

Python 3.6 code to extract QM/MM optimised xyz coordinates from the orca output file (for the structures reported in Figure 6)
with open('orca1.out','r') as file:

```

for line in file:

    if 'CARTESIAN COORDINATES (ANGSTROEM)' in line:
        next(file)

    for line in file:

        if '-----' in line:
            break

        symbol,x,y,z =line.split()

        print(f'{symbol } {x}      {y}      {z}')
```

Cluster 1
RC M=5

C	42.310108	54.485299	33.832495
H	42.309792	54.754320	34.899462
H	41.841960	55.326840	33.297448
C	41.522077	53.222050	33.662774
N	40.913007	52.831257	32.481412
H	40.916425	53.357788	31.604409
C	40.305971	51.638534	32.682649
H	39.749310	51.087973	31.927845
N	40.480995	51.246736	33.936535
C	41.230747	52.218311	34.563298
H	41.504289	52.128168	35.610672
C	42.007082	49.401754	38.692424
H	42.813023	48.764354	39.079909
H	41.148256	49.304873	39.379727
C	41.561804	48.831574	37.343344
O	41.075956	49.622436	36.463785
O	41.650991	47.587591	37.216365
C	44.401119	48.549701	31.102573
H	43.845545	47.940005	30.374044
H	45.344816	48.017769	31.306363
C	43.579694	48.710653	32.340877
N	44.104783	49.083825	33.565247
H	45.092001	49.256547	33.795690
C	43.097035	49.187206	34.450124
H	43.226139	49.494695	35.480052
N	41.942106	48.888856	33.868577
C	42.222484	48.583946	32.553603
H	41.427457	48.305936	31.866649
C	36.625272	45.195974	31.154356
O	35.439578	45.577553	31.302450
O	36.997236	44.094777	30.674420
C	37.745306	46.218362	31.528416
C	37.417330	47.067000	32.771457
C	37.970835	48.486383	32.780308
O	39.255899	48.639872	32.996628
O	37.215290	49.440033	32.575743
H	38.707329	45.694421	31.623777
H	37.829589	46.877902	30.647005

H	36.322903	47.143791	32.817225
H	37.779893	46.548287	33.673864
O	38.629347	49.646751	35.368588
Fe	40.042580	49.269039	34.657211
O	39.985549	47.221278	35.317831
H	39.136834	47.135727	35.775544
H	40.689199	47.211437	36.048337
O	33.081364	51.056089	36.783760
C	33.877209	50.697259	35.863696
O	33.579826	50.664096	34.643428
C	35.312499	50.295168	36.256756
N	35.903518	51.199541	37.254431
C	35.392768	48.826036	36.733591
C	34.578512	48.557675	38.005559
C	35.017500	47.857299	35.610091
H	35.921917	50.365488	35.343053
H	36.464155	48.683705	36.964515
H	34.656385	47.498101	38.300540
H	34.932636	49.162510	38.856226
H	33.513281	48.785818	37.848853
H	35.906158	52.146526	36.865058
H	35.273318	51.248712	38.057581
H	35.140177	46.810389	35.931384
H	33.972073	47.989159	35.290949
H	35.651459	48.014262	34.726896
H	43.338989	54.450958	33.474318
H	42.340798	50.439373	38.699234
H	44.686249	49.485312	30.621533
TS1 M=5			
C	42.196964	54.398651	33.902032
H	42.212299	54.688058	34.963662
H	41.703265	55.223345	33.363850
C	41.412199	53.125476	33.779893
N	40.832103	52.674924	32.604150
H	40.884063	53.140874	31.697946
C	40.173659	51.520227	32.860984
H	39.634131	50.934398	32.120276
N	40.280187	51.203716	34.144895
C	41.048869	52.191408	34.731226
H	41.299516	52.154690	35.788330
C	42.053592	49.358102	38.770622
H	42.877803	48.749424	39.162924
H	41.197891	49.256483	39.461350
C	41.618988	48.772328	37.425249
O	41.007764	49.533684	36.601686
O	41.836971	47.551305	37.244140
C	44.352989	48.558614	31.160372
H	43.790271	47.945268	30.440038
H	45.294550	48.021694	31.362771
C	43.538766	48.730931	32.403101
N	44.069837	49.127262	33.616882
H	45.056314	49.315652	33.833900
C	43.064717	49.213105	34.511660
H	43.204158	49.522791	35.539959
N	41.910337	48.883795	33.952713
C	42.186197	48.576203	32.638201
H	41.392768	48.270900	31.960343
C	36.571606	45.171742	31.165789

