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Discrimination of enzyme–substrate complexes by reactivity using the electron density analysis: peptide bond hydrolysis by the matrix metalloproteinase-2

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Coordinates and absolute PBE0/6-31G** energies of the ES complexes from profiles 1-7

Profile 1 ES

ENERGY = -4285.1648011828 au
Atom nuclear charge X Y Z coordinates in Å

C	6.00	12.274	9.949	15.355
O	8.00	11.743	10.871	14.725
H	1.00	11.710	9.164	15.613
N	7.00	13.578	9.948	15.713
H	1.00	13.958	9.086	16.105
C	6.00	14.518	10.865	15.114
H	1.00	14.045	11.418	14.428
C	6.00	15.661	10.104	14.444
O	8.00	16.031	9.001	14.860
H	1.00	14.892	11.462	15.824
N	7.00	16.211	10.744	13.404
H	1.00	15.735	11.565	13.042
C	6.00	17.242	10.174	12.570
H	1.00	17.709	9.438	13.061
C	6.00	18.227	11.279	12.236
O	8.00	17.885	12.467	12.215
H	1.00	16.839	9.812	11.730
N	7.00	19.493	10.892	11.982
H	1.00	19.732	9.920	12.046
C	6.00	20.587	11.811	11.753
H	1.00	20.234	12.745	11.707
H	1.00	21.039	11.583	10.891
H	1.00	21.245	11.740	12.503
C	6.00	10.308	7.864	7.057
H	1.00	10.753	7.366	7.801
H	1.00	10.719	7.597	6.185
N	7.00	10.004	10.309	6.433
H	1.00	9.483	10.152	5.571
C	6.00	10.486	9.327	7.263
C	6.00	10.344	11.507	6.944
H	1.00	10.060	12.451	6.503

N	7.00	11.030	11.345	8.063
C	6.00	11.123	9.991	8.273
H	1.00	11.627	9.571	9.135
H	1.00	9.332	7.645	7.046
C	6.00	12.981	7.081	11.502
H	1.00	12.407	6.911	10.701
H	1.00	12.588	6.619	12.297
C	6.00	13.052	8.572	11.767
O	8.00	13.693	9.054	12.695
O	8.00	12.373	9.279	10.902
H	1.00	13.901	6.728	11.333
C	6.00	17.309	10.848	7.918
H	1.00	17.987	11.327	8.475
H	1.00	17.125	9.950	8.317
N	7.00	15.990	12.919	7.380
H	1.00	16.782	13.431	6.975
C	6.00	16.054	11.639	7.877
C	6.00	14.757	13.401	7.599
H	1.00	14.448	14.401	7.324
N	7.00	14.013	12.499	8.223
C	6.00	14.812	11.397	8.398
H	1.00	14.439	10.525	8.912
H	1.00	17.662	10.734	6.989
C	6.00	11.649	16.765	5.543
H	1.00	11.717	16.145	4.761
H	1.00	12.379	17.447	5.492
N	7.00	11.729	16.568	8.054
H	1.00	11.706	17.572	8.277
C	6.00	11.782	15.988	6.807
C	6.00	11.772	15.602	8.987
H	1.00	11.717	15.766	10.052
N	7.00	11.850	14.419	8.411
C	6.00	11.857	14.643	7.056
H	1.00	11.936	13.830	6.351
H	1.00	10.761	17.225	5.526
C	6.00	14.181	14.002	12.280
O	8.00	14.536	12.833	12.449
H	1.00	14.879	14.673	12.030
N	7.00	12.921	14.427	12.411
H	1.00	12.744	15.433	12.342
C	6.00	11.899	13.588	12.984
H	1.00	11.366	14.170	13.743
H	1.00	12.360	12.732	13.484
C	6.00	10.854	13.084	12.000
O	8.00	10.689	13.591	10.883
N	7.00	10.079	12.127	12.526
H	1.00	10.367	11.684	13.396
C	6.00	8.863	11.668	11.896
H	1.00	8.609	12.425	11.150
C	6.00	9.001	10.313	11.173

