661300	-2.15552000	-3.41492900

C	-1.08716200	-1.54519300	-1.46662300
O	-0.93093800	-1.63647700	-0.22318500
C	0.56990100	-3.37314300	-1.86650600
H	1.38988900	-3.66781900	-2.53509600
H	1.00420300	-3.15448800	-0.88599600
C	-0.42779700	-4.45781000	-1.69722700
N	-0.97031000	-5.19331100	-2.74506100
H	-0.80111600	-5.03572700	-3.72478000
C	-0.97788500	-5.00287300	-0.56366200
H	-0.78600900	-4.72735400	0.46270500
C	-1.81247000	-6.13083200	-2.20551800
H	-2.39138300	-6.81432600	-2.80045400
N	-1.83126000	-6.04975600	-0.88531500
N	-2.16500000	-0.98305700	-2.03549200
H	-2.22726900	-0.94831200	-3.04697400
C	-3.17447800	-0.27947400	-1.25092500
H	-2.68277200	0.50041200	-0.65776700
C	-3.91507900	-1.14086100	-0.25091100
O	-4.44421200	-0.57218300	0.72832700
C	-4.20582000	0.41614900	-2.15573600
H	-4.91723400	0.89442500	-1.47584500
H	-3.69909900	1.22156700	-2.69537300
C	-4.94153500	-0.47216400	-3.10102700
N	-4.52928100	-0.73494300	-4.40620500
H	-3.68227300	-0.37414900	-4.86541600
C	-6.13789100	-1.13771800	-2.96166500
H	-6.77703300	-1.17180600	-2.09386200
C	-5.49040700	-1.51736000	-4.98397900
H	-5.43500000	-1.84570600	-6.00810800
N	-6.47742900	-1.78751200	-4.13939300
N	-4.01660200	-2.46580200	-0.47304200
H	-3.71166500	-2.88609400	-1.35315900
C	-4.84835300	-3.28686100	0.40008700
H	-5.86736600	-2.88087900	0.42667100
C	-4.36247300	-3.24285400	1.84280200
O	-5.14736600	-3.36954500	2.79230700
C	-4.87829900	-4.73321900	-0.12232500
H	-3.88834900	-5.19011700	-0.00184300
H	-5.58006700	-5.29564900	0.49888500
C	-5.26767700	-4.78813400	-1.55346200
N	-4.37076100	-4.36346800	-2.54488800
C	-6.45063400	-5.15141000	-2.13877500
H	-7.37225400	-5.51333600	-1.71828100
C	-5.01773600	-4.48118000	-3.69532100
H	-4.63488900	-4.21211400	-4.66323700
N	-3.01422100	-3.08612100	1.98702800
H	-2.46376900	-3.02802900	1.13605900
C	-2.40038000	-2.65649900	3.23435500

H	-3.04369600	-2.96428500	4.06090700
C	-2.32592300	-1.12180100	3.27186000
O	-2.84695100	-0.44905400	4.18659800
C	-1.00608500	-3.28935500	3.31676000
H	-1.13470500	-4.37026600	3.44126400
H	-0.52180900	-3.16153600	2.33386700
C	-0.07839100	-2.74823800	4.35107800
N	1.17731700	-3.31903100	4.50729100
H	1.47762100	-4.14864600	3.99608900
C	-0.10066500	-1.68834200	5.23152900
H	-0.91532300	-1.02166600	5.45703700
C	1.85104100	-2.60095100	5.46510600
H	2.85261400	-2.83789700	5.78343300
N	1.11177800	-1.59900200	5.91633100
N	-1.57524400	-0.63223400	2.26366600
H	-1.42644400	-1.23148600	1.45444900
C	-1.05149000	0.70284500	2.02001200
H	-1.63591200	1.20890200	1.24677900
C	0.34531100	0.47556000	1.43845900
O	0.65905900	0.83843100	0.27550800
C	-1.01457800	1.58771800	3.27238900
H	-2.04794400	1.78308300	3.57447100
H	-0.55658900	1.04271900	4.10660200
C	-0.28229000	2.85797200	3.02531200
N	0.25667100	3.62444900	4.05119700
H	0.22613100	3.39065500	5.03064300
C	-0.00247900	3.55740400	1.88236700
H	-0.26055500	3.31191700	0.86968400
C	0.83251500	4.73721600	3.50079400
H	1.31923600	5.50157200	4.08000200
N	0.69648400	4.72507100	2.18183300
N	1.22270200	-0.15467200	2.24970500
H	0.90315200	-0.51112600	3.14779400
C	2.61842500	-0.34110400	1.87811800
H	2.91047700	0.49122600	1.23834300
C	2.82256000	-1.57302800	0.99832400
O	3.05419700	-1.44656200	-0.23228900
C	3.53152700	-0.34720200	3.09844700
H	3.52082800	0.65142500	3.54594500
H	3.18948500	-1.04461900	3.86923800
C	4.94940300	-0.72768700	2.67578500
O	5.33683100	-0.27522500	1.53009800
O	5.59460300	-1.51097800	3.42678600
N	2.78686800	-2.77228100	1.60952600
H	2.58876200	-2.81283300	2.60424000
C	3.16064900	-4.03299700	0.97568600
H	3.17530800	-3.85728100	-0.10569200
C	2.14910300	-5.10479900	1.32863000

O	1.60798300	-5.14450200	2.45494600
C	4.55023900	-4.49918900	1.44737000
H	4.56878600	-4.46272300	2.54469700
H	4.70969200	-5.54278600	1.15269000
C	5.67140200	-3.63778300	0.87832500
H	5.69767100	-3.74017300	-0.21192300
H	5.50991200	-2.59091300	1.13391600
C	7.00882700	-4.10040300	1.41387900
O	7.56024300	-5.12025400	0.95583100
N	7.50491200	-3.35453200	2.42450400
H	8.36868200	-3.65342600	2.84944400
H	6.97351500	-2.57780400	2.83290800
N	1.92721900	-6.04489400	0.39495700
H	2.31206000	-5.98915800	-0.53323600
H	1.28090000	-6.79328600	0.59799800
H	-6.99561100	-5.02331900	-4.19821600
N	-6.27592100	-4.96417400	-3.49896800
Cu	7.50958700	1.94007200	-1.35280900

Structure S2. The Cu²⁺-pHG complex B. Coordinates in Å.

H	-11.72455700	1.62628800	-1.29345100
C	-11.46494800	1.68140900	-0.23485900
H	-11.20443900	2.71119500	0.01428200
C	-10.36288200	0.70131100	0.05120000
O	-10.48640600	-0.51750300	-0.17851300
H	-12.35279400	1.39328700	0.33083700
N	-9.22507900	1.21994600	0.57557900
H	-9.10281800	2.20859900	0.75653300
C	-8.09230400	0.38864600	0.89545800
H	-8.34671300	-0.34930200	1.66610600
H	-7.76365600	-0.19465500	0.02629700
C	-6.96992500	1.27317700	1.37450400
O	-7.09505800	2.51099800	1.48855600
N	-5.81597200	0.63465100	1.67117800
H	-5.72075600	-0.35106400	1.43534000
C	-4.63487300	1.39587900	2.00354500
H	-4.84869300	2.05895500	2.85064500
C	-4.20908700	2.25291100	0.81105500
O	-4.46450200	1.89975600	-0.35979500
C	-3.50705500	0.41849400	2.40486700
H	-3.83954200	-0.15338300	3.27536900
H	-3.35139900	-0.31796200	1.60373600
C	-2.24060800	1.12960100	2.68694800
N	-1.31627600	1.39970200	1.69063800
H	-1.34813200	1.06725600	0.72437000
C	-1.76268700	1.74891500	3.81557300

H	-2.17437800	1.73451000	4.80958200
C	-0.33660300	2.16368500	2.23658000
H	0.55146500	2.43179000	1.69850200
N	-0.56121300	2.39011100	3.53096200
N	-3.47603100	3.36314100	1.06482600
H	-3.30467300	3.68241300	2.00981000
C	-2.93366200	4.13585100	-0.04664200
H	-2.86091000	3.44920500	-0.89537700
C	-1.56599000	4.70310500	0.29486500
O	-1.44379500	5.63742600	1.11950800
C	-3.89386200	5.28380400	-0.41587300
H	-4.84180100	4.82867500	-0.71445600
H	-4.07967100	5.86002800	0.49742700
C	-3.38625300	6.16325400	-1.49813900
N	-2.39894500	7.11821800	-1.27918000
H	-1.95595400	7.28048400	-0.38603300
C	-3.69510800	6.27228700	-2.83064100
H	-4.42043300	5.70834200	-3.39195800
C	-2.16349800	7.75230000	-2.47251700
H	-1.44024500	8.54049300	-2.58843200
N	-2.93194000	7.26519100	-3.43236900
N	-0.51936900	4.20265300	-0.40535100
H	-0.70064900	3.48767300	-1.10285800
C	0.79830000	4.84935300	-0.43324500
H	0.67872000	5.88706900	-0.76351500
C	1.66024500	4.16074100	-1.47871400
O	2.19278700	4.78540300	-2.40560100
C	1.53918400	4.83977700	0.91839600
H	0.89213400	5.28369900	1.67926300
H	1.74754000	3.80742100	1.20578000
C	2.85228500	5.52452600	0.78854700
N	4.03452600	4.78739500	0.69256100
C	3.13887500	6.85334900	0.61878700
H	2.50649500	7.72364300	0.61144900
C	5.00547600	5.65861900	0.46541900
H	6.04724800	5.41962800	0.33857600
N	1.79950200	2.81991800	-1.28638400
H	1.40570800	2.35698100	-0.47390700
C	2.31606300	1.93262800	-2.31963700
H	2.64899400	2.57347600	-3.14079800
C	1.08911800	1.16998600	-2.81472600
O	0.24578900	1.74200800	-3.53496900
C	3.45032000	1.05750000	-1.79350700
H	3.18769900	0.74346900	-0.77728800
H	3.49277800	0.14511500	-2.39901700
C	4.82048600	1.62842600	-1.77141600
N	5.41289200	2.18379600	-0.63262800
C	5.79138100	1.46885200	-2.72159700

