

Structures and Relative Stabilities of Ammonia Clusters at Different Temperatures: DFT Vs Ab-Initio

(Supporting Information)

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Cartesian coordinates for all the isomers of ammonia clusters $(\text{NH}_3)_{n=5-10}$ at MP2/6-31++G(d,p) level of theory**P 85-179**

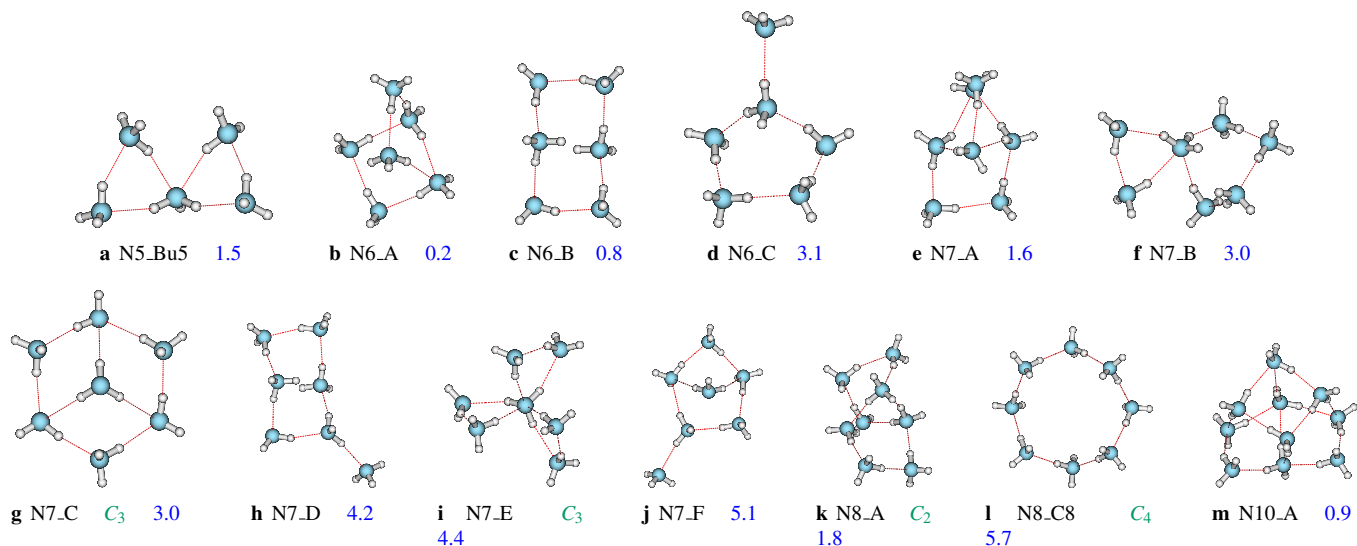


Fig. 1 The MP2/6-31++g(d,p) Optimized isomers of ammonia clusters (NH_3) $_{n=5-10}$ that were not located at the M06-2X/6-31++g(d,p) level of theory. Numbers in blue color represent the zero-point corrected electronic energy differences (in kcal/mol) of the corresponding isomers from the global minimum energy structure for given n . The symmetry point group of each structure is indicated in green color when it is different from the C_1 symmetry point group.

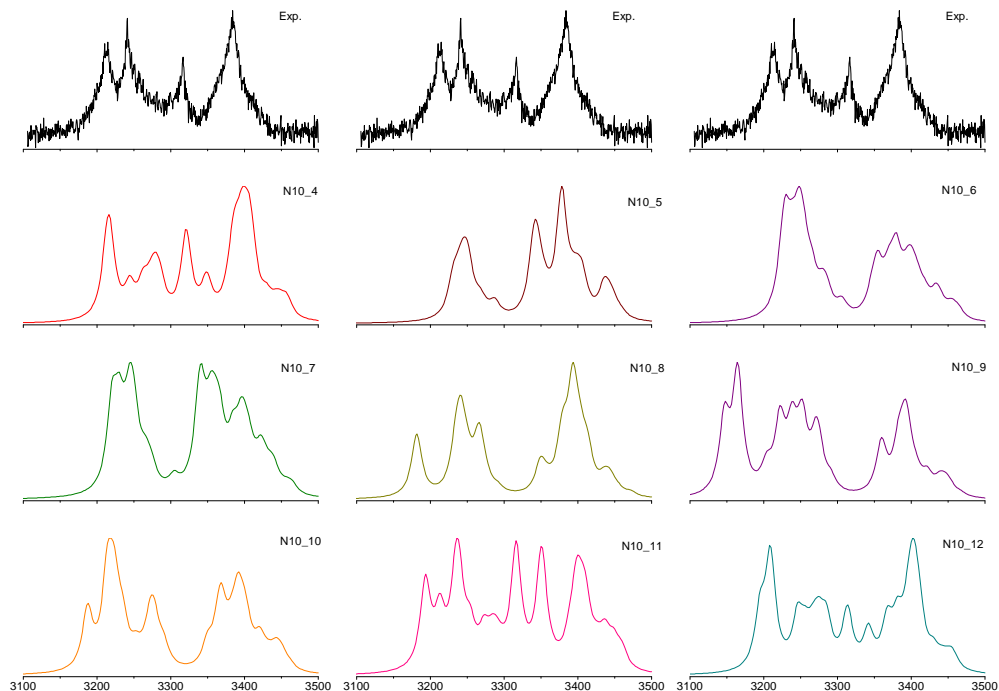


Fig. 2 Comparison of the experimental IR for the ammonia decamer with the Calculated scaled harmonic IR spectra of some of its various isomers (10.4 - 10.12). The calculated IR spectra were performed at the M062X/6-31++G(d,p) level of theory with the scaling factor of 0.948. Experimental data courtesy of Mikhail N. Slipchenko.

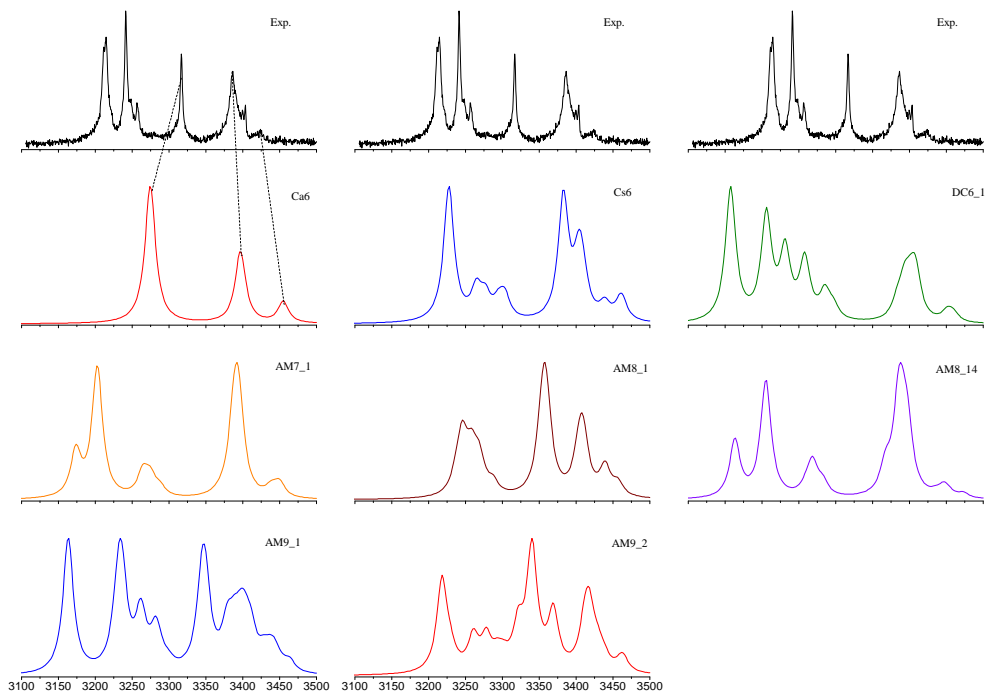


Fig. 3 Comparison of the experimental IR for the ammonia pentamer with the Calculated scaled harmonic IR spectra of all the isomers with $n = 6 - 9$ and that have different hydrogen bond types than those already exhibited by the isomers of pentamer ammonia. The calculated IR spectra were performed at the M062X/6-31++G(d,p) level of theory with the scaling factor of 0.948. Experimental data courtesy of Mikhail N. Slipchenko.

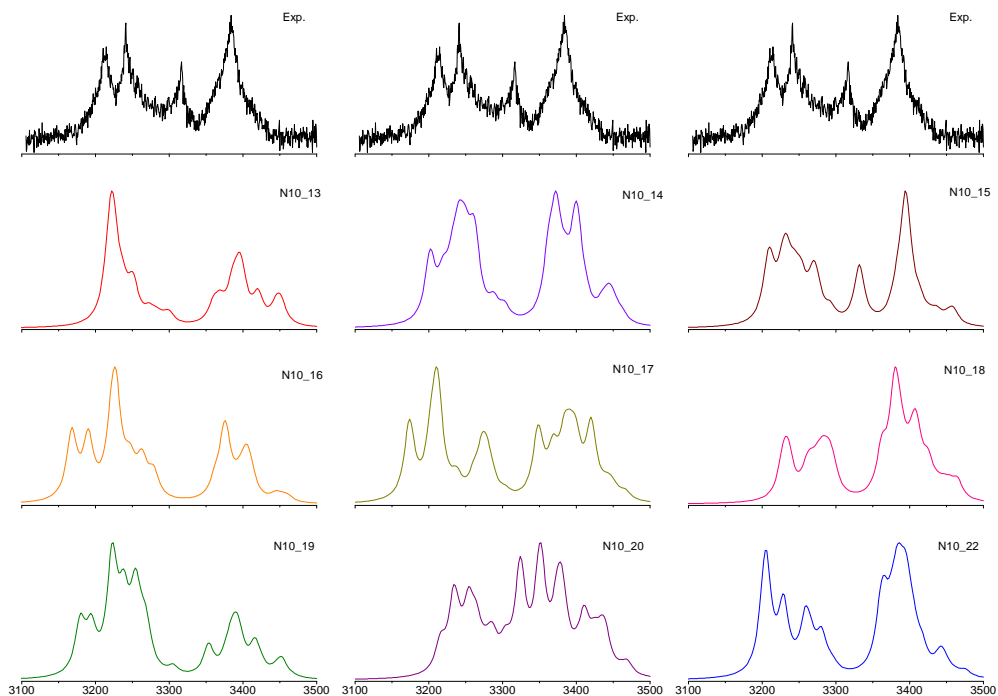


Fig. 4 Comparison of the experimental IR for the ammonia decamer with the Calculated scaled harmonic IR spectra of some of its various isomers (10.13 - 10.22). The calculated IR spectra were performed at the M062X/6-31++G(d,p) level of theory with the scaling factor of 0.948. Experimental data courtesy of Mikhail N. Slipchenko.

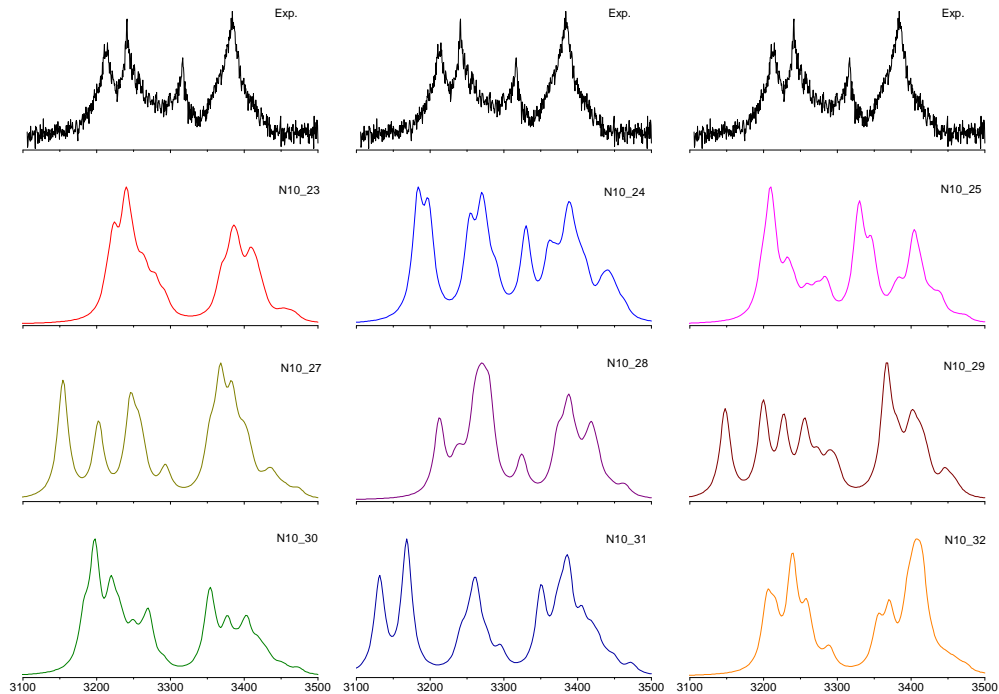


Fig. 5 Comparison of the experimental IR for the ammonia decamer with the Calculated scaled harmonic IR spectra of some of its various isomers (10-23 - 10-32). The calculated IR spectra were performed at the M062X/6-31++G(d,p) level of theory with the scaling factor of 0.948. Experimental data courtesy of Mikhail N. Slipchenko.

