

Structures of the Solvated copper (II) Ion in Ammonia at different temperatures (Supporting information)

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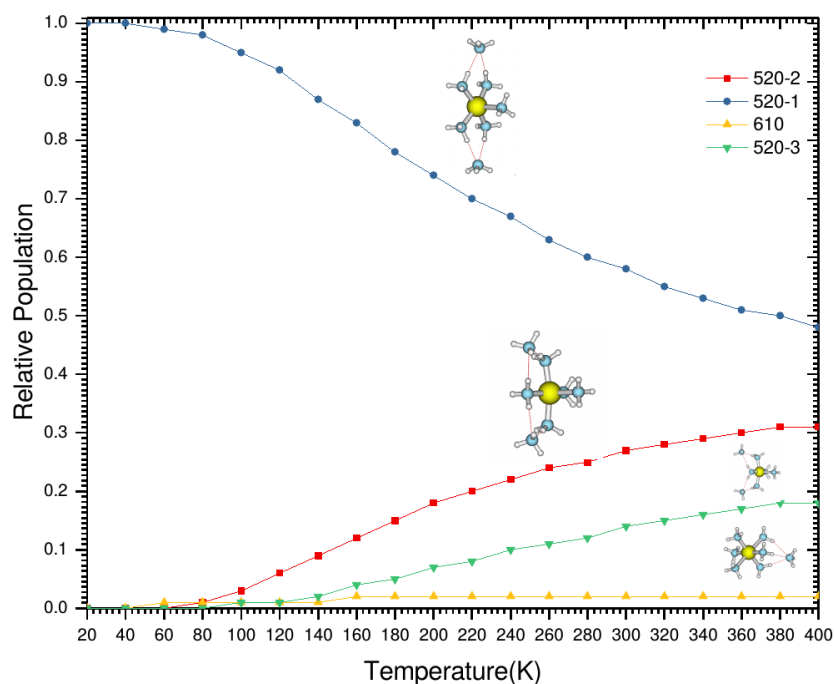


Figure S 1: Temperature dependence of the relative stability of different $\text{Cu}^{2+}(\text{NH}_3)_7$ isomers at M06-2X/6-31++G(d,p) level of theory

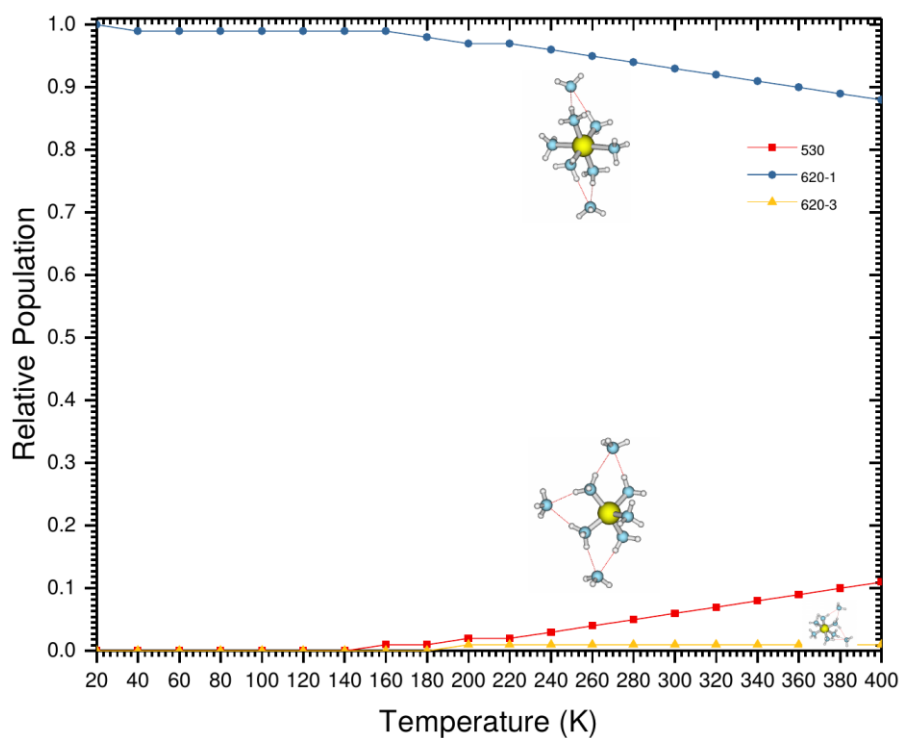


Figure S 2: Temperature dependence of the relative stability of different $\text{Cu}^{2+}(\text{NH}_3)_8$ isomers at M06-2X/6-31++G(d,p) level of theory

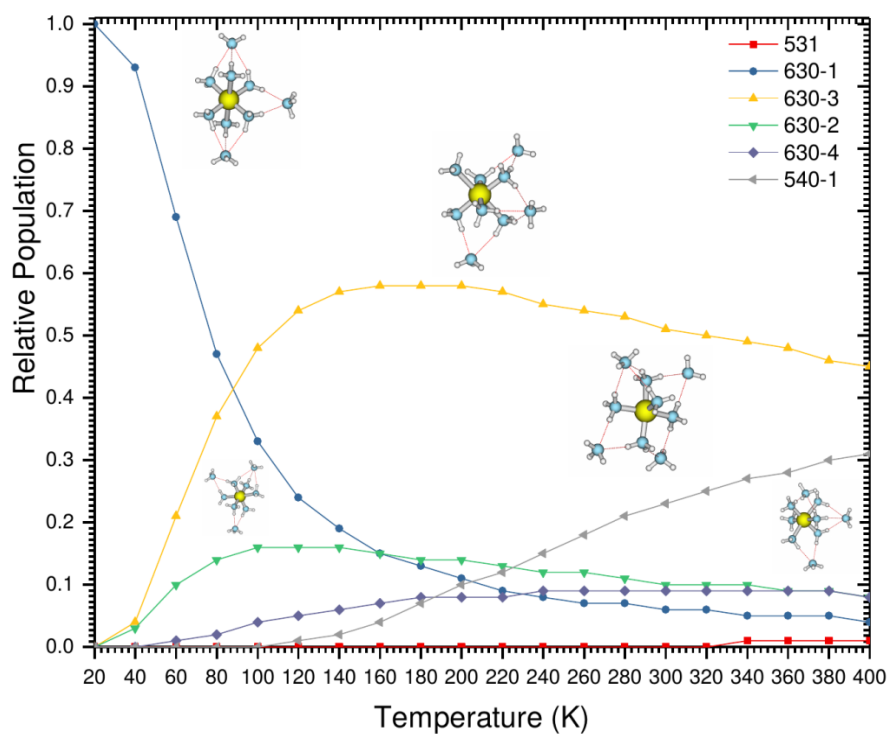


Figure S 3: Temperature dependence of the relative stability of different $\text{Cu}^{2+}(\text{NH}_3)_{n=9}$ isomers at M06-2X/6-31++G(d,p) level of theory

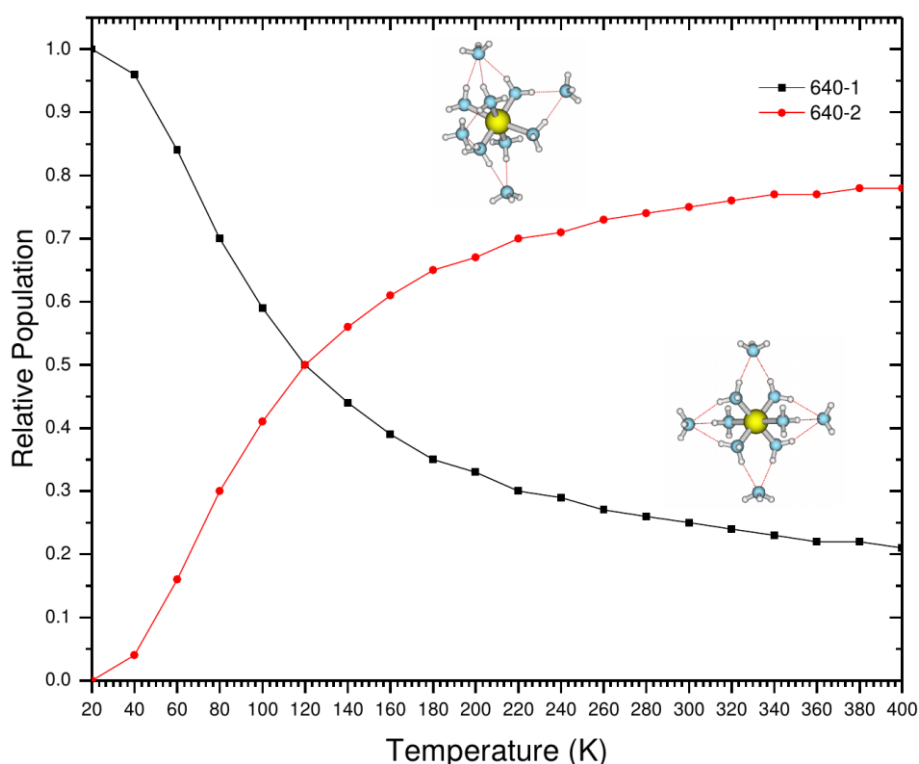


Figure S 4: Temperature dependence of the relative stability of different $\text{Cu}^{2+}(\text{NH}_3)_{n=10}$ isomers at M06-2X/6-31++G(d,p) level of theory

Table S 1: Cartesian coordinates of all the proposed isomers of $\text{Cu}^{2+}(\text{NH}_3)_{n=1-10}$ at MP2/6-31++G(d,p) level of theory

Cartesian coordinates of : 100

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	-0.537548	0.000006	0.000010
7	1.440414	0.000016	0.000027
1	1.834851	-0.890769	-0.335293
1	1.835909	0.154993	0.938708
1	1.835235	0.735496	-0.603893

E+ZPE = -1694.5354250000000

Cartesian coordinates of : 200-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	-0.000000	0.000000	0.000000
7	-1.283800	0.703940	-1.241919
1	-1.811541	-0.022775	-1.741373
1	-0.864982	1.286112	-1.977954
1	-1.996380	1.298935	-0.801134
7	1.283801	-0.703941	1.241919
1	0.864989	-1.286165	1.977916
1	1.811498	0.022775	1.741419
1	1.996417	-1.298884	0.801124

E+ZPE = -1751.0872509999999

Cartesian coordinates of : 200-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	0.000000	0.400012	0.000000
7	-1.706912	-0.523471	0.000000
1	-1.843165	-1.126869	-0.819248
1	-2.511117	0.117847	-0.000005
1	-1.843169	-1.126861	0.819253
7	1.706912	-0.523471	0.000000
1	1.843167	-1.126864	-0.819251
1	1.843166	-1.126866	0.819250

1 2.511117 0.117847 0.000002

E+ZPE = -1751.0672979999999

Cartesian coordinates of : 210

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.783963	-0.140087	0.000000
7	-0.937636	-0.720476	-0.000000
1	-1.108112	-1.321294	0.810003
1	-1.108112	-1.321293	-0.810004
1	-2.732422	0.194122	-0.000000
7	2.595880	0.573312	-0.000000
1	2.806844	1.157320	0.814322
1	2.807095	1.156653	-0.814736
1	3.311801	-0.159525	0.000409
7	-3.730225	0.507367	-0.000000
1	-4.352983	-0.303713	0.000033
1	-3.927590	1.069386	-0.830727
1	-3.927573	1.069441	0.830694

E+ZPE = -1807.5095659999999

Cartesian coordinates of : 220-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.000002	-0.000005	0.000002
7	-1.614807	0.862342	0.000003
1	-1.738087	1.460141	-0.817796
1	-1.738095	1.460126	0.817811
1	-3.245919	0.043281	-0.000006
7	1.614809	-0.862335	0.000003
1	1.738105	-1.460120	-0.817804
1	1.738097	-1.460130	0.817804
1	3.245922	-0.043276	0.000002
7	4.247602	0.316885	-0.000004
1	4.423549	0.885654	-0.829643
1	4.901406	-0.468093	0.000099
7	-4.247600	-0.316879	-0.000005
1	-4.423491	-0.885829	-0.829531
1	-4.423554	-0.885641	0.829637
1	4.423498	0.885829	0.829525
1	-4.901401	0.468101	-0.000118

E+ZPE = -1863.8967130000001

Cartesian coordinates of : 220-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.000001	0.233408	-0.000002
7	-1.776801	0.658901	-0.000016
1	-2.019494	1.225426	0.813820
1	-3.215691	-0.438431	0.000001
1	-2.019485	1.225396	-0.813876
7	1.776802	0.658898	0.000020
1	2.019478	1.225401	0.813876
1	2.019491	1.225420	-0.813819
1	3.215696	-0.438423	0.000004
7	4.151883	-0.950768	-0.000006
1	4.239255	-1.539853	0.829321
1	4.918074	-0.275085	0.000679
7	-4.151880	-0.950769	0.000008
1	-4.239355	-1.539644	0.829475
1	-4.918066	-0.275080	0.000433
1	-4.239709	-1.539003	-0.829877
1	4.239804	-1.538791	-0.830031

E+ZPE = -1863.8951290000000

Cartesian coordinates of : 220-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.925549	-0.468193	0.187672
7	-0.705266	0.045345	-0.548380
1	-0.678214	0.049672	-1.571888
1	-1.032373	1.032605	-0.247222
1	-1.505064	-0.647305	-0.281149
7	2.699623	0.286529	-0.158768
1	2.983096	0.190233	-1.138599
1	3.452276	-0.147686	0.387008
1	2.751212	1.287393	0.052358
7	-1.688867	2.572397	0.148266
1	-2.691859	2.545105	-0.027618
1	-1.343141	3.338244	-0.427064
1	-1.598928	2.896241	1.109317
7	-2.830201	-1.663413	0.045294
1	-3.557472	-1.475116	-0.642957
1	-3.273397	-1.509425	0.949182

1 -2.674092 -2.668370 -0.008743

E+ZPE = -1863.8705880000000

Cartesian coordinates of : 230-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.344973	-0.030116	0.142706
7	-2.066203	-0.078905	0.934744
1	-2.208788	0.683997	1.602932
1	-2.220490	-0.933746	1.477240
1	-2.920988	-0.018772	0.234851
7	-4.278672	0.059139	-0.674418
1	-5.093675	0.048455	-0.062677
1	-4.416336	-0.719483	-1.316277
7	3.013496	-2.206717	-0.039637
1	3.972019	-1.915078	-0.221103
1	2.860122	-3.005735	-0.651558
1	3.028181	-2.589576	0.903172
7	2.925710	2.288486	0.022249
1	2.497310	3.209717	-0.038513
1	3.692764	2.311315	-0.647141
7	1.353792	0.018014	-0.632636
1	1.952761	-0.833137	-0.376505
1	1.916598	0.887413	-0.356630
1	1.317000	0.028561	-1.655472
1	3.371195	2.259305	0.936961
1	-4.380312	0.899996	-1.239866

E+ZPE = -1920.2895360000000

Cartesian coordinates of : 240

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.000007	0.049235	-0.000011
7	1.768976	0.054227	-0.622624
1	1.826459	0.141126	-1.640325
1	2.295630	-0.840745	-0.381474
1	2.343519	0.863738	-0.233099
7	-1.768958	0.054219	0.622606
1	-1.826434	0.141102	1.640309
1	-2.295635	-0.840740	0.381454
1	-2.343495	0.863743	0.233100
7	-3.392775	2.192077	-0.353967

1	-3.016607	3.137179	-0.328347
1	-4.219177	2.221539	0.239935
7	3.392786	2.192045	0.353995
1	3.016820	3.137210	0.327699
1	3.747123	2.069948	1.300093
1	-3.747651	2.069581	-1.299811
1	4.219519	2.221048	-0.239469
7	3.267804	-2.309504	-0.047202
1	3.340091	-2.914786	-0.862390
1	4.223414	-2.025676	0.158726
7	-3.267853	-2.309489	0.047220
1	-3.004344	-2.922058	-0.721153
1	-4.223953	-2.025670	-0.156438
1	3.003032	-2.923347	0.719717
1	-3.338379	-2.916041	0.861616

E+ZPE = -1976.6796240000001

Cartesian coordinates of : 241

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.611301	0.076472	0.081382
7	-2.389651	-0.295808	0.561582
1	-2.530606	-0.301193	1.574515
1	-2.718192	-1.248377	0.221299
1	-3.076182	0.421185	0.180371
7	1.158381	0.436444	-0.385385
1	1.351024	0.268213	-1.375549
1	1.883353	-0.181188	0.169614
1	1.420387	1.446010	-0.208791
7	1.963419	3.179901	0.073865
1	1.902024	3.750891	-0.766079
1	2.953385	3.153355	0.307630
7	-4.317858	1.595078	-0.401333
1	-4.600911	2.246969	0.327191
1	-4.119006	2.171834	-1.215358
1	1.531576	3.735178	0.808523
1	-5.162430	1.080067	-0.640788
7	-3.364686	-2.849836	-0.301683
1	-2.778809	-3.667558	-0.149449
1	-4.213973	-3.030951	0.229474
7	3.025353	-1.051787	0.952176
1	3.875502	-1.083289	0.364065
1	2.810618	-2.022068	1.171675
1	-3.644612	-2.897218	-1.278761
1	3.314737	-0.635819	1.835006
7	5.592851	-1.234053	-0.690929

1	6.166323	-1.900014	-0.180280
1	6.151934	-0.388078	-0.753620
1	5.536920	-1.595208	-1.638813

E+ZPE = -2033.0568029999999

Cartesian coordinates of : 250

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.229063	0.003224	-0.292904
7	1.593196	-0.004166	0.078225
1	1.797605	-0.259648	1.077606
1	2.031822	0.935951	-0.095839
1	2.105465	-0.694653	-0.527931
7	-2.069939	0.005132	-0.685025
1	-2.251651	0.009999	-1.691436
1	-2.573133	0.857933	-0.301909
1	-2.577337	-0.848637	-0.309513
7	-3.537971	-2.277540	0.258905
1	-3.120665	-3.200209	0.161693
1	-4.394507	-2.315651	-0.289753
7	3.060647	-1.894225	-1.612631
1	2.641767	-2.781177	-1.881600
1	3.385360	-1.476951	-2.481777
1	-3.842809	-2.220389	1.227864
1	3.905652	-2.144318	-1.103978
7	2.871775	2.586571	-0.405369
1	2.912438	3.177940	0.421339
1	3.841683	2.386107	-0.638615
7	-3.521694	2.291826	0.275080
1	-3.161143	2.858147	1.039210
1	-4.436058	1.973338	0.588495
1	2.539961	3.191891	-1.152349
1	-3.712128	2.948266	-0.478974
7	2.234209	-0.716358	2.846887
1	3.101395	-0.235541	3.075079
1	1.597395	-0.488181	3.606313
1	2.440165	-1.706379	2.957771

E+ZPE = -2033.0653600000001

Cartesian coordinates of : 300

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
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29	-0.000003	-0.181597	-0.001984
7	-1.907424	-0.668859	0.001818
1	-2.443866	-0.235599	0.758502
1	-2.066140	-1.675909	0.112006
1	-2.397548	-0.419845	-0.862125
7	0.000018	1.806140	-0.000025
1	0.000098	2.203576	0.943932
1	-0.810373	2.223377	-0.464148
1	0.810346	2.223354	-0.464278
7	1.907414	-0.668881	0.001818
1	2.443867	-0.235605	0.758484
1	2.397533	-0.419898	-0.862137
1	2.066119	-1.675929	0.112034

E+ZPE = -1807.5452200000000

Cartesian coordinates of : 310-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.482265	0.056171	-0.019254
7	1.450642	1.776617	-0.000487
1	2.011063	1.940047	-0.840907
1	2.096566	1.877594	0.786356
1	0.829166	2.588263	0.063452
7	1.950963	-1.290325	0.067012
1	1.735180	-2.145998	-0.448915
1	2.149145	-1.597916	1.022738
1	2.849363	-0.975873	-0.304889
7	-1.135846	-0.989348	-0.073303
1	-1.204161	-1.662997	0.692928
1	-2.053836	-0.412040	-0.020400
7	-3.589198	0.340323	0.053746
1	-3.788917	0.874873	0.896904
1	-3.822917	0.958579	-0.720670
1	-4.299533	-0.389787	0.030861
1	-1.222721	-1.544580	-0.927870

E+ZPE = -1863.9427400000000

Cartesian coordinates of : 310-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.684665	-0.226875	-0.000002
7	0.858342	-1.402120	-0.000013

1	0.907949	-2.020865	0.813501
1	1.738195	-0.837758	-0.000013
1	0.907943	-2.020859	-0.813531
7	0.243516	1.523631	-0.000018
1	0.046223	2.110177	0.813669
1	0.046207	2.110172	-0.813704
1	1.256626	1.362611	-0.000026
7	-2.611932	0.183385	0.000018
1	-3.201999	-0.654400	0.000018
1	-2.917181	0.721633	0.814908
7	3.332265	0.270016	0.000016
1	3.645233	0.804817	0.809482
1	3.942746	-0.547380	-0.000190
1	3.645205	0.805192	-0.809212
1	-2.917197	0.721644	-0.814860

E+ZPE = -1863.9411190000001

Cartesian coordinates of : 310-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.729082	-0.000062	-0.002804
7	-1.161102	1.908037	-0.263713
1	-1.941698	2.073860	-0.906013
1	-0.382168	2.448780	-0.646916
1	-1.426957	2.381353	0.603766
7	-1.160383	-1.908352	-0.263568
1	-1.940635	-2.074539	-0.906191
1	-1.426477	-2.381596	0.603878
1	-0.381103	-2.448914	-0.646321
7	0.927385	0.000283	1.015270
1	1.023785	-0.807563	1.633476
1	1.809285	0.000238	0.402978
1	1.023656	0.808373	1.633176
7	3.341269	0.000201	-0.463141
1	3.900447	-0.806896	-0.192070
1	3.900657	0.806964	-0.191509
1	3.354418	0.000555	-1.480867

E+ZPE = -1863.9409280000000

Cartesian coordinates of : 311

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
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29	1.525190	0.000006	0.053849
7	2.089468	-1.907441	-0.058984
1	3.031774	-2.065194	-0.421857
1	1.470825	-2.456894	-0.655742
1	2.071668	-2.357201	0.857551
7	2.089467	1.907423	-0.059498
1	3.031771	2.065079	-0.422418
1	2.071671	2.357428	0.856917
1	1.470820	2.456716	-0.656400
7	-0.285080	0.000065	0.476819
1	-0.525799	0.805296	1.056285
1	-1.960157	-0.000072	-0.609486
1	-0.525803	-0.805012	1.056497
7	-2.881740	-0.000132	-1.098700
1	-2.945720	0.823149	-1.696072
1	-3.721272	-0.000050	-0.406370
1	-2.945717	-0.823555	-1.695876
7	-5.083813	0.000065	0.568877
1	-5.156797	-0.810441	1.179833
1	-5.156805	0.810726	1.179627
1	-5.939075	-0.000009	0.016292

E+ZPE = -1920.3341849999999

Cartesian coordinates of : 320-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.063316	0.313993	0.149557
7	-1.337218	-0.765090	0.937471
1	-1.724325	-0.358747	1.791550
1	-1.006236	-1.691047	1.220475
1	-2.169545	-0.949142	0.291286
7	1.848671	0.607816	-0.535704
1	1.873910	0.735769	-1.549600
1	2.533811	-0.197257	-0.335216
1	2.297590	1.439768	-0.147720
7	-3.593621	-1.370617	-0.674281
1	-3.634885	-1.119060	-1.659434
1	-4.455643	-1.010215	-0.269394
1	-3.700334	-2.383437	-0.657301
7	3.762982	-1.412147	-0.076158
1	3.605040	-2.313188	-0.522298
1	4.633986	-1.068391	-0.476876
1	3.984979	-1.625393	0.893995
7	-0.830030	2.093200	-0.037669
1	-0.499873	2.638340	-0.835802
1	-1.842579	2.029008	-0.153228

1 -0.687554 2.695053 0.776789

E+ZPE = -1920.3369789999999

Cartesian coordinates of : 320-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.118983	0.063530	-0.000002
7	1.850345	0.919618	0.000071
1	2.683367	0.236666	0.000015
1	1.997860	1.522578	0.812089
1	1.997862	1.522714	-0.811847
7	-1.226253	1.526002	0.000062
1	-1.170621	2.142155	-0.812918
1	-1.170610	2.142096	0.813086
1	-2.171032	1.128888	0.000054
7	-3.927054	-0.422366	0.000038
1	-4.320381	-1.363287	-0.000337
1	-4.358723	0.022293	-0.809039
1	-4.358617	0.021621	0.809540
7	4.127898	-0.737831	-0.000062
1	4.931035	-0.111424	-0.000164
1	4.262460	-1.339581	-0.809840
1	4.262584	-1.339476	0.809774
7	-1.102441	-1.453625	-0.000105
1	-2.089856	-1.119625	-0.000064
1	-1.001638	-2.065347	0.813014
1	-1.001661	-2.065218	-0.813323

E+ZPE = -1920.3363310000000

Cartesian coordinates of : 320-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.074114	0.418642	-0.178273
7	0.349120	2.234013	0.485232
1	1.206971	2.267625	1.039849
1	-0.374830	2.635615	1.086833
1	0.478621	2.914856	-0.266870
7	1.613366	-0.172363	-0.962744
1	2.145143	0.572966	-1.415163
1	1.484782	-0.877970	-1.689456
1	2.276374	-0.610105	-0.253075
7	3.487543	-1.381243	0.827031

1	3.669913	-2.332866	0.513938
1	3.310998	-1.461102	1.825886
1	4.384817	-0.905543	0.753159
7	-3.948921	-0.770412	0.536953
1	-4.071264	-0.663548	1.541652
1	-4.420308	-1.643074	0.305416
7	-1.312398	-1.043794	-0.442591
1	-1.456857	-1.259852	-1.431123
1	-2.297171	-0.883409	-0.043934
1	-0.987328	-1.915540	-0.019864
1	-4.521518	-0.042061	0.115520

E+ZPE = -1920.3353700000000

Cartesian coordinates of : 321-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	0.668664	-0.002666	0.000016
7	2.037824	1.423038	-0.000042
1	1.986798	2.038770	0.812211
1	1.986778	2.038725	-0.812329
1	2.985731	1.011418	-0.000043
7	-1.097526	-0.515752	0.000059
1	-1.365010	-1.071853	-0.811262
1	-2.733122	0.608355	0.000062
1	-1.364982	-1.071814	0.811416
7	4.819832	0.073269	-0.000059
1	5.209837	-0.406446	-0.809422
1	5.209876	-0.406797	0.809078
1	5.284815	0.979819	0.000132
7	-3.646138	1.114148	0.000077
1	-3.699458	1.710842	0.824520
1	-3.699417	1.710969	-0.824276
1	-4.492878	0.435379	0.000004
7	1.949274	-1.528713	0.000033
1	2.923115	-1.214110	0.000017
1	1.828542	-2.134580	0.811521
1	1.828526	-2.134611	-0.811430
7	-5.871911	-0.531832	-0.000106
1	-5.948645	-1.141597	-0.811011
1	-5.948665	-1.141755	0.810678
1	-6.722572	0.027492	-0.000062

E+ZPE = -1976.7284860000000

Cartesian coordinates of : 330-1

 Atomic number (AN) and Cartesian coordinates
 AN X Y Z

29	0.138333	-0.054364	-0.042528
7	-0.944842	-1.216867	1.072056
1	-0.399675	-1.735864	1.764167
1	-1.482444	-1.953966	0.523106
1	-1.638635	-0.703428	1.617752
7	1.838518	0.566104	-0.744118
1	1.944481	0.382220	-1.743487
1	2.695314	0.126778	-0.283033
1	1.960866	1.574695	-0.639769
7	-2.407421	-3.264813	-0.277365
1	-3.403655	-3.197573	-0.079181
1	-2.121467	-4.160920	0.112395
1	-2.341951	-3.381723	-1.285836
7	4.213790	-0.522141	0.390884
1	4.378654	-1.515220	0.242654
1	4.987692	-0.052961	-0.075646
1	4.370265	-0.366804	1.384206
7	-1.199033	1.094019	-0.897869
1	-2.092569	0.624720	-1.048572
1	-1.417296	1.959876	-0.327572
1	-0.917496	1.431827	-1.818733
7	-1.865673	3.489657	0.560379
1	-1.637657	4.304469	-0.005597
1	-2.874089	3.535358	0.691666
1	-1.469353	3.683351	1.477018

 E+ZPE = -1976.7273949999999

Cartesian coordinates of : 330-2

 Atomic number (AN) and Cartesian coordinates
 AN X Y Z

29	0.000013	-0.070259	-0.506411
7	1.887637	-0.325112	-0.883234
1	2.387346	-0.982547	-0.211059
1	2.410294	0.552041	-0.865792
1	2.058262	-0.710901	-1.815087
7	-1.887550	-0.325337	-0.883380
1	-2.387269	-0.982696	-0.211141
1	-2.058052	-0.711299	-1.815184
1	-2.410280	0.551777	-0.866138
7	3.357413	-2.097399	0.803104
1	4.207875	-1.645031	1.132348
1	3.677416	-2.881776	0.238354

1	2.940489	-2.518053	1.630082
7	-3.357344	-2.097449	0.803127
1	-2.940450	-2.517978	1.630183
1	-4.207847	-1.645079	1.132263
1	-3.677278	-2.881914	0.238459
7	-0.000115	1.111607	1.055623
1	0.810420	0.981155	1.661595
1	-0.000098	2.135952	0.784628
1	-0.810742	0.981148	1.661470
7	-0.000075	3.923135	0.420015
1	-0.807279	4.370604	0.849481
1	0.807056	4.370619	0.849600
1	-0.000007	4.245370	-0.544937

E+ZPE = -1976.7269790000000

Cartesian coordinates of : 330-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.286221	-0.311627	-0.022915
7	2.047101	-0.957725	-0.514097
1	2.204763	-0.947873	-1.523478
1	2.206847	-1.924866	-0.226714
1	2.857053	-0.402542	-0.092441
7	-0.960550	0.903592	0.816765
1	-1.864173	0.439427	0.936400
1	-1.142095	1.789197	0.258149
1	-0.678123	1.213955	1.748455
7	4.304619	0.406485	0.549060
1	5.119102	0.003281	0.089924
1	4.469029	0.274426	1.544593
1	4.381747	1.408759	0.392330
7	-3.634888	-1.285206	0.602167
1	-4.104063	-2.038239	0.100618
1	-3.699468	-1.556364	1.581769
1	-4.266029	-0.492312	0.502631
7	-0.996478	-1.594349	-0.797672
1	-1.157510	-1.450829	-1.795960
1	-0.720474	-2.572454	-0.706061
1	-1.922166	-1.498879	-0.331486
7	-1.500425	3.340108	-0.593145
1	-1.319656	4.124158	0.030548
1	-2.485223	3.418830	-0.837569
1	-0.995609	3.559164	-1.448736

E+ZPE = -1976.7265290000000

Cartesian coordinates of : 330-4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	-0.206523	-0.247452	0.093655
7	1.598592	0.149820	0.569988
1	1.978259	0.989790	0.061176
1	2.253081	-0.652488	0.362051
1	1.720810	0.344536	1.564605
7	-1.305718	1.173360	0.952907
1	-1.015275	2.118149	0.697579
1	-1.282155	1.145832	1.973497
1	-2.288929	1.082000	0.683384
7	-4.269088	0.137349	-0.265227
1	-4.791121	-0.523876	-0.839430
1	-4.519531	1.046717	-0.650362
1	-4.731535	0.094907	0.641659
7	3.470579	-2.020374	0.072284
1	3.245983	-2.937972	0.449740
1	4.333425	-1.748573	0.538711
1	3.732590	-2.184939	-0.896799
7	-1.645514	-1.250379	-0.762540
1	-2.561049	-0.779892	-0.604474
1	-1.744162	-2.204513	-0.409564
1	-1.536623	-1.346030	-1.774250
7	2.758527	2.451284	-0.798560
1	3.036617	3.170898	-0.134845
1	2.278804	2.947833	-1.545424
1	3.628341	2.126311	-1.215209