H	5.76593200	1.05076100	-3.71109300
C	6.71330700	2.31449800	-0.89640300
H	7.46439300	2.63021900	-0.19598600
N	0.91549200	-0.09851100	-2.36899000
H	1.57212800	-0.55617800	-1.73505100
C	-0.27788200	-0.81552100	-2.73941000
H	-0.54879400	-0.48387100	-3.75081400
C	-1.46554000	-0.41424300	-1.85776000
O	-1.37726700	0.46609000	-0.97572400
C	-0.01030100	-2.32417400	-2.77452000
H	-0.83148700	-2.84929900	-3.28056700
H	0.88190200	-2.47506400	-3.39190800
C	0.20143800	-2.95359100	-1.44704600
N	0.89170800	-4.13809500	-1.32541300
H	1.48461300	-4.58526400	-2.02841200
C	-0.19027200	-2.62097400	-0.17419700
H	-0.67797400	-1.72644700	0.18573500
C	0.90832500	-4.48730100	-0.01647300
H	1.41152700	-5.36882900	0.33980300
N	0.24618000	-3.59720400	0.72040100
N	-2.62626300	-1.07139600	-2.11616100
H	-2.62979100	-1.82763700	-2.79117900
C	-3.88185000	-0.74494000	-1.45692700
H	-3.72116600	0.18507900	-0.90134100
C	-4.31380400	-1.77636500	-0.42976800
O	-5.47931900	-1.76096000	0.02813500
C	-5.01238700	-0.42769700	-2.44375200
H	-5.89748200	-0.21457000	-1.84099800
H	-4.75166200	0.50349400	-2.95557900
C	-5.29222300	-1.51672100	-3.41506600
N	-4.76230400	-1.52338400	-4.70373000
H	-4.23885300	-0.76808700	-5.11665100
C	-6.00982500	-2.68186300	-3.32411300
H	-6.57542200	-3.04397800	-2.48261500
C	-5.18353200	-2.66942200	-5.32984100
H	-4.93413400	-2.91325400	-6.34794800
N	-5.92827400	-3.40084300	-4.51541400
N	-3.36118300	-2.62741100	0.00869100
H	-2.48258400	-2.67232900	-0.49589000
C	-3.65326000	-3.73771700	0.91026600
H	-4.74476700	-3.81045800	0.95501500
C	-3.23277700	-3.38126000	2.33551700
O	-4.04516800	-2.80157800	3.08028200
C	-3.06600100	-5.03033600	0.31844900
H	-1.97217200	-5.01153900	0.36974000
H	-3.41113200	-5.87905400	0.91609600
C	-3.45367900	-5.15964700	-1.11177600
N	-2.61848200	-4.66059400	-2.11533300

C	-4.63088100	-5.59550400	-1.66824400
H	-5.51753300	-6.01609500	-1.22611500
C	-3.29695800	-4.80927200	-3.24849500
H	-2.95581400	-4.52815400	-4.23092600
N	-1.96267900	-3.69107200	2.73522300
H	-1.26135500	-3.97146400	2.04936300
C	-1.51900100	-3.30230100	4.06949900
H	-2.42480000	-3.06258800	4.63025900
C	-0.68486000	-2.02782800	4.09346100
O	-0.79333300	-1.23631200	5.05222000
C	-0.76624300	-4.43032300	4.82479800
H	-0.75214000	-4.14380200	5.88069100
H	-1.35665500	-5.34806700	4.74279100
C	0.63486900	-4.62012800	4.36832900
N	1.00766800	-5.41823900	3.29453900
H	0.40200100	-6.05877100	2.80748000
C	1.76992700	-3.92476500	4.69863600
H	1.88405000	-3.18926700	5.47741100
C	2.32424200	-5.16079000	3.01266500
H	2.87617600	-5.65740800	2.23306600
N	2.81343700	-4.24424600	3.83791800
N	0.20976500	-1.86618200	3.08720100
H	0.28716900	-2.57345900	2.35005400
C	1.02717000	-0.66806300	2.98181100
H	0.36406900	0.18555800	2.89886900
C	1.86367200	-0.67918600	1.70905500
O	1.76414300	0.24172400	0.86553100
C	1.97132900	-0.38433900	4.18994000
H	1.34752100	-0.28549000	5.08046100
H	2.65580100	-1.22414900	4.34090000
C	2.73351700	0.85725500	3.88552700
N	2.17576600	2.12167600	4.02594900
H	1.21399200	2.31992800	4.33323800
C	3.86448600	1.04476000	3.13180700
H	4.59641600	0.33415700	2.78693900
C	2.94106400	3.00758000	3.34746500
H	2.73431300	4.06139900	3.28541900
N	3.96665000	2.38031300	2.76499500
N	2.79319300	-1.66188100	1.64881600
H	2.79413700	-2.39048600	2.36091000
C	3.97114500	-1.60437800	0.79071300
H	4.14185000	-0.54350300	0.54957400
C	3.72606600	-2.28678600	-0.55262700
O	2.76104400	-1.94241300	-1.27232900
C	5.20653900	-2.09279000	1.54974000
H	5.22371600	-1.60444400	2.52683000
H	5.17201800	-3.17133600	1.72434100
C	6.46567400	-1.69377300	0.76782700

O	6.73986900	-0.46862600	0.68911700
O	7.07283200	-2.66600500	0.15797300
N	4.63040600	-3.20237400	-0.96569900
H	5.50494900	-3.33510600	-0.43441100
C	4.70803700	-3.61547600	-2.36469000
H	3.93519800	-3.06045500	-2.90757000
C	4.30466600	-5.07706000	-2.44186400
O	3.09978200	-5.41443300	-2.46542300
C	6.10029300	-3.24982000	-2.89655100
H	6.86480600	-3.64609500	-2.21753100
H	6.25842500	-3.70307300	-3.88076300
C	6.24099300	-1.72686400	-2.98925400
H	5.75211700	-1.36294100	-3.89589600
H	5.72658500	-1.26255500	-2.13573500
C	7.64602600	-1.15749800	-2.98295000
O	7.98957300	-0.29000200	-3.82565600
N	8.45107600	-1.57436400	-1.99106600
H	9.37153300	-1.16449300	-1.94603000
H	8.08227700	-2.04825900	-1.14863700
N	5.29313500	-5.99297000	-2.42504600
H	6.26549200	-5.73635000	-2.38907200
H	5.04964500	-6.97101300	-2.43580400
H	-5.26408000	-5.38274900	-3.70863800
N	-4.51393200	-5.37838400	-3.02674100
Cu	4.59591800	2.65036600	0.99806200
H	5.02922500	7.76709900	0.24191200
H	7.86984000	1.74907400	-2.59952100
N	6.97339200	1.89830500	-2.15956300
N	4.50553000	6.92635700	0.41539700

Structure S3. The Cu²⁺-pHG complex C. Coordinates in Å.

H	7.71990900	-1.61637600	-1.73754600
C	8.26202100	-2.10942600	-0.92487100
H	8.35303700	-3.17169400	-1.15552400
C	7.54705200	-1.83688600	0.36428600
O	7.48430300	-0.68795600	0.85110200
H	9.25745800	-1.66642200	-0.88642400
N	6.93070200	-2.90552900	0.94003200
H	6.98218900	-3.82604700	0.52661700
C	6.13280000	-2.77958400	2.14224900
H	6.66413400	-3.18121700	3.01317600
H	5.96088100	-1.71586700	2.31792900
C	4.83935800	-3.54583300	1.98938000
O	4.81970900	-4.67576600	1.44165600
N	3.75336600	-2.92682300	2.48896300
H	3.81597400	-1.92096800	2.64996600

C	2.41656800	-3.51642600	2.53923800
H	2.51530600	-4.56916300	2.82637300
C	1.79036200	-3.43166100	1.14829600
O	0.94050700	-2.55345500	0.84997500
C	1.58536100	-2.75805200	3.56335500
H	2.19437000	-2.62931200	4.46545500
H	1.37075400	-1.75318700	3.17051400
C	0.33010800	-3.47307800	3.90370400
N	-0.42249000	-3.12404800	5.01176700
H	-0.29261800	-2.26640200	5.53335600
C	-0.31158100	-4.55741000	3.35485200
H	-0.04750000	-5.13338900	2.48191500
C	-1.48112000	-3.99636800	5.08645900
H	-2.23983700	-3.94060100	5.84770800
N	-1.44260100	-4.87634600	4.09902900
N	2.28135700	-4.29712000	0.24067700
H	3.04555200	-4.91224800	0.51890000
C	1.89590100	-4.18972600	-1.16256700
H	1.64031100	-3.13175800	-1.31650800
C	0.61491200	-4.98494100	-1.45799700
O	0.63659500	-6.00070000	-2.17027800
C	3.01734600	-4.60940900	-2.12199700
H	3.96080300	-4.71669400	-1.57511800
H	2.75399000	-5.58902800	-2.53468300
C	3.21491500	-3.58927600	-3.18767800
N	2.18154000	-2.87596900	-3.77167600
H	1.17512600	-2.96180900	-3.63141600
C	4.36445300	-2.99262200	-3.64793200
H	5.38519700	-3.24930800	-3.41482900
C	2.72223600	-1.87789400	-4.51983800
H	2.11912600	-1.18047400	-5.07331800
N	4.05396300	-1.90812400	-4.46470900
N	-0.50952500	-4.44869200	-0.92369300
H	-0.43323800	-3.58515400	-0.38923800
C	-1.82990100	-4.84119400	-1.42476100
H	-1.71119700	-5.81975800	-1.89310800
C	-2.10704600	-3.84757600	-2.55181700
O	-1.86561800	-4.12517900	-3.74013500
C	-2.88109100	-4.89580700	-0.32710000
H	-2.52247500	-5.57840000	0.45548100
H	-2.98636300	-3.91488300	0.16070600
C	-4.18293500	-5.34044200	-0.89751500
N	-5.39684900	-5.13293700	-0.26833600
H	-5.52740600	-4.64707200	0.62532400
C	-4.48252000	-6.00939300	-2.06315400
H	-3.81496500	-6.34220300	-2.84115400
C	-6.36547600	-5.67451100	-1.06898500
H	-7.41354500	-5.62613600	-0.83299700