O	35.380292	45.541188	31.305413
O	36.957961	44.078272	30.680097
C	37.674279	46.200856	31.562876
C	37.318288	47.027505	32.812062
C	37.868560	48.447275	32.842453
O	39.124366	48.609859	33.132910
O	37.120228	49.400368	32.576244
H	38.642073	45.688432	31.662253
H	37.759232	46.874097	30.691356
H	36.222813	47.089986	32.837355
H	37.667449	46.500207	33.714642
O	38.397164	49.206314	35.784758
Fe	39.892639	49.134963	34.869067
O	40.133982	47.043535	35.371553
H	39.325602	46.874022	35.877197
H	40.869720	47.096349	36.062714
O	33.335874	51.115107	36.673375
C	34.069448	50.834569	35.680720
O	33.662803	50.716668	34.500796
C	35.599261	50.638277	35.911880
N	36.171961	51.636583	36.819063
C	35.875367	49.217889	36.411291
C	35.549171	49.048973	37.886805
C	35.312189	48.122006	35.529313
H	36.070133	50.742922	34.924599
H	37.107301	49.160688	36.217004
H	35.474062	47.991394	38.175832
H	36.269572	49.560524	38.541258
H	34.556669	49.495146	38.076408
H	36.315124	52.508642	36.303071
H	35.495118	51.839427	37.556536
H	35.724289	47.139776	35.810147
H	34.213778	48.057704	35.628994
H	35.542296	48.299823	34.474285
H	43.220626	54.395604	33.527633
H	42.359047	50.404278	38.753869
H	44.645644	49.484697	30.665608
IM1 M=5			
C	42.325149	54.471985	33.810719
H	42.312812	54.738946	34.878136
H	41.852046	55.308623	33.272488
C	41.558394	53.197546	33.630144
N	40.969520	52.800506	32.441001
H	40.969312	53.333442	31.567956
C	40.395367	51.589180	32.628959
H	39.865672	51.031692	31.859766
N	40.570036	51.190696	33.880544
C	41.286116	52.179560	34.519955
H	41.552058	52.090494	35.569821
C	42.055539	49.375233	38.723657
H	42.871930	48.756076	39.117933
H	41.198820	49.270011	39.412386
C	41.620921	48.787005	37.380458
O	41.144152	49.564248	36.483977
O	41.705857	47.541824	37.265418
C	44.457296	48.537530	31.042149
H	43.894348	47.939012	30.310120
H	45.410629	48.010599	31.212863

C	43.661129	48.655517	32.300211
N	44.204023	48.992479	33.527333
H	45.190978	49.171363	33.752382
C	43.208164	49.047320	34.432940
H	43.357032	49.310795	35.473822
N	42.047401	48.754820	33.864090
C	42.310260	48.503148	32.535608
H	41.510504	48.237070	31.848346
C	36.620633	45.175764	31.133961
O	35.430449	45.558415	31.245039
O	37.005703	44.081345	30.650569
C	37.725349	46.185657	31.580420
C	37.289528	47.040030	32.777506
C	37.878502	48.429993	32.957857
O	39.162060	48.567706	33.039653
O	37.096728	49.394478	33.109088
H	38.666064	45.647005	31.764485
H	37.903363	46.834509	30.704133
H	36.199919	47.148542	32.715624
H	37.518212	46.496070	33.712265
O	38.507426	49.737432	35.546617
Fe	40.094321	49.231170	34.707300
O	39.948294	47.185614	35.418949
H	39.123145	47.193637	35.927061
H	40.684214	47.158287	36.112373
O	32.942289	51.094500	36.894145
C	33.748506	50.712010	35.995150
O	33.469577	50.633721	34.773478
C	35.182079	50.308491	36.433118
N	35.762942	51.251506	37.401234
C	35.127705	48.895656	36.948272
C	34.598363	48.664381	38.328452
C	35.149502	47.794807	35.938156
H	35.788606	50.329575	35.515553
H	37.777301	49.813017	34.905870
H	34.601177	47.595884	38.594953
H	35.189127	49.205776	39.089965
H	33.554663	49.028491	38.426242
H	35.757518	52.184394	36.979366
H	35.132703	51.320688	38.202480
H	35.300818	46.808835	36.407465
H	34.203563	47.732883	35.358731
H	35.943129	47.955788	35.191445
H	43.356893	54.446068	33.460150
H	42.370474	50.418714	38.718300
H	44.722602	49.488021	30.579282
TS2 M=5			
C	42.358056	54.551761	33.803075
H	42.350620	54.836841	34.865763
H	41.909795	55.393350	33.250754
C	41.557735	53.296583	33.642789
N	40.977428	52.881327	32.456224
H	41.002651	53.387839	31.568168
C	40.365151	51.692473	32.674359
H	39.840560	51.123468	31.909774
N	40.507032	51.325471	33.938281
C	41.241469	52.312892	34.555961
H	41.494613	52.253804	35.611235