E+ZPE = -1976.7239440000001

Cartesian coordinates of : 330-5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	0.245089	-0.493562	-0.340865
7	1.035670	-2.082063	-1.224784
1	1.979722	-2.293514	-0.896279
1	1.110376	-1.982852	-2.239365
1	0.501134	-2.941861	-1.078329
7	1.639265	0.865848	-0.535709
1	2.343209	0.849444	0.256884
1	1.244606	1.807054	-0.541159
1	2.185528	0.801379	-1.395393
7	-1.163026	0.394976	0.596373

1	-1.591855	1.169555	0.027929
1	-1.949571	-0.251621	0.871295
7	-3.374535	-1.312220	1.432336
1	-4.002391	-1.641573	0.702824
1	-3.160909	-2.132912	1.994192
1	-3.950035	-0.725766	2.032982
1	-0.847433	0.823138	1.467806
7	-2.425195	2.553397	-0.914604
1	-2.364472	3.437563	-0.414314
1	-3.419225	2.337571	-0.948577
7	3.610152	0.917922	1.563265
1	3.594866	1.833573	2.007843
1	3.591059	0.250488	2.330763
1	-2.171012	2.772173	-1.874892
1	4.542501	0.836448	1.162733

E+ZPE = -1976.7229430000000

Cartesian coordinates of : 330-6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	0.014242	-0.778342	0.014244
7	-1.320082	0.394676	0.743846
1	-2.317359	0.139883	0.491974
1	-1.141658	1.348199	0.392545
1	-1.295205	0.455856	1.763338
7	1.265602	0.507515	-0.742365
1	1.521035	0.338690	-1.715798
1	2.172320	0.571420	-0.208173
1	0.826589	1.434463	-0.714710
7	0.806361	-2.543321	-0.398858
1	0.400142	-3.318227	0.131278
1	0.708280	-2.807813	-1.381380
7	-0.542430	3.200409	-0.430342
1	-0.786002	3.405628	-1.397874
1	-1.286385	3.633300	0.114996
1	0.271776	3.780382	-0.234721
1	1.808346	-2.576224	-0.202231
7	-4.068717	-0.226431	0.142229
1	-4.361658	-1.200522	0.125574
1	-4.637071	0.206546	0.867262
1	-4.405567	0.168958	-0.732656
7	3.802683	0.741438	0.660162
1	3.935907	1.722032	0.898236
1	4.580158	0.513905	0.043827
1	3.989417	0.235452	1.522721

E+ZPE = -1976.7226470000001

Cartesian coordinates of : 331-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.476365	-0.062070	0.037485
7	-1.804019	-1.083490	1.066120
1	-2.473370	-0.476727	1.539428
1	-1.402973	-1.665688	1.801478
1	-2.369619	-1.728324	0.462066
7	1.297479	0.303529	-0.348361
1	1.537410	0.125075	-1.323282
1	2.869667	-0.457281	0.409537
1	1.544490	1.279398	-0.185427
7	-3.421621	-2.921855	-0.542236
1	-3.173526	-3.119671	-1.508249
1	-4.404794	-2.661542	-0.562894
1	-3.396434	-3.823219	-0.070826
7	3.789732	-0.817997	0.768255
1	3.856089	-0.638519	1.769008
1	3.836770	-1.825676	0.625268
1	4.628599	-0.355010	0.273207
7	-1.727578	1.035274	-1.020877
1	-2.519880	0.515500	-1.396402
1	-2.130611	1.828222	-0.469698
1	-1.262730	1.453965	-1.825072
7	6.020899	0.320516	-0.453205
1	6.081291	0.160107	-1.455969
1	6.102393	1.327105	-0.330630
1	6.876285	-0.070347	-0.063882
7	-2.895238	3.307830	0.449436
1	-3.911272	3.264505	0.467548
1	-2.616536	3.514354	1.404999
1	-2.674242	4.147161	-0.081189

E+ZPE = -2033.1127469999999

Cartesian coordinates of : 331-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.723563	-0.201054	-0.154074
7	-2.625796	-0.171999	-0.536680
1	-2.824469	-0.169589	-1.538664
1	-3.083787	0.662863	-0.168149

1	-3.169436	-0.998499	-0.140807
7	0.912682	-0.999721	0.509210
1	1.751691	-0.481125	0.116577
1	1.034813	-1.981627	0.254965
1	1.003089	-0.970185	1.526199
7	-4.198067	-2.339180	0.454995
1	-5.170210	-2.093548	0.279009
1	-4.152529	-2.546300	1.449969
1	-4.060655	-3.231504	-0.014233
7	3.180954	0.371942	-0.540668
1	3.341705	0.451974	-1.543165
1	3.497821	1.255842	-0.146497
1	3.876451	-0.323161	-0.218204
7	-0.035681	1.511873	-0.793867
1	-0.385627	1.788296	-1.711425
1	-0.252002	2.315560	-0.146456
1	0.981859	1.462916	-0.878332
7	-0.591112	3.798639	0.909134
1	0.282902	4.287615	1.089861
1	-1.173215	4.473380	0.417571
1	-1.024901	3.685840	1.822131
7	5.302039	-1.632161	0.374386
1	5.400079	-1.832854	1.365610
1	5.329328	-2.535025	-0.091042
1	6.165278	-1.166071	0.107680

E+ZPE = -2033.1039690000000

Cartesian coordinates of : 331-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.787593	-0.000000	-0.406723
7	-0.282236	1.866630	-0.290333
1	-0.382982	2.373845	-1.170647
1	0.744621	1.960771	-0.006947
1	-0.820912	2.396468	0.396014
7	-2.693985	-0.000001	-0.851144
1	-2.980439	-0.810316	-1.401146
1	-2.980439	0.810314	-1.401147
1	-3.313980	0.000000	0.006269
7	-0.282235	-1.866630	-0.290331
1	0.744622	-1.960771	-0.006946
1	-0.820912	-2.396467	0.396018
7	2.438432	2.116206	0.452333
1	2.843345	2.857669	-0.115580
1	2.526448	2.438618	1.413616
1	3.077002	1.322944	0.364587

1	-0.382983	-2.373846	-1.170645
7	2.438432	-2.116206	0.452332
1	2.526450	-2.438618	1.413616
1	2.843346	-2.857668	-0.115581
7	-4.498545	0.000001	1.403425
1	-5.114672	0.807529	1.338124
1	-4.159740	0.000001	2.362400
1	3.077003	-1.322943	0.364586
1	-5.114673	-0.807526	1.338124
7	4.946384	0.000001	0.175531
1	5.396459	0.803469	0.607866
1	5.272451	0.000001	-0.788185
1	5.396459	-0.803468	0.607865

E+ZPE = -2033.1028429999999

Cartesian coordinates of : 332-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.101491	0.002553	-0.118009
7	-1.410859	1.034378	0.529340
1	-1.368095	2.029738	0.304449
1	-1.536642	0.990293	1.541764
1	-2.303645	0.666381	0.097980
7	1.975674	-0.300863	-0.449258
1	2.294885	-1.209443	-0.110737
1	2.632169	0.439096	0.021249
1	2.212479	-0.285121	-1.442544
7	-3.835677	0.048191	-0.645068
1	-4.300308	-0.789991	-0.300920
1	-3.973346	0.036259	-1.654025
1	-4.422548	0.830360	-0.308762
7	3.701077	1.512229	0.689124
1	4.648495	1.264063	0.358647
1	3.570836	2.489181	0.436178
1	3.753021	1.501370	1.705312
7	-0.842829	-1.562831	-0.810958
1	-0.789608	-2.393151	-0.166621
1	-1.833426	-1.343054	-0.934148
1	-0.503455	-1.886123	-1.716711
7	-5.642919	2.331541	0.312723
1	-5.732421	2.511362	1.308682
1	-5.517423	3.242483	-0.119539
1	-6.561128	2.015120	0.012425
7	6.545676	0.875376	-0.231499
1	6.936478	-0.021772	0.041055
1	7.121995	1.574376	0.229026

1	6.742659	0.971001	-1.223464
7	-0.739652	-3.921452	0.898319
1	-1.687308	-4.251613	1.066402
1	-0.303916	-3.885586	1.816483
1	-0.276426	-4.685265	0.411022

E+ZPE = -2089.4806060000001

Cartesian coordinates of : 3321

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	1.547886	-0.040054	-0.340450
7	2.672014	-0.349970	1.236277
1	3.474286	-0.927950	0.976615
1	2.201706	-0.829709	2.002699
1	3.057329	0.535400	1.637462
7	-0.091930	0.321821	-1.065394
1	-0.169369	1.211050	-1.554756
1	-1.949880	0.528281	-0.115876
1	-0.456300	-0.383286	-1.702754
7	3.797146	2.111141	2.415676
1	4.792318	2.213788	2.234255
1	3.713242	2.053482	3.427609
1	3.381730	3.003092	2.160683
7	-2.926564	0.657673	0.195060
1	-3.493297	-0.247144	0.067020
1	-2.928205	0.906597	1.181456
1	-3.379834	1.435220	-0.344862
7	3.012429	-0.280911	-1.664241
1	3.791657	-0.826653	-1.270931
1	2.689104	-0.760363	-2.502810
1	3.397211	0.605989	-1.987406
7	-4.285801	2.774427	-1.258195
1	-4.327124	2.630721	-2.263585
1	-5.253391	2.826246	-0.950145
1	-3.909038	3.709645	-1.129288
7	-4.469226	-1.640617	-0.120519
1	-5.350133	-1.559014	0.406553
1	-4.037138	-2.505530	0.194057
1	-4.737226	-1.808096	-1.087113
7	5.221469	-1.970301	-0.260252
1	5.003836	-2.964588	-0.263570
1	5.902619	-1.849383	-1.007401
1	5.755304	-1.817904	0.592698
7	-7.150724	-1.526223	1.429160
1	-7.836381	-0.851652	1.103529
1	-7.102511	-1.407042	2.436465

1 -7.570894 -2.438915 1.279442

E+ZPE = -2145.8710179999998

Cartesian coordinates of : 332-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.000001	-0.758530	-0.437556
7	1.874152	-0.301467	-0.340179
1	2.357376	-0.421894	-1.231714
1	2.389528	-0.878682	0.325751
1	2.069565	0.730086	-0.044913
7	-1.874155	-0.301478	-0.340159
1	-2.357390	-0.421915	-1.231686
1	-2.069571	0.730077	-0.044900
1	-2.389519	-0.878690	0.325783
7	2.492472	2.286822	0.388064
1	2.250564	2.560221	1.337686
1	2.131608	3.027894	-0.208230
1	3.521651	2.359920	0.329988
7	-2.492481	2.286814	0.388069
1	-3.521661	2.359908	0.329995
1	-2.250571	2.560220	1.337688
1	-2.131622	3.027883	-0.208231
7	0.000003	-2.675441	-0.868964
1	0.000010	-3.281994	-0.005951
1	-0.810515	-2.966800	-1.415426
1	0.810516	-2.966794	-1.415435
7	5.532857	2.606125	0.238443
1	6.095794	2.028852	0.856327
1	5.959019	2.521934	-0.679865
1	5.704088	3.564253	0.530819
7	-5.532868	2.606105	0.238455
1	-5.959032	2.521909	-0.679852
1	-5.704102	3.564234	0.530828
1	-6.095801	2.028832	0.856343
7	0.000021	-4.445252	1.432015
1	-0.807570	-5.062335	1.380845
1	0.807612	-5.062335	1.380831
1	0.000029	-4.082996	2.382242

E+ZPE = -2089.4801840000000

Cartesian coordinates of : 340-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	0.317617	-0.426676	0.051867
7	-1.341839	-1.200746	-0.550380
1	-1.868346	-0.489713	-1.079901
1	-1.964421	-1.547154	0.227610
1	-1.217750	-1.993579	-1.182089
7	0.081108	1.421239	-0.541521
1	-0.787271	1.490842	-1.080970
1	0.827892	1.755953	-1.150588
1	0.019718	2.109486	0.248714
7	2.071844	-0.436817	0.886476
1	2.285317	0.447454	1.348825
1	2.172679	-1.148621	1.613013
7	-0.074149	3.417445	1.597251
1	0.696327	4.079550	1.538023
1	-0.911418	3.974110	1.440478
1	-0.118574	3.145143	2.576144
1	2.863091	-0.614811	0.200934
7	-2.741572	1.088151	-2.179538
1	-2.411977	1.311794	-3.116874
1	-3.549259	0.486810	-2.333863
1	-3.141918	1.954468	-1.824430
7	4.281442	-0.957868	-0.863730
1	4.675784	-1.870993	-0.647472
1	5.032237	-0.295101	-0.682204
1	4.157712	-0.952853	-1.873266
7	-3.108592	-2.230118	1.508424
1	-3.550381	-3.068460	1.137307
1	-3.875431	-1.599859	1.730786
1	-2.722605	-2.509874	2.406814

E+ZPE = -2033.1130140000000

Cartesian coordinates of : 340-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	-0.164830	-0.238869	-0.436194
7	1.736699	0.016927	-0.614566
1	2.315191	-0.862332	-0.545823
1	2.052393	0.661900	0.125797
1	1.997444	0.452148	-1.500896
7	-0.611849	1.294737	0.689356
1	-1.253457	1.089087	1.454650
1	-1.044796	2.083115	0.144713
1	0.247983	1.654946	1.113827
7	-1.866168	-1.125788	-0.743241

1	-1.854415	-1.754648	-1.549074
1	-2.199267	-1.714975	0.073530
7	2.450481	2.046784	1.664542
1	2.445269	1.731731	2.632853
1	3.432523	2.022743	1.394802
1	2.231341	3.040335	1.707854
1	-2.615451	-0.460682	-0.938573
7	3.424583	-2.341660	-0.490591
1	3.107801	-3.187160	-0.958815
1	4.302172	-2.100604	-0.945959
1	3.682026	-2.634775	0.448786
7	-1.823816	3.523629	-0.759144
1	-1.189697	4.319375	-0.763448
1	-2.648310	3.845791	-0.257035
1	-2.123832	3.419926	-1.725435
7	-2.873610	-2.782348	1.372996
1	-3.018360	-3.718587	1.000641
1	-2.345083	-2.915700	2.231620
1	-3.795657	-2.470410	1.670154

E+ZPE = -2033.1129010000000

Cartesian coordinates of : 341

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.194545	0.028625	0.335358
7	-1.477918	1.463004	0.490283
1	-1.192811	2.199973	1.136906
1	-2.361951	1.080462	0.858092
1	-1.696017	1.945924	-0.418747
7	1.579258	-0.702641	0.115557
1	1.845493	-1.331827	0.873959
1	2.362049	0.053915	0.077548
1	1.678861	-1.253403	-0.738063
7	-2.129447	2.898489	-1.961276
1	-2.143403	3.892816	-1.745532
1	-3.065921	2.684526	-2.295618
1	-1.526805	2.811063	-2.775589
7	3.630781	1.146832	0.030458
1	4.512510	0.608804	0.046038
1	3.677699	1.726057	-0.804678
1	3.692742	1.795422	0.811922
7	-1.391926	-1.501649	0.569029
1	-2.302933	-1.169880	0.898607
1	-1.554349	-2.045486	-0.313406
1	-1.064174	-2.178522	1.257785
7	-1.890259	-3.121340	-1.823324

1	-2.893981	-3.206817	-1.965470
1	-1.515262	-2.854165	-2.729875
1	-1.563045	-4.072033	-1.667253
7	6.306391	-0.344598	0.077926
1	6.530924	-0.859908	0.924038
1	7.005254	0.390326	0.013127
1	6.505288	-0.978049	-0.690824
7	-4.054797	0.109420	1.650972
1	-4.561887	0.991962	1.612584
1	-4.040867	-0.133350	2.639866
1	-4.690184	-0.560562	1.221842

E+ZPE = -2089.4890839999998

Cartesian coordinates of : 350-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	0.029097	-0.008099	-0.181250
7	1.816359	0.668268	0.009755
1	2.188394	0.547561	0.981156
1	1.870732	1.667229	-0.189088
1	2.502976	0.214908	-0.640117
7	-1.327345	-1.274049	-0.722966
1	-2.222260	-1.012637	-0.282798
1	-1.125471	-2.271757	-0.460573
1	-1.494387	-1.277602	-1.729986
7	3.805138	-0.509762	-1.816455
1	4.601538	0.123229	-1.808784
1	3.554133	-0.609463	-2.796776
1	4.179214	-1.413974	-1.539998
7	-0.862779	-4.080997	-0.062420
1	-1.313183	-4.366622	0.803596
1	-1.297805	-4.643819	-0.789893
1	0.091719	-4.424793	0.004949
7	-1.105529	1.364278	0.637125
1	-1.187952	2.223323	0.041940
1	-2.050490	0.995278	0.771684
1	-0.777557	1.678995	1.549591
7	-3.960145	-0.311335	0.680307
1	-4.084225	-0.445149	1.681965
1	-4.502961	0.519528	0.453059
1	-4.483441	-1.074426	0.254640
7	2.947172	0.378040	2.716814
1	3.217480	1.285530	3.088645
1	3.815644	-0.145278	2.634796
1	2.431527	-0.076585	3.465894
7	-1.373179	3.804343	-0.977013

1	-0.856584	3.912041	-1.846229
1	-2.349203	3.939533	-1.230148
1	-1.129518	4.618320	-0.417305

E+ZPE = -2089.4976929999998

Cartesian coordinates of : 350-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.372059	-0.025555	-0.322746
7	1.279492	0.803931	0.175313
1	1.569350	1.561054	-0.485035
1	2.019993	0.098204	0.155370
1	1.277081	1.214923	1.136120
7	-2.286728	-0.089235	-0.672959
1	-2.494204	-0.156466	-1.670402
1	-2.840863	0.740596	-0.321919
1	-2.716274	-0.913451	-0.251495
7	1.370034	1.986136	2.892507
1	2.267884	1.754741	3.310587
1	0.677238	1.732264	3.591857
1	1.349068	3.001958	2.848647
7	-3.925995	2.112769	0.214198
1	-3.616064	3.056745	-0.002632
1	-4.823445	2.012305	-0.255063
1	-4.143289	2.119776	1.207808
7	0.231809	-1.835775	-0.743944
1	1.240860	-1.912684	-0.550525
1	-0.260587	-2.571703	-0.190829
1	0.105546	-2.087608	-1.724284
7	-1.141524	-3.989133	0.765656
1	-0.404059	-4.630633	1.048131
1	-1.671893	-3.808329	1.614152
1	-1.759029	-4.541118	0.174875
7	2.175523	2.932041	-1.681149
1	2.842774	3.510090	-1.175860
1	1.489491	3.582509	-2.055381
1	2.682711	2.582521	-2.490361
7	3.293219	-1.859685	-0.130341
1	3.605502	-1.959438	0.833307
1	4.002450	-1.287984	-0.584591
1	3.418644	-2.784528	-0.537808

E+ZPE = -2089.4961589999998

Cartesian coordinates of : 351-1

Atomic number (AN) and Cartesian coordinates
AN X Y Z

29	0.433921	-0.077547	0.145758
7	2.340485	0.097983	0.307689
1	2.606282	1.047926	0.566669
1	2.836174	-0.106362	-0.590189
1	2.758706	-0.525424	1.037772
7	-0.118865	1.522870	-0.829184
1	0.190113	2.405093	-0.366041
1	-1.146468	1.536698	-0.890998
1	0.239603	1.560576	-1.782834
7	-1.289021	-0.918735	0.388460
1	-2.016296	-0.266896	0.060103
1	-1.399663	-1.809132	-0.154529
7	-1.671561	-3.413197	-1.104431
1	-0.942287	-3.753716	-1.725487
1	-1.859218	-4.181535	-0.464787
1	-2.503911	-3.334970	-1.683623
1	-1.519304	-1.143016	1.356663
7	-3.227816	1.234952	-0.743034
1	-3.525329	1.143036	-1.712425
1	-3.396521	2.211093	-0.507765
7	0.741348	4.067879	0.436026
1	0.931530	4.113742	1.433803
1	1.546598	4.497276	-0.013074
1	-3.921989	0.710652	-0.193065
1	-0.024806	4.719286	0.282172
7	3.593278	-1.597747	2.374292
1	4.576690	-1.338577	2.395349
1	3.263346	-1.470268	3.327619
1	3.583923	-2.602086	2.216344
7	3.826828	-0.462482	-2.185115
1	4.424068	0.327122	-2.418559
1	3.350745	-0.704218	-3.050223
1	4.463650	-1.235016	-2.005357
7	-5.343914	-0.292947	0.960504
1	-6.161497	-0.211419	0.361796
1	-5.331364	-1.261626	1.265994
1	-5.561816	0.250580	1.791235

E+ZPE = -2145.8727909999998

Cartesian coordinates of : 351-2

Atomic number (AN) and Cartesian coordinates
AN X Y Z

29	-0.401955	0.528491	0.006802
7	1.441189	0.796315	-0.502855
1	1.834034	1.717357	-0.190677
1	1.612706	0.735713	-1.506489
1	2.000893	0.049009	-0.064617
7	-2.231822	1.030110	0.332151
1	-2.687702	0.386116	1.011230
1	-2.815401	1.041721	-0.537669
1	-2.323685	1.964308	0.734115
7	2.811125	-1.565228	0.973577
1	2.775394	-2.580110	0.898226
1	3.028509	-1.384504	1.951787
1	3.658122	-1.297997	0.452210
7	-3.937852	1.196753	-2.061955
1	-3.565070	0.985427	-2.983814
1	-4.763493	0.611223	-1.963567
1	-4.291169	2.148445	-2.128207
7	-0.307299	-1.328153	0.590618
1	-0.606787	-2.007899	-0.144693
1	0.671131	-1.542864	0.822705
1	-0.876915	-1.519504	1.413281
7	5.404064	-0.850862	-0.589113
1	5.698389	-1.729441	-1.006943
1	5.526482	-0.152814	-1.316699
1	6.106117	-0.636425	0.113839
7	2.572445	3.365229	0.346675
1	3.220489	3.242092	1.120707
1	3.129300	3.745745	-0.414801
7	-1.091199	-3.331018	-1.433448
1	-0.421762	-3.447508	-2.189956
1	-1.995594	-3.228178	-1.886167
1	-1.126435	-4.233861	-0.966046
7	-3.594546	-0.701625	2.355119
1	-3.246964	-0.663910	3.310513
1	-3.797037	-1.682433	2.178239
1	-4.505660	-0.249377	2.391246
1	1.956084	4.122766	0.629605

E+ZPE = -2145.8720619999999

Cartesian coordinates of : 351-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	0.271434	0.262133	0.118758
7	1.667756	1.486249	0.628627
1	2.442028	0.993743	1.117736
1	1.346196	2.208014	1.275474

1	2.080860	2.002286	-0.184147
7	-1.508006	-0.276393	-0.376298
1	-1.706226	-0.205926	-1.374541
1	-2.271320	0.283265	0.121610
1	-1.627710	-1.264379	-0.122926
7	2.827733	3.061709	-1.570451
1	2.717268	4.045744	-1.337146
1	2.470609	2.970141	-2.517850
1	3.831352	2.915342	-1.644643
7	-3.543299	1.188031	0.916109
1	-4.410906	1.066464	0.373248
1	-3.758937	0.863927	1.855936
1	-3.416963	2.193463	1.003884
7	1.135080	-1.486702	0.231709
1	1.833412	-1.538529	0.971854
1	0.422486	-2.199006	0.419094
1	1.617116	-1.762250	-0.654812
7	-1.509194	-3.340626	0.609106
1	-1.012009	-4.177864	0.311909
1	-1.645467	-3.454895	1.611445
1	-2.438716	-3.447521	0.207486
7	-6.211832	0.922148	-0.622539
1	-6.222312	1.038188	-1.631374
1	-6.782751	1.677593	-0.254136
1	-6.733516	0.070466	-0.437788
7	3.894892	0.156700	2.139925
1	4.485453	0.969532	2.303161
1	4.513083	-0.533147	1.719952
1	3.681326	-0.199718	3.068646
7	2.487089	-2.362096	-2.238253
1	3.045003	-3.182256	-2.012451
1	1.855729	-2.663777	-2.976197
1	3.131809	-1.713899	-2.682939

E+ZPE = -2145.8715840000000

Cartesian coordinates of : 360-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.183818	0.022208	-0.004192
7	1.493219	-0.902352	-0.133105
1	2.176325	-0.282730	-0.575754
1	1.454030	-1.770606	-0.710229
1	1.886310	-1.170848	0.795123
7	0.361300	1.820861	-0.553958
1	0.322705	2.509430	0.228959
1	-0.218960	2.205193	-1.298531

1	1.327227	1.799410	-0.906650
7	-2.070239	0.209287	0.332885
1	-2.608966	0.345844	-0.551657
1	-2.499392	-0.605994	0.827985
7	-3.383348	-2.025565	1.759208
1	-3.512689	-2.883935	1.230033
1	-2.980895	-2.312323	2.647649
1	-4.321860	-1.703161	1.982510
1	-2.272218	1.022900	0.913567
7	-3.664755	0.598838	-2.134916
1	-4.405801	-0.097800	-2.120051
1	-3.244337	0.521371	-3.057284
7	0.256389	3.844391	1.616754
1	-0.075442	3.610265	2.548714
1	1.193308	4.216054	1.752932
1	-4.142842	1.496593	-2.130578
1	-0.305720	4.639684	1.323085
7	2.680725	-1.708360	2.474431
1	3.669494	-1.470880	2.482380
1	2.308749	-1.336975	3.344465
1	2.646839	-2.719576	2.576305
7	1.480869	-3.382320	-1.778819
1	2.328909	-3.893932	-1.547769
1	1.527735	-3.223244	-2.781948
1	0.722759	-4.046401	-1.646080
7	3.319958	1.499681	-1.577586
1	3.600411	0.908860	-2.357431
1	4.100669	1.473205	-0.925212
1	3.335558	2.444323	-1.957208

E+ZPE = -2145.8798029999998

Cartesian coordinates of : 360-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.001497	-0.349500	-0.306943
7	-1.892335	-0.201324	-0.015409
1	-2.452626	-0.800828	-0.660665
1	-2.173611	0.766500	-0.188711
1	-2.193583	-0.438981	0.954628
7	1.660277	-1.253482	-0.685512
1	1.541983	-2.050472	-1.312761
1	2.135121	-1.637584	0.163641
1	2.332503	-0.618992	-1.161826
7	-2.877457	-0.905655	2.699726
1	-3.420363	-0.143393	3.097479
1	-2.232842	-1.188229	3.432986

1	-3.530825	-1.679016	2.603294
7	3.057958	-2.487550	1.603975
1	3.127231	-3.485623	1.420007
1	4.018472	-2.158411	1.660423
1	2.690698	-2.414292	2.548858
7	0.510068	1.535190	-0.297978
1	-0.319242	2.115674	-0.481118
1	0.912919	1.852072	0.611108
1	1.205358	1.752595	-1.010400
7	1.639659	2.569053	2.240419
1	0.919492	2.892395	2.881293
1	2.248675	1.973962	2.795462
1	2.194360	3.393564	2.023439
7	-3.529115	-1.895274	-1.832590
1	-4.505051	-1.704783	-1.619096
1	-3.422378	-2.900453	-1.723060
1	-3.433934	-1.720608	-2.829676
7	-2.196307	3.065295	-0.780425
1	-2.898494	3.231456	-0.062719
1	-2.719247	2.937946	-1.644212
1	-1.730956	3.963849	-0.892610
7	3.620063	0.477627	-2.158487
1	4.097228	1.250886	-1.701736
1	3.353039	0.826612	-3.075977
1	4.349802	-0.207515	-2.342725

E+ZPE = -2145.8789889999998

Cartesian coordinates of : 361-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.808455	0.282317	0.050798
7	2.649989	-0.222797	0.342866
1	2.911216	-0.216624	1.329001
1	3.334952	0.401266	-0.142586
1	2.819481	-1.189360	0.004580
7	-0.101838	-1.432349	0.004824
1	-0.930366	-1.425335	-0.625752
1	-0.423046	-1.720969	0.949370
1	0.516638	-2.174046	-0.321362
7	-0.627201	1.526349	-0.227953
1	-1.501211	1.179854	0.238017
1	-0.433407	2.485481	0.134180
7	-0.139008	4.275660	0.795885
1	0.775108	4.549917	1.145468
1	-0.360170	4.946473	0.064280
1	-0.787700	4.476519	1.552636

1	-0.857853	1.631921	-1.215843
7	-3.047702	0.503704	1.006044
1	-3.467646	1.148264	1.671132
1	-2.964837	-0.382229	1.496729
7	-2.416688	-1.479250	-1.865827
1	-2.197249	-1.248961	-2.831734
1	-2.730487	-2.446635	-1.890469
1	-3.741761	0.356498	0.270292
1	-3.240498	-0.927977	-1.623893
7	3.174128	-3.029853	-0.641259
1	2.830404	-3.845188	-0.139668
1	3.024604	-3.234097	-1.626457
1	4.184002	-3.056900	-0.517763
7	4.638174	1.496391	-1.006279
1	5.439216	1.603240	-0.388646
1	4.385145	2.441157	-1.283152
1	5.002810	1.057959	-1.848206
7	-5.326853	0.052108	-1.276152
1	-5.756481	0.939656	-1.027225
1	-5.419460	-0.007072	-2.287082
1	-5.951906	-0.660727	-0.907929
7	-0.924069	-2.414347	2.738204
1	-0.189077	-3.021373	3.092874
1	-1.745419	-3.010004	2.666785
1	-1.122702	-1.767203	3.496817

E+ZPE = -2202.2531260000001

Cartesian coordinates of : 361-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.716988	0.476811	-0.501608
7	2.633247	0.297001	-0.666836
1	2.887451	-0.667569	-0.955684
1	3.151000	0.509378	0.216136
1	3.033637	0.914489	-1.374331
7	0.142504	-1.348766	-0.169404
1	0.774072	-2.025031	-0.596808
1	-0.807013	-1.527555	-0.556511
1	0.116862	-1.580021	0.842657
7	-0.950540	1.426590	-0.537834
1	-1.588272	1.078463	0.218630
1	-0.863116	2.461799	-0.438998
7	-0.767746	4.384243	-0.312495
1	-0.789863	4.727780	0.644051
1	0.011115	4.864280	-0.755541
1	-1.601607	4.762173	-0.755262

1	-1.447902	1.264948	-1.413687
7	-2.755078	0.365560	1.472942
1	-3.105611	1.069109	2.118096
1	-2.412944	-0.394081	2.054445
7	3.411112	-2.460603	-1.601369
1	3.028230	-2.786556	-2.485649
1	4.398385	-2.298495	-1.788153
1	-3.569346	-0.000660	0.975544
1	3.392128	-3.267709	-0.982924
7	4.219516	0.958714	1.736782
1	4.760675	0.159873	2.057458
1	3.766075	1.330885	2.566799
1	4.907377	1.658835	1.469688
7	-5.414679	-0.750926	-0.048419
1	-5.782132	-1.505609	0.525910
1	-5.918094	0.081158	0.249142
1	-5.756183	-0.939050	-0.987617
7	-2.547488	-1.891240	-1.331908
1	-2.642165	-1.742215	-2.333481
1	-3.353182	-1.437717	-0.900100
1	-2.691879	-2.889721	-1.200713
7	0.147344	-2.199695	2.724748
1	-0.599270	-2.872191	2.881936
1	0.074677	-1.529431	3.485599
1	1.006910	-2.713242	2.902558

E+ZPE = -2202.2526840000000

Cartesian coordinates of : 361-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.153816	-0.035307	0.008088
7	1.513175	-1.384775	0.005450
1	2.429781	-0.923105	0.038888
1	1.498077	-1.975775	-0.851544
1	1.464825	-2.026771	0.823738
7	-1.670803	0.621935	0.006334
1	-1.855207	1.222603	0.809928
1	-2.420351	-0.143020	0.022559
1	-1.866568	1.197723	-0.812619
7	1.462790	-3.251825	2.342529
1	1.831503	-4.146658	2.030632
1	0.578668	-3.468459	2.794704
1	2.082070	-2.950379	3.090340
7	-3.686131	-1.340494	0.046750
1	-4.592255	-0.851026	0.005429
1	-3.691223	-1.994111	-0.732386