Cartesian coordinates of all the proposed isomers of ammonia clusters (NH₃)_n=2-10 at M06-2X/6-31++G(d,p) level of theory

Cartesian coordinates of ammonia dimer: (NH₃)₂

Cartesian coordinates of : L2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.532828	0.000000	-0.036650
1	1.460179	-0.000002	0.976177
1	2.067569	-0.818490	-0.307694
1	2.067568	0.818493	-0.307691
7	-1.639027	0.000000	0.097840
1	-0.664789	0.000000	-0.202499
1	-2.093566	-0.817937	-0.293310
1	-2.093566	0.817937	-0.293310

Cartesian coordinates of : CY2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.528693	0.000000	0.071602
1	0.824301	0.000000	-0.662480
1	2.115410	0.818125	-0.052028
1	2.115410	-0.818126	-0.052028
7	-1.528694	0.000000	-0.071602
1	-0.824299	0.000000	0.662478
1	-2.115410	0.818126	0.052030
1	-2.115410	-0.818126	0.052030

Cartesian coordinates of ammonia trimer: (NH₃)₃

Cartesian coordinates of : CY3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.775767	-0.274740	0.000001
1	-2.345702	-0.472846	-0.816085
1	-2.345728	-0.472846	0.816069
1	-0.984287	-0.924159	0.000013
7	1.125813	-1.400425	0.000002
1	1.292056	-0.390206	0.000008
1	1.582611	-1.794704	-0.816047
1	1.582654	-1.794721	0.816018
7	0.649930	1.675106	0.000000
1	0.763398	2.267747	0.816063
1	-0.308228	1.314405	0.000004
1	0.763393	2.267741	-0.816068

Cartesian coordinates of : Asym

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.932289	-0.828088	0.000000
1	1.399530	0.042963	0.000000
1	1.712581	-1.370841	-0.826460
1	1.712581	-1.370840	0.826460
7	0.016920	1.709171	0.000000

1	0.041103	2.311078	0.816623
1	0.041102	2.311078	-0.816623
1	-0.868399	1.201970	0.000000
7	-1.773762	-0.819238	0.000000
1	-2.229615	-1.210234	0.817953
1	-2.229614	-1.210232	-0.817954
1	-0.807390	-1.137860	0.000000

Cartesian coordinates of : L3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.608510	-0.548585	-0.014454
1	-3.262696	-0.451315	0.755126
1	-2.205125	-1.478343	0.042807
1	-3.142720	-0.501037	-0.875950
7	0.082019	1.171624	0.005390
1	0.205312	1.639451	0.897989
1	-0.834100	0.720349	0.010146
1	0.070619	1.892473	-0.708988
7	2.747246	-0.573378	0.071906
1	3.223535	-0.561625	-0.823460
1	1.865661	-0.067001	-0.028406
1	2.534227	-1.540575	0.290841

Cartesian coordinates of ammonia tetramer: (NH3)4

Cartesian coordinates of : CY4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.153123	2.196951	0.002461
1	-0.109140	2.798622	0.819179
1	-0.108689	2.803252	-0.810798
1	0.690447	1.612349	0.001045
7	2.196951	0.153123	-0.002461
1	1.612349	-0.690446	-0.001045
1	2.803253	0.108689	0.810798
1	2.798622	0.109139	-0.819180
7	0.153123	-2.196951	0.002461
1	0.108689	-2.803252	-0.810798
1	-0.690447	-1.612349	0.001045
1	0.109140	-2.798623	0.819179
7	-2.196951	-0.153123	-0.002461
1	-2.798623	-0.109139	-0.819179
1	-1.612349	0.690446	-0.001045
1	-2.803253	-0.108689	0.810798

Cartesian coordinates of : P4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.625433	0.539004	-0.904715
1	2.314587	1.270887	-0.759476
1	1.984641	-0.051360	-1.649548
1	1.583630	-0.031394	-0.052548
7	0.542825	-1.067676	1.449492
1	0.114959	-1.714142	0.787270
1	-0.171692	-0.367957	1.644818
1	0.749228	-1.567380	2.307621
7	-1.156225	-1.145314	-1.054614
1	-1.774061	-1.453597	-1.797576

1	-0.452347	-0.529079	-1.456146
1	-1.691956	-0.571681	-0.406713
7	-1.011436	1.576103	0.536107
1	-1.742222	2.075132	0.037835
1	-0.233707	1.430887	-0.112114
1	-0.685240	2.194859	1.272685

Cartesian coordinates of : BC4_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.750749	-0.287466	0.012130
1	-2.253338	0.606462	0.016113
1	-3.344587	-0.322086	0.834465
1	-3.362269	-0.305249	-0.797685
7	-0.388546	1.719226	-0.001954
1	-0.083843	2.216842	-0.832565
1	0.075683	0.809329	0.005676
1	-0.053792	2.245246	0.799012
7	0.145255	-1.427771	-0.014894
1	0.384699	-1.957154	-0.848693
1	-0.871912	-1.297294	-0.011643
1	0.380322	-2.019605	0.777024
7	3.071355	-0.086711	-0.009396
1	3.195050	0.612357	-0.733668
1	3.304202	0.344640	0.878453
1	2.088583	-0.354440	0.012311

Cartesian coordinates of : BC4_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.950001	-1.581048	-0.240438
1	-1.949329	-2.061492	-1.134332
1	-2.193692	-0.600832	-0.407263
1	-2.687342	-1.996262	0.319901
7	0.436415	0.080516	1.022633
1	1.371501	0.003988	0.621721
1	-0.112168	-0.727731	0.722086
1	0.533856	0.026786	2.031620
7	3.341115	-0.049482	-0.413085
1	4.109356	-0.509983	0.063461
1	3.628425	0.903159	-0.611895
1	3.204705	-0.520874	-1.301320
7	-1.923443	1.541277	-0.316825
1	-1.703106	2.100595	-1.134540
1	-1.045415	1.322204	0.166900
1	-2.485397	2.121599	0.297669

Cartesian coordinates of : BC4_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.348045	-1.674750	0.057890
1	-1.512745	-2.293101	0.845519
1	-1.247039	-2.259474	-0.765456
1	-2.172677	-1.085634	-0.065972
7	-3.067918	0.906941	-0.198629
1	-3.333354	1.251498	-1.115643
1	-2.172467	1.325234	0.038909
1	-3.754575	1.250555	0.464872
7	0.780509	0.633116	0.372401
1	0.537753	1.152133	1.209412

1	0.149448	-0.168023	0.287060
1	0.650643	1.242707	-0.428457
7	3.848082	0.116090	-0.296845
1	4.464773	0.370027	0.467535
1	4.017641	-0.860948	-0.510794
1	2.884201	0.205250	0.029294

Cartesian coordinates of ammonia pentamer: (NH3)₅

Cartesian coordinates of : P5_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.201330	0.691937	0.186480
1	2.921346	1.101644	0.773468
1	1.349417	1.251646	0.292330
1	2.511584	0.788730	-0.775828
7	-0.396593	-0.074497	-1.884331
1	-0.023320	-0.829212	-1.310145
1	-0.194229	0.789584	-1.386440
1	0.112349	-0.061671	-2.761902
7	0.800160	-2.041160	0.563738
1	1.261561	-2.770056	0.027337
1	0.768427	-2.367343	1.525502
1	1.399387	-1.208242	0.540393
7	-0.617044	2.042757	0.607511
1	-1.193856	1.202787	0.746578
1	-1.154796	2.679047	0.025221
1	-0.516904	2.497701	1.510598
7	-2.094581	-0.642579	0.494413
1	-1.302799	-1.284342	0.566710
1	-2.295529	-0.560701	-0.500302
1	-2.895544	-1.064782	0.951805

Cartesian coordinates of : P5_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.215217	-0.455281	1.083633
1	2.845261	-1.248274	1.156403
1	2.695718	0.343302	1.487661
1	2.073626	-0.258740	0.091053
7	-0.334972	-1.749252	-0.217807
1	-0.333796	-2.741006	-0.434517
1	0.169857	-1.622679	0.657940
1	0.229942	-1.272901	-0.920849
7	-0.239863	1.556157	0.801170
1	-0.254819	2.395596	1.371593
1	0.217073	0.822549	1.340995
1	-1.208967	1.261875	0.651208
7	1.157503	0.654515	-1.747987
1	0.533061	0.561794	-2.544274
1	1.942102	1.217874	-2.062719
1	0.657687	1.185013	-1.022171
7	-2.867518	0.023662	0.112993
1	-2.168221	-0.706371	-0.056309
1	-3.386720	0.173654	-0.745812
1	-3.524375	-0.320293	0.805781

Cartesian coordinates of : DC5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.088158	1.181347	1.234911
1	-0.127688	0.163973	1.250786
1	-0.087151	1.503234	2.197671
1	0.817265	1.422442	0.823104
7	2.593528	1.116016	-0.340551
1	2.324695	0.129457	-0.409667
1	3.535879	1.163035	0.032830
1	2.621660	1.503472	-1.278029
7	1.443957	-1.805813	-0.306005
1	1.540313	-2.313053	-1.180731
1	0.442140	-1.747871	-0.096321
1	1.868593	-2.382909	0.414039
7	-2.309956	1.194501	-0.875353
1	-3.160909	1.719046	-0.700428
1	-1.965071	1.479296	-1.786519
1	-1.611766	1.467590	-0.174640
7	-1.653016	-1.596907	0.292423
1	-2.043856	-1.543433	1.229171
1	-2.066895	-2.416270	-0.143114
1	-1.991688	-0.772023	-0.216134

Cartesian coordinates of : BC5_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.326460	1.628638	0.338822
1	0.523196	1.818625	1.316967
1	0.963523	2.202172	-0.205712
1	0.569441	0.649829	0.163698
7	0.904726	-1.455940	-0.181040
1	-0.099671	-1.622917	-0.040573
1	1.408413	-2.036201	0.484682
1	1.140654	-1.811392	-1.103613
7	-2.163813	-1.683977	0.234581
1	-2.682385	-2.296897	-0.387215
1	-2.464252	-0.721633	0.043521
1	-2.457155	-1.911758	1.179821
7	-2.701405	1.330484	-0.320223
1	-2.909339	1.600792	-1.276434
1	-1.728827	1.590340	-0.125776
1	-3.300792	1.886959	0.281054
7	3.707389	0.104478	-0.060514
1	3.986525	0.507121	-0.948593
1	3.816925	0.818707	0.651249
1	2.720245	-0.139541	-0.114452

Cartesian coordinates of : BC5_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.065498	-0.046907	1.189814
1	-1.353121	0.030272	2.160482
1	-1.910445	-0.003359	0.619427
1	-0.493874	0.774606	0.973458
7	1.025972	2.206957	0.405400
1	1.641242	1.562043	-0.101874
1	1.558426	2.595985	1.177383
1	0.803611	2.977662	-0.216732
7	2.708894	-0.005659	-1.029516
1	2.626681	-0.076884	-2.039019
1	2.203410	-0.800158	-0.620253
1	3.693045	-0.119032	-0.806991
7	0.992662	-2.187803	0.368724
1	0.552810	-2.942365	-0.149169

1	0.249309	-1.547772	0.679978
1	1.402924	-2.604601	1.199025
7	-3.589245	0.036472	-0.857926
1	-4.137407	0.890136	-0.848787
1	-4.234504	-0.744993	-0.810450
1	-3.111605	-0.012953	-1.751946

Cartesian coordinates of : BC5_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.943507	1.841536	0.093913
1	-1.204486	2.102166	1.039469
1	-1.207372	0.864588	-0.043632
1	-1.505549	2.405079	-0.536206
7	1.573709	0.325111	-1.047428
1	2.390655	0.136004	-0.465464
1	1.059109	1.107238	-0.639586
1	1.911562	0.620541	-1.957934
7	4.080000	-0.393267	0.864976
1	4.841790	0.276707	0.886180
1	4.471300	-1.295264	0.613863
1	3.715015	-0.470883	1.808763
7	-1.028864	-1.273216	-0.687712
1	-0.927848	-2.111283	-0.121888
1	-0.083993	-0.925894	-0.897239
1	-1.449441	-1.568836	-1.564357
7	-3.841995	-0.548352	0.705013
1	-2.911798	-0.660663	0.303003
1	-3.744731	-0.466377	1.711338
1	-4.229604	0.324194	0.362350

Cartesian coordinates of : BC5_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.720862	1.439148	0.034429
1	-0.813456	1.914139	0.006801
1	-2.221298	1.779052	0.850849
1	-2.255243	1.740317	-0.775823
7	1.328665	2.024208	-0.023827
1	1.826092	2.358792	-0.842948
1	1.375058	1.004427	-0.023184
1	1.835046	2.359581	0.789467
7	0.329355	-0.988352	-0.077161
1	0.260612	-1.505375	-0.949466
1	-0.481022	-0.366123	-0.024596
1	0.237268	-1.672142	0.669103
7	3.520958	-1.337158	0.052480
1	4.007760	-0.906855	-0.726109
1	3.940356	-0.992034	0.908802
1	2.547180	-1.040108	0.027788
7	-3.540404	-1.217336	-0.007533
1	-2.799146	-0.521429	0.046404
1	-3.275137	-1.912629	-0.696571
1	-3.608056	-1.683183	0.890765