H	1.00	9.731	10.491	10.376
C	6.00	9.553	9.226	12.084
H	1.00	9.883	8.368	11.493
H	1.00	10.432	9.580	12.628
H	1.00	8.800	8.904	12.810
C	6.00	7.656	9.931	10.540
H	1.00	6.928	9.734	11.338
H	1.00	7.260	10.792	9.985
C	6.00	7.717	8.732	9.603
H	1.00	6.728	8.506	9.191
H	1.00	8.390	8.933	8.766
H	1.00	8.081	7.836	10.115
C	6.00	7.793	11.608	12.980
O	8.00	8.027	11.055	14.060
N	7.00	6.622	12.188	12.670
H	1.00	6.557	12.657	11.764
C	6.00	5.551	12.377	13.617
H	1.00	5.749	11.863	14.452
H	1.00	4.693	12.050	13.220
H	1.00	5.467	13.349	13.837
Zn	30.00	12.146	12.600	9.194
O	8.00	12.698	11.627	10.734
H	1.00	13.461	11.908	11.259
H	1.00	12.539	10.407	10.933

Profile 2 ES

ENERGY = -4361.5273749449 au
Atom nuclear charge X Y Z coordinates in Å

C	6.00	8.750	5.531	16.758
O	8.00	9.190	4.576	17.392
H	1.00	7.791	5.784	16.887
N	7.00	9.491	6.255	15.898
H	1.00	9.087	7.030	15.385
C	6.00	10.878	5.910	15.637
H	1.00	11.270	5.475	16.448
C	6.00	11.669	7.163	15.306
O	8.00	11.099	8.200	14.936
H	1.00	10.922	5.276	14.865
N	7.00	13.002	7.075	15.470
H	1.00	13.425	6.184	15.733
C	6.00	13.898	8.146	15.095
H	1.00	13.482	8.682	14.360
C	6.00	15.234	7.578	14.611
O	8.00	15.618	6.461	14.958

H	1.00	14.058	8.735	15.887
N	7.00	15.959	8.417	13.845
H	1.00	15.441	9.143	13.359
C	6.00	17.250	8.036	13.299
H	1.00	17.653	7.318	13.866
H	1.00	17.856	8.831	13.289
H	1.00	17.131	7.696	12.366
C	6.00	10.503	5.553	7.377
H	1.00	10.896	5.444	6.464
H	1.00	11.094	5.107	8.049
N	7.00	9.648	7.907	6.973
H	1.00	9.118	7.706	6.120
C	6.00	10.389	7.002	7.700
C	6.00	9.735	9.109	7.568
H	1.00	9.204	9.984	7.230
N	7.00	10.500	9.029	8.645
C	6.00	10.909	7.719	8.741
H	1.00	11.491	7.362	9.580
H	1.00	9.596	5.133	7.401
C	6.00	13.216	5.047	11.756
H	1.00	12.365	4.565	11.549
H	1.00	13.579	4.722	12.630
C	6.00	12.945	6.545	11.843
O	8.00	13.853	7.356	12.091
O	8.00	11.719	6.882	11.631
H	1.00	13.883	4.870	11.032
C	6.00	16.789	9.340	8.765
H	1.00	17.418	10.051	9.081
H	1.00	16.804	8.574	9.407
N	7.00	15.048	10.961	7.890
H	1.00	15.626	11.396	7.166
C	6.00	15.412	9.895	8.686
C	6.00	13.778	11.288	8.170
H	1.00	13.242	12.068	7.653
N	7.00	13.299	10.500	9.118
C	6.00	14.307	9.620	9.445
H	1.00	14.183	8.875	10.221
H	1.00	17.073	9.022	7.860
C	6.00	10.489	14.808	6.306
H	1.00	11.237	15.469	6.245
H	1.00	10.470	14.250	5.476
N	7.00	10.767	14.417	8.777
H	1.00	10.660	15.387	9.074
C	6.00	10.697	13.927	7.494
C	6.00	10.895	13.390	9.634
H	1.00	10.950	13.511	10.703
N	7.00	10.910	12.244	8.974
C	6.00	10.787	12.565	7.640
H	1.00	10.797	11.810	6.869
H	1.00	9.621	15.295	6.400