1	-3.724439	-1.918476	0.882693
7	1.216278	1.588068	0.022155
1	2.208522	1.345110	0.063184
1	1.069032	2.160911	-0.830770
1	1.005019	2.193375	0.837699
7	0.816924	3.284772	-2.438789
1	1.740556	3.459883	-2.826754
1	0.252343	2.978982	-3.226857
1	0.454935	4.200898	-2.186402
7	-6.461507	0.010904	-0.068168
1	-6.717632	0.604988	0.714704
1	-7.118810	-0.763634	-0.050997
1	-6.686484	0.542622	-0.903672
7	4.248878	0.273219	0.120353
1	4.761867	-0.601325	0.209998
1	4.572039	0.839721	0.901524
1	4.635292	0.714474	-0.711217
7	0.622390	3.375350	2.384150
1	1.508954	3.826578	2.595887
1	-0.022409	4.136679	2.188160
1	0.310547	2.976042	3.265496
7	1.527571	-3.108544	-2.439981
1	0.888115	-2.920040	-3.207182
1	1.359715	-4.077249	-2.180634
1	2.455903	-3.096927	-2.854565

E+ZPE = -2202.2523350000001

Cartesian coordinates of : 370

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.004288	-0.220763	-0.028132
7	-1.895295	-0.530993	0.071422
1	-2.185336	-1.491829	-0.205184
1	-2.348205	0.117090	-0.580105
1	-2.301357	-0.355069	1.013539
7	1.878034	-0.583522	0.055732
1	2.138571	-1.560592	-0.191803
1	2.300539	-0.386973	0.986517
1	2.339566	0.031186	-0.621535
7	-3.165153	-0.112871	2.744863
1	-3.803350	0.678474	2.749005
1	-2.589646	-0.001944	3.575122
1	-3.745329	-0.927933	2.926747
7	3.187810	-0.105439	2.699515
1	3.603977	-0.981840	3.004021
1	3.964105	0.545191	2.611741

1	2.645421	0.225298	3.492734
7	0.018872	1.564480	-0.813470
1	-0.820201	1.703139	-1.383490
1	0.039611	2.330593	-0.109802
1	0.851354	1.672523	-1.399600
7	0.084417	3.857140	1.100600
1	-0.535768	4.584089	0.752822
1	-0.183468	3.714254	2.070415
1	1.006505	4.284135	1.133347
7	-2.827832	-3.265107	-0.709581
1	-3.843364	-3.231082	-0.747763
1	-2.607978	-4.002821	-0.045698
1	-2.536170	-3.619105	-1.616646
7	-2.920715	1.621893	-2.186082
1	-3.719118	1.997957	-1.679404
1	-3.306699	0.922853	-2.816875
1	-2.624210	2.380294	-2.796708
7	2.923897	1.500738	-2.260413
1	3.781720	1.778019	-1.788354
1	2.665002	2.312698	-2.816896
1	3.206363	0.801595	-2.943754
7	2.726935	-3.366381	-0.642200
1	2.475451	-3.708071	-1.565884
1	2.436126	-4.093635	0.005701
1	3.743451	-3.375941	-0.619087

E+ZPE = -2202.2592380000001

Cartesian coordinates of : 400

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.000002	-0.000002	-0.000018
7	-1.122671	-1.610985	0.541760
1	-0.612776	-2.292084	1.107317
1	-1.496215	-2.146861	-0.244347
1	-1.938089	-1.368428	1.107446
7	-1.611041	1.122626	-0.541742
1	-1.368526	1.938147	-1.107297
1	-2.146993	1.496008	0.244388
1	-2.292057	0.612748	-1.107412
7	1.122659	1.610989	0.541762
1	1.938177	1.368431	1.107304
1	1.496051	2.146972	-0.244343
7	1.611049	-1.122626	-0.541736
1	2.292056	-0.612750	-1.107420
1	2.147010	-1.495993	0.244395
1	1.368536	-1.938157	-1.107279

1 0.612799 2.291993 1.107465

E+ZPE = -1863.9746849999999

Cartesian coordinates of : 410

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.546912	-0.000534	-0.046909
7	-1.698889	-1.535028	0.646116
1	-1.181091	-2.165297	1.260901
1	-2.073007	-2.131679	-0.094212
7	0.803365	1.476502	0.223717
1	0.643412	2.045154	1.056350
7	0.888319	-1.200889	-0.811675
1	0.948713	-1.122915	-1.829019
1	1.810618	-0.910438	-0.455920
1	0.808430	-2.200787	-0.629944
7	3.591156	-0.004373	0.298888
1	3.975592	-0.940308	0.421744
1	3.889241	0.489534	1.139143
1	1.744984	1.071749	0.323867
1	4.148899	0.402382	-0.450934
1	0.870093	2.142028	-0.547546
1	-2.511150	-1.250329	1.194802
7	-2.134811	1.266445	-0.240262
1	-2.486461	1.627474	0.648506
1	-1.927007	2.096049	-0.797730
1	-2.944785	0.844285	-0.697141

E+ZPE = -1920.3655340000000

Cartesian coordinates of : 420-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.000000	0.000000	-0.112010
7	-1.470101	1.335485	-0.523714
1	-1.543639	1.537380	-1.522405
1	-1.373956	2.245514	-0.074374
1	-2.390093	0.971022	-0.241645
7	-1.377169	-1.428197	0.288731
1	-1.196065	-1.932690	1.157492
1	-1.451551	-2.147804	-0.430989
1	-2.318829	-1.023940	0.381197
7	1.470101	-1.335485	-0.523715

1	1.543639	-1.537380	-1.522405
1	2.390093	-0.971022	-0.241645
7	1.377169	1.428197	0.288731
1	2.318829	1.023940	0.381197
1	1.451551	2.147804	-0.430989
1	1.196065	1.932690	1.157492
1	1.373956	-2.245514	-0.074375
7	4.190919	-0.000281	0.381411
1	4.503524	0.573702	1.163204
1	4.581967	-0.919163	0.584160
1	4.726699	0.335696	-0.417488
7	-4.190919	0.000280	0.381411
1	-4.581970	0.919164	0.584146
1	-4.503522	-0.573691	1.163213
1	-4.726698	-0.335710	-0.417483

E+ZPE = -1976.7553069999999

Cartesian coordinates of : 420-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.005758	-0.727221	0.071153
7	1.987322	-0.600273	-0.302259
1	2.283970	0.387455	-0.330038
1	2.275778	-1.013233	-1.189818
1	2.575213	-1.042929	0.404938
7	-0.011697	1.132249	0.839861
1	0.814575	1.665862	0.551310
1	-0.017695	1.148319	1.860647
1	-0.842899	1.652993	0.541537
7	-2.815053	2.367405	-0.221212
1	-3.546585	2.221079	-0.915423
1	-2.368444	3.233581	-0.517397
1	-3.318236	2.610173	0.630779
7	0.021871	-2.773601	0.049586
1	0.043341	-3.167439	-0.892563
1	-0.791672	-3.197508	0.496446
7	-1.975386	-0.630613	-0.314238
1	-2.284796	0.352721	-0.351920
1	-2.560616	-1.074229	0.394600
1	-2.254137	-1.055829	-1.199049
7	2.779178	2.410555	-0.226341
1	2.769022	3.087100	0.535284
1	2.562355	2.951821	-1.061459
1	3.765081	2.172782	-0.326424
1	0.825119	-3.183357	0.527344

E+ZPE = -1976.7546600000001

Cartesian coordinates of : 420-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.739165	-0.120194	0.027403
7	0.890049	0.618952	0.900593
1	1.283973	1.422980	0.351776
1	1.623379	-0.093505	0.927938
1	0.795499	0.963277	1.854831
7	-1.946530	0.142427	1.659783
1	-2.887079	-0.244891	1.580354
1	-2.080062	1.123576	1.909654
1	-1.553966	-0.295359	2.494362
7	2.039345	2.911734	-0.531676
1	1.515149	3.409764	-1.246940
1	2.937032	2.697703	-0.960207
1	2.247524	3.612231	0.176938
7	-2.309700	-0.032965	-1.280484
1	-2.903292	-0.863972	-1.266815
1	-2.941548	0.751567	-1.115120
7	0.395510	-1.265397	-1.180838
1	0.731905	-0.779216	-2.012711
1	1.245380	-1.570994	-0.672067
1	-0.054363	-2.113489	-1.525903
7	2.898174	-2.060186	0.366848
1	2.837088	-2.509956	1.278350
1	3.155020	-2.814004	-0.268844
1	3.733226	-1.479178	0.412992
1	-2.017013	0.067124	-2.252845

E+ZPE = -1976.7529589999999

Cartesian coordinates of : 421-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.573795	0.151089	0.161244
7	1.580505	-1.546981	-0.294096
1	1.249881	-1.995568	-1.148977
1	1.526675	-2.266069	0.427722
1	2.582375	-1.360212	-0.433203
7	-0.422813	1.858678	-0.216448
1	-0.393039	2.537436	0.544783
1	-1.426212	1.662053	-0.387407

1	-0.082497	2.359003	-1.038112
7	4.636094	-0.765816	-0.521930
1	5.128689	-1.240341	0.233133
1	5.204111	0.055789	-0.723004
1	4.773688	-1.361751	-1.336802
7	-3.329964	1.106567	-0.611672
1	-3.769586	1.892594	-0.135319
1	-3.476993	1.286681	-1.603491
1	-3.933108	0.298891	-0.396739
7	2.320863	1.083749	0.613314
1	2.467033	1.163749	1.620993
1	3.125666	0.554623	0.253279
1	2.415130	2.032872	0.254296
7	-5.180425	-1.293823	0.038815
1	-5.232027	-1.746189	0.947300
1	-5.231954	-2.045370	-0.643497
7	-1.167391	-0.802324	0.562872
1	-1.962544	-0.266573	0.187146
1	-1.342656	-0.886711	1.565439
1	-1.262556	-1.747919	0.195588
1	-6.058220	-0.788926	-0.055200

E+ZPE = -2033.1326690000001

Cartesian coordinates of : 422

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.004754	-0.517512	-0.207552
7	-1.281321	-1.846475	0.596014
1	-0.962827	-2.234242	1.484353
1	-1.469312	-2.653128	0.000541
7	1.390714	0.956039	-0.178851
1	1.261498	1.628889	0.576849
7	1.442339	-1.887348	-0.582111
1	1.476428	-2.155613	-1.566784
1	2.375915	-1.498146	-0.360252
1	1.361851	-2.764375	-0.069885
7	4.099273	-0.558817	0.068214
1	4.410661	-1.104195	0.870218
1	4.453730	0.393064	0.242850
1	2.335293	0.564992	-0.056703
1	4.654016	-0.903237	-0.713773
1	1.427313	1.511577	-1.033507
1	-2.198673	-1.403260	0.779379
7	-1.533466	0.717928	-0.676242
1	-1.385237	1.708750	-0.491906
1	-1.787898	0.664923	-1.663684

1	-2.381258	0.450161	-0.156674
7	-3.926630	-0.394099	0.977426
1	-3.997906	-0.274923	1.986518
1	-4.542594	-1.176612	0.762551
1	-4.401683	0.428119	0.576743
7	5.224157	2.283787	0.583608
1	5.139743	3.030905	-0.099903
1	6.207599	2.025337	0.574794
1	5.071901	2.721487	1.488004
7	-5.423230	2.035368	-0.233027
1	-5.096754	2.997500	-0.233732
1	-5.811200	1.878461	-1.159221
1	-6.221317	2.026736	0.397021

E+ZPE = -2089.5094840000002

Cartesian coordinates of : 430-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.073668	-0.429413	0.289842
7	-1.295526	1.167437	0.410690
1	-1.594864	1.375495	1.363748
1	-2.155465	1.026839	-0.123716
1	-0.827127	2.016184	0.071982
7	1.145933	-1.884448	-0.408797
1	1.208572	-2.692309	0.211368
1	2.110580	-1.543406	-0.528384
1	0.859202	-2.258175	-1.313756
7	0.540905	3.644841	-0.373755
1	-0.142070	4.315603	-0.025532
1	0.537224	3.768668	-1.384453
1	1.434890	4.027710	-0.071064
7	4.054391	-0.744379	-0.631563
1	4.659648	-0.800329	0.185771
1	4.331886	-1.539074	-1.205554
1	4.386553	0.064776	-1.153090
7	-1.680570	-1.649097	0.421238
1	-1.946315	-1.836295	1.389275
1	-2.500807	-1.194022	-0.013155
1	-1.592803	-2.567197	-0.011457
7	-4.081356	-0.177939	-0.848054
1	-4.617440	-1.038900	-0.944234
1	-4.688251	0.433526	-0.305070
1	-4.073642	0.218486	-1.785841
7	1.507383	0.748524	0.701661
1	1.340519	1.699751	0.355543
1	2.374716	0.401431	0.281329

1 1.693247 0.839637 1.700955

E+ZPE = -2033.1413889999999

Cartesian coordinates of : 430-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.001220	0.854334	-0.008097
7	1.980993	0.886924	-0.398870
1	2.292063	-0.018027	-0.794740
1	2.558767	1.034279	0.429144
1	2.271794	1.605328	-1.062142
7	0.001364	-1.125223	0.173128
1	0.002216	-1.437979	1.170492
1	0.821522	-1.545014	-0.267023
1	-0.818044	-1.547149	-0.266376
7	-2.907030	-1.821693	-1.463730
1	-3.814149	-1.483391	-1.780641
1	-3.131024	-2.598424	-0.844852
1	-2.492886	-2.247709	-2.290238
7	-0.003626	2.820364	0.588546
1	0.804740	3.078707	1.154435
1	-0.813533	3.077376	1.152825
7	-1.983570	0.881910	-0.398526
1	-2.292499	-0.023940	-0.794014
1	-2.276181	1.599376	-1.062017
1	-2.561603	1.028152	0.429503
7	2.910518	-1.813861	-1.466044
1	2.502278	-2.230271	-2.300353
1	3.125770	-2.597422	-0.852703
1	3.821902	-1.476213	-1.771199
1	-0.003393	3.477244	-0.193127
7	0.004520	-2.074325	2.983740
1	0.826016	-1.849010	3.539357
1	-0.789685	-1.809354	3.561087
1	-0.020872	-3.090897	2.949698

E+ZPE = -2033.1396270000000

Cartesian coordinates of : 431

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.763333	0.398279	-0.334661
7	1.238128	0.453857	-0.568071

1	1.536259	0.461252	-1.543703
1	1.670297	-0.375996	-0.147083
1	1.656729	1.280879	-0.134878
7	-0.792379	2.341781	0.231202
1	-1.389676	2.522776	1.037919
1	-1.125616	2.969513	-0.500753
1	0.149400	2.675455	0.483353
7	-2.740219	0.335200	-0.733005
1	-2.925739	0.105115	-1.710180
1	-3.193316	-0.415151	-0.177195
7	-0.710782	-1.604897	-0.210625
1	-1.477172	-1.976127	0.351101
1	-0.782883	-2.071865	-1.114685
1	0.184733	-1.918232	0.202983
1	-3.269375	1.187733	-0.557905
7	-4.048092	-1.885729	0.861232
1	-5.001293	-1.532868	0.797432
1	-4.100770	-2.826456	0.476069
1	-3.889055	-2.012375	1.858402
7	2.116542	3.270206	0.858039
1	2.621538	3.725726	0.100066
1	2.833209	2.823369	1.426596
1	1.781855	4.037908	1.437982
7	4.869300	-1.674530	-0.383449
1	5.279510	-0.793187	-0.678173
1	5.017276	-2.313379	-1.160144
1	5.470847	-2.012810	0.363129
7	2.063609	-2.306513	0.805632
1	1.975575	-3.305084	0.624818
1	2.987205	-2.056607	0.426085
1	2.154352	-2.235313	1.817243

E+ZPE = -2089.5174179999999

Cartesian coordinates of : 432-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.131119	0.755203	0.072206
7	-2.128421	1.013805	-0.097719
1	-2.438962	1.418994	-0.979936
1	-2.534718	1.602661	0.629068
1	-2.594378	0.096051	-0.012582
7	1.707723	0.155836	-0.494035
1	1.818077	0.075842	-1.504796
1	1.942752	-0.768341	-0.105656
1	2.420734	0.820043	-0.189310
7	-3.279187	-1.802445	0.283245

1	-3.524360	-2.236580	1.171297
1	-3.072082	-2.579013	-0.341858
1	-4.164733	-1.408648	-0.067384
7	2.097034	-2.668611	0.729830
1	2.941990	-2.719438	0.143019
1	2.430999	-2.792684	1.683870
1	1.586131	-3.523634	0.517688
7	0.337819	2.681062	-0.317922
1	1.336585	2.850506	-0.110110
1	0.202247	2.946486	-1.293383
1	-0.192739	3.362793	0.223121
7	-5.984122	-0.672853	-0.736357
1	-6.430354	0.113733	-0.273455
1	-6.095245	-0.504584	-1.732158
1	-6.574060	-1.474958	-0.531418
7	4.656359	-2.944729	-1.017723
1	4.547151	-3.072787	-2.019654
1	4.970626	-3.844221	-0.663405
1	5.449608	-2.320168	-0.905488
7	3.313307	3.086406	0.300159
1	4.045218	2.907056	-0.384069
1	3.252265	4.102135	0.342878
1	3.711013	2.816953	1.197397
7	-0.409696	-0.877815	1.193958
1	-1.295709	-1.331786	0.938747
1	0.358376	-1.552024	1.076805
1	-0.469687	-0.679862	2.192742

E+ZPE = -2145.8935600000000

Cartesian coordinates of : 432-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.037919	0.139941	-0.480903
7	1.361418	1.638431	-0.302213
1	0.945773	2.435388	0.190410
1	1.687022	2.003147	-1.197326
7	-1.302087	-1.319572	-0.078510
1	-1.100646	-1.840351	0.774750
7	-1.443381	1.467116	-0.756731
1	-1.563415	1.746106	-1.730451
1	-2.352505	1.100115	-0.445330
1	-1.242775	2.327223	-0.235613
7	-4.052799	0.035064	0.170399
1	-4.327203	0.592683	0.977044
1	-4.404501	-0.912662	0.371234
1	-2.249792	-0.928677	0.037750

1	-4.637781	0.370021	-0.593123
1	-1.376560	-2.021383	-0.814690
1	2.201839	1.322602	0.198101
7	1.581361	-1.149807	-0.715189
1	1.430790	-2.112330	-0.419221
1	1.895798	-1.213184	-1.684101
1	2.390830	-0.796877	-0.180266
7	3.861201	0.163577	0.887898
1	3.795615	0.243018	1.900896
1	4.511324	0.896397	0.609262
1	4.374742	-0.713980	0.720032
7	-5.198249	-2.788315	0.760509
1	-5.231689	-3.468876	0.006862
1	-6.165475	-2.522928	0.926316
1	-4.917008	-3.307423	1.587279
7	5.487383	-2.429143	0.370259
1	5.163389	-3.356181	0.630326
1	5.881965	-2.528176	-0.560844
1	6.278599	-2.241217	0.980263
7	-0.399875	4.045669	0.896928
1	-1.299200	4.489981	0.722037
1	0.282277	4.753005	0.630076
1	-0.335878	3.985136	1.911056

E+ZPE = -2145.8932629999999

Cartesian coordinates of : 433

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.213320	-0.435682	0.022158
7	1.949556	-1.460670	-0.119013
1	2.093554	-1.947143	-1.002826
1	2.074143	-2.168574	0.604149
1	2.736713	-0.799797	-0.010666
7	-1.216394	0.842737	-0.568497
1	-1.222274	1.019520	-1.572682
1	-1.122098	1.759996	-0.118687
1	-2.139087	0.453656	-0.342209
7	4.110509	0.658658	0.306990
1	4.481894	0.971255	1.202170
1	4.219508	1.455489	-0.317271
1	4.792154	-0.037438	-0.028699
7	-0.496655	3.550944	0.894661
1	-1.217062	3.930036	0.265465
1	-0.837927	3.737439	1.835644
1	0.301592	4.172084	0.777380
7	-0.982627	-2.005048	-0.420147

1	-1.963795	-1.722748	-0.265441
1	-0.924711	-2.313171	-1.390348
1	-0.825993	-2.841198	0.140761
7	6.229199	-1.394085	-0.662778
1	6.353133	-2.269036	-0.161712
1	6.268347	-1.633837	-1.649201
1	7.073169	-0.857391	-0.481593
7	-2.639533	4.797335	-1.001255
1	-2.301832	5.058486	-1.923257
1	-2.774895	5.673600	-0.504122
1	-3.572885	4.423826	-1.146198
7	-3.798050	-0.890466	0.052994
1	-4.389566	-0.495278	-0.675494
1	-4.101948	-1.871604	0.134098
1	-4.108112	-0.448006	0.915891
7	1.076395	0.921723	1.212573
1	2.069891	1.014378	0.972607
1	0.622011	1.843285	1.129762
1	1.045839	0.672893	2.201089
7	-4.779207	-3.828896	0.279287
1	-4.749543	-4.224597	1.214672
1	-4.473268	-4.571531	-0.342648
1	-5.765575	-3.695434	0.073092

E+ZPE = -2202.2686910000002

Cartesian coordinates of : 440-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.055537	0.271121	-0.064931
7	-1.747724	-0.226191	0.912322
1	-1.722920	0.011842	1.903934
1	-1.897225	-1.242195	0.867107
1	-2.575745	0.237822	0.529176
7	-1.021686	1.778422	-1.021704
1	-0.865800	1.778508	-2.029580
1	-0.733324	2.702832	-0.701458
1	-2.040603	1.731550	-0.885156
7	1.758732	0.934157	-0.578801
1	2.269187	1.338218	0.238360
1	2.324333	0.151707	-0.917927
7	0.748300	-1.509444	0.421524
1	1.502922	-1.768499	-0.227664
1	1.165962	-1.514324	1.351960
1	0.040756	-2.248581	0.427206
1	1.794741	1.646640	-1.305436
7	3.180930	-1.943130	-1.504171

1	2.821464	-2.519867	-2.262200
1	3.879424	-1.348932	-1.946363
1	3.723586	-2.578686	-0.922434
7	-4.106266	1.534829	-0.481419
1	-4.574174	1.747636	0.397630
1	-4.665089	0.799877	-0.910575
1	-4.279023	2.354667	-1.060727
7	3.265508	2.138834	1.678590
1	3.788371	2.920676	1.290583
1	3.969678	1.516857	2.067995
1	2.771966	2.521623	2.480877
7	-1.908770	-3.393959	0.744330
1	-1.403430	-4.066283	1.318278
1	-2.845282	-3.381552	1.144070
1	-2.022360	-3.848685	-0.159352

E+ZPE = -2089.5255020000000

Cartesian coordinates of : 442-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.077603	-0.409121	0.083191
7	-2.083486	-0.319651	0.317595
1	-2.404222	-0.508314	1.266150
1	-2.571578	-0.991281	-0.273573
1	-2.433575	0.616481	0.064873
7	1.855060	-0.093933	0.538396
1	2.016509	0.072594	1.531131
1	2.240820	0.719531	0.046651
1	2.407640	-0.923615	0.297163
7	-2.838028	2.555095	-0.515136
1	-3.082515	2.831458	-1.464157
1	-2.473307	3.399808	-0.079298
1	-3.740652	2.387191	-0.048652
7	2.612891	2.554312	-1.008754
1	3.436670	2.532734	-0.393079
1	2.983273	2.503277	-1.955716
1	2.249194	3.501156	-0.920192
7	0.041507	-2.323316	0.657981
1	0.975330	-2.681272	0.439394
1	-0.083643	-2.462026	1.660105
1	-0.654398	-2.936708	0.194110
7	-5.598586	2.136461	0.860019
1	-6.216348	1.381529	0.576762
1	-5.639238	2.159813	1.874816
1	-6.056074	2.989894	0.551050
7	5.124061	2.604682	0.848733

1	4.974945	3.181599	1.671774
1	5.752893	3.137277	0.253676
1	5.666632	1.807760	1.168186
7	3.183860	-2.947562	-0.062331
1	4.009928	-2.514696	-0.470278
1	3.524810	-3.423703	0.770297
1	2.941938	-3.690966	-0.713969
7	-0.118076	1.113891	-1.217299
1	-0.927820	1.718337	-1.034922
1	0.743582	1.675900	-1.168828
1	-0.205935	0.809185	-2.186492
7	-1.977836	-4.146608	-0.655689
1	-1.608383	-5.066414	-0.426172
1	-2.048614	-4.134777	-1.670023
1	-2.936947	-4.160842	-0.317942

E+ZPE = -2202.2758450000001

Cartesian coordinates of : 442-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.000001	0.000000	-0.482816
7	-1.874042	-0.743452	-0.515066
1	-1.920114	-1.638206	-0.017277
1	-2.228424	-0.920904	-1.454505
7	1.874041	0.743452	-0.515072
1	1.920114	1.638206	-0.017283
7	0.740338	-1.863426	-0.395018
1	0.878984	-2.282173	-1.314499
1	1.662886	-1.871787	0.064818
1	0.106908	-2.490739	0.108888
7	3.578092	-1.594642	0.791299
1	3.598634	-1.532609	1.807097
1	4.386302	-1.049285	0.462660
1	2.537451	0.093559	-0.079735
1	3.821104	-2.561918	0.585989
1	2.228420	0.920904	-1.454511
1	-2.537451	-0.093560	-0.079728
7	-0.740340	1.863426	-0.395014
1	-0.106909	2.490738	0.108892
1	-0.878988	2.282174	-1.314494
1	-1.662887	1.871787	0.064823
7	-3.578092	1.594640	0.791306
1	-3.821103	2.561918	0.585999
1	-3.598636	1.532604	1.807103
1	-4.386303	1.049286	0.462663
7	6.088252	-0.056077	-0.237478

1	6.480945	-0.591473	-1.006838
1	6.739091	-0.171480	0.534645
1	6.169245	0.917418	-0.515398
7	-6.088252	0.056081	-0.237483
1	-6.169245	-0.917412	-0.515405
1	-6.739093	0.171484	0.534639
1	-6.480943	0.591480	-1.006843
7	-1.627358	-3.588745	0.975767
1	-0.962076	-4.060788	1.584689
1	-1.944429	-4.307054	0.327853
1	-2.427769	-3.401369	1.575920
7	1.627364	3.588741	0.975764
1	0.962074	4.060810	1.584657
1	2.427751	3.401356	1.575947
1	1.944473	4.307033	0.327851

E+ZPE = -2202.2757689999999

Cartesian coordinates of : 442-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.000087	0.358785	-0.500885
7	1.422632	1.776591	-0.484524
1	1.096488	2.622688	-0.007553
1	1.707914	2.070336	-1.418481
7	-1.423673	-1.066682	-0.457934
1	-1.104418	-1.887519	0.065259
7	-1.422811	1.776581	-0.484027
1	-1.708422	2.070322	-1.417885
1	-2.275019	1.434835	-0.017368
1	-1.096506	2.622681	-0.007172
7	-3.920737	0.429634	0.767532
1	-3.915021	0.410055	1.785264
1	-4.458531	-0.398071	0.476429
1	-2.285784	-0.715274	-0.025746
1	-4.517617	1.219016	0.527704
1	-1.690662	-1.404689	-1.382151
1	2.275007	1.434850	-0.018164
7	1.423525	-1.066671	-0.458436
1	1.104459	-1.887512	0.064869
1	1.690191	-1.404676	-1.382747
1	2.285785	-0.715258	-0.026550
7	3.921007	0.429661	0.766158
1	3.915646	0.410100	1.783892
1	4.517803	1.219040	0.526108
1	4.458700	-0.398048	0.474881
7	-5.662858	-1.989715	-0.141792

1	-6.206400	-1.704786	-0.951748
1	-6.329713	-2.063615	0.621667
1	-5.366603	-2.941823	-0.334558
7	5.662816	-1.989699	-0.143733
1	5.366497	-2.941812	-0.336376
1	6.206073	-1.704785	-0.953884
1	6.329937	-2.063583	0.619495
7	0.000121	4.346196	0.849893
1	-0.803241	4.532022	1.446721
1	-0.000192	5.100518	0.166241
1	0.803869	4.532182	1.446152
7	0.000202	-3.530110	1.069813
1	0.803936	-3.659125	1.680882
1	-0.803323	-3.659140	1.681152
1	0.000107	-4.344192	0.458682

E+ZPE = -2202.2757080000001

Cartesian coordinates of : 442-4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.219625	0.932365	-0.158565
7	-0.603569	-0.859842	0.103192
1	0.090441	-1.548925	0.406341
1	-1.005569	-1.213084	-0.764388
7	1.111905	2.723051	0.184749
1	0.699612	3.245804	0.956438
7	1.999779	0.097713	-0.595271
1	2.784820	0.647788	-0.242185
1	2.059920	-0.846411	-0.181960
1	2.160360	-0.019484	-1.595462
7	1.975564	-2.690188	0.687087
1	1.399205	-3.514358	0.528843
1	2.167246	-2.694499	1.686846
1	2.112722	2.609943	0.402532
1	2.873161	-2.914004	0.234959
1	1.069419	3.347738	-0.620341
1	-1.389276	-0.837386	0.782050
7	-1.620182	1.727705	-0.280005
1	-2.053234	1.771943	0.642423
1	-1.694341	2.665479	-0.670390
1	-2.248055	1.114723	-0.845088
7	-2.994899	-0.784788	1.886162
1	-3.255894	-0.050152	2.538889
1	-2.903598	-1.619425	2.460656
1	-3.811928	-0.940483	1.293348
7	4.145203	2.289613	0.704933

1	4.768723	2.437162	-0.086103
1	4.591080	1.569708	1.269443
1	4.232343	3.137609	1.261971
7	-3.495261	0.002455	-1.769562
1	-4.094634	0.667723	-2.253038
1	-3.240629	-0.678854	-2.480131
1	-4.101695	-0.485614	-1.107802
7	-5.753364	-1.421384	0.163859
1	-6.438926	-0.690811	0.339119
1	-5.903867	-2.109746	0.897176
1	-6.062322	-1.880378	-0.689497
7	4.650109	-3.522201	-0.675730
1	4.436377	-4.196163	-1.405473
1	5.133655	-4.046992	0.047807
1	5.348752	-2.902358	-1.074492

E+ZPE = -2202.2746450000000

Cartesian coordinates of : 450

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	0.001052	0.005109	0.001708
7	-1.415414	1.372200	-0.427950
1	-1.715285	1.330132	-1.401617
1	-1.096738	2.332145	-0.265678
1	-2.258839	1.204319	0.135201
7	1.456059	-1.338451	-0.284235
1	1.205191	-2.085108	-0.930250
1	1.744405	-1.804869	0.600082
1	2.288447	-0.885010	-0.667114
7	-3.945871	0.533029	1.264236
1	-4.445429	1.391791	1.041703
1	-3.873556	0.531385	2.279419
1	-4.609180	-0.206820	1.043463
7	2.308691	-2.723552	2.229615
1	2.225066	-3.730153	2.108931
1	3.301546	-2.556899	2.374888
1	1.870973	-2.523057	3.125062
7	1.366657	1.427964	0.413601
1	1.007903	2.375375	0.262509
1	1.686428	1.393018	1.381183
1	2.205084	1.295074	-0.166180
7	-2.160449	-2.869018	-2.189464
1	-2.041372	-3.868727	-2.043814
1	-3.156745	-2.742801	-2.351070
1	-1.718606	-2.673314	-3.083943
7	-0.106055	4.278336	0.011443

1	-0.783718	4.658347	0.669215
1	0.769929	4.733471	0.260460
7	3.896534	0.678622	-1.322742
1	4.623558	0.029096	-1.030110
1	4.316360	1.597913	-1.199539
1	3.824480	0.562177	-2.331238
1	-0.354102	4.680683	-0.890199
7	-1.400905	-1.390695	0.301571
1	-1.657144	-1.889341	-0.574945
1	-1.126973	-2.110991	0.967888
1	-2.256915	-0.965051	0.663653