Cartesian coordinates of : BC5_5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.588786	0.606054	0.872177
1	2.269813	-0.038507	0.471544

1	2.047126	1.092847	1.636145
1	1.346047	1.305120	0.167421
7	-0.134829	2.553221	-0.961869
1	-0.817281	1.990701	-0.442241
1	-0.328364	2.448493	-1.952560
1	-0.289989	3.528997	-0.729742
7	-1.550929	0.532213	0.909113
1	-1.939264	0.823727	1.800650
1	-0.573136	0.275324	1.069410
1	-2.066899	-0.294917	0.610118
7	3.503908	-1.699044	-0.382963
1	4.473348	-1.825563	-0.112527
1	3.467970	-1.667735	-1.396385
1	2.987693	-2.518236	-0.079665
7	-3.378060	-1.844498	-0.346107
1	-4.030096	-1.274720	-0.875144
1	-3.918279	-2.498527	0.210171
1	-2.830824	-2.382623	-1.009652

Cartesian coordinates of ammonia hexamer: (NH₃)₆

Cartesian coordinates of : Ca6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.223605	1.226693	1.441171
1	-1.394542	1.353944	0.440591
1	-0.298637	1.614109	1.613449
1	-1.894678	1.790304	1.953516
7	1.223605	-1.226693	-1.441171
1	1.894678	-1.790304	-1.953516
1	0.298637	-1.614109	-1.613449
1	1.394543	-1.353944	-0.440591
7	-1.445857	-1.710080	0.296621
1	-1.544429	-0.890699	0.901018
1	-0.575262	-2.155601	0.577464
1	-2.203027	-2.353213	0.505351
7	1.305021	-0.750259	1.678983
1	0.421624	-0.623875	2.167870
1	1.532455	0.163538	1.279431
1	2.011118	-0.980691	2.370921
7	1.445857	1.710080	-0.296621
1	2.203027	2.353213	-0.505351
1	0.575262	2.155601	-0.577464
1	1.544429	0.890699	-0.901018
7	-1.305021	0.750259	-1.678983
1	-1.532455	-0.163538	-1.279431
1	-0.421624	0.623875	-2.167870
1	-2.011118	0.980691	-2.370921

Cartesian coordinates of : P6_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.532795	-0.759084	1.588549
1	-0.308220	0.235592	1.555934
1	0.209393	-1.249974	1.087755
1	-0.493838	-1.054229	2.559073
7	-0.157058	-0.139007	-1.664107
1	-1.154527	-0.321753	-1.518506
1	0.348292	-0.865479	-1.154813
1	0.036301	-0.271603	-2.652485
7	-2.910198	-0.765233	-0.373632
1	-2.274673	-0.860243	0.426861

1	-3.307451	-1.679036	-0.567983
1	-3.678931	-0.159665	-0.104437
7	2.215042	1.285232	-0.093968
1	1.637274	1.673549	0.648939
1	1.589811	1.180516	-0.893194
1	2.929553	1.967787	-0.324475
7	2.127197	-1.772020	0.082928
1	2.551494	-2.181266	-0.744428
1	2.519116	-2.261756	0.881883
7	-0.752930	2.137871	0.471637
1	-0.628100	1.557856	-0.362547
1	-0.595405	3.104536	0.202455
1	-1.728648	2.062091	0.745052
1	2.423762	-0.791231	0.135067

Cartesian coordinates of : P6_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.336754	0.963298	-1.463861
1	0.517646	1.264792	-0.994871
1	-0.237006	1.180950	-2.450260
1	-0.401724	-0.052480	-1.372513
7	1.958554	-1.584699	-0.126734
1	1.319580	-1.837749	-0.876353
1	1.371866	-1.327489	0.670148
1	2.495966	-2.411256	0.113238
7	-1.332014	-1.847577	-0.393863
1	-1.797057	-2.708866	-0.662642
1	-2.046762	-1.177765	-0.105612
1	-0.778538	-2.035714	0.438339
7	-2.819029	0.941967	0.285993
1	-2.099057	1.235867	-0.385182
1	-2.957504	1.696975	0.951229
1	-3.693469	0.837386	-0.220348
7	0.025770	0.103411	1.663299
1	0.055047	0.290345	2.660995
1	-0.942547	0.219859	1.362716
1	0.573190	0.829522	1.199141
7	2.506782	1.424182	0.000351
1	2.963726	1.937168	-0.747737
1	2.612550	0.421616	-0.187936
1	3.020937	1.632762	0.851364

Cartesian coordinates of : P6_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.231605	0.627689	1.877814
1	-0.523992	-0.324483	1.661430
1	-0.172502	0.714484	2.887257
1	0.709735	0.751817	1.499696
7	2.357380	1.244309	0.150347
1	1.747158	1.143349	-0.668428
1	3.286366	0.941286	-0.128119
1	2.426488	2.233738	0.369710
7	0.349487	0.196520	-1.930347
1	0.282223	0.150821	-2.941691
1	-0.591577	0.317291	-1.559899
1	0.713835	-0.695251	-1.588188
7	-2.150941	1.461575	-0.337768
1	-1.831598	2.198229	-0.960654
1	-1.542986	1.468389	0.489997
1	-3.087211	1.717196	-0.038293
7	1.452616	-1.860091	0.087988
1	0.501446	-1.962571	0.441565

1	1.855926	-1.032714	0.525125
1	1.991705	-2.666907	0.384068
7	-1.727838	-1.661879	0.134241
1	-1.583166	-2.209706	-0.710027
1	-2.010609	-0.724274	-0.163110
1	-2.514937	-2.077554	0.623638

Cartesian coordinates of : Cs6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.000001	0.479719	-1.573818
1	0.000000	0.788556	-2.541507
1	0.818430	0.895282	-1.125539
1	-0.818431	0.895277	-1.125539
7	1.772706	-1.668325	0.000008
1	1.936057	-2.669519	0.000015
1	1.197929	-1.434525	-0.809052
1	1.197930	-1.434514	0.809065
7	2.796721	1.163378	-0.000004
1	3.303330	1.498478	-0.814129
1	2.838137	0.138942	-0.000002
1	3.303334	1.498481	0.814118
7	0.000000	0.479746	1.573809
1	-0.000002	0.788582	2.541498
1	-0.818429	0.895306	1.125529
1	0.818431	0.895305	1.125531
7	-2.796721	1.163379	-0.000004
1	-3.303332	1.498483	0.814118
1	-2.838138	0.138943	0.000000
1	-3.303331	1.498478	-0.814128
7	-1.772707	-1.668325	0.000007
1	-1.197935	-1.434533	-0.809058
1	-1.936057	-2.669519	0.000025
1	-1.197925	-1.434505	0.809058

Cartesian coordinates of : P6_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.380396	1.407057	0.014031
1	2.903950	1.764427	0.808152
1	2.853843	1.750152	-0.817216
1	2.470818	0.383739	0.017154
7	-0.250225	0.204188	1.620545
1	-0.068461	-0.141004	2.557927
1	0.510873	0.833588	1.369974
1	-0.178114	-0.585360	0.978429
7	-0.653638	1.728494	-0.979878
1	-0.862613	2.521576	-1.577995
1	0.332723	1.783281	-0.714617
1	-1.179118	1.842298	-0.116435
7	-0.677053	-1.421086	-1.107450
1	-1.584651	-1.574715	-0.664856
1	-0.667095	-1.960471	-1.968314
1	-0.667435	-0.428228	-1.361189
7	-3.109412	-0.274445	0.391618
1	-2.365586	0.090996	0.988536
1	-3.988977	-0.210606	0.892674
1	-3.170213	0.327144	-0.424779
7	2.219510	-1.684904	0.048891
1	1.265919	-1.741701	-0.325918
1	2.209379	-2.103776	0.974171
1	2.817710	-2.266473	-0.530001

Cartesian coordinates of : P6_5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.988102	-1.847360	0.736630
1	1.916426	-1.524096	0.994692
1	0.768819	-1.427398	-0.168238
1	1.035521	-2.853199	0.605508
7	-2.078106	-1.418511	0.261825
1	-2.162280	-0.410932	0.134927
1	-1.273857	-1.580172	0.866121
1	-2.909694	-1.746825	0.740883
7	0.521412	1.031282	1.778978
1	1.341030	1.035779	1.167537
1	0.324056	0.048766	1.960571
1	0.776203	1.467725	2.659144
7	-1.679624	1.893019	-0.163993
1	-2.576591	2.069567	0.279468
1	-1.426340	2.751610	-0.644817
1	-0.985575	1.736980	0.578988
7	-0.280352	-0.392766	-1.904736
1	-0.892651	-1.181476	-1.692466
1	-0.220212	-0.315296	-2.915845
1	-0.792879	0.422620	-1.557364
7	2.459727	0.669383	-0.686709
1	2.670806	1.586397	-1.068716
1	1.641146	0.304698	-1.182543
1	3.247962	0.069926	-0.911813

Cartesian coordinates of : P6_6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.499657	-1.142643	-0.320169
1	3.332246	-1.695900	-0.492532
1	1.880725	-1.221570	-1.128142
1	1.980602	-1.565324	0.448271
7	0.001435	-0.840710	1.609584
1	0.330433	0.072158	1.295542
1	0.288353	-0.950172	2.577622
1	-1.020581	-0.803234	1.587671
7	-1.046458	1.832678	-0.825049
1	-0.850769	2.027131	-1.803610
1	-0.140557	1.786106	-0.344772
1	-1.529653	2.650386	-0.462878
7	1.839840	1.725570	0.441076
1	2.275584	2.450997	-0.121775
1	2.251192	0.826611	0.155253
1	2.125632	1.899919	1.400690
7	-0.347872	-1.297646	-1.480885
1	-0.921289	-1.937899	-2.020308
1	-0.810802	-0.391083	-1.467981
1	-0.327140	-1.617179	-0.512001
7	-2.883742	-0.380180	0.573189
1	-3.751797	-0.003117	0.939434
1	-3.122551	-1.149639	-0.044480
1	-2.429639	0.342329	0.009775

Cartesian coordinates of : P6_7

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.838560	-1.964876	-0.495856
1	1.220385	-2.330556	-1.363734

1	0.507499	-2.766917	0.032994
1	1.619615	-1.549666	0.025657
7	-0.411888	0.667810	1.207025
1	-1.427854	0.590631	1.305844
1	-0.028185	0.825939	2.134032
1	-0.076997	-0.242625	0.892716
7	-3.469362	0.008630	0.855582
1	-3.864544	-0.846748	1.232070
1	-3.092288	-0.191651	-0.074930
1	-4.230063	0.672197	0.752024
7	-1.548302	-0.090020	-1.551677
1	-1.611199	-0.126816	-2.563905
1	-0.799663	-0.720975	-1.253399
1	-1.260644	0.849296	-1.288548
7	1.559851	1.702070	-0.912997
1	1.304688	1.127557	-1.711254
1	1.635057	2.661001	-1.235740
1	0.792232	1.637395	-0.236954
7	2.991469	-0.274499	0.938902
1	3.981832	-0.474206	0.839572
1	2.846474	0.025624	1.898075
1	2.761358	0.516719	0.328625

Cartesian coordinates of : TC6_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.642123	-1.253585	-1.151119
1	0.796793	-1.768509	-2.012337
1	0.677469	-0.260527	-1.376170
1	-0.305737	-1.468113	-0.827411
7	-2.249017	-1.698386	0.046310
1	-2.725079	-0.797387	-0.070064
1	-2.369520	-1.978567	1.015452
1	-2.746228	-2.383508	-0.515131
7	-0.324707	0.864836	1.075000
1	0.395297	1.170497	0.416295
1	-0.385208	-0.148536	0.995702
1	0.010857	1.079383	2.009037
7	2.898659	-0.810152	0.912878
1	2.161391	-1.197656	0.313316
1	2.540664	-0.776375	1.862342
1	3.682190	-1.455347	0.912272
7	-3.146844	1.264794	-0.097327
1	-3.126234	1.753011	-0.986979
1	-2.232913	1.386888	0.351241
1	-3.849107	1.718857	0.477480
7	2.163328	1.638660	-0.799125
1	2.496248	1.541664	-1.753881
1	2.677432	0.966490	-0.220344
1	2.416886	2.574565	-0.497143

Cartesian coordinates of : DC6_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.800982	0.092238	0.213451
1	3.710061	0.338075	-0.166265
1	2.902155	0.050222	1.223133
1	2.152730	0.857719	0.000992
7	-2.191762	1.520463	-0.182650
1	-2.278405	0.559650	-0.526890
1	-3.005946	2.039620	-0.496088
1	-2.246282	1.441217	0.830059
7	-2.185432	-1.578776	-0.255263
1	-2.202432	-1.376223	0.741918

1	-1.238756	-1.904353	-0.456606
1	-2.831261	-2.339302	-0.439364
7	0.960723	-2.215273	-0.730635
1	1.311886	-3.138126	-0.492558
1	1.688469	-1.533499	-0.487773
1	0.858120	-2.193016	-1.741489
7	0.726209	2.296592	-0.680300
1	0.958980	2.272441	-1.669521
1	0.890895	3.249458	-0.368241
1	-0.285736	2.122918	-0.608417
7	-0.228643	-0.131164	1.628319
1	0.271425	-0.111872	2.511835
1	0.043834	0.699101	1.103871
1	0.125719	-0.922586	1.090951