C	6.00	13.573	11.591	12.985
O	8.00	13.899	10.403	12.938
H	1.00	14.288	12.281	12.870
N	7.00	12.315	12.010	13.181
H	1.00	12.123	13.009	13.297
C	6.00	11.286	11.108	13.636
H	1.00	10.729	11.610	14.434
H	1.00	11.728	10.201	14.059
C	6.00	10.259	10.707	12.593
O	8.00	10.115	11.323	11.512
N	7.00	9.450	9.734	12.990
H	1.00	9.698	9.188	13.814
C	6.00	8.238	9.396	12.278
H	1.00	8.001	10.257	11.647
C	6.00	8.368	8.164	11.362
H	1.00	9.227	8.382	10.718
C	6.00	8.677	6.887	12.128
H	1.00	7.793	6.511	12.651
H	1.00	9.039	6.128	11.434
H	1.00	9.483	7.047	12.848
C	6.00	7.124	8.038	10.473
H	1.00	6.226	7.971	11.102
H	1.00	7.015	8.959	9.885
C	6.00	7.158	6.850	9.519
H	1.00	8.069	6.857	8.913
H	1.00	7.125	5.897	10.057
H	1.00	6.304	6.881	8.834
C	6.00	7.165	9.220	13.341
O	8.00	7.392	8.584	14.377
N	7.00	5.995	9.817	13.059
H	1.00	5.929	10.366	12.203
C	6.00	4.905	9.866	14.001
H	1.00	5.114	9.280	14.784
H	1.00	4.067	9.545	13.559
H	1.00	4.776	10.807	14.314
Zn	30.00	11.367	10.427	9.823
O	8.00	11.899	9.290	11.350
H	1.00	12.738	9.455	11.818
H	1.00	11.743	8.228	11.509
O	8.00	9.058	13.941	11.982
H	1.00	9.135	13.030	11.668
H	1.00	8.813	13.834	12.927

Profile 3 ES

ENERGY = -4361.5172348147 au
Atom nuclear charge X Y Z coordinates in Å

C	6.00	12.154	9.674	15.325

O	8.00	11.633	10.710	14.892
H	1.00	11.562	8.926	15.624
N	7.00	13.491	9.518	15.408
H	1.00	13.884	8.620	15.698
C	6.00	14.402	10.477	14.816
H	1.00	13.952	10.926	14.044
C	6.00	15.667	9.773	14.322
O	8.00	16.018	8.688	14.789
H	1.00	14.652	11.161	15.501
N	7.00	16.373	10.444	13.391
H	1.00	15.894	11.182	12.885
C	6.00	17.551	9.855	12.786
H	1.00	18.068	9.344	13.472
C	6.00	18.399	10.991	12.238
O	8.00	17.915	12.094	11.971
H	1.00	17.283	9.241	12.044
N	7.00	19.716	10.739	12.084
H	1.00	20.052	9.817	12.293
C	6.00	20.709	11.738	11.732
H	1.00	20.255	12.609	11.547
H	1.00	21.206	11.442	10.916
H	1.00	21.351	11.852	12.490
C	6.00	10.355	7.383	7.570
H	1.00	10.667	7.159	6.647
H	1.00	10.942	6.928	8.239
N	7.00	9.733	9.778	7.022
H	1.00	9.128	9.569	6.219
C	6.00	10.420	8.857	7.773
C	6.00	10.005	11.006	7.487
H	1.00	9.556	11.905	7.094
N	7.00	10.843	10.928	8.512
C	6.00	11.100	9.592	8.704
H	1.00	11.698	9.245	9.536
H	1.00	9.412	7.071	7.687
C	6.00	13.178	7.135	11.914
H	1.00	12.266	6.750	11.776
H	1.00	13.523	6.861	12.812
C	6.00	13.105	8.652	11.839
O	8.00	14.111	9.365	11.979
O	8.00	11.926	9.120	11.612
H	1.00	13.794	6.795	11.203
C	6.00	17.315	10.643	8.423
H	1.00	18.026	11.315	8.633
H	1.00	17.314	9.929	9.124
N	7.00	15.676	12.346	7.536
H	1.00	16.255	12.646	6.743
C	6.00	15.985	11.317	8.398
C	6.00	14.430	12.764	7.789
H	1.00	13.920	13.518	7.209
N	7.00	13.918	12.081	8.800