N	-5.85060200	-6.21671700	-2.16251800
N	-2.45716400	-2.60408100	-2.13467200
H	-2.71989800	-2.40514400	-1.17467700
C	-2.44825500	-1.47514300	-3.04582800
H	-2.45718300	-1.90242300	-4.05596400
C	-1.07868600	-0.81714100	-2.88235100
O	-0.03503400	-1.41491000	-3.25264400
C	-3.63503000	-0.53513400	-2.84653700
H	-3.49491200	-0.00033700	-1.90440500
H	-3.60911900	0.22072000	-3.64377000
C	-4.96154000	-1.21145300	-2.78810600
N	-6.08110100	-0.53483300	-2.31722300
H	-6.16118700	0.43426200	-1.98783200
C	-5.40119600	-2.47850700	-3.09577300
H	-4.84173700	-3.32090400	-3.46896800
C	-7.13071000	-1.41132500	-2.36525700
H	-8.12749300	-1.13610700	-2.06630400
N	-6.76009600	-2.59481300	-2.82995600
N	-0.98341700	0.40912900	-2.30711400
H	-1.75593800	0.87687500	-1.82704900
C	0.30472900	1.05873200	-2.22379600
H	0.87136600	0.74475800	-3.10945300
C	1.09764800	0.62956100	-0.98869900
O	0.63547400	0.73748900	0.16777000
C	0.14927600	2.59736800	-2.23830000
H	-0.57060500	2.85301700	-3.02302300
H	-0.29614000	2.93358000	-1.29850900
C	1.47042500	3.22703700	-2.46660100
N	2.10834500	3.20180800	-3.70208600
H	1.67896700	2.92227900	-4.57006800
C	2.40620300	3.71427800	-1.59724200
H	2.28092500	3.92763100	-0.54732400
C	3.38456000	3.65279900	-3.54976200
H	4.09300200	3.75346000	-4.35128300
N	3.60944300	3.94628300	-2.27286600
N	2.36274000	0.19896500	-1.22366700
H	2.64496000	0.09068300	-2.19106000
C	3.19803400	-0.47462900	-0.22945700
H	2.61209600	-1.29810400	0.19477400
C	3.60792900	0.35210700	0.97762900
O	4.02592400	-0.24138000	1.99946100
C	4.44679100	-1.05000200	-0.93755300
H	5.07195400	-1.52946200	-0.18077500
H	4.12105400	-1.83292800	-1.62726400
C	5.18820900	0.02627200	-1.65415900
N	5.17102000	0.22531400	-3.03422500
H	4.86771000	-0.47665300	-3.74170600
C	5.74943900	1.15812100	-1.13056200

H	5.98138200	1.35736300	-0.10037500
C	5.68372300	1.45805100	-3.28017900
H	5.81090600	1.85726100	-4.27082800
N	6.00542300	2.07955800	-2.14147600
N	3.51496800	1.69544500	0.95145200
H	3.24993600	2.15310100	0.08912300
C	3.80128400	2.47830000	2.14918400
H	4.46186000	1.84995800	2.75963300
C	2.56319800	2.69289500	3.02754400
O	2.60239000	3.52266500	3.95393300
C	4.52014900	3.79863000	1.85393300
H	4.01765100	4.33714500	1.04159000
H	4.41100500	4.41191200	2.75293600
C	5.95279400	3.62104800	1.49370900
N	6.42485800	3.82653700	0.19176000
C	6.99876500	3.19513200	2.26674500
H	7.04628900	2.92006700	3.30510500
C	7.72265900	3.52871500	0.19081000
H	8.36352300	3.54337200	-0.67148500
N	1.50686800	1.88884000	2.77378500
H	1.48122900	1.33511600	1.92156100
C	0.28897500	1.94359500	3.58217500
H	0.57243100	2.22089400	4.59990100
C	-0.33859900	0.54871000	3.66859200
O	-0.35569000	-0.09178600	4.74124000
C	-0.65176800	2.99700800	2.97734400
H	-0.17137100	3.97503100	3.10048600
H	-0.70727200	2.82681400	1.89036300
C	-2.03474000	3.01288200	3.52513500
N	-3.00922400	3.80152500	2.93372200
H	-2.82051500	4.44259900	2.15930800
C	-2.68536600	2.31907300	4.52134900
H	-2.27519800	1.61608400	5.22737400
C	-4.18989400	3.56402900	3.58491100
H	-5.11409800	4.05274600	3.32307800
N	-4.03680700	2.65809100	4.54401200
N	-0.89861900	0.13252100	2.51148800
H	-0.60993600	0.59634200	1.65197200
C	-1.87495500	-0.93666200	2.30583400
H	-1.39027200	-1.86510600	1.97818800
C	-2.77366000	-0.46388100	1.16874600
O	-2.99809400	-1.16084200	0.16070700
C	-2.77588800	-1.22011800	3.53518900
H	-2.19093000	-1.72734600	4.29471500
H	-3.10234200	-0.27220800	3.97548900
C	-3.95915200	-2.01921600	3.11762100
N	-5.19383000	-1.42035800	2.88938900
H	-5.42990500	-0.47129200	3.13851200

C	-4.09630700	-3.30771700	2.66785900
H	-3.37007500	-4.10555300	2.69569900
C	-6.01308400	-2.34770600	2.30995400
H	-7.03041300	-2.14690600	2.02310600
N	-5.37620000	-3.49958300	2.15753600
N	-3.33986500	0.75141300	1.36258300
H	-3.09805700	1.27668700	2.19861200
C	-4.23831300	1.36235900	0.39347300
H	-4.36575900	0.62136000	-0.40019800
C	-3.50057400	2.52068800	-0.26984000
O	-2.42756500	2.28345600	-0.89073500
C	-5.62927500	1.62968200	0.97069400
H	-6.10413200	0.65280500	1.10655600
H	-5.57668000	2.13554300	1.93711900
C	-6.45060300	2.45948200	-0.01642900
O	-6.60931300	1.98470100	-1.17985300
O	-6.76908400	3.64090400	0.37591100
N	-3.99184100	3.76535200	-0.20966100
H	-4.89830200	3.95011200	0.23402100
C	-3.41734800	4.82891200	-1.00965200
H	-3.17498000	4.42125300	-2.00155100
C	-2.13135500	5.34099900	-0.39001500
O	-1.87309000	5.24923000	0.82605700
C	-4.46032100	5.94343400	-1.15729000
H	-4.84059600	6.19171000	-0.15749200
H	-4.00314000	6.85609300	-1.55215800
C	-5.61425300	5.51038600	-2.07113900
H	-5.30802700	5.59955400	-3.11656900
H	-5.90111900	4.47193600	-1.88297100
C	-6.79241200	6.43168500	-1.84807600
O	-6.84141100	7.55605400	-2.38638400
N	-7.70996600	5.95933700	-0.97991500
H	-8.50014400	6.54217900	-0.75552700
H	-7.59089400	5.04999700	-0.52349500
N	-1.27567300	5.94107800	-1.25095600
H	-1.49096900	6.05173300	-2.22780000
H	-0.45514900	6.39532400	-0.88218600
Ni	5.25212400	3.85308900	-1.30952600
H	9.01677400	2.81625400	1.69462800
N	8.10208100	3.14318600	1.43320800

Structure S4. The Ni²⁺-pHG complex A. Coordinates in Å.

H	6.78911200	-0.57434600	-1.50475200
C	6.71296900	-0.47254100	-2.58749500
H	7.68486200	-0.72696700	-3.01627300
C	6.41435700	0.94983000	-2.93624000

O	7.20625500	1.88141500	-2.69408700
H	5.96680100	-1.18050300	-2.94712800
N	5.23860000	1.19479000	-3.59734300
H	4.58052900	0.44399800	-3.78377700
C	5.07167800	2.47400100	-4.25019400
H	5.97787200	2.74784400	-4.79644200
H	4.25451700	2.38848400	-4.97376600
C	4.77891100	3.65848600	-3.35145400
O	5.08542200	4.81021000	-3.71162900
N	4.09221700	3.38751600	-2.20926100
H	3.97732600	2.41985000	-1.91920400
C	3.68287400	4.41321300	-1.26697800
H	4.56479200	4.90504600	-0.82875900
C	2.91682400	3.71104400	-0.15615900
O	2.66561000	2.48246400	-0.23311400
C	2.84860700	5.52072900	-1.97984000
H	3.52826800	5.96641400	-2.70768400
H	2.05870500	5.02218200	-2.54698300
C	2.28803000	6.54099400	-1.05939500
N	0.94000100	6.61297000	-0.74071900
H	0.20733900	6.05557800	-1.18753200
C	2.89970500	7.47043000	-0.24753100
H	3.94352100	7.73489200	-0.20529900
C	0.79514000	7.56395700	0.23387100
H	-0.15221100	7.80499000	0.68156300
N	1.96087600	8.10283400	0.56363500
N	2.51232300	4.43133800	0.91942900
H	2.65887400	5.43627100	0.94888900
C	1.73240800	3.78200400	1.96365100
H	1.89336200	2.71051200	1.82304100
C	0.24608900	4.07411100	1.81096000
O	-0.24346500	5.16339300	2.16857400
C	2.16855400	4.15913500	3.39382500
H	3.23604300	4.39530900	3.38526200
H	1.62923100	5.05609700	3.71112200
C	1.96306400	2.97875100	4.27766700
N	0.75778000	2.30187000	4.41434700
H	-0.18240400	2.59559800	4.14037900
C	2.90089000	2.15170600	4.83792900
H	3.96510400	2.30788500	4.91215600
C	1.00946600	1.10752900	5.02426500
H	0.23315800	0.39674200	5.26041000
N	2.30809900	0.97668000	5.28941100
N	-0.51325200	3.05386600	1.33178100
H	-0.11180300	2.19458700	0.95599000
C	-1.95994400	3.11511100	1.45936800
H	-2.13787000	4.04889900	2.00722300
C	-2.33626900	2.03454300	2.46941500

