

Supplementary material

Reactivity of polynuclear zinc-thiolate sites

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a) Absolute electronic energies and correction to Gibbs free energies for all the molecules depicted in Scheme 1 and their related protonated species.

System	Electronic Energy ^{a,b}	Correction to G_{gaz} ^{b,c}	Gas phase Electronic Energy ^{b,d}	COSMO Electronic Energy ^{b,e}
1	-3531.495938	0.097832	-3531.654123	-3531.926378
1H	-3532.167332	0.104055	-3532.316052	-3532.393217
2	-3319.639427	0.128544	-3319.828248	-3319.930474
2H	-3320.176339	0.138046	-3320.359517	-3320.385078
3	-3107.668585	0.161027	-3107.892209	-3107.931560
3H	-3108.077899	0.172201	-3108.301085	-3108.380165
4	-6187.063718	0.159653	-6187.240346	-6187.482207
4H_t	-6187.682707	0.167153	-6187.853256	-6187.933752
4H_b	-6187.687835	0.168624	-6187.858394	-6187.934850
5	-6201.231596	0.251919	-6201.539752	-6201.664197
5H_{t1}	-6201.776900	0.259221	-6202.080757	-6202.124116
5H_{t2}	-6201.761105	-	-	-
5H_b	-6201.781312	-	-	-
6	-9280.492479	0.250245	-9280.759292	-9281.216725
6H_t	-9281.195557	0.261815	-9281.453029	-9281.676000
6H_b	-9281.185552	0.257470	-9281.443210	-9281.664007
7	-11936.045965	0.313720	-11936.332029	-11936.765276
7H_{t1}	-11936.728035	0.318640	-11937.009636	-11937.222512
7H_{t1}	-11936.724215	0.323378	-11937.000639	-11937.217089
7H_{b1}	-11936.723020	0.321364	-11937.001765	-11937.212436
7H_{b2}	-11936.724164	0.322935	-11936.997782	-11937.208777
8	-11512.304088	0.377766	-11512.657668	-11512.770801
8H_{t1}	-11512.792590	0.386946	-11513.145994	-11513.212637
8H_{t2}	-11512.815284	0.387523	-11513.165967	-11513.219960
8H_{b1}	-11512.790362	0.386864	-11513.142952	-11513.200568
8H_{b2}	-11512.798559	0.386524	-11513.151226	-11513.203408
9	-3093.557462	0.066752	-3093.655544	-3093.740827

9H	-3094.068278	0.075472	-3094.163233	-3094.183020
10	-8418.698512	0.285485	-8418.966835	-8419.024585
10H_t	-8419.115899	0.296370	-8419.384432	-8419.467174
10H_{b1}	-8419.090657	0.295010	-8419.360903	-8419.447381
10H_{b2}	-8419.100697	0.292506	-8419.374120	-8419.458631
11	-11498.149159	0.284435	-11498.373298	-11498.589701
11H_t	-11498.733726	0.293241	-11498.952672	-11499.035411
11H_b	-11498.718156	0.291922	-11498.939731	-11499.019781
12	-21642.389659	0.475915	-21642.629221	-21642.826613
12H_t	-21642.948857	0.483027	-21643.185154	-21643.270621
12H_b	-21642.930632	0.480458	-21643.167742	-21643.249924

^a Electronic energy at the MARIJ-BP86/def2-SVP level

^b Values are given in a.u.

^c Thermal correction to gas phase Gibbs free energy computed at the MARIJ-BP86/def2-SVP level

^d Electronic energy at the RI-B3LYP/def2-TZVPP//MARIJ-BP86/def2-SVP level

^e Electronic energy at the COSMO/RI-B3LYP/def2-TZVPP//MARIJ-BP86/def2-SVP level ($\epsilon=78.4$).

b) Cartesian coordinates of the optimized geometries for all the molecules depicted in Scheme 1 and their related protonated species at the MARIJ-BP86/def2-SVP level of theory.

1

Zn 0.0000050 -0.0000045 -0.0000005
S 1.4192404 -1.4263941 1.3420965
S -1.4192276 1.4263810 1.3421101
S 1.4263866 1.4192384 -1.3421030
S -1.4263979 -1.4192356 -1.3421038
C 2.2035927 2.2010073 0.1345496
H 1.4298489 2.6894901 0.7678747
H 2.6995554 1.4312681 0.7669245
H 2.9613685 2.9655415 -0.1643047
C 2.2011057 -2.2035006 -0.1345591
H 2.9655428 -2.9613745 0.1642921
H 1.4313902 -2.6993332 -0.7670661
H 2.6897170 -1.4297313 -0.7677514
C -2.2036167 -2.2009894 0.1345492
H -2.6995269 -1.4312060 0.7669092
H -2.9614231 -2.9654758 -0.1643046
H -1.4298785 -2.6895305 0.7678680
C -2.2011031 2.2034927 -0.1345369
H -2.6897151 1.4297246 -0.7677299
H -2.9655404 2.9613629 0.1643229
H -1.4313918 2.6993300 -0.7670452

1H⁺

Zn 0.1562961 -0.2032308 -0.2798399
S 1.3547867 -1.3573387 1.3297895
S -1.8369884 3.0083569 1.2447678
S 0.8942982 1.8388092 -1.0291085
S -1.6483020 -1.2518003 -1.2178012
C 2.3580790 2.0757185 0.0711090
H 2.1415861 2.8308895 0.8554929
H 2.6295287 1.1197619 0.5658725
H 3.2206334 2.4367349 -0.5275280
C 1.8343445 -2.7642708 0.2332181
H 2.0850904 -3.6479291 0.8574417
H 1.0070622 -3.0424283 -0.4525916

H	2.7250370	-2.5198994	-0.3837984
C	-2.0856691	-2.4146356	0.1493003
H	-3.0189565	-2.0899484	0.6557482
H	-2.2524419	-3.4349587	-0.2564347
H	-1.2710459	-2.4535214	0.9029507
C	-3.0949001	2.2512757	0.1412485
H	-2.7610061	1.2522093	-0.2114780
H	-4.0254794	2.1316166	0.7309018
H	-3.3128684	2.8959947	-0.7350086
H	-0.7503755	2.6942374	0.4265335

2

Zn	-0.0960838	0.1750158	-0.4335356
S	-0.9319916	2.0235919	-1.5849240
S	-1.3743258	-1.7899684	-0.5160633
S	2.2780220	-0.0156023	-0.4311231
C	2.4401903	-1.8496927	-0.5555388
H	2.8889153	-2.2802526	0.3671513
H	1.4420951	-2.3149629	-0.7091871
H	3.0989992	-2.1254776	-1.4080674
C	0.4033075	2.2511568	-2.8369172
H	0.0723008	1.9174681	-3.8453885
H	0.6842458	3.3249622	-2.9148337
H	1.3086104	1.6709089	-2.5598184
C	-2.1454567	-1.5560897	-2.1730288
H	-1.5760912	-2.0837165	-2.9698724
H	-3.1806032	-1.9634809	-2.1754154
H	-2.1825391	-0.4747391	-2.4287011
N	-0.3288086	0.4783977	1.7472505
C	0.7451039	0.5344698	2.5220750
C	-1.4287411	0.4812193	2.5741814
H	1.7712873	0.4964174	2.1125661
C	-1.0147603	0.5483917	3.8938674
H	-2.4406432	0.4043797	2.1603654
H	-1.5624286	0.5651040	4.8420972
N	0.3733238	0.5813590	3.8380084
H	1.0064532	0.6160863	4.6369153

2H⁺

Zn	-0.0463313	0.0862898	-0.0541471
S	-0.6159927	2.5916210	-1.0429140
S	-1.9616474	-0.7576782	-0.9689154
S	2.2014563	-0.1150596	-0.3834275
C	2.3819547	-1.9185439	-0.7304532
H	1.9984895	-2.5463075	0.0985623
H	1.8644481	-2.2119654	-1.6648726
H	3.4621627	-2.1339855	-0.8536119
C	0.5498374	2.5592062	-2.4640596
H	1.1245583	1.6118460	-2.4732676
H	0.0063617	2.7190018	-3.4139875
H	1.2517095	3.3998176	-2.3073123
C	-1.3224181	-1.6609637	-2.4451113
H	-0.8589616	-2.6253279	-2.1561536
H	-2.1797683	-1.8774547	-3.1129014
H	-0.5805511	-1.0660305	-3.0126760
N	-0.2778070	0.4866185	1.9901042
C	0.8076724	0.5182065	2.7612609
C	-1.3657506	0.7251252	2.8064680
H	1.8287910	0.3540660	2.3846726
C	-0.9265211	0.9091930	4.1039252

H	-2.3880123	0.7439184	2.4142273
H	-1.4598953	1.1166628	5.0364277
N	0.4514877	0.7737198	4.0492366
H	1.0946168	0.8481462	4.8388181
H	-1.4966672	1.6137971	-1.4841132

3

Zn	1.3255905	-0.0244433	0.3056013
N	3.3738047	-0.3657958	-0.2414519
S	1.4407360	2.1387730	1.0653024
S	-0.1934738	-0.8497108	-1.2212828
C	0.8445917	-1.9698278	-2.2512479
C	4.1320906	0.7209546	-0.3753073
C	0.2476647	2.9482257	-0.0876941
H	-0.7950888	2.8321215	0.2708429
H	0.3073583	2.5241384	-1.1090761
H	0.4774458	4.0320766	-0.1335464
H	1.6776125	-1.4287629	-2.7444742
H	0.2055888	-2.4045873	-3.0468816
H	1.2742430	-2.8138332	-1.6700072
N	5.3830408	0.3680494	-0.7815855
H	3.7623783	1.7372278	-0.1515802
H	6.1527452	1.0148896	-0.9586241
C	5.4271160	-1.0103097	-0.9164842
C	4.1612354	-1.4501173	-0.5752473
H	6.3290449	-1.5416044	-1.2356510
H	3.7751691	-2.4744993	-0.5523292
N	1.1894861	-1.4609652	1.8858128
C	1.7895705	-1.6267898	3.1178290
C	0.2316624	-2.3806473	1.7912625
C	1.1832762	-2.6755412	3.7847527
H	2.6083350	-0.9804869	3.4521448
H	-0.4287095	-2.4697658	0.9114069
H	1.3558766	-3.1187543	4.7702875
N	0.2000142	-3.1370809	2.9237855
H	-0.4494135	-3.9029449	3.1077419

3H⁺

Zn	1.7630578	-0.5916201	0.2285077
N	3.7673544	-0.7258229	-0.1853790
S	1.1683950	1.5835740	0.2691804
S	0.7115412	-1.8352549	-1.6942541
C	1.0937227	-0.5893751	-2.9931202
C	4.4171424	0.3639955	-0.6115919
C	-0.6405050	1.5692084	-0.0972359
H	-1.2092634	0.9473831	0.6220245
H	-0.8627060	1.2291543	-1.1292816
H	-1.0008258	2.6119537	-0.0060046
H	1.1135741	0.4268236	-2.5537001
H	0.3580014	-0.6736039	-3.8133059
H	2.0955841	-0.8545618	-3.3781106
N	5.7351476	0.0818681	-0.7621422
H	3.9548620	1.3409250	-0.8051537
H	6.4504209	0.7437518	-1.0734806
C	5.9478045	-1.2411273	-0.4195719
C	4.7089682	-1.7339992	-0.0600792
H	6.9365301	-1.7082073	-0.4589124
H	4.4468066	-2.7411304	0.2793908
N	1.2598218	-1.6578014	1.9004265
C	1.2107624	-2.9979129	2.2483005

C	0.8721178	-0.9600664	2.9746157
C	0.7861823	-3.1068071	3.5580159
H	1.4741129	-3.7961458	1.5464313
H	0.7987962	0.1352525	3.0154976
H	0.6159946	-3.9760403	4.2004710
N	0.5807376	-1.8093079	3.9907275
H	0.2596861	-1.5308498	4.9213769
H	-0.5550334	-1.4186524	-1.4050292

4

C	1.4381993	-2.0916196	-1.1605152
S	0.6775743	-0.4192270	-0.9893646
H	0.6355044	-2.8548792	-1.2571426
H	2.0610180	-2.3112157	-0.2687454
C	2.9095187	1.6556229	1.3583399
S	1.2749126	1.8564392	2.1830567
H	2.7860341	1.4814478	0.2676758
H	3.4670596	0.7859805	1.7691567
C	1.9760533	-1.1783471	4.1138898
S	1.5322529	-2.0244083	2.5377329
H	1.9494181	-0.0732798	3.9749296
H	2.9968133	-1.4789607	4.4434991
C	-2.2118791	-2.1177005	2.2866645
S	-2.0168769	-0.4377215	1.5489892
H	-2.8562791	-2.0530802	3.1901629
H	-1.2135088	-2.5124429	2.5759590
C	-4.6562394	-0.0332892	-1.2330568
S	-3.1180782	0.3815907	-2.1571313
H	-4.8935719	-1.1170763	-1.3055923
H	-5.5176121	0.5418463	-1.6433457
C	-2.7389423	-3.1742655	-2.9560935
S	-2.1249120	-3.2825887	-1.2216638
H	-3.0670430	-2.1335788	-3.1813424
H	-3.5972718	-3.8676033	-3.1103635
H	1.2699353	-1.4440993	4.9331421
H	3.5284705	2.5701074	1.5041580
H	2.0778647	-2.1157342	-2.0693480
H	-1.9483478	-3.4559543	-3.6883037
H	-2.6850762	-2.7965532	1.5471272
H	-4.5500851	0.2088105	-0.1535897
Zn	0.4351644	-0.2205567	1.4629918
Zn	-1.7162728	-0.9786880	-0.8456044