Cartesian coordinates of : DC6_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.982139	-2.030927	-0.368657
1	2.699326	-1.322779	-0.182606
1	1.965395	-2.192117	-1.371079
1	2.284325	-2.899003	0.062618
7	-0.628136	-0.681918	0.760779
1	-0.591097	-0.771579	1.772704
1	0.159957	-1.225175	0.391465
1	-1.496128	-1.132338	0.458223
7	1.051988	1.756601	-0.389492
1	0.886851	1.774991	-1.391477
1	0.714968	2.638691	-0.016108
1	0.467564	1.011253	0.000330
7	-3.596532	-1.249578	-0.221662
1	-3.606395	-0.227959	-0.257621
1	-4.363521	-1.554200	0.368731
1	-3.780071	-1.600443	-1.156025
7	3.797965	0.435270	0.222721
1	4.083989	0.568398	1.187497
1	2.983134	1.032819	0.050253
1	4.560389	0.762204	-0.361927
7	-2.608176	1.689598	0.016192
1	-2.332883	2.274099	-0.766593
1	-1.800155	1.122060	0.282517
1	-2.830388	2.307753	0.789935

Cartesian coordinates of : TC6_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.579006	-1.343036	1.032828
1	-2.447928	-1.214119	0.026727
1	-3.576948	-1.413828	1.207581
1	-2.172654	-2.239079	1.284706
7	0.405115	-0.460311	0.220955
1	-0.254191	-0.658245	-0.530031
1	-0.072811	-0.714966	1.082001
1	1.217901	-1.071855	0.110511
7	-1.763618	1.696726	0.649700
1	-2.085732	0.887770	1.182639
1	-1.993817	2.539538	1.164805
1	-0.750115	1.613561	0.601727
7	3.368447	-1.452285	-0.134635
1	3.929072	-1.856767	0.608388
1	3.494970	-0.437310	-0.110626
1	3.744783	-1.795688	-1.012373
7	-2.149913	-0.038488	-1.827591
1	-1.455853	0.116363	-2.553098

1	-2.152580	0.785438	-1.216896
1	-3.050894	-0.086458	-2.293904
7	2.744922	1.598481	0.071548
1	2.895183	2.132551	0.921328
1	1.828399	1.146352	0.135260
1	2.721584	2.259127	-0.698376

Cartesian coordinates of : CY6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.681320	0.869313	0.671658
1	3.610120	1.270795	0.586266
1	2.463514	0.842784	1.663289
1	2.021616	1.522573	0.233398
7	-2.681320	-0.869313	-0.671658
1	-2.021616	-1.522573	-0.233398
1	-2.463514	-0.842784	-1.663289
1	-3.610120	-1.270795	-0.586266
7	-0.586872	-2.753289	0.672084
1	-0.500579	-2.548430	1.663089
1	0.309048	-2.511117	0.233150
1	-0.704826	-3.758526	0.589884
7	2.093243	-1.885723	-0.671807
1	2.905002	-2.490078	-0.588451
1	2.330449	-0.988596	-0.232594
1	1.960259	-1.708644	-1.662986
7	-2.093243	1.885723	0.671807
1	-2.905002	2.490078	0.588451
1	-1.960259	1.708645	1.662986
1	-2.330449	0.988596	0.232594
7	0.586872	2.753289	-0.672084
1	0.500579	2.548430	-1.663089
1	0.704826	3.758526	-0.589884
1	-0.309048	2.511117	-0.233150

Cartesian coordinates of : BP6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.625156	-2.201269	0.470351
1	0.397887	-2.493994	1.416420
1	0.634716	-3.043668	-0.097351
1	-0.145186	-1.606465	0.136828
7	1.919156	0.037129	-1.702852
1	1.298470	0.780787	-1.388248
1	1.626829	-0.801382	-1.202804
1	1.752111	-0.114223	-2.692235
7	0.645547	2.154435	0.402713
1	0.062349	2.555450	1.131506
1	1.158297	2.926496	-0.014193
1	1.337773	1.544904	0.855967
7	-1.334345	-0.137219	-0.683401
1	-0.806129	0.695049	-0.411506
1	-2.306513	-0.012306	-0.398612
1	-1.318621	-0.179394	-1.698289
7	-4.407138	0.092535	0.325974
1	-4.847339	1.003949	0.253964
1	-4.395417	-0.165842	1.307321
1	-5.001279	-0.573362	-0.157113
7	2.777999	0.073560	1.153356
1	3.264369	0.207154	0.268803
1	2.234354	-0.785359	1.044663
1	3.468710	-0.071992	1.881902

Cartesian coordinates of : BDC6_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.932873	-1.047710	-0.966327
1	-2.430784	-1.216392	-1.834497
1	-1.105368	-0.494181	-1.183570
1	-2.526787	-0.463043	-0.372974
7	-0.462744	2.225917	-0.365429
1	0.110873	1.389960	-0.527043
1	0.135924	2.927414	0.059879
1	-0.730681	2.584534	-1.277496
7	1.284629	-0.338622	-0.861217
1	1.432187	-0.703902	-1.798226
1	1.041685	-1.139246	-0.270134
1	2.185681	0.018630	-0.538499
7	-0.021487	-2.771503	0.696949
1	0.104941	-3.745834	0.442527
1	-0.836302	-2.410685	0.188524
1	-0.238807	-2.748098	1.688159
7	-3.059898	1.137136	0.979656
1	-2.949503	0.920060	1.964799
1	-3.841752	1.778728	0.898291
1	-2.213548	1.619740	0.661188
7	4.033513	0.702286	0.487186
1	3.778651	0.708869	1.469652
1	4.429129	1.610178	0.266546
1	4.766473	0.010745	0.367147

Cartesian coordinates of : BDC6_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.176001	2.160300	0.482657
1	0.195059	2.872403	-0.139130
1	-0.376350	2.618722	1.366526
1	-1.070103	1.848828	0.091205
7	-2.947209	1.121401	-0.644714
1	-3.119200	0.277522	-0.086496
1	-3.120824	0.870761	-1.614193
1	-3.653841	1.806728	-0.393811
7	-0.549718	-1.135018	-1.075696
1	0.310694	-1.113083	-0.518321
1	-0.832955	-0.163426	-1.188353
1	-0.315914	-1.494026	-1.996051
7	1.754525	-0.365172	0.834154
1	1.242995	0.520339	0.807072
1	2.731508	-0.189584	0.601228
1	1.724512	-0.709834	1.788360
7	-2.943374	-1.633735	0.765129
1	-2.638106	-1.715744	1.729741
1	-2.116410	-1.736138	0.165496
1	-3.570269	-2.410535	0.582326
7	4.777662	-0.213604	-0.307143
1	4.715285	-1.122872	-0.753653
1	5.645363	-0.184599	0.217502
1	4.837361	0.485343	-1.040165

Cartesian coordinates of : BC6_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.875452	-1.662663	0.129126
1	1.621964	-2.191979	-0.311607

1	0.958459	-1.815683	1.129971
1	1.064659	-0.670414	-0.039957
7	-1.403253	2.387182	-0.432791
1	-1.995246	1.717642	0.072293
1	-1.743068	2.422054	-1.389453
1	-1.572306	3.304667	-0.031164
7	-3.131954	0.229395	1.007431
1	-2.844803	0.051398	1.965031
1	-2.887957	-0.599811	0.454536
1	-4.143841	0.311682	1.013646
7	-2.091725	-2.123796	-0.741342
1	-2.358816	-3.093149	-0.601276
1	-1.096569	-2.036089	-0.508993
1	-2.192462	-1.929724	-1.732908
7	1.555515	1.421661	-0.284538
1	2.014341	1.766346	-1.123762
1	2.001479	1.899079	0.494921
1	0.580951	1.746173	-0.324101
7	4.242446	-0.174164	0.356945
1	4.741051	-0.513346	-0.458629
1	3.274589	-0.001512	0.093347
1	4.252205	-0.910631	1.054277

Cartesian coordinates of : BC6_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.192433	-1.538219	0.406654
1	1.823562	-2.166397	-0.081999
1	1.372910	-1.656213	1.399324
1	1.464006	-0.582540	0.161312
7	1.830874	1.494686	-0.302848
1	0.839028	1.647490	-0.086058
1	1.982831	1.799473	-1.260254
1	2.377209	2.116435	0.287283
7	-1.192429	1.538215	0.406673
1	-1.372897	1.656211	1.399345
1	-1.464004	0.582536	0.161335
1	-1.823564	2.166392	-0.081974
7	-1.830878	-1.494688	-0.302834
1	-2.377207	-2.116441	0.287297
1	-0.839030	-1.647493	-0.086055
1	-1.982845	-1.799467	-1.260241
7	4.608310	-0.105262	-0.094510
1	4.680022	-0.782812	0.656794
1	4.903862	-0.559693	-0.951659
1	3.630050	0.160596	-0.189926
7	-4.608311	0.105266	-0.094528
1	-4.680047	0.782778	0.656809
1	-4.903828	0.559744	-0.951665
1	-3.630050	-0.160595	-0.189920

Cartesian coordinates of : BC6_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.889958	-0.734532	1.540208
1	1.283410	-1.669272	1.491193
1	1.283615	-0.291057	2.364642
1	1.227685	-0.217197	0.725267
7	1.798232	0.988312	-1.006876
1	0.989564	1.584116	-0.786070
1	1.668877	0.646582	-1.955327
1	2.621020	1.584946	-1.029272
7	-0.711105	2.585164	-0.152894
1	-0.541517	3.280060	0.568322

1	-1.279848	1.839078	0.269667
1	-1.277822	3.037680	-0.863860
7	-2.115020	0.166514	1.131703
1	-2.643400	0.242209	1.995160
1	-1.232181	-0.302988	1.347999
1	-2.648939	-0.430482	0.499315
7	3.970492	-1.302748	-0.446882
1	4.284846	-1.381086	0.514275
1	3.685048	-2.225638	-0.755927
1	3.155860	-0.691123	-0.463748
7	-3.697596	-1.636348	-1.052842
1	-4.455393	-1.121849	-1.489401
1	-4.066972	-2.532451	-0.752871
1	-2.998589	-1.816052	-1.766283

Cartesian coordinates of : BC6_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.132235	1.412095	-0.368276
1	2.984256	1.395297	0.183651
1	2.410971	1.384464	-1.344262
1	1.613561	0.552739	-0.169192
7	0.279354	-1.070462	0.284165
1	-0.549214	-0.490798	0.114823
1	0.221527	-1.397015	1.245166
1	0.200182	-1.896869	-0.303153
7	-2.223041	0.806035	-0.176366
1	-2.652863	0.898593	-1.092861
1	-1.673537	1.658790	-0.014003
1	-2.986595	0.800213	0.495145
7	-0.318756	3.221799	0.286162
1	-0.402567	4.031347	-0.320863
1	0.574885	2.764845	0.077741
1	-0.269849	3.572593	1.237817
7	3.249313	-2.222425	0.034030
1	3.844413	-1.927821	-0.732615
1	3.798794	-2.179823	0.885480
1	2.482564	-1.558120	0.112959
7	-3.243033	-2.233020	-0.050203
1	-3.261487	-2.724263	-0.937447
1	-2.836490	-2.856923	0.638575
1	-2.631062	-1.425409	-0.143546

Cartesian coordinates of : BC6_5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.070451	-0.092109	0.811579
1	-2.156632	-0.046061	1.822453
1	-3.012137	-0.029862	0.424654
1	-1.545920	0.737012	0.518306
7	-0.038690	2.170780	-0.070314
1	0.744879	1.565221	0.206284
1	0.075155	3.062704	0.400925
1	0.047481	2.349203	-1.066043
7	2.070452	0.092189	0.811568
1	3.012138	0.029925	0.424647
1	1.545917	-0.736938	0.518318
1	2.156631	0.046169	1.822444
7	0.038686	-2.170729	-0.070246
1	-0.047494	-2.349188	-1.065968
1	-0.744879	-1.565156	0.206336
1	-0.075160	-3.062634	0.401026
7	-4.962935	0.025067	-0.680782
1	-5.840909	0.026904	-0.172663

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1   -4.956183   -0.791220   -1.283340
1   -4.948367    0.847889   -1.274290
7    4.962939   -0.025183   -0.680778
1    4.948501   -0.848251   -1.273948
1    5.840910   -0.026679   -0.172651
1    4.956069    0.790855   -1.283673

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Cartesian coordinates of ammonia heptamer: (NH3)7

Cartesian coordinates of : AM7_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.794645	-1.230003	0.353964
1	-2.709212	-0.316571	-0.107777
1	-3.297160	-1.093915	1.226412
1	-3.384490	-1.815623	-0.230227
7	0.000107	-1.538300	-1.319088
1	-0.000008	-2.262894	-2.030856
1	-0.820567	-1.692054	-0.730950
1	0.820676	-1.692365	-0.730886
7	0.000006	-0.649360	1.839927
1	0.825010	-1.024783	1.370089
1	-0.824916	-1.024919	1.370055
1	0.000018	-1.018946	2.785892
7	1.752678	1.157322	-1.218324
1	1.133469	0.460397	-1.632749
1	2.096683	1.755354	-1.962758
1	1.170987	1.730421	-0.605738
7	-0.000043	2.365299	1.192063
1	0.814827	2.827481	1.585633
1	-0.814510	2.827643	1.586275
1	-0.000002	1.394052	1.530973
7	2.794682	-1.229898	0.353975
1	3.384403	-1.815369	-0.230495
1	3.297425	-1.093986	1.226320
1	2.709125	-0.316378	-0.107567
7	-1.752817	1.157245	-1.218327
1	-1.171272	1.730171	-0.605430
1	-1.133460	0.460595	-1.632983
1	-2.096797	1.755555	-1.962551