E+ZPE = -2145.9089540000000

Cartesian coordinates of : 460

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	-0.162413	-0.004162	0.218836
7	1.712114	-0.684894	0.237405
1	2.124505	-0.707097	-0.714981
1	1.775153	-1.635815	0.602458
1	2.317125	-0.085417	0.802591
7	-1.919778	0.603641	-0.528412
1	-1.825652	1.341843	-1.223677
1	-2.544350	0.977818	0.211761
1	-2.412056	-0.172693	-0.975782
7	3.360710	1.648441	1.882760
1	4.242605	1.379179	1.452469
1	3.410353	1.299387	2.837361
1	3.420009	2.660441	1.973704
7	-3.736441	1.706363	1.605451
1	-3.964193	2.678223	1.410405
1	-4.622656	1.210519	1.548323
1	-3.479537	1.682286	2.588766
7	-0.940596	-1.826626	0.601176
1	-0.226204	-2.557734	0.699400
1	-1.479924	-1.837026	1.466263
1	-1.596801	-2.095358	-0.139947
7	0.325583	3.670573	-1.861988
1	-0.379160	4.396487	-1.758240
1	1.215101	4.163798	-1.859305
1	0.217492	3.322858	-2.811038
7	1.372683	-3.913941	1.082624
1	1.977583	-3.878485	1.900214
1	0.720374	-4.669728	1.281107
7	-3.164734	-2.265755	-1.645087
1	-3.986297	-2.570033	-1.127101

1	-2.772625	-3.116381	-2.043157
1	-3.534331	-1.759024	-2.446526
1	1.957188	-4.268136	0.328978
7	0.432284	1.874524	0.584235
1	0.429853	2.460801	-0.269324
1	-0.176068	2.351702	1.247988
1	1.376469	1.897840	0.982423
7	2.981232	-0.794602	-2.498806
1	2.392154	-0.981204	-3.305665
1	3.672061	-1.540722	-2.491671
1	3.500384	0.048319	-2.729525

E+ZPE = -2202.2885339999998

Cartesian coordinates of : 500

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.002206	0.003003	-0.122482
7	0.642283	1.935205	-0.625336
1	1.151197	2.399270	0.128115
1	-0.092265	2.594217	-0.882417
7	-0.660258	-1.922721	-0.639177
1	-1.147547	-1.942793	-1.536428
7	0.031605	-0.022546	2.112499
1	-0.680601	0.557175	2.556211
1	-0.107586	-0.948556	2.517444
1	0.908333	0.302136	2.520431
7	1.955375	-0.640070	-0.292578
1	2.655470	0.045332	-0.008352
1	2.217888	-0.901078	-1.244568
1	0.066175	-2.632421	-0.731379
1	2.160161	-1.464046	0.273353
1	-1.322639	-2.321046	0.027149
1	1.279448	1.949335	-1.422779
7	-1.963502	0.643362	-0.245838
1	-2.276753	0.821979	-1.201498
1	-2.645725	-0.013208	0.133862
1	-2.140119	1.514008	0.255852

E+ZPE = -1920.3753280000001

Cartesian coordinates of : 510

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
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29	0.484342	0.000000	-0.131116
7	0.616282	0.000000	2.110743
1	-0.302424	0.000001	2.553096
1	1.094052	0.806154	2.512674
7	1.932410	-1.451177	-0.518744
1	2.816755	-1.303769	-0.032727
7	-0.979848	1.433181	-0.342176
1	-0.914117	2.209181	0.315646
1	-0.995914	1.866435	-1.265967
1	-1.917348	1.032395	-0.213021
7	-0.979849	-1.433180	-0.342172
1	-1.917348	-1.032393	-0.213017
1	-0.914117	-2.209179	0.315652
1	1.652547	-2.398066	-0.265041
1	-0.995915	-1.866436	-1.265962
1	2.182942	-1.510956	-1.506782
1	1.094052	-0.806154	2.512674
7	1.932412	1.451176	-0.518740
1	2.816756	1.303767	-0.032724
1	2.182944	1.510956	-1.506778
1	1.652549	2.398064	-0.265036
7	-3.798014	-0.000000	-0.060135
1	-4.203865	0.802404	0.418831
1	-4.237373	-0.000002	-0.979420
1	-4.203865	-0.802403	0.418834

E+ZPE = -1976.7647239999999

Cartesian coordinates of : 520-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.004436	0.000007	0.157408
7	1.448442	-1.420382	0.517020
1	2.377650	-1.057086	0.274531
1	1.337210	-2.294939	0.006677
7	-1.471681	1.434820	0.363767
1	-1.501823	1.846707	1.296440
7	0.097764	-0.000094	-2.096495
1	0.579380	-0.806093	-2.492873
1	-0.819007	-0.000115	-2.542131
1	0.579379	0.805869	-2.492945
7	1.448442	1.420428	0.516893
1	2.377650	1.057111	0.274437
1	1.510201	1.692666	1.498197
1	-1.381106	2.225011	-0.273098
1	1.337210	2.294940	0.006473
1	-2.407695	1.043955	0.204620

1	1.510201	-1.692532	1.498348
7	-1.471681	-1.434787	0.363897
1	-1.501823	-1.846590	1.296608
1	-2.407695	-1.043937	0.204715
1	-1.381106	-2.225036	-0.272895
7	4.251840	-0.000002	-0.050645
1	4.617892	-0.802789	-0.559544
1	4.761432	0.000038	0.831466
7	-4.295280	0.000000	0.000152
1	-4.688748	-0.802850	-0.487833
1	-4.688748	0.802804	-0.487908
1	-4.754623	0.000043	0.909387
1	4.617892	0.802738	-0.559617

E+ZPE = -2033.1520579999999

Cartesian coordinates of : 520-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.000000	-0.641923	-0.156438
7	2.044267	-0.620980	-0.366933
1	2.366261	-0.891632	-1.296326
1	2.555281	-1.222803	0.277243
7	0.000000	-0.404238	2.081092
1	-0.807193	0.115504	2.423093
7	-2.044267	-0.620980	-0.366933
1	-2.366261	-0.891633	-1.296326
1	-2.555280	-1.222804	0.277244
1	-2.402927	0.331451	-0.214207
7	-0.000000	1.334297	-0.704943
1	-0.830992	1.824571	-0.365532
1	-0.000000	1.466408	-1.716306
1	-0.000001	-1.269741	2.619638
1	0.830991	1.824571	-0.365532
1	0.807195	0.115502	2.423094
1	2.402927	0.331452	-0.214207
7	0.000001	-2.723599	-0.324262
1	0.808333	-3.179563	0.096972
1	-0.808334	-3.179563	0.096969
1	0.000003	-3.034939	-1.296335
7	-3.025766	2.347065	0.032496
1	-3.333996	2.727329	-0.860775
1	-3.885196	2.060589	0.498175
1	-2.713273	3.156364	0.565672
7	3.025765	2.347066	0.032496
1	2.713272	3.156364	0.565674
1	3.333994	2.727331	-0.860775

1 3.885196 2.060590 0.498173

E+ZPE = -2033.1512319999999

Cartesian coordinates of : 520-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.594837	-0.125360	-0.086425
7	0.895208	1.905331	-0.340503
1	0.004665	2.417266	-0.278013
1	1.295450	2.169224	-1.240100
1	1.509679	2.324049	0.357109
7	-1.278360	0.289187	0.622838
1	-1.617615	1.199649	0.298996
1	-1.318796	0.331227	1.640360
1	-1.967923	-0.416562	0.348211
7	-3.154518	-2.237121	-0.162628
1	-3.116814	-3.254523	-0.129222
1	-3.649561	-2.026202	-1.027173
1	-3.806085	-1.990175	0.580010
7	2.356116	-0.490448	-1.134426
1	2.254366	-0.396062	-2.145582
1	2.733126	-1.426998	-0.992934
7	-0.031192	-2.046860	-0.525116
1	-1.043658	-2.152575	-0.376584
1	0.413583	-2.769701	0.039700
1	0.129122	-2.327353	-1.492221
7	-1.890923	3.366484	-0.198183
1	-2.166716	3.759529	0.699869
1	-2.766037	3.157129	-0.674925
1	-1.510071	4.156675	-0.715995
1	3.116363	0.141105	-0.884232
7	1.549250	-0.458630	1.953201
1	1.096892	-1.199122	2.488494
1	1.505142	0.359251	2.560305
1	2.535557	-0.716001	1.943965

E+ZPE = -2033.1501920000001

Cartesian coordinates of : 522-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.000762	0.005222	-0.175502
7	-1.848613	-0.878058	-0.392652

1	-2.019003	-1.226664	-1.335544
7	1.832346	0.888846	-0.525427
1	1.997278	1.767106	-0.037455
7	0.925886	-1.790772	-0.544764
1	0.939657	-2.044218	-1.532546
1	1.915187	-1.739896	-0.255532
1	0.521562	-2.595886	-0.070216
7	3.888102	-1.383131	0.200570
1	4.025074	-1.756954	1.137663
1	4.564940	-0.611470	0.117279
1	2.590823	0.254041	-0.248089
1	4.244733	-2.106920	-0.421225
1	1.998801	1.097063	-1.509833
7	-0.927894	1.831068	-0.319089
1	-0.578993	2.533523	0.330757
1	-0.840911	2.254915	-1.242402
1	-1.940985	1.747971	-0.142297
7	-3.944142	1.394485	0.121823
1	-4.264491	2.063262	-0.576520
1	-4.133789	1.842314	1.016459
1	-4.615719	0.615558	0.065462
7	5.992775	0.886501	-0.102980
1	6.282344	1.043937	-1.064283
1	6.779868	0.422782	0.343179
1	5.949481	1.807653	0.323184
7	-6.040368	-0.892305	-0.087466
1	-6.179800	-1.337959	-0.989852
1	-6.094456	-1.639571	0.598701
1	-6.872243	-0.328081	0.064900
7	0.112798	-0.068570	2.082263
1	0.820035	0.546337	2.481943
1	-0.758671	0.201293	2.536363
1	0.330863	-0.990573	2.456880
1	-2.012075	-1.675525	0.219436
1	-2.607820	-0.211927	-0.202803

E+ZPE = -2145.90394699999998

Cartesian coordinates of : 522-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.000708	-0.464014	-0.190476
7	-1.458415	-1.889846	-0.434509
1	-1.502064	-2.260909	-1.383263
7	1.450097	0.972725	-0.482070
1	1.323330	1.837349	0.040421
7	1.458857	-1.854015	-0.599484

1	1.554793	-2.058724	-1.593991
1	2.377820	-1.495987	-0.297843
1	1.334943	-2.760901	-0.153244
7	4.129499	-0.520830	0.192642
1	4.374753	-0.856258	1.122185
1	4.532257	0.425258	0.133461
1	2.371926	0.603646	-0.216735
1	4.695957	-1.081255	-0.442021
1	1.543477	1.261954	-1.455573
7	-1.472048	0.969989	-0.324938
1	-1.378323	1.738170	0.337178
1	-1.520685	1.412766	-1.242096
1	-2.403669	0.565773	-0.164076
7	-4.183510	-0.538692	0.075874
1	-4.506959	-0.953108	0.947985
1	-4.690922	-1.038052	-0.652685
1	-4.582500	0.410940	0.067610
7	5.435675	2.291110	-0.035729
1	5.646310	2.569014	-0.990217
1	6.334650	2.075186	0.387084
1	5.117131	3.135519	0.430591
7	-5.484465	2.283754	0.010800
1	-5.310250	2.975683	0.733970
1	-5.477552	2.796066	-0.866574
1	-6.449355	1.992973	0.144839
7	0.115824	-0.557251	2.066521
1	0.652169	0.198589	2.489616
1	-0.797365	-0.518219	2.517129
1	0.547419	-1.409589	2.420547
1	-1.354424	-2.705974	0.166031
1	-2.394020	-1.502123	-0.240274

E+ZPE = -2145.9038270000001

Cartesian coordinates of : 530

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.000000	-0.395433	0.039714
7	-1.412621	0.985609	0.588175
1	-1.121430	1.915521	0.270069
1	-1.536467	1.065350	1.596158
1	-2.342500	0.793140	0.207892
7	-1.458811	-1.441006	-0.980939
1	-1.481758	-2.438093	-0.772876
1	-1.360613	-1.383070	-1.994061
1	-2.399099	-1.077485	-0.780220
7	1.458811	-1.441006	-0.980938

1	1.360614	-1.383071	-1.994060
1	2.399100	-1.077485	-0.780220
7	1.412621	0.985609	0.588175
1	2.342500	0.793140	0.207892
1	1.121430	1.915521	0.270069
1	1.536467	1.065350	1.596158
1	1.481759	-2.438093	-0.772875
7	4.280305	-0.099385	-0.521928
1	4.754300	0.303276	0.284136
1	4.768887	-0.977913	-0.685223
1	4.546173	0.492226	-1.306811
7	-4.280305	-0.099385	-0.521928
1	-4.754300	0.303277	0.284135
1	-4.768887	-0.977913	-0.685222
1	-4.546173	0.492226	-1.306811
7	-0.000000	-1.652498	1.941857
1	0.000001	-1.095115	2.794969
1	0.808048	-2.266013	2.038050
1	-0.808051	-2.266010	2.038050
7	0.000000	3.782869	-0.218823
1	0.000005	4.376298	0.608521
1	0.802757	4.093425	-0.762501
1	-0.802762	4.093427	-0.762493

E+ZPE = -2089.5349620000002

Cartesian coordinates of : 531

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.416787	-0.280807	0.171549
7	2.196705	0.719095	0.346525
1	2.098895	1.656669	-0.060970
7	-1.401900	-0.980334	-0.500635
1	-1.651758	-1.905226	-0.154536
7	-0.497963	1.451975	0.757943
1	-0.074745	2.242924	0.267205
1	-1.507795	1.456297	0.567854
1	-0.395999	1.658124	1.750198
7	-3.563790	1.119443	0.235571
1	-3.908877	1.328670	1.170396
1	-4.231020	0.434350	-0.146575
1	-2.168289	-0.350021	-0.225953
1	-3.728898	1.969143	-0.300821
1	-1.465552	-1.050269	-1.515488
7	1.384243	-1.750044	-0.909723
1	1.163712	-2.699639	-0.614644
1	1.163147	-1.721768	-1.904480

1	2.406410	-1.654668	-0.857175
7	4.496483	-1.238404	-0.928064
1	4.842237	-0.711431	-1.727584
1	4.688382	-2.211074	-1.160491
1	5.143724	-1.028306	-0.171007
7	-5.657140	-0.873267	-0.922543
1	-5.705653	-0.956972	-1.933898
1	-6.502286	-0.377636	-0.651691
1	-5.771919	-1.816454	-0.563211
7	1.522465	3.649817	-0.705321
1	2.508160	3.896717	-0.768213
1	1.164399	3.773653	-1.649813
1	1.109806	4.406092	-0.163067
7	0.394060	-1.344477	2.191754
1	0.802569	-2.277877	2.193552
1	0.899804	-0.842640	2.920112
1	-0.545226	-1.467486	2.567422
1	2.488191	0.867585	1.311068
1	2.979619	0.248029	-0.111660

E+ZPE = -2145.9100950000002

Cartesian coordinates of : 532

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.094344	-0.302139	-0.242754
7	1.737371	0.569516	-0.519957
1	2.042245	0.611166	-1.491315
7	-1.936447	-1.190679	-0.460015
1	-2.124991	-1.970815	0.166287
7	-0.953900	1.464522	-0.787492
1	-0.976816	1.625233	-1.793497
1	-1.929622	1.512905	-0.471337
1	-0.433360	2.248759	-0.387639
7	-3.982401	1.137352	-0.003718
1	-4.124800	1.632784	0.874042
1	-4.676599	0.377121	0.002027
1	-2.675557	-0.496162	-0.291203
1	-4.309668	1.781003	-0.721863
1	-2.104164	-1.553877	-1.397658
7	0.854274	-2.114810	-0.146401
1	0.394201	-2.822441	0.422852
1	0.991123	-2.550838	-1.057709
1	1.798056	-1.980688	0.249544
7	3.688600	-1.543293	0.913227
1	3.935468	-2.530945	0.882431
1	3.845815	-1.273733	1.882070

1	4.426253	-1.072861	0.371431
7	-6.142674	-1.108851	-0.039894
1	-6.321762	-1.558466	-0.933197
1	-6.962194	-0.536088	0.143391
1	-6.173717	-1.851636	0.652365
7	5.995194	-0.219262	-0.714620
1	6.299152	-0.874359	-1.429596
1	6.008235	0.693726	-1.159357
1	6.745934	-0.196627	-0.029802
7	-0.192428	0.093725	1.983568
1	-1.122485	0.010616	2.390417
1	0.403840	-0.509849	2.547112
1	0.109185	1.043176	2.195752
1	1.717569	1.536278	-0.186167
1	2.473308	0.064037	-0.019761
7	1.165437	3.662592	0.380038
1	1.441162	4.198492	-0.440660
1	1.962640	3.723182	1.010081
1	0.446343	4.227257	0.827693

E+ZPE = -2202.2861160000002

Cartesian coordinates of : 540

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.087952	-0.131117	-0.020327
7	-0.416912	1.740676	0.664159
1	0.374837	2.379388	0.546523
1	-0.653721	1.767076	1.654426
1	-1.220048	2.140913	0.170288
7	-1.718973	-0.243589	-0.984714
1	-2.325653	-0.926333	-0.514988
1	-1.682165	-0.522570	-1.963139
1	-2.209293	0.655639	-0.970456
7	0.849159	-1.613331	-1.251448
1	0.851364	-1.351178	-2.236479
1	1.825809	-1.838157	-1.027567
7	1.980146	0.222455	0.677083
1	2.691534	-0.381478	0.259182
1	2.247115	1.197580	0.508936
1	2.052179	0.086055	1.683918
1	0.327461	-2.486893	-1.204293
7	3.934750	-2.035422	-0.658671
1	4.517601	-2.026080	0.175837
1	3.904240	-3.015723	-0.932192
1	4.495633	-1.583091	-1.377832
7	-3.031244	2.717274	-0.934389

1	-3.239505	3.422629	-0.230484
1	-3.939975	2.326035	-1.173888
1	-2.747722	3.242611	-1.758841
7	-0.615763	-1.460813	1.661494
1	-0.747323	-1.012740	2.566481
1	-0.032684	-2.273473	1.853153
1	-1.533198	-1.825227	1.394931
7	2.365066	3.408129	0.376493
1	2.470173	3.863451	1.280896
1	3.315981	3.296702	0.030667
1	1.958920	4.116282	-0.231345
7	-3.563397	-2.394450	0.507844
1	-4.292751	-1.883466	1.000903
1	-3.441789	-3.253117	1.041115
1	-3.997457	-2.698919	-0.361228

E+ZPE = -2145.9169689999999

Cartesian coordinates of : 541-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.309433	0.041141	0.123920
7	1.906557	1.314845	0.364256
1	1.599574	2.284740	0.237128
7	-1.390175	-0.806025	-0.694149
1	-1.467058	-1.808856	-0.534416
7	-0.857876	1.477439	0.986271
1	-0.583310	2.406989	0.659694
1	-1.858702	1.348717	0.796858
1	-0.761096	1.501958	1.999765
7	-3.855921	0.749973	0.399279
1	-4.210494	0.678961	1.350932
1	-4.417739	0.082132	-0.146406
1	-2.246150	-0.379434	-0.315312
1	-4.156264	1.667093	0.074734
1	-1.456165	-0.686611	-1.704100
7	1.494188	-1.188277	-1.016342
1	1.727158	-2.037804	-0.488984
1	1.086824	-1.502107	-1.894762
1	2.379269	-0.735684	-1.263648
7	4.186721	0.453261	-1.751806
1	4.130806	1.201320	-2.439667
1	4.512098	-0.355554	-2.277180
1	4.971585	0.699196	-1.152159
7	-5.650358	-1.197068	-1.248993
1	-5.729841	-0.986491	-2.239638
1	-6.554633	-0.963494	-0.848110

1	-5.580777	-2.208462	-1.187288
7	0.621428	4.257705	0.075831
1	1.540162	4.687207	0.162725
1	0.299828	4.514198	-0.854879
1	0.034723	4.788864	0.715893
7	0.495587	-1.302813	1.932037
1	0.999059	-2.143396	1.640626
1	1.015691	-0.926053	2.722209
1	-0.387703	-1.621688	2.325797
1	2.330772	1.272605	1.289132
1	2.661429	1.133844	-0.302868
7	2.194910	-3.832088	0.659864
1	3.185334	-3.763788	0.884195
1	2.150027	-4.436853	-0.157672
1	1.796592	-4.393293	1.409981

E+ZPE = -2202.2913140000001

Cartesian coordinates of : 541-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.488778	-0.027102	0.518192
7	-2.344964	-0.824748	0.143752
1	-2.276800	-1.643847	-0.468440
7	1.387466	0.783497	0.350273
1	1.796814	1.087139	1.231728
7	0.319611	-1.884728	0.233115
1	-0.268658	-2.456121	-0.378778
1	1.254157	-1.824099	-0.191304
1	0.436763	-2.420016	1.091470
7	3.202853	-1.475488	-0.902648
1	3.485056	-2.417527	-0.638905
1	4.004957	-0.884333	-0.646609
1	2.054323	0.118594	-0.057440
1	3.185409	-1.484376	-1.920338
1	1.370337	1.611470	-0.250703
7	-1.263596	1.854360	0.241479
1	-1.366281	2.384850	1.104700
1	-0.646202	2.412838	-0.356383
1	-2.189533	1.836157	-0.195320
7	-4.198786	1.532349	-1.082573
1	-4.152829	1.533541	-2.099206
1	-4.431460	2.490096	-0.828090
1	-5.037766	1.002078	-0.856536
7	5.737750	0.180210	-0.132515
1	5.797513	1.177858	0.047491
1	6.347475	0.010992	-0.927752

1	6.191009	-0.267426	0.659057
7	-1.854079	-3.507664	-1.569010
1	-2.686772	-3.344240	-2.130969
1	-1.146931	-3.794193	-2.242490
1	-2.063222	-4.345596	-1.030336
7	-0.639755	-0.095144	2.823123
1	-1.384019	0.486528	3.205023
1	-0.828544	-1.027869	3.187101
1	0.202721	0.205896	3.310319
1	-2.822366	-1.144828	0.984526
1	-2.976108	-0.151450	-0.299251
7	0.947762	3.476454	-1.437769
1	1.330699	4.243405	-0.889042
1	0.243211	3.906986	-2.032853
1	1.691773	3.209764	-2.078813

E+ZPE = -2202.2912790000000

Cartesian coordinates of : 600

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.000002	0.000001	0.001957
7	-0.047640	1.489217	-1.459224
1	-0.435484	1.193054	-2.354331
1	0.868451	1.877782	-1.683396
7	-0.104539	-1.461641	1.490714
1	-0.684900	-1.181875	2.281169
7	0.047631	-1.489672	-1.458759
1	0.435485	-1.193791	-2.353955
1	0.620078	-2.289991	-1.191119
1	-0.868465	-1.878291	-1.682817
7	-2.496078	0.033408	-0.033367
1	-2.885669	0.054903	-0.975466
1	-2.933899	0.830743	0.427464
1	-0.506480	-2.347011	1.183940
1	-2.942627	-0.774639	0.399430
1	0.797429	-1.708707	1.897769
1	-0.620101	2.289610	-1.191834
7	0.104546	1.462114	1.490251
1	-0.797425	1.709334	1.897205
1	0.684882	1.182589	2.280810
1	0.506516	2.347375	1.183201
7	2.496075	-0.033427	-0.033366
1	2.933885	-0.830666	0.427641
1	2.885664	-0.055137	-0.975461
1	2.942635	0.774709	0.399251

E+ZPE = -1976.7616470000000

Cartesian coordinates of : 610-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.451064	0.001087	0.000092
7	0.439302	-2.500437	-0.037584
1	0.802479	-2.941454	-0.881934
1	-0.510115	-2.862752	0.041323
1	0.945425	-2.959319	0.719020
7	1.947222	-0.034281	1.460026
1	1.618271	-0.272239	2.394777
1	2.423767	0.860353	1.569047
1	2.686297	-0.709258	1.266663
7	0.395265	2.502089	0.035702
1	0.880703	2.970191	-0.728767
1	-0.563612	2.841097	-0.032022
7	-1.015699	0.005072	-1.458158
1	-1.956256	-0.009802	-1.047130
1	-0.994719	0.822600	-2.066144
1	-0.972975	-0.798527	-2.083399
1	0.758887	2.954679	0.873713
7	-3.864685	-0.009508	0.000111
1	-4.258146	-0.948683	-0.022420
1	-4.293238	0.429191	0.813498
1	-4.292265	0.467956	-0.791642
7	1.947906	0.059629	-1.458344
1	1.614837	0.275317	-2.397024
1	2.450974	-0.821835	-1.554661
1	2.665991	0.758766	-1.271753
7	-1.015554	-0.023496	1.458177
1	-1.956069	0.001517	1.047526
1	-0.970277	0.768867	2.097396
1	-0.997106	-0.851644	2.051745

E+ZPE = -2033.1489839999999

Cartesian coordinates of : 620-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.008480	0.064226	0.000000
7	1.461375	0.400460	-1.435733
1	1.526260	1.375668	-1.723434
1	1.351611	-0.128606	-2.298859

1	2.387397	0.159226	-1.066268
7	1.461375	0.400460	1.435733
1	1.351611	-0.128606	2.298859
1	1.526260	1.375668	1.723434
1	2.387397	0.159226	1.066268
7	-1.425521	-0.250565	1.457557
1	-1.459950	0.486200	2.160075
1	-2.367875	-0.303217	1.055958
7	-1.425521	-0.250565	-1.457557
1	-2.367875	-0.303217	-1.055958
1	-1.459950	0.486201	-2.160075
1	-1.295912	-1.116775	-1.977900
1	-1.295912	-1.116775	1.977900
7	-4.279349	-0.463998	-0.000000
1	-4.568017	-1.440637	-0.000000
1	-4.753087	-0.054661	0.803284
1	-4.753087	-0.054661	-0.803285
7	4.283018	-0.154798	-0.000000
1	4.654980	-0.658355	-0.803220
1	4.654979	-0.658365	0.803214
1	4.779986	0.734240	0.000006
7	0.598580	-2.353354	0.000000
1	1.154645	-2.639098	-0.804470
1	-0.194932	-2.992928	-0.000000
1	1.154645	-2.639098	0.804471
7	-0.694085	2.511958	0.000000
1	-0.403766	3.068353	-0.802935
1	-1.710659	2.582129	-0.000000
1	-0.403766	3.068353	0.802936

E+ZPE = -2089.5342550000000

Cartesian coordinates of : 620-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	0.000001	-0.591408	0.074788
7	0.000006	-1.825401	-2.133968
1	0.000009	-2.842946	-2.077424
1	0.803532	-1.607823	-2.721882
1	-0.803521	-1.607828	-2.721883
7	-2.064795	-0.539080	0.125633
1	-2.521247	-1.096603	-0.594623
1	-2.396079	0.423998	-0.007216
1	-2.468163	-0.851643	1.007326
7	-0.000003	0.679799	2.222405
1	-0.000000	0.193639	3.118141
1	0.806421	1.300542	2.270188

7	2.064797	-0.539073	0.125637
1	2.396078	0.424005	-0.007212
1	2.468164	-0.851634	1.007331
1	2.521251	-1.096595	-0.594617
1	-0.806432	1.300535	2.270190
7	2.967438	2.482430	-0.319051
1	3.329931	2.599193	-1.263579
1	2.615366	3.402172	-0.060579
1	3.796314	2.360984	0.260167
7	0.000003	-2.451757	1.022536
1	0.807342	-3.027730	0.788557
1	-0.807333	-3.027733	0.788553
1	0.000000	-2.388853	2.039895
7	-0.000001	1.214070	-0.911555
1	0.827717	1.770040	-0.684333
1	-0.827721	1.770038	-0.684333
1	-0.000001	1.118888	-1.925625
7	-2.967446	2.482421	-0.319052
1	-3.329937	2.599184	-1.263581
1	-3.796322	2.360970	0.260163
1	-2.615378	3.402163	-0.060578

E+ZPE = -2089.5335470000000

Cartesian coordinates of : 620-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.000000	0.000000	0.000000
7	-0.541769	-2.465262	0.000125
1	-0.207199	-2.996889	0.802500
1	-0.207250	-2.996959	-0.802226
1	-1.549773	-2.614495	0.000164
7	-1.452948	0.236268	-1.453294
1	-2.395553	0.183170	-1.052210
1	-1.418957	-0.470288	-2.186108
1	-1.409382	1.131474	-1.937332
7	0.541769	2.465261	-0.000124
1	0.207255	2.996957	0.802230
1	1.549773	2.614494	-0.000169
7	1.452948	-0.236269	1.453294
1	2.395554	-0.183170	1.052210
1	1.418957	0.470287	2.186109
1	1.409383	-1.131475	1.937331
1	0.207194	2.996890	-0.802496
7	4.311973	-0.155988	-0.000140
1	4.682694	-1.104546	-0.000113
1	4.748956	0.292393	-0.803405

1	4.749010	0.292461	0.803057
7	-1.452849	0.236392	1.453374
1	-1.418808	-0.470102	2.186247
1	-2.395482	0.183259	1.052359
1	-1.409251	1.131639	1.937332
7	1.452849	-0.236392	-1.453374
1	2.395481	-0.183259	-1.052359
1	1.418807	0.470101	-2.186247
1	1.409251	-1.131639	-1.937332
7	-4.311973	0.155989	0.000139
1	-4.748956	-0.292391	0.803404
1	-4.682694	1.104548	0.000110
1	-4.749010	-0.292460	-0.803058

E+ZPE = -2089.5335380000001

Cartesian coordinates of : 621

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.502079	0.063771	-0.000004
7	1.956646	-0.124328	1.456064
1	1.876792	-0.984195	1.996011
1	1.948643	0.630671	2.139531
1	2.899568	-0.134736	1.053067
7	1.956663	-0.124355	-1.456053
1	1.948668	0.630631	-2.139535
1	1.876815	-0.984232	-1.995986
1	2.899580	-0.134755	-1.053046
7	-0.992007	0.251411	-1.421083
1	-0.786865	-0.127773	-2.343455
1	-1.819191	-0.251942	-1.079585
7	-0.992024	0.251438	1.421056
1	-1.819203	-0.251921	1.079559
1	-0.786892	-0.127729	2.343437
1	-1.293195	1.210910	1.583065
1	-1.293176	1.210880	-1.583113
7	-3.383669	-1.268150	-0.000015
1	-4.099253	-0.525052	-0.000002
1	-3.617260	-1.851687	-0.802160
1	-3.617252	-1.851707	0.802116
7	4.816179	-0.222136	0.000025
1	5.274427	0.204092	0.803369
1	5.274436	0.204076	-0.803322
1	5.137250	-1.188477	0.000036
7	0.964007	2.561472	-0.000025
1	1.967271	2.739193	-0.000022
1	0.615321	3.081164	0.804054

1	0.615330	3.081149	-0.804117
7	-0.001919	-2.355792	0.000017
1	0.287034	-2.910871	0.803724
1	-1.020764	-2.394300	0.000005
1	0.287054	-2.910889	-0.803671
7	-5.653842	0.840493	0.000025
1	-6.466748	0.230185	0.000065
1	-5.769440	1.443814	0.809196
1	-5.769483	1.443766	-0.809176

E+ZPE = -2145.9092110000001

Cartesian coordinates of : 630-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.100178	-0.010109	0.414325
7	-0.574230	-0.039327	2.939273
1	0.217700	-0.068575	3.579418
1	-1.148126	-0.835733	3.212204
1	-1.113192	0.770410	3.242507
7	0.104276	2.062665	0.433354
1	0.028824	2.469217	1.364111
1	-0.690137	2.429331	-0.104188
1	0.938334	2.476939	0.021061
7	0.793625	0.015569	-1.886085
1	1.813925	0.006969	-1.896282
1	0.502899	-0.779665	-2.451531
7	0.040401	-2.081462	0.372201
1	-0.769763	-2.408499	-0.167463
1	0.857445	-2.508556	-0.060526
1	-0.038498	-2.512415	1.291627
1	0.516582	0.833162	-2.425922
7	-2.528501	-2.968077	-1.294193
1	-3.411961	-3.073897	-0.799455
1	-2.787034	-2.720024	-2.246917
1	-2.164012	-3.915852	-1.369580
7	2.071936	-0.048169	1.022735
1	2.313926	-0.871365	1.571361
1	2.330326	0.740941	1.612438
1	2.726399	-0.034714	0.226704
7	-1.891397	0.028974	-0.086211
1	-2.162112	-0.789041	-0.635528
1	-2.132615	0.866606	-0.619483
1	-2.502020	0.032034	0.728619
7	-2.422638	3.072133	-1.227827
1	-3.280688	3.231947	-0.703715
1	-2.007142	3.996635	-1.325014