O	-1.90949000	2.19270900	3.64113300
C	-2.69589200	3.21845300	0.11851400
H	-2.20206200	4.00904100	-0.46085500
H	-2.57712200	2.30198900	-0.46300300
C	-4.13052900	3.51147400	0.34581000
N	-4.55572500	4.65612200	1.01895600
H	-3.96851300	5.43912500	1.26177900
C	-5.24891600	2.75088000	0.17777600
H	-5.34710100	1.79562600	-0.32596900
C	-5.88379000	4.55050400	1.26961200
H	-6.46162900	5.28726000	1.79761800
N	-6.33533700	3.39601700	0.78417200
N	-3.03909600	0.92892300	2.14129000
H	-3.25266000	0.67731400	1.17983900
C	-3.23194600	-0.07210100	3.18910400
H	-3.42843400	0.46800700	4.11749700
C	-1.96879700	-0.89269400	3.44015200
O	-1.77175100	-1.43582000	4.54438300
C	-4.37191400	-1.07992200	2.91929400
H	-4.00876900	-1.83245900	2.21235400
H	-4.55483100	-1.58847900	3.86979300
C	-5.64094000	-0.51559600	2.38564500
N	-5.94363900	-0.60126600	1.03559800
H	-5.32611300	-0.86410700	0.26848800
C	-6.71867600	0.10456300	2.96484300
H	-6.89235500	0.33946900	3.99997400
C	-7.15594800	-0.06056800	0.81118700
H	-7.64189600	-0.11415800	-0.14754200
N	-7.68066100	0.39331500	1.98182100
N	-1.15597900	-1.07214000	2.36775400
H	-1.43723300	-0.71116000	1.45807500
C	-0.11262400	-2.08831800	2.37232300
H	0.25825100	-2.18287200	3.39827300
C	0.97103800	-1.60234000	1.43558600
O	0.81827600	-1.73162000	0.19590500
C	-0.68426500	-3.42756500	1.87872300
H	-1.50273000	-3.70374700	2.55753500
H	-1.12117100	-3.23440800	0.89326000
C	0.31470800	-4.51499400	1.73705300
N	0.86295100	-5.21328900	2.80664100
H	0.68769100	-5.03068500	3.78094000
C	0.87610800	-5.08339100	0.62058400
H	0.68487300	-4.83813200	-0.41358400
C	1.72148300	-6.15249500	2.29619700
H	2.30684500	-6.81173900	2.91192800
N	1.74480800	-6.10733500	0.97456500
N	2.03451900	-0.99721600	1.98967100
H	2.10681700	-0.95004500	2.99959500

C	3.02949700	-0.28249400	1.19464300
H	2.52675500	0.48171200	0.59064700
C	3.79467100	-1.14773800	0.21487200
O	4.31172800	-0.60304200	-0.78540400
C	4.03105100	0.45049100	2.10343000
H	4.70349500	0.98554500	1.42604900
H	3.48379700	1.21234300	2.66899400
C	4.81961500	-0.41717900	3.02615900
N	4.49811500	-0.61039900	4.36765900
H	3.70395200	-0.19065500	4.87064300
C	5.97781700	-1.13364300	2.82726900
H	6.54314100	-1.23916200	1.91433400
C	5.47157100	-1.40338900	4.90719600
H	5.48197200	-1.68700100	5.94588900
N	6.38138400	-1.74778700	4.00375400
N	3.92384500	-2.46212800	0.48894600
H	3.60479100	-2.85368400	1.37682200
C	4.77070100	-3.30998900	-0.34116300
H	5.79110900	-2.90887700	-0.36268400
C	4.30098600	-3.31192900	-1.78878700
O	5.09764500	-3.41386300	-2.73225100
C	4.78632500	-4.73972900	0.22537400
H	3.79873100	-5.19864500	0.09554700
H	5.49961000	-5.32269500	-0.36323100
C	5.14288300	-4.75951700	1.66579800
N	4.22892400	-4.30267400	2.62679900
C	6.30477500	-5.13131200	2.28653000
H	7.23020100	-5.51526900	1.89500500
C	4.84589100	-4.41019800	3.79468100
H	4.44273700	-4.12036100	4.74854300
N	2.94790700	-3.22395200	-1.94511600
H	2.39418900	-3.13671000	-1.09804500
C	2.33790900	-2.81316200	-3.20215500
H	2.98368200	-3.13499300	-4.02127000
C	2.29701300	-1.27837500	-3.24568300
O	2.93127900	-0.61314900	-4.09112300
C	0.94107900	-3.43649400	-3.28683900
H	1.06139300	-4.51772000	-3.41848200
H	0.44746400	-3.31557000	-2.30776900
C	0.02804900	-2.87565500	-4.32304000
N	-1.25052000	-3.39444300	-4.46585400
H	-1.58982600	-4.19361800	-3.93208500
C	0.08983100	-1.82622700	-5.21292000
H	0.92808900	-1.19186200	-5.44660000
C	-1.90062400	-2.65626900	-5.42431200
H	-2.91203800	-2.85552700	-5.73714700
N	-1.12234000	-1.69037500	-5.89012900
N	1.46874600	-0.77518100	-2.30918000

H	1.21612000	-1.38271400	-1.53431600
C	1.03013200	0.59058600	-2.07026800
H	1.64888900	1.07210100	-1.30801500
C	-0.37281600	0.43769200	-1.48434500
O	-0.66703100	0.81120600	-0.32113700
C	1.03735400	1.45898400	-3.33585400
H	2.08175200	1.61145200	-3.62659900
H	0.56990100	0.91538400	-4.16640100
C	0.34344700	2.75575000	-3.11911200
N	-0.16110800	3.51978700	-4.16364500
H	-0.12519600	3.26869400	-5.13857100
C	0.07516300	3.48438300	-1.99140900
H	0.31755300	3.25110400	-0.97189200
C	-0.70442300	4.66133900	-3.63958300
H	-1.15938500	5.43081400	-4.23753900
N	-0.58079300	4.66915100	-2.31934200
N	-1.27794200	-0.15639900	-2.29568500
H	-0.97368600	-0.52900100	-3.19214300
C	-2.67826600	-0.28583700	-1.92033500
H	-2.94874200	0.57508000	-1.30916800
C	-2.91184300	-1.48283700	-1.00246100
O	-3.12420600	-1.31445900	0.22703400
C	-3.59339800	-0.30931100	-3.13816200
H	-3.55260900	0.66976900	-3.62512200
H	-3.27712500	-1.04758500	-3.88142600
C	-5.02074600	-0.62781200	-2.69619400
O	-5.37687000	-0.14310300	-1.55346100
O	-5.70562700	-1.39408600	-3.42817600
N	-2.91064000	-2.70023400	-1.57588800
H	-2.70816700	-2.77840700	-2.56711000
C	-3.31494700	-3.93044500	-0.90249100
H	-3.32071600	-3.72102700	0.17277100
C	-2.32966600	-5.03509400	-1.22477400
O	-1.78375700	-5.11583300	-2.34651500
C	-4.71892900	-4.37100300	-1.35474200
H	-4.74299500	-4.36046900	-2.45252700
H	-4.90559400	-5.40213600	-1.03364500
C	-5.81290300	-3.46423900	-0.80226900
H	-5.84061700	-3.53978900	0.28996500
H	-5.62097600	-2.42799100	-1.07791300
C	-7.16392900	-3.90104000	-1.32477400
O	-7.73815300	-4.89993100	-0.84830100
N	-7.64719000	-3.15998400	-2.34500300
H	-8.52049600	-3.44511800	-2.75985800
H	-7.09919800	-2.40561300	-2.77290000
N	-2.13192600	-5.95490900	-0.26544100
H	-2.53281800	-5.87606800	0.65425200
H	-1.50256200	-6.72308100	-0.44625300

H	6.80218200	-4.97881400	4.35398200
N	6.09918100	-4.92024400	3.63812500
Ni	-7.63128300	2.16068200	1.38571000

Structure S5. The Ni²⁺-pHG complex B. Coordinates in Å.

H	-11.35754300	-1.85391300	-0.03826900
C	-10.96795400	-1.58457600	0.94508600
H	-11.01073000	-0.50026500	1.05796200
C	-9.58260600	-2.14653500	1.09373800
O	-9.35409200	-3.36944300	1.01805800
H	-11.62044000	-2.04552600	1.68850200
N	-8.59427000	-1.24405600	1.31282900
H	-8.76446800	-0.24810300	1.37371700
C	-7.21936100	-1.64991400	1.46294100
H	-7.09967400	-2.33373700	2.31263500
H	-6.86168400	-2.20771300	0.58886100
C	-6.37538500	-0.41819900	1.66428300
O	-6.86639600	0.73076400	1.70064000
N	-5.04689000	-0.63310200	1.80928100
H	-4.68121200	-1.57880100	1.75569200
C	-4.14387800	0.48831400	1.93252000
H	-4.45224400	1.10425800	2.78747600
C	-4.22635100	1.36920800	0.68181000
O	-4.59307000	0.91983200	-0.42043100
C	-2.71513700	-0.02566600	2.18476100
H	-2.75066700	-0.70979800	3.03760300
H	-2.37329100	-0.61453400	1.32434300
C	-1.77761000	1.09569000	2.42917300
N	-0.84602900	1.50608500	1.49581400
H	-0.67195600	1.04368600	0.60431000
C	-1.67410700	1.99174200	3.46949400
H	-2.22227800	2.00232600	4.39698100
C	-0.21453100	2.60544800	1.99681500
H	0.62032100	3.08909400	1.50992600
N	-0.69532300	2.94005700	3.19127700
N	-3.87742300	2.67396100	0.83393400
H	-3.60804900	3.02242400	1.74486700
C	-4.17907300	3.63009600	-0.22959500
H	-4.19192800	3.05010400	-1.16030800
C	-3.09079000	4.68790300	-0.33762200
O	-3.32339900	5.90657100	-0.16814600
C	-5.58098800	4.22200700	-0.01655900
H	-6.23244400	3.38155200	0.24622600
H	-5.55082400	4.89501500	0.84809300
C	-6.14894700	4.90205900	-1.20788200
N	-5.69388900	6.12432900	-1.67729100