4H⁺ site of protonation : S_t

C	1.2017876	-2.4238112	-1.1353568
S	0.5047459	-0.7105814	-1.1025772
H	0.3932017	-3.1709234	-1.2629402
H	1.7359309	-2.6167040	-0.1821801
C	2.7789677	1.6778487	0.9824158
S	1.1731120	1.8298006	1.8749609
H	2.6267175	1.4514772	-0.0937284
H	3.4151762	0.8754938	1.4117525
C	1.8979409	-1.3207504	3.9563149
S	1.2414355	-2.1614846	2.4485758
H	1.9649396	-0.2235722	3.7943195
H	2.9083158	-1.7138124	4.1982188
C	-2.4212991	-1.8900154	2.5966877
S	-2.1626379	-0.3557938	1.6046185
H	-2.8445240	-1.5970176	3.5784726
H	-1.4390259	-2.3867847	2.7555011

C	-4.6824902	0.1256267	-1.1205754
S	-3.0938995	0.8462948	-1.6876451
H	-4.6708460	-0.9658278	-1.3245938
H	-5.5462070	0.6374403	-1.5870299
C	-2.1519748	-2.7199128	-3.2722226
S	-2.7610143	-2.9770572	-1.5491911
H	-2.8346412	-2.0682699	-3.8597490
H	-2.0980439	-3.6995494	-3.7906283
H	1.2403906	-1.5062783	4.8321316
H	3.3318301	2.6378930	1.0642850
H	1.9113572	-2.5026258	-1.9833865
H	-1.1418833	-2.2614715	-3.2797750
H	-3.1280079	-2.5760283	2.0901185
H	-4.6829175	0.2784869	-0.0238329
Zn	0.3824553	-0.2751789	1.4041292
Zn	-1.7301697	-1.1902320	-0.5484228
H	-3.0987137	0.3083918	-2.9407155

4H⁺ site of protonation : S_b

C	1.3678382	-3.0911422	-0.9225683
S	1.0280119	-1.2750045	-0.9247416
H	0.6083372	-3.5785008	-1.5667469
H	1.2982209	-3.5084732	0.1004857
C	0.3314739	2.1930570	0.4899355
S	0.6115341	1.2756008	2.0689626
H	-0.3535464	1.6536244	-0.1994368
H	1.2890766	2.3763660	-0.0360550
C	1.9758425	-1.4746326	4.3100998
S	2.2024871	-2.3243088	2.6875317
H	2.3694191	-0.4388469	4.2901368
H	2.5298475	-2.0452458	5.0838694
C	-1.9668197	-2.1749259	2.0946838
S	-2.3404683	-0.5989436	1.2322612
H	-2.4717367	-2.2084514	3.0796011
H	-0.8722322	-2.3063133	2.2272197
C	-3.7207327	0.9087217	-1.8993044
S	-1.9767269	0.6138021	-2.4137414
H	-4.4024937	0.1085680	-2.2557934
H	-4.0613657	1.8697377	-2.3385694
C	-3.4996351	-2.9924662	-2.6725270
S	-2.2074690	-3.3593315	-1.4081746
H	-3.2122585	-2.1194309	-3.2943475
H	-4.4806439	-2.7742586	-2.1996720
H	0.9086239	-1.4342417	4.6085176
H	-0.1223495	3.1735297	0.7392395
H	2.3860733	-3.2692959	-1.3202791
H	-3.6283318	-3.8748837	-3.3339393
H	-2.3494800	-2.9761904	1.4295449
H	-3.8234698	0.9799468	-0.7971503
Zn	1.3621732	-0.7435455	1.3074161
Zn	-1.4126276	-1.2094866	-1.1314696
H	-1.2627782	0.1714992	1.7392232

5

S	6.5495740	-1.1334423	7.7166178
C	3.3094805	-0.7245761	4.1766415
N	4.1372346	-0.6763268	5.2863856
C	3.3174467	0.5208570	3.5746772
C	4.6425956	0.5526959	5.3633939
N	4.1643495	1.3139697	4.3396638

S	3.0904258	-7.3293916	4.4242968
S	3.9012061	-4.2031532	6.1614058
C	2.2653691	-2.3793379	8.7229543
N	3.3317382	-1.6072612	8.3114802
C	1.7202079	-1.8270527	9.8679555
C	3.4514825	-0.6074970	9.1761072
N	2.4879697	-0.7026295	10.1393712
S	1.9675728	-3.6763228	2.8662913
S	5.7158753	-4.9367374	2.7328299
Zn	4.7006533	-2.1266326	6.7095413
Zn	3.5990264	-5.1559991	3.7283283
C	7.8391433	-1.1988135	6.4033636
H	7.4892707	-0.7624777	5.4445477
H	8.7276154	-0.6260790	6.7421396
H	8.1567514	-2.2417584	6.2043564
C	6.0574796	-3.1712591	3.1049696
H	7.1167013	-2.9370989	2.8629049
H	5.4111765	-2.4888171	2.5115486
H	5.8876490	-2.9405391	4.1792269
C	4.4823425	-8.2406907	3.6329963
H	5.4285848	-7.6628516	3.6917140
H	4.6305088	-9.2147823	4.1488684
H	4.2830541	-8.4547925	2.5604180
C	2.7115751	-3.3494935	1.2100932
H	3.7190998	-3.8158117	1.1438019
H	2.0747453	-3.7694738	0.4013468
H	2.8119041	-2.2562612	1.0254453
C	5.2228396	-5.3817910	6.6619904
H	5.4904367	-5.2633176	7.7308211
H	4.7936883	-6.3866284	6.4633140
H	6.1144682	-5.2515660	6.0187610
H	2.7988467	-1.6660444	3.8533013
H	2.0041603	-3.2892536	8.1648688
H	2.8127977	0.8980734	2.6799193
H	5.3568984	0.8703746	6.1385369
H	4.4142034	2.2856481	4.1553397
H	2.3703447	-0.0699704	10.9313103
H	0.8793353	-2.1257338	10.5012901
H	4.2332305	0.1622301	9.1440683

5H⁺ site of protonation : S_{II}

S	6.3646433	-1.1727189	7.8470123
C	3.0680996	-0.7760097	4.3135430
N	3.9162898	-0.7247698	5.4069548
C	3.1336913	0.4331950	3.6462910
C	4.4885681	0.4802629	5.4116841
N	4.0344978	1.2105897	4.3584519
S	3.0104415	-7.3404586	4.3710329
S	3.9194823	-4.2873941	6.6493974
C	1.8852171	-2.1047782	8.8723518
N	3.0404697	-1.4696012	8.4616564
C	1.3859617	-1.4625860	9.9900238
C	3.2546283	-0.4636061	9.3066206
N	2.2696620	-0.4269157	10.2463008
S	1.8884933	-4.0347053	3.3247842
S	5.9102213	-4.9955880	3.2941123
Zn	4.4240749	-2.0281870	6.9625990
Zn	3.8775479	-4.7255395	4.2961621
C	7.5623634	-1.3305691	6.4545914
H	7.2398453	-0.7723831	5.5505001

H	8.5355843	-0.9158322	6.7849924
H	7.7169259	-2.3898413	6.1705789
C	6.2020112	-3.3166239	2.5907992
H	7.2029389	-3.3157255	2.1139638
H	5.4529237	-3.0479988	1.8191819
H	6.1978327	-2.5338476	3.3759560
C	3.8627210	-8.0058644	2.8858211
H	4.5995022	-8.7433314	3.2562072
H	3.1428648	-8.5205404	2.2217929
H	4.4041243	-7.1968973	2.3561738
C	2.4288292	-3.8551124	1.5682375
H	3.2540780	-4.5534587	1.3265718
H	1.5695725	-4.0687469	0.9014186
H	2.7762295	-2.8216854	1.3621579
C	5.5487267	-5.0386695	7.0952145
H	6.0066256	-4.4630226	7.9219641
H	5.3736316	-6.0844457	7.4120243
H	6.2099943	-5.0275912	6.2052624
H	2.4986533	-1.6898060	4.0604716
H	1.5053546	-2.9893230	8.3492280
H	2.6322154	0.7961087	2.7440658
H	5.2246327	0.8058219	6.1621926
H	4.3261006	2.1610871	4.1263127
H	2.2076668	0.2397176	11.0172292
H	0.5050015	-1.6488466	10.6112748
H	4.1152208	0.2164900	9.2712899
H	2.1047112	-6.5218458	3.7233896

5H⁺ site of protonation : S_{p2}

S	6.2195382	-1.9569880	7.3381980
C	3.6169409	-0.4607434	3.5087257
N	4.0058146	-0.8739667	4.7746841
C	3.0922742	0.8121257	3.6021712
C	3.7200802	0.1158565	5.6293639
N	3.1695496	1.1514104	4.9435710
S	3.8440072	-7.2252245	3.9548466
S	3.0736040	-4.0956855	6.1596388
C	2.7717063	-1.4595765	9.0260716
N	3.4104894	-0.2564923	8.7851584
C	2.4323303	-1.5563588	10.3662457
C	3.4603775	0.3698976	9.9531384
N	2.8784946	-0.3797192	10.9413201
S	2.7354346	-3.5821764	2.2476324
S	6.1731962	-3.9796145	4.0337660
Zn	4.7289531	-2.6972949	5.3070029
Zn	3.6958607	-4.9620504	3.8100310
C	7.9046777	-2.3711447	6.7374602
H	8.3100906	-1.4329496	6.3139366
H	8.5407115	-2.6890863	7.5839778
H	7.8485299	-3.1391189	5.9385200
C	6.3714620	-3.0421489	2.4623113
H	7.0332445	-3.6293102	1.7965296
H	5.3722550	-2.9281083	1.9891430
H	6.8313192	-2.0499240	2.6374107
C	5.4639481	-7.5532411	3.1398049
H	6.2312199	-6.8124358	3.4422163
H	5.8061310	-8.5634474	3.4432059
H	5.3749521	-7.5380036	2.0342296
C	2.9397107	-4.6812314	0.7769108
H	3.9646317	-4.6267229	0.3563205

H	2.7232498	-5.7335510	1.0471221
H	2.2240531	-4.3583981	-0.0056161
C	4.0173257	-5.3704880	7.1072497
H	3.3461156	-5.7786593	7.8874973
H	4.3134759	-6.1874073	6.4135670
H	4.9145018	-4.9460078	7.6038104
H	3.6725646	-1.1427797	2.6467511
H	2.6028235	-2.1961493	8.2255053
H	2.6693304	1.4820163	2.8482144
H	3.8285027	0.0940146	6.7325250
H	2.8442689	2.0221789	5.3654463
H	2.7884128	-0.1192245	11.9244335
H	1.9239586	-2.3345895	10.9440749
H	3.9038725	1.3555300	10.1432671
H	5.9593482	-3.1294841	7.9852909

5H⁺ site of protonation : S_b

S	5.9096632	-1.0282224	8.7356089
C	3.9139755	-0.2599699	4.4035985
N	4.5950800	-0.4460585	5.5955030
C	4.4180156	0.8637206	3.7768174
C	5.4961764	0.5328898	5.6972254
N	5.4142680	1.3471866	4.6116766
S	2.6519065	-6.7706822	5.1297932
S	4.8116396	-4.0259834	6.1750859
C	1.3390492	-2.1894957	7.5436783
N	2.6177975	-1.8733174	7.9725410
C	0.4676800	-2.0501479	8.6071044
C	2.5362708	-1.5524037	9.2649193
N	1.2458988	-1.6473302	9.6817608
S	1.5911975	-3.0023023	4.0883559
S	4.6177883	-5.0572022	2.3704279
Zn	4.5146199	-1.8873062	7.1055401
Zn	3.4267473	-4.3590636	4.1966560
C	7.0333762	-2.4432689	9.0970473
H	7.7681350	-2.5990592	8.2819887
H	7.5936615	-2.2161163	10.0261181
H	6.4728171	-3.3868388	9.2472276
C	4.9998204	-3.4149444	1.6229775
H	5.3563284	-3.5778785	0.5858698
H	4.1009115	-2.7676779	1.5873474
H	5.7969803	-2.8813686	2.1800705
C	3.7722486	-7.8880157	4.2006899
H	4.7308342	-7.3827628	3.9778364
H	3.9309104	-8.8308709	4.7570315
H	3.2622582	-8.1048357	3.2441035
C	0.7345934	-3.7483069	2.6350154
H	1.4718524	-4.1379190	1.9052478
H	0.0739430	-4.5810507	2.9501520
H	0.1120738	-2.9735279	2.1447577
C	6.4797339	-3.9253568	5.3912279
H	6.7407139	-2.8773162	5.1511154
H	7.2370604	-4.3398331	6.0839314
H	6.4443525	-4.5174774	4.4530778
H	3.1207816	-0.9544991	4.0755684
H	1.1321062	-2.5023343	6.5062464
H	4.1617793	1.3463682	2.8290506
H	6.1929246	0.6420695	6.5419212
H	5.9959999	2.1688660	4.4431389
H	0.9148387	-1.4575673	10.6285111

