

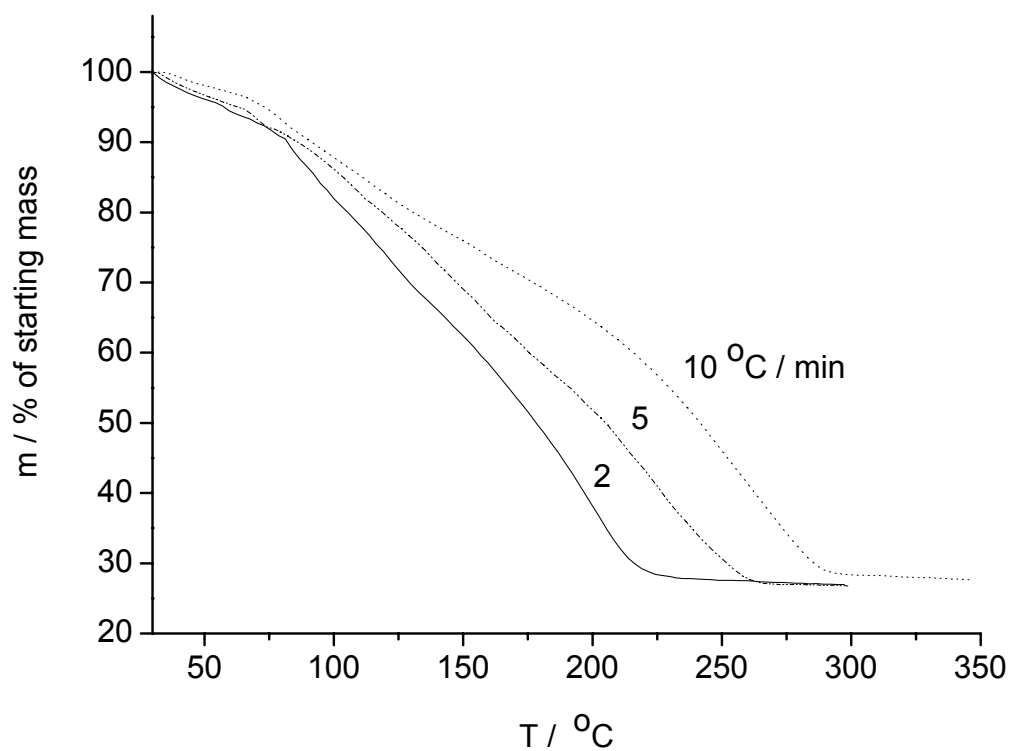
**Supplementary Material (ESI) for Dalton Trans.**

**Electronic supplementary information**

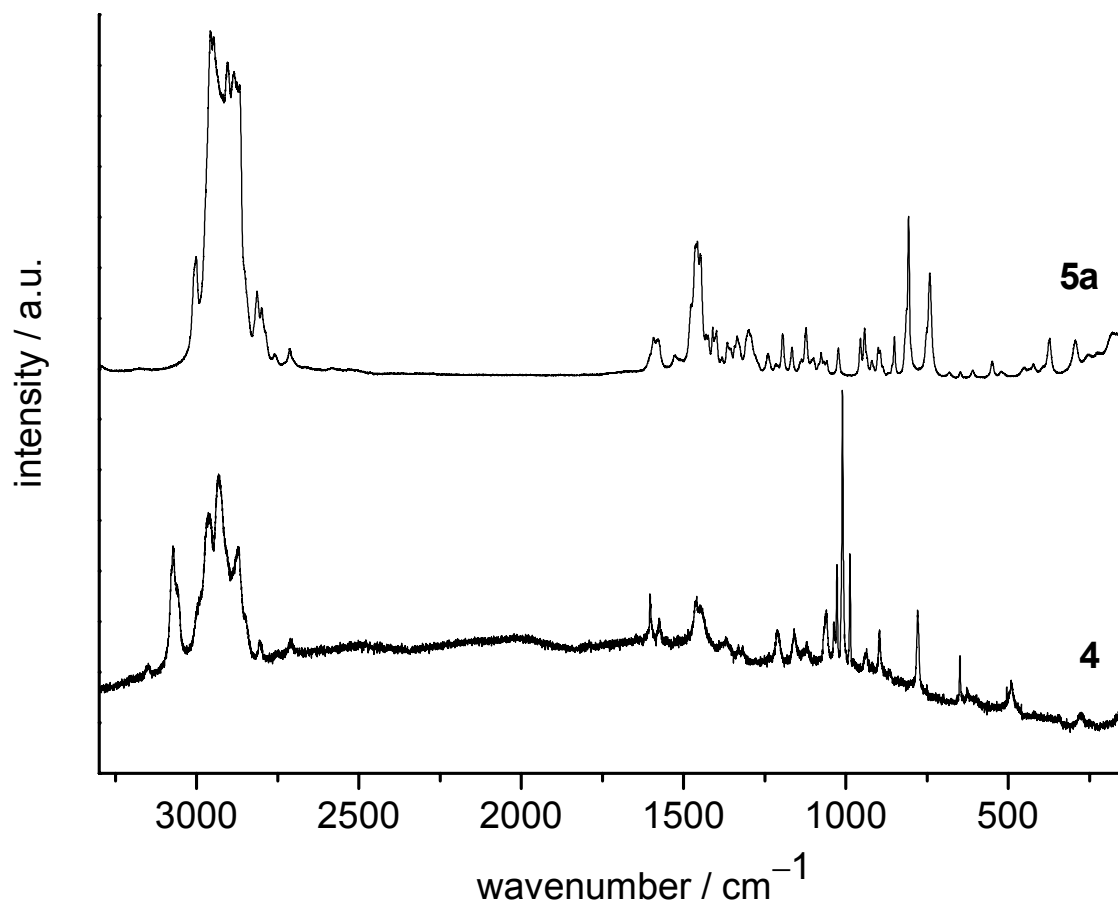
**Electron Density Controlled Carbamate Ligand Binding Mode:  
Towards a Better Understanding of Metalloenzyme Activity**

C. Neuhäuser, D. Domide, J. Mautz, E. Kaifer, H.-J. Himmel\*

**Fig. S1** TG curve obtained for **4** at different heating rates



**Fig. S2** Raman spectra for **4** and **5a**, excited at 514 nm.



SCF energies, coordinates (in bor and Angstrom) and vibrational properties for compounds **1b**, **5b**, **6a** and **6b**

**1b**

BP/SVP

SCF energy = -2615.8091885210

Coordinates in bor

-0.55528575264386	0.00359163269114	0.00067694654117	zn
-3.86175150799926	1.31213424570560	6.34115030605720	n
-3.88043521176800	-1.30365308839945	-6.33155984498681	n
2.61679606400444	-2.39520385965341	1.47334889937146	n
2.62754170347716	2.38626218236569	-1.47818302531046	n
-1.08195927924396	2.47463727342560	3.21912093192007	o
-3.07431874222142	-1.24413308667054	2.92604718666223	o
-1.09745289015795	-2.47240075966598	-3.21472223243673	o
-3.07217576599071	1.25578177611818	-2.92433651936602	o
-2.66031134896179	0.84399548044259	4.07231972787951	c
-2.67059181738584	-0.83753108935733	-4.06733990378496	c
2.85223327432362	-2.04385070354303	4.22386617149623	c
2.06549611455098	-5.05917429555168	0.87560401149979	c
4.85311058453675	-1.45694959347570	0.09595719861437	c
4.86267292791849	1.43369652313688	-0.10818691711741	c
2.09279669406336	5.05297214618987	-0.87745003411390	c
2.85587988136635	2.03576448084971	-4.22986965649906	c
-3.87304322911575	3.13621362005072	6.96134381091674	h
-5.41852154048431	0.24615808066342	6.73293839894529	h
-3.90314650305514	-3.12919811504957	-6.94713158161683	h
-5.43465693156282	-0.23277635173374	-6.72027079006724	h
3.04311296698361	-0.01676404471285	4.68882875681921	h
4.50255279679228	-3.10714164789212	4.99893091081919	h
1.10149213294036	-2.72833212649970	5.13465753913759	h
1.70365032333936	-5.24909363852853	-1.17237659420996	h
0.32099813533328	-5.62127790218519	1.88241311959699	h
3.64155636358715	-6.33225851454949	1.46492661838702	h
4.81936588566402	-2.30348056525738	-1.81977833094813	h
6.64359163085349	-2.10118601853212	1.01279171013801	h
6.65359280869831	2.06532077816884	-1.03284893871548	h
4.84332000287704	2.28168525865192	1.80725344535730	h
1.73431456846800	5.24319984902027	1.17117383766744	h
0.35065215573547	5.62678567194969	-1.88184931180191	h
3.67560171708848	6.31746326345090	-1.46732882213318	h
3.03499229480711	0.00797066136374	-4.69633879791572	h
4.51072053118052	3.09005354222698	-5.00727849799835	h
1.10721105409325	2.73005030514943	-5.13709853213772	h

Coordinates in Angstrom

HETATM	1	zn	1	-0.294	0.002	0.000
HETATM	2	n	1	-2.044	0.694	3.356
HETATM	3	n	1	-2.053	-0.690	-3.351
HETATM	4	n	1	1.385	-1.267	0.780
HETATM	5	n	1	1.390	1.263	-0.782
HETATM	6	o	1	-0.573	1.310	1.703
HETATM	7	o	1	-1.627	-0.658	1.548
HETATM	8	o	1	-0.581	-1.308	-1.701
HETATM	9	o	1	-1.626	0.665	-1.547
HETATM	10	c	1	-1.408	0.447	2.155
HETATM	11	c	1	-1.413	-0.443	-2.152
HETATM	12	c	1	1.509	-1.082	2.235
HETATM	13	c	1	1.093	-2.677	0.463
HETATM	14	c	1	2.568	-0.771	0.051
HETATM	15	c	1	2.573	0.759	-0.057
HETATM	16	c	1	1.107	2.674	-0.464
HETATM	17	c	1	1.511	1.077	-2.238
HETATM	18	h	1	-2.050	1.660	3.684
HETATM	19	h	1	-2.867	0.130	3.563
HETATM	20	h	1	-2.065	-1.656	-3.676
HETATM	21	h	1	-2.876	-0.123	-3.556
HETATM	22	h	1	1.610	-0.009	2.481
HETATM	23	h	1	2.383	-1.644	2.645
HETATM	24	h	1	0.583	-1.444	2.717
HETATM	25	h	1	0.902	-2.778	-0.620
HETATM	26	h	1	0.170	-2.975	0.996
HETATM	27	h	1	1.927	-3.351	0.775
HETATM	28	h	1	2.550	-1.219	-0.963
HETATM	29	h	1	3.516	-1.112	0.536
HETATM	30	h	1	3.521	1.093	-0.547
HETATM	31	h	1	2.563	1.207	0.956
HETATM	32	h	1	0.918	2.775	0.620
HETATM	33	h	1	0.186	2.978	-0.996
HETATM	34	h	1	1.945	3.343	-0.776
HETATM	35	h	1	1.606	0.004	-2.485
HETATM	36	h	1	2.387	1.635	-2.650
HETATM	37	h	1	0.586	1.445	-2.718