H	-4.91955000	6.61759400	-1.25497500
C	-7.16368400	4.54635700	-2.06256400
H	-7.77686900	3.66163300	-2.03122300
C	-6.43879700	6.45041500	-2.77832800
H	-6.29013400	7.35325600	-3.34463600
N	-7.34156700	5.51627000	-3.04095400
N	-1.85135800	4.25159200	-0.67438800
H	-1.70734200	3.27021000	-0.88971800
C	-0.80327200	5.22310200	-0.98643400
H	-1.25687700	6.02425600	-1.57798600
C	0.26370900	4.62269800	-1.88928500
O	0.56743400	5.17561600	-2.95714000
C	-0.18967700	5.87902000	0.27407400
H	-0.96824300	6.47485800	0.75431800
H	0.12415500	5.10709700	0.98165200
C	0.99716900	6.67430900	-0.12598000
N	2.28184200	6.13420400	-0.00960200
C	1.07842100	7.82903900	-0.85343700
H	0.31593600	8.50758800	-1.19125000
C	3.11157600	6.94808200	-0.65626900
H	4.17224300	6.80341100	-0.75949400
N	0.87474300	3.49152800	-1.43960000
H	0.68593900	3.12479000	-0.51549300
C	1.67872600	2.66016500	-2.33059400
H	1.91579600	3.28237800	-3.19775300
C	0.71275500	1.56049200	-2.80787100
O	-0.32801500	1.87112400	-3.41905500
C	2.91170700	2.08471000	-1.66016900
H	2.56435500	1.53862700	-0.77801700
H	3.31936900	1.31991700	-2.32969100
C	4.08924600	2.88068500	-1.21393300
N	4.13492700	3.72761400	-0.09764800
C	5.38114400	2.54117200	-1.53605100
H	5.75984400	1.82273400	-2.24253500
C	5.42659600	3.86945200	0.22104100
H	5.79508600	4.42027600	1.06955100
N	0.97813300	0.26478600	-2.47921400
H	1.81023700	-0.01685000	-1.96222100
C	-0.00225100	-0.74457400	-2.80252200
H	-0.39870300	-0.51131700	-3.79907500
C	-1.20774700	-0.67546800	-1.85615400
O	-1.28915500	0.14594500	-0.91916700
C	0.63694500	-2.13833000	-2.84293800
H	-0.03120300	-2.84697100	-3.35084300
H	1.54018400	-2.05557500	-3.45943500
C	0.99879100	-2.69631800	-1.51420700
N	1.73147400	-3.86502300	-1.41314900
H	1.93200000	-4.49145300	-2.17637800

C	0.78681900	-2.29176100	-0.22202100
H	0.30725100	-1.39435900	0.13743700
C	1.94944000	-4.12667300	-0.09382500
H	2.53424100	-4.96218000	0.24910800
N	1.38941600	-3.19123100	0.66093800
N	-2.18759000	-1.58415800	-2.09715200
H	-2.06160800	-2.28269600	-2.81883200
C	-3.42791200	-1.61852600	-1.33539300
H	-3.47445200	-0.67849300	-0.77600900
C	-3.46877100	-2.73229900	-0.30335000
O	-4.55790000	-3.11494100	0.17926600
C	-4.67376000	-1.61194800	-2.22517000
H	-5.53726900	-1.58890800	-1.55758500
H	-4.68190900	-0.66391900	-2.77084000
C	-4.75779600	-2.77551700	-3.14504400
N	-4.38846500	-2.70584200	-4.48675100
H	-4.15041300	-1.85845700	-4.97694500
C	-5.10884400	-4.08456600	-2.94312100
H	-5.44915700	-4.53463600	-2.02617000
C	-4.53834000	-3.95595200	-5.03279700
H	-4.34175600	-4.17780000	-6.06730600
N	-4.95919900	-4.81747900	-4.11890400
N	-2.27429500	-3.19667200	0.13043800
H	-1.43087300	-2.94187900	-0.37098400
C	-2.17151400	-4.29125500	1.08600000
H	-3.20053300	-4.64170100	1.23005100
C	-1.76222600	-3.74048900	2.45312600
O	-2.59943500	-3.09958200	3.11714600
C	-1.33380900	-5.43191700	0.47898900
H	-0.27777700	-5.14971400	0.42885800
H	-1.41196500	-6.31014600	1.12726700
C	-1.79909300	-5.72201000	-0.90600800
N	-1.18746400	-5.11841200	-2.01015500
C	-2.90840100	-6.41730400	-1.32058400
H	-3.64439200	-6.97878600	-0.77135600
C	-1.93415800	-5.45694800	-3.05783500
H	-1.76795200	-5.15600000	-4.07910900
N	-0.49610200	-3.96661700	2.91120200
H	0.22940100	-4.20639200	2.24280200
C	-0.10164200	-3.46555100	4.22402200
H	-0.99383600	-3.48325500	4.85315400
C	0.35906100	-2.01015900	4.22373600
O	0.17447300	-1.29762500	5.23089500
C	0.99278000	-4.34419500	4.88666200
H	1.06091400	-4.02276300	5.93009900
H	0.64530600	-5.38230500	4.88744900
C	2.32765300	-4.19922800	4.24612000
N	2.74751500	-4.93361300	3.14018800

H	2.31831800	-5.78073000	2.80442100
C	3.26938000	-3.21374400	4.38378800
H	3.29883500	-2.43446200	5.12740400
C	3.89418100	-4.36162600	2.65211100
H	4.42558100	-4.73923100	1.79125700
N	4.22507500	-3.29699500	3.37563900
N	1.05465000	-1.60878600	3.13426700
H	1.23033800	-2.26709000	2.36892700
C	1.58612500	-0.26221600	2.98813000
H	0.75107200	0.44157800	2.92897700
C	2.31358000	-0.17404900	1.65343900
O	1.84055600	0.50696500	0.71738400
C	2.52583400	0.25990200	4.11346100
H	2.02070600	0.11933800	5.07129000
H	3.46232100	-0.30213000	4.13728800
C	2.75751400	1.70609400	3.82704000
N	1.98202700	2.69272200	4.42142500
H	1.28060000	2.53430700	5.12721600
C	3.39196500	2.33486500	2.78502700
H	4.08250700	1.94014300	2.05995400
C	2.13102600	3.84723000	3.73252000
H	1.58674000	4.74878700	3.94704700
N	2.97408000	3.66127600	2.71383700
N	3.50814300	-0.80104600	1.57529500
H	3.81181900	-1.45849300	2.29666400
C	4.47848800	-0.49589200	0.52056200
H	4.22216300	0.49547400	0.13453100
C	4.29900900	-1.41488000	-0.68595900
O	3.56774700	-1.07505600	-1.64656100
C	5.88094500	-0.42956800	1.13319300
H	5.82903300	0.14284500	2.06320300
H	6.25310600	-1.42546800	1.40254400
C	6.85304200	0.27353900	0.18557500
O	7.54091700	1.23323000	0.64182700
O	6.82716300	-0.13832500	-1.03062900
N	4.90737600	-2.62232200	-0.64366600
H	5.50345800	-2.85047800	0.13990600
C	5.00217800	-3.48712600	-1.80312400
H	4.17472200	-3.20454100	-2.46546200
C	4.82435700	-4.93320000	-1.39384500
O	4.85414100	-5.32294400	-0.21090600
C	6.33348200	-3.27039000	-2.55115900
H	7.13242700	-3.19320900	-1.80370700
H	6.57594800	-4.12674500	-3.19092500
C	6.30341400	-2.00135600	-3.40380400
H	5.62699700	-2.14347600	-4.25176300
H	5.95764500	-1.16152100	-2.80232000
C	7.68872700	-1.73686600	-3.94382200

O	8.13314200	-2.36999600	-4.92389500
N	8.39806700	-0.82396300	-3.24589100
H	9.34837500	-0.64285900	-3.52679300
H	8.00607600	-0.37775700	-2.41113800
N	4.59973100	-5.79802400	-2.41861700
H	4.67503800	-5.51539700	-3.38273500
H	4.56815900	-6.78497000	-2.21379600
H	-3.77317700	-6.44284200	-3.28841000
N	-2.97718300	-6.24872500	-2.68823400
Ni	2.84228500	4.66731000	1.08189300
H	2.79642000	8.73442500	-1.73533300
H	7.14034500	2.80658100	-0.40057300
N	6.21027600	3.16886600	-0.63290500
N	2.41428700	7.99077500	-1.17700700

Structure S6. The Ni²⁺-pHG complex C. Coordinates in Å.

H	7.72507500	-1.30648900	-1.79360700
C	8.27825400	-1.88635500	-1.04789800
H	8.33932200	-2.92296400	-1.38188700
C	7.60339600	-1.72637400	0.28120100
O	7.57917600	-0.62623500	0.87695400
H	9.28451500	-1.46980400	-0.99616800
N	6.97818000	-2.83160300	0.76804000
H	7.00717200	-3.71144400	0.27080000
C	6.20644000	-2.81151100	1.99455900
H	6.77117200	-3.25344500	2.82407500
H	6.00259300	-1.76902000	2.24601500
C	4.93251500	-3.60913200	1.81970600
O	4.93212400	-4.69818700	1.19507300
N	3.84574200	-3.05825200	2.39179000
H	3.89210400	-2.06320000	2.61177100
C	2.51902500	-3.67156600	2.44167100
H	2.63822300	-4.73575400	2.67454000
C	1.85011600	-3.52612400	1.07572700
O	0.98169900	-2.64629200	0.84802100
C	1.70934400	-2.97376200	3.52299000
H	2.31418000	-2.95676000	4.43769000
H	1.54631200	-1.92743300	3.22362900
C	0.41048000	-3.64338800	3.77645000
N	-0.48752900	-3.13996900	4.70076000
H	-0.41988800	-2.21726000	5.12335600
C	-0.16750800	-4.79022500	3.28807900
H	0.20375100	-5.47708100	2.54447600
C	-1.55919000	-3.99744500	4.74013500
H	-2.41439200	-3.84732200	5.37697500
N	-1.40089800	-5.00261400	3.89396400