1	-2.728536	2.832662	-2.168655
7	4.151788	-0.016440	-1.326162
1	4.931297	0.110149	-0.683544
1	4.274476	0.716937	-2.021123
1	4.361719	-0.883488	-1.816135

E+ZPE = -2145.9161210000002

Cartesian coordinates of : 630-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.063694	-0.503894	0.272258
7	-1.233139	-1.639102	-1.454282
1	-0.878816	-1.596224	-2.408094
1	-2.128424	-1.148775	-1.468201
1	-1.462620	-2.621318	-1.313016
7	-0.609447	-1.937465	1.646482
1	-1.622278	-2.046863	1.632161
1	-0.372552	-1.706202	2.610125
1	-0.241490	-2.875387	1.495799
7	1.364752	0.732695	2.055101
1	2.357311	0.781217	1.831753
1	1.045435	1.699726	2.044286
7	0.733430	0.941342	-1.040443
1	0.511657	1.877824	-0.691993
1	1.743637	0.889750	-1.189143
1	0.310506	0.880192	-1.964681
1	1.337530	0.461529	3.036821
7	-0.427487	3.734324	0.126490
1	-0.948528	4.097221	-0.669491
1	-0.919388	4.093412	0.942413
1	0.451046	4.248808	0.115658
7	1.759613	-1.616391	-0.105223
1	1.595812	-2.400606	-0.734443
1	2.196579	-2.012812	0.724829
1	2.479655	-1.037915	-0.552817
7	-1.549381	0.691956	0.700217
1	-1.296867	1.670430	0.540050
1	-1.881542	0.647791	1.661646
1	-2.363964	0.489669	0.105787
7	-4.102032	0.088740	-1.081509
1	-4.174460	0.688573	-1.900544
1	-4.553855	-0.781917	-1.353426
1	-4.737211	0.500060	-0.400537
7	3.905432	0.260036	-1.539069
1	4.214776	1.223460	-1.428051
1	3.921981	0.093445	-2.543398

1 4.676765 -0.295099 -1.173323

E+ZPE = -2145.9151579999998

Cartesian coordinates of : 640-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.000000	-0.000000	-0.000000
7	-1.120735	-1.272712	-1.811552
1	-1.919176	-1.693919	-1.336595
1	-0.599113	-2.046653	-2.218525
1	-1.511491	-0.775878	-2.609731
7	-0.351070	1.807968	-0.959267
1	-0.397852	1.719314	-1.972390
1	0.380951	2.491746	-0.776047
1	-1.236588	2.237332	-0.670529
7	1.120735	1.272711	1.811552
1	0.599113	2.046652	2.218526
1	1.511492	0.775877	2.609730
7	0.351070	-1.807969	0.959267
1	1.236589	-2.237332	0.670530
1	0.397851	-1.719315	1.972390
1	-0.380950	-2.491747	0.776046
1	1.919176	1.693919	1.336595
7	3.191924	-2.947517	0.043008
1	3.563017	-3.130279	-0.886977
1	3.992028	-2.644356	0.594112
1	2.960763	-3.868961	0.409027
7	-1.823638	0.118003	0.925413
1	-1.752095	0.152992	1.940174
1	-2.412305	-0.691983	0.700637
1	-2.341352	0.955686	0.650736
7	1.823638	-0.118003	-0.925413
1	2.341353	-0.955686	-0.650735
1	2.412304	0.691983	-0.700638
1	1.752095	-0.152994	-1.940174
7	3.593120	2.447576	-0.227403
1	3.851635	2.670570	-1.186329
1	3.454942	3.352957	0.216403
1	4.444138	2.080008	0.193041
7	-3.593122	-2.447574	0.227401
1	-3.454945	-3.352955	-0.216405
1	-4.444140	-2.080005	-0.193045
1	-3.851639	-2.670567	1.186327
7	-3.191922	2.947518	-0.043005
1	-3.563015	3.130280	0.886979
1	-3.992027	2.644357	-0.594109

1 -2.960760 3.868962 -0.409024

E+ZPE = -2202.2962539999999

Table S 2: Cartesian coordinates of all the proposed isomers of $\text{Cu}^{2+}(\text{NH}_3)_{n=1-10}$ at M06-2X/6-31++G(d,p) level of theory

Cartesian coordinates of : 100

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.537548	0.000006	0.000010
7	1.440414	0.000016	0.000027
1	1.834851	-0.890769	-0.335293
1	1.835909	0.154993	0.938708
1	1.835235	0.735496	-0.603893

E+ZPE = -1694.5354250000000

Cartesian coordinates of : 200-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.000000	0.000000	0.000000
7	-1.283800	0.703940	-1.241919
1	-1.811541	-0.022775	-1.741373
1	-0.864982	1.286112	-1.977954
1	-1.996380	1.298935	-0.801134
7	1.283801	-0.703941	1.241919
1	0.864989	-1.286165	1.977916
1	1.811498	0.022775	1.741419
1	1.996417	-1.298884	0.801124

E+ZPE = -1751.0872509999999

Cartesian coordinates of : 200-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.000000	0.400012	0.000000
7	-1.706912	-0.523471	0.000000
1	-1.843165	-1.126869	-0.819248
1	-2.511117	0.117847	-0.000005

1	-1.843169	-1.126861	0.819253
7	1.706912	-0.523471	0.000000
1	1.843167	-1.126864	-0.819251
1	1.843166	-1.126866	0.819250
1	2.511117	0.117847	0.000002

E+ZPE = -1751.0672979999999

Cartesian coordinates of : 210

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.783963	-0.140087	0.000000
7	-0.937636	-0.720476	-0.000000
1	-1.108112	-1.321294	0.810003
1	-1.108112	-1.321293	-0.810004
1	-2.732422	0.194122	-0.000000
7	2.595880	0.573312	-0.000000
1	2.806844	1.157320	0.814322
1	2.807095	1.156653	-0.814736
1	3.311801	-0.159525	0.000409
7	-3.730225	0.507367	-0.000000
1	-4.352983	-0.303713	0.000033
1	-3.927590	1.069386	-0.830727
1	-3.927573	1.069441	0.830694

E+ZPE = -1807.5095659999999

Cartesian coordinates of : 220-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.000002	-0.000005	0.000002
7	-1.614807	0.862342	0.000003
1	-1.738087	1.460141	-0.817796
1	-1.738095	1.460126	0.817811
1	-3.245919	0.043281	-0.000006
7	1.614809	-0.862335	0.000003
1	1.738105	-1.460120	-0.817804
1	1.738097	-1.460130	0.817804
1	3.245922	-0.043276	0.000002
7	4.247602	0.316885	-0.000004
1	4.423549	0.885654	-0.829643
1	4.901406	-0.468093	0.000099
7	-4.247600	-0.316879	-0.000005
1	-4.423491	-0.885829	-0.829531

1	-4.423554	-0.885641	0.829637
1	4.423498	0.885829	0.829525
1	-4.901401	0.468101	-0.000118

E+ZPE = -1863.8967130000001

Cartesian coordinates of : 220-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.000001	0.233408	-0.000002
7	-1.776801	0.658901	-0.000016
1	-2.019494	1.225426	0.813820
1	-3.215691	-0.438431	0.000001
1	-2.019485	1.225396	-0.813876
7	1.776802	0.658898	0.000020
1	2.019478	1.225401	0.813876
1	2.019491	1.225420	-0.813819
1	3.215696	-0.438423	0.000004
7	4.151883	-0.950768	-0.000006
1	4.239255	-1.539853	0.829321
1	4.918074	-0.275085	0.000679
7	-4.151880	-0.950769	0.000008
1	-4.239355	-1.539644	0.829475
1	-4.918066	-0.275080	0.000433
1	-4.239709	-1.539003	-0.829877
1	4.239804	-1.538791	-0.830031

E+ZPE = -1863.8951290000000

Cartesian coordinates of : 220-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.925549	-0.468193	0.187672
7	-0.705266	0.045345	-0.548380
1	-0.678214	0.049672	-1.571888
1	-1.032373	1.032605	-0.247222
1	-1.505064	-0.647305	-0.281149
7	2.699623	0.286529	-0.158768
1	2.983096	0.190233	-1.138599
1	3.452276	-0.147686	0.387008
1	2.751212	1.287393	0.052358
7	-1.688867	2.572397	0.148266
1	-2.691859	2.545105	-0.027618
1	-1.343141	3.338244	-0.427064

1	-1.598928	2.896241	1.109317
7	-2.830201	-1.663413	0.045294
1	-3.557472	-1.475116	-0.642957
1	-3.273397	-1.509425	0.949182
1	-2.674092	-2.668370	-0.008743

E+ZPE = -1863.8705880000000

Cartesian coordinates of : 230-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.344973	-0.030116	0.142706
7	-2.066203	-0.078905	0.934744
1	-2.208788	0.683997	1.602932
1	-2.220490	-0.933746	1.477240
1	-2.920988	-0.018772	0.234851
7	-4.278672	0.059139	-0.674418
1	-5.093675	0.048455	-0.062677
1	-4.416336	-0.719483	-1.316277
7	3.013496	-2.206717	-0.039637
1	3.972019	-1.915078	-0.221103
1	2.860122	-3.005735	-0.651558
1	3.028181	-2.589576	0.903172
7	2.925710	2.288486	0.022249
1	2.497310	3.209717	-0.038513
1	3.692764	2.311315	-0.647141
7	1.353792	0.018014	-0.632636
1	1.952761	-0.833137	-0.376505
1	1.916598	0.887413	-0.356630
1	1.317000	0.028561	-1.655472
1	3.371195	2.259305	0.936961
1	-4.380312	0.899996	-1.239866

E+ZPE = -1920.2895360000000

Cartesian coordinates of : 240

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.000007	0.049235	-0.000011
7	1.768976	0.054227	-0.622624
1	1.826459	0.141126	-1.640325
1	2.295630	-0.840745	-0.381474
1	2.343519	0.863738	-0.233099
7	-1.768958	0.054219	0.622606

1	-1.826434	0.141102	1.640309
1	-2.295635	-0.840740	0.381454
1	-2.343495	0.863743	0.233100
7	-3.392775	2.192077	-0.353967
1	-3.016607	3.137179	-0.328347
1	-4.219177	2.221539	0.239935
7	3.392786	2.192045	0.353995
1	3.016820	3.137210	0.327699
1	3.747123	2.069948	1.300093
1	-3.747651	2.069581	-1.299811
1	4.219519	2.221048	-0.239469
7	3.267804	-2.309504	-0.047202
1	3.340091	-2.914786	-0.862390
1	4.223414	-2.025676	0.158726
7	-3.267853	-2.309489	0.047220
1	-3.004344	-2.922058	-0.721153
1	-4.223953	-2.025670	-0.156438
1	3.003032	-2.923347	0.719717
1	-3.338379	-2.916041	0.861616

E+ZPE = -1976.6796240000001

Cartesian coordinates of : 241

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.611301	0.076472	0.081382
7	-2.389651	-0.295808	0.561582
1	-2.530606	-0.301193	1.574515
1	-2.718192	-1.248377	0.221299
1	-3.076182	0.421185	0.180371
7	1.158381	0.436444	-0.385385
1	1.351024	0.268213	-1.375549
1	1.883353	-0.181188	0.169614
1	1.420387	1.446010	-0.208791
7	1.963419	3.179901	0.073865
1	1.902024	3.750891	-0.766079
1	2.953385	3.153355	0.307630
7	-4.317858	1.595078	-0.401333
1	-4.600911	2.246969	0.327191
1	-4.119006	2.171834	-1.215358
1	1.531576	3.735178	0.808523
1	-5.162430	1.080067	-0.640788
7	-3.364686	-2.849836	-0.301683
1	-2.778809	-3.667558	-0.149449
1	-4.213973	-3.030951	0.229474
7	3.025353	-1.051787	0.952176
1	3.875502	-1.083289	0.364065

1	2.810618	-2.022068	1.171675
1	-3.644612	-2.897218	-1.278761
1	3.314737	-0.635819	1.835006
7	5.592851	-1.234053	-0.690929
1	6.166323	-1.900014	-0.180280
1	6.151934	-0.388078	-0.753620
1	5.536920	-1.595208	-1.638813

E+ZPE = -2033.0568029999999

Cartesian coordinates of : 250

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.229063	0.003224	-0.292904
7	1.593196	-0.004166	0.078225
1	1.797605	-0.259648	1.077606
1	2.031822	0.935951	-0.095839
1	2.105465	-0.694653	-0.527931
7	-2.069939	0.005132	-0.685025
1	-2.251651	0.009999	-1.691436
1	-2.573133	0.857933	-0.301909
1	-2.577337	-0.848637	-0.309513
7	-3.537971	-2.277540	0.258905
1	-3.120665	-3.200209	0.161693
1	-4.394507	-2.315651	-0.289753
7	3.060647	-1.894225	-1.612631
1	2.641767	-2.781177	-1.881600
1	3.385360	-1.476951	-2.481777
1	-3.842809	-2.220389	1.227864
1	3.905652	-2.144318	-1.103978
7	2.871775	2.586571	-0.405369
1	2.912438	3.177940	0.421339
1	3.841683	2.386107	-0.638615
7	-3.521694	2.291826	0.275080
1	-3.161143	2.858147	1.039210
1	-4.436058	1.973338	0.588495
1	2.539961	3.191891	-1.152349
1	-3.712128	2.948266	-0.478974
7	2.234209	-0.716358	2.846887
1	3.101395	-0.235541	3.075079
1	1.597395	-0.488181	3.606313
1	2.440165	-1.706379	2.957771

E+ZPE = -2033.0653600000001

Cartesian coordinates of : 300

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.000003	-0.181597	-0.001984
7	-1.907424	-0.668859	0.001818
1	-2.443866	-0.235599	0.758502
1	-2.066140	-1.675909	0.112006
1	-2.397548	-0.419845	-0.862125
7	0.000018	1.806140	-0.000025
1	0.000098	2.203576	0.943932
1	-0.810373	2.223377	-0.464148
1	0.810346	2.223354	-0.464278
7	1.907414	-0.668881	0.001818
1	2.443867	-0.235605	0.758484
1	2.397533	-0.419898	-0.862137
1	2.066119	-1.675929	0.112034

E+ZPE = -1807.5452200000000

Cartesian coordinates of : 310-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.482265	0.056171	-0.019254
7	1.450642	1.776617	-0.000487
1	2.011063	1.940047	-0.840907
1	2.096566	1.877594	0.786356
1	0.829166	2.588263	0.063452
7	1.950963	-1.290325	0.067012
1	1.735180	-2.145998	-0.448915
1	2.149145	-1.597916	1.022738
1	2.849363	-0.975873	-0.304889
7	-1.135846	-0.989348	-0.073303
1	-1.204161	-1.662997	0.692928
1	-2.053836	-0.412040	-0.020400
7	-3.589198	0.340323	0.053746
1	-3.788917	0.874873	0.896904
1	-3.822917	0.958579	-0.720670
1	-4.299533	-0.389787	0.030861
1	-1.222721	-1.544580	-0.927870

E+ZPE = -1863.9427400000000

Cartesian coordinates of : 310-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	-0.684665	-0.226875	-0.000002
7	0.858342	-1.402120	-0.000013
1	0.907949	-2.020865	0.813501
1	1.738195	-0.837758	-0.000013
1	0.907943	-2.020859	-0.813531
7	0.243516	1.523631	-0.000018
1	0.046223	2.110177	0.813669
1	0.046207	2.110172	-0.813704
1	1.256626	1.362611	-0.000026
7	-2.611932	0.183385	0.000018
1	-3.201999	-0.654400	0.000018
1	-2.917181	0.721633	0.814908
7	3.332265	0.270016	0.000016
1	3.645233	0.804817	0.809482
1	3.942746	-0.547380	-0.000190
1	3.645205	0.805192	-0.809212
1	-2.917197	0.721644	-0.814860

E+ZPE = -1863.9411190000001

Cartesian coordinates of : 310-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	-0.729082	-0.000062	-0.002804
7	-1.161102	1.908037	-0.263713
1	-1.941698	2.073860	-0.906013
1	-0.382168	2.448780	-0.646916
1	-1.426957	2.381353	0.603766
7	-1.160383	-1.908352	-0.263568
1	-1.940635	-2.074539	-0.906191
1	-1.426477	-2.381596	0.603878
1	-0.381103	-2.448914	-0.646321
7	0.927385	0.000283	1.015270
1	1.023785	-0.807563	1.633476
1	1.809285	0.000238	0.402978
1	1.023656	0.808373	1.633176
7	3.341269	0.000201	-0.463141
1	3.900447	-0.806896	-0.192070
1	3.900657	0.806964	-0.191509
1	3.354418	0.000555	-1.480867

E+ZPE = -1863.9409280000000

Cartesian coordinates of : 311

Atomic number (AN) and Cartesian coordinates
AN X Y Z

29	1.525190	0.000006	0.053849
7	2.089468	-1.907441	-0.058984
1	3.031774	-2.065194	-0.421857
1	1.470825	-2.456894	-0.655742
1	2.071668	-2.357201	0.857551
7	2.089467	1.907423	-0.059498
1	3.031771	2.065079	-0.422418
1	2.071671	2.357428	0.856917
1	1.470820	2.456716	-0.656400
7	-0.285080	0.000065	0.476819
1	-0.525799	0.805296	1.056285
1	-1.960157	-0.000072	-0.609486
1	-0.525803	-0.805012	1.056497
7	-2.881740	-0.000132	-1.098700
1	-2.945720	0.823149	-1.696072
1	-3.721272	-0.000050	-0.406370
1	-2.945717	-0.823555	-1.695876
7	-5.083813	0.000065	0.568877
1	-5.156797	-0.810441	1.179833
1	-5.156805	0.810726	1.179627
1	-5.939075	-0.000009	0.016292

E+ZPE = -1920.3341849999999

Cartesian coordinates of : 320-1

Atomic number (AN) and Cartesian coordinates
AN X Y Z

29	0.063316	0.313993	0.149557
7	-1.337218	-0.765090	0.937471
1	-1.724325	-0.358747	1.791550
1	-1.006236	-1.691047	1.220475
1	-2.169545	-0.949142	0.291286
7	1.848671	0.607816	-0.535704
1	1.873910	0.735769	-1.549600
1	2.533811	-0.197257	-0.335216
1	2.297590	1.439768	-0.147720
7	-3.593621	-1.370617	-0.674281
1	-3.634885	-1.119060	-1.659434
1	-4.455643	-1.010215	-0.269394
1	-3.700334	-2.383437	-0.657301
7	3.762982	-1.412147	-0.076158
1	3.605040	-2.313188	-0.522298
1	4.633986	-1.068391	-0.476876

1	3.984979	-1.625393	0.893995
7	-0.830030	2.093200	-0.037669
1	-0.499873	2.638340	-0.835802
1	-1.842579	2.029008	-0.153228
1	-0.687554	2.695053	0.776789

E+ZPE = -1920.3369789999999

Cartesian coordinates of : 320-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.118983	0.063530	-0.000002
7	1.850345	0.919618	0.000071
1	2.683367	0.236666	0.000015
1	1.997860	1.522578	0.812089
1	1.997862	1.522714	-0.811847
7	-1.226253	1.526002	0.000062
1	-1.170621	2.142155	-0.812918
1	-1.170610	2.142096	0.813086
1	-2.171032	1.128888	0.000054
7	-3.927054	-0.422366	0.000038
1	-4.320381	-1.363287	-0.000337
1	-4.358723	0.022293	-0.809039
1	-4.358617	0.021621	0.809540
7	4.127898	-0.737831	-0.000062
1	4.931035	-0.111424	-0.000164
1	4.262460	-1.339581	-0.809840
1	4.262584	-1.339476	0.809774
7	-1.102441	-1.453625	-0.000105
1	-2.089856	-1.119625	-0.000064
1	-1.001638	-2.065347	0.813014
1	-1.001661	-2.065218	-0.813323

E+ZPE = -1920.3363310000000

Cartesian coordinates of : 320-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.074114	0.418642	-0.178273
7	0.349120	2.234013	0.485232
1	1.206971	2.267625	1.039849
1	-0.374830	2.635615	1.086833
1	0.478621	2.914856	-0.266870
7	1.613366	-0.172363	-0.962744

1	2.145143	0.572966	-1.415163
1	1.484782	-0.877970	-1.689456
1	2.276374	-0.610105	-0.253075
7	3.487543	-1.381243	0.827031
1	3.669913	-2.332866	0.513938
1	3.310998	-1.461102	1.825886
1	4.384817	-0.905543	0.753159
7	-3.948921	-0.770412	0.536953
1	-4.071264	-0.663548	1.541652
1	-4.420308	-1.643074	0.305416
7	-1.312398	-1.043794	-0.442591
1	-1.456857	-1.259852	-1.431123
1	-2.297171	-0.883409	-0.043934
1	-0.987328	-1.915540	-0.019864
1	-4.521518	-0.042061	0.115520

E+ZPE = -1920.3353700000000

Cartesian coordinates of : 321-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.668664	-0.002666	0.000016
7	2.037824	1.423038	-0.000042
1	1.986798	2.038770	0.812211
1	1.986778	2.038725	-0.812329
1	2.985731	1.011418	-0.000043
7	-1.097526	-0.515752	0.000059
1	-1.365010	-1.071853	-0.811262
1	-2.733122	0.608355	0.000062
1	-1.364982	-1.071814	0.811416
7	4.819832	0.073269	-0.000059
1	5.209837	-0.406446	-0.809422
1	5.209876	-0.406797	0.809078
1	5.284815	0.979819	0.000132
7	-3.646138	1.114148	0.000077
1	-3.699458	1.710842	0.824520
1	-3.699417	1.710969	-0.824276
1	-4.492878	0.435379	0.000004
7	1.949274	-1.528713	0.000033
1	2.923115	-1.214110	0.000017
1	1.828542	-2.134580	0.811521
1	1.828526	-2.134611	-0.811430
7	-5.871911	-0.531832	-0.000106
1	-5.948645	-1.141597	-0.811011
1	-5.948665	-1.141755	0.810678
1	-6.722572	0.027492	-0.000062

E+ZPE = -1976.7284860000000

Cartesian coordinates of : 330-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.138333	-0.054364	-0.042528
7	-0.944842	-1.216867	1.072056
1	-0.399675	-1.735864	1.764167
1	-1.482444	-1.953966	0.523106
1	-1.638635	-0.703428	1.617752
7	1.838518	0.566104	-0.744118
1	1.944481	0.382220	-1.743487
1	2.695314	0.126778	-0.283033
1	1.960866	1.574695	-0.639769
7	-2.407421	-3.264813	-0.277365
1	-3.403655	-3.197573	-0.079181
1	-2.121467	-4.160920	0.112395
1	-2.341951	-3.381723	-1.285836
7	4.213790	-0.522141	0.390884
1	4.378654	-1.515220	0.242654
1	4.987692	-0.052961	-0.075646
1	4.370265	-0.366804	1.384206
7	-1.199033	1.094019	-0.897869
1	-2.092569	0.624720	-1.048572
1	-1.417296	1.959876	-0.327572
1	-0.917496	1.431827	-1.818733
7	-1.865673	3.489657	0.560379
1	-1.637657	4.304469	-0.005597
1	-2.874089	3.535358	0.691666
1	-1.469353	3.683351	1.477018

E+ZPE = -1976.7273949999999

Cartesian coordinates of : 330-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.000013	-0.070259	-0.506411
7	1.887637	-0.325112	-0.883234
1	2.387346	-0.982547	-0.211059
1	2.410294	0.552041	-0.865792
1	2.058262	-0.710901	-1.815087
7	-1.887550	-0.325337	-0.883380
1	-2.387269	-0.982696	-0.211141
1	-2.058052	-0.711299	-1.815184

1	-2.410280	0.551777	-0.866138
7	3.357413	-2.097399	0.803104
1	4.207875	-1.645031	1.132348
1	3.677416	-2.881776	0.238354
1	2.940489	-2.518053	1.630082
7	-3.357344	-2.097449	0.803127
1	-2.940450	-2.517978	1.630183
1	-4.207847	-1.645079	1.132263
1	-3.677278	-2.881914	0.238459
7	-0.000115	1.111607	1.055623
1	0.810420	0.981155	1.661595
1	-0.000098	2.135952	0.784628
1	-0.810742	0.981148	1.661470
7	-0.000075	3.923135	0.420015
1	-0.807279	4.370604	0.849481
1	0.807056	4.370619	0.849600
1	-0.000007	4.245370	-0.544937

E+ZPE = -1976.7269790000000

Cartesian coordinates of : 330-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.286221	-0.311627	-0.022915
7	2.047101	-0.957725	-0.514097
1	2.204763	-0.947873	-1.523478
1	2.206847	-1.924866	-0.226714
1	2.857053	-0.402542	-0.092441
7	-0.960550	0.903592	0.816765
1	-1.864173	0.439427	0.936400
1	-1.142095	1.789197	0.258149
1	-0.678123	1.213955	1.748455
7	4.304619	0.406485	0.549060
1	5.119102	0.003281	0.089924
1	4.469029	0.274426	1.544593
1	4.381747	1.408759	0.392330
7	-3.634888	-1.285206	0.602167
1	-4.104063	-2.038239	0.100618
1	-3.699468	-1.556364	1.581769
1	-4.266029	-0.492312	0.502631
7	-0.996478	-1.594349	-0.797672
1	-1.157510	-1.450829	-1.795960
1	-0.720474	-2.572454	-0.706061
1	-1.922166	-1.498879	-0.331486
7	-1.500425	3.340108	-0.593145
1	-1.319656	4.124158	0.030548
1	-2.485223	3.418830	-0.837569

1 -0.995609 3.559164 -1.448736

E+ZPE = -1976.7265290000000

Cartesian coordinates of : 330-4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.206523	-0.247452	0.093655
7	1.598592	0.149820	0.569988
1	1.978259	0.989790	0.061176
1	2.253081	-0.652488	0.362051
1	1.720810	0.344536	1.564605
7	-1.305718	1.173360	0.952907
1	-1.015275	2.118149	0.697579
1	-1.282155	1.145832	1.973497
1	-2.288929	1.082000	0.683384
7	-4.269088	0.137349	-0.265227
1	-4.791121	-0.523876	-0.839430
1	-4.519531	1.046717	-0.650362
1	-4.731535	0.094907	0.641659
7	3.470579	-2.020374	0.072284
1	3.245983	-2.937972	0.449740
1	4.333425	-1.748573	0.538711
1	3.732590	-2.184939	-0.896799
7	-1.645514	-1.250379	-0.762540
1	-2.561049	-0.779892	-0.604474
1	-1.744162	-2.204513	-0.409564
1	-1.536623	-1.346030	-1.774250
7	2.758527	2.451284	-0.798560
1	3.036617	3.170898	-0.134845
1	2.278804	2.947833	-1.545424
1	3.628341	2.126311	-1.215209

E+ZPE = -1976.7239440000001

Cartesian coordinates of : 330-5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.245089	-0.493562	-0.340865
7	1.035670	-2.082063	-1.224784
1	1.979722	-2.293514	-0.896279
1	1.110376	-1.982852	-2.239365
1	0.501134	-2.941861	-1.078329
7	1.639265	0.865848	-0.535709

1	2.343209	0.849444	0.256884
1	1.244606	1.807054	-0.541159
1	2.185528	0.801379	-1.395393
7	-1.163026	0.394976	0.596373
1	-1.591855	1.169555	0.027929
1	-1.949571	-0.251621	0.871295
7	-3.374535	-1.312220	1.432336
1	-4.002391	-1.641573	0.702824
1	-3.160909	-2.132912	1.994192
1	-3.950035	-0.725766	2.032982
1	-0.847433	0.823138	1.467806
7	-2.425195	2.553397	-0.914604
1	-2.364472	3.437563	-0.414314
1	-3.419225	2.337571	-0.948577
7	3.610152	0.917922	1.563265
1	3.594866	1.833573	2.007843
1	3.591059	0.250488	2.330763
1	-2.171012	2.772173	-1.874892
1	4.542501	0.836448	1.162733

E+ZPE = -1976.7229430000000

Cartesian coordinates of : 330-6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.014242	-0.778342	0.014244
7	-1.320082	0.394676	0.743846
1	-2.317359	0.139883	0.491974
1	-1.141658	1.348199	0.392545
1	-1.295205	0.455856	1.763338
7	1.265602	0.507515	-0.742365
1	1.521035	0.338690	-1.715798
1	2.172320	0.571420	-0.208173
1	0.826589	1.434463	-0.714710
7	0.806361	-2.543321	-0.398858
1	0.400142	-3.318227	0.131278
1	0.708280	-2.807813	-1.381380
7	-0.542430	3.200409	-0.430342
1	-0.786002	3.405628	-1.397874
1	-1.286385	3.633300	0.114996
1	0.271776	3.780382	-0.234721
1	1.808346	-2.576224	-0.202231
7	-4.068717	-0.226431	0.142229
1	-4.361658	-1.200522	0.125574
1	-4.637071	0.206546	0.867262
1	-4.405567	0.168958	-0.732656
7	3.802683	0.741438	0.660162

1	3.935907	1.722032	0.898236
1	4.580158	0.513905	0.043827
1	3.989417	0.235452	1.522721

E+ZPE = -1976.7226470000001

Cartesian coordinates of : 331-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.476365	-0.062070	0.037485
7	-1.804019	-1.083490	1.066120
1	-2.473370	-0.476727	1.539428
1	-1.402973	-1.665688	1.801478
1	-2.369619	-1.728324	0.462066
7	1.297479	0.303529	-0.348361
1	1.537410	0.125075	-1.323282
1	2.869667	-0.457281	0.409537
1	1.544490	1.279398	-0.185427
7	-3.421621	-2.921855	-0.542236
1	-3.173526	-3.119671	-1.508249
1	-4.404794	-2.661542	-0.562894
1	-3.396434	-3.823219	-0.070826
7	3.789732	-0.817997	0.768255
1	3.856089	-0.638519	1.769008
1	3.836770	-1.825676	0.625268
1	4.628599	-0.355010	0.273207
7	-1.727578	1.035274	-1.020877
1	-2.519880	0.515500	-1.396402
1	-2.130611	1.828222	-0.469698
1	-1.262730	1.453965	-1.825072
7	6.020899	0.320516	-0.453205
1	6.081291	0.160107	-1.455969
1	6.102393	1.327105	-0.330630
1	6.876285	-0.070347	-0.063882
7	-2.895238	3.307830	0.449436
1	-3.911272	3.264505	0.467548
1	-2.616536	3.514354	1.404999
1	-2.674242	4.147161	-0.081189

E+ZPE = -2033.1127469999999

Cartesian coordinates of : 331-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
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29	-0.723563	-0.201054	-0.154074
7	-2.625796	-0.171999	-0.536680
1	-2.824469	-0.169589	-1.538664
1	-3.083787	0.662863	-0.168149
1	-3.169436	-0.998499	-0.140807
7	0.912682	-0.999721	0.509210
1	1.751691	-0.481125	0.116577
1	1.034813	-1.981627	0.254965
1	1.003089	-0.970185	1.526199
7	-4.198067	-2.339180	0.454995
1	-5.170210	-2.093548	0.279009
1	-4.152529	-2.546300	1.449969
1	-4.060655	-3.231504	-0.014233
7	3.180954	0.371942	-0.540668
1	3.341705	0.451974	-1.543165
1	3.497821	1.255842	-0.146497
1	3.876451	-0.323161	-0.218204
7	-0.035681	1.511873	-0.793867
1	-0.385627	1.788296	-1.711425
1	-0.252002	2.315560	-0.146456
1	0.981859	1.462916	-0.878332
7	-0.591112	3.798639	0.909134
1	0.282902	4.287615	1.089861
1	-1.173215	4.473380	0.417571
1	-1.024901	3.685840	1.822131
7	5.302039	-1.632161	0.374386
1	5.400079	-1.832854	1.365610
1	5.329328	-2.535025	-0.091042
1	6.165278	-1.166071	0.107680