C	6.00	14.878	11.174	9.195
H	1.00	14.712	10.516	10.041
H	1.00	17.498	10.232	7.530
C	6.00	11.179	16.478	5.974
H	1.00	11.033	15.877	5.188
H	1.00	11.977	17.057	5.806
N	7.00	11.642	16.204	8.435
H	1.00	11.773	17.206	8.613
C	6.00	11.411	15.652	7.198
C	6.00	11.760	15.223	9.345
H	1.00	11.909	15.376	10.403
N	7.00	11.613	14.047	8.756
C	6.00	11.397	14.299	7.420
H	1.00	11.263	13.504	6.703
H	1.00	10.372	17.053	6.108
C	6.00	14.192	13.748	12.443
O	8.00	14.456	12.542	12.470
H	1.00	14.922	14.378	12.178
N	7.00	12.997	14.270	12.744
H	1.00	12.849	15.276	12.598
C	6.00	11.961	13.511	13.402
H	1.00	11.590	14.108	14.242
H	1.00	12.380	12.590	13.811
C	6.00	10.755	13.187	12.535
O	8.00	10.478	13.865	11.533
N	7.00	9.986	12.210	13.016
H	1.00	10.335	11.647	13.789
C	6.00	8.740	11.825	12.388
H	1.00	8.508	12.610	11.665
C	6.00	8.838	10.479	11.638
H	1.00	9.685	10.599	10.952
C	6.00	9.153	9.324	12.572
H	1.00	9.540	8.487	11.993
H	1.00	9.941	9.589	13.278
H	1.00	8.265	9.013	13.129
C	6.00	7.574	10.219	10.807
H	1.00	6.684	10.319	11.443
H	1.00	7.487	11.000	10.044
C	6.00	7.548	8.857	10.123
H	1.00	8.456	8.698	9.532
H	1.00	7.476	8.041	10.850
H	1.00	6.694	8.779	9.445
C	6.00	7.688	11.792	13.486
O	8.00	7.928	11.252	14.573
N	7.00	6.529	12.396	13.186
H	1.00	6.430	12.801	12.252
C	6.00	5.449	12.548	14.130
H	1.00	5.693	12.102	14.991
H	1.00	4.621	12.127	13.760
H	1.00	5.284	13.520	14.294

Zn	30.00	12.017	12.226	9.480
O	8.00	12.257	11.478	11.220
H	1.00	13.127	11.633	11.635
H	1.00	12.052	10.400	11.438
O	8.00	8.894	15.911	12.698
H	1.00	9.241	15.159	12.194
H	1.00	9.367	16.669	12.305

Profile 4 ES

ENERGY = -4361.5173654822 au
Atom nuclear charge X Y Z coordinates in Å

C	6.00	9.571	8.809	16.986
O	8.00	9.964	7.884	17.696
H	1.00	8.613	9.087	17.058
N	7.00	10.359	9.464	16.121
H	1.00	9.988	10.196	15.524
C	6.00	11.753	9.082	15.951
H	1.00	12.123	8.780	16.829
C	6.00	12.555	10.267	15.448
O	8.00	12.012	11.209	14.859
H	1.00	11.814	8.335	15.289
N	7.00	13.875	10.224	15.725
H	1.00	14.258	9.353	16.091
C	6.00	14.813	11.121	15.092
H	1.00	14.347	11.629	14.367
C	6.00	15.971	10.327	14.489
O	8.00	16.314	9.228	14.944
H	1.00	15.170	11.761	15.773
N	7.00	16.563	10.931	13.450
H	1.00	16.104	11.741	13.043
C	6.00	17.603	10.308	12.665
H	1.00	17.977	9.528	13.166
H	1.00	18.331	10.971	12.489
H	1.00	17.222	9.994	11.795
C	6.00	10.361	8.070	7.186
H	1.00	10.715	7.823	6.284
H	1.00	10.869	7.574	7.890
N	7.00	9.954	10.510	6.611
H	1.00	9.380	10.342	5.780
C	6.00	10.520	9.537	7.398
C	6.00	10.296	11.713	7.106
H	1.00	9.963	12.648	6.683
N	7.00	11.060	11.566	8.179
C	6.00	11.201	10.214	8.372
H	1.00	11.756	9.810	9.209
H	1.00	9.392	7.828	7.241