C	42.119356	49.388994	38.826307
H	42.965925	48.773182	39.154888
H	41.311281	49.263572	39.568638
C	41.602163	48.832497	37.493220
O	41.063591	49.647099	36.664379
O	41.682256	47.596774	37.325562
C	44.355104	48.544451	31.150478
H	43.791192	47.937257	30.425797
H	45.294113	48.001979	31.349830
C	43.541768	48.706870	32.394925
N	44.078338	49.070457	33.617058
H	45.066694	49.245904	33.836175
C	43.076237	49.139207	34.517353
H	43.217660	49.430092	35.551893
N	41.917680	48.832052	33.952943
C	42.188691	48.555671	32.630067
H	41.390311	48.273762	31.946860
C	36.534004	45.173362	31.193403
O	35.332234	45.525384	31.297578
O	36.945761	44.094566	30.696361
C	37.608456	46.199312	31.665391
C	37.132226	47.050515	32.846263
C	37.718596	48.442025	33.052405
O	38.981791	48.603298	33.090406
O	36.905368	49.386546	33.267922
H	38.553631	45.677565	31.873913
H	37.800862	46.849027	30.792323
H	36.044101	47.152181	32.751240
H	37.335934	46.507039	33.787612
O	38.285196	50.025073	35.578871
Fe	39.953185	49.383451	34.795552
O	39.697170	47.337036	35.617395
H	38.961666	47.497376	36.226078
H	40.499645	47.268981	36.214422
O	33.053952	50.952776	36.881717
C	33.687530	50.475281	35.898576
O	33.428144	50.712156	34.695640
C	34.880941	49.541319	36.162101
N	35.825791	50.000458	37.175237
C	34.591123	48.216997	36.803251
C	33.713139	48.097536	37.995369
C	35.365412	47.051876	36.316348
H	35.395674	49.393947	35.203694
H	37.650753	49.993787	34.834085
H	33.005787	47.256751	37.868494
H	34.307954	47.844949	38.893642
H	33.155348	49.022537	38.183725
H	36.772433	50.146127	36.800417
H	35.463683	50.744774	37.766155
H	35.337547	46.202588	37.013571
H	34.967307	46.722215	35.335326
H	36.412563	47.341447	36.118435
H	43.389296	54.491085	33.455326
H	42.427918	50.434245	38.808809
H	44.654164	49.470826	30.660111
PC M=5			
C	42.307462	54.498071	33.828849
H	42.305085	54.783194	34.891726