N	2.32692600	-4.33868800	0.11187200
H	3.10937700	-4.95225300	0.33525800
C	1.88967200	-4.18169000	-1.27181500
H	1.63474300	-3.11831900	-1.38536200
C	0.59361800	-4.96121500	-1.54723500
O	0.58924100	-5.96553000	-2.27572200
C	2.97531100	-4.57617600	-2.28357200
H	3.92644000	-4.75321800	-1.76945500
H	2.66756200	-5.51888300	-2.74859200
C	3.18996800	-3.49913600	-3.28703900
N	2.16969500	-2.72901800	-3.81944800
H	1.16230000	-2.80189700	-3.67540200
C	4.35040100	-2.90685400	-3.72575100
H	5.36605700	-3.20390000	-3.52009800
C	2.72890100	-1.70480300	-4.51765100
H	2.13992300	-0.96478700	-5.02959500
N	4.06008400	-1.77159600	-4.47825800
N	-0.51332500	-4.41981900	-0.98182500
H	-0.40923800	-3.58051900	-0.41453400
C	-1.84592900	-4.77191300	-1.48014700
H	-1.74702100	-5.73842900	-1.97742200
C	-2.10809700	-3.74133100	-2.57696900
O	-1.84950000	-3.98364500	-3.76981400
C	-2.89776100	-4.84567000	-0.38389900
H	-2.54014000	-5.54118700	0.38710400
H	-3.00973800	-3.87318000	0.11989300
C	-4.19490200	-5.28704200	-0.96977600
N	-5.41321900	-5.11773300	-0.33729700
H	-5.56213300	-4.66238500	0.56862000
C	-4.48318000	-5.92640700	-2.15513300
H	-3.81068000	-6.22756300	-2.94172900
C	-6.37203200	-5.65160900	-1.15517100
H	-7.42085900	-5.62689500	-0.91891200
N	-5.84739500	-6.15307500	-2.26288100
N	-2.45983200	-2.50696000	-2.13142000
H	-2.75954900	-2.33503200	-1.17618200
C	-2.44827200	-1.36391600	-3.02752100
H	-2.43639600	-1.78055000	-4.04195600
C	-1.08776500	-0.69900900	-2.83428500
O	-0.03343600	-1.26925100	-3.22100500
C	-3.64776900	-0.43458000	-2.84614900
H	-3.52808100	0.11917400	-1.91078100
H	-3.61926300	0.31146000	-3.65271600
C	-4.96577600	-1.12975400	-2.80379500
N	-6.10081000	-0.47396700	-2.34132300
H	-6.20385100	0.49423000	-2.01582600
C	-5.38237100	-2.40234200	-3.12188500
H	-4.80821800	-3.23483700	-3.49448900

C	-7.13576800	-1.36672000	-2.40406200
H	-8.13986400	-1.10794800	-2.11499300
N	-6.74160000	-2.54167900	-2.87016800
N	-1.00427900	0.50035300	-2.20411700
H	-1.78131700	0.93898300	-1.70410800
C	0.29147400	1.12232800	-2.06074300
H	0.85114800	0.89897000	-2.97759000
C	1.07530500	0.55527600	-0.88068300
O	0.61360200	0.57595000	0.27960200
C	0.17949900	2.65394700	-1.88513100
H	-0.52104500	3.03631700	-2.63476000
H	-0.26256900	2.87584800	-0.91099100
C	1.52412500	3.26902800	-2.00854900
N	2.22144800	3.27777900	-3.21180000
H	1.83659300	3.02403400	-4.10837900
C	2.41953700	3.73168800	-1.07910700
H	2.23203400	3.93260200	-0.03539700
C	3.48590900	3.71953500	-2.97615300
H	4.24205400	3.84263900	-3.73416300
N	3.65450700	3.98108300	-1.68604200
N	2.33580600	0.14083500	-1.15913100
H	2.58989700	0.06241000	-2.13666700
C	3.21246900	-0.54988000	-0.21640200
H	2.67484300	-1.41835500	0.17714200
C	3.60650700	0.24198500	1.01827100
O	4.07821600	-0.36129300	2.01160900
C	4.46620700	-1.03165100	-0.97591600
H	5.11861800	-1.53330100	-0.25538400
H	4.15821400	-1.78883000	-1.70181100
C	5.17695600	0.09463400	-1.64878900
N	5.25168700	0.29881900	-3.02505500
H	4.93186100	-0.37857800	-3.75100500
C	5.74795900	1.20216200	-1.08423000
H	5.92023100	1.38515800	-0.04130600
C	5.84131300	1.50416800	-3.23253400
H	6.03705300	1.91151000	-4.20959500
N	6.12916100	2.09952300	-2.07096600
N	3.44090300	1.57412500	1.02699000
H	3.12236200	2.02851600	0.18140600
C	3.68194100	2.36141600	2.22883900
H	4.26460900	1.70603100	2.88746000
C	2.40332600	2.64018400	3.02168500
O	2.37711600	3.55683000	3.86232000
C	4.50029300	3.62108300	1.94135400
H	4.10422100	4.16218100	1.07573100
H	4.39027400	4.28289100	2.80517800
C	5.92514100	3.28942200	1.67080100
N	6.55878100	3.63205700	0.47750900

C	6.80877800	2.56916000	2.43245500
H	6.70353400	2.10354000	3.39609600
C	7.79640300	3.13898100	0.53167500
H	8.52355800	3.19817900	-0.25971900
N	1.38893700	1.76842700	2.81725800
H	1.40355800	1.14435800	2.01442600
C	0.14957100	1.84591400	3.59001800
H	0.40472000	2.13665000	4.61215300
C	-0.49131100	0.45641800	3.68527300
O	-0.51318000	-0.17285900	4.76668500
C	-0.77187500	2.89606200	2.95271900
H	-0.27843400	3.86920200	3.05891600
H	-0.83115800	2.70403200	1.86922700
C	-2.15133900	2.94320900	3.50691800
N	-3.11252300	3.75093700	2.92128400
H	-2.91389700	4.39056700	2.14726300
C	-2.80706300	2.27249900	4.51599500
H	-2.40571400	1.56759000	5.22547000
C	-4.29126700	3.54792000	3.58775900
H	-5.20535900	4.05852900	3.33236400
N	-4.14983000	2.64534900	4.55178700
N	-1.06438800	0.03466000	2.53859100
H	-0.75261700	0.46688700	1.67033500
C	-2.09631200	-0.98538300	2.35809400
H	-1.66306100	-1.94237300	2.04073900
C	-2.97569400	-0.48023600	1.21492600
O	-3.16390300	-1.14411000	0.17748800
C	-3.01214100	-1.21677900	3.58352700
H	-2.44451500	-1.67939500	4.38304600
H	-3.36198500	-0.25547800	3.97300100
C	-4.16901800	-2.05050300	3.15437300
N	-5.42587100	-1.49598400	2.94141800
H	-5.69609400	-0.56168900	3.20866000
C	-4.25270100	-3.32831500	2.66063400
H	-3.49181400	-4.09385500	2.64469200
C	-6.20620600	-2.43677400	2.33031900
H	-7.22993300	-2.26759200	2.04651700
N	-5.52292400	-3.55628900	2.14351900
N	-3.55243200	0.72729000	1.42706700
H	-3.33438100	1.24635200	2.27422600
C	-4.39220800	1.37736600	0.43159500
H	-4.50593700	0.65218300	-0.38032800
C	-3.59455600	2.52405700	-0.18224500
O	-2.47297000	2.26970800	-0.70326200
C	-5.79762100	1.67389900	0.95569900
H	-6.29515600	0.70692300	1.07845400
H	-5.77039300	2.18483200	1.92055400
C	-6.57178700	2.51027400	-0.06385500

O	-6.70011200	2.03140500	-1.22949800
O	-6.88547200	3.69920100	0.30858400
N	-4.09079100	3.76767600	-0.20289000
H	-5.01676200	3.96960800	0.19131600
C	-3.48271000	4.80522200	-1.01306200
H	-3.19854600	4.36535900	-1.98006200
C	-2.22132700	5.34405000	-0.36509100
O	-1.96650900	5.22500800	0.84927800
C	-4.52511600	5.90630200	-1.24718600
H	-4.94992200	6.18884000	-0.27510500
H	-4.05709100	6.80761500	-1.65497200
C	-5.63528400	5.43403500	-2.19521300
H	-5.27873400	5.47819500	-3.22755800
H	-5.93411600	4.40465600	-1.97847900
C	-6.82000500	6.36493300	-2.07054000
O	-6.84781200	7.45571800	-2.67544200
N	-7.77047500	5.94411500	-1.21082600
H	-8.56754200	6.53918500	-1.05228500
H	-7.67105000	5.06382700	-0.69598000
N	-1.37833200	5.99350100	-1.20245500
H	-1.59646400	6.14092700	-2.17397600
H	-0.57092000	6.45497800	-0.81393600
Zn	5.89031200	4.17010500	-1.41042200
H	8.77851800	1.93000900	1.94671900
N	7.97913300	2.49060500	1.70178400

Structure S7. The Zn^{2+} -pHG complex A. Coordinates in Å.