Cartesian coordinates of : AM7_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.592587	-0.026241	-1.857642
1	0.037763	0.767960	-1.519823
1	0.570424	-0.001331	-2.872981
1	1.549770	0.169138	-1.569534
7	2.401280	1.479118	0.208399
1	1.592198	1.268673	0.801794
1	3.113736	1.908432	0.790860
1	2.102960	2.179567	-0.465349
7	0.010096	0.169283	1.703743
1	0.595888	-0.650932	1.529720
1	-0.821563	0.071087	1.122540
1	-0.296915	0.134483	2.671108
7	-1.080216	-2.207855	-0.373040
1	-1.315673	-3.021960	-0.932274
1	-0.493605	-2.526200	0.394139
1	-0.503118	-1.581868	-0.946457
7	-3.092560	0.017242	0.297006
1	-3.821553	0.120237	-0.402994
1	-3.560646	-0.106183	1.189942

1	-2.582692	-0.849312	0.087287
7	-0.961113	2.277933	-0.381924
1	-1.778523	1.701994	-0.162649
1	-1.284746	3.202631	-0.646859
1	-0.437377	2.362130	0.485824
7	2.148509	-1.711994	0.408349
1	1.745550	-1.965716	-0.490135
1	2.887299	-2.374837	0.619726
1	2.570742	-0.790395	0.281881

Cartesian coordinates of : AM7_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.496014	1.281148	1.425624
1	0.574724	1.918050	2.212649
1	-0.311438	1.576559	0.877238
1	1.323488	1.407340	0.841206
7	1.436170	-1.666744	0.770916
1	0.762422	-2.029305	0.096394
1	0.979949	-0.891796	1.256571
1	1.619360	-2.400664	1.447667
7	-1.232296	-2.288784	-0.949876
1	-1.675853	-1.760709	-0.187416
1	-1.316619	-3.277254	-0.730677
1	-1.779495	-2.131851	-1.791673
7	3.181501	0.608160	-0.255241
1	3.707727	0.518397	-1.119366
1	3.837739	0.923977	0.453112
1	2.853420	-0.326057	0.017377
7	-2.017514	2.072220	-0.589357
1	-1.818974	3.067903	-0.621134
1	-2.905121	1.937047	-1.064736
1	-1.291209	1.588643	-1.133687
7	0.303537	0.423100	-1.730965
1	0.498990	0.391807	-2.727437
1	1.176782	0.674791	-1.266767
1	0.072331	-0.529586	-1.444334
7	-2.144385	-0.451138	1.345234
1	-2.318129	0.449433	0.894908
1	-2.881767	-0.615979	2.022807
1	-1.269514	-0.336482	1.852946

Cartesian coordinates of : AM7_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.287466	0.030453	-0.100866
1	-3.489195	0.087001	-1.094188
1	-4.156952	-0.192701	0.372576
1	-2.634209	-0.742864	0.044383
7	-0.879472	1.884843	0.637858
1	-0.381057	1.269325	1.283881
1	-1.813019	1.488405	0.498773
1	-0.996069	2.781235	1.101252
7	1.386756	0.014605	1.964372
1	1.816374	0.291024	2.841854
1	1.820219	0.557824	1.212229
1	1.636588	-0.956200	1.789908
7	-0.380601	-0.041435	-1.865554
1	-0.879035	-0.807367	-1.413857
1	-0.809377	0.124516	-2.770757
1	-0.553987	0.779134	-1.280934
7	2.017624	1.649403	-0.644785
1	1.851562	1.109740	-1.491138
1	2.652409	2.406939	-0.875645

1	1.111286	2.050677	-0.395295
7	-0.866142	-1.848533	0.703058
1	0.031520	-2.136779	0.306917
1	-1.234633	-2.637700	1.226330
1	-0.619894	-1.124760	1.379198
7	2.016439	-1.664302	-0.672698
1	2.475553	-2.378191	-1.229850
1	1.389787	-1.136218	-1.285741
1	2.732162	-1.008291	-0.369590

Cartesian coordinates of : AM7_5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.946599	-1.327477	0.520574
1	-3.130794	-0.323725	0.424623
1	-3.180541	-1.593321	1.472681
1	-3.587860	-1.828040	-0.087362
7	-0.618107	-0.480007	-1.660549
1	-0.899717	-0.630510	-2.624993
1	-1.357263	-0.861379	-1.068000
1	0.207947	-1.063185	-1.487245
7	-0.102951	-0.053145	1.435528
1	0.653679	-0.056756	0.753440
1	-0.789331	-0.739866	1.119068
1	0.289867	-0.391169	2.309203
7	1.048407	2.023889	-0.710970
1	0.462678	1.299381	-1.139005
1	1.199946	2.753260	-1.400697
1	0.502405	2.427211	0.045768
7	3.188435	0.368374	0.754700
1	2.630562	1.037768	0.211122
1	3.161367	0.666227	1.725456
1	4.154513	0.446507	0.451535
7	-2.368597	1.621619	0.127976
1	-1.914325	1.504655	-0.775548
1	-2.673542	2.585449	0.210825
1	-1.645782	1.437497	0.826356
7	1.776301	-2.125718	-0.489701
1	2.351544	-1.430277	-0.004612
1	2.395458	-2.728562	-1.022526
1	1.330965	-2.703905	0.217005

Cartesian coordinates of : AM7_6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.042043	0.700447	-0.512495
1	3.845832	0.980155	0.042353
1	3.306270	0.817294	-1.486356
1	2.888348	-0.301547	-0.346282
7	2.058168	-2.124114	0.160310
1	1.323883	-1.725747	0.760144
1	2.598250	-2.779321	0.717199
1	1.593888	-2.664728	-0.563702
7	-0.218551	-0.642946	1.614204
1	-1.045336	-0.964210	1.110309
1	-0.089841	0.354607	1.423927
1	-0.403833	-0.744749	2.607063
7	0.558943	2.276824	0.654346
1	0.025756	2.548301	-0.167451
1	1.435791	1.874014	0.309335
1	0.783998	3.124285	1.166311
7	-0.152674	-0.027158	-1.453694
1	-0.653967	-0.828198	-1.067697
1	0.156561	-0.277466	-2.388094

1	0.685227	0.102038	-0.887584
7	-2.575211	1.433883	-0.169129
1	-2.144012	1.732322	0.702058
1	-3.111382	2.214567	-0.533214
1	-1.807214	1.227100	-0.813190
7	-2.728418	-1.612265	-0.246212
1	-2.998468	-1.939548	-1.169179
1	-3.011874	-0.629844	-0.170993
1	-3.267975	-2.152018	0.423728

Cartesian coordinates of : AM7_7

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.786238	-1.648033	-0.574274
1	2.713987	-2.517344	-0.055161
1	3.442613	-1.803959	-1.332337
1	1.870654	-1.440183	-0.982091
7	-0.301685	-1.427407	1.379011
1	-0.233869	-2.040747	2.186069
1	0.385941	-0.671041	1.505470
1	0.032045	-1.948922	0.570341
7	1.858306	0.739258	1.221155
1	1.619534	1.513434	0.597816
1	2.487915	0.111157	0.716902
1	2.365815	1.125382	2.010884
7	0.441022	2.882867	-0.637292
1	0.608122	3.812269	-0.263899
1	0.342875	2.982808	-1.642955
1	-0.452369	2.544128	-0.263112
7	-1.942756	1.353502	0.589114
1	-1.453801	0.619960	1.103469
1	-2.506172	0.870658	-0.107756
1	-2.575563	1.814362	1.235592
7	0.060313	-0.359333	-1.466169
1	0.260400	0.400708	-0.815103
1	-0.936732	-0.560539	-1.377682
1	0.204605	0.018732	-2.398551
7	-2.820794	-1.477226	-0.492856
1	-3.782219	-1.395646	-0.176374
1	-2.743073	-2.368456	-0.973960
1	-2.215214	-1.512163	0.331624

Cartesian coordinates of : AM7_8

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.585906	0.436231	1.567310
1	-0.588183	0.735078	2.538122
1	-1.432295	0.809993	1.134400
1	0.198455	0.904758	1.108648
7	1.882761	1.948297	0.000327
1	2.646937	1.261661	-0.000116
1	2.017408	2.545915	0.811636
1	2.016647	2.546185	-0.810908
7	3.889113	-0.394304	-0.000528
1	4.448897	-0.619433	-0.816775
1	3.064046	-1.006692	-0.000075
1	4.449612	-0.619181	0.815298
7	1.146655	-1.765270	0.000596
1	0.653568	-1.376645	-0.804027
1	0.653525	-1.375553	0.804673
1	0.985629	-2.768094	0.001273
7	-2.325792	-1.760803	0.000231
1	-1.748376	-1.527750	0.807726
1	-1.748370	-1.528163	-0.807378

1	-2.488046	-2.762309	0.000489
7	-0.585501	0.435419	-1.567347
1	-0.587235	0.734279	-2.538156
1	-1.431954	0.809475	-1.134813
1	0.198803	0.903683	-1.108335
7	-3.421776	1.042335	-0.000580
1	-3.429171	0.017039	-0.000302
1	-3.938473	1.361431	0.813566
1	-3.938300	1.360987	-0.815010

Cartesian coordinates of : AM7_9

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.827374	1.380711	-0.006958
1	3.218342	0.432876	0.022683
1	3.113030	1.795980	-0.889043
1	3.274869	1.918441	0.729365
7	3.349955	-1.704642	0.150847
1	3.789461	-2.153462	0.948182
1	2.335336	-1.774865	0.268197
1	3.608893	-2.240541	-0.671388
7	-2.090578	0.859192	1.841819
1	-3.013305	1.281210	1.899181
1	-1.653534	1.006703	2.747381
1	-1.552235	1.400222	1.152225
7	-0.399011	2.200564	-0.400830
1	0.598631	2.064920	-0.233686
1	-0.684572	1.522374	-1.111681
1	-0.523150	3.130979	-0.787559
7	-2.493361	-1.825651	0.223310
1	-2.448738	-1.040570	0.880465
1	-3.340833	-2.350937	0.412042
1	-1.705996	-2.436838	0.423498
7	-1.635371	-0.148192	-2.223710
1	-1.187202	-0.736033	-2.920404
1	-2.085869	-0.766418	-1.539545
1	-2.368915	0.365243	-2.703457
7	0.431043	-0.781567	0.431421
1	-0.128681	-0.644014	-0.410299
1	1.049787	0.029878	0.471632
1	-0.225679	-0.668056	1.200917

Cartesian coordinates of : AM7_10

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.774451	-0.879919	1.557719
1	2.709483	-0.520421	1.383258
1	1.689488	-1.030958	2.558081
1	1.125447	-0.135346	1.291585
7	-0.224542	0.874612	-0.096116
1	0.264699	0.547008	-0.930831
1	-0.836492	1.649291	-0.355340
1	-0.872040	0.127674	0.152909
7	2.219957	-0.577477	-1.541642
1	2.772843	-0.764981	-2.372080
1	2.343884	-1.360208	-0.903585
1	2.620675	0.238733	-1.073192
7	-0.284250	-2.333041	-0.365296
1	0.422883	-2.165526	0.354207
1	0.063574	-1.861190	-1.198728
1	-0.294996	-3.329153	-0.562922
7	2.670142	1.978333	0.295637
1	2.803781	2.815324	-0.264019
1	3.069039	2.170949	1.209420

1	1.662788	1.842430	0.415198
7	-3.057196	-1.085550	0.390587
1	-3.823805	-1.483351	-0.144270
1	-3.246774	-1.288950	1.367676
1	-2.205655	-1.597320	0.132900
7	-3.091090	2.061420	-0.288975
1	-3.154598	1.067817	-0.051153
1	-3.528755	2.592100	0.457096
1	-3.637777	2.217422	-1.129617

Cartesian coordinates of : AM7_11

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.862446	1.411970	-1.055166
1	2.235713	1.860218	-1.885936
1	1.478776	0.510677	-1.334471
1	2.646704	1.209392	-0.428991
7	1.950460	-2.154194	-0.073918
1	1.120377	-1.669367	-0.432420
1	1.622338	-2.854209	0.585123
1	2.359798	-2.660892	-0.853589
7	-0.618018	-0.647944	-1.087577
1	-0.847482	-0.522809	-2.069724
1	-0.743950	0.258689	-0.637286
1	-1.328189	-1.270100	-0.690441
7	-0.554266	2.255075	0.622253
1	-0.747193	3.252275	0.659018
1	0.290897	2.131539	0.047375
1	-0.302939	1.975073	1.566793
7	3.857338	0.100572	0.949089
1	3.757322	0.283564	1.942291
1	4.833301	-0.122140	0.782468
1	3.297104	-0.726739	0.718057
7	-3.460025	1.045592	0.132478
1	-4.127785	1.644268	0.608679
1	-3.655489	1.117183	-0.861982
1	-2.526097	1.439099	0.282788
7	-2.974295	-2.002202	0.495449
1	-3.731212	-2.584037	0.151462
1	-3.303595	-1.032423	0.528247
1	-2.773892	-2.301339	1.444285