H	41.844349	55.334845	33.281447
C	41.513500	53.236208	33.677161
N	40.934571	52.811673	32.494421
H	40.968410	53.307868	31.601765
C	40.309861	51.629912	32.725897
H	39.787443	51.059311	31.960771
N	40.438457	51.275114	33.995380
C	41.182629	52.265133	34.600744
H	41.433437	52.218356	35.657374
C	42.087146	49.397686	38.830925
H	42.929863	48.778712	39.163249
H	41.281590	49.289238	39.579075
C	41.557782	48.827552	37.509455
O	40.957428	49.623064	36.700754
O	41.678231	47.598270	37.332765
C	44.391428	48.545184	31.150973
H	43.822021	47.936303	30.431971
H	45.338890	48.010677	31.331537
C	43.596414	48.689539	32.409204
N	44.142574	49.027769	33.632822
H	45.130484	49.210398	33.847158
C	43.145661	49.067991	34.544901
H	43.303330	49.320513	35.588049
N	41.984505	48.769820	33.984761
C	42.246514	48.527730	32.654169
H	41.448729	48.254596	31.966611
C	36.505002	45.171387	31.193608
O	35.303333	45.528307	31.274364
O	36.924915	44.093353	30.702963
C	37.572292	46.190980	31.695548
C	37.038084	47.081670	32.818487
C	37.689216	48.425426	33.097302
O	38.951876	48.522631	33.186164
O	36.917509	49.407592	33.332860
H	38.490933	45.656368	31.977213
H	37.833194	46.810342	30.818077
H	35.970310	47.241872	32.628863
H	37.108980	46.533587	33.777114
O	37.966232	50.148297	35.642308
Fe	40.018004	49.259608	34.813205
O	39.619258	47.258663	35.715111
H	38.899400	47.300663	36.359295
H	40.447296	47.206113	36.274214
O	33.080547	50.910757	36.864549
C	33.659147	50.436819	35.847577
O	33.411473	50.767527	34.660200
C	34.754947	49.403576	35.987453
N	35.712623	49.424683	37.113485
C	34.784287	48.287136	36.981447
C	33.717831	48.121918	38.044274
C	35.409106	46.992237	36.505022
H	35.239719	49.205322	35.028913
H	37.545316	50.053859	34.743407
H	32.984725	47.358565	37.741109
H	34.177341	47.777072	38.986022
H	33.186222	49.063513	38.223948
H	37.291443	49.744351	36.255153
H	35.363945	50.077665	37.821999

H	35.645187	46.330829	37.353661
H	34.709966	46.457002	35.843721
H	36.326800	47.184036	35.930545
H	43.337653	54.457939	33.475065
H	42.403373	50.440472	38.805146
H	44.673033	49.477032	30.660641

Cluster 2

RC M=5

C	41.279563	55.221379	36.170179
H	41.461209	55.345953	37.248159
H	40.686339	56.093226	35.851489
C	40.527548	53.945141	35.960156
N	39.661267	53.704282	34.907180
H	39.440886	54.357499	34.154436
C	39.167590	52.449555	35.031987
H	38.459758	51.990372	34.345850
N	39.674232	51.875103	36.114957
C	40.514457	52.788971	36.709366
H	41.045675	52.545441	37.625763
C	42.254370	49.512482	40.162086
H	43.058828	48.803552	40.392469
H	41.437514	49.355362	40.887615
C	41.700852	49.157882	38.780809
O	41.008113	50.043580	38.174792
O	41.926607	48.002620	38.356120
C	42.739232	49.964626	31.986547
H	41.960050	49.589523	31.305784
H	43.626796	49.332533	31.816581
C	42.271076	49.844926	33.402050
N	43.125485	49.695750	34.480554
H	44.153088	49.715527	34.492261
C	42.391902	49.575661	35.603286
H	42.822173	49.409841	36.583541
N	41.098339	49.631883	35.314279
C	41.005600	49.794138	33.946073
H	40.042063	49.861551	33.450963
C	34.532002	46.831955	33.593402
O	33.404864	47.383106	33.661824
O	34.869989	45.922535	32.791642
C	35.631884	47.326811	34.558215
C	36.727735	48.119149	33.813894
C	37.969705	48.253795	34.679055
O	38.241624	49.420383	35.163058
O	38.635347	47.224462	34.909052
H	35.191024	47.942827	35.357566
H	36.107348	46.441246	35.009109
H	37.002492	47.538111	32.918649
H	36.357254	49.109045	33.508594
O	38.354023	50.128217	37.793972
Fe	39.525436	49.848056	36.702428
O	39.614748	47.851649	37.116356
H	40.552356	47.680986	37.386116
H	39.371551	47.434379	36.216438
O	34.947940	53.884275	39.316145
C	34.835940	53.657933	38.078385
O	33.822025	53.950775	37.395611
C	35.993662	52.941433	37.345140
N	37.166504	52.831322	38.216331