H	-6.85604800	-0.04709400	1.43978500
C	-6.78017200	0.01279800	2.52593000
H	-7.77360000	-0.17094000	2.94115000
C	-6.36517800	1.39407100	2.91895200
O	-7.07336600	2.39503600	2.69412100
H	-6.09904300	-0.76733600	2.86362700
N	-5.17899900	1.52411500	3.59351200
H	-4.58943100	0.71732200	3.77598700
C	-4.90922600	2.77421600	4.26935300
H	-5.79202800	3.11332900	4.81753200
H	-4.10482600	2.60775100	4.99299100
C	-4.51457700	3.94461900	3.39133800
O	-4.72113200	5.11248400	3.76975400
N	-3.85040100	3.63583400	2.24566400
H	-3.80927600	2.66590200	1.94422300
C	-3.34353000	4.63824300	1.32564900
H	-4.17291600	5.21869600	0.89461600
C	-2.63398900	3.89142200	0.20795300
O	-2.47697300	2.64713800	0.27759900

C	-2.41235000	5.64970900	2.06209300
H	-3.04439600	6.12746100	2.81352900
H	-1.65628900	5.07107400	2.59947200
C	-1.78062800	6.64667500	1.16184700
N	-0.42939800	6.63270200	0.84707500
H	0.26310000	6.01716900	1.28015000
C	-2.32343000	7.63590600	0.37211400
H	-3.34613900	7.97349500	0.33528300
C	-0.21618500	7.59511200	-0.10386500
H	0.74740300	7.78373400	-0.54188900
N	-1.34033900	8.22169000	-0.42102100
N	-2.17111700	4.58472900	-0.86236700
H	-2.23529600	5.59831400	-0.88605800
C	-1.43259700	3.88191100	-1.90326100
H	-1.64574500	2.82203900	-1.74496500
C	0.06614400	4.10136400	-1.76249900
O	0.60407100	5.16445000	-2.12733700
C	-1.85813500	4.25568400	-3.33860700
H	-2.91051400	4.55220700	-3.32679200
H	-1.27216200	5.11460100	-3.67751600
C	-1.72604400	3.04897700	-4.20129400
N	-0.55704500	2.31437100	-4.35103100
H	0.40090500	2.57447400	-4.10383100
C	-2.71278400	2.25761100	-4.72633800
H	-3.76794900	2.46912500	-4.79218400
C	-0.87618600	1.12185100	-4.93204300
H	-0.13922100	0.36789100	-5.16562200
N	-2.18610600	1.04582200	-5.16446100
N	0.77617300	3.04581500	-1.28227400
H	0.33591700	2.20830400	-0.89726900
C	2.22152900	3.02309600	-1.43414000
H	2.45204300	3.96394000	-1.94844800
C	2.49813000	1.95038000	-2.47924500
O	2.11449300	2.17886200	-3.65390800
C	2.99507500	2.99538700	-0.11313000
H	2.57210600	3.77759200	0.53109900
H	2.83027900	2.05361800	0.41671100
C	4.44388400	3.20391200	-0.35680300
N	4.93605200	4.35148400	-0.97530300
H	4.39027400	5.16705800	-1.20823200
C	5.52321000	2.38121900	-0.20736400
H	5.55213700	1.40595500	0.25907800
C	6.26552800	4.19095100	-1.19138900
H	6.89581900	4.92395200	-1.66348800
N	6.65207500	2.99794900	-0.75032300
N	3.05946700	0.76705600	-2.15883800
H	3.28619200	0.50402700	-1.20580000
C	3.18453900	-0.23527500	-3.21067700

H	3.42998000	0.29535500	-4.13351900
C	1.87113900	-0.96095700	-3.47648800
O	1.67079900	-1.52662300	-4.56954600
C	4.26247500	-1.30183600	-2.91717700
H	3.84126500	-2.05095500	-2.23996200
H	4.47500800	-1.80220800	-3.86533100
C	5.50435500	-0.76227900	-2.30119000
N	5.80416700	-1.01229200	-0.97232100
H	5.19627600	-1.41299800	-0.26187900
C	6.52511700	0.03521300	-2.75554400
H	6.67443600	0.46115800	-3.73255600
C	6.95758100	-0.40029300	-0.65329000
H	7.36117500	-0.41541200	0.34492400
N	7.42108200	0.26717500	-1.71364800
N	1.00379000	-1.02935500	-2.43542700
H	1.27593200	-0.64547300	-1.53318500
C	-0.09779700	-1.98475200	-2.44599200
H	-0.48185700	-2.04144200	-3.47034000
C	-1.15127800	-1.45981100	-1.49620800
O	-1.00732500	-1.62177100	-0.25964800
C	0.39481500	-3.36614100	-1.97952700
H	1.18876300	-3.68367900	-2.66832900
H	0.85054600	-3.22020100	-0.99473600
C	-0.67256900	-4.38874200	-1.85236000
N	-1.26928100	-5.02935900	-2.93267700
H	-1.08163000	-4.84319900	-3.90403900
C	-1.26885000	-4.93873600	-0.74512100
H	-1.06367600	-4.72181900	0.29250300
C	-2.18420100	-5.92172400	-2.43615800
H	-2.81331300	-6.52964600	-3.06136800
N	-2.20110200	-5.89902300	-1.11371600
N	-2.18692700	-0.79591400	-2.03587200
H	-2.24786500	-0.71034700	-3.04447900
C	-3.14027200	-0.05616200	-1.21291900
H	-2.59310800	0.67204100	-0.60360200
C	-3.91933600	-0.90106400	-0.22820100
O	-4.35885700	-0.34676200	0.80363900
C	-4.13709300	0.73634200	-2.07819500
H	-4.80481500	1.23861600	-1.37155700
H	-3.58596100	1.52504600	-2.59982000
C	-4.94774300	-0.06393700	-3.04048100
N	-4.57057300	-0.31371000	-4.35845200
H	-3.71054600	0.01105300	-4.82040400
C	-6.18623700	-0.64877600	-2.90519700
H	-6.81709300	-0.66437200	-2.03058900
C	-5.58943800	-1.01048900	-4.94596900
H	-5.56864300	-1.30990800	-5.98015200
N	-6.58242300	-1.23973000	-4.09615800

N	-4.15386200	-2.19575900	-0.52619200
H	-3.89343500	-2.59043200	-1.43236500
C	-5.04882600	-2.99155800	0.30817900
H	-6.04167100	-2.52658800	0.33742900
C	-4.57484500	-3.02865700	1.75355800
O	-5.37385000	-3.07090500	2.69964900
C	-5.16039000	-4.41501300	-0.26272900
H	-4.19725700	-4.92906100	-0.15965900
H	-5.89243000	-4.95865700	0.34034800
C	-5.55246500	-4.40272400	-1.69374700
N	-4.63506800	-3.99332500	-2.67218400
C	-6.75140000	-4.69023800	-2.28831600
H	-7.68987900	-5.01892600	-1.87797400
C	-5.28616700	-4.04485100	-3.82500500
H	-4.88865200	-3.77028700	-4.78535200
N	-3.21899600	-3.04604200	1.90441200
H	-2.66619400	-2.98998100	1.05455300
C	-2.57562600	-2.69011000	3.16125400
H	-3.24328000	-2.96523400	3.97985600
C	-2.41743400	-1.16276500	3.21656200
O	-2.99861600	-0.45769100	4.06734200
C	-1.23368000	-3.42665000	3.23865500
H	-1.44438400	-4.49531100	3.35864600
H	-0.72870700	-3.34009300	2.26134700
C	-0.28366400	-2.95463700	4.28496900
N	0.94853800	-3.57491200	4.43382300
H	1.22523500	-4.39232500	3.89203400
C	-0.27736800	-1.92155400	5.19551600
H	-1.06844300	-1.22737100	5.42641100
C	1.63865700	-2.90916300	5.41762000
H	2.63077900	-3.18746100	5.73238100
N	0.93052700	-1.89519400	5.89272500
N	-1.55562700	-0.71757600	2.28038800
H	-1.36329500	-1.33554900	1.49748900
C	-1.02592900	0.61415500	2.03357200
H	-1.60837000	1.13273000	1.26823600
C	0.36682200	0.37078900	1.45625600
O	0.71685800	0.77639300	0.31850900
C	-0.98054000	1.48414600	3.29889500
H	-2.01296700	1.74966200	3.54915800
H	-0.60261800	0.89496500	4.14291600
C	-0.14602200	2.70066400	3.11512500
N	0.43965100	3.37865700	4.17675100
H	0.38369600	3.10415000	5.14448600
C	0.19246600	3.42887000	2.00644600
H	-0.07654700	3.24350900	0.98442100
C	1.09720300	4.47126500	3.68003800
H	1.63307300	5.17141200	4.29589100

N	0.96949100	4.52954100	2.36087200
N	1.19809900	-0.33045000	2.25595500
H	0.83505600	-0.71545600	3.12523900
C	2.58799000	-0.58117700	1.90678300
H	2.94582300	0.25929200	1.31081600
C	2.72294100	-1.78467400	0.97664800
O	2.94646100	-1.61989400	-0.25083200
C	3.45913300	-0.69946600	3.15257400
H	3.52530100	0.28538900	3.62453100
H	3.02807000	-1.37849800	3.89414000
C	4.84797800	-1.19709600	2.76240600
O	5.31803900	-0.72737800	1.65680600
O	5.38485100	-2.07945200	3.48985200
N	2.62076100	-3.00557600	1.53652700
H	2.43968800	-3.08027500	2.53209900
C	2.90276700	-4.25368200	0.83756500
H	2.91130500	-4.02528900	-0.23384200
C	1.82910200	-5.27385900	1.15844500
O	1.27549500	-5.30977900	2.27905300
C	4.26789800	-4.83061000	1.25719300
H	4.29749700	-4.87536000	2.35366700
H	4.36382700	-5.85818800	0.88756200
C	5.43291000	-3.99589500	0.73618300
H	5.46121900	-4.04363700	-0.35764900
H	5.32285800	-2.95666400	1.04685500
C	6.74274300	-4.54969800	1.25246100
O	7.28579400	-5.52718900	0.70036200
N	7.22044400	-3.93751400	2.35682600
H	8.06330000	-4.30410400	2.77028800
H	6.70809600	-3.17968600	2.82199900
N	1.56213000	-6.17606900	0.19910400
H	1.95488300	-6.11641000	-0.72561300
H	0.87402000	-6.89225100	0.37864100
H	-7.28745500	-4.48013700	-4.34293800
N	-6.56678700	-4.47173800	-3.64236200
Zn	8.38484200	2.00362200	-1.31023700

Structure S8. The Zn^{2+} -pHG complex B. Coordinates in Å.