Vibrational Properties

#	mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-

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7	a	41.11	0.04762	YES	YES
8	a	47.88	0.02770	YES	YES
9	a	62.10	0.20206	YES	YES
10	a	65.28	2.42003	YES	YES
11	a	88.63	0.38545	YES	YES
12	a	93.73	0.05319	YES	YES
13	a	106.84	0.62015	YES	YES
14	a	131.84	2.34786	YES	YES
15	a	136.04	8.73453	YES	YES
16	a	148.35	2.50136	YES	YES
17	a	161.42	18.57397	YES	YES
18	a	175.12	9.34323	YES	YES
19	a	178.96	12.98142	YES	YES
20	a	184.34	8.60932	YES	YES
21	a	190.96	1.64520	YES	YES
22	a	197.54	4.28346	YES	YES
23	a	232.38	0.18450	YES	YES
24	a	256.13	31.73510	YES	YES
25	a	258.66	0.23235	YES	YES
26	a	269.95	7.69031	YES	YES
27	a	273.49	0.88456	YES	YES
28	a	287.31	3.07168	YES	YES
29	a	313.58	160.56893	YES	YES
30	a	353.84	4.14124	YES	YES
31	a	378.45	4.55832	YES	YES
32	a	408.28	322.06689	YES	YES
33	a	412.08	53.74901	YES	YES
34	a	420.33	16.33399	YES	YES
35	a	434.33	18.82791	YES	YES
36	a	435.90	3.52074	YES	YES
37	a	456.78	17.37498	YES	YES
38	a	479.02	2.91378	YES	YES
39	a	480.29	8.59952	YES	YES
40	a	536.66	0.93924	YES	YES
41	a	537.16	6.36706	YES	YES
42	a	570.64	7.28127	YES	YES
43	a	696.32	64.28967	YES	YES
44	a	699.95	31.45597	YES	YES
45	a	768.62	20.62346	YES	YES
46	a	775.64	23.24705	YES	YES
47	a	777.12	17.38806	YES	YES
48	a	793.65	42.39161	YES	YES
49	a	930.40	6.69011	YES	YES
50	a	942.79	48.98254	YES	YES
51	a	1016.50	15.53826	YES	YES
52	a	1016.83	10.61135	YES	YES
53	a	1026.40	28.25097	YES	YES
54	a	1028.92	0.52668	YES	YES
55	a	1029.22	0.73586	YES	YES
56	a	1030.40	0.25645	YES	YES
57	a	1053.65	11.29007	YES	YES

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58	a	1057.64	11.70622	YES	YES
59	a	1058.11	18.84795	YES	YES
60	a	1075.69	2.21819	YES	YES
61	a	1078.74	0.16671	YES	YES
62	a	1117.67	19.81652	YES	YES
63	a	1144.35	3.34546	YES	YES
64	a	1169.62	3.80487	YES	YES
65	a	1214.25	0.38099	YES	YES
66	a	1239.07	0.19745	YES	YES
67	a	1239.99	5.84993	YES	YES
68	a	1267.19	1.65251	YES	YES
69	a	1277.31	26.01853	YES	YES
70	a	1325.23	4.97380	YES	YES
71	a	1358.12	6.57088	YES	YES
72	a	1371.34	0.17601	YES	YES
73	a	1373.73	1.80914	YES	YES
74	a	1399.34	0.02980	YES	YES
75	a	1400.20	14.43632	YES	YES
76	a	1405.56	1.45349	YES	YES
77	a	1407.11	4.11786	YES	YES
78	a	1418.07	24.26856	YES	YES
79	a	1423.70	36.61325	YES	YES
80	a	1424.82	8.69532	YES	YES
81	a	1425.06	8.96668	YES	YES
82	a	1431.25	9.97071	YES	YES
83	a	1431.70	66.09949	YES	YES
84	a	1443.05	115.82512	YES	YES
85	a	1443.51	55.39607	YES	YES
86	a	1444.51	259.53810	YES	YES
87	a	1450.80	52.13003	YES	YES
88	a	1562.15	570.71888	YES	YES
89	a	1566.33	417.57898	YES	YES
90	a	1585.42	28.03294	YES	YES
91	a	1598.52	406.31687	YES	YES
92	a	2900.72	2.31035	YES	YES
93	a	2903.57	11.73411	YES	YES
94	a	2904.03	41.86399	YES	YES
95	a	2907.12	5.25128	YES	YES
96	a	2908.27	199.93460	YES	YES
97	a	2915.22	189.23016	YES	YES
98	a	3015.42	0.63025	YES	YES
99	a	3031.60	18.41230	YES	YES
100	a	3045.75	4.93727	YES	YES
101	a	3046.11	6.26335	YES	YES
102	a	3049.58	4.34690	YES	YES
103	a	3049.94	8.87351	YES	YES
104	a	3094.21	4.33589	YES	YES
105	a	3094.39	4.16259	YES	YES
106	a	3095.80	2.27918	YES	YES
107	a	3096.24	2.56034	YES	YES
108	a	3502.55	27.11903	YES	YES

109	a	3502.69	34.60703	YES	YES
110	a	3629.91	31.70055	YES	YES
111	a	3630.31	33.28482	YES	YES

## BP/TZVPP

SCF energy = -2617.0176242360

### Coordinates in bor

-0.55212682850428	0.00018601768898	0.00011422069075	zn
-3.96968510174439	1.35306455472193	6.28438646493943	n
-3.97073155580357	-1.35286701476256	-6.28376175025016	n
2.65614340905170	-2.36275372154049	1.50548669271036	n
2.65716318514204	2.36194257265587	-1.50537438797353	n
-1.15383635203516	2.50381003135610	3.19600265028110	o
-3.11182739584214	-1.23406070162595	2.91641626362621	o
-1.15565407033488	-2.50392821574307	-3.19464060330913	o
-3.10931472546198	1.23651918368315	-2.91849439331578	o
-2.72911890587474	0.86792882671598	4.04014431525953	c
-2.72923493948367	-0.86692090232921	-4.04004373948012	c
2.94222948742051	-1.99998830528705	4.25515853347419	c
2.17703959636402	-5.05690926437674	0.96518673422734	c
4.89536718694031	-1.44150135863523	0.11308876081764	c
4.89678156256209	1.43832140707831	-0.11538463543504	c
2.18037259420786	5.05600939454059	-0.96334969340851	c
2.94128124690484	2.00029598036998	-4.25554211956484	c
-4.03294331903879	3.18450594212542	6.83661066107546	h
-5.53623381848220	0.30598183145967	6.62088681680815	h
-4.03656479006133	-3.18486802088918	-6.83409668187927	h
-5.53618275108163	-0.30423318677919	-6.62058477796889	h
3.17426797413437	0.00653154251097	4.70427285784173	h
4.58350398845486	-3.07205904266365	4.98219394345170	h
1.22141742537528	-2.66312421215814	5.19543994787839	h
1.83965395665381	-5.30496713705390	-1.06124138763829	h
0.47030844842328	-5.64516546459370	1.98153551804454	h
3.78162747781678	-6.24876974196030	1.57741743804456	h
4.85326294314238	-2.30109160698632	-1.77541001527084	h
6.66245293399389	-2.07165983443019	1.03820749496332	h
6.66364613867770	2.06637047542951	-1.04231517813727	h
4.85787765873610	2.29789294831029	1.77317691021846	h
1.84403047680149	5.30327292331339	1.06330651124391	h
0.47370998824534	5.64620104973208	-1.97857190456159	h
3.78549295286955	6.24714584475576	-1.57554123883329	h
3.17153074478312	-0.00622081045061	-4.70554806856069	h
4.58298699163075	3.07134339807002	-4.98291203938164	h
1.22037570721266	2.66516761917255	-5.19426970924824	h

### Coordinates in Angstrom

HETATM	1	zn	1	-0.292	0.000	0.000
HETATM	2	n	1	-2.101	0.716	3.326
HETATM	3	n	1	-2.101	-0.716	-3.325
HETATM	4	n	1	1.406	-1.250	0.797
HETATM	5	n	1	1.406	1.250	-0.797
HETATM	6	o	1	-0.611	1.325	1.691
HETATM	7	o	1	-1.647	-0.653	1.543
HETATM	8	o	1	-0.612	-1.325	-1.691
HETATM	9	o	1	-1.645	0.654	-1.544
HETATM	10	c	1	-1.444	0.459	2.138
HETATM	11	c	1	-1.444	-0.459	-2.138
HETATM	12	c	1	1.557	-1.058	2.252
HETATM	13	c	1	1.152	-2.676	0.511
HETATM	14	c	1	2.591	-0.763	0.060
HETATM	15	c	1	2.591	0.761	-0.061
HETATM	16	c	1	1.154	2.676	-0.510
HETATM	17	c	1	1.556	1.059	-2.252
HETATM	18	h	1	-2.134	1.685	3.618
HETATM	19	h	1	-2.930	0.162	3.504
HETATM	20	h	1	-2.136	-1.685	-3.616
HETATM	21	h	1	-2.930	-0.161	-3.503
HETATM	22	h	1	1.680	0.003	2.489
HETATM	23	h	1	2.425	-1.626	2.636
HETATM	24	h	1	0.646	-1.409	2.749
HETATM	25	h	1	0.974	-2.807	-0.562
HETATM	26	h	1	0.249	-2.987	1.049
HETATM	27	h	1	2.001	-3.307	0.835
HETATM	28	h	1	2.568	-1.218	-0.940
HETATM	29	h	1	3.526	-1.096	0.549
HETATM	30	h	1	3.526	1.093	-0.552
HETATM	31	h	1	2.571	1.216	0.938
HETATM	32	h	1	0.976	2.806	0.563
HETATM	33	h	1	0.251	2.988	-1.047
HETATM	34	h	1	2.003	3.306	-0.834
HETATM	35	h	1	1.678	-0.003	-2.490
HETATM	36	h	1	2.425	1.625	-2.637
HETATM	37	h	1	0.646	1.410	-2.749

### B3LYP/SVP

SCF energy = -2614.9462270240

Coordinates in bor

-0.56560023173991	0.00067588781973	0.00033973181699	zn
-3.89808998857298	1.32930259811476	6.29820703878865	n
-3.90666808084204	-1.32820306418963	-6.29311867479047	n
2.64536647699297	-2.38761080306890	1.47975748013904	n
2.64613215400690	2.38678419552917	-1.48295106262938	n
-1.11448650087742	2.45907114651816	3.20339910858507	o



-3.07158090790507	-1.22918399452501	2.92780010541587	o
-1.11260992343733	-2.45532106364839	-3.20661713412817	o
-3.08067525635584	1.22623353495493	-2.91962612955760	o
-2.68119119026161	0.84749724466311	4.06113381600497	c
-2.68625205209524	-0.84705822775022	-4.05784041966301	c
2.88296933769463	-2.04720238889995	4.22582992229367	c
2.10315065055221	-5.04699952991707	0.87922814844397	c
4.87441655526763	-1.44468686021936	0.10831296487664	c
4.87670844309471	1.43940532867192	-0.11696720829369	c
2.10951431427432	5.04655961483586	-0.87896432935869	c
2.87763584767438	2.04827057593677	-4.22988526908392	c
-3.88422260773963	3.13033195146695	6.94068266641278	h
-5.41205889889584	0.24162269918045	6.72518708115423	h
-3.88844031684659	-3.12792316382455	-6.93925263774104	h
-5.42543338552052	-0.24465526059603	-6.71418891909496	h
3.08081181092730	-0.03804040570119	4.69895574879785	h
4.52417958094832	-3.10685993222430	4.98372739868581	h
1.15060999083175	-2.73332584075271	5.13641167518334	h
1.75155439821570	-5.24174136630583	-1.15474768781411	h
0.37329088112737	-5.61727927210830	1.87726527945298	h
3.67462007002078	-6.30248561278342	1.46542226684514	h
4.85978531324607	-2.29631476636472	-1.78799439775181	h
6.64892494698523	-2.06678804209937	1.03471722252085	h
6.65007516980862	2.05814631749049	-1.04780665065316	h
4.86852830328892	2.29095472451971	1.77935202719120	h
1.76126164488736	5.23992900087430	1.15572061047893	h
0.37921560574199	5.62123655578751	-1.87369842760044	h
3.68233471214246	6.29986297371556	-1.46618717647790	h
3.07134176998707	0.03921450992217	-4.70491157473711	h
4.51880508567129	3.10624848872220	-4.99020602937402	h
1.14445375405403	2.73776576661019	-5.13641487344257	h

### Coordinates in Angstrom

HETATM	1	zn	1	-0.299	0.000	0.000
HETATM	2	n	1	-2.063	0.703	3.333
HETATM	3	n	1	-2.067	-0.703	-3.330
HETATM	4	n	1	1.400	-1.263	0.783
HETATM	5	n	1	1.400	1.263	-0.785
HETATM	6	o	1	-0.590	1.301	1.695
HETATM	7	o	1	-1.625	-0.650	1.549
HETATM	8	o	1	-0.589	-1.299	-1.697
HETATM	9	o	1	-1.630	0.649	-1.545
HETATM	10	c	1	-1.419	0.448	2.149
HETATM	11	c	1	-1.422	-0.448	-2.147
HETATM	12	c	1	1.526	-1.083	2.236
HETATM	13	c	1	1.113	-2.671	0.465
HETATM	14	c	1	2.579	-0.764	0.057
HETATM	15	c	1	2.581	0.762	-0.062
HETATM	16	c	1	1.116	2.671	-0.465