C	35.545605	51.563509	36.753555
C	34.735649	50.732220	37.752153
C	34.835791	51.682443	35.404801
H	36.262690	53.585518	36.487099
H	36.482526	51.013280	36.571544
H	33.733665	51.162367	37.916539
H	34.602396	49.706004	37.374493
H	35.246659	50.664718	38.724696
H	36.839502	52.454823	39.109403
H	37.783630	52.101969	37.850515
H	35.514730	52.098067	34.641275
H	34.497633	50.698734	35.043257
H	33.954022	52.334336	35.474937
H	42.228892	55.295451	35.639751
H	42.635785	50.526108	40.285183
H	43.032675	50.961880	31.658765
TS1 M=5			
C	41.338381	55.259129	36.155917
H	41.524718	55.338698	37.237105
H	40.775152	56.162259	35.870699
C	40.548254	54.015939	35.897452
N	39.721486	53.824424	34.804345
H	39.546154	54.510506	34.066897
C	39.189190	52.579494	34.883599
H	38.506178	52.160647	34.147646
N	39.627973	51.965818	35.973069
C	40.468574	52.844097	36.618056
H	40.957241	52.565599	37.548650
C	42.060680	49.578836	40.137597
H	42.815229	48.823503	40.391300
H	41.225437	49.489083	40.853601
C	41.507703	49.225405	38.754156
O	40.764377	50.085323	38.166236
O	41.778783	48.086671	38.315217
C	42.788879	49.983749	31.938244
H	42.023591	49.597832	31.247838
H	43.687165	49.363944	31.779712
C	42.301282	49.864596	33.346321
N	43.133732	49.727839	34.443260
H	44.160292	49.748154	34.475378
C	42.369814	49.608284	35.549722
H	42.777388	49.441461	36.541188
N	41.085058	49.655105	35.232952
C	41.025005	49.809938	33.864741
H	40.072337	49.869165	33.346494
C	34.503186	46.780701	33.570497
O	33.385140	47.348503	33.649459
O	34.811506	45.844715	32.787752
C	35.633739	47.291152	34.486424
C	36.730567	48.012169	33.675602
C	37.970094	48.196953	34.531559
O	38.208929	49.376148	34.995852
O	38.654903	47.186265	34.792585
H	35.226369	47.957598	35.262790
H	36.097748	46.419076	34.974530
H	36.990056	47.363346	32.824452
H	36.366830	48.980782	33.301008
O	37.997152	50.277627	37.638439

Fe	39.371822	49.870538	36.617099
O	39.482140	47.867415	37.052782
H	40.414978	47.721638	37.351586
H	39.296604	47.438833	36.143165
O	34.923264	53.887964	39.378914
C	34.892254	53.629123	38.143824
O	33.921192	53.868164	37.383960
C	36.119263	52.914181	37.518689
N	37.264884	52.945365	38.421514
C	35.730809	51.472248	37.062658
C	34.783033	50.733400	37.996991
C	35.302395	51.393260	35.607975
H	36.384829	53.476795	36.607097
H	36.749074	50.884252	37.165756
H	33.755251	51.122176	37.896863
H	34.761471	49.661175	37.748072
H	35.084811	50.836413	39.048638
H	36.953714	52.554466	39.315082
H	37.948028	52.261791	38.083580
H	36.084896	51.780993	34.937888
H	35.066914	50.363983	35.300765
H	34.393358	52.002794	35.461973
H	42.287016	55.317603	35.622306
H	42.504152	50.567438	40.256193
H	43.071255	50.985739	31.615216
IM1 M=5			
C	41.271863	55.186147	36.155650
H	41.446850	55.303127	37.235815
H	40.673437	56.056585	35.841879
C	40.530875	53.905340	35.931832
N	39.700593	53.654238	34.852492
H	39.504217	54.300530	34.088281
C	39.204837	52.398938	34.975404
H	38.522630	51.937193	34.265181
N	39.671553	51.831125	36.078235
C	40.491368	52.753934	36.688283
H	40.992178	52.523557	37.625413
C	42.201917	49.499271	40.170317
H	42.993782	48.787568	40.433145
H	41.368888	49.371477	40.883268
C	41.673847	49.118045	38.787538
O	40.928383	49.964372	38.182052
O	41.962839	47.982948	38.354283
C	42.787333	49.966379	31.930297
H	42.008841	49.592458	31.248086
H	43.681903	49.349118	31.742350
C	42.329070	49.815018	33.345385
N	43.186063	49.671359	34.422425
H	44.212064	49.716158	34.438880
C	42.447510	49.509715	35.540940
H	42.878923	49.335222	36.521457
N	41.155963	49.535516	35.251955
C	41.065048	49.719538	33.889278
H	40.102462	49.767820	33.387685
C	34.515355	46.782384	33.603990
O	33.406098	47.368331	33.671868
O	34.827008	45.864453	32.801974
C	35.633941	47.244063	34.562530