H	-0.6127838	-2.2016744	8.6885932
H	3.4031664	-1.2633766	9.8789585
H	3.4972806	-6.5005699	6.1691489

6

S	1.9085893	5.5152195	7.3508259
S	3.3966408	3.3139586	10.3195062
S	5.2504675	0.9408627	12.8926690
S	5.7945576	0.2823232	9.0354885
S	2.5851197	-1.8179897	8.2228138
S	-0.2017633	2.6817581	8.7587188
S	3.2491748	1.9211215	6.6791059
S	7.3446428	3.4192903	10.8294791
S	5.0189078	-1.0908621	5.3007751
Zn	4.1058233	-0.2781940	7.3426258
Zn	5.4135636	1.9951393	10.7629376
C	6.2304747	0.2627754	5.0043125
H	7.0163952	0.2889803	5.7907767
H	6.7331330	0.1276941	4.0174815
H	5.7243875	1.2518380	5.0100597
C	8.0707316	3.1473104	9.1613502
H	9.1585053	3.3933611	9.1686942
H	7.9453021	2.0899653	8.8445772
H	7.5854150	3.7847213	8.3902171
C	5.7980710	-1.2768632	10.0193110
H	4.9817094	-1.9321748	9.6426869
H	6.7760812	-1.7951283	9.9160108
H	5.6115346	-1.0199675	11.0852026
C	7.0385706	0.6205051	13.2032057
H	7.3451960	-0.3965410	12.8637016
H	7.6620481	1.3656042	12.6606074
H	7.2634853	0.6895730	14.2937627
C	4.0712988	5.0307699	10.3036537
H	3.7543643	5.5312154	9.3628816
H	3.6773796	5.6010909	11.1737818
H	5.1797705	4.9830309	10.3733721
C	0.7792344	6.2544272	8.6034591
H	0.0705138	5.4812866	8.9761208
H	1.3387169	6.6547106	9.4799534
H	0.1977946	7.0981614	8.1621373
C	-0.9795316	3.1463656	7.1550038
H	-0.9313624	2.3204186	6.4102430
H	-2.0550463	3.4010069	7.3050861
H	-0.4595170	4.0305159	6.7231680
C	1.9305187	1.2371654	5.5943259
H	2.4074202	0.4857267	4.9301037
H	1.1491168	0.7383840	6.2018790
H	1.4685044	2.0471637	4.9916438
C	1.9206500	-0.8252123	9.6298592
H	1.3220371	0.0401588	9.2753459
H	1.2641601	-1.4685487	10.2581333
H	2.7377412	-0.4374577	10.2736373
Zn	2.0525125	3.2969457	8.2739953

6H⁺ site of protonation : S_t

S	1.9637776	5.6559574	7.4876878
S	3.4461333	3.2230781	10.2253071
S	4.9151240	0.3882794	12.5929339
S	5.9525029	0.5100264	8.8362986
S	2.0242373	-0.7015832	8.5952376

S	0.0999117	2.3722252	8.3896934
S	3.4457927	2.2312136	6.3419843
S	7.2528037	3.2346768	11.3217209
S	4.3054248	-1.6856348	6.0971339
Zn	4.1344309	0.2645996	7.3853130
Zn	5.3821072	1.8982823	10.8509682
C	5.9609185	-1.3421466	5.3636416
H	6.6800972	-0.9966813	6.1354621
H	6.3616601	-2.2686385	4.8982386
H	5.9045981	-0.5598111	4.5772756
C	7.9773103	3.4485634	9.6434278
H	9.0092104	3.8543627	9.7331357
H	8.0220826	2.4841468	9.0958232
H	7.3847130	4.1573716	9.0265267
C	6.0911500	-1.1976159	9.5105069
H	5.7034139	-1.9144006	8.7566707
H	7.1572803	-1.4222222	9.7189249
H	5.5162924	-1.2597921	10.4600544
C	6.6452568	-0.0910139	13.0208219
H	6.9508694	-1.0367010	12.5204238
H	7.3540984	0.7083966	12.7153550
H	6.7319460	-0.2451970	14.1189770
C	4.0644039	4.9437228	10.4633517
H	3.8859564	5.5227675	9.5329994
H	3.5150497	5.4228136	11.3004829
H	5.1446154	4.8990297	10.7187634
C	0.8178459	6.1806916	8.8328333
H	0.0946568	5.3722495	9.0712170
H	1.3671275	6.4311855	9.7665539
H	0.2518803	7.0851707	8.5173345
C	-0.8179935	3.1757368	7.0065596
H	-0.8378460	2.5375533	6.0955232
H	-1.8701523	3.3666243	7.3117169
H	-0.3359973	4.1426309	6.7433214
C	2.0473113	1.4850592	5.3999173
H	2.3894566	0.5429063	4.9256955
H	1.2130038	1.2771378	6.1031775
H	1.7061404	2.2014173	4.6254479
C	1.9726794	-0.0654634	10.3148353
H	1.5893457	0.9701389	10.2439469
H	1.2752234	-0.6758835	10.9202658
H	2.9836904	-0.0551878	10.7700815
Zn	2.2056468	3.4128603	8.1363361
H	2.7752621	-1.8168207	8.8538731

6H⁺ site of protonation : S_b

S	2.1932484	5.6592359	7.9202609
S	3.6756972	3.0365498	10.1417315
S	4.7073500	0.7143228	12.7589220
S	6.0650520	0.2789353	8.9037348
S	2.5560911	-1.5923838	8.8477843
S	-0.3790335	2.8875949	8.8527802
S	3.0125255	1.8990052	6.8333162
S	7.5083005	3.0746604	11.3374719
S	4.8139610	-1.2081988	5.6607640
Zn	3.9657212	-0.2468663	7.6133961
Zn	5.9522931	1.4281853	10.9312157
C	5.9023969	0.1651553	5.0944035
H	6.7182885	0.3605884	5.8216422
H	6.3598698	-0.1012726	4.1156620

H	5.3275966	1.1067438	4.9701850
C	7.8984389	3.5198476	9.5905113
H	8.8350569	4.1167441	9.5660189
H	8.0349229	2.6109911	8.9696647
H	7.0896220	4.1262809	9.1330810
C	6.2578995	-1.4821885	9.4131542
H	5.3221401	-1.8443294	9.8856650
H	6.4202627	-2.0631311	8.4829411
H	7.1233396	-1.6038620	10.0948314
C	5.3769155	1.8445519	14.0529490
H	4.6143787	1.9864276	14.8483214
H	6.2884885	1.4189223	14.5234256
H	5.6444700	2.8359203	13.6337296
C	4.0480868	4.6527339	10.9137241
H	3.9064822	5.3834937	10.0894726
H	3.3338765	4.8739260	11.7292309
H	5.0954762	4.6366249	11.2817104
C	1.0094217	6.3411613	9.1613631
H	0.2402383	5.5804842	9.4174520
H	1.5295540	6.6401181	10.0983146
H	0.5051420	7.2437141	8.7522978
C	-1.1660589	3.6589469	7.3724775
H	-1.1468585	2.9782077	6.4943242
H	-2.2296949	3.8909579	7.5984240
H	-0.6503112	4.6011480	7.0889947
C	1.6283308	1.0880383	5.9270181
H	2.0610033	0.2324640	5.3689233
H	0.8589528	0.7242140	6.6358245
H	1.1693301	1.8069492	5.2175295
C	1.8165414	-0.3926603	10.0337133
H	1.4680405	0.5288875	9.5220354
H	0.9310810	-0.8600119	10.5158255
H	2.5295260	-0.1118683	10.8373690
Zn	1.8093626	3.3802052	8.2455385
H	3.5107804	2.2733628	11.2959307

7

S	-0.1647082	-0.5880633	-6.5801776
S	-3.8789933	-1.7501777	-6.8554610
S	-6.0201492	-5.0507918	-6.7404339
S	-2.8261560	-4.8338064	-8.9532203
S	-0.1203439	-4.4770891	-11.8457654
S	-1.5782781	-1.2639743	-10.1562723
S	-2.8919532	1.8423777	-7.7976432
S	-6.1139789	-2.6660867	-9.8627298
S	-6.6983302	-6.3158403	-11.8947150
S	-7.8101624	-2.9166907	-13.2003255
S	-3.7872892	-3.7880367	-12.5299530
C	-1.0359613	-0.1897219	-5.0054391
H	-1.6646128	0.7184422	-5.1318389
H	-1.7114804	-1.0158816	-4.6979941
H	-0.2966652	-0.0087624	-4.1915470
C	-5.9625232	-6.5600453	-7.8018109
H	-4.9373377	-6.9854042	-7.8388693
H	-6.6477907	-7.3320200	-7.3843359
H	-6.2660334	-6.3544289	-8.8506388
C	-8.4913724	-6.1726700	-11.4959370
H	-8.9102162	-5.2461138	-11.9467095
H	-9.0433761	-7.0530709	-11.8980591
H	-8.6648619	-6.1354059	-10.3986257

C -7.9068181 -4.1026928 -14.6058980
H -8.9392078 -4.1362163 -15.0263643
H -7.2185098 -3.8180845 -15.4348018
H -7.6252637 -5.1234581 -14.2625062
C -3.4330838 -5.5512305 -12.9337654
H -2.3331282 -5.6668231 -13.0325257
H -3.8045397 -6.2202523 -12.1321981
H -3.9466958 -5.8211054 -13.8791084
C 0.3343322 -5.7672861 -10.6151411
H -0.5684915 -6.1623351 -10.1024142
H 0.8462573 -6.6161042 -11.1224945
H 1.0248794 -5.3772965 -9.8344728
C -1.2659564 2.7050760 -7.7363422
H -1.3337952 3.6186442 -7.1011645
H -0.4897784 2.0272173 -7.3138203
H -0.9308050 3.0275052 -8.7489732
C -7.8090204 -2.9169079 -9.1841201
H -8.5047670 -3.1074872 -10.0256166
H -7.8022709 -3.7627570 -8.4633960
H -8.1324535 -1.9987689 -8.6487552
C -5.3217498 -0.6140820 -6.9425917
H -6.1179964 -0.9725256 -6.2571887
H -4.9889703 0.4000370 -6.6400121
H -5.7245269 -0.5825873 -7.9759313
C 0.2569812 -1.3526321 -10.0108892
H 0.6257479 -2.1406205 -10.7019725
H 0.6975087 -0.3682011 -10.2733569
H 0.5537183 -1.6045375 -8.9723164
C -1.6482600 -4.3777266 -7.6127405
H -2.0921573 -4.6682207 -6.6395328
H -0.6930124 -4.9233130 -7.7550192
H -1.4380377 -3.2886154 -7.5969582
Zn -2.1337102 -0.4073725 -7.9171855
Zn -2.0707505 -3.5336525 -10.8332439
Zn -4.7598494 -3.6309520 -8.1164978
Zn -6.1418186 -4.0027031 -11.8879109

7H⁺ site of protonation : S₁₁

S -0.0559345 -1.1174196 -7.2574555
S -3.9198700 -1.3381894 -6.9236377
S -6.2773589 -4.5205855 -6.7063695
S -3.1954180 -4.5345162 -9.0207858
S -0.4088329 -4.2461471 -11.8969020
S -2.1262844 -0.9339812 -10.5181142
S -2.3613437 1.9948858 -7.7398691
S -6.3757216 -2.2044337 -9.8353954
S -7.3889433 -5.8203907 -11.7195943
S -6.4061461 -2.8640604 -15.3915878
S -4.1196161 -3.8130633 -12.4085209
C -0.3794363 -0.5308613 -5.5376419
H -0.8994966 0.4505415 -5.5548641
H -1.0257682 -1.2450610 -4.9855352
H 0.5795984 -0.4265004 -4.9843231
C -6.2425165 -6.0843448 -7.6827100
H -5.2173986 -6.5040662 -7.7375256
H -6.9051864 -6.8297848 -7.1926596
H -6.5927727 -5.9462602 -8.7276677
C -8.9768548 -5.5325583 -10.8293029
H -9.5157799 -4.6442163 -11.2158910
H -9.6231803 -6.4207999 -10.9877879