Cartesian coordinates of : AM7_12

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.735171	-0.848542	-0.097639
1	-3.922292	-0.712511	-1.086764
1	-3.599878	0.082057	0.312508
1	-4.576084	-1.247607	0.308030
7	-2.838455	1.949949	0.879098
1	-2.519148	2.081244	1.833628
1	-3.259356	2.824710	0.582884
1	-2.015560	1.772849	0.290388
7	-0.610203	0.883149	-0.958733
1	-0.652898	-0.095697	-0.673484
1	-0.872291	0.912846	-1.939922
1	0.367558	1.176007	-0.903910
7	-0.951696	-2.133326	0.324495
1	-0.949993	-3.133818	0.146707
1	-1.918640	-1.804679	0.208203
1	-0.712002	-2.012751	1.304851
7	2.466541	1.818322	-0.628917
1	3.150000	1.986676	-1.361572
1	2.204384	2.729862	-0.264312

1	2.946999	1.312832	0.123293
7	3.692749	-0.232150	1.368900
1	3.313229	-0.336768	2.304394
1	4.672438	-0.493204	1.413094
1	3.210628	-0.894876	0.752926
7	1.969468	-1.433576	-0.871724
1	1.942734	-0.471233	-1.206337
1	1.015639	-1.676761	-0.596463
1	2.221895	-2.025966	-1.656511

Cartesian coordinates of : AM7_13

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.389282	0.270266	-0.417704
1	3.270426	-0.743117	-0.332153
1	4.051077	0.562905	0.295333
1	3.819850	0.456679	-1.318184
7	1.461946	2.938814	0.248306
1	2.063578	2.176225	-0.058546
1	0.499585	2.660842	0.066143
1	1.667548	3.750743	-0.324608
7	2.213829	-2.589238	0.077149
1	1.364709	-2.066623	0.297032
1	2.444059	-3.167317	0.879063
1	2.001187	-3.215994	-0.692452
7	-1.680890	-2.363915	-0.185907
1	-0.942357	-1.712134	0.096434
1	-1.644410	-3.169155	0.431036
1	-1.464388	-2.693058	-1.121595
7	-1.800630	2.140954	-0.214425
1	-2.561646	1.452708	-0.173867
1	-1.993537	2.848187	0.489372
1	-1.858457	2.601537	-1.118071
7	-3.893573	-0.164494	-0.033431
1	-3.273561	-0.979102	-0.088727
1	-4.392743	-0.219687	0.849167
1	-4.587805	-0.254832	-0.768877
7	0.339140	-0.105700	0.605339
1	-0.359388	0.572837	0.287204
1	0.473710	0.093229	1.594470
1	1.218839	0.158320	0.156543

Cartesian coordinates of : AM7_14

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.918735	-0.258339	-0.193068
1	-1.927846	-0.404996	-0.249392
1	-0.464954	-1.123293	-0.482433
1	-0.652084	0.432463	-0.898965
7	0.849911	1.972407	-1.497868
1	1.741499	1.562460	-1.226520
1	0.503239	2.464791	-0.671522
1	1.026229	2.656705	-2.226058
7	2.124118	0.397992	0.855597
1	2.324645	-0.413273	1.439421
1	1.106464	0.439342	0.784886
1	2.434411	1.235266	1.338936
7	1.109208	-2.401760	1.403131
1	0.241706	-1.907217	1.595564
1	1.216973	-2.423914	0.388349
1	1.007647	-3.354329	1.736427
7	-4.123956	-0.765340	-0.317046
1	-4.298283	-1.728353	-0.585878
1	-4.583458	-0.171116	-0.999444

1	-4.577051	-0.611414	0.577813
7	-0.505071	2.430014	1.350291
1	-1.347460	2.993777	1.407055
1	-0.783862	1.463564	1.165168
1	-0.065883	2.458273	2.265253
7	1.668408	-1.391505	-1.601893
1	1.149170	-0.789008	-2.236447
1	2.166798	-0.769290	-0.961105
1	2.354914	-1.894727	-2.155118

Cartesian coordinates of : AM7_15

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.675656	2.238932	-1.231554
1	-0.814121	2.074312	-2.224207
1	-0.781435	3.238522	-1.086392
1	-1.429910	1.762387	-0.722159
7	-2.294928	0.372674	0.566444
1	-1.581831	-0.309168	0.295815
1	-3.209963	-0.077306	0.529204
1	-2.119295	0.626009	1.534150
7	0.135827	-0.992839	-0.909063
1	1.037978	-1.451103	-0.740737
1	0.325889	-0.049328	-1.244807
1	-0.315884	-1.494575	-1.668275
7	2.935036	-2.244051	-0.235584
1	2.923726	-2.788405	0.621420
1	3.441436	-2.789405	-0.926034
1	3.473534	-1.390594	-0.052946
7	4.111940	0.560828	0.370416
1	4.365213	1.136896	-0.426293
1	4.771581	0.772992	1.112116
1	3.178093	0.852755	0.681270
7	-5.219157	-1.009697	0.308350
1	-5.911193	-0.692410	0.979153
1	-5.555385	-0.764090	-0.617074
1	-5.180848	-2.022219	0.362957
7	1.156274	1.086948	1.140302
1	0.889538	1.539405	2.009177
1	0.754508	0.151466	1.142266
1	0.693011	1.584287	0.376224

Cartesian coordinates of : AM7_16

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.415721	-1.334234	-0.501869
1	-1.921368	-2.166737	-0.214219
1	-1.388680	-1.343328	-1.517163
1	-1.974667	-0.526374	-0.219797
7	-2.897926	1.360130	0.388704
1	-3.581882	1.916574	-0.116621
1	-1.964326	1.711290	0.146594
1	-3.047056	1.542734	1.376921
7	1.373670	-0.662400	0.802004
1	1.283701	-0.742466	1.811108
1	2.165051	-1.250774	0.527044
1	0.519638	-1.057611	0.396706
7	3.673414	1.351328	-0.059088
1	3.471852	1.898309	-0.889982
1	3.991717	1.996188	0.657038
1	2.798759	0.926099	0.257029
7	-5.091538	-0.956846	-0.029490
1	-4.937402	-1.524683	-0.855653
1	-4.267981	-0.374158	0.112984

1	-5.184633	-1.581840	0.763807
7	4.215069	-1.711098	-0.121905
1	4.914777	-2.093046	0.506021
1	4.364642	-2.137190	-1.030729
1	4.380242	-0.706061	-0.210691
7	0.029512	1.923104	-0.453570
1	0.522821	2.775209	-0.204544
1	0.520944	1.141097	-0.011401
1	0.128495	1.806878	-1.457957

Cartesian coordinates of ammonia octamer: (NH₃)₈

Cartesian coordinates of : AM8_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.523140	-0.428678	-1.580651
1	-1.659312	-0.130291	-2.035604
1	-3.247280	-0.497662	-2.288145
1	-2.788662	0.306064	-0.928190
7	0.501183	0.242218	2.096237
1	0.724151	0.611732	3.015729
1	1.305962	-0.305612	1.782216
1	0.410646	1.036604	1.459475
7	-0.534203	2.122722	-0.237363
1	-0.379640	1.492849	-1.027596
1	-0.731193	3.044053	-0.616774
1	-1.377382	1.800922	0.242303
7	2.532390	-1.571045	0.449727
1	2.920261	-1.156448	-0.394094
1	3.154623	-2.320384	0.736028
1	1.634696	-1.987562	0.191706
7	-0.578227	-2.106195	0.202318
1	-1.367636	-1.794900	-0.370800
1	-0.809235	-3.022481	0.574570
1	-0.500018	-1.463163	0.991765
7	2.603762	1.517554	-0.369588
1	3.330273	2.218496	-0.473415
1	1.734258	1.994306	-0.125931
1	2.850739	0.924717	0.419548
7	0.609772	-0.189465	-2.094155
1	1.434320	0.320675	-1.767201
1	0.823227	-0.569942	-3.011239
1	0.463452	-0.977773	-1.461450
7	-2.611319	0.411158	1.499194
1	-1.703840	0.192897	1.917617
1	-3.007050	-0.467723	1.174944
1	-3.216874	0.762740	2.234502

Cartesian coordinates of : AM8_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.935714	0.963209	1.682618
1	1.183814	1.137786	2.651646
1	0.470147	0.053603	1.645682
1	0.241697	1.658774	1.411621
7	-0.543150	-1.855828	1.077356
1	-1.174888	-1.942569	0.280269
1	-0.832413	-2.539499	1.770597
1	0.394510	-2.116528	0.755296
7	2.435551	-2.092222	0.048166
1	2.760832	-1.181104	-0.292453
1	3.025886	-2.343780	0.835789

1	2.614146	-2.774904	-0.682469
7	2.908202	0.891114	-0.687907
1	3.775058	1.415596	-0.630543
1	2.365949	1.055514	0.168739
1	2.367747	1.270159	-1.460513
7	-2.873850	-1.277922	-1.196646
1	-3.020837	-0.520316	-0.518840
1	-3.183432	-0.948248	-2.106346
1	-3.488275	-2.046076	-0.943120
7	-2.492628	0.737819	1.045651
1	-1.966301	1.541901	0.700176
1	-1.809219	0.062667	1.390607
1	-3.047856	1.050716	1.835663
7	0.106017	-0.097303	-1.495851
1	0.592265	-0.417931	-2.329002
1	-0.784687	-0.596949	-1.459173
1	0.657910	-0.425538	-0.704306
7	-0.495977	2.751123	-0.465325
1	-0.268006	1.884219	-0.967473
1	-1.100549	3.308455	-1.061459
1	0.367351	3.274104	-0.346813

Cartesian coordinates of : AM8_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.510915	2.282914	-0.544712
1	1.900292	3.116240	-0.974881
1	2.287550	1.651262	-0.324150
1	1.105556	2.558532	0.346329
7	3.587961	0.058006	0.259542
1	3.922267	-0.028644	1.214773
1	4.410494	0.129115	-0.332238
1	3.104072	-0.815109	0.016825
7	1.675605	-2.223629	-0.465985
1	1.004654	-1.621345	-0.957472
1	1.916567	-3.000583	-1.073278
1	1.188855	-2.602915	0.342092
7	-0.346994	-0.103705	-1.521169
1	-0.708577	-0.028385	-2.467576
1	0.216973	0.733451	-1.342874
1	-1.149433	-0.059119	-0.894274
7	-1.510918	-2.282909	0.544718
1	-1.900298	-3.116232	0.974891
1	-2.287552	-1.651258	0.324148
1	-1.105555	-2.558535	-0.346319
7	-3.587960	-0.058007	-0.259553
1	-3.104071	0.815108	-0.016833
1	-4.410496	-0.129116	0.332223
1	-3.922261	0.028646	-1.214786
7	0.346997	0.103705	1.521173
1	-0.216973	-0.733449	1.342877
1	0.708588	0.028377	2.467576
1	1.149431	0.059120	0.894272
7	-1.675606	2.223626	0.465987
1	-1.004659	1.621346	0.957484
1	-1.188848	2.602908	-0.342087
1	-1.916576	3.000582	1.073273

Cartesian coordinates of : AM8_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.527787	1.685689	-1.279682
1	0.437310	2.248801	-2.119497
1	0.283254	0.720577	-1.519147

1	-0.160827	2.019738	-0.605529
7	-0.033570	-1.424054	-1.542632
1	-0.102157	-1.933985	-2.418381
1	0.875759	-1.647001	-1.124848
1	-0.751104	-1.793911	-0.919630
7	3.154960	1.315932	0.302645
1	3.978177	1.708231	-0.144678
1	3.042862	1.803489	1.186766
1	2.340093	1.551233	-0.278691
7	2.672561	-1.732324	0.050867
1	2.534000	-2.154018	0.964778
1	2.996720	-0.769149	0.195990
1	3.422088	-2.246850	-0.401349
7	-2.802667	0.092317	-0.968701
1	-2.732580	-0.768750	-0.422768
1	-2.002410	0.082624	-1.598149
1	-3.644188	0.041154	-1.533889
7	-1.859604	2.319702	0.909363
1	-2.362835	1.644387	0.320233
1	-2.090553	3.252994	0.581427
1	-2.229613	2.244077	1.852615
7	-1.900053	-2.201587	1.042880
1	-1.181874	-1.538890	1.362479
1	-2.662003	-2.181392	1.714519
1	-1.501079	-3.134993	1.084073
7	0.246418	-0.041072	1.443209
1	0.803882	-0.189025	0.603001
1	-0.242427	0.846903	1.312352
1	0.908673	0.091533	2.202673