C	36.742273	48.002551	33.802730
C	37.986719	48.128395	34.662590
O	38.222461	49.280077	35.207510
O	38.684005	47.114179	34.844174
H	35.216498	47.872724	35.365218
H	36.088857	46.346582	35.011534
H	37.000590	47.403029	32.915787
H	36.387890	48.994351	33.483980
O	38.078495	50.075598	37.929562
Fe	39.484546	49.746374	36.729024
O	39.642099	47.709928	37.100386
H	40.579701	47.567913	37.375885
H	39.433168	47.303558	36.196267
O	34.919583	53.929357	39.366323
C	34.814680	53.688141	38.132563
O	33.811427	53.959950	37.428424
C	35.970461	52.936058	37.417929
N	37.136989	52.805522	38.295217
C	35.423070	51.627876	36.874940
C	34.765075	50.675059	37.823842
C	35.085912	51.531808	35.424867
H	36.251998	53.560220	36.550657
H	37.220574	49.974242	37.488953
H	33.694692	50.935855	37.974012
H	34.776837	49.642765	37.433831
H	35.241151	50.678436	38.815683
H	36.794967	52.471966	39.199864
H	37.724899	52.032838	37.964836
H	35.876840	51.967835	34.791746
H	34.908392	50.495413	35.098356
H	34.151483	52.090386	35.202223
H	42.223154	55.274234	35.630909
H	42.591950	50.511153	40.280024
H	43.065614	50.972861	31.617855
TS2 M=5			
C	41.301102	55.262404	36.225392
H	41.517816	55.372199	37.298624
H	40.737027	56.162966	35.931177
C	40.490643	54.019419	36.026470
N	39.678733	53.788881	34.929291
H	39.543500	54.429897	34.146660
C	39.116151	52.558319	35.070951
H	38.449302	52.110332	34.336829
N	39.509943	51.991775	36.198601
C	40.364571	52.884925	36.806956
H	40.867262	52.619208	37.736577
C	42.292334	49.478384	40.206174
H	43.114578	48.782056	40.412549
H	41.497055	49.299952	40.950363
C	41.709037	49.144166	38.822788
O	41.034814	50.041248	38.237620
O	41.919296	47.980756	38.395818
C	42.760095	49.995351	31.947602
H	41.984751	49.618066	31.263288
H	43.651869	49.369561	31.774885
C	42.288407	49.871434	33.360686
N	43.136179	49.710801	34.443548
H	44.162235	49.725192	34.463144