C	6.00	13.030	7.408	11.693
H	1.00	12.351	7.228	10.981
H	1.00	12.744	6.969	12.545
C	6.00	13.150	8.905	11.911
O	8.00	13.913	9.402	12.730
O	8.00	12.373	9.595	11.115
H	1.00	13.916	7.040	11.410
C	6.00	17.443	11.141	8.148
H	1.00	18.115	11.671	8.665
H	1.00	17.277	10.271	8.613
N	7.00	16.063	13.143	7.473
H	1.00	16.831	13.665	7.028
C	6.00	16.173	11.905	8.057
C	6.00	14.815	13.594	7.662
H	1.00	14.459	14.548	7.303
N	7.00	14.103	12.715	8.351
C	6.00	14.941	11.657	8.600
H	1.00	14.603	10.812	9.179
H	1.00	17.793	10.965	7.228
C	6.00	11.681	16.948	5.608
H	1.00	12.436	17.595	5.506
H	1.00	11.685	16.307	4.840
N	7.00	11.873	16.794	8.123
H	1.00	11.961	17.796	8.341
C	6.00	11.840	16.197	6.883
C	6.00	11.895	15.832	9.063
H	1.00	11.904	16.015	10.124
N	7.00	11.881	14.640	8.497
C	6.00	11.847	14.852	7.141
H	1.00	11.837	14.030	6.441
H	1.00	10.814	17.447	5.620
C	6.00	14.549	14.212	12.213
O	8.00	14.894	13.038	12.375
H	1.00	15.250	14.879	11.959
N	7.00	13.288	14.643	12.358
H	1.00	13.080	15.630	12.168
C	6.00	12.288	13.835	13.014
H	1.00	11.819	14.459	13.782
H	1.00	12.761	12.987	13.510
C	6.00	11.154	13.345	12.129
O	8.00	10.850	13.939	11.074
N	7.00	10.399	12.386	12.671
H	1.00	10.731	11.908	13.507
C	6.00	9.138	11.992	12.079
H	1.00	8.896	12.765	11.345
C	6.00	9.200	10.636	11.342
H	1.00	10.018	10.745	10.622
C	6.00	9.556	9.489	12.275
H	1.00	9.910	8.635	11.693
H	1.00	10.373	9.767	12.946

H	1.00	8.695	9.188	12.880
C	6.00	7.895	10.403	10.568
H	1.00	7.041	10.448	11.257
H	1.00	7.759	11.236	9.867
C	6.00	7.833	9.095	9.792
H	1.00	6.941	9.062	9.158
H	1.00	8.705	8.984	9.145
H	1.00	7.796	8.229	10.458
C	6.00	8.083	11.968	13.176
O	8.00	8.323	11.470	14.281
N	7.00	6.898	12.510	12.835
H	1.00	6.809	12.916	11.902
C	6.00	5.793	12.641	13.751
H	1.00	6.023	12.198	14.618
H	1.00	4.982	12.206	13.360
H	1.00	5.606	13.610	13.912
Zn	30.00	12.238	12.823	9.253
O	8.00	12.766	11.934	10.857
H	1.00	13.616	12.158	11.266
H	1.00	12.571	10.704	11.098
O	8.00	10.360	16.309	12.526
H	1.00	10.272	17.050	11.899
H	1.00	10.387	15.531	11.946

Profile 5 ES

ENERGY = -4361.5228109905 au
Atom nuclear charge X Y Z coordinates in Å

C	6.00	8.500	6.775	16.600
O	8.00	8.879	5.751	17.162
H	1.00	7.544	7.050	16.702
N	7.00	9.314	7.544	15.853
H	1.00	8.979	8.382	15.396
C	6.00	10.710	7.175	15.691
H	1.00	11.037	6.743	16.532
C	6.00	11.548	8.404	15.402
O	8.00	11.057	9.405	14.862
H	1.00	10.795	6.531	14.930
N	7.00	12.841	8.308	15.769
H	1.00	13.201	7.415	16.111
C	6.00	13.819	9.310	15.420
H	1.00	13.434	9.924	14.731
C	6.00	15.069	8.638	14.858
O	8.00	15.375	7.486	15.176
H	1.00	14.062	9.835	16.236
N	7.00	15.793	9.388	14.014
H	1.00	15.420	10.281	13.713