HETATM	17	c	1	1.523	1.084	-2.238
HETATM	18	h	1	-2.055	1.656	3.673
HETATM	19	h	1	-2.864	0.128	3.559
HETATM	20	h	1	-2.058	-1.655	-3.672
HETATM	21	h	1	-2.871	-0.129	-3.553
HETATM	22	h	1	1.630	-0.020	2.487
HETATM	23	h	1	2.394	-1.644	2.637
HETATM	24	h	1	0.609	-1.446	2.718
HETATM	25	h	1	0.927	-2.774	-0.611
HETATM	26	h	1	0.198	-2.973	0.993
HETATM	27	h	1	1.945	-3.335	0.775
HETATM	28	h	1	2.572	-1.215	-0.946
HETATM	29	h	1	3.518	-1.094	0.548
HETATM	30	h	1	3.519	1.089	-0.554
HETATM	31	h	1	2.576	1.212	0.942
HETATM	32	h	1	0.932	2.773	0.612
HETATM	33	h	1	0.201	2.975	-0.992
HETATM	34	h	1	1.949	3.334	-0.776
HETATM	35	h	1	1.625	0.021	-2.490
HETATM	36	h	1	2.391	1.644	-2.641
HETATM	37	h	1	0.606	1.449	-2.718

## 5b

### BP/SVP

SCF energy = -2993.0330521570

### Coordinates in bo:

-0.00763148482948	0.02935114170741	1.85036217872102	zn
-0.60577745575163	3.03536289564632	3.99178006073891	o
-4.32368330460880	4.36146671474397	2.21590202666917	o
0.59566182534912	-2.90329563056155	4.08951220468083	o
4.28987071019478	-4.31336789900257	2.32938056560625	o
3.27049007844818	0.13745163989470	-0.10594516728605	n
4.16709976116375	-1.49626903476884	0.59762188267949	h
6.51021240840299	0.34143668890101	-3.19825974054577	n
3.73313513070971	3.76641811029638	-2.64214603261289	n
-3.28789345299171	-0.14801095509396	-0.09548445179371	n
-4.19477533445983	1.49834113443627	0.56361505584813	h
-3.70364663199462	-3.83400519586664	-2.55502267525716	n
-6.50155849985970	-0.44333764617411	-3.20799007803443	n
-2.56566715070551	6.51409922793900	5.51213988056722	n
2.54029709876053	-6.34653904839579	5.70498362382435	n
4.45302171257592	1.36124558391330	-1.89583300959692	c
6.96169885830653	-2.37035133059765	-3.02370400067293	c
7.94800669450612	-2.93073069387066	-1.24956937336836	h
8.13264767658406	-2.97063204877433	-4.65517916140121	h

5.15025532936834	-3.40774991785838	-3.07303317270463	h
8.77417546083871	1.85636888019420	-3.63883420348513	c
8.35656899518236	3.87847436290346	-3.33841551914328	h
9.50032192704306	1.60092862201592	-5.59384175881664	h
10.31103569113057	1.31152904612100	-2.30441065912068	h
3.73920600945036	4.50818778221658	-5.29405224538184	c
4.65115601532381	3.03087133097041	-6.45167230165441	h
4.75211947337673	6.32595589216439	-5.59392469419223	h
1.76691934898304	4.76066101576395	-5.98965010856154	h
2.09673627742121	5.26589873783622	-1.01564212673257	c
0.05262467678718	4.95749072830766	-1.41760222366646	h
2.51698485498663	7.30020152718102	-1.30692298558218	h
2.40846463963831	4.78041534558318	0.99013037251801	h
-4.44738763694112	-1.41783934026660	-1.86811597363007	c
-2.07212669128054	-5.28361608072265	-0.87879188589281	c
-0.02587947291281	-4.96329999160536	-1.26102779739075	h
-2.46879699641982	-7.32749080722378	-1.13370153430521	h
-2.41474317465493	-4.76028380227725	1.11227590932062	h
-3.67157522849063	-4.63003589077900	-5.19103429917150	c
-4.58404536185334	-3.18609166762949	-6.38972497675405	h
-4.66347820295336	-6.46339438678734	-5.46475719018693	h
-1.68907482863792	-4.87689858188210	-5.85904589896107	h
-8.74422155083189	-1.98915903725490	-3.64883851319957	c
-8.31303110481793	-3.99954276759820	-3.29426716893552	h
-9.44251475369665	-1.78619417493944	-5.62011129486171	h
-10.30629932471653	-1.42727010551849	-2.35135603842458	h
-6.98197687874933	2.26631083388165	-3.09357094427286	c
-8.00891951475640	2.84860435428116	-1.34973139330469	h
-8.12714263014102	2.82511755450329	-4.75787312515938	h
-5.18036049139494	3.32110828070665	-3.12569488714197	h
-2.55710036909394	4.51691759347234	3.79894396148564	c
-4.25987863945695	7.39743200944500	5.76488763038846	h
-1.44357572602403	6.32367029538539	7.06877503344626	h
2.53411000664545	-4.40442360782257	3.92992133943447	c
4.22850520091983	-7.23648555561177	5.97383968909265	h
1.42871964297633	-6.09913090352051	7.26099136656774	h

### Coordinates in Angstrom:

REMARK test basis

HETATM	1	zn	1	-0.004	0.016	0.979
HETATM	2	o	1	-0.321	1.606	2.112
HETATM	3	o	1	-2.288	2.308	1.173
HETATM	4	o	1	0.315	-1.536	2.164
HETATM	5	o	1	2.270	-2.283	1.233
HETATM	6	n	1	1.731	0.073	-0.056
HETATM	7	h	1	2.205	-0.792	0.316
HETATM	8	n	1	3.445	0.181	-1.692
HETATM	9	n	1	1.975	1.993	-1.398
HETATM	10	n	1	-1.740	-0.078	-0.051

HETATM	11	h	1	-2.220	0.793	0.298
HETATM	12	n	1	-1.960	-2.029	-1.352
HETATM	13	n	1	-3.440	-0.235	-1.698
HETATM	14	n	1	-1.358	3.447	2.917
HETATM	15	n	1	1.344	-3.358	3.019
HETATM	16	c	1	2.356	0.720	-1.003
HETATM	17	c	1	3.684	-1.254	-1.600
HETATM	18	h	1	4.206	-1.551	-0.661
HETATM	19	h	1	4.304	-1.572	-2.463
HETATM	20	h	1	2.725	-1.803	-1.626
HETATM	21	c	1	4.643	0.982	-1.926
HETATM	22	h	1	4.422	2.052	-1.767
HETATM	23	h	1	5.027	0.847	-2.960
HETATM	24	h	1	5.456	0.694	-1.219
HETATM	25	c	1	1.979	2.386	-2.801
HETATM	26	h	1	2.461	1.604	-3.414
HETATM	27	h	1	2.515	3.348	-2.960
HETATM	28	h	1	0.935	2.519	-3.170
HETATM	29	c	1	1.110	2.787	-0.537
HETATM	30	h	1	0.028	2.623	-0.750
HETATM	31	h	1	1.332	3.863	-0.692
HETATM	32	h	1	1.275	2.530	0.524
HETATM	33	c	1	-2.353	-0.750	-0.989
HETATM	34	c	1	-1.097	-2.796	-0.465
HETATM	35	h	1	-0.014	-2.626	-0.667
HETATM	36	h	1	-1.306	-3.878	-0.600
HETATM	37	h	1	-1.278	-2.519	0.589
HETATM	38	c	1	-1.943	-2.450	-2.747
HETATM	39	h	1	-2.426	-1.686	-3.381
HETATM	40	h	1	-2.468	-3.420	-2.892
HETATM	41	h	1	-0.894	-2.581	-3.100
HETATM	42	c	1	-4.627	-1.053	-1.931
HETATM	43	h	1	-4.399	-2.116	-1.743
HETATM	44	h	1	-4.997	-0.945	-2.974
HETATM	45	h	1	-5.454	-0.755	-1.244
HETATM	46	c	1	-3.695	1.199	-1.637
HETATM	47	h	1	-4.238	1.507	-0.714
HETATM	48	h	1	-4.301	1.495	-2.518
HETATM	49	h	1	-2.741	1.757	-1.654
HETATM	50	c	1	-1.353	2.390	2.010
HETATM	51	h	1	-2.254	3.915	3.051
HETATM	52	h	1	-0.764	3.346	3.741
HETATM	53	c	1	1.341	-2.331	2.080
HETATM	54	h	1	2.238	-3.829	3.161
HETATM	55	h	1	0.756	-3.228	3.842

### Vibrational Properties:

#	mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR	RAMAN

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1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	5.89	0.02282	YES	YES
8	a	15.83	1.43108	YES	YES
9	a	16.74	1.49606	YES	YES
10	a	33.78	0.51365	YES	YES
11	a	35.37	0.19863	YES	YES
12	a	42.51	1.01760	YES	YES
13	a	54.53	0.89882	YES	YES
14	a	58.46	7.68669	YES	YES
15	a	65.72	1.46270	YES	YES
16	a	71.75	2.52039	YES	YES
17	a	89.86	3.84772	YES	YES
18	a	105.16	0.03687	YES	YES
19	a	111.16	3.46862	YES	YES
20	a	113.82	2.52335	YES	YES
21	a	115.12	3.76261	YES	YES
22	a	127.28	2.70542	YES	YES
23	a	133.74	0.05473	YES	YES
24	a	138.58	2.63392	YES	YES
25	a	142.77	0.56264	YES	YES
26	a	146.13	1.23913	YES	YES
27	a	149.46	13.23689	YES	YES
28	a	157.31	13.22938	YES	YES
29	a	162.42	13.28089	YES	YES
30	a	171.64	6.19474	YES	YES
31	a	175.19	6.72304	YES	YES
32	a	183.50	1.54161	YES	YES
33	a	193.31	29.06001	YES	YES
34	a	207.68	0.63781	YES	YES
35	a	221.06	10.43380	YES	YES
36	a	237.74	1.08814	YES	YES
37	a	242.06	1.14184	YES	YES
38	a	251.88	0.65992	YES	YES
39	a	255.84	20.45163	YES	YES
40	a	283.28	22.77103	YES	YES
41	a	284.49	25.14583	YES	YES
42	a	288.75	16.11391	YES	YES
43	a	305.93	16.65063	YES	YES
44	a	308.65	4.61889	YES	YES
45	a	309.46	49.89551	YES	YES
46	a	360.71	1.10456	YES	YES
47	a	361.39	1.16251	YES	YES
48	a	371.84	9.58132	YES	YES
49	a	372.93	4.52661	YES	YES
50	a	404.26	298.27689	YES	YES
51	a	405.80	153.68046	YES	YES

