Electronic Supplementary Material for PCCP

Toward a DFT-based molecular dynamics description of Co(II) binding in sulfur-rich peptides: Supplementary material

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Cartesian coordinates of the DFT/B3LYP(AE) optimized structures of [Co–(Cys-H)]$^+$ and DFT/BLYP(AE) optimized structures of [Co–(Glutathione-H)]$^+$ complexes, respectively shown in figures 3 and 4 of the paper, are provided here.
We also give the energy differences between the two [Co–(Glutathione-H)]$^+$ structures when calculations are done using different atomic basis sets with BLYP and B3LYP functionals on the optimized structures (i.e. BLYP/6-31G(d)/Wachters).

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$[Co–(Cys-H)]^+$ 1S	x(Å)	y(Å)	z(Å)
C	-0.015355	1.760002	0.188729
S	1.475144	1.056867	-0.666192
Co	0.997744	-0.975620	-0.042394
O	-0.989197	-1.164954	-0.661926
C	-1.576755	-0.179381	-0.195496
O	-2.759512	0.221874	-0.592381
C	-0.915622	0.688257	0.866936
N	-0.053426	-0.239398	1.653508
H	-0.602295	2.336085	-0.531316
H	0.333157	2.454616	0.959426
H	-1.679568	1.184419	1.474404
H	0.530075	0.287889	2.303625
H	-0.615358	-0.882981	2.212460
H	-3.097370	-0.341009	-1.315996

$[Co–(Cys-H)]^+$ 2S	x(Å)	y(Å)	z(Å)
C	-0.051441	1.762996	0.231101
S	1.424489	1.091668	-0.674690
Co	1.039939	-0.939561	-0.027312
C	-0.946088	0.673497	0.878565
C	-1.723025	-0.076993	-0.200233
O	-1.023559	-1.220013	-0.611928
N	-0.088416	-0.294514	1.626813
O	-2.756789	0.249606	-0.696659
H	-0.648405	2.364061	-0.459392
H	0.320315	2.429895	1.015595
H	-1.684304	1.159975	1.524867
H	0.460926	0.202154	2.329834
H	-0.659591	-0.974744	2.130718
H	-1.474085	-1.612028	-1.384738

$[Co–(Cys-H)]^+$ 3S	x(Å)	y(Å)	z(Å)
C	0.388080	1.541758	-0.393322
C	1.349307	0.603143	0.376870
N	2.764561	0.915051	0.145217
S	-1.419334	1.421478	0.011446
Co	-1.647741	-0.709348	0.022906
O	0.092455	-1.511218	0.060915
C	1.184179	-0.893657	0.025859
O	2.268109	-1.515797	-0.282242
H	2.923151	1.504728	-0.668504
H	3.220701	1.338204	0.947841
H	1.128388	0.679218	1.449132
H	0.512663	1.424367	-1.475209
H	0.663158	2.568115	-0.135543
H	2.984449	-0.802587	-0.221676

$[Co–(Cys-H)]^+$ 4S	x(Å)	y(Å)	z(Å)
C	0.233989	1.251126	0.378933
S	-1.592838	1.381474	0.100605
Co	-1.843838	-0.741734	-0.044807
N	0.159968	-1.202211	-0.166201
C	0.872301	0.096445	-0.422277
C	2.375279	0.044164	-0.114468
O	2.717711	-1.065862	0.574665
O	3.130302	0.923684	-0.437874
H	0.684245	2.193493	0.059485
H	0.411272	1.140192	1.454096
H	0.771314	0.316686	-1.488622
H	0.513715	-1.604997	0.707665
H	0.422004	-1.880522	-0.884068
H	3.673171	-1.039130	0.767500

$[Co–(Cys-H)]^+$ 5S	x(Å)	y(Å)	z(Å)
C	0.000000	0.000000	0.000000
S	0.000000	0.000000	1.855588
Co	2.097311	0.000000	2.241690
O	3.035601	0.011344	0.531576
C	2.480216	0.220784	-0.574834
O	3.082772	-0.111832	-1.681056
C	1.096429	0.854039	-0.726785
N	0.817629	1.130562	-2.111145
H	0.019709	-1.039742	-0.342562
H	-0.964976	0.425360	-0.285738
H	1.166429	1.815018	-0.200113
H	0.087771	1.822604	-2.235980
H	0.626092	0.311784	-2.679506
H	3.958514	-0.504560	-1.497176