E+ZPE = -2033.1039690000000

Cartesian coordinates of : 331-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.787593	-0.000000	-0.406723
7	-0.282236	1.866630	-0.290333
1	-0.382982	2.373845	-1.170647
1	0.744621	1.960771	-0.006947
1	-0.820912	2.396468	0.396014
7	-2.693985	-0.000001	-0.851144
1	-2.980439	-0.810316	-1.401146
1	-2.980439	0.810314	-1.401147
1	-3.313980	0.000000	0.006269
7	-0.282235	-1.866630	-0.290331
1	0.744622	-1.960771	-0.006946
1	-0.820912	-2.396467	0.396018

7	2.438432	2.116206	0.452333
1	2.843345	2.857669	-0.115580
1	2.526448	2.438618	1.413616
1	3.077002	1.322944	0.364587
1	-0.382983	-2.373846	-1.170645
7	2.438432	-2.116206	0.452332
1	2.526450	-2.438618	1.413616
1	2.843346	-2.857668	-0.115581
7	-4.498545	0.000001	1.403425
1	-5.114672	0.807529	1.338124
1	-4.159740	0.000001	2.362400
1	3.077003	-1.322943	0.364586
1	-5.114673	-0.807526	1.338124
7	4.946384	0.000001	0.175531
1	5.396459	0.803469	0.607866
1	5.272451	0.000001	-0.788185
1	5.396459	-0.803468	0.607865

E+ZPE = -2033.1028429999999

Cartesian coordinates of : 332-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.101491	0.002553	-0.118009
7	-1.410859	1.034378	0.529340
1	-1.368095	2.029738	0.304449
1	-1.536642	0.990293	1.541764
1	-2.303645	0.666381	0.097980
7	1.975674	-0.300863	-0.449258
1	2.294885	-1.209443	-0.110737
1	2.632169	0.439096	0.021249
1	2.212479	-0.285121	-1.442544
7	-3.835677	0.048191	-0.645068
1	-4.300308	-0.789991	-0.300920
1	-3.973346	0.036259	-1.654025
1	-4.422548	0.830360	-0.308762
7	3.701077	1.512229	0.689124
1	4.648495	1.264063	0.358647
1	3.570836	2.489181	0.436178
1	3.753021	1.501370	1.705312
7	-0.842829	-1.562831	-0.810958
1	-0.789608	-2.393151	-0.166621
1	-1.833426	-1.343054	-0.934148
1	-0.503455	-1.886123	-1.716711
7	-5.642919	2.331541	0.312723
1	-5.732421	2.511362	1.308682
1	-5.517423	3.242483	-0.119539

1	-6.561128	2.015120	0.012425
7	6.545676	0.875376	-0.231499
1	6.936478	-0.021772	0.041055
1	7.121995	1.574376	0.229026
1	6.742659	0.971001	-1.223464
7	-0.739652	-3.921452	0.898319
1	-1.687308	-4.251613	1.066402
1	-0.303916	-3.885586	1.816483
1	-0.276426	-4.685265	0.411022

E+ZPE = -2089.4806060000001

Cartesian coordinates of : 3321

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	1.547886	-0.040054	-0.340450
7	2.672014	-0.349970	1.236277
1	3.474286	-0.927950	0.976615
1	2.201706	-0.829709	2.002699
1	3.057329	0.535400	1.637462
7	-0.091930	0.321821	-1.065394
1	-0.169369	1.211050	-1.554756
1	-1.949880	0.528281	-0.115876
1	-0.456300	-0.383286	-1.702754
7	3.797146	2.111141	2.415676
1	4.792318	2.213788	2.234255
1	3.713242	2.053482	3.427609
1	3.381730	3.003092	2.160683
7	-2.926564	0.657673	0.195060
1	-3.493297	-0.247144	0.067020
1	-2.928205	0.906597	1.181456
1	-3.379834	1.435220	-0.344862
7	3.012429	-0.280911	-1.664241
1	3.791657	-0.826653	-1.270931
1	2.689104	-0.760363	-2.502810
1	3.397211	0.605989	-1.987406
7	-4.285801	2.774427	-1.258195
1	-4.327124	2.630721	-2.263585
1	-5.253391	2.826246	-0.950145
1	-3.909038	3.709645	-1.129288
7	-4.469226	-1.640617	-0.120519
1	-5.350133	-1.559014	0.406553
1	-4.037138	-2.505530	0.194057
1	-4.737226	-1.808096	-1.087113
7	5.221469	-1.970301	-0.260252
1	5.003836	-2.964588	-0.263570
1	5.902619	-1.849383	-1.007401

1	5.755304	-1.817904	0.592698
7	-7.150724	-1.526223	1.429160
1	-7.836381	-0.851652	1.103529
1	-7.102511	-1.407042	2.436465
1	-7.570894	-2.438915	1.279442

E+ZPE = -2145.8710179999998

Cartesian coordinates of : 332-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.000001	-0.758530	-0.437556
7	1.874152	-0.301467	-0.340179
1	2.357376	-0.421894	-1.231714
1	2.389528	-0.878682	0.325751
1	2.069565	0.730086	-0.044913
7	-1.874155	-0.301478	-0.340159
1	-2.357390	-0.421915	-1.231686
1	-2.069571	0.730077	-0.044900
1	-2.389519	-0.878690	0.325783
7	2.492472	2.286822	0.388064
1	2.250564	2.560221	1.337686
1	2.131608	3.027894	-0.208230
1	3.521651	2.359920	0.329988
7	-2.492481	2.286814	0.388069
1	-3.521661	2.359908	0.329995
1	-2.250571	2.560220	1.337688
1	-2.131622	3.027883	-0.208231
7	0.000003	-2.675441	-0.868964
1	0.000010	-3.281994	-0.005951
1	-0.810515	-2.966800	-1.415426
1	0.810516	-2.966794	-1.415435
7	5.532857	2.606125	0.238443
1	6.095794	2.028852	0.856327
1	5.959019	2.521934	-0.679865
1	5.704088	3.564253	0.530819
7	-5.532868	2.606105	0.238455
1	-5.959032	2.521909	-0.679852
1	-5.704102	3.564234	0.530828
1	-6.095801	2.028832	0.856343
7	0.000021	-4.445252	1.432015
1	-0.807570	-5.062335	1.380845
1	0.807612	-5.062335	1.380831
1	0.000029	-4.082996	2.382242

E+ZPE = -2089.4801840000000

Cartesian coordinates of : 340-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	0.317617	-0.426676	0.051867
7	-1.341839	-1.200746	-0.550380
1	-1.868346	-0.489713	-1.079901
1	-1.964421	-1.547154	0.227610
1	-1.217750	-1.993579	-1.182089
7	0.081108	1.421239	-0.541521
1	-0.787271	1.490842	-1.080970
1	0.827892	1.755953	-1.150588
1	0.019718	2.109486	0.248714
7	2.071844	-0.436817	0.886476
1	2.285317	0.447454	1.348825
1	2.172679	-1.148621	1.613013
7	-0.074149	3.417445	1.597251
1	0.696327	4.079550	1.538023
1	-0.911418	3.974110	1.440478
1	-0.118574	3.145143	2.576144
1	2.863091	-0.614811	0.200934
7	-2.741572	1.088151	-2.179538
1	-2.411977	1.311794	-3.116874
1	-3.549259	0.486810	-2.333863
1	-3.141918	1.954468	-1.824430
7	4.281442	-0.957868	-0.863730
1	4.675784	-1.870993	-0.647472
1	5.032237	-0.295101	-0.682204
1	4.157712	-0.952853	-1.873266
7	-3.108592	-2.230118	1.508424
1	-3.550381	-3.068460	1.137307
1	-3.875431	-1.599859	1.730786
1	-2.722605	-2.509874	2.406814

E+ZPE = -2033.1130140000000

Cartesian coordinates of : 340-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	-0.164830	-0.238869	-0.436194
7	1.736699	0.016927	-0.614566
1	2.315191	-0.862332	-0.545823
1	2.052393	0.661900	0.125797
1	1.997444	0.452148	-1.500896
7	-0.611849	1.294737	0.689356

1	-1.253457	1.089087	1.454650
1	-1.044796	2.083115	0.144713
1	0.247983	1.654946	1.113827
7	-1.866168	-1.125788	-0.743241
1	-1.854415	-1.754648	-1.549074
1	-2.199267	-1.714975	0.073530
7	2.450481	2.046784	1.664542
1	2.445269	1.731731	2.632853
1	3.432523	2.022743	1.394802
1	2.231341	3.040335	1.707854
1	-2.615451	-0.460682	-0.938573
7	3.424583	-2.341660	-0.490591
1	3.107801	-3.187160	-0.958815
1	4.302172	-2.100604	-0.945959
1	3.682026	-2.634775	0.448786
7	-1.823816	3.523629	-0.759144
1	-1.189697	4.319375	-0.763448
1	-2.648310	3.845791	-0.257035
1	-2.123832	3.419926	-1.725435
7	-2.873610	-2.782348	1.372996
1	-3.018360	-3.718587	1.000641
1	-2.345083	-2.915700	2.231620
1	-3.795657	-2.470410	1.670154

E+ZPE = -2033.1129010000000

Cartesian coordinates of : 341

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	-0.194545	0.028625	0.335358
7	-1.477918	1.463004	0.490283
1	-1.192811	2.199973	1.136906
1	-2.361951	1.080462	0.858092
1	-1.696017	1.945924	-0.418747
7	1.579258	-0.702641	0.115557
1	1.845493	-1.331827	0.873959
1	2.362049	0.053915	0.077548
1	1.678861	-1.253403	-0.738063
7	-2.129447	2.898489	-1.961276
1	-2.143403	3.892816	-1.745532
1	-3.065921	2.684526	-2.295618
1	-1.526805	2.811063	-2.775589
7	3.630781	1.146832	0.030458
1	4.512510	0.608804	0.046038
1	3.677699	1.726057	-0.804678
1	3.692742	1.795422	0.811922
7	-1.391926	-1.501649	0.569029

1	-2.302933	-1.169880	0.898607
1	-1.554349	-2.045486	-0.313406
1	-1.064174	-2.178522	1.257785
7	-1.890259	-3.121340	-1.823324
1	-2.893981	-3.206817	-1.965470
1	-1.515262	-2.854165	-2.729875
1	-1.563045	-4.072033	-1.667253
7	6.306391	-0.344598	0.077926
1	6.530924	-0.859908	0.924038
1	7.005254	0.390326	0.013127
1	6.505288	-0.978049	-0.690824
7	-4.054797	0.109420	1.650972
1	-4.561887	0.991962	1.612584
1	-4.040867	-0.133350	2.639866
1	-4.690184	-0.560562	1.221842

E+ZPE = -2089.4890839999998

Cartesian coordinates of : 350-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	0.029097	-0.008099	-0.181250
7	1.816359	0.668268	0.009755
1	2.188394	0.547561	0.981156
1	1.870732	1.667229	-0.189088
1	2.502976	0.214908	-0.640117
7	-1.327345	-1.274049	-0.722966
1	-2.222260	-1.012637	-0.282798
1	-1.125471	-2.271757	-0.460573
1	-1.494387	-1.277602	-1.729986
7	3.805138	-0.509762	-1.816455
1	4.601538	0.123229	-1.808784
1	3.554133	-0.609463	-2.796776
1	4.179214	-1.413974	-1.539998
7	-0.862779	-4.080997	-0.062420
1	-1.313183	-4.366622	0.803596
1	-1.297805	-4.643819	-0.789893
1	0.091719	-4.424793	0.004949
7	-1.105529	1.364278	0.637125
1	-1.187952	2.223323	0.041940
1	-2.050490	0.995278	0.771684
1	-0.777557	1.678995	1.549591
7	-3.960145	-0.311335	0.680307
1	-4.084225	-0.445149	1.681965
1	-4.502961	0.519528	0.453059
1	-4.483441	-1.074426	0.254640
7	2.947172	0.378040	2.716814

1	3.217480	1.285530	3.088645
1	3.815644	-0.145278	2.634796
1	2.431527	-0.076585	3.465894
7	-1.373179	3.804343	-0.977013
1	-0.856584	3.912041	-1.846229
1	-2.349203	3.939533	-1.230148
1	-1.129518	4.618320	-0.417305

E+ZPE = -2089.4976929999998

Cartesian coordinates of : 350-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.372059	-0.025555	-0.322746
7	1.279492	0.803931	0.175313
1	1.569350	1.561054	-0.485035
1	2.019993	0.098204	0.155370
1	1.277081	1.214923	1.136120
7	-2.286728	-0.089235	-0.672959
1	-2.494204	-0.156466	-1.670402
1	-2.840863	0.740596	-0.321919
1	-2.716274	-0.913451	-0.251495
7	1.370034	1.986136	2.892507
1	2.267884	1.754741	3.310587
1	0.677238	1.732264	3.591857
1	1.349068	3.001958	2.848647
7	-3.925995	2.112769	0.214198
1	-3.616064	3.056745	-0.002632
1	-4.823445	2.012305	-0.255063
1	-4.143289	2.119776	1.207808
7	0.231809	-1.835775	-0.743944
1	1.240860	-1.912684	-0.550525
1	-0.260587	-2.571703	-0.190829
1	0.105546	-2.087608	-1.724284
7	-1.141524	-3.989133	0.765656
1	-0.404059	-4.630633	1.048131
1	-1.671893	-3.808329	1.614152
1	-1.759029	-4.541118	0.174875
7	2.175523	2.932041	-1.681149
1	2.842774	3.510090	-1.175860
1	1.489491	3.582509	-2.055381
1	2.682711	2.582521	-2.490361
7	3.293219	-1.859685	-0.130341
1	3.605502	-1.959438	0.833307
1	4.002450	-1.287984	-0.584591
1	3.418644	-2.784528	-0.537808

E+ZPE = -2089.4961589999998

Cartesian coordinates of : 351-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.433921	-0.077547	0.145758
7	2.340485	0.097983	0.307689
1	2.606282	1.047926	0.566669
1	2.836174	-0.106362	-0.590189
1	2.758706	-0.525424	1.037772
7	-0.118865	1.522870	-0.829184
1	0.190113	2.405093	-0.366041
1	-1.146468	1.536698	-0.890998
1	0.239603	1.560576	-1.782834
7	-1.289021	-0.918735	0.388460
1	-2.016296	-0.266896	0.060103
1	-1.399663	-1.809132	-0.154529
7	-1.671561	-3.413197	-1.104431
1	-0.942287	-3.753716	-1.725487
1	-1.859218	-4.181535	-0.464787
1	-2.503911	-3.334970	-1.683623
1	-1.519304	-1.143016	1.356663
7	-3.227816	1.234952	-0.743034
1	-3.525329	1.143036	-1.712425
1	-3.396521	2.211093	-0.507765
7	0.741348	4.067879	0.436026
1	0.931530	4.113742	1.433803
1	1.546598	4.497276	-0.013074
1	-3.921989	0.710652	-0.193065
1	-0.024806	4.719286	0.282172
7	3.593278	-1.597747	2.374292
1	4.576690	-1.338577	2.395349
1	3.263346	-1.470268	3.327619
1	3.583923	-2.602086	2.216344
7	3.826828	-0.462482	-2.185115
1	4.424068	0.327122	-2.418559
1	3.350745	-0.704218	-3.050223
1	4.463650	-1.235016	-2.005357
7	-5.343914	-0.292947	0.960504
1	-6.161497	-0.211419	0.361796
1	-5.331364	-1.261626	1.265994
1	-5.561816	0.250580	1.791235

E+ZPE = -2145.8727909999998

Cartesian coordinates of : 351-2

Atomic number (AN) and Cartesian coordinates
AN X Y Z

29	-0.401955	0.528491	0.006802
7	1.441189	0.796315	-0.502855
1	1.834034	1.717357	-0.190677
1	1.612706	0.735713	-1.506489
1	2.000893	0.049009	-0.064617
7	-2.231822	1.030110	0.332151
1	-2.687702	0.386116	1.011230
1	-2.815401	1.041721	-0.537669
1	-2.323685	1.964308	0.734115
7	2.811125	-1.565228	0.973577
1	2.775394	-2.580110	0.898226
1	3.028509	-1.384504	1.951787
1	3.658122	-1.297997	0.452210
7	-3.937852	1.196753	-2.061955
1	-3.565070	0.985427	-2.983814
1	-4.763493	0.611223	-1.963567
1	-4.291169	2.148445	-2.128207
7	-0.307299	-1.328153	0.590618
1	-0.606787	-2.007899	-0.144693
1	0.671131	-1.542864	0.822705
1	-0.876915	-1.519504	1.413281
7	5.404064	-0.850862	-0.589113
1	5.698389	-1.729441	-1.006943
1	5.526482	-0.152814	-1.316699
1	6.106117	-0.636425	0.113839
7	2.572445	3.365229	0.346675
1	3.220489	3.242092	1.120707
1	3.129300	3.745745	-0.414801
7	-1.091199	-3.331018	-1.433448
1	-0.421762	-3.447508	-2.189956
1	-1.995594	-3.228178	-1.886167
1	-1.126435	-4.233861	-0.966046
7	-3.594546	-0.701625	2.355119
1	-3.246964	-0.663910	3.310513
1	-3.797037	-1.682433	2.178239
1	-4.505660	-0.249377	2.391246
1	1.956084	4.122766	0.629605

E+ZPE = -2145.8720619999999

Cartesian coordinates of : 351-3

Atomic number (AN) and Cartesian coordinates
AN X Y Z

29	0.271434	0.262133	0.118758
7	1.667756	1.486249	0.628627
1	2.442028	0.993743	1.117736
1	1.346196	2.208014	1.275474
1	2.080860	2.002286	-0.184147
7	-1.508006	-0.276393	-0.376298
1	-1.706226	-0.205926	-1.374541
1	-2.271320	0.283265	0.121610
1	-1.627710	-1.264379	-0.122926
7	2.827733	3.061709	-1.570451
1	2.717268	4.045744	-1.337146
1	2.470609	2.970141	-2.517850
1	3.831352	2.915342	-1.644643
7	-3.543299	1.188031	0.916109
1	-4.410906	1.066464	0.373248
1	-3.758937	0.863927	1.855936
1	-3.416963	2.193463	1.003884
7	1.135080	-1.486702	0.231709
1	1.833412	-1.538529	0.971854
1	0.422486	-2.199006	0.419094
1	1.617116	-1.762250	-0.654812
7	-1.509194	-3.340626	0.609106
1	-1.012009	-4.177864	0.311909
1	-1.645467	-3.454895	1.611445
1	-2.438716	-3.447521	0.207486
7	-6.211832	0.922148	-0.622539
1	-6.222312	1.038188	-1.631374
1	-6.782751	1.677593	-0.254136
1	-6.733516	0.070466	-0.437788
7	3.894892	0.156700	2.139925
1	4.485453	0.969532	2.303161
1	4.513083	-0.533147	1.719952
1	3.681326	-0.199718	3.068646
7	2.487089	-2.362096	-2.238253
1	3.045003	-3.182256	-2.012451
1	1.855729	-2.663777	-2.976197
1	3.131809	-1.713899	-2.682939

E+ZPE = -2145.8715840000000

Cartesian coordinates of : 360-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.183818	0.022208	-0.004192
7	1.493219	-0.902352	-0.133105
1	2.176325	-0.282730	-0.575754
1	1.454030	-1.770606	-0.710229

1	1.886310	-1.170848	0.795123
7	0.361300	1.820861	-0.553958
1	0.322705	2.509430	0.228959
1	-0.218960	2.205193	-1.298531
1	1.327227	1.799410	-0.906650
7	-2.070239	0.209287	0.332885
1	-2.608966	0.345844	-0.551657
1	-2.499392	-0.605994	0.827985
7	-3.383348	-2.025565	1.759208
1	-3.512689	-2.883935	1.230033
1	-2.980895	-2.312323	2.647649
1	-4.321860	-1.703161	1.982510
1	-2.272218	1.022900	0.913567
7	-3.664755	0.598838	-2.134916
1	-4.405801	-0.097800	-2.120051
1	-3.244337	0.521371	-3.057284
7	0.256389	3.844391	1.616754
1	-0.075442	3.610265	2.548714
1	1.193308	4.216054	1.752932
1	-4.142842	1.496593	-2.130578
1	-0.305720	4.639684	1.323085
7	2.680725	-1.708360	2.474431
1	3.669494	-1.470880	2.482380
1	2.308749	-1.336975	3.344465
1	2.646839	-2.719576	2.576305
7	1.480869	-3.382320	-1.778819
1	2.328909	-3.893932	-1.547769
1	1.527735	-3.223244	-2.781948
1	0.722759	-4.046401	-1.646080
7	3.319958	1.499681	-1.577586
1	3.600411	0.908860	-2.357431
1	4.100669	1.473205	-0.925212
1	3.335558	2.444323	-1.957208

E+ZPE = -2145.8798029999998

Cartesian coordinates of : 360-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.001497	-0.349500	-0.306943
7	-1.892335	-0.201324	-0.015409
1	-2.452626	-0.800828	-0.660665
1	-2.173611	0.766500	-0.188711
1	-2.193583	-0.438981	0.954628
7	1.660277	-1.253482	-0.685512
1	1.541983	-2.050472	-1.312761
1	2.135121	-1.637584	0.163641

1	2.332503	-0.618992	-1.161826
7	-2.877457	-0.905655	2.699726
1	-3.420363	-0.143393	3.097479
1	-2.232842	-1.188229	3.432986
1	-3.530825	-1.679016	2.603294
7	3.057958	-2.487550	1.603975
1	3.127231	-3.485623	1.420007
1	4.018472	-2.158411	1.660423
1	2.690698	-2.414292	2.548858
7	0.510068	1.535190	-0.297978
1	-0.319242	2.115674	-0.481118
1	0.912919	1.852072	0.611108
1	1.205358	1.752595	-1.010400
7	1.639659	2.569053	2.240419
1	0.919492	2.892395	2.881293
1	2.248675	1.973962	2.795462
1	2.194360	3.393564	2.023439
7	-3.529115	-1.895274	-1.832590
1	-4.505051	-1.704783	-1.619096
1	-3.422378	-2.900453	-1.723060
1	-3.433934	-1.720608	-2.829676
7	-2.196307	3.065295	-0.780425
1	-2.898494	3.231456	-0.062719
1	-2.719247	2.937946	-1.644212
1	-1.730956	3.963849	-0.892610
7	3.620063	0.477627	-2.158487
1	4.097228	1.250886	-1.701736
1	3.353039	0.826612	-3.075977
1	4.349802	-0.207515	-2.342725

E+ZPE = -2145.8789889999998

Cartesian coordinates of : 361-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.808455	0.282317	0.050798
7	2.649989	-0.222797	0.342866
1	2.911216	-0.216624	1.329001
1	3.334952	0.401266	-0.142586
1	2.819481	-1.189360	0.004580
7	-0.101838	-1.432349	0.004824
1	-0.930366	-1.425335	-0.625752
1	-0.423046	-1.720969	0.949370
1	0.516638	-2.174046	-0.321362
7	-0.627201	1.526349	-0.227953
1	-1.501211	1.179854	0.238017
1	-0.433407	2.485481	0.134180

7	-0.139008	4.275660	0.795885
1	0.775108	4.549917	1.145468
1	-0.360170	4.946473	0.064280
1	-0.787700	4.476519	1.552636
1	-0.857853	1.631921	-1.215843
7	-3.047702	0.503704	1.006044
1	-3.467646	1.148264	1.671132
1	-2.964837	-0.382229	1.496729
7	-2.416688	-1.479250	-1.865827
1	-2.197249	-1.248961	-2.831734
1	-2.730487	-2.446635	-1.890469
1	-3.741761	0.356498	0.270292
1	-3.240498	-0.927977	-1.623893
7	3.174128	-3.029853	-0.641259
1	2.830404	-3.845188	-0.139668
1	3.024604	-3.234097	-1.626457
1	4.184002	-3.056900	-0.517763
7	4.638174	1.496391	-1.006279
1	5.439216	1.603240	-0.388646
1	4.385145	2.441157	-1.283152
1	5.002810	1.057959	-1.848206
7	-5.326853	0.052108	-1.276152
1	-5.756481	0.939656	-1.027225
1	-5.419460	-0.007072	-2.287082
1	-5.951906	-0.660727	-0.907929
7	-0.924069	-2.414347	2.738204
1	-0.189077	-3.021373	3.092874
1	-1.745419	-3.010004	2.666785
1	-1.122702	-1.767203	3.496817

E+ZPE = -2202.2531260000001

Cartesian coordinates of : 361-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	0.716988	0.476811	-0.501608
7	2.633247	0.297001	-0.666836
1	2.887451	-0.667569	-0.955684
1	3.151000	0.509378	0.216136
1	3.033637	0.914489	-1.374331
7	0.142504	-1.348766	-0.169404
1	0.774072	-2.025031	-0.596808
1	-0.807013	-1.527555	-0.556511
1	0.116862	-1.580021	0.842657
7	-0.950540	1.426590	-0.537834
1	-1.588272	1.078463	0.218630
1	-0.863116	2.461799	-0.438998

7	-0.767746	4.384243	-0.312495
1	-0.789863	4.727780	0.644051
1	0.011115	4.864280	-0.755541
1	-1.601607	4.762173	-0.755262
1	-1.447902	1.264948	-1.413687
7	-2.755078	0.365560	1.472942
1	-3.105611	1.069109	2.118096
1	-2.412944	-0.394081	2.054445
7	3.411112	-2.460603	-1.601369
1	3.028230	-2.786556	-2.485649
1	4.398385	-2.298495	-1.788153
1	-3.569346	-0.000660	0.975544
1	3.392128	-3.267709	-0.982924
7	4.219516	0.958714	1.736782
1	4.760675	0.159873	2.057458
1	3.766075	1.330885	2.566799
1	4.907377	1.658835	1.469688
7	-5.414679	-0.750926	-0.048419
1	-5.782132	-1.505609	0.525910
1	-5.918094	0.081158	0.249142
1	-5.756183	-0.939050	-0.987617
7	-2.547488	-1.891240	-1.331908
1	-2.642165	-1.742215	-2.333481
1	-3.353182	-1.437717	-0.900100
1	-2.691879	-2.889721	-1.200713
7	0.147344	-2.199695	2.724748
1	-0.599270	-2.872191	2.881936
1	0.074677	-1.529431	3.485599
1	1.006910	-2.713242	2.902558

E+ZPE = -2202.2526840000000

Cartesian coordinates of : 361-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.153816	-0.035307	0.008088
7	1.513175	-1.384775	0.005450
1	2.429781	-0.923105	0.038888
1	1.498077	-1.975775	-0.851544
1	1.464825	-2.026771	0.823738
7	-1.670803	0.621935	0.006334
1	-1.855207	1.222603	0.809928
1	-2.420351	-0.143020	0.022559
1	-1.866568	1.197723	-0.812619
7	1.462790	-3.251825	2.342529
1	1.831503	-4.146658	2.030632
1	0.578668	-3.468459	2.794704

1	2.082070	-2.950379	3.090340
7	-3.686131	-1.340494	0.046750
1	-4.592255	-0.851026	0.005429
1	-3.691223	-1.994111	-0.732386
1	-3.724439	-1.918476	0.882693
7	1.216278	1.588068	0.022155
1	2.208522	1.345110	0.063184
1	1.069032	2.160911	-0.830770
1	1.005019	2.193375	0.837699
7	0.816924	3.284772	-2.438789
1	1.740556	3.459883	-2.826754
1	0.252343	2.978982	-3.226857
1	0.454935	4.200898	-2.186402
7	-6.461507	0.010904	-0.068168
1	-6.717632	0.604988	0.714704
1	-7.118810	-0.763634	-0.050997
1	-6.686484	0.542622	-0.903672
7	4.248878	0.273219	0.120353
1	4.761867	-0.601325	0.209998
1	4.572039	0.839721	0.901524
1	4.635292	0.714474	-0.711217
7	0.622390	3.375350	2.384150
1	1.508954	3.826578	2.595887
1	-0.022409	4.136679	2.188160
1	0.310547	2.976042	3.265496
7	1.527571	-3.108544	-2.439981
1	0.888115	-2.920040	-3.207182
1	1.359715	-4.077249	-2.180634
1	2.455903	-3.096927	-2.854565

E+ZPE = -2202.2523350000001

Cartesian coordinates of : 370

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	-0.004288	-0.220763	-0.028132
7	-1.895295	-0.530993	0.071422
1	-2.185336	-1.491829	-0.205184
1	-2.348205	0.117090	-0.580105
1	-2.301357	-0.355069	1.013539
7	1.878034	-0.583522	0.055732
1	2.138571	-1.560592	-0.191803
1	2.300539	-0.386973	0.986517
1	2.339566	0.031186	-0.621535
7	-3.165153	-0.112871	2.744863
1	-3.803350	0.678474	2.749005
1	-2.589646	-0.001944	3.575122

1	-3.745329	-0.927933	2.926747
7	3.187810	-0.105439	2.699515
1	3.603977	-0.981840	3.004021
1	3.964105	0.545191	2.611741
1	2.645421	0.225298	3.492734
7	0.018872	1.564480	-0.813470
1	-0.820201	1.703139	-1.383490
1	0.039611	2.330593	-0.109802
1	0.851354	1.672523	-1.399600
7	0.084417	3.857140	1.100600
1	-0.535768	4.584089	0.752822
1	-0.183468	3.714254	2.070415
1	1.006505	4.284135	1.133347
7	-2.827832	-3.265107	-0.709581
1	-3.843364	-3.231082	-0.747763
1	-2.607978	-4.002821	-0.045698
1	-2.536170	-3.619105	-1.616646
7	-2.920715	1.621893	-2.186082
1	-3.719118	1.997957	-1.679404
1	-3.306699	0.922853	-2.816875
1	-2.624210	2.380294	-2.796708
7	2.923897	1.500738	-2.260413
1	3.781720	1.778019	-1.788354
1	2.665002	2.312698	-2.816896
1	3.206363	0.801595	-2.943754
7	2.726935	-3.366381	-0.642200
1	2.475451	-3.708071	-1.565884
1	2.436126	-4.093635	0.005701
1	3.743451	-3.375941	-0.619087

E+ZPE = -2202.2592380000001

Cartesian coordinates of : 400

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.000002	-0.000002	-0.000018
7	-1.122671	-1.610985	0.541760
1	-0.612776	-2.292084	1.107317
1	-1.496215	-2.146861	-0.244347
1	-1.938089	-1.368428	1.107446
7	-1.611041	1.122626	-0.541742
1	-1.368526	1.938147	-1.107297
1	-2.146993	1.496008	0.244388
1	-2.292057	0.612748	-1.107412
7	1.122659	1.610989	0.541762
1	1.938177	1.368431	1.107304
1	1.496051	2.146972	-0.244343

7	1.611049	-1.122626	-0.541736
1	2.292056	-0.612750	-1.107420
1	2.147010	-1.495993	0.244395
1	1.368536	-1.938157	-1.107279
1	0.612799	2.291993	1.107465

E+ZPE = -1863.9746849999999

Cartesian coordinates of : 410

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.546912	-0.000534	-0.046909
7	-1.698889	-1.535028	0.646116
1	-1.181091	-2.165297	1.260901
1	-2.073007	-2.131679	-0.094212
7	0.803365	1.476502	0.223717
1	0.643412	2.045154	1.056350
7	0.888319	-1.200889	-0.811675
1	0.948713	-1.122915	-1.829019
1	1.810618	-0.910438	-0.455920
1	0.808430	-2.200787	-0.629944
7	3.591156	-0.004373	0.298888
1	3.975592	-0.940308	0.421744
1	3.889241	0.489534	1.139143
1	1.744984	1.071749	0.323867
1	4.148899	0.402382	-0.450934
1	0.870093	2.142028	-0.547546
1	-2.511150	-1.250329	1.194802
7	-2.134811	1.266445	-0.240262
1	-2.486461	1.627474	0.648506
1	-1.927007	2.096049	-0.797730
1	-2.944785	0.844285	-0.697141