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52	a	425.23	8.99224	YES	YES
53	a	427.39	8.19205	YES	YES
54	a	506.57	9.73827	YES	YES
55	a	508.91	12.11646	YES	YES
56	a	540.44	5.40771	YES	YES
57	a	540.88	5.54708	YES	YES
58	a	570.39	0.78964	YES	YES
59	a	571.45	1.83570	YES	YES
60	a	608.15	2.81346	YES	YES
61	a	611.66	24.52128	YES	YES
62	a	668.75	53.31484	YES	YES
63	a	668.97	51.99213	YES	YES
64	a	725.82	5.88676	YES	YES
65	a	726.76	1.79296	YES	YES
66	a	759.41	3.38401	YES	YES
67	a	761.11	8.21703	YES	YES
68	a	773.95	10.27700	YES	YES
69	a	774.57	27.77911	YES	YES
70	a	916.83	7.02285	YES	YES
71	a	917.24	43.47860	YES	YES
72	a	976.73	15.95855	YES	YES
73	a	984.11	134.65957	YES	YES
74	a	1015.96	45.16681	YES	YES
75	a	1018.34	67.63492	YES	YES
76	a	1025.68	3.19097	YES	YES
77	a	1026.93	1.80023	YES	YES
78	a	1044.22	2.70178	YES	YES
79	a	1044.50	23.28943	YES	YES
80	a	1051.47	3.48245	YES	YES
81	a	1052.07	6.88228	YES	YES
82	a	1077.18	45.28808	YES	YES
83	a	1078.31	9.32284	YES	YES
84	a	1088.73	4.14151	YES	YES
85	a	1089.47	4.95630	YES	YES
86	a	1091.89	5.26486	YES	YES
87	a	1092.13	1.38593	YES	YES
88	a	1117.97	21.42644	YES	YES
89	a	1121.71	252.88914	YES	YES
90	a	1129.66	3.83099	YES	YES
91	a	1129.91	3.96067	YES	YES
92	a	1132.66	16.12888	YES	YES
93	a	1132.93	6.89582	YES	YES
94	a	1236.27	6.38679	YES	YES
95	a	1238.22	69.74346	YES	YES
96	a	1254.32	58.53340	YES	YES
97	a	1255.55	61.65390	YES	YES
98	a	1307.77	136.83040	YES	YES
99	a	1308.59	112.01417	YES	YES
100	a	1330.54	184.04204	YES	YES
101	a	1332.40	359.81329	YES	YES
102	a	1381.56	17.74449	YES	YES

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103	a	1381.82	57.10805	YES	YES
104	a	1387.95	29.04201	YES	YES
105	a	1388.97	18.89557	YES	YES
106	a	1394.69	323.35515	YES	YES
107	a	1395.77	215.63189	YES	YES
108	a	1403.35	209.41858	YES	YES
109	a	1408.04	4.25342	YES	YES
110	a	1408.74	1.83644	YES	YES
111	a	1409.01	87.98617	YES	YES
112	a	1419.78	30.68769	YES	YES
113	a	1419.97	36.21399	YES	YES
114	a	1423.62	23.38238	YES	YES
115	a	1425.93	39.25876	YES	YES
116	a	1429.02	53.19107	YES	YES
117	a	1430.80	62.12457	YES	YES
118	a	1436.77	4.20238	YES	YES
119	a	1437.14	0.89771	YES	YES
120	a	1440.49	89.32684	YES	YES
121	a	1444.03	27.75481	YES	YES
122	a	1444.15	0.49974	YES	YES
123	a	1444.66	0.44451	YES	YES
124	a	1448.74	11.81071	YES	YES
125	a	1448.95	25.52470	YES	YES
126	a	1466.08	12.19045	YES	YES
127	a	1467.02	17.69386	YES	YES
128	a	1520.12	62.77694	YES	YES
129	a	1521.62	496.15445	YES	YES
130	a	1559.47	344.38418	YES	YES
131	a	1563.64	250.94444	YES	YES
132	a	1623.48	819.82118	YES	YES
133	a	1641.96	92.41575	YES	YES
134	a	1650.62	190.04763	YES	YES
135	a	1658.91	494.14145	YES	YES
136	a	2900.77	130.61540	YES	YES
137	a	2900.95	27.54641	YES	YES
138	a	2902.38	108.35104	YES	YES
139	a	2902.81	82.57098	YES	YES
140	a	2915.35	47.02653	YES	YES
141	a	2916.31	100.54396	YES	YES
142	a	2918.00	33.20293	YES	YES
143	a	2918.32	23.08605	YES	YES
144	a	2959.95	94.67173	YES	YES
145	a	2960.69	49.93689	YES	YES
146	a	2967.02	39.61090	YES	YES
147	a	2967.49	75.22146	YES	YES
148	a	2973.69	761.70386	YES	YES
149	a	2987.79	689.02597	YES	YES
150	a	2988.57	29.12372	YES	YES
151	a	2989.46	154.95548	YES	YES
152	a	2997.04	23.28174	YES	YES
153	a	2997.35	74.69884	YES	YES

154	a	3066.47	8.76394	YES	YES
155	a	3067.24	8.29860	YES	YES
156	a	3072.69	10.17985	YES	YES
157	a	3073.25	12.32328	YES	YES
158	a	3075.37	1.49347	YES	YES
159	a	3076.07	3.06846	YES	YES
160	a	3081.62	1.54922	YES	YES
161	a	3083.69	1.53296	YES	YES
162	a	3449.31	17.53832	YES	YES
163	a	3450.56	18.14975	YES	YES
164	a	3565.11	19.33244	YES	YES
165	a	3566.04	18.05999	YES	YES

## BP/TZVPP

SCF energy = -2994.6592422710

### Coordinates in bor

-0.00078841948073	-0.01120280034866	1.79694789842220	zn
-0.51133888636031	2.92832105808776	4.06892177623913	o
-4.21007414206205	4.42538991410974	2.40114778182014	o
0.52185816655934	-2.96594814283548	4.04713640627436	o
4.20644049279739	-4.45481116240332	2.34073180593220	o
3.28393182306395	0.09777315782018	-0.13971021317585	n
4.15171102883516	-1.54611754404000	0.50630910708425	h
6.47921189976850	0.26215907074625	-3.26103548951842	n
3.85259759394959	3.75689533295034	-2.58744261172522	n
-3.29452669310883	-0.10549853322347	-0.12480955643456	n
-4.16621680126422	1.52661280456265	0.54524286285468	h
-3.86269078128293	-3.73282417871880	-2.61974579401452	n
-6.47130244621455	-0.21852063578743	-3.26586263458475	n
-2.35633221402661	6.38181167699489	5.76626729439989	n
2.36393109254085	-6.44626307158149	5.69156685611033	n
4.48612289078530	1.32161712857103	-1.91310226860350	c
6.89425108001023	-2.45658238561333	-3.07690968338477	c
7.89859486703135	-3.00359822479368	-1.33320478056501	h
8.02464871547892	-3.06095010877505	-4.70989946722283	h
5.08546488387802	-3.45897926594443	-3.10208609216537	h
8.78473365932781	1.71561296787771	-3.71002531638857	c
8.42558623948640	3.73105942001829	-3.42904090733993	h
9.47893776909889	1.41686206205674	-5.64769271844454	h
10.28653360059423	1.13030591780774	-2.38519039876272	h
3.87131643154027	4.57529680997941	-5.21684201035794	c
4.71839562921908	3.11853637668351	-6.41350496669197	h
4.93827248341026	6.34776761737843	-5.44798908884203	h
1.92072747668599	4.91528641800115	-5.87346046893194	h
2.29195434991865	5.28953176243721	-0.91746270807812	c
0.25677514866414	5.08209025485410	-1.31926858973732	h
2.80236900478223	7.28730955507985	-1.17682102402466	h



2.60797401643805	4.75884117226558	1.05488072365090	h
-4.49121907295068	-1.30282842230936	-1.91909897733675	c
-2.32051807421048	-5.29363732773460	-0.95803646563118	c
-0.28189833333316	-5.09365624957006	-1.34545225496770	h
-2.84229650744978	-7.28468621283366	-1.24440189342199	h
-2.64633341164070	-4.78349132365894	1.01799479994406	h
-3.86423920948567	-4.51620360818192	-5.26008895007593	c
-4.70019288575452	-3.04175004694374	-6.44259922738792	h
-4.93254107616784	-6.28367141942423	-5.52156328494822	h
-1.91000658753891	-4.85123421641781	-5.90759649341492	h
-8.77761853171255	-1.65818333149064	-3.75390748092511	c
-8.42887337129474	-3.67940576097331	-3.50296767494316	h
-9.45772435777880	-1.32638869499645	-5.69130216660432	h
-10.28847179116949	-1.09140085328134	-2.43103543202641	h
-6.87832440094294	2.49848402823132	-3.04807528489174	c
-7.89730026276465	3.02449783178012	-1.30607126095475	h
-7.99113509280967	3.13125620548372	-4.68278971324812	h
-5.06523207444754	3.49391500983328	-3.04166053025062	h
-2.42576459246027	4.45830039280700	3.96420152602258	c
-4.03297533384813	7.24558054382160	6.09438724747720	h
-1.26607241869686	6.04598061495359	7.30507127098970	h
2.42960474266757	-4.50145891272913	3.91268914084241	c
4.03913285468469	-7.32074873125286	6.00033094815792	h
1.28239418397825	-6.12545648884147	7.24005540837945	h

### Coordinates in Angstrom

HETATM	1	zn	1	-0.000	-0.006	0.951
HETATM	2	o	1	-0.271	1.550	2.153
HETATM	3	o	1	-2.228	2.342	1.271
HETATM	4	o	1	0.276	-1.570	2.142
HETATM	5	o	1	2.226	-2.357	1.239
HETATM	6	n	1	1.738	0.052	-0.074
HETATM	7	h	1	2.197	-0.818	0.268
HETATM	8	n	1	3.429	0.139	-1.726
HETATM	9	n	1	2.039	1.988	-1.369
HETATM	10	n	1	-1.743	-0.056	-0.066
HETATM	11	h	1	-2.205	0.808	0.289
HETATM	12	n	1	-2.044	-1.975	-1.386
HETATM	13	n	1	-3.424	-0.116	-1.728
HETATM	14	n	1	-1.247	3.377	3.051
HETATM	15	n	1	1.251	-3.411	3.012
HETATM	16	c	1	2.374	0.699	-1.012
HETATM	17	c	1	3.648	-1.300	-1.628
HETATM	18	h	1	4.180	-1.589	-0.706
HETATM	19	h	1	4.246	-1.620	-2.492
HETATM	20	h	1	2.691	-1.830	-1.642
HETATM	21	c	1	4.649	0.908	-1.963
HETATM	22	h	1	4.459	1.974	-1.815

HETATM	23	h	1	5.016	0.750	-2.989
HETATM	24	h	1	5.443	0.598	-1.262
HETATM	25	c	1	2.049	2.421	-2.761
HETATM	26	h	1	2.497	1.650	-3.394
HETATM	27	h	1	2.613	3.359	-2.883
HETATM	28	h	1	1.016	2.601	-3.108
HETATM	29	c	1	1.213	2.799	-0.486
HETATM	30	h	1	0.136	2.689	-0.698
HETATM	31	h	1	1.483	3.856	-0.623
HETATM	32	h	1	1.380	2.518	0.558
HETATM	33	c	1	-2.377	-0.689	-1.016
HETATM	34	c	1	-1.228	-2.801	-0.507
HETATM	35	h	1	-0.149	-2.695	-0.712
HETATM	36	h	1	-1.504	-3.855	-0.659
HETATM	37	h	1	-1.400	-2.531	0.539
HETATM	38	c	1	-2.045	-2.390	-2.784
HETATM	39	h	1	-2.487	-1.610	-3.409
HETATM	40	h	1	-2.610	-3.325	-2.922
HETATM	41	h	1	-1.011	-2.567	-3.126
HETATM	42	c	1	-4.645	-0.877	-1.986
HETATM	43	h	1	-4.460	-1.947	-1.854
HETATM	44	h	1	-5.005	-0.702	-3.012
HETATM	45	h	1	-5.444	-0.578	-1.286
HETATM	46	c	1	-3.640	1.322	-1.613
HETATM	47	h	1	-4.179	1.600	-0.691
HETATM	48	h	1	-4.229	1.657	-2.478
HETATM	49	h	1	-2.680	1.849	-1.610
HETATM	50	c	1	-1.284	2.359	2.098
HETATM	51	h	1	-2.134	3.834	3.225
HETATM	52	h	1	-0.670	3.199	3.866
HETATM	53	c	1	1.286	-2.382	2.071
HETATM	54	h	1	2.137	-3.874	3.175
HETATM	55	h	1	0.679	-3.241	3.831

### B3LYP/SVP

SCF energy = -2991.9159862000

### Coordinates in bor

-0.00312416080952	0.00834452278442	1.91579200504905	zn
-0.61126984608674	3.00528919956784	4.03690392791444	o
-4.24103008851024	4.40678428847270	2.24504602777323	o
0.61550599169187	-2.96902685421834	4.06181109425045	o
4.23856634941125	-4.39175929082111	2.27271924395732	o
3.26625546243320	0.18021299645467	-0.11592802886870	n
4.17397631554195	-1.43133675819514	0.53072301254342	h
6.45749486870299	0.39639918183549	-3.21570122034223	n
3.67323981168530	3.79172175243224	-2.64132601391710	n