H -8.8201463 -5.4100530 -9.7396006
C -7.1806565 -4.5282996 -15.3949276
H -8.1243844 -4.4445967 -15.9700104
H -6.5349982 -5.2828008 -15.8894571
H -7.4154298 -4.8633029 -14.3623159
C -3.7054180 -5.5789025 -12.7522683
H -2.6013678 -5.6260505 -12.8638400
H -4.0131112 -6.2237931 -11.9076289
H -4.2142399 -5.9120933 -13.6778704
C 0.2511409 -5.2775730 -10.5215939
H -0.5362802 -5.9308691 -10.0913294
H 1.0653625 -5.9263950 -10.9104338
H 0.6697385 -4.6536243 -9.7052078
C -0.6213015 2.5636740 -7.9500330
H -0.4222501 3.4320141 -7.2835451
H 0.0908650 1.7478794 -7.6989330
H -0.4183449 2.8877816 -8.9949533
C -8.0188567 -2.3968349 -9.0215425
H -8.8042594 -2.6137568 -9.7699344
H -7.9545165 -3.1968484 -8.2502525
H -8.2561273 -1.4363247 -8.5215126
C -5.2235851 -0.0481046 -7.0410421
H -6.0660047 -0.3030905 -6.3660801
H -4.7749566 0.9157799 -6.7270157
H -5.6021776 0.0461131 -8.0784873
C -0.3511613 -0.6222590 -10.9329889
H 0.0643745 -1.5081523 -11.4552234
H -0.2836374 0.2719998 -11.5850427
H 0.2248632 -0.4411646 -10.0032910
C -2.0514690 -4.4542460 -7.5704627
H -2.6373264 -4.6789121 -6.6572554
H -1.2586167 -5.2181059 -7.6945156
H -1.5772870 -3.4529701 -7.4768021
Zn -2.0727966 -0.2989280 -8.1446403
Zn -2.2230857 -3.2686377 -10.8080503
Zn -4.9132032 -3.1735807 -8.0241603
Zn -6.0951030 -4.0251239 -11.2114599
H -5.4754369 -3.1275777 -14.4065597

7H⁺ site of protonation : S₁₂

S -0.0363468 -1.1077521 -6.7645824
S -3.8460435 -1.7962564 -6.7832720
S -6.1067840 -4.7152055 -6.6151421
S -3.0447906 -4.9373761 -8.8736714
S -0.4001720 -4.8321994 -11.8981901
S -1.7711070 -1.5194482 -10.2335110
S -2.5929112 1.6648676 -7.7969565
S -6.1952197 -2.3517956 -9.8601804
S -6.8585994 -6.0656259 -10.4818482
S -7.8838065 -3.4437364 -13.2463305
S -4.0383843 -4.0713600 -12.4703168
C -0.7350672 -0.6965313 -5.1091536
H -1.2817399 0.2695561 -5.1424338
H -1.4514358 -1.4719101 -4.7654966
H 0.0870324 -0.6180844 -4.3644393
C -5.7720349 -6.4544614 -7.0793883
H -4.7187914 -6.5556278 -7.4075289
H -6.0229561 -7.1424400 -6.2482533
H -6.4128086 -6.6378846 -7.9707263
C -8.3907663 -6.5784829 -11.3666174

H	-8.6631846	-5.8010221	-12.1149525
H	-8.2391760	-7.5471278	-11.8916976
H	-9.2356389	-6.7060444	-10.6553145
C	-7.0307890	-4.0828199	-14.7478626
H	-7.5001464	-3.6420991	-15.6545094
H	-5.9539951	-3.8125295	-14.7448615
H	-7.1062324	-5.1887336	-14.8325625
C	-3.8301178	-5.8779673	-12.7917249
H	-2.7494896	-6.1181062	-12.7137772
H	-4.4240097	-6.4640947	-12.0613416
H	-4.1937161	-6.1043453	-13.8148843
C	0.3152938	-5.7582391	-10.4793904
H	-0.4551846	-6.3625939	-9.9560145
H	1.0981422	-6.4525112	-10.8547016
H	0.7904194	-5.0836885	-9.7359747
C	-0.9262315	2.4067226	-7.5288386
H	-0.9758362	3.1880273	-6.7383135
H	-0.1973125	1.6253222	-7.2204229
H	-0.5483719	2.8885237	-8.4573723
C	-7.8032875	-2.7606053	-9.0627199
H	-8.6078640	-2.2941775	-9.6657656
H	-7.9415537	-3.8625821	-9.0617988
H	-7.8441093	-2.3594744	-8.0306038
C	-5.1645151	-0.5104052	-6.7592220
H	-5.9193921	-0.7563878	-5.9845875
H	-4.6757443	0.4579689	-6.5255111
H	-5.6585411	-0.4426872	-7.7491835
C	0.0714088	-1.5477705	-10.3226845
H	0.3747502	-2.3019481	-11.0784632
H	0.4358880	-0.5413306	-10.6102825
H	0.5069367	-1.8173315	-9.3396289
C	-1.7866056	-4.5019144	-7.5967744
H	-2.2059452	-4.6669903	-6.5840568
H	-0.9071106	-5.1612471	-7.7303202
H	-1.4556330	-3.4452181	-7.6738612
Zn	-1.9888558	-0.5878996	-7.9663827
Zn	-2.2353736	-3.7818444	-10.8999568
Zn	-4.6454213	-3.2929596	-8.4027675
Zn	-6.3109743	-4.0682503	-11.6356085
H	-5.0607503	-4.5153628	-5.7627742

7H⁺ site of protonation : S_{b1}

S	0.2286797	-1.4806222	-7.4857900
S	-3.4071379	-2.4899290	-6.6964984
S	-6.2487926	-5.2230243	-6.8842805
S	-2.6040807	-5.5686123	-8.8286524
S	0.2319864	-4.5943920	-11.6568677
S	-2.5302049	-2.0441807	-10.3451037
S	-2.7468140	1.0880760	-8.2732404
S	-5.4544819	-3.7345149	-10.1238226
S	-6.7156636	-7.0294017	-12.2502491
S	-6.8922735	-3.3146312	-13.5014895
S	-3.2891142	-5.1218020	-12.6327841
C	0.0182984	-1.4777822	-5.6550827
H	-0.0546162	-0.4446561	-5.2511166
H	-0.8962617	-2.0299044	-5.3537370
H	0.8978163	-1.9665429	-5.1832482
C	-6.4284648	-6.7178081	-7.9529351
H	-5.6465378	-7.4718755	-7.7280516
H	-7.4195297	-7.1778095	-7.7553421

H	-6.3685321	-6.4887023	-9.0378632
C	-8.3712589	-6.4366545	-11.6882536
H	-8.5790799	-5.4166319	-12.0730915
H	-9.1605102	-7.1262929	-12.0573184
H	-8.4312568	-6.4079878	-10.5797104
C	-7.7942427	-4.3339426	-14.7480299
H	-8.8604592	-4.0243884	-14.8000820
H	-7.3526154	-4.2044815	-15.7598938
H	-7.7467495	-5.4114765	-14.4827669
C	-2.9852105	-6.9223756	-12.3839526
H	-1.8957824	-7.0639046	-12.2372984
H	-3.5336773	-7.2993568	-11.4997489
H	-3.3185079	-7.4816183	-13.2808501
C	1.3528479	-4.4896961	-10.1963267
H	1.3780070	-5.4420561	-9.6241728
H	2.3840939	-4.2898611	-10.5590418
H	1.0726994	-3.6734682	-9.4992519
C	-1.4382993	1.9054828	-7.2648783
H	-1.7362080	1.9982657	-6.1972692
H	-0.4927519	1.3229900	-7.3141328
H	-1.2477441	2.9306220	-7.6518625
C	-6.9448468	-2.7488352	-9.7347203
H	-7.5654684	-2.6799145	-10.6502579
H	-7.4561447	-3.3001167	-8.9203917
H	-6.6472770	-1.7451943	-9.3777456
C	-4.8220005	-1.3800575	-6.2871717
H	-4.9733076	-1.3632881	-5.1887840
H	-4.5699056	-0.3595620	-6.6492274
H	-5.7550883	-1.7358017	-6.7640704
C	-1.5653831	-1.0595150	-11.5582213
H	-0.5820219	-1.5463575	-11.7164023
H	-2.1107578	-1.0216472	-12.5213192
H	-1.4495671	-0.0368439	-11.1483802
C	-1.2437538	-5.2272899	-7.6291947
H	-1.5698214	-5.5320123	-6.6153615
H	-0.3592260	-5.8273769	-7.9186348
H	-0.9591615	-4.1541994	-7.6180236
Zn	-1.9742998	-1.1070175	-8.1583523
Zn	-1.8870466	-4.3194506	-10.8006408
Zn	-4.3579482	-4.3247394	-7.8187921
Zn	-5.6606597	-4.9882512	-12.4753926
H	-4.5478238	-2.7304210	-10.5167307

7H⁺ site of protonation : S_{b2}

S	-0.4276666	-2.6370075	-7.2926826
S	-4.3228860	-1.4127683	-7.0750383
S	-6.1769436	-4.7133890	-6.6361369
S	-3.5094613	-4.3380836	-9.4678968
S	-0.3704193	-3.8632523	-12.1745317
S	-1.9384754	-0.8106685	-10.2050102
S	-1.7000076	1.1182510	-6.7289655
S	-6.6807261	-2.6165596	-10.0730007
S	-5.2450181	-6.1990546	-11.7033330
S	-8.0885572	-4.0954491	-13.2365512
S	-4.0940319	-2.8655443	-12.8078032
C	0.2151322	-2.0432168	-5.6725009
H	0.1238222	-0.9373496	-5.6124358
H	-0.3468667	-2.4846725	-4.8211669
H	1.2840993	-2.3277981	-5.5618736
C	-6.6496192	-6.2005336	-7.6097156

H	-6.9086227	-7.0200571	-6.9057971
H	-7.5326013	-6.0165508	-8.2570053
H	-5.8221544	-6.5576178	-8.2568006
C	-6.7943647	-7.0807677	-11.2421739
H	-7.6581590	-6.5706343	-11.7187436
H	-6.7408883	-8.1321096	-11.5940858
H	-6.9455926	-7.0851449	-10.1457136
C	-7.6146116	-5.3119967	-14.5359476
H	-8.5252190	-5.8220970	-14.9192442
H	-7.1159812	-4.8163645	-15.3965014
H	-6.9196272	-6.0807307	-14.1370540
C	-3.5170903	-4.1191338	-14.0384399
H	-2.4221402	-4.2579739	-13.9351407
H	-4.0163210	-5.0918207	-13.8565384
H	-3.7660485	-3.7625679	-15.0581734
C	0.3056019	-4.7571136	-10.7112393
H	-0.3102626	-5.6446827	-10.4562102
H	1.3283995	-5.1129799	-10.9585137
H	0.3706448	-4.1072142	-9.8139433
C	-0.8397587	2.0712984	-8.0462262
H	-0.8507789	3.1527088	-7.7862059
H	0.2218051	1.7635202	-8.1627736
H	-1.3407153	1.9483394	-9.0291624
C	-8.3423149	-3.2434547	-9.5643561
H	-8.7241203	-3.9364465	-10.3396582
H	-8.2630382	-3.7544298	-8.5833132
H	-9.0405827	-2.3873724	-9.4703194
C	-5.1030060	0.0842219	-7.8130104
H	-6.0949041	0.2555007	-7.3474396
H	-4.4233723	0.9335293	-7.5927898
H	-5.2349900	-0.0253830	-8.9063911
C	-0.1030786	-0.6716192	-10.3889087
H	0.2257513	-1.3192760	-11.2274034
H	0.1601207	0.3869925	-10.5859395
H	0.3798290	-1.0188408	-9.4518940
C	-2.6989065	-5.3789218	-8.1945043
H	-3.4687848	-5.6523190	-7.4446584
H	-2.2474165	-6.2706706	-8.6686830
H	-1.9182440	-4.7455898	-7.7169969
Zn	-2.0154971	-0.9796662	-7.7497190
Zn	-2.2589927	-2.9014215	-11.2614839
Zn	-5.3590127	-3.2075477	-8.1794738
Zn	-6.1155815	-3.9604208	-12.0117030
H	-4.2998364	-5.3239086	-10.2543797

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C	-0.5210049	2.6010004	0.1966807
S	-0.0821500	0.9904123	-0.5867083
H	-0.0029635	3.4182492	-0.3469611
H	-0.2088448	2.6355282	1.2593354
C	-4.2526569	0.1555085	-0.8090813
S	-5.1902664	-0.7890800	0.4700266
H	-3.2182091	0.3942526	-0.4874952
H	-4.7863350	1.1089866	-0.9999587
C	-2.7620203	1.1840106	2.9167879
S	-1.1206460	0.4066972	3.2343549
H	-3.4340438	0.5218733	2.3335089
H	-2.6144173	2.1304274	2.3619018
C	1.2762424	0.8107170	6.3039309
S	2.7855059	0.0008171	5.6160555