$[Co–(Cys-H)]^+$ 6S	x(Å)	y(Å)	z(Å)
C	-0.840759	-0.143777	-0.999895
C	-0.839751	-0.133348	0.546809
N	0.559777	-0.136813	1.087415
Co	1.742664	0.912325	-0.213956
S	0.249241	1.166014	-1.731318
C	-1.539357	-1.409362	1.074497
O	-0.878298	-2.344646	1.460536
O	-2.872955	-1.456195	1.035989
H	0.549716	0.219904	2.045373
H	0.815954	-1.131357	1.191868
H	-1.334182	0.775075	0.905481
H	-1.850541	0.038163	-1.376690
H	-0.514667	-1.116259	-1.382902
H	-3.291240	-0.624548	0.763630

$[Co–(Cys-H)]^+$ 7S	x(Å)	y(Å)	z(Å)
C	-1.530971	-0.239560	-0.605813
S	-1.469631	-0.402443	1.238765
Co	0.594207	-0.119012	1.681752
O	1.581699	0.068802	-0.059274
C	0.897988	0.040543	-1.341341
O	1.455770	-0.468783	-2.255984
C	-0.480292	0.695070	-1.292404
N	-0.809024	1.068933	-2.643446
H	-1.501987	-1.248119	-1.031249
H	-2.518870	0.181000	-0.812511
H	-0.393857	1.610314	-0.694135
H	-1.624912	1.666983	-2.707035
H	-0.877628	0.291344	-3.292234
H	2.486930	-0.265048	-0.222911

$[Co–(Cys-H)]^+$ 1O	x(Å)	y(Å)	z(Å)
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.540208
N	1.413078	0.000000	2.042660
Co	1.777677	-1.990025	1.502147
O	0.130327	-2.306136	2.261860
C	-0.708425	-1.276217	2.085871
O	-1.898609	-1.299546	2.267008
S	1.111901	-1.326172	-0.728874
H	1.951830	0.771720	1.645786
H	1.420378	0.134616	3.055629
H	-0.557088	0.878561	1.880772
H	0.329991	0.957420	-0.409674
H	-1.005231	-0.206853	-0.372493
H	2.142219	-0.532833	-1.095684

$[Co–(Cys-H)]^+$ 2O	x(Å)	y(Å)	z(Å)
C	-1.488088	-0.140993	-1.054763
S	-1.642474	0.293837	0.785724
Co	0.684457	-0.067411	1.498042
O	1.084600	1.208868	0.035686
C	0.882724	0.173505	-0.690251
O	1.181127	-0.972778	-0.185583
C	-0.147780	0.257149	-1.801538
N	-0.029749	-0.620406	-2.929406
H	0.335383	-1.540344	-2.702770
H	0.477033	-0.216853	-3.708740
H	-0.208430	1.294666	-2.135306
H	-1.604488	-1.222154	-1.121206
H	-2.328990	0.357809	-1.537562
H	-2.269973	-0.838257	1.171200

$[Co–(Cys-H)]^+$ 1N	x(Å)	y(Å)	z(Å)
C	-1.580314	-0.290156	-0.834308
S	-1.628029	-0.337123	1.031099
C	-0.116519	-0.237052	-1.373454
C	0.482591	1.119164	-0.995643
O	0.987150	1.280347	0.124856
Co	0.812531	-0.637046	1.038316
N	0.684172	-1.243087	-0.689378
O	0.371608	2.076708	-1.888120
H	1.084523	-1.965493	-1.279187
H	-0.144522	-0.348262	-2.462309
H	-2.207237	0.533491	-1.184216
H	-2.029335	-1.234095	-1.148716
H	0.759666	2.910131	-1.558157
H	-1.726764	0.991872	1.252638

$[Co–(Cys-H)]^+$ 2N	x(Å)	y(Å)	z(Å)
C	-1.530327	-0.510476	-0.811056
S	-1.551378	-0.528481	1.056180
Co	0.876994	-0.560047	1.051895
O	0.795793	1.438602	0.063772
C	0.254278	1.234256	-1.210483
O	0.085279	2.132263	-1.979358
C	-0.110621	-0.248599	-1.391312
N	0.861207	-1.084496	-0.700559
H	1.435366	-1.670356	-1.300092
H	-0.151353	-0.431711	-2.469984
H	-2.276284	0.205753	-1.162971
H	-1.844490	-1.516372	-1.096459
H	1.025764	2.379857	0.176685
H	-1.802804	0.783272	1.258495

$[Co–(Cys-H)]^+$ 3N	x(Å)	y(Å)	z(Å)
C	-1.230709	0.869892	1.043983
S	-0.900331	1.663451	2.656781
C	-0.004632	0.732203	0.077614
C	0.859194	-0.474499	0.408235
Co	0.089884	-0.961620	-2.122309
O	1.045106	-1.408325	-0.404284
N	-0.422127	0.576698	-1.311471
O	1.398280	-0.495046	1.598966
H	-0.919500	1.389385	-1.667898
H	0.621816	1.627132	0.207707
H	-1.737013	-0.091555	1.165793
H	-1.938151	1.541489	0.550062
H	1.938124	-1.300404	1.722151
H	-0.322171	0.606997	3.259864