H	-12.04946500	0.08290800	0.12705700
C	-11.59346600	0.20555800	1.11103600
H	-11.48409600	1.27053300	1.32160700
C	-10.29339400	-0.54651300	1.14628200
O	-10.23425200	-1.77329900	0.93357900
H	-12.27697500	-0.23193300	1.84080900
N	-9.18755900	0.18719600	1.42384200
H	-9.21688100	1.18621400	1.58533900

C	-7.87863600	-0.41155700	1.48739300
H	-7.83935500	-1.19664200	2.25173400
H	-7.61351000	-0.90312900	0.54245600
C	-6.87013100	0.66673200	1.78955500
O	-7.18934700	1.86812600	1.90660600
N	-5.59371400	0.23923200	1.91960200
H	-5.37224000	-0.72554500	1.68278900
C	-4.51484500	1.19271400	2.01823400
H	-4.72758800	1.90794500	2.82109000
C	-4.36556600	1.95091600	0.69988200
O	-4.77129300	1.46004800	-0.37644000
C	-3.21114300	0.42879100	2.34655900
H	-3.39298500	-0.17319700	3.24222200
H	-2.99840200	-0.29012900	1.54294000
C	-2.04777500	1.32344400	2.53913400
N	-1.18073700	1.65581400	1.50672400
H	-1.20485500	1.28162900	0.55876100
C	-1.61743800	2.04062800	3.62827800
H	-2.00446400	2.02154700	4.63206000
C	-0.27764000	2.54773600	1.99767700
H	0.60252700	2.87811300	1.45656200
N	-0.50243100	2.79786900	3.28775100
N	-3.68473400	3.11974600	0.71698500
H	-3.41153700	3.56405900	1.58491100
C	-3.30172300	3.74461500	-0.54456400
H	-3.09606700	2.93985300	-1.25823600
C	-2.07395600	4.60890200	-0.33185400
O	-2.14875400	5.62438700	0.39449400
C	-4.44528800	4.61916000	-1.10077500
H	-5.28742100	3.95873200	-1.31662700
H	-4.75258300	5.29783600	-0.29831700
C	-4.05788000	5.37665600	-2.31691300
N	-3.28741500	6.53352000	-2.25614700
H	-2.95071400	6.95029300	-1.40010900
C	-4.28227700	5.17108400	-3.65491000
H	-4.84613100	4.38012000	-4.11940700
C	-3.09145700	6.96966700	-3.54274900
H	-2.53036800	7.85500000	-3.78628000
N	-3.68008700	6.16729500	-4.41357200
N	-0.95543500	4.25741300	-1.01616200
H	-1.03073500	3.49783600	-1.68701900
C	0.23337700	5.11492500	-1.10885400
H	0.00361000	5.98596300	-1.73560000
C	1.34281600	4.39426500	-1.86784600
O	2.00307300	4.99831600	-2.72166000
C	0.71271200	5.64024300	0.27210100
H	0.00666000	6.39714200	0.60873600
H	0.66314600	4.82681000	1.00219000

C	2.09827000	6.16269900	0.21849100
N	3.17942300	5.28647400	0.30605200
C	2.57952400	7.42655500	0.01879100
H	2.07693300	8.36865800	-0.10745500
C	4.28453400	6.00275300	0.16327500
H	5.28975000	5.61996200	0.18411200
N	1.59272900	3.08111800	-1.53131500
H	0.96304200	2.61424500	-0.88208400
C	2.22142900	2.19751800	-2.53406700
H	2.51208600	2.85162400	-3.35963100
C	1.05201700	1.33063200	-3.01596900
O	0.12973700	1.83993200	-3.68453400
C	3.39134200	1.35597600	-2.04604900
H	3.00969300	0.68892300	-1.27019000
H	3.69666700	0.71062800	-2.87726200
C	4.62540100	1.93179500	-1.44816200
N	4.61516600	2.64961300	-0.25033500
C	5.90961000	1.49965900	-1.66279500
H	6.31976500	0.85638900	-2.42160100
C	5.85926800	2.63416200	0.23653800
H	6.14570000	3.03753800	1.19488200
N	1.00383700	0.04000000	-2.59284000
H	1.74253300	-0.37716300	-2.02554900
C	-0.15400300	-0.76677200	-2.89454000
H	-0.47885300	-0.51079100	-3.91155000
C	-1.34076400	-0.41507900	-1.98500600
O	-1.30394900	0.52464900	-1.16086700
C	0.21439300	-2.25368100	-2.84796500
H	-0.57180900	-2.86387500	-3.31281700
H	1.11368200	-2.37732800	-3.46345100
C	0.47716100	-2.76971100	-1.48081900
N	1.01707300	-4.02758100	-1.28706000
H	1.15732900	-4.72005900	-2.00547100
C	0.31187500	-2.24882600	-0.22367300
H	-0.03224900	-1.26854200	0.07278200
C	1.16268600	-4.23404500	0.05082200
H	1.60838500	-5.12488700	0.45907200
N	0.74386400	-3.17304300	0.72755900
N	-2.43757500	-1.19705100	-2.14907400
H	-2.40137800	-1.98453100	-2.78526000
C	-3.68430900	-0.96566800	-1.43558800
H	-3.59472900	0.00693100	-0.94251800
C	-3.94729000	-1.97012700	-0.32645600
O	-5.08781000	-2.06974200	0.17794100
C	-4.88814700	-0.83245000	-2.37529200
H	-5.75072500	-0.61658700	-1.74293000
H	-4.72683200	0.05586400	-2.99373300
C	-5.13961000	-2.03303000	-3.21445700

N	-4.76245000	-2.11137000	-4.55395100
H	-4.37852500	-1.35165400	-5.09261600
C	-5.70982100	-3.24887500	-2.93763100
H	-6.13415600	-3.57838800	-2.00455500
C	-5.12497000	-3.34794800	-5.02518100
H	-4.96948900	-3.66275800	-6.04252000
N	-5.68689900	-4.06715100	-4.06614300
N	-2.88302800	-2.67276800	0.12703800
H	-2.00799600	-2.62773700	-0.38388100
C	-3.02952100	-3.74084200	1.11255800
H	-4.10714300	-3.90903000	1.20621600
C	-2.60513200	-3.25591600	2.49855500
O	-3.45207200	-2.71155200	3.23128000
C	-2.35625700	-5.02116000	0.58906100
H	-1.26807600	-4.91078800	0.58500000
H	-2.59793400	-5.84311100	1.26972900
C	-2.80171800	-5.30567100	-0.80140000
N	-2.07316300	-4.83801500	-1.90080100
C	-3.97351800	-5.87336800	-1.23637300
H	-4.79484000	-6.31413100	-0.69812100
C	-2.81559900	-5.12849700	-2.96630200
H	-2.56936700	-4.90242600	-3.99058900
N	-1.30317400	-3.42349500	2.87314500
H	-0.60411900	-3.65482300	2.17046900
C	-0.84752300	-2.93523500	4.17078600
H	-1.74638300	-2.78145000	4.77092700
C	-0.17110700	-1.56860200	4.11016800
O	-0.35495400	-0.74745900	5.03091100
C	0.06511800	-3.94870500	4.91540000
H	0.14163700	-3.59763000	5.94917800
H	-0.45066200	-4.91391700	4.93624900
C	1.43397400	-4.05510200	4.34468700
N	1.77460000	-4.86405700	3.26375500
H	1.20924600	-5.61245700	2.89700400
C	2.52567000	-3.24993600	4.53147500
H	2.64895500	-2.47418500	5.26918500
C	3.02597500	-4.50407500	2.83161000
H	3.51970200	-4.96190000	1.98559900
N	3.50138100	-3.50854800	3.57321700
N	0.67296400	-1.35701000	3.07061400
H	0.79870500	-2.08573100	2.36419900
C	1.38873800	-0.10017300	2.88123800
H	0.66234800	0.69184900	2.72483800
C	2.21710400	-0.17275600	1.61292700
O	2.01461200	0.63457000	0.67097200
C	2.29801600	0.33665100	4.06143700
H	1.67346600	0.38697900	4.95631500
H	3.07335100	-0.41602400	4.23374200

C	2.94644400	1.64770900	3.77625700
N	2.28205700	2.85781200	3.90137300
H	1.27074600	2.96685800	4.05936600
C	4.19580700	1.96834800	3.29289700
H	5.02314900	1.31013600	3.07814900
C	3.12071800	3.83938800	3.46466500
H	2.85127000	4.88184100	3.45379600
N	4.30531400	3.34182800	3.09458300
N	3.21660200	-1.08121200	1.62053100
H	3.31060100	-1.74868700	2.38804200
C	4.31933200	-1.07597800	0.65946900
H	4.34809000	-0.07590100	0.21389600
C	3.98584200	-2.01139500	-0.50043700
O	3.18680900	-1.64795500	-1.39938500
C	5.63844300	-1.30847500	1.40468800
H	5.62153800	-0.71697200	2.32171400
H	5.74481800	-2.35223200	1.72355600
C	6.81863800	-0.85037800	0.55029600
O	7.57458800	0.05582100	1.01041100
O	6.88104600	-1.37557400	-0.62042500
N	4.52917700	-3.24575200	-0.49626000
H	5.26068300	-3.44979700	0.16902800
C	4.41954200	-4.13433700	-1.63374000
H	3.62836000	-3.71268200	-2.26868400
C	3.97250600	-5.51333600	-1.18962800
O	3.82508500	-5.84127100	0.00225600
C	5.73856200	-4.14808000	-2.42699900
H	6.56270900	-4.32384900	-1.72380500
H	5.76474200	-4.96602300	-3.15551800
C	5.96143600	-2.82069500	-3.15402700
H	5.26125800	-2.73379000	-3.98987500
H	5.80699700	-1.99523500	-2.45838900
C	7.36681300	-2.77926800	-3.70493700
O	7.66852800	-3.38394600	-4.75432300
N	8.24754300	-2.09235700	-2.94416500
H	9.21300200	-2.07898700	-3.23223100
H	7.96506200	-1.68329200	-2.04715700
N	3.68333700	-6.37735300	-2.20034900
H	3.88733000	-6.16572300	-3.16359100
H	3.44713000	-7.32830800	-1.96177500
H	-4.76356900	-5.86848300	-3.22979800
N	-3.96519100	-5.76425400	-2.61164200
Zn	2.97501900	3.23976400	0.71013500
H	4.61005000	8.06765500	-0.14612000
H	7.52955600	1.49350600	-0.27771300
N	6.67051400	1.95133000	-0.60057300
N	3.96102700	7.31122300	-0.01044600

Structure S9. The Zn^{2+} -pHG complex C. Coordinates in Å.

Corresponding authors

*E-mail: henryk.kozlowski@chem.uni.wroc.pl. Tel: (+48) (71) 375 72 51. Fax: (+48) (71) 375 72 51.

(H.K.).

*E-mail: ymiller@bgu.ac.il. Tel: 972-86428705. Fax: 972-86428709 (Y.M.).