C	6.00	17.016	8.892	13.421
H	1.00	17.247	8.006	13.824
H	1.00	17.758	9.540	13.594
H	1.00	16.890	8.786	12.435
C	6.00	10.254	6.323	7.270
H	1.00	10.613	6.145	6.354
H	1.00	10.876	5.938	7.952
N	7.00	9.357	8.633	6.715
H	1.00	8.842	8.382	5.867
C	6.00	10.135	7.792	7.480
C	6.00	9.420	9.870	7.242
H	1.00	8.860	10.707	6.858
N	7.00	10.202	9.873	8.310
C	6.00	10.650	8.584	8.468
H	1.00	11.276	8.304	9.301
H	1.00	9.353	5.898	7.363
C	6.00	13.049	6.063	11.776
H	1.00	12.188	5.579	11.621
H	1.00	13.413	5.814	12.673
C	6.00	12.806	7.558	11.726
O	8.00	13.679	8.409	11.882
O	8.00	11.549	7.858	11.484
H	1.00	13.706	5.808	11.067
C	6.00	16.491	10.101	8.488
H	1.00	17.114	10.793	8.853
H	1.00	16.436	9.333	9.126
N	7.00	14.844	11.769	7.499
H	1.00	15.448	12.152	6.763
C	6.00	15.142	10.694	8.308
C	6.00	13.563	12.116	7.711
H	1.00	13.066	12.928	7.201
N	7.00	13.020	11.334	8.629
C	6.00	13.993	10.439	9.003
H	1.00	13.820	9.693	9.766
H	1.00	16.834	9.777	7.606
C	6.00	10.433	15.424	5.700
H	1.00	11.240	16.002	5.583
H	1.00	10.346	14.810	4.915
N	7.00	10.712	15.196	8.186
H	1.00	10.796	16.199	8.393
C	6.00	10.574	14.620	6.947
C	6.00	10.735	14.233	9.118
H	1.00	10.813	14.415	10.175
N	7.00	10.620	13.044	8.551
C	6.00	10.519	13.271	7.197
H	1.00	10.424	12.460	6.492
H	1.00	9.618	16.000	5.764
C	6.00	13.795	12.796	12.921
O	8.00	14.258	11.980	13.721
H	1.00	14.431	13.428	12.479

N	7.00	12.492	12.892	12.604
H	1.00	12.194	13.727	12.086
C	6.00	11.470	12.111	13.261
H	1.00	11.102	12.634	14.156
H	1.00	11.881	11.159	13.603
C	6.00	10.274	11.852	12.362
O	8.00	10.116	12.465	11.283
N	7.00	9.361	11.017	12.856
H	1.00	9.597	10.465	13.678
C	6.00	8.146	10.693	12.130
H	1.00	7.943	11.536	11.463
C	6.00	8.298	9.414	11.271
H	1.00	9.192	9.594	10.662
C	6.00	8.548	8.170	12.113
H	1.00	7.634	7.845	12.620
H	1.00	8.912	7.363	11.474
H	1.00	9.321	8.343	12.864
C	6.00	7.100	9.257	10.325
H	1.00	6.166	9.292	10.902
H	1.00	7.072	10.121	9.650
C	6.00	7.125	7.980	9.494
H	1.00	6.966	7.091	10.114
H	1.00	6.342	8.006	8.730
H	1.00	8.085	7.858	8.985
C	6.00	7.016	10.535	13.137
O	8.00	7.193	9.896	14.178
N	7.00	5.837	11.090	12.791
H	1.00	5.797	11.642	11.939
C	6.00	4.701	11.066	13.685
H	1.00	4.905	10.479	14.469
H	1.00	3.903	10.708	13.201
H	1.00	4.508	11.994	14.005
Zn	30.00	11.124	11.294	9.450
O	8.00	11.631	10.230	10.972
H	1.00	12.529	10.361	11.296
H	1.00	11.500	8.928	11.312
O	8.00	8.441	14.682	11.299
H	1.00	8.890	13.836	11.137
H	1.00	8.615	14.844	12.247