-3.28112962521259	-0.18808099924232	-0.09887242679532	n
-4.19061699742030	1.42724000162895	0.53437805322884	h
-3.66915573418501	-3.81130053626158	-2.60979791416517	n
-6.45976881859689	-0.42590690635819	-3.21044868366796	n
-2.53245944377877	6.46024751775620	5.59664873746150	n
2.54239919485360	-6.40530178031405	5.65489083873994	n
4.41495961072899	1.40366997428933	-1.90513736314442	c
6.93375506470567	-2.30659350155261	-3.04159236609975	c
7.91398779293505	-2.85225647384753	-1.27738618083818	h
8.10971595859078	-2.88585361945347	-4.65860951885120	h
5.14891322026018	-3.36067189516399	-3.10075449243195	h
8.70158127468678	1.92002521822521	-3.69222759199137	c
8.28771806114448	3.92915923090642	-3.40394654948460	h
9.39644732207056	1.65367704220252	-5.64156820304780	h
10.24612126610382	1.39110453518906	-2.38395383299974	h
3.63818174682731	4.53223817916084	-5.28830669430210	c
4.52946963153381	3.07450285163642	-6.45975835565417	h
4.63436335230050	6.34148401195674	-5.59433224039809	h
1.66809435483640	4.77868546626237	-5.94614009730497	h
2.06079754848662	5.29315951012928	-0.99860839984467	c
0.02645416867083	4.94800879028110	-1.33149987414028	h
2.43905469793267	7.31221386101545	-1.34590318513664	h
2.44336094076125	4.86601602056273	0.99151060904862	h
-4.42004101316699	-1.42159507023696	-1.88763421670553	c
-2.06291662614597	-5.30220001533617	-0.95135085190558	c
-0.02728614985960	-4.96040610459747	-1.27995770533223	h
-2.44090346468171	-7.32358271855964	-1.28577482150099	h
-2.45197665074547	-4.86034469874294	1.03423020312115	h
-3.61483197673763	-4.56137656098894	-5.25365384567835	c
-4.50475103247320	-3.11209328657747	-6.43672440659937	h
-4.60176850438762	-6.37580025027408	-5.55899055295161	h
-1.63987087143358	-4.80223943259001	-5.89902389515185	h
-8.69285766449795	-1.96049488551320	-3.70251012018622	c
-8.27522657932397	-3.96603763420112	-3.39554564180841	h
-9.36733625833365	-1.71010460310398	-5.66118883586411	h
-10.25344399583532	-1.42779057545675	-2.41511678294700	h
-6.94868313359219	2.27555572353870	-3.04906718909784	c
-7.95230504198154	2.82095700629251	-1.29780973102224	h
-8.10845963082270	2.84622362374149	-4.68083446870961	h
-5.16800141307766	3.33733721500703	-3.08911081382109	h
-2.52058627432582	4.51328998482871	3.84955816796767	c
-4.18420037667866	7.40031019768986	5.81309138043677	h
-1.42182035820843	6.25728941012262	7.14157322572439	h
2.52378935084578	-4.47929315198675	3.88467807387934	c
4.19485365064512	-7.34292926347750	5.87639701801111	h
1.43665703361040	-6.18456679705508	7.20087315715465	h

### Coordinates in Angstrom

HETATM 1 zn 1 -0.002 0.004 1.014

HETATM	2	o	1	-0.323	1.590	2.136
HETATM	3	o	1	-2.244	2.332	1.188
HETATM	4	o	1	0.326	-1.571	2.149
HETATM	5	o	1	2.243	-2.324	1.203
HETATM	6	n	1	1.728	0.095	-0.061
HETATM	7	h	1	2.209	-0.757	0.281
HETATM	8	n	1	3.417	0.210	-1.702
HETATM	9	n	1	1.944	2.006	-1.398
HETATM	10	n	1	-1.736	-0.100	-0.052
HETATM	11	h	1	-2.218	0.755	0.283
HETATM	12	n	1	-1.942	-2.017	-1.381
HETATM	13	n	1	-3.418	-0.225	-1.699
HETATM	14	n	1	-1.340	3.419	2.962
HETATM	15	n	1	1.345	-3.390	2.992
HETATM	16	c	1	2.336	0.743	-1.008
HETATM	17	c	1	3.669	-1.221	-1.610
HETATM	18	h	1	4.188	-1.509	-0.676
HETATM	19	h	1	4.291	-1.527	-2.465
HETATM	20	h	1	2.725	-1.778	-1.641
HETATM	21	c	1	4.605	1.016	-1.954
HETATM	22	h	1	4.386	2.079	-1.801
HETATM	23	h	1	4.972	0.875	-2.985
HETATM	24	h	1	5.422	0.736	-1.262
HETATM	25	c	1	1.925	2.398	-2.798
HETATM	26	h	1	2.397	1.627	-3.418
HETATM	27	h	1	2.452	3.356	-2.960
HETATM	28	h	1	0.883	2.529	-3.147
HETATM	29	c	1	1.091	2.801	-0.528
HETATM	30	h	1	0.014	2.618	-0.705
HETATM	31	h	1	1.291	3.869	-0.712
HETATM	32	h	1	1.293	2.575	0.525
HETATM	33	c	1	-2.339	-0.752	-0.999
HETATM	34	c	1	-1.092	-2.806	-0.503
HETATM	35	h	1	-0.014	-2.625	-0.677
HETATM	36	h	1	-1.292	-3.875	-0.680
HETATM	37	h	1	-1.298	-2.572	0.547
HETATM	38	c	1	-1.913	-2.414	-2.780
HETATM	39	h	1	-2.384	-1.647	-3.406
HETATM	40	h	1	-2.435	-3.374	-2.942
HETATM	41	h	1	-0.868	-2.541	-3.122
HETATM	42	c	1	-4.600	-1.037	-1.959
HETATM	43	h	1	-4.379	-2.099	-1.797
HETATM	44	h	1	-4.957	-0.905	-2.996
HETATM	45	h	1	-5.426	-0.756	-1.278
HETATM	46	c	1	-3.677	1.204	-1.613
HETATM	47	h	1	-4.208	1.493	-0.687
HETATM	48	h	1	-4.291	1.506	-2.477
HETATM	49	h	1	-2.735	1.766	-1.635
HETATM	50	c	1	-1.334	2.388	2.037
HETATM	51	h	1	-2.214	3.916	3.076
HETATM	52	h	1	-0.752	3.311	3.779

HETATM	53	c	1	1.336	-2.370	2.056
HETATM	54	h	1	2.220	-3.886	3.110
HETATM	55	h	1	0.760	-3.273	3.811

## 6a

### BP/SVP

SCF energy = -2756.1782869450

### Coordinates in bor:

0.19219437952396	-0.23723243089447	-0.06320837320866	zn
-5.48945188132566	-1.31475772276645	-1.55561077319621	o
3.65175292790213	-4.24678507561725	0.15628431040492	o
-1.46811996771918	-1.29014569359285	-3.16544837193501	o
0.36134593001890	-2.91130060939625	2.55692677885177	o
-3.90020301694303	-1.68953618429362	-3.26430337159635	c
2.13423765909225	-4.50335760057749	1.97315805302674	c
-4.71922058589944	-2.54138541269347	-5.62173384260490	n
-6.47047849978435	-3.34469301430551	-5.65630776094116	h
-3.38529215329325	-3.32239669763256	-6.77453474279083	h
2.34471116261482	-6.58931895302223	3.53368007488764	n
0.84476774323125	-7.01892390097299	4.66340312302226	h
3.42067642897755	-8.04984215055460	2.88776861353336	h
-1.66853700280248	2.69341733379093	1.69833010203905	n
-4.02784092261027	2.31223567692517	2.36067448145510	c
-4.72312851574376	0.08879999221312	3.55359665269447	n
-3.14633424715362	-1.01828975928527	3.85857862097995	h
-5.87928513217328	-0.90031602801784	2.31860492197067	h
-5.90822721538598	4.06670411773016	2.03544959031278	n
-5.77619448878513	5.24182355418441	0.51080896157746	h
-7.69718324007011	3.49542154195982	2.47696746276026	h
-0.79971620839116	5.03186884920270	0.58215249414694	c
-1.37314350873146	6.72702065699739	1.69661321485436	h
-1.58595644621804	5.27648255051552	-1.36732652076881	h
2.11264357517666	4.94290692766345	0.39891194435939	c
2.92471848334965	5.33963200580348	2.30570757875499	h
2.72032778228350	6.52313312851295	-0.86799655933652	h
2.94313109455338	2.47880698516579	-0.51107039610697	n
5.33449056360413	2.11947348558050	-1.12521488048517	c
7.09536663510614	4.05401591259820	-1.06736095497883	n
6.40782517096367	5.85437183009072	-1.13870343025927	h
8.71822851316214	3.80128977333354	-2.07938869395905	h
6.16298066265382	-0.21081921307562	-1.81211640686481	n
5.08941279198997	-1.77386153703847	-1.17792121791995	h
8.06884804595867	-0.49602424672673	-1.84827665132825	h

### Coordinates in Angstrom

HETATM	1	zn	1	0.102	-0.126	-0.033
HETATM	2	o	1	-2.905	-0.696	-0.823
HETATM	3	o	1	1.932	-2.247	0.083
HETATM	4	o	1	-0.777	-0.683	-1.675
HETATM	5	o	1	0.191	-1.541	1.353
HETATM	6	c	1	-2.064	-0.894	-1.727
HETATM	7	c	1	1.129	-2.383	1.044
HETATM	8	n	1	-2.497	-1.345	-2.975
HETATM	9	h	1	-3.424	-1.770	-2.993
HETATM	10	h	1	-1.791	-1.758	-3.585
HETATM	11	n	1	1.241	-3.487	1.870
HETATM	12	h	1	0.447	-3.714	2.468
HETATM	13	h	1	1.810	-4.260	1.528
HETATM	14	n	1	-0.883	1.425	0.899
HETATM	15	c	1	-2.131	1.224	1.249
HETATM	16	n	1	-2.499	0.047	1.880
HETATM	17	h	1	-1.665	-0.539	2.042
HETATM	18	h	1	-3.111	-0.476	1.227
HETATM	19	n	1	-3.126	2.152	1.077
HETATM	20	h	1	-3.057	2.774	0.270
HETATM	21	h	1	-4.073	1.850	1.311
HETATM	22	c	1	-0.423	2.663	0.308
HETATM	23	h	1	-0.727	3.560	0.898
HETATM	24	h	1	-0.839	2.792	-0.724
HETATM	25	c	1	1.118	2.616	0.211
HETATM	26	h	1	1.548	2.826	1.220
HETATM	27	h	1	1.440	3.452	-0.459
HETATM	28	n	1	1.557	1.312	-0.270
HETATM	29	c	1	2.823	1.122	-0.595
HETATM	30	n	1	3.755	2.145	-0.565
HETATM	31	h	1	3.391	3.098	-0.603
HETATM	32	h	1	4.613	2.012	-1.100
HETATM	33	n	1	3.261	-0.112	-0.959
HETATM	34	h	1	2.693	-0.939	-0.623
HETATM	35	h	1	4.270	-0.262	-0.978

### Vibrational Properties

#	mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	4.19	14.17008	YES	YES
8	a	32.07	8.18339	YES	YES
9	a	32.55	7.31578	YES	YES
10	a	38.40	2.78306	YES	YES