Cartesian coordinates of : AM8_5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.102379	0.196486	-2.006145
1	-1.230985	-0.716947	-1.568941
1	-1.487180	0.139413	-2.944270
1	-0.098047	0.348849	-2.102290
7	2.121448	-0.115774	2.161884
1	3.046020	-0.459567	1.917874
1	1.909575	0.681524	1.547023
1	2.181798	0.234533	3.113523
7	-2.121448	2.161884	0.115774
1	-2.181798	3.113523	-0.234533
1	-3.046020	1.917875	0.459567
1	-1.909575	1.547023	-0.681524
7	1.102379	2.006145	0.196486
1	1.487180	2.944270	0.139413
1	0.098046	2.102290	0.348850
1	1.230984	1.568941	-0.716947
7	1.102379	-2.006145	-0.196486
1	0.098047	-2.102290	-0.348850
1	1.230985	-1.568941	0.716947
1	1.487180	-2.944270	-0.139413
7	2.121448	0.115774	-2.161884
1	1.909575	-0.681524	-1.547023
1	3.046020	0.459567	-1.917874
1	2.181798	-0.234533	-3.113523
7	-2.121448	-2.161885	-0.115774
1	-1.909575	-1.547023	0.681524
1	-3.046020	-1.917875	-0.459567
1	-2.181798	-3.113523	0.234533
7	-1.102379	-0.196486	2.006145
1	-1.487180	-0.139413	2.944270
1	-0.098047	-0.348849	2.102290
1	-1.230985	0.716947	1.568941

Cartesian coordinates of : AM8_6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.065824	1.755158	-1.263051
1	3.030793	1.507030	-1.462702
1	1.976660	2.747573	-1.462444
1	1.914688	1.626533	-0.253352
7	1.756241	-2.066134	1.261387
1	2.748815	-1.976953	1.459977
1	1.508331	-3.031156	1.461048
1	1.626771	-1.914792	0.251827
7	-1.112815	1.308419	-1.640764
1	-1.486747	1.747888	-2.476433
1	-1.348620	0.316308	-1.691374
1	-0.095672	1.380579	-1.692318
7	-2.067219	-1.755900	-1.260310
1	-1.978286	-2.748422	-1.459272
1	-3.032388	-1.507852	-1.459087
1	-1.915020	-1.626737	-0.250841
7	-1.754826	2.066902	1.261974
1	-2.747187	1.977963	1.461736
1	-1.626502	1.914913	0.252365
1	-1.506582	3.032023	1.460743
7	1.309741	1.112402	1.640150
1	0.317663	1.348182	1.691526
1	1.749824	1.486201	2.475555
1	1.381962	0.095252	1.691472
7	-1.308037	-1.111499	1.641712
1	-1.380191	-0.094319	1.692532
1	-1.747267	-1.484805	2.477787
1	-0.315909	-1.347248	1.692233
7	1.111080	-1.309364	-1.641098
1	1.346799	-0.317267	-1.692386
1	1.484253	-1.749206	-2.476911
1	0.093893	-1.381584	-1.691684

Cartesian coordinates of : AM8_7-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.399881	0.509968	-1.733594
1	2.941528	0.213730	-0.913486
1	2.757806	1.413438	-2.029790
1	2.604548	-0.146104	-2.482055
7	-0.773651	0.102343	-1.680414
1	-1.240560	0.734761	-1.029039
1	-1.152695	0.304340	-2.601634
1	0.216614	0.362929	-1.703078
7	-1.957306	2.672053	-0.004702
1	-1.991484	3.153072	-0.898500
1	-0.976241	2.616674	0.290966
1	-2.455403	3.254654	0.661659
7	0.696325	1.543201	0.947634
1	1.381457	1.850541	1.631060
1	1.212859	1.095125	0.191451
1	0.122491	0.819341	1.384228
7	-2.505226	-2.309968	-0.593324
1	-3.337636	-2.402741	-1.166825
1	-2.064867	-3.223517	-0.552763
1	-1.861978	-1.669171	-1.067080
7	0.636431	-1.801452	0.563752
1	0.551289	-2.812656	0.612110
1	0.412828	-1.521596	-0.391077
1	-0.114636	-1.406479	1.133403
7	-1.944013	-0.170502	1.592492
1	-2.383233	-0.114140	2.506486
1	-2.361811	-0.959912	1.092734

1	-2.206048	0.671838	1.077032
7	3.419232	-0.545675	0.968123
1	4.143669	-1.253129	1.044582
1	2.507931	-1.020634	0.995506
1	3.491858	0.039866	1.794339

Cartesian coordinates of : AM8_8

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.709735	-0.010186	0.172890
1	-4.586752	-0.216178	-0.295054
1	-3.898325	0.003782	1.170536
1	-3.064553	-0.783049	-0.008049
7	-1.374867	-2.032292	-0.682506
1	-0.453087	-2.309324	-0.327686
1	-1.184409	-1.381346	-1.443984
1	-1.811730	-2.857722	-1.081704
7	1.474747	-2.076986	0.702085
1	2.319464	-1.634269	0.330378
1	1.766568	-2.882916	1.246750
1	1.058984	-1.402523	1.345992
7	-1.495125	2.022578	-0.704731
1	-1.057326	1.396389	-1.381964
1	-1.684765	2.902269	-1.175618
1	-2.396224	1.598149	-0.467300
7	1.474042	2.051344	0.711458
1	1.854602	2.880324	1.157872
1	1.222070	1.389223	1.444665
1	0.583286	2.313895	0.282756
7	3.672536	-0.014788	-0.277476
1	3.038041	0.763193	-0.072738
1	4.512663	0.116502	0.277719
1	3.949592	0.057270	-1.251749
7	-0.722042	0.030852	1.662189
1	-1.155838	-0.755687	1.176709
1	-1.092516	0.053617	2.607753
1	-1.049106	0.871370	1.182043
7	0.679994	0.015952	-1.630615
1	1.193552	-0.807025	-1.938468
1	1.264489	0.822208	-1.840383
1	0.674469	-0.043475	-0.611540

Cartesian coordinates of : AM8_9

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.484823	0.837872	-1.768769
1	2.597385	0.879035	-0.754627
1	3.400380	0.929183	-2.196678
1	1.940198	1.659206	-2.016578
7	-2.582720	-1.474519	-0.935930
1	-2.954861	-1.564723	-1.876975
1	-2.800081	-2.341180	-0.452193
1	-1.562155	-1.424455	-1.017210
7	1.754126	1.519193	1.230916
1	1.173889	1.074441	1.943012
1	1.092874	1.864778	0.529052
1	2.214254	2.319421	1.653784
7	-0.487565	1.590660	-0.942664
1	-1.325824	1.633349	-0.360722
1	-0.318404	0.606283	-1.153507
1	-0.713871	2.048679	-1.820887
7	0.596003	-1.565836	-1.269851
1	1.229990	-0.887383	-1.705171
1	1.106357	-1.902262	-0.446783

1	0.511735	-2.349838	-1.911836
7	2.210823	-1.622082	1.377594
1	3.083828	-2.092577	1.592793
1	2.412686	-0.635707	1.203507
1	1.631817	-1.638059	2.212982
7	-0.601830	-0.365049	1.753460
1	-0.223397	-0.691594	0.863389
1	-1.127832	-1.143352	2.142164
1	-1.283846	0.359262	1.528178
7	-3.268581	1.127125	0.608546
1	-3.738789	0.959593	1.493228
1	-3.224953	0.239470	0.095004
1	-3.856934	1.766890	0.082955

Cartesian coordinates of : AM8_10

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.617792	2.421095	0.733674
1	2.305528	1.872343	0.204111
1	1.648286	3.374504	0.385156
1	1.936216	2.449755	1.698223
7	-0.530046	-1.960847	1.415044
1	-0.509866	-2.620928	2.186657
1	-1.362328	-2.159570	0.854622
1	-0.681148	-1.024543	1.804141
7	3.363498	0.486863	-0.938623
1	3.259516	0.588499	-1.944228
1	2.972399	-0.426970	-0.677752
1	4.362000	0.451725	-0.754874
7	2.199694	-2.289206	-0.081998
1	2.013725	-2.970254	-0.813111
1	1.319462	-2.159632	0.433727
1	2.856850	-2.729380	0.556236
7	-1.168484	1.073582	1.742791
1	-0.364411	1.584160	1.373071
1	-1.920070	1.140588	1.057156
1	-1.480067	1.552123	2.582022
7	-0.036186	0.155566	-1.061294
1	-0.170039	-0.569017	-0.354427
1	0.582814	-0.248891	-1.759210
1	0.506549	0.882402	-0.591999
7	-2.778227	-1.540541	-0.712353
1	-3.026925	-0.600314	-0.405868
1	-3.631203	-2.014402	-0.991288
1	-2.202517	-1.419472	-1.541194
7	-2.750284	1.610581	-1.009341
1	-2.615545	2.602257	-0.834715
1	-1.843327	1.213336	-1.279594
1	-3.380191	1.532044	-1.802168

Cartesian coordinates of : AM8_11

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.727662	-2.666042	-0.493819
1	1.973868	-3.588312	-0.147486
1	1.868688	-2.678434	-1.499918
1	2.397623	-1.995746	-0.100688
7	-0.724526	2.863129	0.084687
1	-1.139475	3.789054	0.048920
1	-1.320575	2.230890	-0.460428
1	-0.778487	2.543394	1.048554
7	-1.500051	-2.215861	-0.888701
1	-1.952093	-3.069583	-1.200155
1	-1.966868	-1.917685	-0.032320

1	-0.530252	-2.442154	-0.662155
7	-2.565253	0.642598	-1.228040
1	-3.014190	0.305718	-0.375178
1	-2.193660	-0.201083	-1.668093
1	-3.287582	1.019247	-1.834212
7	2.219800	2.213116	-0.713310
1	2.865467	2.996370	-0.751290
1	1.288663	2.588643	-0.497185
1	2.165787	1.829978	-1.653431
7	3.331914	-0.340047	0.847885
1	3.058044	0.521502	0.364869
1	4.343298	-0.333690	0.938868
1	2.952159	-0.285604	1.789365
7	0.115485	-0.001765	0.567550
1	-0.437974	0.166374	-0.273047
1	0.836000	0.716517	0.571042
1	0.593934	-0.889154	0.415347
7	-2.642212	-0.506020	1.777293
1	-2.702416	-1.258946	2.456308
1	-1.651303	-0.267283	1.656427
1	-3.108386	0.296228	2.191070

Cartesian coordinates of : AM8_12

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.024094	-0.082053	0.271799
1	-0.758491	-0.598565	-0.209373
1	0.859905	-0.344031	-0.161339
1	-0.177625	0.907002	0.082746
7	2.668427	-1.761764	-0.775565
1	3.528176	-2.278816	-0.615222
1	2.588836	-1.640466	-1.781151
1	1.889053	-2.360243	-0.475167
7	0.130962	-3.061316	0.414564
1	0.126754	-2.389755	1.179686
1	-0.714704	-2.867999	-0.128174
1	0.041307	-3.990879	0.812011
7	1.513926	2.659447	-0.861810
1	1.993812	2.157047	-0.104833
1	1.635287	2.098037	-1.700781
1	2.019049	3.526959	-1.018107
7	-1.529513	3.022600	-0.285058
1	-2.007382	3.283331	-1.142631
1	-1.686443	3.774518	0.379708
1	-0.523700	3.000895	-0.489168
7	-2.569265	-1.953520	-0.950939
1	-2.886958	-1.180293	-0.353819
1	-2.620667	-1.636729	-1.914746
1	-3.240552	-2.710058	-0.856621
7	-2.880870	0.424955	0.992970
1	-2.531278	1.285223	0.560217
1	-3.685318	0.668424	1.562175
1	-2.141843	0.108621	1.617197
7	2.700290	0.738140	1.253959
1	1.859603	0.501368	1.775865
1	3.465338	0.844340	1.911555
1	2.898795	-0.063357	0.650529

Cartesian coordinates of : AM8_13

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.226871	2.517180	0.403103
1	-0.597874	2.976274	0.779701
1	0.858241	3.249951	0.093460

1	-0.070124	1.982748	-0.419829
7	-0.082329	-2.576588	0.379205
1	0.195736	-3.551935	0.401067
1	-0.797788	-2.463851	-0.338015
1	0.726214	-2.017255	0.108724
7	-1.197137	-0.011479	1.773314
1	-0.800715	-0.932867	1.568291
1	-1.355652	0.036922	2.775466
1	-0.482883	0.680753	1.547466
7	-2.889205	-1.492690	-0.634437
1	-3.434286	-0.685027	-0.936719
1	-2.699416	-1.325035	0.353143
1	-3.473849	-2.319400	-0.707970
7	2.018106	-0.167631	0.588896
1	2.995120	-0.080695	0.303489
1	2.006481	-0.636649	1.491241
1	1.648656	0.771325	0.748130
7	-0.332509	0.217419	-1.587544
1	0.478370	-0.122264	-1.065902
1	-0.127957	0.099946	-2.575585
1	-1.113997	-0.406852	-1.371985
7	5.054209	-0.023707	-0.486379
1	4.985662	-0.220359	-1.479777
1	5.524951	0.869399	-0.383226
1	5.653869	-0.732563	-0.076585
7	-3.045033	1.492337	-0.428721
1	-2.294291	1.677764	-1.089010
1	-3.487626	2.371245	-0.183404
1	-2.607658	1.094538	0.405775