H	0.5714939	0.0887596	6.7637160
H	0.7225836	1.3600408	5.5172339
C	2.8964797	0.2140262	1.7317029
S	1.8881942	-1.3271652	1.8646204
H	3.9455839	-0.0511178	1.4905448
H	2.8752897	0.7632652	2.6946685
C	-1.4536507	-2.3265859	-1.3388025
S	-1.3917407	-2.5317474	0.4906660
H	-0.5316288	-2.7582235	-1.7763274
H	-1.5028142	-1.2503337	-1.6002132
C	-5.7602084	-5.6437757	-0.5596998
N	-4.6870650	-6.3042956	0.0222148
C	-5.5556559	-4.3017376	-0.2908052
C	-3.8851423	-5.3696534	0.6112990
N	-4.3917352	-4.1570396	0.4339861
H	-4.5245437	-7.3119434	0.0162771
H	-6.1429867	-3.4101212	-0.5514969
H	-2.9564231	-5.5976227	1.1471557
C	-0.1091474	-4.1595876	3.6527975
S	0.0549665	-2.8984228	4.9825045
H	0.7340447	-4.8766573	3.7216600
H	-0.1184806	-3.7035566	2.6429178
C	5.2175312	-4.3412016	4.9961426
N	5.0865353	-4.4443911	3.6181665
C	4.2234279	-3.4652156	5.3943103
C	4.0455969	-3.6496641	3.2309004
N	3.5109521	-3.0528799	4.2888333
H	5.6715766	-5.0049010	2.9980125
H	3.9787366	-3.0764570	6.3897285
H	3.7058164	-3.4947879	2.1971040
C	-2.8528550	-2.3057654	7.4702703
S	-2.6502732	-0.6693665	6.6466017
H	-1.9087094	-2.8877681	7.4530933
H	-3.6425905	-2.9194874	6.9866857
C	-5.0548841	-1.9133830	4.1751466
S	-3.5432194	-2.7693072	3.5463549
H	-5.4069127	-1.1660553	3.4366177
H	-4.7825224	-1.3989757	5.1223461
Zn	-0.2926248	-0.4748409	1.1880389
Zn	-3.6249710	-2.2881577	1.2302010
Zn	1.9076714	-1.6016600	4.2530755
Zn	-1.8112368	-1.4099078	4.6296503
H	-4.1952610	-0.4016227	-1.7666703
H	-6.5495790	-6.1769781	-1.0982190
H	-2.3335779	-2.8610141	-1.7475692
H	2.4690551	0.8274839	0.9121922
H	-1.6127018	2.7945700	0.1466224
H	1.5972562	1.5333209	7.0825514
H	5.9916771	-4.8801900	5.5510339
H	-3.1453550	-2.1415755	8.5287786
H	-1.0619543	-4.7050488	3.8029675
H	-5.8540502	-2.6599996	4.3537069
H	-3.2317797	1.4055293	3.8948159

8H⁺ site of protonation : S₁₁

C	-0.1937287	2.8220142	0.7255601
S	-0.4781401	1.2401983	-0.1829002
H	0.8315993	3.1964978	0.5335253
H	-0.3144786	2.6939691	1.8194528
C	-4.0016010	0.4873389	-0.6602248

S	-4.8400304	-0.4183467	0.6970093
H	-2.9910899	0.7903064	-0.2868634
H	-4.5982210	1.3813033	-0.9194388
C	-2.6585796	1.2022838	3.2058385
S	-1.0395241	0.4142308	3.5638947
H	-3.3781402	0.4692275	2.7914829
H	-2.5172496	2.0243999	2.4782758
C	1.3415561	0.6388763	6.5703978
S	2.8439016	0.0104774	5.7052494
H	0.7660037	-0.1674461	7.0673283
H	0.6624795	1.1657816	5.8717450
C	3.0001913	0.2751564	1.8843376
S	1.9553400	-1.2470286	1.9451262
H	4.0621405	-0.0228426	1.7857885
H	2.8786057	0.8573996	2.8196097
C	-1.1904778	-2.0752853	-1.2516746
S	-1.2221070	-2.4030105	0.5589055
H	-0.1429110	-2.2035489	-1.5847286
H	-1.5003341	-1.0385234	-1.4839372
C	-5.6899134	-5.4474467	-0.6511692
N	-5.6599703	-5.8218557	0.6808098
C	-5.0084651	-4.2463427	-0.7092766
C	-4.9843999	-4.8724683	1.3814321
N	-4.5800533	-3.9029182	0.5598102
H	-6.0704646	-6.6693845	1.0771939
H	-4.7988915	-3.6217731	-1.5840973
H	-4.7843902	-4.8880535	2.4627983
C	-0.0595701	-4.1337649	3.7041298
S	0.1693144	-2.9273593	5.0737404
H	0.7873653	-4.8478582	3.7132075
H	-0.1030695	-3.6413577	2.7129391
C	5.4305255	-4.1745431	5.0373843
N	5.2532559	-4.3750135	3.6768437
C	4.4161166	-3.3161133	5.4187113
C	4.1670687	-3.6531411	3.2784070
N	3.6443476	-3.0080518	4.3166541
H	5.8413938	-4.9500329	3.0720716
H	4.1961686	-2.8670247	6.3944617
H	3.7964044	-3.5895912	2.2474986
C	-2.8589770	-2.5922682	7.5996583
S	-2.7699850	-0.9080024	6.8511505
H	-1.8580092	-3.0643810	7.6551330
H	-3.5315465	-3.2655002	7.0283835
C	-5.0146580	-1.8291149	4.2205578
S	-3.5017725	-2.7071822	3.6327379
H	-5.2902564	-0.9910388	3.5517333
H	-4.7557300	-1.4213542	5.2246827
Zn	-0.1891353	-0.3320621	1.4753742
Zn	-3.3688565	-2.3666382	1.3536507
Zn	2.0323785	-1.6139958	4.3435775
Zn	-1.6810434	-1.4382140	4.9184662
H	-3.8718790	-0.1638671	-1.5425654
H	-6.1774369	-6.0518727	-1.4219444
H	-1.8269699	-2.8049278	-1.7890308
H	2.7051428	0.8739510	1.0011207
H	-0.9135614	3.5871506	0.3712683
H	1.6732070	1.3563265	7.3478232
H	6.2465512	-4.6422203	5.5963724
H	-3.2601623	-2.4954297	8.6288321
H	-1.0000060	-4.6944341	3.8710644

H	-5.8622108	-2.5380552	4.2933373
H	-3.0748069	1.6100673	4.1467813
H	-5.7926414	-1.0697803	-0.0326117

8H⁺ site of protonation : S₁₂

C	-0.3461552	2.6931514	0.2739502
S	-0.0438275	1.0248562	-0.4507205
H	0.1076230	3.4495761	-0.3975278
H	0.1154437	2.8014737	1.2752235
C	-4.0874358	0.3463553	-0.6349767
S	-4.9543361	-0.4287457	0.8009557
H	-3.0180184	0.5547194	-0.4239388
H	-4.5961355	1.3049731	-0.8598656
C	-2.5401707	1.4560646	3.0771361
S	-0.9633378	0.5709623	3.4446587
H	-3.2174781	0.8539129	2.4360257
H	-2.2860488	2.3996774	2.5593505
C	1.4036268	0.6071788	6.5610922
S	2.9249265	-0.0568468	5.7729243
H	0.9006112	-0.1673958	7.1863331
H	0.6834950	0.9959722	5.8128951
C	3.0330448	0.2982844	1.8212684
S	2.0184127	-1.2382085	1.9622435
H	4.0943442	0.0247520	1.6637144
H	2.9481278	0.9003415	2.7468098
C	-1.1463523	-2.4165204	-0.9877553
S	-1.2667422	-2.4740591	0.8510446
H	-0.1264121	-2.7327033	-1.2791638
H	-1.3200994	-1.3849579	-1.3524531
C	-5.9164688	-5.1615897	-0.5750289
N	-4.8271960	-5.9299428	-0.1947343
C	-5.6342718	-3.8795441	-0.1415792
C	-3.9359361	-5.1193512	0.4422819
N	-4.4046082	-3.8758635	0.4864662
H	-4.7075547	-6.9296676	-0.3658500
H	-6.2042782	-2.9450174	-0.2307483
H	-2.9727778	-5.4524469	0.8461481
C	-0.0021385	-4.2553222	3.9534651
S	0.1492414	-2.7915760	5.0614738
H	0.8727502	-4.9117263	4.1232751
H	-0.0450437	-3.9537196	2.8884075
C	5.3521758	-4.3685197	5.0290584
N	5.2191815	-4.4650516	3.6525328
C	4.3534089	-3.5033988	5.4355463
C	4.1746971	-3.6790498	3.2679189
N	3.6341797	-3.0906850	4.3316383
H	5.8116518	-5.0145137	3.0282943
H	4.1159532	-3.1202411	6.4344673
H	3.8425912	-3.5260188	2.2326461
C	-2.4157332	-2.3071878	7.6177214
S	-2.3723093	-0.6746309	6.7812021
H	-1.5597582	-2.9229205	7.2798146
H	-3.3595676	-2.7885303	7.3004939
C	-4.9634854	-1.5194819	4.2594347
S	-3.5694465	-2.6145295	3.7422556
H	-5.0267857	-0.6286906	3.6040428
H	-4.8357079	-1.2036537	5.3129806
Zn	-0.1509995	-0.3645753	1.3592600
Zn	-3.5456859	-2.1364362	1.3479227
Zn	2.1226819	-1.6031086	4.3051914

Zn	-1.6530439	-1.4282231	4.4004405
H	-4.1510176	-0.2946647	-1.5369252
H	-6.7725087	-5.5853156	-1.1084631
H	-1.8851158	-3.1092720	-1.4348248
H	2.6569402	0.8650958	0.9458489
H	-1.4301274	2.9137448	0.3532718
H	1.6917755	1.4391502	7.2349944
H	6.1308527	-4.9032996	5.5811022
H	-2.4158861	-2.1746537	8.7154744
H	-0.9256142	-4.8073663	4.2141727
H	-5.9031179	-2.0980959	4.1719295
H	-3.0464430	1.6990804	4.0312635
H	-1.0878094	-0.3319218	7.1048114

8H⁺ site of protonation : S_{b1}

C	-0.7233091	2.5800084	-0.0728464
S	0.0061857	0.9239251	-0.4231247
H	-0.5416906	3.2236690	-0.9568627
H	-0.2498700	3.0615421	0.8054470
C	-3.8801981	0.1172558	-0.7741387
S	-4.6662961	-0.2504892	0.8570852
H	-2.7938828	0.3210101	-0.6759955
H	-4.3727777	1.0168334	-1.1941101
C	-2.4314540	1.8233982	3.2085076
S	-0.9545043	0.7804382	3.5920930
H	-3.1355387	1.2917904	2.5344948
H	-2.0844198	2.7570824	2.7281759
C	1.3892264	0.7824537	6.7977983
S	2.6303503	-0.5592824	6.5322997
H	0.3546132	0.3867873	6.8387199
H	1.4512693	1.5594888	6.0131882
C	2.7661506	1.1021234	2.0816380
S	2.1765462	-0.6414363	2.1856280
H	3.8651548	1.1450522	2.2046254
H	2.2753483	1.7291413	2.8495456
C	-0.8157690	-2.6586202	-0.5158869
S	-1.0703600	-2.4388503	1.2966630
H	0.2074456	-3.0447209	-0.6877573
H	-0.9250660	-1.6849288	-1.0334931
C	-5.8340850	-4.8542066	-0.4804874
N	-4.8211383	-5.7072154	-0.0715431
C	-5.4722871	-3.6022716	-0.0193328
C	-3.8958832	-4.9726862	0.6089431
N	-4.2691250	-3.6974002	0.6519223
H	-4.7740762	-6.7121568	-0.2476499
H	-5.9684817	-2.6249856	-0.1033255
H	-2.9829252	-5.3879236	1.0505116
C	-0.4313808	-4.2459180	4.5301292
S	0.1220465	-2.5299345	4.8682658
H	0.3507869	-4.9679389	4.8283481
H	-0.5868468	-4.2731381	3.4336787
C	5.2415456	-4.4888155	4.7162880
N	5.2510700	-4.2243860	3.3560498
C	4.3303411	-3.6020096	5.2578213
C	4.3737041	-3.2143189	3.1082462
N	3.8025610	-2.8228246	4.2458335
H	5.8242850	-4.6977062	2.6556813
H	4.0267051	-3.4597730	6.3012048
H	4.1646669	-2.7771780	2.1226584
C	-2.8196005	-2.0822792	7.7089310

S	-2.4597088	-0.3991059	7.0485832
H	-1.8918723	-2.6714942	7.8655364
H	-3.4920725	-2.6570906	7.0402627
C	-5.0830314	-1.4861705	4.4398743
S	-3.5595079	-2.4106980	3.9464208
H	-5.2815856	-0.6606542	3.7297428
H	-4.9272845	-1.0691096	5.4548178
Zn	-0.1961599	-0.1961741	1.5609881
Zn	-3.3958654	-1.9948802	1.5979149
Zn	2.4765364	-1.2024524	4.3980980
Zn	-1.9859252	-0.8953805	4.8885366
H	-4.0225632	-0.7163535	-1.4920008
H	-6.7001745	-5.2059617	-1.0489108
H	-1.5514783	-3.3845659	-0.9127444
H	2.4727782	1.4616483	1.0747721
H	-1.8173601	2.5238382	0.0926873
H	1.6268073	1.2458983	7.7752914
H	5.8723566	-5.2598747	5.1684281
H	-3.3166114	-1.9713078	8.6935732
H	-1.3902297	-4.4426456	5.0440985
H	-5.9419089	-2.1842756	4.4403406
H	-2.9339225	2.0738775	4.1624153
H	0.3842991	-2.6041039	6.2052424