C	42.384323	49.591224	35.560316
H	42.796816	49.410149	36.547475
N	41.097517	49.660442	35.263684
C	41.019288	49.829596	33.900349
H	40.058834	49.897570	33.396418
C	34.446591	46.744351	33.653439
O	33.387720	47.426232	33.695752
O	34.662185	45.762921	32.897928
C	35.619744	47.176473	34.549683
C	36.669241	47.955170	33.731671
C	37.927911	48.197128	34.560827
O	38.050238	49.344985	35.131592
O	38.728524	47.251545	34.678395
H	35.257835	47.790218	35.391060
H	36.108965	46.276230	34.953698
H	36.939229	47.337314	32.861737
H	36.244881	48.905336	33.372060
O	38.037520	49.865872	38.118247
Fe	39.463660	49.783119	36.752309
O	39.574396	47.654361	37.099491
H	40.507288	47.571455	37.408742
H	39.469035	47.343258	36.159484
O	34.758720	53.934481	39.082040
C	34.673990	53.618586	37.869771
O	33.842432	54.050539	37.036560
C	35.665419	52.579883	37.306260
N	36.411281	51.870535	38.307286
C	35.025052	51.416896	36.643779
C	33.925170	50.689078	37.330587
C	35.511791	50.904439	35.366780
H	36.342808	53.099862	36.607208
H	37.615122	48.998867	38.042521
H	33.024130	50.763354	36.694448
H	34.150092	49.610232	37.390620
H	33.701065	51.072332	38.335896
H	35.849995	51.615929	39.120715
H	37.106063	51.084386	38.069951
H	35.769353	51.727694	34.679560
H	36.474783	50.319229	35.483072
H	34.798742	50.207198	34.902579
H	42.238940	55.314300	35.672368
H	42.657498	50.498703	40.323095
H	43.047621	50.996553	31.626683
PC M=5			
C	41.372250	55.312181	36.179972
H	41.586468	55.421366	37.253507
H	40.812538	56.213809	35.881715
C	40.565095	54.069407	35.972168
N	39.737319	53.849429	34.886610
H	39.566208	54.511749	34.127766
C	39.209274	52.601067	35.002849
H	38.527338	52.160150	34.278011
N	39.643992	52.013033	36.105246
C	40.485014	52.912491	36.723558
H	41.009371	52.641392	37.639164
C	42.314596	49.491702	40.146846
H	43.146539	48.804019	40.343920
H	41.530480	49.297761	40.899334

C	41.721097	49.135579	38.775259
O	41.083255	50.036367	38.146471
O	41.862534	47.947974	38.402736
C	42.833524	49.997301	31.851921
H	42.055151	49.627335	31.167412
H	43.732525	49.391173	31.650394
C	42.384513	49.832044	33.266922
N	43.243283	49.640541	34.334265
H	44.268860	49.657932	34.349379
C	42.502718	49.508791	35.459321
H	42.928986	49.316373	36.439265
N	41.214505	49.600553	35.180070
C	41.121614	49.795672	33.821335
H	40.156381	49.889023	33.329303
C	34.506606	46.651218	33.600631
O	33.460211	47.350560	33.657679
O	34.715377	45.700282	32.803616
C	35.667346	47.009025	34.541935
C	36.602727	48.063759	33.919390
C	37.869960	48.233160	34.755928
O	38.132493	49.403196	35.226118
O	38.555488	47.213438	34.966145
H	35.270846	47.382488	35.497033
H	36.263164	46.105928	34.734478
H	36.907391	47.700131	32.922498
H	36.086423	49.025610	33.789862
O	38.218904	49.918321	38.320101
Fe	39.617308	49.857609	36.625183
O	39.392446	47.732388	37.329638
H	40.330749	47.579472	37.590663
H	39.222961	47.356905	36.414790
O	34.711542	53.755127	39.283188
C	34.553136	53.448567	38.064909
O	33.814351	54.045504	37.251257
C	35.290065	52.243366	37.509425
N	35.978519	51.328455	38.417285
C	34.771104	50.851329	37.720112
C	33.531342	50.602459	38.546739
C	35.041172	49.801603	36.667054
H	35.803353	52.438002	36.560705
H	38.051361	48.966868	38.205108
H	32.648060	50.509886	37.896246
H	33.642302	49.652256	39.094603
H	33.348390	51.392095	39.285856
H	35.763582	51.595257	39.383340
H	37.359745	50.436038	38.240168
H	35.971152	50.001900	36.116840
H	35.149213	48.816581	37.152080
H	34.212265	49.722437	35.946933
H	42.311006	55.352317	35.627529
H	42.670564	50.514477	40.270482
H	43.100180	51.012664	31.558662