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11	a	47.86	10.19720	YES	YES
12	a	50.59	1.06194	YES	YES
13	a	72.57	4.50400	YES	YES
14	a	79.31	28.98562	YES	YES
15	a	91.79	1.62312	YES	YES
16	a	98.72	6.19560	YES	YES
17	a	121.43	7.73091	YES	YES
18	a	140.16	0.43518	YES	YES
19	a	157.36	4.75605	YES	YES
20	a	164.87	13.63971	YES	YES
21	a	179.88	21.73959	YES	YES
22	a	197.44	7.87465	YES	YES
23	a	218.06	38.77743	YES	YES
24	a	231.72	15.32734	YES	YES
25	a	264.96	12.38992	YES	YES
26	a	280.29	10.65228	YES	YES
27	a	299.17	49.07130	YES	YES
28	a	316.42	21.80202	YES	YES
29	a	322.84	111.02485	YES	YES
30	a	326.68	77.82115	YES	YES
31	a	362.25	190.43971	YES	YES
32	a	388.47	49.74738	YES	YES
33	a	409.66	167.79307	YES	YES
34	a	427.21	105.07899	YES	YES
35	a	446.48	72.11211	YES	YES
36	a	454.77	138.18268	YES	YES
37	a	461.65	174.03770	YES	YES
38	a	496.86	78.97840	YES	YES
39	a	498.84	28.33771	YES	YES
40	a	505.09	3.10579	YES	YES
41	a	526.74	27.41132	YES	YES
42	a	557.30	1.33025	YES	YES
43	a	567.98	2.47062	YES	YES
44	a	570.19	0.11291	YES	YES
45	a	582.47	7.52025	YES	YES
46	a	604.27	23.57475	YES	YES
47	a	655.37	17.59948	YES	YES
48	a	668.89	19.81248	YES	YES
49	a	684.76	34.99639	YES	YES
50	a	701.96	7.13672	YES	YES
51	a	766.73	25.28005	YES	YES
52	a	770.33	16.84974	YES	YES
53	a	826.56	19.83174	YES	YES
54	a	840.46	137.60483	YES	YES
55	a	919.09	141.99424	YES	YES
56	a	932.22	224.80744	YES	YES
57	a	984.67	7.95470	YES	YES
58	a	1008.52	4.17429	YES	YES
59	a	1021.48	4.28252	YES	YES
60	a	1031.00	8.55167	YES	YES
61	a	1055.09	2.20330	YES	YES

62	a	1056.02	8.33805	YES	YES
63	a	1064.39	13.11418	YES	YES
64	a	1068.59	26.58595	YES	YES
65	a	1070.26	9.52844	YES	YES
66	a	1090.63	29.51790	YES	YES
67	a	1112.55	32.46973	YES	YES
68	a	1191.25	35.47755	YES	YES
69	a	1209.65	3.27011	YES	YES
70	a	1223.38	2.05916	YES	YES
71	a	1247.69	0.70323	YES	YES
72	a	1327.11	47.53926	YES	YES
73	a	1339.28	34.87243	YES	YES
74	a	1383.16	476.42239	YES	YES
75	a	1411.46	28.48980	YES	YES
76	a	1419.39	73.90883	YES	YES
77	a	1422.42	292.03821	YES	YES
78	a	1439.80	27.32737	YES	YES
79	a	1472.56	56.13026	YES	YES
80	a	1532.01	248.16035	YES	YES
81	a	1545.98	344.10138	YES	YES
82	a	1571.43	39.15642	YES	YES
83	a	1576.38	234.08118	YES	YES
84	a	1593.52	136.32255	YES	YES
85	a	1597.41	90.85742	YES	YES
86	a	1638.21	162.37973	YES	YES
87	a	1655.39	98.49052	YES	YES
88	a	1680.28	1313.61922	YES	YES
89	a	1698.29	241.92768	YES	YES
90	a	2868.99	18.80678	YES	YES
91	a	2876.47	119.83379	YES	YES
92	a	2925.37	103.17985	YES	YES
93	a	2931.44	1193.17139	YES	YES
94	a	2945.68	52.63461	YES	YES
95	a	3329.02	147.21695	YES	YES
96	a	3411.77	117.00178	YES	YES
97	a	3488.88	38.68474	YES	YES
98	a	3491.16	13.24912	YES	YES
99	a	3491.62	20.87722	YES	YES
100	a	3505.59	23.62689	YES	YES
101	a	3560.19	41.88133	YES	YES
102	a	3599.86	34.86345	YES	YES
103	a	3604.98	37.48439	YES	YES
104	a	3622.64	19.19205	YES	YES
105	a	3637.45	29.90904	YES	YES

BP/TZVPP

SCF energy = -2757.5557522230

**Coordinates in bor**



0.16785537595136	-0.27108045571210	-0.06071945611375	zn
-5.15932718502256	-1.60176774232132	-1.75700263217469	o
4.05180285110043	-4.05918033373442	0.26501744903146	o
-1.15726869899283	-1.29021190591500	-3.33965278006043	o
0.54137222442081	-2.97904247031545	2.48683868164946	o
-3.56326997772617	-1.82480636947091	-3.47671542609755	c
2.45798124301815	-4.43056877311655	1.98461114843305	c
-4.32026592054418	-2.62484540559437	-5.87559668423037	n
-5.98563870049086	-3.56876267723586	-5.91614122320742	h
-2.93450678577515	-3.32394312998638	-6.99870211150558	h
2.73915613678012	-6.49700778326783	3.56688736370353	n
1.19062011136104	-7.05330294064478	4.54391138766217	h
3.89536202827047	-7.88076181815121	2.92789680092476	h
-1.95463395305472	2.48308859271754	1.69556321101438	n
-4.26744451239078	2.01695753410335	2.40745884999860	c
-4.81279424263679	-0.16786711362720	3.71809500939866	n
-3.25174258685658	-1.29651376104311	3.88350779857519	h
-6.24599931230460	-1.16126127881121	2.89629109512357	h
-6.23286550233302	3.68261556266773	2.09872053415440	n
-6.20635534686574	4.75598638951114	0.51154070487315	h
-7.97172490335103	3.05821098100030	2.60764995059495	h
-1.23651664931989	4.89046486899728	0.59320897696478	c
-1.97187422082559	6.50876329695316	1.68569736798767	h
-1.96459748212254	5.05940730789431	-1.36237151136330	h
1.67020709845642	5.03375817769202	0.51389464410561	c
2.37819147025099	5.44656302541933	2.43441470148340	h
2.18322266786973	6.65369954586562	-0.70774976488869	h
2.71991717746860	2.65302071875175	-0.40061367077846	n
5.11142827410584	2.51094185287340	-1.03302437076178	c
6.72587189106608	4.56959492051499	-0.95139419465095	n
5.89809814439848	6.29691835607398	-0.99720995298865	h
8.30251238494558	4.45575747317951	-2.03643358240265	h
6.13153021947830	0.27544428540035	-1.77761622783814	n
5.21743058053585	-1.36238085881738	-1.15738814180760	h
8.04335960312788	0.15768425794268	-1.76941758365267	h

### Coordinates in Angstrom

HETATM	1	zn	1	0.089	-0.143	-0.032
HETATM	2	o	1	-2.730	-0.848	-0.930
HETATM	3	o	1	2.144	-2.148	0.140
HETATM	4	o	1	-0.612	-0.683	-1.767
HETATM	5	o	1	0.286	-1.576	1.316
HETATM	6	c	1	-1.886	-0.966	-1.840
HETATM	7	c	1	1.301	-2.345	1.050
HETATM	8	n	1	-2.286	-1.389	-3.109
HETATM	9	h	1	-3.167	-1.889	-3.131
HETATM	10	h	1	-1.553	-1.759	-3.704
HETATM	11	n	1	1.449	-3.438	1.888

HETATM	12	h	1	0.630	-3.732	2.405
HETATM	13	h	1	2.061	-4.170	1.549
HETATM	14	n	1	-1.034	1.314	0.897
HETATM	15	c	1	-2.258	1.067	1.274
HETATM	16	n	1	-2.547	-0.089	1.968
HETATM	17	h	1	-1.721	-0.686	2.055
HETATM	18	h	1	-3.305	-0.615	1.533
HETATM	19	n	1	-3.298	1.949	1.111
HETATM	20	h	1	-3.284	2.517	0.271
HETATM	21	h	1	-4.218	1.618	1.380
HETATM	22	c	1	-0.654	2.588	0.314
HETATM	23	h	1	-1.043	3.444	0.892
HETATM	24	h	1	-1.040	2.677	-0.721
HETATM	25	c	1	0.884	2.664	0.272
HETATM	26	h	1	1.258	2.882	1.288
HETATM	27	h	1	1.155	3.521	-0.375
HETATM	28	n	1	1.439	1.404	-0.212
HETATM	29	c	1	2.705	1.329	-0.547
HETATM	30	n	1	3.559	2.418	-0.503
HETATM	31	h	1	3.121	3.332	-0.528
HETATM	32	h	1	4.393	2.358	-1.078
HETATM	33	n	1	3.245	0.146	-0.941
HETATM	34	h	1	2.761	-0.721	-0.612
HETATM	35	h	1	4.256	0.083	-0.936

## B3LYP/SVP

SCF energy = -2756.1782805940

## Coordinates in bor

0.18909410776431	-0.23723109509706	-0.07077408916454	zn
-5.45674185071442	-1.32881821868116	-1.57236578286500	o
3.73660984475775	-4.23274765174182	0.17517373530613	o
-1.43941022760183	-1.29724506345508	-3.18990561895686	o
0.39346040801665	-2.92307188594988	2.52109282484934	o
-3.87501487519935	-1.68304696944753	-3.29062199447583	c
2.18306758172370	-4.50499955308875	1.95839852981985	c
-4.70117476032459	-2.49263684673131	-5.66092753695003	n
-6.45400907130967	-3.29220869577244	-5.70354169075279	h
-3.37213953234145	-3.25914128186185	-6.82907958878517	h
2.37238997163396	-6.59850741440777	3.51181204754673	n
0.85166950212520	-7.04168846205149	4.60752749755939	h
3.46632535861228	-8.05080461214955	2.87790342667048	h
-1.70225720359774	2.65729717127513	1.69947186361257	n
-4.05051429863616	2.25376477827927	2.38257690836718	c
-4.71488700042363	0.01755141107045	3.56866362654027	n
-3.13048531114801	-1.08629118634400	3.84327788855730	h
-5.89337487976892	-0.96681345766117	2.35438611418923	h

-5.94649794761126	3.99868346724990	2.09364602149411	n
-5.84643001855216	5.17431205593877	0.56686881440927	h
-7.72491891846366	3.41544360734010	2.56093818565345	h
-0.85324013485005	5.01627068118482	0.60633511012291	c
-1.44650011751102	6.69430522304932	1.73505879589332	h
-1.63644779011843	5.26968138341358	-1.34244095020545	h
2.05972556914803	4.95451979995793	0.43245859881373	c
2.86215019584182	5.33725112533161	2.34577898127951	h
2.65744710797758	6.55382425419925	-0.81509573058902	h
2.91405475824276	2.50710349469707	-0.50035691914099	n
5.30867356923407	2.17050593844423	-1.11445462704369	c
7.05174978263539	4.12130326056475	-1.04674260116012	n
6.34755246669788	5.91515450505854	-1.10825781861430	h
8.67745912974415	3.88895867754819	-2.05845694090730	h
6.15870125938980	-0.14894517692032	-1.81178277202142	n
5.10843521525582	-1.72767818980140	-1.17460420637197	h
8.06794949504073	-0.41184938651633	-1.85156274361285	h

### Coordinates in Angstrom

HETATM	1	zn	1	0.100	-0.126	-0.037
HETATM	2	o	1	-2.888	-0.703	-0.832
HETATM	3	o	1	1.977	-2.240	0.093
HETATM	4	o	1	-0.762	-0.686	-1.688
HETATM	5	o	1	0.208	-1.547	1.334
HETATM	6	c	1	-2.051	-0.891	-1.741
HETATM	7	c	1	1.155	-2.384	1.036
HETATM	8	n	1	-2.488	-1.319	-2.996
HETATM	9	h	1	-3.415	-1.742	-3.018
HETATM	10	h	1	-1.784	-1.725	-3.614
HETATM	11	n	1	1.255	-3.492	1.858
HETATM	12	h	1	0.451	-3.726	2.438
HETATM	13	h	1	1.834	-4.260	1.523
HETATM	14	n	1	-0.901	1.406	0.899
HETATM	15	c	1	-2.143	1.193	1.261
HETATM	16	n	1	-2.495	0.009	1.888
HETATM	17	h	1	-1.657	-0.575	2.034
HETATM	18	h	1	-3.119	-0.512	1.246
HETATM	19	n	1	-3.147	2.116	1.108
HETATM	20	h	1	-3.094	2.738	0.300
HETATM	21	h	1	-4.088	1.807	1.355
HETATM	22	c	1	-0.452	2.654	0.321
HETATM	23	h	1	-0.765	3.542	0.918
HETATM	24	h	1	-0.866	2.789	-0.710
HETATM	25	c	1	1.090	2.622	0.229
HETATM	26	h	1	1.515	2.824	1.241
HETATM	27	h	1	1.406	3.468	-0.431
HETATM	28	n	1	1.542	1.327	-0.265
HETATM	29	c	1	2.809	1.149	-0.590
HETATM	30	n	1	3.732	2.181	-0.554
HETATM	31	h	1	3.359	3.130	-0.586