Profile 6 ES

ENERGY = -4361.5273749449
Atom nuclear charge X Y Z coordinates in Å

C	6.00	8.750	5.531	16.758
O	8.00	9.190	4.576	17.392
H	1.00	7.791	5.784	16.887
N	7.00	9.491	6.255	15.898

H	1.00	9.087	7.030	15.385
C	6.00	10.878	5.910	15.637
H	1.00	11.270	5.475	16.448
C	6.00	11.669	7.163	15.306
O	8.00	11.099	8.200	14.936
H	1.00	10.922	5.276	14.865
N	7.00	13.002	7.075	15.470
H	1.00	13.425	6.184	15.733
C	6.00	13.898	8.146	15.095
H	1.00	13.482	8.682	14.360
C	6.00	15.234	7.578	14.611
O	8.00	15.618	6.461	14.958
H	1.00	14.058	8.735	15.887
N	7.00	15.959	8.417	13.845
H	1.00	15.441	9.143	13.359
C	6.00	17.250	8.036	13.299
H	1.00	17.653	7.318	13.866
H	1.00	17.856	8.831	13.289
H	1.00	17.131	7.696	12.366
C	6.00	10.503	5.553	7.377
H	1.00	10.896	5.444	6.464
H	1.00	11.094	5.107	8.049
N	7.00	9.648	7.907	6.973
H	1.00	9.118	7.706	6.120
C	6.00	10.389	7.002	7.700
C	6.00	9.735	9.109	7.568
H	1.00	9.204	9.984	7.230
N	7.00	10.500	9.029	8.645
C	6.00	10.909	7.719	8.741
H	1.00	11.491	7.362	9.580
H	1.00	9.596	5.133	7.401
C	6.00	13.216	5.047	11.756
H	1.00	12.365	4.565	11.549
H	1.00	13.579	4.722	12.630
C	6.00	12.945	6.545	11.843
O	8.00	13.853	7.356	12.091
O	8.00	11.719	6.882	11.631
H	1.00	13.883	4.870	11.032
C	6.00	16.789	9.340	8.765
H	1.00	17.418	10.051	9.081
H	1.00	16.804	8.574	9.407
N	7.00	15.048	10.961	7.890
H	1.00	15.626	11.396	7.166
C	6.00	15.412	9.895	8.686
C	6.00	13.778	11.288	8.170
H	1.00	13.242	12.068	7.653
N	7.00	13.299	10.500	9.118
C	6.00	14.307	9.620	9.445
H	1.00	14.183	8.875	10.221
H	1.00	17.073	9.022	7.860

C	6.00	10.489	14.808	6.306
H	1.00	11.237	15.469	6.245
H	1.00	10.470	14.250	5.476
N	7.00	10.767	14.417	8.777
H	1.00	10.660	15.387	9.074
C	6.00	10.697	13.927	7.494
C	6.00	10.895	13.390	9.634
H	1.00	10.950	13.511	10.703
N	7.00	10.910	12.244	8.974
C	6.00	10.787	12.565	7.640
H	1.00	10.797	11.810	6.869
H	1.00	9.621	15.295	6.400
C	6.00	13.573	11.591	12.985
O	8.00	13.899	10.403	12.938
H	1.00	14.288	12.281	12.870
N	7.00	12.315	12.010	13.181
H	1.00	12.123	13.009	13.297
C	6.00	11.286	11.108	13.636
H	1.00	10.729	11.610	14.434
H	1.00	11.728	10.201	14.059
C	6.00	10.259	10.707	12.593
O	8.00	10.115	11.323	11.512
N	7.00	9.450	9.734	12.990
H	1.00	9.698	9.188	13.814
C	6.00	8.238	9.396	12.278
H	1.00	8.001	10.257	11.647
C	6.00	8.368	8.164	11.362
H	1.00	9.227	8.382	10.718
C	6.00	8.677	6.887	12.128
H	1.00	7.793	6.511	12.651
H	1.00	9.039	6.128	11.434
H	1.00	9.483	7.047	12.848
C	6.00	7.124	8.038	10.473
H	1.00	6.226	7.971	11.102
H	1.00	7.015	8.959	9.885
C	6.00	7.158	6.850	9.519
H	1.00	8.069	6.857	8.913
H	1.00	7.125	5.897	10.057
H	1.00	6.304	6.881	8.834
C	6.00	7.165	9.220	13.341
O	8.00	7.392	8.584	14.377
N	7.00	5.995	9.817	13.059
H	1.00	5.929	10.366	12.203
C	6.00	4.905	9.866	14.001
H	1.00	5.114	9.280	14.784
H	1.00	4.067	9.545	13.559
H	1.00	4.776	10.807	14.314
Zn	30.00	11.367	10.427	9.823
O	8.00	11.899	9.290	11.350
H	1.00	12.738	9.455	11.818