8H⁺ site of protonation : S_{b2}

C	0.1003112	2.2396851	-0.2347605
S	0.0431367	0.6145105	-1.1028064
H	0.2631577	3.0220603	-1.0024780
H	0.9326658	2.3005153	0.4948276
C	-4.0513405	0.2972427	-0.7438308
S	-4.8444711	-0.3593468	0.7884808
H	-2.9512156	0.4000243	-0.6471273
H	-4.4793933	1.2992579	-0.9461814
C	-2.5190771	1.4478870	3.0069976
S	-1.2657118	0.1214772	2.8269582
H	-3.4093808	1.0660170	2.4577607
H	-2.1518747	2.3781311	2.5369846
C	3.9124706	-2.8910508	6.5060992
S	4.0143767	-2.5702537	4.6923258
H	3.7015607	-1.9699290	7.0906293
H	4.8894144	-3.2915864	6.8441334
C	2.9008671	-0.0605866	1.6260816
S	1.7259499	-1.4452678	1.9234528
H	3.9187382	-0.3994745	1.8972647
H	2.6461610	0.8348964	2.2270794
C	-1.7225689	-2.7443706	-1.4574160
S	-1.4734623	-2.7840976	0.3715100
H	-0.8473056	-3.2175391	-1.9419706
H	-1.8205965	-1.7029303	-1.8193598
C	-6.4811341	-4.9496841	-0.5098602
N	-5.4992042	-5.8531705	-0.1357070
C	-5.9911006	-3.7054981	-0.1595591
C	-4.4664408	-5.1574954	0.4162239
N	-4.7423710	-3.8559880	0.4107663
H	-5.5391057	-6.8672108	-0.2518350
H	-6.4301094	-2.7044698	-0.2617196
H	-3.5493732	-5.6156590	0.8038277
C	-0.1257593	-4.3061481	3.8578143
S	-0.0168465	-2.9448391	5.0967594
H	0.8005044	-4.9068933	3.9297702

H	-0.2297262	-3.9216014	2.8249187
C	1.5750866	1.9414707	6.5417276
N	2.9272219	1.7321770	6.3240810
C	0.9286427	0.8884368	5.9201246
C	3.0741179	0.5911069	5.5979892
N	1.8774575	0.0630146	5.3369760
H	3.6905777	2.3203189	6.6619170
H	-0.1525447	0.6616366	5.8934898
H	4.0234156	0.1190764	5.2961171
C	-1.8843437	-0.9240089	7.8523705
S	-2.5990427	-0.1637508	6.3296667
H	-0.7770956	-0.9650239	7.8185810
H	-2.2709178	-1.9485515	8.0155982
C	-5.1156374	-1.9663006	4.1450456
S	-3.6003359	-2.8438076	3.5532029
H	-5.2917110	-1.0472693	3.5528890
H	-4.9765548	-1.6905271	5.2081962
Zn	-0.1369700	-0.8427102	0.6154915
Zn	-3.6322081	-2.2469240	1.2315085
Zn	1.9003949	-1.7891509	4.2974872
Zn	-1.9418491	-1.6547046	4.7309227
H	-4.2686350	-0.3485215	-1.6178853
H	-7.4172021	-5.2649525	-0.9801339
H	-2.6333661	-3.3184245	-1.7132383
H	2.8640179	0.2003062	0.5507676
H	-0.8526245	2.4667831	0.2843573
H	3.1303380	-3.6383742	6.7459312
H	1.1960816	2.7920196	7.1164586
H	-2.1857286	-0.2975848	8.7153122
H	-1.0002254	-4.9373614	4.1039728
H	-5.9824921	-2.6457338	4.0366666
H	-2.7377807	1.5920346	4.0826525
H	-0.1948191	0.7367468	3.4026538

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Zn	-0.0002469	0.0004103	0.2194423
S	-1.1677879	1.9681952	0.1232594
S	2.2887880	0.0234782	0.1322975
S	-1.1215043	-1.9952757	0.1288167
C	0.1464636	3.0730192	-0.5560738
H	-0.2654950	3.6937206	-1.3814686
H	0.5342660	3.7625571	0.2250282
H	1.0025640	2.4842819	-0.9458882
C	-2.7324444	-1.4108887	-0.5580460
H	-2.6473269	-0.3782008	-0.9553631
H	-3.0627754	-2.0835643	-1.3792298
H	-3.5252774	-1.4120901	0.2212616
C	2.5851470	-1.6581849	-0.5707521
H	1.6440140	-2.1026609	-0.9556490
H	3.3186983	-1.5995779	-1.4040867
H	2.9990693	-2.3469558	0.1973319

9H⁺

Zn	-0.3728608	-0.0171907	-0.0466210
S	-1.3691586	1.8991355	0.4627914
S	2.1911381	0.6064233	-0.0871245
S	-0.3106851	-2.2156628	-0.3045428
C	-0.5149110	3.0748051	-0.6755628
H	-0.8076693	2.9155028	-1.7321097
H	-0.8264617	4.0966645	-0.3823140

H	0.5909409	3.0230637	-0.6013075
C	-2.0242381	-2.6852633	0.2015005
H	-2.7904369	-2.1418938	-0.3843361
H	-2.1372177	-3.7690073	0.0027212
H	-2.1980581	-2.5090160	1.2808740
C	2.9440840	-0.9769409	0.4600360
H	3.2426112	-1.5018151	-0.4663384
H	3.8425211	-0.7787834	1.0728141
H	2.1993264	-1.5966780	0.9949635
H	1.9758337	1.1546556	1.1431925

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Zn	-0.1375353	1.0234422	-0.2995034
N	-2.2076309	0.8851536	-0.4687861
C	-3.1171434	1.3250458	0.4010989
C	-2.8975920	0.3762509	-1.5569020
H	-2.9092757	1.7905109	1.3707384
C	-4.2533244	0.5154196	-1.3320334
H	-2.3573992	-0.0704432	-2.4065312
H	-5.1241397	0.2422763	-1.9349612
N	0.0548580	2.2207425	1.4438037
C	0.6552729	1.7577595	2.5400454
C	-0.1638788	3.5720985	1.6429817
H	0.9873004	0.7185035	2.6731738
C	0.3094594	3.9302008	2.8916341
H	-0.6271393	4.1972679	0.8715979
H	0.3339611	4.8878228	3.4204172
N	0.8218931	2.7656275	3.4385831
N	-4.3685003	1.1172853	-0.0902141
H	-5.2408654	1.3624789	0.3806354
H	1.2703367	2.6768780	4.3523743
S	0.5908155	2.3704857	-2.0478576
S	0.8711749	-0.9567275	0.4019359
Zn	1.7406301	-1.7727874	-1.7608803
Zn	1.4282465	0.6424828	-3.6039297
S	1.7854389	1.0832834	-5.8022026
S	2.2097571	-3.9924102	-1.7037221
S	-0.1494409	-1.1468531	-3.1725962
S	3.4066051	-0.1846311	-2.4201672
C	-0.4971717	-2.1903266	0.4887673
H	-1.0840401	-2.0554837	1.4177727
H	-1.1534685	-2.1056966	-0.3983592
H	-0.0219265	-3.1904687	0.4711892
C	2.1772569	3.0724659	-1.4192708
H	2.0151040	3.5912940	-0.4543012
H	2.9475348	2.2849211	-1.3070331
H	2.5335781	3.8102598	-2.1635050
C	4.1637594	-1.1534568	-3.8064968
H	3.7288670	-0.8165744	-4.7700113
H	5.2572449	-0.9805297	-3.8044532
H	3.9560375	-2.2318850	-3.6582624
C	0.0584816	-2.2156338	-4.6673803
H	-0.9363028	-2.3975173	-5.1171189
H	0.7077731	-1.7056333	-5.4048897
H	0.5145588	-3.1800871	-4.3738656
C	3.7748020	-3.9530495	-0.7268886
H	3.6010372	-3.6104136	0.3132751
H	4.1844058	-4.9827219	-0.6878806
H	4.5375454	-3.2943817	-1.1892762
C	3.2598851	2.1848073	-5.6804204

H	3.7282708	2.2545973	-6.6830793
H	2.9775639	3.2094648	-5.3622294
H	4.0161495	1.7922297	-4.9700253

10H⁺ site of protonation : S_t

Zn	-0.0256530	1.3011320	0.0209699
N	-2.0417843	1.1857183	-0.3896730
C	-3.0487453	1.5432961	0.4126287
C	-2.6082941	0.7054777	-1.5603048
H	-2.9551994	1.9616478	1.4207967
C	-3.9833855	0.7797144	-1.4564330
H	-1.9877753	0.3261345	-2.3840339
H	-4.7833257	0.5011077	-2.1488267
N	0.0880197	2.3415665	1.8167925
C	0.6162376	1.8026251	2.9195282
C	-0.2184466	3.6589579	2.1187111
H	0.9780733	0.7695025	3.0036277
C	0.1286902	3.9143509	3.4315951
H	-0.6562756	4.3373225	1.3783593
H	0.0532466	4.8163432	4.0464685
N	0.6522208	2.7278644	3.9123925
N	-4.2357123	1.3115650	-0.2050292
H	-5.1590817	1.4963992	0.1935855
H	1.0160286	2.5705157	4.8553999
S	0.9441501	2.7014015	-1.6277011
S	0.9035453	-0.7846285	0.5426888
Zn	2.0256595	-1.4924584	-1.4662176
Zn	1.9922513	0.9972216	-2.9132883
S	2.4286431	2.1513140	-5.0842094
S	2.4796662	-3.6361150	-1.9578725
S	0.3691894	-0.6710338	-3.2120742
S	3.8332591	0.1606792	-1.7498629
C	-0.5131312	-1.9644670	0.4498371
H	-1.1906780	-1.8059296	1.3094564
H	-1.0656047	-1.8472936	-0.5009790
H	-0.0901229	-2.9856990	0.4894615
C	2.4026420	3.4486872	-0.7725980
H	2.0504570	4.0738910	0.0691579
H	3.1015733	2.6732335	-0.4071062
H	2.9315206	4.0939347	-1.4987651
C	4.8644051	-0.7425348	-2.9925526
H	5.0634295	-0.1071965	-3.8758035
H	5.8296936	-0.9793376	-2.5068606
H	4.3648408	-1.6871238	-3.2877496
C	0.8584636	-1.7239722	-4.6496188
H	1.7250344	-2.3587802	-4.3794481
H	-0.0002212	-2.3781753	-4.8904782
H	1.0909829	-1.1031148	-5.5361269
C	3.9654817	-3.9765560	-0.9178063
H	3.7281242	-3.9267134	0.1626623
H	4.3010494	-5.0058502	-1.1516321
H	4.8010552	-3.2823255	-1.1348511
C	0.6796784	2.4841623	-5.5386287
H	0.6204364	2.7671531	-6.6053165
H	0.0449111	1.6082026	-5.3084544
H	0.3697709	3.3376885	-4.9075510
H	2.6270411	1.0573506	-5.8761807

10H⁺ site of protonation : S_{b1}

Zn	-0.5513718	1.6314245	0.1493333
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N	-2.0069091	0.2520091	0.4979704
C	-2.8660586	0.2320854	1.5238083
C	-2.2581253	-0.8778109	-0.2694394
H	-2.9344608	0.9745006	2.3263954
C	-3.2935036	-1.5836183	0.3102496
H	-1.6632663	-1.0995077	-1.1717576
H	-3.7875032	-2.5168644	0.0240093
N	-0.6009294	2.9839414	1.7223321
C	0.4629635	3.1694783	2.5107351
C	-1.5552871	3.9114780	2.1100238
H	1.4043928	2.6093844	2.4416459
C	-1.0560084	4.6639227	3.1550713
H	-2.5240152	3.9979765	1.6065078
H	-1.4845875	5.4894150	3.7313091
N	0.2165916	4.1753744	3.3870381
N	-3.6576921	-0.8657824	1.4354535
H	-4.3972659	-1.1185343	2.0951732
H	0.8734019	4.5214817	4.0907722
S	-1.2190282	3.1238943	-1.6579296
S	1.6499846	0.9162630	0.0638092
Zn	1.9184368	0.4907385	-2.3357742
Zn	4.2212202	1.9875761	-3.6444742
S	5.3005917	2.9792138	-5.2826570
S	0.1191576	-0.7441724	-2.9921573
S	1.9583215	2.7698882	-3.2324189
S	4.2743920	0.0170415	-2.3740442
C	1.5713218	-0.8522250	0.5883595
H	2.6068253	-1.2417377	0.5792279
H	1.1642990	-0.9318936	1.6137657
H	0.9549985	-1.4334365	-0.1247230
C	-2.1515914	2.1294004	-2.8933497
H	-1.5950374	1.2100074	-3.1708817
H	-3.1217187	1.8684644	-2.4319816
H	-2.3306999	2.7651386	-3.7797670
C	4.6332136	-1.2387143	-3.6832123
H	5.7167227	-1.2143199	-3.9031592
H	4.3706602	-2.2366653	-3.2857261
H	4.0645779	-1.0529599	-4.6124022
C	1.3308940	2.5483759	-4.9629791
H	0.7238471	3.4337377	-5.2297949
H	2.1904274	2.4831983	-5.6578824
H	0.7163796	1.6294965	-5.0210678
C	0.7027457	-2.1324463	-4.0526368
H	1.4040918	-2.7921121	-3.5070937
H	-0.1828722	-2.7286420	-4.3451741
H	1.1883319	-1.7591658	-4.9742784
C	6.7178940	1.8412974	-5.6127088
H	7.3658531	2.3513430	-6.3517063
H	7.3186435	1.6480605	-4.7035492
H	6.3845890	0.8809217	-6.0509839
H	0.0529462	3.0887521	-2.2799467