E+ZPE = -1920.3655340000000

Cartesian coordinates of : 420-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.000000	0.000000	-0.112010
7	-1.470101	1.335485	-0.523714
1	-1.543639	1.537380	-1.522405
1	-1.373956	2.245514	-0.074374
1	-2.390093	0.971022	-0.241645
7	-1.377169	-1.428197	0.288731

1	-1.196065	-1.932690	1.157492
1	-1.451551	-2.147804	-0.430989
1	-2.318829	-1.023940	0.381197
7	1.470101	-1.335485	-0.523715
1	1.543639	-1.537380	-1.522405
1	2.390093	-0.971022	-0.241645
7	1.377169	1.428197	0.288731
1	2.318829	1.023940	0.381197
1	1.451551	2.147804	-0.430989
1	1.196065	1.932690	1.157492
1	1.373956	-2.245514	-0.074375
7	4.190919	-0.000281	0.381411
1	4.503524	0.573702	1.163204
1	4.581967	-0.919163	0.584160
1	4.726699	0.335696	-0.417488
7	-4.190919	0.000280	0.381411
1	-4.581970	0.919164	0.584146
1	-4.503522	-0.573691	1.163213
1	-4.726698	-0.335710	-0.417483

E+ZPE = -1976.7553069999999

Cartesian coordinates of : 420-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.005758	-0.727221	0.071153
7	1.987322	-0.600273	-0.302259
1	2.283970	0.387455	-0.330038
1	2.275778	-1.013233	-1.189818
1	2.575213	-1.042929	0.404938
7	-0.011697	1.132249	0.839861
1	0.814575	1.665862	0.551310
1	-0.017695	1.148319	1.860647
1	-0.842899	1.652993	0.541537
7	-2.815053	2.367405	-0.221212
1	-3.546585	2.221079	-0.915423
1	-2.368444	3.233581	-0.517397
1	-3.318236	2.610173	0.630779
7	0.021871	-2.773601	0.049586
1	0.043341	-3.167439	-0.892563
1	-0.791672	-3.197508	0.496446
7	-1.975386	-0.630613	-0.314238
1	-2.284796	0.352721	-0.351920
1	-2.560616	-1.074229	0.394600
1	-2.254137	-1.055829	-1.199049
7	2.779178	2.410555	-0.226341
1	2.769022	3.087100	0.535284

1	2.562355	2.951821	-1.061459
1	3.765081	2.172782	-0.326424
1	0.825119	-3.183357	0.527344

E+ZPE = -1976.7546600000001

Cartesian coordinates of : 420-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.739165	-0.120194	0.027403
7	0.890049	0.618952	0.900593
1	1.283973	1.422980	0.351776
1	1.623379	-0.093505	0.927938
1	0.795499	0.963277	1.854831
7	-1.946530	0.142427	1.659783
1	-2.887079	-0.244891	1.580354
1	-2.080062	1.123576	1.909654
1	-1.553966	-0.295359	2.494362
7	2.039345	2.911734	-0.531676
1	1.515149	3.409764	-1.246940
1	2.937032	2.697703	-0.960207
1	2.247524	3.612231	0.176938
7	-2.309700	-0.032965	-1.280484
1	-2.903292	-0.863972	-1.266815
1	-2.941548	0.751567	-1.115120
7	0.395510	-1.265397	-1.180838
1	0.731905	-0.779216	-2.012711
1	1.245380	-1.570994	-0.672067
1	-0.054363	-2.113489	-1.525903
7	2.898174	-2.060186	0.366848
1	2.837088	-2.509956	1.278350
1	3.155020	-2.814004	-0.268844
1	3.733226	-1.479178	0.412992
1	-2.017013	0.067124	-2.252845

E+ZPE = -1976.75295899999999

Cartesian coordinates of : 421-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.573795	0.151089	0.161244
7	1.580505	-1.546981	-0.294096
1	1.249881	-1.995568	-1.148977
1	1.526675	-2.266069	0.427722

1	2.582375	-1.360212	-0.433203
7	-0.422813	1.858678	-0.216448
1	-0.393039	2.537436	0.544783
1	-1.426212	1.662053	-0.387407
1	-0.082497	2.359003	-1.038112
7	4.636094	-0.765816	-0.521930
1	5.128689	-1.240341	0.233133
1	5.204111	0.055789	-0.723004
1	4.773688	-1.361751	-1.336802
7	-3.329964	1.106567	-0.611672
1	-3.769586	1.892594	-0.135319
1	-3.476993	1.286681	-1.603491
1	-3.933108	0.298891	-0.396739
7	2.320863	1.083749	0.613314
1	2.467033	1.163749	1.620993
1	3.125666	0.554623	0.253279
1	2.415130	2.032872	0.254296
7	-5.180425	-1.293823	0.038815
1	-5.232027	-1.746189	0.947300
1	-5.231954	-2.045370	-0.643497
7	-1.167391	-0.802324	0.562872
1	-1.962544	-0.266573	0.187146
1	-1.342656	-0.886711	1.565439
1	-1.262556	-1.747919	0.195588
1	-6.058220	-0.788926	-0.055200

E+ZPE = -2033.1326690000001

Cartesian coordinates of : 422

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.004754	-0.517512	-0.207552
7	-1.281321	-1.846475	0.596014
1	-0.962827	-2.234242	1.484353
1	-1.469312	-2.653128	0.000541
7	1.390714	0.956039	-0.178851
1	1.261498	1.628889	0.576849
7	1.442339	-1.887348	-0.582111
1	1.476428	-2.155613	-1.566784
1	2.375915	-1.498146	-0.360252
1	1.361851	-2.764375	-0.069885
7	4.099273	-0.558817	0.068214
1	4.410661	-1.104195	0.870218
1	4.453730	0.393064	0.242850
1	2.335293	0.564992	-0.056703
1	4.654016	-0.903237	-0.713773
1	1.427313	1.511577	-1.033507

1	-2.198673	-1.403260	0.779379
7	-1.533466	0.717928	-0.676242
1	-1.385237	1.708750	-0.491906
1	-1.787898	0.664923	-1.663684
1	-2.381258	0.450161	-0.156674
7	-3.926630	-0.394099	0.977426
1	-3.997906	-0.274923	1.986518
1	-4.542594	-1.176612	0.762551
1	-4.401683	0.428119	0.576743
7	5.224157	2.283787	0.583608
1	5.139743	3.030905	-0.099903
1	6.207599	2.025337	0.574794
1	5.071901	2.721487	1.488004
7	-5.423230	2.035368	-0.233027
1	-5.096754	2.997500	-0.233732
1	-5.811200	1.878461	-1.159221
1	-6.221317	2.026736	0.397021

E+ZPE = -2089.5094840000002

Cartesian coordinates of : 430-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.073668	-0.429413	0.289842
7	-1.295526	1.167437	0.410690
1	-1.594864	1.375495	1.363748
1	-2.155465	1.026839	-0.123716
1	-0.827127	2.016184	0.071982
7	1.145933	-1.884448	-0.408797
1	1.208572	-2.692309	0.211368
1	2.110580	-1.543406	-0.528384
1	0.859202	-2.258175	-1.313756
7	0.540905	3.644841	-0.373755
1	-0.142070	4.315603	-0.025532
1	0.537224	3.768668	-1.384453
1	1.434890	4.027710	-0.071064
7	4.054391	-0.744379	-0.631563
1	4.659648	-0.800329	0.185771
1	4.331886	-1.539074	-1.205554
1	4.386553	0.064776	-1.153090
7	-1.680570	-1.649097	0.421238
1	-1.946315	-1.836295	1.389275
1	-2.500807	-1.194022	-0.013155
1	-1.592803	-2.567197	-0.011457
7	-4.081356	-0.177939	-0.848054
1	-4.617440	-1.038900	-0.944234
1	-4.688251	0.433526	-0.305070

1	-4.073642	0.218486	-1.785841
7	1.507383	0.748524	0.701661
1	1.340519	1.699751	0.355543
1	2.374716	0.401431	0.281329
1	1.693247	0.839637	1.700955

E+ZPE = -2033.1413889999999

Cartesian coordinates of : 430-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.001220	0.854334	-0.008097
7	1.980993	0.886924	-0.398870
1	2.292063	-0.018027	-0.794740
1	2.558767	1.034279	0.429144
1	2.271794	1.605328	-1.062142
7	0.001364	-1.125223	0.173128
1	0.002216	-1.437979	1.170492
1	0.821522	-1.545014	-0.267023
1	-0.818044	-1.547149	-0.266376
7	-2.907030	-1.821693	-1.463730
1	-3.814149	-1.483391	-1.780641
1	-3.131024	-2.598424	-0.844852
1	-2.492886	-2.247709	-2.290238
7	-0.003626	2.820364	0.588546
1	0.804740	3.078707	1.154435
1	-0.813533	3.077376	1.152825
7	-1.983570	0.881910	-0.398526
1	-2.292499	-0.023940	-0.794014
1	-2.276181	1.599376	-1.062017
1	-2.561603	1.028152	0.429503
7	2.910518	-1.813861	-1.466044
1	2.502278	-2.230271	-2.300353
1	3.125770	-2.597422	-0.852703
1	3.821902	-1.476213	-1.771199
1	-0.003393	3.477244	-0.193127
7	0.004520	-2.074325	2.983740
1	0.826016	-1.849010	3.539357
1	-0.789685	-1.809354	3.561087
1	-0.020872	-3.090897	2.949698

E+ZPE = -2033.1396270000000

Cartesian coordinates of : 431

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	-0.763333	0.398279	-0.334661
7	1.238128	0.453857	-0.568071
1	1.536259	0.461252	-1.543703
1	1.670297	-0.375996	-0.147083
1	1.656729	1.280879	-0.134878
7	-0.792379	2.341781	0.231202
1	-1.389676	2.522776	1.037919
1	-1.125616	2.969513	-0.500753
1	0.149400	2.675455	0.483353
7	-2.740219	0.335200	-0.733005
1	-2.925739	0.105115	-1.710180
1	-3.193316	-0.415151	-0.177195
7	-0.710782	-1.604897	-0.210625
1	-1.477172	-1.976127	0.351101
1	-0.782883	-2.071865	-1.114685
1	0.184733	-1.918232	0.202983
1	-3.269375	1.187733	-0.557905
7	-4.048092	-1.885729	0.861232
1	-5.001293	-1.532868	0.797432
1	-4.100770	-2.826456	0.476069
1	-3.889055	-2.012375	1.858402
7	2.116542	3.270206	0.858039
1	2.621538	3.725726	0.100066
1	2.833209	2.823369	1.426596
1	1.781855	4.037908	1.437982
7	4.869300	-1.674530	-0.383449
1	5.279510	-0.793187	-0.678173
1	5.017276	-2.313379	-1.160144
1	5.470847	-2.012810	0.363129
7	2.063609	-2.306513	0.805632
1	1.975575	-3.305084	0.624818
1	2.987205	-2.056607	0.426085
1	2.154352	-2.235313	1.817243

E+ZPE = -2089.5174179999999

Cartesian coordinates of : 432-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	-0.131119	0.755203	0.072206
7	-2.128421	1.013805	-0.097719
1	-2.438962	1.418994	-0.979936
1	-2.534718	1.602661	0.629068
1	-2.594378	0.096051	-0.012582
7	1.707723	0.155836	-0.494035

1	1.818077	0.075842	-1.504796
1	1.942752	-0.768341	-0.105656
1	2.420734	0.820043	-0.189310
7	-3.279187	-1.802445	0.283245
1	-3.524360	-2.236580	1.171297
1	-3.072082	-2.579013	-0.341858
1	-4.164733	-1.408648	-0.067384
7	2.097034	-2.668611	0.729830
1	2.941990	-2.719438	0.143019
1	2.430999	-2.792684	1.683870
1	1.586131	-3.523634	0.517688
7	0.337819	2.681062	-0.317922
1	1.336585	2.850506	-0.110110
1	0.202247	2.946486	-1.293383
1	-0.192739	3.362793	0.223121
7	-5.984122	-0.672853	-0.736357
1	-6.430354	0.113733	-0.273455
1	-6.095245	-0.504584	-1.732158
1	-6.574060	-1.474958	-0.531418
7	4.656359	-2.944729	-1.017723
1	4.547151	-3.072787	-2.019654
1	4.970626	-3.844221	-0.663405
1	5.449608	-2.320168	-0.905488
7	3.313307	3.086406	0.300159
1	4.045218	2.907056	-0.384069
1	3.252265	4.102135	0.342878
1	3.711013	2.816953	1.197397
7	-0.409696	-0.877815	1.193958
1	-1.295709	-1.331786	0.938747
1	0.358376	-1.552024	1.076805
1	-0.469687	-0.679862	2.192742

E+ZPE = -2145.8935600000000

Cartesian coordinates of : 432-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	0.037919	0.139941	-0.480903
7	1.361418	1.638431	-0.302213
1	0.945773	2.435388	0.190410
1	1.687022	2.003147	-1.197326
7	-1.302087	-1.319572	-0.078510
1	-1.100646	-1.840351	0.774750
7	-1.443381	1.467116	-0.756731
1	-1.563415	1.746106	-1.730451
1	-2.352505	1.100115	-0.445330
1	-1.242775	2.327223	-0.235613

7	-4.052799	0.035064	0.170399
1	-4.327203	0.592683	0.977044
1	-4.404501	-0.912662	0.371234
1	-2.249792	-0.928677	0.037750
1	-4.637781	0.370021	-0.593123
1	-1.376560	-2.021383	-0.814690
1	2.201839	1.322602	0.198101
7	1.581361	-1.149807	-0.715189
1	1.430790	-2.112330	-0.419221
1	1.895798	-1.213184	-1.684101
1	2.390830	-0.796877	-0.180266
7	3.861201	0.163577	0.887898
1	3.795615	0.243018	1.900896
1	4.511324	0.896397	0.609262
1	4.374742	-0.713980	0.720032
7	-5.198249	-2.788315	0.760509
1	-5.231689	-3.468876	0.006862
1	-6.165475	-2.522928	0.926316
1	-4.917008	-3.307423	1.587279
7	5.487383	-2.429143	0.370259
1	5.163389	-3.356181	0.630326
1	5.881965	-2.528176	-0.560844
1	6.278599	-2.241217	0.980263
7	-0.399875	4.045669	0.896928
1	-1.299200	4.489981	0.722037
1	0.282277	4.753005	0.630076
1	-0.335878	3.985136	1.911056

E+ZPE = -2145.8932629999999

Cartesian coordinates of : 433

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.213320	-0.435682	0.022158
7	1.949556	-1.460670	-0.119013
1	2.093554	-1.947143	-1.002826
1	2.074143	-2.168574	0.604149
1	2.736713	-0.799797	-0.010666
7	-1.216394	0.842737	-0.568497
1	-1.222274	1.019520	-1.572682
1	-1.122098	1.759996	-0.118687
1	-2.139087	0.453656	-0.342209
7	4.110509	0.658658	0.306990
1	4.481894	0.971255	1.202170
1	4.219508	1.455489	-0.317271
1	4.792154	-0.037438	-0.028699
7	-0.496655	3.550944	0.894661

1	-1.217062	3.930036	0.265465
1	-0.837927	3.737439	1.835644
1	0.301592	4.172084	0.777380
7	-0.982627	-2.005048	-0.420147
1	-1.963795	-1.722748	-0.265441
1	-0.924711	-2.313171	-1.390348
1	-0.825993	-2.841198	0.140761
7	6.229199	-1.394085	-0.662778
1	6.353133	-2.269036	-0.161712
1	6.268347	-1.633837	-1.649201
1	7.073169	-0.857391	-0.481593
7	-2.639533	4.797335	-1.001255
1	-2.301832	5.058486	-1.923257
1	-2.774895	5.673600	-0.504122
1	-3.572885	4.423826	-1.146198
7	-3.798050	-0.890466	0.052994
1	-4.389566	-0.495278	-0.675494
1	-4.101948	-1.871604	0.134098
1	-4.108112	-0.448006	0.915891
7	1.076395	0.921723	1.212573
1	2.069891	1.014378	0.972607
1	0.622011	1.843285	1.129762
1	1.045839	0.672893	2.201089
7	-4.779207	-3.828896	0.279287
1	-4.749543	-4.224597	1.214672
1	-4.473268	-4.571531	-0.342648
1	-5.765575	-3.695434	0.073092

E+ZPE = -2202.2686910000002

Cartesian coordinates of : 440-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.055537	0.271121	-0.064931
7	-1.747724	-0.226191	0.912322
1	-1.722920	0.011842	1.903934
1	-1.897225	-1.242195	0.867107
1	-2.575745	0.237822	0.529176
7	-1.021686	1.778422	-1.021704
1	-0.865800	1.778508	-2.029580
1	-0.733324	2.702832	-0.701458
1	-2.040603	1.731550	-0.885156
7	1.758732	0.934157	-0.578801
1	2.269187	1.338218	0.238360
1	2.324333	0.151707	-0.917927
7	0.748300	-1.509444	0.421524
1	1.502922	-1.768499	-0.227664

1	1.165962	-1.514324	1.351960
1	0.040756	-2.248581	0.427206
1	1.794741	1.646640	-1.305436
7	3.180930	-1.943130	-1.504171
1	2.821464	-2.519867	-2.262200
1	3.879424	-1.348932	-1.946363
1	3.723586	-2.578686	-0.922434
7	-4.106266	1.534829	-0.481419
1	-4.574174	1.747636	0.397630
1	-4.665089	0.799877	-0.910575
1	-4.279023	2.354667	-1.060727
7	3.265508	2.138834	1.678590
1	3.788371	2.920676	1.290583
1	3.969678	1.516857	2.067995
1	2.771966	2.521623	2.480877
7	-1.908770	-3.393959	0.744330
1	-1.403430	-4.066283	1.318278
1	-2.845282	-3.381552	1.144070
1	-2.022360	-3.848685	-0.159352

E+ZPE = -2089.5255020000000

Cartesian coordinates of : 442-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.077603	-0.409121	0.083191
7	-2.083486	-0.319651	0.317595
1	-2.404222	-0.508314	1.266150
1	-2.571578	-0.991281	-0.273573
1	-2.433575	0.616481	0.064873
7	1.855060	-0.093933	0.538396
1	2.016509	0.072594	1.531131
1	2.240820	0.719531	0.046651
1	2.407640	-0.923615	0.297163
7	-2.838028	2.555095	-0.515136
1	-3.082515	2.831458	-1.464157
1	-2.473307	3.399808	-0.079298
1	-3.740652	2.387191	-0.048652
7	2.612891	2.554312	-1.008754
1	3.436670	2.532734	-0.393079
1	2.983273	2.503277	-1.955716
1	2.249194	3.501156	-0.920192
7	0.041507	-2.323316	0.657981
1	0.975330	-2.681272	0.439394
1	-0.083643	-2.462026	1.660105
1	-0.654398	-2.936708	0.194110
7	-5.598586	2.136461	0.860019

1	-6.216348	1.381529	0.576762
1	-5.639238	2.159813	1.874816
1	-6.056074	2.989894	0.551050
7	5.124061	2.604682	0.848733
1	4.974945	3.181599	1.671774
1	5.752893	3.137277	0.253676
1	5.666632	1.807760	1.168186
7	3.183860	-2.947562	-0.062331
1	4.009928	-2.514696	-0.470278
1	3.524810	-3.423703	0.770297
1	2.941938	-3.690966	-0.713969
7	-0.118076	1.113891	-1.217299
1	-0.927820	1.718337	-1.034922
1	0.743582	1.675900	-1.168828
1	-0.205935	0.809185	-2.186492
7	-1.977836	-4.146608	-0.655689
1	-1.608383	-5.066414	-0.426172
1	-2.048614	-4.134777	-1.670023
1	-2.936947	-4.160842	-0.317942

E+ZPE = -2202.2758450000001

Cartesian coordinates of : 442-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.000001	0.000000	-0.482816
7	-1.874042	-0.743452	-0.515066
1	-1.920114	-1.638206	-0.017277
1	-2.228424	-0.920904	-1.454505
7	1.874041	0.743452	-0.515072
1	1.920114	1.638206	-0.017283
7	0.740338	-1.863426	-0.395018
1	0.878984	-2.282173	-1.314499
1	1.662886	-1.871787	0.064818
1	0.106908	-2.490739	0.108888
7	3.578092	-1.594642	0.791299
1	3.598634	-1.532609	1.807097
1	4.386302	-1.049285	0.462660
1	2.537451	0.093559	-0.079735
1	3.821104	-2.561918	0.585989
1	2.228420	0.920904	-1.454511
1	-2.537451	-0.093560	-0.079728
7	-0.740340	1.863426	-0.395014
1	-0.106909	2.490738	0.108892
1	-0.878988	2.282174	-1.314494
1	-1.662887	1.871787	0.064823
7	-3.578092	1.594640	0.791306

1	-3.821103	2.561918	0.585999
1	-3.598636	1.532604	1.807103
1	-4.386303	1.049286	0.462663
7	6.088252	-0.056077	-0.237478
1	6.480945	-0.591473	-1.006838
1	6.739091	-0.171480	0.534645
1	6.169245	0.917418	-0.515398
7	-6.088252	0.056081	-0.237483
1	-6.169245	-0.917412	-0.515405
1	-6.739093	0.171484	0.534639
1	-6.480943	0.591480	-1.006843
7	-1.627358	-3.588745	0.975767
1	-0.962076	-4.060788	1.584689
1	-1.944429	-4.307054	0.327853
1	-2.427769	-3.401369	1.575920
7	1.627364	3.588741	0.975764
1	0.962074	4.060810	1.584657
1	2.427751	3.401356	1.575947
1	1.944473	4.307033	0.327851

E+ZPE = -2202.2757689999999

Cartesian coordinates of : 442-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	-0.000087	0.358785	-0.500885
7	1.422632	1.776591	-0.484524
1	1.096488	2.622688	-0.007553
1	1.707914	2.070336	-1.418481
7	-1.423673	-1.066682	-0.457934
1	-1.104418	-1.887519	0.065259
7	-1.422811	1.776581	-0.484027
1	-1.708422	2.070322	-1.417885
1	-2.275019	1.434835	-0.017368
1	-1.096506	2.622681	-0.007172
7	-3.920737	0.429634	0.767532
1	-3.915021	0.410055	1.785264
1	-4.458531	-0.398071	0.476429
1	-2.285784	-0.715274	-0.025746
1	-4.517617	1.219016	0.527704
1	-1.690662	-1.404689	-1.382151
1	2.275007	1.434850	-0.018164
7	1.423525	-1.066671	-0.458436
1	1.104459	-1.887512	0.064869
1	1.690191	-1.404676	-1.382747
1	2.285785	-0.715258	-0.026550
7	3.921007	0.429661	0.766158

1	3.915646	0.410100	1.783892
1	4.517803	1.219040	0.526108
1	4.458700	-0.398048	0.474881
7	-5.662858	-1.989715	-0.141792
1	-6.206400	-1.704786	-0.951748
1	-6.329713	-2.063615	0.621667
1	-5.366603	-2.941823	-0.334558
7	5.662816	-1.989699	-0.143733
1	5.366497	-2.941812	-0.336376
1	6.206073	-1.704785	-0.953884
1	6.329937	-2.063583	0.619495
7	0.000121	4.346196	0.849893
1	-0.803241	4.532022	1.446721
1	-0.000192	5.100518	0.166241
1	0.803869	4.532182	1.446152
7	0.000202	-3.530110	1.069813
1	0.803936	-3.659125	1.680882
1	-0.803323	-3.659140	1.681152
1	0.000107	-4.344192	0.458682

E+ZPE = -2202.2757080000001

Cartesian coordinates of : 442-4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.219625	0.932365	-0.158565
7	-0.603569	-0.859842	0.103192
1	0.090441	-1.548925	0.406341
1	-1.005569	-1.213084	-0.764388
7	1.111905	2.723051	0.184749
1	0.699612	3.245804	0.956438
7	1.999779	0.097713	-0.595271
1	2.784820	0.647788	-0.242185
1	2.059920	-0.846411	-0.181960
1	2.160360	-0.019484	-1.595462
7	1.975564	-2.690188	0.687087
1	1.399205	-3.514358	0.528843
1	2.167246	-2.694499	1.686846
1	2.112722	2.609943	0.402532
1	2.873161	-2.914004	0.234959
1	1.069419	3.347738	-0.620341
1	-1.389276	-0.837386	0.782050
7	-1.620182	1.727705	-0.280005
1	-2.053234	1.771943	0.642423
1	-1.694341	2.665479	-0.670390
1	-2.248055	1.114723	-0.845088
7	-2.994899	-0.784788	1.886162

1	-3.255894	-0.050152	2.538889
1	-2.903598	-1.619425	2.460656
1	-3.811928	-0.940483	1.293348
7	4.145203	2.289613	0.704933
1	4.768723	2.437162	-0.086103
1	4.591080	1.569708	1.269443
1	4.232343	3.137609	1.261971
7	-3.495261	0.002455	-1.769562
1	-4.094634	0.667723	-2.253038
1	-3.240629	-0.678854	-2.480131
1	-4.101695	-0.485614	-1.107802
7	-5.753364	-1.421384	0.163859
1	-6.438926	-0.690811	0.339119
1	-5.903867	-2.109746	0.897176
1	-6.062322	-1.880378	-0.689497
7	4.650109	-3.522201	-0.675730
1	4.436377	-4.196163	-1.405473
1	5.133655	-4.046992	0.047807
1	5.348752	-2.902358	-1.074492

E+ZPE = -2202.2746450000000

Cartesian coordinates of : 450

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.001052	0.005109	0.001708
7	-1.415414	1.372200	-0.427950
1	-1.715285	1.330132	-1.401617
1	-1.096738	2.332145	-0.265678
1	-2.258839	1.204319	0.135201
7	1.456059	-1.338451	-0.284235
1	1.205191	-2.085108	-0.930250
1	1.744405	-1.804869	0.600082
1	2.288447	-0.885010	-0.667114
7	-3.945871	0.533029	1.264236
1	-4.445429	1.391791	1.041703
1	-3.873556	0.531385	2.279419
1	-4.609180	-0.206820	1.043463
7	2.308691	-2.723552	2.229615
1	2.225066	-3.730153	2.108931
1	3.301546	-2.556899	2.374888
1	1.870973	-2.523057	3.125062
7	1.366657	1.427964	0.413601
1	1.007903	2.375375	0.262509
1	1.686428	1.393018	1.381183
1	2.205084	1.295074	-0.166180
7	-2.160449	-2.869018	-2.189464

1	-2.041372	-3.868727	-2.043814
1	-3.156745	-2.742801	-2.351070
1	-1.718606	-2.673314	-3.083943
7	-0.106055	4.278336	0.011443
1	-0.783718	4.658347	0.669215
1	0.769929	4.733471	0.260460
7	3.896534	0.678622	-1.322742
1	4.623558	0.029096	-1.030110
1	4.316360	1.597913	-1.199539
1	3.824480	0.562177	-2.331238
1	-0.354102	4.680683	-0.890199
7	-1.400905	-1.390695	0.301571
1	-1.657144	-1.889341	-0.574945
1	-1.126973	-2.110991	0.967888
1	-2.256915	-0.965051	0.663653

E+ZPE = -2145.9089540000000

Cartesian coordinates of : 460

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.162413	-0.004162	0.218836
7	1.712114	-0.684894	0.237405
1	2.124505	-0.707097	-0.714981
1	1.775153	-1.635815	0.602458
1	2.317125	-0.085417	0.802591
7	-1.919778	0.603641	-0.528412
1	-1.825652	1.341843	-1.223677
1	-2.544350	0.977818	0.211761
1	-2.412056	-0.172693	-0.975782
7	3.360710	1.648441	1.882760
1	4.242605	1.379179	1.452469
1	3.410353	1.299387	2.837361
1	3.420009	2.660441	1.973704
7	-3.736441	1.706363	1.605451
1	-3.964193	2.678223	1.410405
1	-4.622656	1.210519	1.548323
1	-3.479537	1.682286	2.588766
7	-0.940596	-1.826626	0.601176
1	-0.226204	-2.557734	0.699400
1	-1.479924	-1.837026	1.466263
1	-1.596801	-2.095358	-0.139947
7	0.325583	3.670573	-1.861988
1	-0.379160	4.396487	-1.758240
1	1.215101	4.163798	-1.859305
1	0.217492	3.322858	-2.811038
7	1.372683	-3.913941	1.082624

1	1.977583	-3.878485	1.900214
1	0.720374	-4.669728	1.281107
7	-3.164734	-2.265755	-1.645087
1	-3.986297	-2.570033	-1.127101
1	-2.772625	-3.116381	-2.043157
1	-3.534331	-1.759024	-2.446526
1	1.957188	-4.268136	0.328978
7	0.432284	1.874524	0.584235
1	0.429853	2.460801	-0.269324
1	-0.176068	2.351702	1.247988
1	1.376469	1.897840	0.982423
7	2.981232	-0.794602	-2.498806
1	2.392154	-0.981204	-3.305665
1	3.672061	-1.540722	-2.491671
1	3.500384	0.048319	-2.729525

E+ZPE = -2202.2885339999998

Cartesian coordinates of : 500

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.002206	0.003003	-0.122482
7	0.642283	1.935205	-0.625336
1	1.151197	2.399270	0.128115
1	-0.092265	2.594217	-0.882417
7	-0.660258	-1.922721	-0.639177
1	-1.147547	-1.942793	-1.536428
7	0.031605	-0.022546	2.112499
1	-0.680601	0.557175	2.556211
1	-0.107586	-0.948556	2.517444
1	0.908333	0.302136	2.520431
7	1.955375	-0.640070	-0.292578
1	2.655470	0.045332	-0.008352
1	2.217888	-0.901078	-1.244568
1	0.066175	-2.632421	-0.731379
1	2.160161	-1.464046	0.273353
1	-1.322639	-2.321046	0.027149
1	1.279448	1.949335	-1.422779
7	-1.963502	0.643362	-0.245838
1	-2.276753	0.821979	-1.201498
1	-2.645725	-0.013208	0.133862
1	-2.140119	1.514008	0.255852

E+ZPE = -1920.3753280000001

Cartesian coordinates of : 510

Atomic number (AN) and Cartesian coordinates
AN X Y Z

29	0.484342	0.000000	-0.131116
7	0.616282	0.000000	2.110743
1	-0.302424	0.000001	2.553096
1	1.094052	0.806154	2.512674
7	1.932410	-1.451177	-0.518744
1	2.816755	-1.303769	-0.032727
7	-0.979848	1.433181	-0.342176
1	-0.914117	2.209181	0.315646
1	-0.995914	1.866435	-1.265967
1	-1.917348	1.032395	-0.213021
7	-0.979849	-1.433180	-0.342172
1	-1.917348	-1.032393	-0.213017
1	-0.914117	-2.209179	0.315652
1	1.652547	-2.398066	-0.265041
1	-0.995915	-1.866436	-1.265962
1	2.182942	-1.510956	-1.506782
1	1.094052	-0.806154	2.512674
7	1.932412	1.451176	-0.518740
1	2.816756	1.303767	-0.032724
1	2.182944	1.510956	-1.506778
1	1.652549	2.398064	-0.265036
7	-3.798014	-0.000000	-0.060135
1	-4.203865	0.802404	0.418831
1	-4.237373	-0.000002	-0.979420
1	-4.203865	-0.802403	0.418834

E+ZPE = -1976.7647239999999

Cartesian coordinates of : 520-1

Atomic number (AN) and Cartesian coordinates
AN X Y Z

29	-0.004436	0.000007	0.157408
7	1.448442	-1.420382	0.517020
1	2.377650	-1.057086	0.274531
1	1.337210	-2.294939	0.006677
7	-1.471681	1.434820	0.363767
1	-1.501823	1.846707	1.296440
7	0.097764	-0.000094	-2.096495
1	0.579380	-0.806093	-2.492873
1	-0.819007	-0.000115	-2.542131
1	0.579379	0.805869	-2.492945
7	1.448442	1.420428	0.516893
1	2.377650	1.057111	0.274437