$[Co–(Gluthation-H)]^+$ Structure I	x(Å)	y(Å)	z(Å)
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.548906
N	1.392088	0.000000	2.154983
O	4.297909	1.593215	0.923919
C	4.357161	2.645167	0.203235
N	5.437565	2.957402	-0.514263
C	6.639737	2.120474	-0.600139
C	7.609162	2.831031	-1.554212
O	8.765805	2.142397	-1.672028
C	0.180004	1.381801	-0.697619
C	1.616269	1.911429	-0.706304
N	1.933741	2.835516	0.343375
C	3.187402	3.646814	0.252970
C	3.253087	4.534512	1.535353
S	2.910370	3.537339	3.090949
O	2.483419	1.532066	-1.487049
C	-0.865803	-1.176408	2.083868
O	-1.876541	-1.583187	1.543404
O	-0.372371	-1.656764	3.269560
O	7.341931	3.882453	-2.123144
H	1.887243	-0.831120	1.788659
H	1.270532	-0.216362	3.158636
H	-0.493969	0.916289	1.920455
H	0.755099	-0.711664	-0.380894
H	-0.981074	-0.395227	-0.303235
H	-0.099873	1.260981	-1.755841
H	-0.517315	2.114402	-0.253593
H	1.136487	3.391007	0.672908
H	3.181174	4.278626	-0.651961
H	2.511012	5.345256	1.451851
H	5.459645	3.781982	-1.127315
H	7.102668	1.989493	0.392045
H	6.394110	1.116546	-0.986593
H	9.344542	2.642744	-2.298130
H	-0.994367	-2.359885	3.579265
H	4.246797	4.999976	1.619063

$[Co–(Gluthation-H)]^+$ Structure II	x(Å)	y(Å)	z(Å)
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.567981
N	1.406041	0.000000	2.107090
S	3.772123	-3.082929	2.875391
C	4.502888	-3.751196	1.284448
C	4.109612	-2.886080	0.060628
C	4.335188	-3.673733	-1.261283
O	3.393483	-4.320697	-1.747505
C	0.679290	-1.221496	-0.681932
C	2.183871	-1.296919	-0.370642
N	2.638150	-2.580599	0.107270
O	2.931347	-0.315322	-0.426242
C	-0.647307	-1.292248	2.108503
O	0.060096	-2.253811	2.459585
O	-1.975995	-1.410195	2.156641
N	5.585954	-3.588375	-1.798713
C	6.059377	-4.517930	-2.826413
C	7.093629	-5.485666	-2.224220
O	7.507527	-6.382940	-3.157667
O	7.496759	-5.432163	-1.072676
H	1.991383	0.637990	1.546166
H	1.410900	0.370932	3.069692
H	-0.558360	0.890792	1.907549
H	-1.044801	0.064799	-0.344459
H	0.503440	0.923408	-0.330196
H	0.164985	-2.162799	-0.426556
H	0.580723	-1.093004	-1.774489
H	2.151503	-3.373112	-0.358533
H	4.640200	-1.922760	0.070208
H	4.133271	-4.781236	1.158501
H	5.596921	-3.791713	1.390446
H	6.316091	-3.153935	-1.230721
H	5.193730	-5.069216	-3.221588
H	6.521563	-3.970337	-3.665592
H	8.179886	-6.961097	-2.721644
H	-2.427497	-0.568599	1.911551

Energy differences between Structure I and Structure II of [Co–(Gluthation-H)]$^+$ obtained from BLYP/6-31G(d)/Wachters geometry optimization.

	ΔE (kcal/mol)
BLYP(AE)/3-21G	–5.78
BLYP(AE)/6-31G	+9.52
BLYP(AE)/6-31G(d)	+5.15
BLYP(AE)/6-31+G(d)	+10.99
BLYP(AE)/6-311G	+10.22
BLYP(AE)/6-311G(d)	+7.15
BLYP(AE)/6-311+G(d)	+11.27
B3LYP(AE)/3-21G	+5.45
B3LYP(AE)/6-31G	+8.85
B3LYP(AE)/6-31G(d)	+8.53
B3LYP(AE)/6-31+G(d)	+30.31
B3LYP(AE)/6-311G	+13.34
B3LYP(AE)/6-311G(d)	+15.94
B3LYP(AE)/6-311+G(d)	+12.09
BLYP/PW-PP	+7.60