10H⁺ site of protonation : S_{b2}

Zn	-1.6663560	1.3721923	-0.2379202
N	-3.5996476	1.7425127	0.3936652
C	-4.1012509	1.7864579	1.6310969
C	-4.6515302	1.9736955	-0.4781007
H	-3.5414989	1.6452912	2.5622766
C	-5.8083439	2.1610333	0.2524220
H	-4.4931275	1.9906784	-1.5629645

H	-6.8392420	2.3654669	-0.0515445
N	-0.4877104	2.6442449	0.8804379
C	0.5383557	2.2427127	1.6369681
C	-0.5218098	4.0280134	0.9510087
H	0.8395421	1.2014636	1.8033653
C	0.5037310	4.4647083	1.7662619
H	-1.2723827	4.6199319	0.4174522
H	0.8166206	5.4670344	2.0736977
N	1.1560336	3.3196470	2.1850343
N	-5.4347109	2.0386673	1.5785436
H	-6.0560629	2.1230537	2.3865879
H	1.9717014	3.2848276	2.8011417
S	-1.6967238	1.7644825	-2.5256872
S	-0.9732224	-0.7598217	0.5383481
Zn	0.0580555	-1.7699155	-1.3078744
Zn	-0.0457058	0.5310983	-3.8078001
S	0.5932036	1.6976020	-5.6304763
S	-0.7613652	-3.7405106	-2.0133370
S	-1.4911977	-1.3153902	-4.6952132
S	1.5726854	-0.2709825	-2.1878454
C	-2.4925766	-1.7866719	0.7529383
H	-2.9361091	-1.5679297	1.7421846
H	-3.2331961	-1.5871723	-0.0428467
H	-2.1919915	-2.8504769	0.7105551
C	-0.9942998	3.4581166	-2.7476598
H	-1.7834965	4.2105430	-2.5605172
H	-0.1331999	3.6332714	-2.0756430
H	-0.6467983	3.5190944	-3.7992671
C	2.7145331	-1.2909581	-3.2196513
H	3.3464477	-0.6011453	-3.8087049
H	3.3607929	-1.8973082	-2.5583825
H	2.1573958	-1.9519006	-3.9078541
C	-0.4945745	-1.8564551	-6.1423651
H	-1.1339994	-2.4454269	-6.8250482
H	-0.1358257	-0.9297440	-6.6327575
H	0.3734245	-2.4593470	-5.8197504
C	0.7159168	-4.7180459	-2.5349784
H	1.3341851	-4.9950715	-1.6603371
H	0.3350943	-5.6472543	-3.0002036
H	1.3421898	-4.1844141	-3.2737391
C	2.4085598	1.9257852	-5.3994446
H	2.7337104	2.7256838	-6.0932092
H	2.6671249	2.2371571	-4.3686102
H	2.9728741	1.0066420	-5.6551110
H	-1.2408992	-2.3853461	-3.8189107

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Zn	-0.5429024	0.1177690	0.0869161
S	0.1419994	1.2740120	-1.9342498
S	0.4721586	-2.0428012	-0.1770574
S	0.1031259	0.9452635	2.2606212
S	-2.8759307	0.2427486	0.1274695
Zn	2.5034463	1.7365447	-1.8192742
Zn	2.4370401	1.4829180	2.1831494
Zn	2.8592518	-1.7926233	-0.0243836
S	4.1934505	-3.6940696	-0.1631808
S	3.6642078	3.0974713	-3.3158305
S	3.5371901	2.5050257	3.9623505
S	2.5816864	2.9375779	0.2896254
S	3.2646127	-0.7793020	2.1091901

S	3.3484813	-0.4902610	-1.9981825
C	-3.2500165	-0.2609237	-1.6052266
H	-3.1660138	-1.3609545	-1.7367711
H	-4.2885459	0.0383104	-1.8672977
H	-2.5517007	0.2177391	-2.3234858
C	0.1024680	-2.8059318	1.4582815
H	-0.9960686	-2.8968759	1.5720262
H	0.5714378	-3.8091887	1.4989013
H	0.4999765	-2.1916286	2.2895213
C	3.7247972	-4.2571404	-1.8548209
H	3.7065915	-3.4077616	-2.5696191
H	4.4623077	-5.0069591	-2.2167599
H	2.7197246	-4.7308261	-1.8681936
C	5.1724924	-0.3174878	-1.8235510
H	5.4340576	0.4837185	-1.1056127
H	5.5667075	-1.2882260	-1.4575740
H	5.6187237	-0.0656929	-2.8064033
C	5.0834567	-0.5045918	2.1776455
H	5.4897093	-0.2344353	1.1845528
H	5.2684415	0.3299262	2.8856162
H	5.5875752	-1.4285827	2.5245188
C	2.7940318	4.7014533	-3.0680703
H	1.8277415	4.7381899	-3.6163507
H	2.5822922	4.8869659	-1.9937961
H	3.4289431	5.5327346	-3.4456853
C	4.2848818	3.6389728	0.3409196
H	4.6820954	3.6398968	-0.6964671
H	4.2515226	4.6749296	0.7348035
H	4.9323527	3.0345964	1.0051333
C	-0.6697968	2.8984574	-1.6274615
H	-0.7966035	3.4390288	-2.5873538
H	-1.6613089	2.6999908	-1.1702755
H	-0.0590174	3.5190547	-0.9425701
C	-0.7095608	2.5981321	2.2830667
H	-1.7262133	2.5034738	1.8520016
H	-0.7768396	2.9565608	3.3300534
H	-0.1215628	3.3295621	1.6943383
C	3.1802030	1.2553615	5.2695912
H	3.8700148	1.4051975	6.1290186
H	2.1384472	1.3405974	5.6468818
H	3.3141900	0.2225358	4.8852819

11H⁺ site of protonation : S_t

Zn	-0.1011476	0.2067524	0.1170612
S	0.2867810	1.3820168	-1.8673399
S	0.4970094	-2.0437350	-0.0787720
S	-0.0812050	0.9467601	2.3163578
S	-2.7328697	-0.2707343	-0.3260184
Zn	2.7551568	1.7215918	-1.6222140
Zn	2.3505645	1.3549059	2.4160579
Zn	2.9485384	-1.8617889	0.1015787
S	4.1229765	-3.8217720	-0.0420869
S	3.9734044	3.0934248	-2.9964162
S	3.1393127	2.3772964	4.3087843
S	2.5878014	2.8078031	0.5294979
S	3.2212490	-0.8613602	2.2536219
S	3.3773691	-0.5492216	-1.8603147
C	-2.4914878	-0.9909978	-1.9954404
H	-1.9549511	-1.9433103	-1.8205031
H	-3.4638833	-1.1769229	-2.4891757

H	-1.8381843	-0.3275264	-2.5951357
C	0.1344398	-2.7293481	1.5949939
H	-0.9588551	-2.8396586	1.7314797
H	0.6211764	-3.7216469	1.6586374
H	0.5419689	-2.0833095	2.3956032
C	3.6064448	-4.3565328	-1.7304557
H	3.6625739	-3.5211293	-2.4583307
H	4.2817197	-5.1680060	-2.0738609
H	2.5674293	-4.7470957	-1.7362715
C	5.2217067	-0.5226285	-1.8542935
H	5.6114458	0.3172519	-1.2484989
H	5.5678434	-1.4878568	-1.4318924
H	5.5868127	-0.4063794	-2.8930919
C	5.0161416	-0.4503487	2.2949132
H	5.3327708	0.0493273	1.3594675
H	5.1879868	0.2378366	3.1460562
H	5.6018354	-1.3811573	2.4220571
C	3.1479610	4.7208098	-2.7417180
H	2.2163977	4.8082734	-3.3398999
H	2.8929206	4.8929314	-1.6755815
H	3.8366633	5.5279573	-3.0679050
C	4.2356478	3.6067590	0.7450537
H	4.7482511	3.5987089	-0.2392837
H	4.0975599	4.6494761	1.0917811
H	4.8307772	3.0596288	1.5000920
C	-0.3839521	3.0661015	-1.5364302
H	-0.3818702	3.6312080	-2.4886062
H	-1.4245103	3.0029399	-1.1607908
H	0.2512562	3.5948381	-0.7990509
C	-0.6089945	2.7120581	2.3463666
H	-1.6885870	2.7975321	2.1131410
H	-0.4208792	3.0891029	3.3701855
H	-0.0084089	3.3160283	1.6399964
C	2.8347541	1.0285098	5.5301889
H	3.4436183	1.2202857	6.4382955
H	1.7679521	0.9852852	5.8339721
H	3.1154189	0.0363405	5.1212572
H	-3.1466401	0.9664677	-0.7249185

11H⁺ site of protonation : S_b

Zn	-0.8022895	0.4501107	0.3825157
S	0.0583630	0.9443831	-1.7839707
S	0.6136574	-1.8192639	0.1993636
S	0.2234903	0.9606283	2.4331208
S	-3.0657787	0.3516441	0.4006530
Zn	2.4179358	1.4783953	-1.8372841
Zn	2.5935944	1.3471766	2.1398822
Zn	3.2880206	-1.9527651	-0.0594391
S	3.5756917	-4.2069907	-0.1748798
S	3.3649915	2.6909913	-3.5478266
S	3.6539965	2.3410447	3.9191367
S	2.6055795	2.7242539	0.2039870
S	3.4697407	-0.9245474	2.0425926
S	3.5384802	-0.6648978	-2.0137862
C	-3.4505162	-0.2298450	-1.3089295
H	-3.6302484	-1.3253757	-1.3244187
H	-4.3724974	0.2721238	-1.6677147
H	-2.6253121	-0.0008338	-2.0134904
C	0.3855713	-3.1791623	1.4003949
H	-0.6741025	-3.4902789	1.4378341

H	1.0806940	-3.9971627	1.1170590
H	0.6917166	-2.7552415	2.3750332
C	3.2781278	-4.4975500	-1.9733356
H	3.6035662	-3.6314073	-2.5836671
H	3.8503744	-5.3923474	-2.2935033
H	2.2048523	-4.6881216	-2.1838421
C	5.2571912	-0.0393516	-1.7694949
H	5.3797698	0.3958949	-0.7592270
H	5.9786484	-0.8681083	-1.9070779
H	5.4387591	0.7535265	-2.5209370
C	5.2608131	-0.6341024	2.3676221
H	5.8186546	-0.4201640	1.4363008
H	5.3224034	0.2498808	3.0372519
H	5.6980642	-1.5275795	2.8536455
C	2.7548372	4.4005739	-3.2269637
H	1.7505638	4.5635003	-3.6710006
H	2.6912125	4.6228994	-2.1423153
H	3.4544944	5.1260356	-3.6917965
C	4.2975771	3.4553057	0.1309279
H	4.6433888	3.4208869	-0.9222021
H	4.2591512	4.5047838	0.4821770
H	4.9940527	2.8916932	0.7803039
C	-0.6848285	2.6284807	-1.9291393
H	-0.7040129	2.9201295	-2.9967280
H	-1.7162877	2.5958825	-1.5247307
H	-0.0856340	3.3636333	-1.3581570
C	-0.3022593	2.7159162	2.6521861
H	-1.4067826	2.7766431	2.6124139
H	0.0635994	3.0616597	3.6376425
H	0.1431233	3.3566843	1.8669282
C	3.1976387	1.1325805	5.2365360
H	3.6910121	1.4355333	6.1834743
H	2.1022458	1.1070998	5.4093716
H	3.5267014	0.1031255	4.9852765
H	0.1852275	-2.4558235	-0.9271427

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C	0.3006998	1.7243503	-1.6131737
S	-0.9761411	1.5336028	-0.3048286
H	0.0478032	1.0861868	-2.4828295
H	1.3048343	1.4443500	-1.2423222
C	-4.7996328	0.6967629	-0.1623252
S	-4.9491345	0.1261370	1.5854227
H	-5.1050020	-0.1547777	-0.8052371
H	-3.7574617	0.9857287	-0.4027539
S	-1.4358444	0.2756150	3.1792748
C	3.3075461	1.1836564	4.9880899
S	1.7539671	0.2176818	5.1838081
H	3.1823101	1.9687086	4.2154871
H	4.1034573	0.4731955	4.6826954
C	2.8226178	0.3692239	1.2290766
S	1.7225071	-1.1104552	1.2607493
H	3.7817004	0.0913423	1.7090634
H	2.3805146	1.2284333	1.7696834
C	-1.9943236	-1.8119312	-1.5120315
S	-1.7520970	-2.2132541	0.2678820
H	-1.1531241	-2.2325593	-2.0984515
H	-2.0304665	-0.7138192	-1.6578158
C	0.0359754	-4.2239685	3.0530231
S	0.2550023	-3.0213298	4.4307682