HETATM	32	h	1	4.592	2.058	-1.089
HETATM	33	n	1	3.259	-0.079	-0.959
HETATM	34	h	1	2.703	-0.914	-0.622
HETATM	35	h	1	4.269	-0.218	-0.980

## 6b

### BP/SVP

SCF energy = -3069.1983011220

### Coordinates in bor

-0.03234708307209	0.94980699940924	-0.16641225573834	zn
-2.62817180571522	-2.00402597407019	0.37672970785667	n
-6.09481997173177	-0.21675045944055	2.44171121200286	n
-6.75223943822999	-3.56984607095963	-0.35758545437955	n
-1.43560812715560	-4.34043910031191	-0.47413485852648	c
-1.47819261746650	-4.53038776550418	-2.55552911898422	h
-2.39936641816754	-6.01534795428143	0.31724038601694	h
-5.07315519867768	-1.90554252492848	0.78331935993456	c
-4.44606963165803	3.74221334474291	-1.35620138860951	o
-0.69050126122241	3.00419170149825	-3.19691907951847	o
-2.88504198058763	4.08567169589847	-3.06657712428397	c
-3.44857907384721	5.66316671943625	-5.07815760102279	n
-1.98437811598803	6.28036776621368	-6.14414673556003	h
-4.89861387566650	6.88077682686475	-4.80632756671599	h
0.89065868157742	3.08388100237002	2.69871288430982	o
5.05494109260423	2.11844856018830	2.92020109930870	o
3.16020591775982	3.32263641338313	3.58448794760122	c
3.35397839713126	5.08353982540175	5.51767251890781	n
5.12372328450508	5.66997803484604	5.94580427707660	h
1.94600278301404	6.37042255044489	5.67089268119939	h
-4.50316585956132	1.06943620887752	4.28166636429496	c
-2.92686407881930	-0.15360219192399	4.84025032266714	h
-5.65706255981699	1.51397447527552	5.95960465007362	h
-3.70672646433703	2.82896304056753	3.51066148056789	h
-8.43880956507849	1.11740422615603	1.86227754974534	c
-7.99304797404455	3.07973905201922	1.33230890471125	h
-9.72488850280306	1.09475989154420	3.50494538687783	h
-9.39172326470753	0.24438653750511	0.24526321860937	h
-8.88573536605877	-4.66086696196683	0.97457423893960	c
-8.74591500878115	-4.23427208960460	2.99934215040575	h
-8.89061087822526	-6.73688244462177	0.73841454283648	h
-10.72299674495358	-3.94403775372457	0.27628512083305	h
-6.55339568636599	-4.16595092175168	-3.02737497331000	c
-5.19317737794361	-2.89329934472247	-3.93654590315068	h

-8.40565647774800	-3.88261657086715	-3.95098747841433	h
-5.96564996740846	-6.14153379873849	-3.37600675155471	h
2.50501104174894	-2.04193863995481	-0.69152459831304	n
3.42274337876641	2.31565616895069	-4.54490963858469	h
1.33850206949195	-4.30319614019683	0.34940907869842	c
4.96473478854830	-1.85365289454563	-0.95271563572627	c
4.49980626065610	0.56542540051490	-4.89023716616752	c
1.38977581551951	-4.33243743129484	2.43934620518222	h
2.30381954701933	-6.03497008394172	-0.31114099585893	h
5.96838559397738	-0.23856763717549	-2.70801149794066	n
6.66422036259451	-3.30532014568455	0.39014588324719	n
3.12927164807400	-0.90702790992800	-5.39283671024867	h
5.79785655295759	0.86802023164130	-6.49433189764722	h
8.14301371494856	1.33603731048125	-2.09810330287730	c
9.00787794749523	-4.20779709804028	-0.71205154522926	c
6.35307318898284	-3.71724995947270	3.09119769822241	c
7.61533848812869	3.34431453445671	-2.28337883143012	h
9.75790378706635	0.95949860710615	-3.36919600463304	h
8.69775038245280	1.05251481631564	-0.12510696000334	h
8.94440417698981	-4.01506072157635	-2.77596763384169	h
9.27119987405698	-6.22699184418557	-0.25170293255531	h
10.68205372448272	-3.17533350705763	-0.00219808820508	h
5.01650382245748	-2.32795481482544	3.84609353347988	h
8.17806537963384	-3.38136655725590	4.04273538285649	h
5.73725722191753	-5.66143860640107	3.54766942827069	h

### Coordinates in Angstrom

HETATM	1	zn	1	-0.017	0.503	-0.088
HETATM	2	n	1	-1.391	-1.060	0.199
HETATM	3	n	1	-3.225	-0.115	1.292
HETATM	4	n	1	-3.573	-1.889	-0.189
HETATM	5	c	1	-0.760	-2.297	-0.251
HETATM	6	h	1	-0.782	-2.397	-1.352
HETATM	7	h	1	-1.270	-3.183	0.168
HETATM	8	c	1	-2.685	-1.008	0.415
HETATM	9	o	1	-2.353	1.980	-0.718
HETATM	10	o	1	-0.365	1.590	-1.692
HETATM	11	c	1	-1.527	2.162	-1.623
HETATM	12	n	1	-1.825	2.997	-2.687
HETATM	13	h	1	-1.050	3.323	-3.251
HETATM	14	h	1	-2.592	3.641	-2.543
HETATM	15	o	1	0.471	1.632	1.428
HETATM	16	o	1	2.675	1.121	1.545
HETATM	17	c	1	1.672	1.758	1.897
HETATM	18	n	1	1.775	2.690	2.920
HETATM	19	h	1	2.711	3.000	3.146
HETATM	20	h	1	1.030	3.371	3.001
HETATM	21	c	1	-2.383	0.566	2.266
HETATM	22	h	1	-1.549	-0.081	2.561

HETATM	23	h	1	-2.994	0.801	3.154
HETATM	24	h	1	-1.962	1.497	1.858
HETATM	25	c	1	-4.466	0.591	0.985
HETATM	26	h	1	-4.230	1.630	0.705
HETATM	27	h	1	-5.146	0.579	1.855
HETATM	28	h	1	-4.970	0.129	0.130
HETATM	29	c	1	-4.702	-2.466	0.516
HETATM	30	h	1	-4.628	-2.241	1.587
HETATM	31	h	1	-4.705	-3.565	0.391
HETATM	32	h	1	-5.674	-2.087	0.146
HETATM	33	c	1	-3.468	-2.205	-1.602
HETATM	34	h	1	-2.748	-1.531	-2.083
HETATM	35	h	1	-4.448	-2.055	-2.091
HETATM	36	h	1	-3.157	-3.250	-1.787
HETATM	37	n	1	1.326	-1.081	-0.366
HETATM	38	h	1	1.811	1.225	-2.405
HETATM	39	c	1	0.708	-2.277	0.185
HETATM	40	c	1	2.627	-0.981	-0.504
HETATM	41	c	1	2.381	0.299	-2.588
HETATM	42	h	1	0.735	-2.293	1.291
HETATM	43	h	1	1.219	-3.194	-0.165
HETATM	44	n	1	3.158	-0.126	-1.433
HETATM	45	n	1	3.527	-1.749	0.206
HETATM	46	h	1	1.656	-0.480	-2.854
HETATM	47	h	1	3.068	0.459	-3.437
HETATM	48	c	1	4.309	0.707	-1.110
HETATM	49	c	1	4.767	-2.227	-0.377
HETATM	50	c	1	3.362	-1.967	1.636
HETATM	51	h	1	4.030	1.770	-1.208
HETATM	52	h	1	5.164	0.508	-1.783
HETATM	53	h	1	4.603	0.557	-0.066
HETATM	54	h	1	4.733	-2.125	-1.469
HETATM	55	h	1	4.906	-3.295	-0.133
HETATM	56	h	1	5.653	-1.680	-0.001
HETATM	57	h	1	2.655	-1.232	2.035
HETATM	58	h	1	4.328	-1.789	2.139
HETATM	59	h	1	3.036	-2.996	1.877

## BP/TZVPP

SCF energy = -3072.0735297590

## Coordinates in bor

-0.03210910891534	0.94950108029048	-0.16435232018028	zn
-2.61244601453960	-1.97802048560574	0.40928458963106	n
-6.11832167991709	-0.25137561524889	2.47802008138266	n
-6.72550392360536	-3.58536509668323	-0.35780618325826	n
-1.40870656858674	-4.32968451658241	-0.41641497798478	c
-1.43551139756630	-4.53241392826879	-2.49346280972870	h

-2.37803165614772	-5.98905107000947	0.38898960895145	h
-5.07322746112051	-1.91390922430760	0.80413175419945	c
-4.41917718335761	3.80981067350047	-1.38799179048780	o
-0.68600230367557	2.89992492832243	-3.29378942638530	o
-2.87617973180923	4.02381549520684	-3.15645655205148	c
-3.48109485380654	5.48429439513107	-5.27103579680151	n
-1.99653400600822	6.07588630575046	-6.32777713873982	h
-4.85034752152695	6.78873275012473	-4.96951142799175	h
0.80265307491553	3.19898024061166	2.65819967976946	o
5.03893649989560	2.36937279753118	2.77349330011609	o
3.10061203714576	3.49608401024546	3.49555200666236	c
3.26548369044585	5.23044802234513	5.48684833975787	n
5.02424565082074	5.92507672231362	5.79018041956953	h
1.84081302821291	6.50777755373681	5.59633683431472	h
-4.54799692323766	1.01672374045396	4.35581945075588	c
-2.97209560880822	-0.20770466720177	4.89526143011946	h
-5.71987351765693	1.41121956474636	6.02726308327834	h
-3.76864707941258	2.79807128428223	3.62690507443697	h
-8.46647420965292	1.08272201916611	1.89536228794507	c
-8.02662880932168	3.05052478486471	1.39345719601475	h
-9.74748383935501	1.04262946806570	3.53395634268022	h
-9.40632314822645	0.21330581539876	0.27499495821566	h
-8.91037559349733	-4.65042225945113	0.92055119454088	c
-8.82313434007679	-4.20294109552911	2.93807096146837	h
-8.91437584204844	-6.72214969504779	0.69857906710252	h
-10.71205737297366	-3.92713652705206	0.15578972513376	h
-6.47916429943259	-4.18015536255562	-3.03024599572544	c
-5.08832698734536	-2.92123365280608	-3.89915616509761	h
-8.30713780590824	-3.87346736750521	-3.98109859399676	h
-5.90766236006239	-6.15817066209217	-3.35853095634306	h
2.51922933439298	-2.00928660622434	-0.63038437954831	n
3.60518816360780	2.28847860435892	-4.56292510039378	h
1.35390918412658	-4.27335848696046	0.43664239708733	c
4.99373993501965	-1.87387606015932	-0.89782799730174	c
4.55483252227636	0.46742931363465	-4.88774374516335	c
1.38724202377337	-4.27136877299545	2.52431541425655	h
2.33511948801134	-5.99865602573861	-0.20095012910864	h
6.03426419378244	-0.35295860977712	-2.71441122803456	n
6.65863419460096	-3.30439484064456	0.51070988198535	n
3.09336818462858	-0.93494863674695	-5.30082619060853	h
5.82705541160456	0.64768717391555	-6.52360050344535	h
8.26476689602630	1.17849403578021	-2.17778578262218	c
8.99752430303404	-4.30325541012210	-0.52926694928503	c
6.30235138590606	-3.60766380747685	3.22522780247183	c
7.76336810804361	3.19288199629038	-2.29849802601064	h
9.79498805770257	0.78785249447062	-3.53532322439671	h
8.91601463946045	0.83120539458284	-0.24964759145632	h
8.95957258885409	-4.16925890638441	-2.59351719720368	h
9.19254627085616	-6.30750905068075	-0.00025072304848	h
10.68071546087143	-3.29231577816174	0.17545810897036	h
4.97004573448890	-2.17529064180769	3.89578571389878	h