H	1.00	11.743	8.228	11.509
O	8.00	9.058	13.941	11.982
H	1.00	9.135	13.030	11.668
H	1.00	8.813	13.834	12.927

Profile 7 ES

ENERGY = -4361.5273080473 au
Atom nuclear charge X Y Z coordinates in Å

C	6.00	63.170	21.234	13.225
O	8.00	62.545	22.166	12.718
H	1.00	62.647	20.440	13.537
N	7.00	64.507	21.206	13.390
H	1.00	64.941	20.363	13.763
C	6.00	65.381	22.194	12.796
H	1.00	64.949	22.565	11.974
C	6.00	66.714	21.562	12.422
O	8.00	67.144	20.566	13.019
H	1.00	65.538	22.932	13.452
N	7.00	67.388	22.222	11.472
H	1.00	66.873	22.884	10.902
C	6.00	68.665	21.774	10.981
H	1.00	69.111	21.214	11.679
C	6.00	69.541	22.970	10.659
O	8.00	69.090	24.035	10.226
H	1.00	68.530	21.229	10.153
N	7.00	70.856	22.754	10.878
H	1.00	71.116	21.855	11.279
C	6.00	71.876	23.745	10.672
H	1.00	71.468	24.567	10.275
H	1.00	72.571	23.384	10.050
H	1.00	72.300	23.974	11.548
C	6.00	61.818	19.299	5.303
H	1.00	62.422	18.904	5.995
H	1.00	62.175	19.091	4.392
N	7.00	61.010	21.624	4.700
H	1.00	60.466	21.354	3.872
C	6.00	61.752	20.774	5.485
C	6.00	61.132	22.873	5.181
H	1.00	60.620	23.727	4.766
N	7.00	61.926	22.873	6.243
C	6.00	62.316	21.570	6.441
H	1.00	62.925	21.277	7.283
H	1.00	60.902	18.910	5.399
C	6.00	64.487	18.973	9.745
H	1.00	63.607	18.530	9.576
H	1.00	64.824	18.711	10.649
C	6.00	64.314	20.487	9.686

O	8.00	65.282	21.255	9.867
O	8.00	63.124	20.887	9.429
H	1.00	65.144	18.685	9.048
C	6.00	68.185	22.865	6.537
H	1.00	68.814	23.531	6.938
H	1.00	68.072	22.095	7.164
N	7.00	66.640	24.599	5.489
H	1.00	67.288	24.978	4.791
C	6.00	66.868	23.508	6.299
C	6.00	65.373	25.008	5.675
H	1.00	64.949	25.872	5.186
N	7.00	64.769	24.248	6.574
C	6.00	65.691	23.301	6.960
H	1.00	65.469	22.552	7.707
H	1.00	68.557	22.536	5.669
C	6.00	62.007	28.114	3.176
H	1.00	62.671	28.858	3.100
H	1.00	62.169	27.448	2.448
N	7.00	61.989	28.119	5.700
H	1.00	61.669	29.085	5.830
C	6.00	62.156	27.445	4.509
C	6.00	62.139	27.258	6.720
H	1.00	62.083	27.548	7.762
N	7.00	62.400	26.045	6.261
C	6.00	62.406	26.149	4.885
H	1.00	62.588	25.292	4.254
H	1.00	61.082	28.483	3.089
C	6.00	65.095	25.611	10.378
O	8.00	65.591	24.492	10.507
H	1.00	65.688	26.343	10.042
N	7.00	63.817	25.924	10.654
H	1.00	63.414	26.818	10.351
C	6.00	62.861	24.944	11.117
H	1.00	62.309	25.361	11.966
H	1.00	63.375	24.051	11.473
C	6.00	61.821	24.539	10.084
O	8.00	61.673	25.167	9.002
N	7.00	61.017	23.570	10.482
H	1.00	61.205	23.093	11.362
C	6.00	59.767	23.267	9.817
H	1.00	59.574	24.100	9.135
C	6.00	59.799	21.974	8.984
H	1.00	60.672	22.077	8.330
C	6.00	60.000	20.727	9.829
H	1.00	60.847	20.831	10.511
H	1.00	59.096	20.489	10.398
H	1.00	60.227	19.890	9.166
C	6.00	58.550	21.894	8.099
H	1.00	57.647	21.924	8.724
H	1.00	58.517	22.793	7.471

C	6.00	58.498	20.666	7.207
H	1.00	58.340	19.744	7.773
H	1.00	57.687	20.740	6.479
H	1.00	59.423	20.536	6.641
C	6.00	58.713	23.226	10.914
O	8.00	58.958	22.711	12.009
N	7.00	57.540	23.791	10.585
H	1.00	57.421	24.153	9.646
C	6.00	56.446	23.896	11.520
H	1.00	56.716	23.497	12.396
H	1.00	55.652	23.405	11.161
H	1.00	56.210	24.859	11.651
Zn	30.00	62.821	24.317	7.309
O	8.00	63.483	23.221	8.872
H	1.00	64.362	23.334	9.260
H	1.00	63.238	22.197	9.154
O	8.00	61.941	27.772	9.815
H	1.00	61.291	28.500	9.907
H	1.00	61.427	26.984	9.580