H	0.9704222	-4.8098088	2.9523667
H	-0.1818295	-3.7185325	2.0910880
C	-0.9585674	-1.2722867	7.5378631
S	-2.5159848	-1.2283068	6.5546034
H	-0.1770412	-0.6150935	7.1071118
H	-0.5760005	-2.3109980	7.5558569
C	-4.9240219	-2.6557601	4.3379129
S	-3.4603532	-3.1106908	3.3227143
H	-5.8085568	-3.2104476	3.9690205
H	-5.1258953	-1.5701389	4.2720014
Zn	-0.5105046	-0.3426972	1.0859837
Zn	-3.9596528	-2.0922009	1.2020955
Zn	2.0230540	-1.6144029	3.6133795
Zn	-1.7713706	-1.7624309	4.3590821
H	-5.4725906	1.5603527	-0.3311433
H	-2.9502049	-2.2580879	-1.8493593
H	3.0160284	0.6659130	0.1788673
H	0.2999928	2.7930141	-1.9109136
H	3.5714409	1.6608242	5.9531071
H	-1.1900662	-0.9396182	8.5684633
H	-0.8067096	-4.8997973	3.2951326
H	-4.7314122	-2.9140569	5.3969859
S	-5.3951334	-3.0553877	-0.3452701
S	4.2112096	-2.3393058	3.8204685
Zn	-3.4737586	1.4437403	2.8797368
Zn	-0.0026917	1.6573100	4.4648398
C	-7.0535074	-2.5996601	0.3150194
H	-7.7973067	-2.6276381	-0.5099355
H	-7.3907734	-3.3102497	1.0997664
H	-7.0503722	-1.5795254	0.7517543
C	4.2336261	-2.6558964	5.6369899
H	3.5972540	-3.5240942	5.9072961
H	5.2747417	-2.8748324	5.9574376
H	3.8671243	-1.7794581	6.2114637
S	-1.0399050	2.4343457	6.4664982
S	-4.4783342	2.0256621	4.9650177
S	0.9019509	3.2394048	2.9084131
S	-2.7367459	3.6437560	2.2043186
Zn	-3.0746002	1.1089322	6.7162555
S	-4.3294486	1.2758113	8.6582039
C	-4.6797565	3.0833447	8.7072894
H	-5.5256629	3.2748000	9.4023273
H	-3.8078204	3.6690394	9.0714748
H	-4.9645026	3.4689529	7.7058816
C	-1.8031740	4.0709945	6.0936824
H	-1.0088425	4.8422018	6.0610140
H	-2.3525460	4.0679287	5.1318938
H	-2.5107686	4.3223838	6.9062822
C	-6.0360955	1.0911894	5.2559657
H	-6.1176198	0.9342043	6.3522958
H	-6.8955125	1.6841876	4.8857769
H	-6.0362694	0.1120512	4.7402452
C	-3.9297071	4.2325714	0.9366703
H	-4.9598813	4.1349590	1.3324162
H	-3.7260380	5.2991605	0.7166347
H	-3.8382747	3.6486672	0.0010374
C	0.7121512	4.9474734	3.5666158
H	1.3795481	5.0896641	4.4391532
H	0.9790085	5.6553324	2.7573997
H	-0.3360074	5.1407838	3.8602819

Zn	-0.6397343	3.4833569	1.0548957
S	0.0636334	5.2850798	-0.2200668
C	1.8889427	5.0175650	-0.2217619
H	2.2006960	4.2826171	-0.9936698
H	2.3945541	5.9808728	-0.4456935
H	2.2519911	4.6511805	0.7606888

12H⁺ site of protonation : S_t

C	0.1144243	1.6959311	-1.6978415
S	-1.0899496	1.5412368	-0.3179340
H	-0.2043267	1.0616082	-2.5471652
H	1.1347060	1.4015684	-1.3884328
C	-4.9077070	0.7407186	-0.0053278
S	-4.9355835	0.1320592	1.7362917
H	-5.2228968	-0.1091074	-0.6455214
H	-3.8919202	1.0682128	-0.3008149
S	-1.3758599	0.2536576	3.2163636
C	3.3596217	1.2945865	4.7072151
S	1.8656291	0.3046155	5.1245093
H	3.1495159	1.9821306	3.8643071
H	4.2065682	0.6259396	4.4561767
C	2.7217763	0.4589952	1.0459320
S	1.6858367	-1.0615374	1.1843815
H	3.7168887	0.2737385	1.4947770
H	2.2521699	1.3337155	1.5361043
C	-2.0944000	-1.8798920	-1.4639040
S	-1.8118467	-2.2394749	0.3208149
H	-1.2359208	-2.2598175	-2.0518447
H	-2.2010553	-0.7892907	-1.6249411
C	-0.0661426	-4.2050036	3.0473786
S	0.1903500	-3.0012298	4.4216041
H	0.8667487	-4.7801146	2.8915035
H	-0.3559892	-3.7019421	2.1039217
C	-0.9273721	-1.2677879	7.5734410
S	-2.5077734	-1.1613604	6.6341613
H	-0.1292531	-0.6523593	7.1133978
H	-0.5952640	-2.3230270	7.6123585
C	-4.9857714	-2.9075491	4.4206528
S	-3.4772564	-3.1308972	3.3889452
H	-5.6853806	-3.7362313	4.1990495
H	-5.4874304	-1.9474965	4.1926069
Zn	-0.6441741	-0.3271905	1.0347223
Zn	-4.0287505	-2.0907708	1.2794891
Zn	1.5685311	-1.3541400	3.4963966
Zn	-1.9003460	-1.7220385	4.4366491
H	-5.6188704	1.5826101	-0.1143614
H	-3.0261095	-2.3873134	-1.7796714
H	2.8629044	0.6833975	-0.0289765
H	0.1130010	2.7635401	-1.9976698
H	3.6326389	1.8916705	5.5989627
H	-1.1197489	-0.8999186	8.5998413
H	-0.8821844	-4.8898835	3.3450733
H	-4.7074110	-2.9305445	5.4917502
S	-5.4560147	-3.0269022	-0.2562396
S	3.8065937	-2.7529610	3.9590351
Zn	-3.4489353	1.4605119	2.9864670
Zn	-0.0173820	1.7621690	4.4386642
C	-7.1155591	-2.5800749	0.4092999
H	-7.8560870	-2.6315621	-0.4156539
H	-7.4387332	-3.2857707	1.2028147

H	-7.1275138	-1.5540136	0.8301834
C	3.6214571	-2.8726973	5.7797353
H	2.7616562	-3.5523221	5.9320275
H	4.5340060	-3.2962263	6.2395451
H	3.3599789	-1.8839066	6.2031907
S	-0.8911087	2.4910592	6.4851106
S	-4.3947654	2.0484028	5.0805949
S	0.9068275	3.2358689	2.8323521
S	-2.6709918	3.6349877	2.3288272
Zn	-2.9554446	1.2156735	6.8244875
S	-4.0473672	1.3895264	8.8348273
C	-4.3177194	3.2070813	8.9638376
H	-5.0589807	3.4015007	9.7670122
H	-3.3863654	3.7515224	9.2294722
H	-4.7181587	3.6303492	8.0195765
C	-1.6526954	4.1387735	6.1514578
H	-0.8520897	4.8989334	6.0720822
H	-2.2557773	4.1359376	5.2228352
H	-2.3058912	4.3943706	7.0064343
C	-5.8509217	0.9785036	5.4307201
H	-5.9905558	0.9727128	6.5310293
H	-6.7437696	1.3936134	4.9253017
H	-5.6908855	-0.0588379	5.0824273
C	-4.0025514	4.3505041	1.2836018
H	-4.9595890	4.2941057	1.8373826
H	-3.7642782	5.4116966	1.0771689
H	-4.0973225	3.8069211	0.3244695
C	0.7699187	4.9592747	3.4656816
H	1.4645698	5.1070923	4.3147156
H	1.0230016	5.6431804	2.6323140
H	-0.2681496	5.1703173	3.7817344
Zn	-0.6928401	3.5090624	1.0023895
S	0.0168994	5.2697279	-0.2876111
C	1.8318451	4.9465972	-0.3536080
H	2.0846524	4.1258728	-1.0568774
H	2.3380882	5.8673842	-0.7101095
H	2.2457461	4.6839944	0.6418838
H	4.7638959	-1.7809717	3.9358244

12H⁺ site of protonation : S_b

C	-0.1097541	1.9759781	-1.6428938
S	-1.2843821	1.8302226	-0.2345477
H	-0.5356785	1.4701754	-2.5306122
H	0.8700839	1.5221514	-1.4033030
C	-5.0528413	1.0413800	-0.1919216
S	-5.0203182	0.3818425	1.5301896
H	-5.3177237	0.1889752	-0.8513900
H	-4.0580198	1.4311901	-0.4828746
S	-1.6488243	0.5574107	3.2451967
C	3.0219585	1.4881519	5.3268127
S	1.5517008	0.3897036	5.1879694
H	3.0125382	2.2429842	4.5159961
H	3.9437369	0.8783393	5.2681903
C	2.6826091	0.9743856	1.0212183
S	1.6466338	-0.5482262	1.1466592
H	3.7224081	0.7126034	1.2971440
H	2.3125894	1.7856675	1.6775961
C	-1.4930301	-2.2419509	-1.1277301
S	-1.6496695	-2.0644994	0.6966411
H	-0.4202726	-2.2962488	-1.3951522

H	-1.9644733	-1.3834741	-1.6415752
C	0.0988945	-4.1343922	3.3257434
S	-0.1167734	-2.4776987	4.0682928
H	1.1864674	-4.3486671	3.3150838
H	-0.2959257	-4.0267837	2.2964963
C	-1.3878563	-1.0855706	7.4496207
S	-3.0050527	-0.9979471	6.5705651
H	-0.5906776	-0.5210192	6.9268024
H	-1.0829588	-2.1447015	7.5646283
C	-5.4613589	-2.6381731	4.1065807
S	-3.8553951	-2.8792936	3.2337769
H	-6.1147163	-3.4998766	3.8704330
H	-5.9599100	-1.7093815	3.7692205
Zn	-0.6711679	0.0412847	1.1394829
Zn	-4.0226728	-1.7952511	1.0496446
Zn	2.0628484	-1.0871048	3.4002932
Zn	-2.5143100	-1.3178809	4.3175873
H	-5.8149502	1.8410243	-0.2679693
H	-2.0046157	-3.1726866	-1.4387648
H	2.6731025	1.3269672	-0.0279102
H	0.0142398	3.0597328	-1.8457050
H	2.9832479	2.0028410	6.3061384
H	-1.5370808	-0.6458754	8.4546968
H	-0.4865677	-4.8881841	3.8819390
H	-5.2901845	-2.5972428	5.1997609
S	-5.1914253	-2.6627249	-0.7159408
S	3.6724340	-2.6421845	3.7522801
Zn	-3.6737493	1.8028623	2.8526062
Zn	-0.2401966	1.9150405	4.5780927
C	-6.9015087	-2.6387141	-0.0262510
H	-7.6191737	-2.8013021	-0.8565655
H	-7.0568312	-3.4443336	0.7212178
H	-7.1371887	-1.6656482	0.4513021
C	3.8344016	-2.6450927	5.5933816
H	3.6340490	-3.6607098	5.9930400
H	4.8665192	-2.3615320	5.8848437
H	3.1330111	-1.9304544	6.0701632
S	-1.2533312	2.5921414	6.5925937
S	-4.7059835	2.2940581	4.9408427
S	0.7084411	3.4373990	3.0312203
S	-2.8790690	3.9815090	2.2787708
Zn	-3.3878877	1.4203544	6.7531466
S	-4.5954046	1.5166973	8.6963153
C	-4.7935110	3.3343027	8.9238628
H	-5.5533063	3.5136640	9.7127610
H	-3.8492288	3.8187561	9.2512122
H	-5.1430659	3.8284632	7.9940623
C	-1.9222910	4.2779710	6.2509055
H	-1.0842893	5.0001853	6.2229684
H	-2.4810717	4.3185247	5.2958267
H	-2.6033647	4.5532468	7.0777702
C	-6.1940100	1.2386702	5.1871280
H	-6.3842894	1.2000037	6.2791259
H	-7.0559151	1.6879484	4.6576201
H	-6.0363537	0.2116172	4.8084752
C	-4.0466828	4.6242705	1.0118940
H	-5.0791035	4.5718877	1.4083679
H	-3.7935776	5.6811274	0.8006175
H	-3.9778446	4.0403035	0.0748477
C	0.5700219	5.1644752	3.6552268

H	1.2575759	5.3131955	4.5099212
H	0.8389849	5.8396298	2.8192131
H	-0.4687454	5.3892344	3.9588469
Zn	-0.7891248	3.7586999	1.1245406
S	0.0507748	5.4837446	-0.1371670
C	1.8484270	5.0699723	-0.1410728
H	2.0791200	4.2171993	-0.8132314
H	2.4088925	5.9536808	-0.5095426
H	2.2203626	4.8184282	0.8731515
H	0.3491052	-2.7485381	5.3215443