1	1.510201	1.692666	1.498197
1	-1.381106	2.225011	-0.273098
1	1.337210	2.294940	0.006473
1	-2.407695	1.043955	0.204620
1	1.510201	-1.692532	1.498348
7	-1.471681	-1.434787	0.363897
1	-1.501823	-1.846590	1.296608
1	-2.407695	-1.043937	0.204715
1	-1.381106	-2.225036	-0.272895
7	4.251840	-0.000002	-0.050645
1	4.617892	-0.802789	-0.559544
1	4.761432	0.000038	0.831466
7	-4.295280	0.000000	0.000152
1	-4.688748	-0.802850	-0.487833
1	-4.688748	0.802804	-0.487908
1	-4.754623	0.000043	0.909387
1	4.617892	0.802738	-0.559617

E+ZPE = -2033.1520579999999

Cartesian coordinates of : 520-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.000000	-0.641923	-0.156438
7	2.044267	-0.620980	-0.366933
1	2.366261	-0.891632	-1.296326
1	2.555281	-1.222803	0.277243
7	0.000000	-0.404238	2.081092
1	-0.807193	0.115504	2.423093
7	-2.044267	-0.620980	-0.366933
1	-2.366261	-0.891633	-1.296326
1	-2.555280	-1.222804	0.277244
1	-2.402927	0.331451	-0.214207
7	-0.000000	1.334297	-0.704943
1	-0.830992	1.824571	-0.365532
1	-0.000000	1.466408	-1.716306
1	-0.000001	-1.269741	2.619638
1	0.830991	1.824571	-0.365532
1	0.807195	0.115502	2.423094
1	2.402927	0.331452	-0.214207
7	0.000001	-2.723599	-0.324262
1	0.808333	-3.179563	0.096972
1	-0.808334	-3.179563	0.096969
1	0.000003	-3.034939	-1.296335
7	-3.025766	2.347065	0.032496
1	-3.333996	2.727329	-0.860775
1	-3.885196	2.060589	0.498175

1	-2.713273	3.156364	0.565672
7	3.025765	2.347066	0.032496
1	2.713272	3.156364	0.565674
1	3.333994	2.727331	-0.860775
1	3.885196	2.060590	0.498173

E+ZPE = -2033.1512319999999

Cartesian coordinates of : 520-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.594837	-0.125360	-0.086425
7	0.895208	1.905331	-0.340503
1	0.004665	2.417266	-0.278013
1	1.295450	2.169224	-1.240100
1	1.509679	2.324049	0.357109
7	-1.278360	0.289187	0.622838
1	-1.617615	1.199649	0.298996
1	-1.318796	0.331227	1.640360
1	-1.967923	-0.416562	0.348211
7	-3.154518	-2.237121	-0.162628
1	-3.116814	-3.254523	-0.129222
1	-3.649561	-2.026202	-1.027173
1	-3.806085	-1.990175	0.580010
7	2.356116	-0.490448	-1.134426
1	2.254366	-0.396062	-2.145582
1	2.733126	-1.426998	-0.992934
7	-0.031192	-2.046860	-0.525116
1	-1.043658	-2.152575	-0.376584
1	0.413583	-2.769701	0.039700
1	0.129122	-2.327353	-1.492221
7	-1.890923	3.366484	-0.198183
1	-2.166716	3.759529	0.699869
1	-2.766037	3.157129	-0.674925
1	-1.510071	4.156675	-0.715995
1	3.116363	0.141105	-0.884232
7	1.549250	-0.458630	1.953201
1	1.096892	-1.199122	2.488494
1	1.505142	0.359251	2.560305
1	2.535557	-0.716001	1.943965

E+ZPE = -2033.1501920000001

Cartesian coordinates of : 522-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	0.000762	0.005222	-0.175502
7	-1.848613	-0.878058	-0.392652
1	-2.019003	-1.226664	-1.335544
7	1.832346	0.888846	-0.525427
1	1.997278	1.767106	-0.037455
7	0.925886	-1.790772	-0.544764
1	0.939657	-2.044218	-1.532546
1	1.915187	-1.739896	-0.255532
1	0.521562	-2.595886	-0.070216
7	3.888102	-1.383131	0.200570
1	4.025074	-1.756954	1.137663
1	4.564940	-0.611470	0.117279
1	2.590823	0.254041	-0.248089
1	4.244733	-2.106920	-0.421225
1	1.998801	1.097063	-1.509833
7	-0.927894	1.831068	-0.319089
1	-0.578993	2.533523	0.330757
1	-0.840911	2.254915	-1.242402
1	-1.940985	1.747971	-0.142297
7	-3.944142	1.394485	0.121823
1	-4.264491	2.063262	-0.576520
1	-4.133789	1.842314	1.016459
1	-4.615719	0.615558	0.065462
7	5.992775	0.886501	-0.102980
1	6.282344	1.043937	-1.064283
1	6.779868	0.422782	0.343179
1	5.949481	1.807653	0.323184
7	-6.040368	-0.892305	-0.087466
1	-6.179800	-1.337959	-0.989852
1	-6.094456	-1.639571	0.598701
1	-6.872243	-0.328081	0.064900
7	0.112798	-0.068570	2.082263
1	0.820035	0.546337	2.481943
1	-0.758671	0.201293	2.536363
1	0.330863	-0.990573	2.456880
1	-2.012075	-1.675525	0.219436
1	-2.607820	-0.211927	-0.202803

E+ZPE = -2145.9039469999998

Cartesian coordinates of : 522-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	0.000708	-0.464014	-0.190476
7	-1.458415	-1.889846	-0.434509

1	-1.502064	-2.260909	-1.383263
7	1.450097	0.972725	-0.482070
1	1.323330	1.837349	0.040421
7	1.458857	-1.854015	-0.599484
1	1.554793	-2.058724	-1.593991
1	2.377820	-1.495987	-0.297843
1	1.334943	-2.760901	-0.153244
7	4.129499	-0.520830	0.192642
1	4.374753	-0.856258	1.122185
1	4.532257	0.425258	0.133461
1	2.371926	0.603646	-0.216735
1	4.695957	-1.081255	-0.442021
1	1.543477	1.261954	-1.455573
7	-1.472048	0.969989	-0.324938
1	-1.378323	1.738170	0.337178
1	-1.520685	1.412766	-1.242096
1	-2.403669	0.565773	-0.164076
7	-4.183510	-0.538692	0.075874
1	-4.506959	-0.953108	0.947985
1	-4.690922	-1.038052	-0.652685
1	-4.582500	0.410940	0.067610
7	5.435675	2.291110	-0.035729
1	5.646310	2.569014	-0.990217
1	6.334650	2.075186	0.387084
1	5.117131	3.135519	0.430591
7	-5.484465	2.283754	0.010800
1	-5.310250	2.975683	0.733970
1	-5.477552	2.796066	-0.866574
1	-6.449355	1.992973	0.144839
7	0.115824	-0.557251	2.066521
1	0.652169	0.198589	2.489616
1	-0.797365	-0.518219	2.517129
1	0.547419	-1.409589	2.420547
1	-1.354424	-2.705974	0.166031
1	-2.394020	-1.502123	-0.240274

E+ZPE = -2145.9038270000001

Cartesian coordinates of : 530

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.000000	-0.395433	0.039714
7	-1.412621	0.985609	0.588175
1	-1.121430	1.915521	0.270069
1	-1.536467	1.065350	1.596158
1	-2.342500	0.793140	0.207892
7	-1.458811	-1.441006	-0.980939

1	-1.481758	-2.438093	-0.772876
1	-1.360613	-1.383070	-1.994061
1	-2.399099	-1.077485	-0.780220
7	1.458811	-1.441006	-0.980938
1	1.360614	-1.383071	-1.994060
1	2.399100	-1.077485	-0.780220
7	1.412621	0.985609	0.588175
1	2.342500	0.793140	0.207892
1	1.121430	1.915521	0.270069
1	1.536467	1.065350	1.596158
1	1.481759	-2.438093	-0.772875
7	4.280305	-0.099385	-0.521928
1	4.754300	0.303276	0.284136
1	4.768887	-0.977913	-0.685223
1	4.546173	0.492226	-1.306811
7	-4.280305	-0.099385	-0.521928
1	-4.754300	0.303277	0.284135
1	-4.768887	-0.977913	-0.685222
1	-4.546173	0.492226	-1.306811
7	-0.000000	-1.652498	1.941857
1	0.000001	-1.095115	2.794969
1	0.808048	-2.266013	2.038050
1	-0.808051	-2.266010	2.038050
7	0.000000	3.782869	-0.218823
1	0.000005	4.376298	0.608521
1	0.802757	4.093425	-0.762501
1	-0.802762	4.093427	-0.762493

E+ZPE = -2089.5349620000002

Cartesian coordinates of : 531

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.416787	-0.280807	0.171549
7	2.196705	0.719095	0.346525
1	2.098895	1.656669	-0.060970
7	-1.401900	-0.980334	-0.500635
1	-1.651758	-1.905226	-0.154536
7	-0.497963	1.451975	0.757943
1	-0.074745	2.242924	0.267205
1	-1.507795	1.456297	0.567854
1	-0.395999	1.658124	1.750198
7	-3.563790	1.119443	0.235571
1	-3.908877	1.328670	1.170396
1	-4.231020	0.434350	-0.146575
1	-2.168289	-0.350021	-0.225953
1	-3.728898	1.969143	-0.300821

1	-1.465552	-1.050269	-1.515488
7	1.384243	-1.750044	-0.909723
1	1.163712	-2.699639	-0.614644
1	1.163147	-1.721768	-1.904480
1	2.406410	-1.654668	-0.857175
7	4.496483	-1.238404	-0.928064
1	4.842237	-0.711431	-1.727584
1	4.688382	-2.211074	-1.160491
1	5.143724	-1.028306	-0.171007
7	-5.657140	-0.873267	-0.922543
1	-5.705653	-0.956972	-1.933898
1	-6.502286	-0.377636	-0.651691
1	-5.771919	-1.816454	-0.563211
7	1.522465	3.649817	-0.705321
1	2.508160	3.896717	-0.768213
1	1.164399	3.773653	-1.649813
1	1.109806	4.406092	-0.163067
7	0.394060	-1.344477	2.191754
1	0.802569	-2.277877	2.193552
1	0.899804	-0.842640	2.920112
1	-0.545226	-1.467486	2.567422
1	2.488191	0.867585	1.311068
1	2.979619	0.248029	-0.111660

E+ZPE = -2145.9100950000002

Cartesian coordinates of : 532

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.094344	-0.302139	-0.242754
7	1.737371	0.569516	-0.519957
1	2.042245	0.611166	-1.491315
7	-1.936447	-1.190679	-0.460015
1	-2.124991	-1.970815	0.166287
7	-0.953900	1.464522	-0.787492
1	-0.976816	1.625233	-1.793497
1	-1.929622	1.512905	-0.471337
1	-0.433360	2.248759	-0.387639
7	-3.982401	1.137352	-0.003718
1	-4.124800	1.632784	0.874042
1	-4.676599	0.377121	0.002027
1	-2.675557	-0.496162	-0.291203
1	-4.309668	1.781003	-0.721863
1	-2.104164	-1.553877	-1.397658
7	0.854274	-2.114810	-0.146401
1	0.394201	-2.822441	0.422852
1	0.991123	-2.550838	-1.057709

1	1.798056	-1.980688	0.249544
7	3.688600	-1.543293	0.913227
1	3.935468	-2.530945	0.882431
1	3.845815	-1.273733	1.882070
1	4.426253	-1.072861	0.371431
7	-6.142674	-1.108851	-0.039894
1	-6.321762	-1.558466	-0.933197
1	-6.962194	-0.536088	0.143391
1	-6.173717	-1.851636	0.652365
7	5.995194	-0.219262	-0.714620
1	6.299152	-0.874359	-1.429596
1	6.008235	0.693726	-1.159357
1	6.745934	-0.196627	-0.029802
7	-0.192428	0.093725	1.983568
1	-1.122485	0.010616	2.390417
1	0.403840	-0.509849	2.547112
1	0.109185	1.043176	2.195752
1	1.717569	1.536278	-0.186167
1	2.473308	0.064037	-0.019761
7	1.165437	3.662592	0.380038
1	1.441162	4.198492	-0.440660
1	1.962640	3.723182	1.010081
1	0.446343	4.227257	0.827693

E+ZPE = -2202.2861160000002

Cartesian coordinates of : 540

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z

29	0.087952	-0.131117	-0.020327
7	-0.416912	1.740676	0.664159
1	0.374837	2.379388	0.546523
1	-0.653721	1.767076	1.654426
1	-1.220048	2.140913	0.170288
7	-1.718973	-0.243589	-0.984714
1	-2.325653	-0.926333	-0.514988
1	-1.682165	-0.522570	-1.963139
1	-2.209293	0.655639	-0.970456
7	0.849159	-1.613331	-1.251448
1	0.851364	-1.351178	-2.236479
1	1.825809	-1.838157	-1.027567
7	1.980146	0.222455	0.677083
1	2.691534	-0.381478	0.259182
1	2.247115	1.197580	0.508936
1	2.052179	0.086055	1.683918
1	0.327461	-2.486893	-1.204293
7	3.934750	-2.035422	-0.658671

1	4.517601	-2.026080	0.175837
1	3.904240	-3.015723	-0.932192
1	4.495633	-1.583091	-1.377832
7	-3.031244	2.717274	-0.934389
1	-3.239505	3.422629	-0.230484
1	-3.939975	2.326035	-1.173888
1	-2.747722	3.242611	-1.758841
7	-0.615763	-1.460813	1.661494
1	-0.747323	-1.012740	2.566481
1	-0.032684	-2.273473	1.853153
1	-1.533198	-1.825227	1.394931
7	2.365066	3.408129	0.376493
1	2.470173	3.863451	1.280896
1	3.315981	3.296702	0.030667
1	1.958920	4.116282	-0.231345
7	-3.563397	-2.394450	0.507844
1	-4.292751	-1.883466	1.000903
1	-3.441789	-3.253117	1.041115
1	-3.997457	-2.698919	-0.361228

E+ZPE = -2145.9169689999999

Cartesian coordinates of : 541-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.309433	0.041141	0.123920
7	1.906557	1.314845	0.364256
1	1.599574	2.284740	0.237128
7	-1.390175	-0.806025	-0.694149
1	-1.467058	-1.808856	-0.534416
7	-0.857876	1.477439	0.986271
1	-0.583310	2.406989	0.659694
1	-1.858702	1.348717	0.796858
1	-0.761096	1.501958	1.999765
7	-3.855921	0.749973	0.399279
1	-4.210494	0.678961	1.350932
1	-4.417739	0.082132	-0.146406
1	-2.246150	-0.379434	-0.315312
1	-4.156264	1.667093	0.074734
1	-1.456165	-0.686611	-1.704100
7	1.494188	-1.188277	-1.016342
1	1.727158	-2.037804	-0.488984
1	1.086824	-1.502107	-1.894762
1	2.379269	-0.735684	-1.263648
7	4.186721	0.453261	-1.751806
1	4.130806	1.201320	-2.439667
1	4.512098	-0.355554	-2.277180

1	4.971585	0.699196	-1.152159
7	-5.650358	-1.197068	-1.248993
1	-5.729841	-0.986491	-2.239638
1	-6.554633	-0.963494	-0.848110
1	-5.580777	-2.208462	-1.187288
7	0.621428	4.257705	0.075831
1	1.540162	4.687207	0.162725
1	0.299828	4.514198	-0.854879
1	0.034723	4.788864	0.715893
7	0.495587	-1.302813	1.932037
1	0.999059	-2.143396	1.640626
1	1.015691	-0.926053	2.722209
1	-0.387703	-1.621688	2.325797
1	2.330772	1.272605	1.289132
1	2.661429	1.133844	-0.302868
7	2.194910	-3.832088	0.659864
1	3.185334	-3.763788	0.884195
1	2.150027	-4.436853	-0.157672
1	1.796592	-4.393293	1.409981

E+ZPE = -2202.2913140000001

Cartesian coordinates of : 541-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	-0.488778	-0.027102	0.518192
7	-2.344964	-0.824748	0.143752
1	-2.276800	-1.643847	-0.468440
7	1.387466	0.783497	0.350273
1	1.796814	1.087139	1.231728
7	0.319611	-1.884728	0.233115
1	-0.268658	-2.456121	-0.378778
1	1.254157	-1.824099	-0.191304
1	0.436763	-2.420016	1.091470
7	3.202853	-1.475488	-0.902648
1	3.485056	-2.417527	-0.638905
1	4.004957	-0.884333	-0.646609
1	2.054323	0.118594	-0.057440
1	3.185409	-1.484376	-1.920338
1	1.370337	1.611470	-0.250703
7	-1.263596	1.854360	0.241479
1	-1.366281	2.384850	1.104700
1	-0.646202	2.412838	-0.356383
1	-2.189533	1.836157	-0.195320
7	-4.198786	1.532349	-1.082573
1	-4.152829	1.533541	-2.099206
1	-4.431460	2.490096	-0.828090

1	-5.037766	1.002078	-0.856536
7	5.737750	0.180210	-0.132515
1	5.797513	1.177858	0.047491
1	6.347475	0.010992	-0.927752
1	6.191009	-0.267426	0.659057
7	-1.854079	-3.507664	-1.569010
1	-2.686772	-3.344240	-2.130969
1	-1.146931	-3.794193	-2.242490
1	-2.063222	-4.345596	-1.030336
7	-0.639755	-0.095144	2.823123
1	-1.384019	0.486528	3.205023
1	-0.828544	-1.027869	3.187101
1	0.202721	0.205896	3.310319
1	-2.822366	-1.144828	0.984526
1	-2.976108	-0.151450	-0.299251
7	0.947762	3.476454	-1.437769
1	1.330699	4.243405	-0.889042
1	0.243211	3.906986	-2.032853
1	1.691773	3.209764	-2.078813

E+ZPE = -2202.2912790000000

Cartesian coordinates of : 600

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.000002	0.000001	0.001957
7	-0.047640	1.489217	-1.459224
1	-0.435484	1.193054	-2.354331
1	0.868451	1.877782	-1.683396
7	-0.104539	-1.461641	1.490714
1	-0.684900	-1.181875	2.281169
7	0.047631	-1.489672	-1.458759
1	0.435485	-1.193791	-2.353955
1	0.620078	-2.289991	-1.191119
1	-0.868465	-1.878291	-1.682817
7	-2.496078	0.033408	-0.033367
1	-2.885669	0.054903	-0.975466
1	-2.933899	0.830743	0.427464
1	-0.506480	-2.347011	1.183940
1	-2.942627	-0.774639	0.399430
1	0.797429	-1.708707	1.897769
1	-0.620101	2.289610	-1.191834
7	0.104546	1.462114	1.490251
1	-0.797425	1.709334	1.897205
1	0.684882	1.182589	2.280810
1	0.506516	2.347375	1.183201
7	2.496075	-0.033427	-0.033366

1	2.933885	-0.830666	0.427641
1	2.885664	-0.055137	-0.975461
1	2.942635	0.774709	0.399251

E+ZPE = -1976.7616470000000

Cartesian coordinates of : 610-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.451064	0.001087	0.000092
7	0.439302	-2.500437	-0.037584
1	0.802479	-2.941454	-0.881934
1	-0.510115	-2.862752	0.041323
1	0.945425	-2.959319	0.719020
7	1.947222	-0.034281	1.460026
1	1.618271	-0.272239	2.394777
1	2.423767	0.860353	1.569047
1	2.686297	-0.709258	1.266663
7	0.395265	2.502089	0.035702
1	0.880703	2.970191	-0.728767
1	-0.563612	2.841097	-0.032022
7	-1.015699	0.005072	-1.458158
1	-1.956256	-0.009802	-1.047130
1	-0.994719	0.822600	-2.066144
1	-0.972975	-0.798527	-2.083399
1	0.758887	2.954679	0.873713
7	-3.864685	-0.009508	0.000111
1	-4.258146	-0.948683	-0.022420
1	-4.293238	0.429191	0.813498
1	-4.292265	0.467956	-0.791642
7	1.947906	0.059629	-1.458344
1	1.614837	0.275317	-2.397024
1	2.450974	-0.821835	-1.554661
1	2.665991	0.758766	-1.271753
7	-1.015554	-0.023496	1.458177
1	-1.956069	0.001517	1.047526
1	-0.970277	0.768867	2.097396
1	-0.997106	-0.851644	2.051745

E+ZPE = -2033.1489839999999

Cartesian coordinates of : 620-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
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29	0.008480	0.064226	0.000000
7	1.461375	0.400460	-1.435733
1	1.526260	1.375668	-1.723434
1	1.351611	-0.128606	-2.298859
1	2.387397	0.159226	-1.066268
7	1.461375	0.400460	1.435733
1	1.351611	-0.128606	2.298859
1	1.526260	1.375668	1.723434
1	2.387397	0.159226	1.066268
7	-1.425521	-0.250565	1.457557
1	-1.459950	0.486200	2.160075
1	-2.367875	-0.303217	1.055958
7	-1.425521	-0.250565	-1.457557
1	-2.367875	-0.303217	-1.055958
1	-1.459950	0.486201	-2.160075
1	-1.295912	-1.116775	-1.977900
1	-1.295912	-1.116775	1.977900
7	-4.279349	-0.463998	-0.000000
1	-4.568017	-1.440637	-0.000000
1	-4.753087	-0.054661	0.803284
1	-4.753087	-0.054661	-0.803285
7	4.283018	-0.154798	-0.000000
1	4.654980	-0.658355	-0.803220
1	4.654979	-0.658365	0.803214
1	4.779986	0.734240	0.000006
7	0.598580	-2.353354	0.000000
1	1.154645	-2.639098	-0.804470
1	-0.194932	-2.992928	-0.000000
1	1.154645	-2.639098	0.804471
7	-0.694085	2.511958	0.000000
1	-0.403766	3.068353	-0.802935
1	-1.710659	2.582129	-0.000000
1	-0.403766	3.068353	0.802936

E+ZPE = -2089.5342550000000

Cartesian coordinates of : 620-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.000001	-0.591408	0.074788
7	0.000006	-1.825401	-2.133968
1	0.000009	-2.842946	-2.077424
1	0.803532	-1.607823	-2.721882
1	-0.803521	-1.607828	-2.721883
7	-2.064795	-0.539080	0.125633
1	-2.521247	-1.096603	-0.594623
1	-2.396079	0.423998	-0.007216

1	-2.468163	-0.851643	1.007326
7	-0.000003	0.679799	2.222405
1	-0.000000	0.193639	3.118141
1	0.806421	1.300542	2.270188
7	2.064797	-0.539073	0.125637
1	2.396078	0.424005	-0.007212
1	2.468164	-0.851634	1.007331
1	2.521251	-1.096595	-0.594617
1	-0.806432	1.300535	2.270190
7	2.967438	2.482430	-0.319051
1	3.329931	2.599193	-1.263579
1	2.615366	3.402172	-0.060579
1	3.796314	2.360984	0.260167
7	0.000003	-2.451757	1.022536
1	0.807342	-3.027730	0.788557
1	-0.807333	-3.027733	0.788553
1	0.000000	-2.388853	2.039895
7	-0.000001	1.214070	-0.911555
1	0.827717	1.770040	-0.684333
1	-0.827721	1.770038	-0.684333
1	-0.000001	1.118888	-1.925625
7	-2.967446	2.482421	-0.319052
1	-3.329937	2.599184	-1.263581
1	-3.796322	2.360970	0.260163
1	-2.615378	3.402163	-0.060578

E+ZPE = -2089.5335470000000

Cartesian coordinates of : 620-3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.000000	0.000000	0.000000
7	-0.541769	-2.465262	0.000125
1	-0.207199	-2.996889	0.802500
1	-0.207250	-2.996959	-0.802226
1	-1.549773	-2.614495	0.000164
7	-1.452948	0.236268	-1.453294
1	-2.395553	0.183170	-1.052210
1	-1.418957	-0.470288	-2.186108
1	-1.409382	1.131474	-1.937332
7	0.541769	2.465261	-0.000124
1	0.207255	2.996957	0.802230
1	1.549773	2.614494	-0.000169
7	1.452948	-0.236269	1.453294
1	2.395554	-0.183170	1.052210
1	1.418957	0.470287	2.186109
1	1.409383	-1.131475	1.937331

1	0.207194	2.996890	-0.802496
7	4.311973	-0.155988	-0.000140
1	4.682694	-1.104546	-0.000113
1	4.748956	0.292393	-0.803405
1	4.749010	0.292461	0.803057
7	-1.452849	0.236392	1.453374
1	-1.418808	-0.470102	2.186247
1	-2.395482	0.183259	1.052359
1	-1.409251	1.131639	1.937332
7	1.452849	-0.236392	-1.453374
1	2.395481	-0.183259	-1.052359
1	1.418807	0.470101	-2.186247
1	1.409251	-1.131639	-1.937332
7	-4.311973	0.155989	0.000139
1	-4.748956	-0.292391	0.803404
1	-4.682694	1.104548	0.000110
1	-4.749010	-0.292460	-0.803058

E+ZPE = -2089.5335380000001

Cartesian coordinates of : 621

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.502079	0.063771	-0.000004
7	1.956646	-0.124328	1.456064
1	1.876792	-0.984195	1.996011
1	1.948643	0.630671	2.139531
1	2.899568	-0.134736	1.053067
7	1.956663	-0.124355	-1.456053
1	1.948668	0.630631	-2.139535
1	1.876815	-0.984232	-1.995986
1	2.899580	-0.134755	-1.053046
7	-0.992007	0.251411	-1.421083
1	-0.786865	-0.127773	-2.343455
1	-1.819191	-0.251942	-1.079585
7	-0.992024	0.251438	1.421056
1	-1.819203	-0.251921	1.079559
1	-0.786892	-0.127729	2.343437
1	-1.293195	1.210910	1.583065
1	-1.293176	1.210880	-1.583113
7	-3.383669	-1.268150	-0.000015
1	-4.099253	-0.525052	-0.000002
1	-3.617260	-1.851687	-0.802160
1	-3.617252	-1.851707	0.802116
7	4.816179	-0.222136	0.000025
1	5.274427	0.204092	0.803369
1	5.274436	0.204076	-0.803322

1	5.137250	-1.188477	0.000036
7	0.964007	2.561472	-0.000025
1	1.967271	2.739193	-0.000022
1	0.615321	3.081164	0.804054
1	0.615330	3.081149	-0.804117
7	-0.001919	-2.355792	0.000017
1	0.287034	-2.910871	0.803724
1	-1.020764	-2.394300	0.000005
1	0.287054	-2.910889	-0.803671
7	-5.653842	0.840493	0.000025
1	-6.466748	0.230185	0.000065
1	-5.769440	1.443814	0.809196
1	-5.769483	1.443766	-0.809176

E+ZPE = -2145.9092110000001

Cartesian coordinates of : 630-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.100178	-0.010109	0.414325
7	-0.574230	-0.039327	2.939273
1	0.217700	-0.068575	3.579418
1	-1.148126	-0.835733	3.212204
1	-1.113192	0.770410	3.242507
7	0.104276	2.062665	0.433354
1	0.028824	2.469217	1.364111
1	-0.690137	2.429331	-0.104188
1	0.938334	2.476939	0.021061
7	0.793625	0.015569	-1.886085
1	1.813925	0.006969	-1.896282
1	0.502899	-0.779665	-2.451531
7	0.040401	-2.081462	0.372201
1	-0.769763	-2.408499	-0.167463
1	0.857445	-2.508556	-0.060526
1	-0.038498	-2.512415	1.291627
1	0.516582	0.833162	-2.425922
7	-2.528501	-2.968077	-1.294193
1	-3.411961	-3.073897	-0.799455
1	-2.787034	-2.720024	-2.246917
1	-2.164012	-3.915852	-1.369580
7	2.071936	-0.048169	1.022735
1	2.313926	-0.871365	1.571361
1	2.330326	0.740941	1.612438
1	2.726399	-0.034714	0.226704
7	-1.891397	0.028974	-0.086211
1	-2.162112	-0.789041	-0.635528
1	-2.132615	0.866606	-0.619483

1	-2.502020	0.032034	0.728619
7	-2.422638	3.072133	-1.227827
1	-3.280688	3.231947	-0.703715
1	-2.007142	3.996635	-1.325014
1	-2.728536	2.832662	-2.168655
7	4.151788	-0.016440	-1.326162
1	4.931297	0.110149	-0.683544
1	4.274476	0.716937	-2.021123
1	4.361719	-0.883488	-1.816135

E+ZPE = -2145.9161210000002

Cartesian coordinates of : 630-2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.063694	-0.503894	0.272258
7	-1.233139	-1.639102	-1.454282
1	-0.878816	-1.596224	-2.408094
1	-2.128424	-1.148775	-1.468201
1	-1.462620	-2.621318	-1.313016
7	-0.609447	-1.937465	1.646482
1	-1.622278	-2.046863	1.632161
1	-0.372552	-1.706202	2.610125
1	-0.241490	-2.875387	1.495799
7	1.364752	0.732695	2.055101
1	2.357311	0.781217	1.831753
1	1.045435	1.699726	2.044286
7	0.733430	0.941342	-1.040443
1	0.511657	1.877824	-0.691993
1	1.743637	0.889750	-1.189143
1	0.310506	0.880192	-1.964681
1	1.337530	0.461529	3.036821
7	-0.427487	3.734324	0.126490
1	-0.948528	4.097221	-0.669491
1	-0.919388	4.093412	0.942413
1	0.451046	4.248808	0.115658
7	1.759613	-1.616391	-0.105223
1	1.595812	-2.400606	-0.734443
1	2.196579	-2.012812	0.724829
1	2.479655	-1.037915	-0.552817
7	-1.549381	0.691956	0.700217
1	-1.296867	1.670430	0.540050
1	-1.881542	0.647791	1.661646
1	-2.363964	0.489669	0.105787
7	-4.102032	0.088740	-1.081509
1	-4.174460	0.688573	-1.900544
1	-4.553855	-0.781917	-1.353426

1	-4.737211	0.500060	-0.400537
7	3.905432	0.260036	-1.539069
1	4.214776	1.223460	-1.428051
1	3.921981	0.093445	-2.543398
1	4.676765	-0.295099	-1.173323

E+ZPE = -2145.9151579999998

Cartesian coordinates of : 640-1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
29	0.000000	-0.000000	-0.000000
7	-1.120735	-1.272712	-1.811552
1	-1.919176	-1.693919	-1.336595
1	-0.599113	-2.046653	-2.218525
1	-1.511491	-0.775878	-2.609731
7	-0.351070	1.807968	-0.959267
1	-0.397852	1.719314	-1.972390
1	0.380951	2.491746	-0.776047
1	-1.236588	2.237332	-0.670529
7	1.120735	1.272711	1.811552
1	0.599113	2.046652	2.218526
1	1.511492	0.775877	2.609730
7	0.351070	-1.807969	0.959267
1	1.236589	-2.237332	0.670530
1	0.397851	-1.719315	1.972390
1	-0.380950	-2.491747	0.776046
1	1.919176	1.693919	1.336595
7	3.191924	-2.947517	0.043008
1	3.563017	-3.130279	-0.886977
1	3.992028	-2.644356	0.594112
1	2.960763	-3.868961	0.409027
7	-1.823638	0.118003	0.925413
1	-1.752095	0.152992	1.940174
1	-2.412305	-0.691983	0.700637
1	-2.341352	0.955686	0.650736
7	1.823638	-0.118003	-0.925413
1	2.341353	-0.955686	-0.650735
1	2.412304	0.691983	-0.700638
1	1.752095	-0.152994	-1.940174
7	3.593120	2.447576	-0.227403
1	3.851635	2.670570	-1.186329
1	3.454942	3.352957	0.216403
1	4.444138	2.080008	0.193041
7	-3.593122	-2.447574	0.227401
1	-3.454945	-3.352955	-0.216405
1	-4.444140	-2.080005	-0.193045

1	-3.851639	-2.670567	1.186327
7	-3.191922	2.947518	-0.043005
1	-3.563015	3.130280	0.886979
1	-3.992027	2.644357	-0.594109
1	-2.960760	3.868962	-0.409024

E+ZPE = -2202.2962539999999