8.11617184870526 -3.26560946091967 4.18412918645246 h  
5.64623522860499 -5.51852067195371 3.73731131466102 h

### Coordinates in Angstrom

HETATM	1	zn	1	-0.017	0.502	-0.087
HETATM	2	n	1	-1.382	-1.047	0.217
HETATM	3	n	1	-3.238	-0.133	1.311
HETATM	4	n	1	-3.559	-1.897	-0.189
HETATM	5	c	1	-0.745	-2.291	-0.220
HETATM	6	h	1	-0.760	-2.398	-1.319
HETATM	7	h	1	-1.258	-3.169	0.206
HETATM	8	c	1	-2.685	-1.013	0.426
HETATM	9	o	1	-2.339	2.016	-0.734
HETATM	10	o	1	-0.363	1.535	-1.743
HETATM	11	c	1	-1.522	2.129	-1.670
HETATM	12	n	1	-1.842	2.902	-2.789
HETATM	13	h	1	-1.057	3.215	-3.349
HETATM	14	h	1	-2.567	3.592	-2.630
HETATM	15	o	1	0.425	1.693	1.407
HETATM	16	o	1	2.666	1.254	1.468
HETATM	17	c	1	1.641	1.850	1.850
HETATM	18	n	1	1.728	2.768	2.904
HETATM	19	h	1	2.659	3.135	3.064
HETATM	20	h	1	0.974	3.444	2.961
HETATM	21	c	1	-2.407	0.538	2.305
HETATM	22	h	1	-1.573	-0.110	2.590
HETATM	23	h	1	-3.027	0.747	3.189
HETATM	24	h	1	-1.994	1.481	1.919
HETATM	25	c	1	-4.480	0.573	1.003
HETATM	26	h	1	-4.248	1.614	0.737
HETATM	27	h	1	-5.158	0.552	1.870
HETATM	28	h	1	-4.978	0.113	0.146
HETATM	29	c	1	-4.715	-2.461	0.487
HETATM	30	h	1	-4.669	-2.224	1.555
HETATM	31	h	1	-4.717	-3.557	0.370
HETATM	32	h	1	-5.669	-2.078	0.082
HETATM	33	c	1	-3.429	-2.212	-1.604
HETATM	34	h	1	-2.693	-1.546	-2.063
HETATM	35	h	1	-4.396	-2.050	-2.107
HETATM	36	h	1	-3.126	-3.259	-1.777
HETATM	37	n	1	1.333	-1.063	-0.334
HETATM	38	h	1	1.908	1.211	-2.415
HETATM	39	c	1	0.716	-2.261	0.231
HETATM	40	c	1	2.643	-0.992	-0.475
HETATM	41	c	1	2.410	0.247	-2.586
HETATM	42	h	1	0.734	-2.260	1.336
HETATM	43	h	1	1.236	-3.174	-0.106
HETATM	44	n	1	3.193	-0.187	-1.436
HETATM	45	n	1	3.524	-1.749	0.270



HETATM	46	h	1	1.637	-0.495	-2.805
HETATM	47	h	1	3.084	0.343	-3.452
HETATM	48	c	1	4.374	0.624	-1.152
HETATM	49	c	1	4.761	-2.277	-0.280
HETATM	50	c	1	3.335	-1.909	1.707
HETATM	51	h	1	4.108	1.690	-1.216
HETATM	52	h	1	5.183	0.417	-1.871
HETATM	53	h	1	4.718	0.440	-0.132
HETATM	54	h	1	4.741	-2.206	-1.372
HETATM	55	h	1	4.864	-3.338	-0.000
HETATM	56	h	1	5.652	-1.742	0.093
HETATM	57	h	1	2.630	-1.151	2.062
HETATM	58	h	1	4.295	-1.728	2.214
HETATM	59	h	1	2.988	-2.920	1.978

### B3LYP/SVP

SCF energy = -3069.1983011220

### Coordinates in bor

-0.03234708307209	0.94980699940924	-0.16641225573834	zn
-2.62817180571522	-2.00402597407019	0.37672970785667	n
-6.09481997173177	-0.21675045944055	2.44171121200286	n
-6.75223943822999	-3.56984607095963	-0.35758545437955	n
-1.43560812715560	-4.34043910031191	-0.47413485852648	c
-1.47819261746650	-4.53038776550418	-2.55552911898422	h
-2.39936641816754	-6.01534795428143	0.31724038601694	h
-5.07315519867768	-1.90554252492848	0.78331935993456	c
-4.44606963165803	3.74221334474291	-1.35620138860951	o
-0.69050126122241	3.00419170149825	-3.19691907951847	o
-2.88504198058763	4.08567169589847	-3.06657712428397	c
-3.44857907384721	5.66316671943625	-5.07815760102279	n
-1.98437811598803	6.28036776621368	-6.14414673556003	h
-4.89861387566650	6.88077682686475	-4.80632756671599	h
0.89065868157742	3.08388100237002	2.69871288430982	o
5.05494109260423	2.11844856018830	2.92020109930870	o
3.16020591775982	3.32263641338313	3.58448794760122	c
3.35397839713126	5.08353982540175	5.51767251890781	n
5.12372328450508	5.66997803484604	5.94580427707660	h
1.94600278301404	6.37042255044489	5.67089268119939	h
-4.50316585956132	1.06943620887752	4.28166636429496	c
-2.92686407881930	-0.15360219192399	4.84025032266714	h
-5.65706255981699	1.51397447527552	5.95960465007362	h
-3.70672646433703	2.82896304056753	3.51066148056789	h
-8.43880956507849	1.11740422615603	1.86227754974534	c
-7.99304797404455	3.07973905201922	1.33230890471125	h
-9.72488850280306	1.09475989154420	3.50494538687783	h
-9.39172326470753	0.24438653750511	0.24526321860937	h

-8.88573536605877	-4.66086696196683	0.97457423893960	c
-8.74591500878115	-4.23427208960460	2.99934215040575	h
-8.89061087822526	-6.73688244462177	0.73841454283648	h
-10.72299674495358	-3.94403775372457	0.27628512083305	h
-6.55339568636599	-4.16595092175168	-3.02737497331000	c
-5.19317737794361	-2.89329934472247	-3.93654590315068	h
-8.40565647774800	-3.88261657086715	-3.95098747841433	h
-5.96564996740846	-6.14153379873849	-3.37600675155471	h
2.50501104174894	-2.04193863995481	-0.69152459831304	n
3.42274337876641	2.31565616895069	-4.54490963858469	h
1.33850206949195	-4.30319614019683	0.34940907869842	c
4.96473478854830	-1.85365289454563	-0.95271563572627	c
4.49980626065610	0.56542540051490	-4.89023716616752	c
1.38977581551951	-4.33243743129484	2.43934620518222	h
2.30381954701933	-6.03497008394172	-0.31114099585893	h
5.96838559397738	-0.23856763717549	-2.70801149794066	n
6.66422036259451	-3.30532014568455	0.39014588324719	n
3.12927164807400	-0.90702790992800	-5.39283671024867	h
5.79785655295759	0.86802023164130	-6.49433189764722	h
8.14301371494856	1.33603731048125	-2.09810330287730	c
9.00787794749523	-4.20779709804028	-0.71205154522926	c
6.35307318898284	-3.71724995947270	3.09119769822241	c
7.61533848812869	3.34431453445671	-2.28337883143012	h
9.75790378706635	0.95949860710615	-3.36919600463304	h
8.69775038245280	1.05251481631564	-0.12510696000334	h
8.94440417698981	-4.01506072157635	-2.77596763384169	h
9.27119987405698	-6.22699184418557	-0.25170293255531	h
10.68205372448272	-3.17533350705763	-0.00219808820508	h
5.01650382245748	-2.32795481482544	3.84609353347988	h
8.17806537963384	-3.38136655725590	4.04273538285649	h
5.73725722191753	-5.66143860640107	3.54766942827069	h

### Coordinates in Angstrom

HETATM	1	zn	1	-0.017	0.503	-0.088
HETATM	2	n	1	-1.391	-1.060	0.199
HETATM	3	n	1	-3.225	-0.115	1.292
HETATM	4	n	1	-3.573	-1.889	-0.189
HETATM	5	c	1	-0.760	-2.297	-0.251
HETATM	6	h	1	-0.782	-2.397	-1.352
HETATM	7	h	1	-1.270	-3.183	0.168
HETATM	8	c	1	-2.685	-1.008	0.415
HETATM	9	o	1	-2.353	1.980	-0.718
HETATM	10	o	1	-0.365	1.590	-1.692
HETATM	11	c	1	-1.527	2.162	-1.623
HETATM	12	n	1	-1.825	2.997	-2.687
HETATM	13	h	1	-1.050	3.323	-3.251
HETATM	14	h	1	-2.592	3.641	-2.543
HETATM	15	o	1	0.471	1.632	1.428
HETATM	16	o	1	2.675	1.121	1.545

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HETATM	17	c	1	1.672	1.758	1.897
HETATM	18	n	1	1.775	2.690	2.920
HETATM	19	h	1	2.711	3.000	3.146
HETATM	20	h	1	1.030	3.371	3.001
HETATM	21	c	1	-2.383	0.566	2.266
HETATM	22	h	1	-1.549	-0.081	2.561
HETATM	23	h	1	-2.994	0.801	3.154
HETATM	24	h	1	-1.962	1.497	1.858
HETATM	25	c	1	-4.466	0.591	0.985
HETATM	26	h	1	-4.230	1.630	0.705
HETATM	27	h	1	-5.146	0.579	1.855
HETATM	28	h	1	-4.970	0.129	0.130
HETATM	29	c	1	-4.702	-2.466	0.516
HETATM	30	h	1	-4.628	-2.241	1.587
HETATM	31	h	1	-4.705	-3.565	0.391
HETATM	32	h	1	-5.674	-2.087	0.146
HETATM	33	c	1	-3.468	-2.205	-1.602
HETATM	34	h	1	-2.748	-1.531	-2.083
HETATM	35	h	1	-4.448	-2.055	-2.091
HETATM	36	h	1	-3.157	-3.250	-1.787
HETATM	37	n	1	1.326	-1.081	-0.366
HETATM	38	h	1	1.811	1.225	-2.405
HETATM	39	c	1	0.708	-2.277	0.185
HETATM	40	c	1	2.627	-0.981	-0.504
HETATM	41	c	1	2.381	0.299	-2.588
HETATM	42	h	1	0.735	-2.293	1.291
HETATM	43	h	1	1.219	-3.194	-0.165
HETATM	44	n	1	3.158	-0.126	-1.433
HETATM	45	n	1	3.527	-1.749	0.206
HETATM	46	h	1	1.656	-0.480	-2.854
HETATM	47	h	1	3.068	0.459	-3.437
HETATM	48	c	1	4.309	0.707	-1.110
HETATM	49	c	1	4.767	-2.227	-0.377
HETATM	50	c	1	3.362	-1.967	1.636
HETATM	51	h	1	4.030	1.770	-1.208
HETATM	52	h	1	5.164	0.508	-1.783
HETATM	53	h	1	4.603	0.557	-0.066
HETATM	54	h	1	4.733	-2.125	-1.469
HETATM	55	h	1	4.906	-3.295	-0.133
HETATM	56	h	1	5.653	-1.680	-0.001
HETATM	57	h	1	2.655	-1.232	2.035
HETATM	58	h	1	4.328	-1.789	2.139
HETATM	59	h	1	3.036	-2.996	1.877