Cartesian coordinates of : AM8_14

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	4.589426	0.001180	0.393227
1	4.805910	-0.714555	1.079295
1	5.162782	-0.174652	-0.425318
1	4.876894	0.893112	0.782641
7	-0.683567	1.744095	1.593598
1	-0.560313	2.056721	2.551417
1	-1.534183	1.180908	1.561948
1	0.086219	1.112489	1.365796
7	-0.685960	-1.742099	1.594586
1	-0.562771	-2.053555	2.552795
1	-1.536209	-1.178398	1.562369
1	0.084186	-1.111263	1.365833
7	-0.033115	2.820453	-1.178957
1	0.809751	3.386801	-1.155670
1	-0.724847	3.349282	-1.702039
1	-0.370516	2.723154	-0.214074
7	-3.242564	0.002366	0.702077
1	-3.848036	0.818162	0.719305
1	-3.850377	-0.811652	0.720749
1	-2.748363	0.000865	-0.200729
7	-0.032480	-2.823413	-1.175309
1	-0.723289	-3.352974	-1.698869
1	0.810219	-3.389904	-1.149358
1	-0.371698	-2.724443	-0.211238
7	1.385600	-0.000921	-0.134870
1	1.138883	-0.818475	-0.693260
1	2.399495	-0.000073	-0.014963
1	1.137724	0.815532	-0.694350
7	-1.439455	-0.001796	-1.790487
1	-0.846047	0.823962	-1.694510
1	-0.845901	-0.827236	-1.692753
1	-1.794698	-0.002868	-2.742073

Cartesian coordinates of : AM8_15

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-4.141179	-1.700758	0.300892
1	-4.395261	-0.739535	0.062251
1	-4.553850	-2.317621	-0.391284
1	-4.566635	-1.926851	1.194106
7	-0.121828	2.389553	0.378464
1	-0.374191	2.782317	1.280649
1	-0.367358	3.082429	-0.322473
1	-0.703822	1.561386	0.221965
7	4.358895	-0.210604	0.315689
1	3.788527	0.231994	-0.413964
1	5.043380	0.468316	0.633682
1	4.875468	-0.976631	-0.104523
7	1.556252	-0.121575	1.657863
1	1.323065	0.815381	1.327557
1	1.422946	-0.131445	2.664743
1	2.555885	-0.253869	1.476647
7	-3.813851	1.308039	-0.422120
1	-2.861397	0.955400	-0.306413
1	-3.945218	2.075797	0.228539
1	-3.897790	1.689692	-1.358756
7	1.360333	-2.101059	-0.807073
1	0.728242	-2.893896	-0.747350
1	2.285754	-2.471040	-1.003591
1	1.397281	-1.662468	0.116812
7	-1.235872	-0.489481	0.045808
1	-0.780322	-0.795211	-0.812387
1	-2.038610	-1.104566	0.205671
1	-0.546181	-0.655016	0.780029
7	2.089588	0.863599	-1.463665
1	1.525082	1.453160	-0.851723
1	2.095357	1.290400	-2.384420
1	1.623290	-0.042119	-1.536766

Cartesian coordinates of : AM8_16-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.056623	-0.458051	0.732617
1	-2.798539	-1.445051	0.796115
1	-2.963720	-0.195628	-0.249879
1	-4.037633	-0.378873	0.981957
7	-2.155103	1.124722	-1.995400
1	-3.056719	1.308405	-2.425689
1	-1.452923	1.307067	-2.706518
1	-2.020216	1.806418	-1.240038
7	-1.595085	2.398077	0.729846
1	-2.025426	1.548098	1.099432
1	-0.582743	2.293816	0.802256
1	-1.873772	3.176923	1.317484
7	-1.447593	-3.163531	0.351266
1	-0.695126	-2.517694	0.112365
1	-1.668427	-3.708144	-0.476091
1	-1.095728	-3.806441	1.053132
7	2.450108	-2.239221	-0.181740
1	1.556454	-1.739081	-0.127795
1	2.406023	-2.878699	-0.968887
1	2.542787	-2.804479	0.656485
7	1.732850	2.291639	0.693257
1	2.541379	1.743224	0.375053
1	1.733943	3.160485	0.166143
1	1.903045	2.538388	1.664188
7	4.031276	0.445692	-0.317811
1	3.622285	-0.494593	-0.289348
1	4.313467	0.622936	-1.277262

1	4.881868	0.425606	0.236697
7	-0.033895	-0.380545	0.029517
1	0.588904	0.422573	0.142269
1	-0.637887	-0.161602	-0.765055
1	-0.662843	-0.355135	0.832125

Cartesian coordinates of : AM8_17

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.900429	2.364557	1.540587
1	-0.829409	3.133805	2.198336
1	-0.342837	1.590798	1.899001
1	-0.483965	2.662956	0.657248
7	-0.263177	2.440588	-1.602267
1	0.417879	2.043873	-2.243753
1	-0.684987	3.238632	-2.067410
1	-0.994781	1.736786	-1.462305
7	-0.398276	-1.258886	-2.298627
1	0.277667	-0.800571	-1.673775
1	0.059839	-1.476859	-3.177171
1	-1.134704	-0.582308	-2.481964
7	1.224169	0.128245	-0.069439
1	1.060317	1.125364	-0.194160
1	0.746299	-0.149673	0.789486
1	2.225752	-0.008017	0.070931
7	-0.739684	-0.748779	2.375237
1	-1.592606	-0.221638	2.545091
1	-0.450903	-1.148897	3.262706
1	-0.979741	-1.521681	1.745178
7	-1.259191	-2.905247	0.142774
1	-0.602892	-3.652109	0.352437
1	-2.171926	-3.339859	0.042554
1	-0.996052	-2.523260	-0.774196
7	-2.226092	0.368528	-0.386956
1	-3.166384	-0.009864	-0.449112
1	-2.201909	1.044966	0.379236
1	-1.612769	-0.401885	-0.122745
7	4.431127	-0.327867	0.271229
1	4.966975	0.476006	-0.039057
1	4.699283	-0.522808	1.230201
1	4.712723	-1.121727	-0.294516

Cartesian coordinates of : AM8_18

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.879033	2.034214	0.597814
1	3.571140	2.139214	1.333967
1	2.672424	2.968537	0.257252
1	3.316627	1.506640	-0.164758
7	3.822285	-0.220495	-1.308362
1	3.472165	-0.765319	-0.512465
1	4.799044	-0.459709	-1.447877
1	3.323819	-0.525198	-2.138623
7	2.491931	-1.123023	1.316817
1	1.584391	-1.556083	1.131651
1	2.332814	-0.131432	1.489503
1	2.862172	-1.531684	2.169022
7	0.266850	0.561082	-0.520865
1	0.682361	0.418027	-1.438076
1	0.151108	-0.367893	-0.113427
1	0.978654	1.044333	0.030687
7	-2.352093	-1.168274	-1.283106
1	-1.849374	-0.287257	-1.374017
1	-3.206503	-0.955515	-0.760362

1	-2.625331	-1.464637	-2.214863
7	-2.306467	2.272013	0.072207
1	-2.504478	2.869122	-0.725363
1	-2.078904	2.887319	0.847691
1	-1.458944	1.738608	-0.150131
7	-0.322879	-2.522810	0.574299
1	-0.770438	-2.734839	1.461634
1	-1.066212	-2.227243	-0.072900
1	0.053628	-3.398190	0.221139
7	-4.526078	0.117956	0.538370
1	-4.578554	-0.174616	1.508738
1	-3.879414	0.911416	0.479090
1	-5.450272	0.441764	0.272271

Cartesian coordinates of : AM8_19

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	4.598860	-0.971579	-0.032672
1	4.386745	-1.958614	0.071154
1	5.135529	-0.860736	-0.886584
1	5.197923	-0.703506	0.741324
7	-1.067242	-0.704788	1.647780
1	-0.957259	-0.707957	2.657891
1	-1.444576	-1.616837	1.377120
1	-0.131763	-0.629074	1.242210
7	-0.483955	-1.097985	-1.546221
1	-1.180974	-0.355042	-1.549949
1	0.269240	-0.779016	-0.931284
1	-0.106971	-1.176807	-2.485650
7	-0.155196	2.368844	1.675884
1	-0.631226	3.163300	2.089709
1	-0.000772	2.564857	0.687487
1	-0.774057	1.561517	1.724749
7	-1.908012	-3.299646	0.104385
1	-1.431812	-2.730146	-0.602842
1	-1.380480	-4.157383	0.229938
1	-2.821341	-3.557633	-0.254554
7	-0.060886	2.324840	-1.633315
1	0.322077	1.815657	-2.425027
1	-0.959387	1.892340	-1.399512
1	-0.243755	3.271364	-1.953297
7	1.677452	0.383902	0.310332
1	1.468613	1.128368	-0.355608
1	2.624864	0.045811	0.138018
1	1.664978	0.844207	1.219374
7	-2.646913	1.010844	-0.386537
1	-2.233882	0.456609	0.374852
1	-2.981709	1.877435	0.026762
1	-3.468768	0.510269	-0.713733

Cartesian coordinates of : AM8_20

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.365780	-0.603967	0.484973
1	-0.266741	-0.594744	1.497277
1	0.436441	-1.128757	0.124575
1	-1.211634	-1.146740	0.275325
7	-3.065020	-2.089117	-0.162117
1	-3.776735	-1.351972	-0.127963
1	-3.342069	-2.815393	0.491239
1	-3.098613	-2.501856	-1.089333
7	-4.922013	0.413651	-0.037986
1	-4.109826	1.039001	-0.042108
1	-5.449577	0.592637	0.810588

1	-5.519405	0.669597	-0.817665
7	1.377583	1.830684	-0.552029
1	1.387886	1.873349	-1.567604
1	0.995132	2.713775	-0.226488
1	0.712896	1.096282	-0.290640
7	4.259788	0.423007	-0.691419
1	5.068718	0.801389	-1.172161
1	4.511900	0.238270	0.277761
1	3.533147	1.138705	-0.656028
7	2.278480	-1.926866	-0.785784
1	2.752607	-2.767407	-0.467120
1	1.863897	-2.155543	-1.684954
1	3.002202	-1.216961	-0.950549
7	-2.205990	1.952634	-0.055228
1	-2.008406	2.606977	0.695957
1	-1.570718	1.157617	0.054710
1	-1.960625	2.417014	-0.924456
7	2.765936	-0.064587	1.841269
1	2.407989	-0.869155	1.330048
1	2.403396	-0.100421	2.788102
1	2.377260	0.756271	1.379730

Cartesian coordinates of : AM8_21

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.844304	2.308780	-0.915470
1	-1.199656	3.124902	-1.402112
1	-1.640603	1.757844	-0.582687
1	-0.327116	1.742035	-1.585602
7	-2.620815	0.321583	0.675067
1	-3.515601	-0.164895	0.617182
1	-2.549416	0.730726	1.601774
1	-1.869507	-0.363286	0.588303
7	-0.195331	-1.461387	-0.446723
1	-0.178825	-0.795039	-1.218192
1	0.751850	-1.845909	-0.403545
1	-0.820301	-2.218370	-0.708546
7	1.730358	0.564209	-1.676754
1	2.158396	-0.341919	-1.490256
1	2.342186	1.073930	-2.306451
1	1.716291	1.060021	-0.786371
7	0.776691	1.008783	1.361631
1	0.380215	0.108972	1.082447
1	0.567926	1.142967	2.346654
1	0.259498	1.719776	0.835391
7	2.927305	-2.199558	-0.194124
1	3.366195	-1.394596	0.269111
1	2.817998	-2.927186	0.506908
1	3.585622	-2.557882	-0.879951
7	3.830737	0.469211	1.052762
1	2.860949	0.761111	1.223629
1	4.347913	0.573859	1.920250
1	4.233940	1.122851	0.387991
7	-5.551255	-0.919344	0.139776
1	-6.206158	-0.189026	0.399822
1	-5.919426	-1.799431	0.484987
1	-5.536075	-0.967388	-0.873890

Cartesian coordinates of : AM8_22

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.049612	-0.288495	0.069913
1	2.740271	-1.029147	0.190756
1	1.432867	-0.295018	0.879769

1	2.530909	0.611129	0.072752
7	-0.284484	2.129702	1.396012
1	-1.178820	2.597465	1.515529
1	0.284953	2.391193	2.196751
1	-0.463643	1.120470	1.472605
7	-0.932242	-0.882415	1.183555
1	-0.809692	-0.907451	0.172419
1	-0.515945	-1.729827	1.558181
1	-1.939576	-0.927781	1.362575
7	-0.333679	0.700520	-1.585015
1	-0.177224	1.140394	-2.487434
1	0.537038	0.231627	-1.308423
1	-0.463891	1.445264	-0.900674
7	-4.062820	-0.821911	1.091751
1	-4.696626	-1.581354	1.318344
1	-4.540672	0.044536	1.317112
1	-3.889465	-0.839361	0.081301
7	-2.993822	-0.949328	-1.824728
1	-3.520823	-0.617279	-2.626858
1	-2.728913	-1.909267	-2.026197
1	-2.126934	-0.401651	-1.775764
7	4.299476	-2.630053	0.163065
1	4.368291	-3.288776	0.931596
1	4.121458	-3.160959	-0.683188
1	5.204692	-2.182986	0.060757
7	2.237721	2.779100	-0.436018
1	1.332072	2.682048	0.029004
1	2.546194	3.740432	-0.334256
1	2.095141	2.606459	-1.426399

Cartesian coordinates of : AM8_23

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.437707	-1.664689	0.317387
1	0.793378	-2.592216	0.106625
1	0.476581	-1.554446	1.326360
1	1.086799	-0.984854	-0.086344
7	2.306056	0.649463	-0.844171
1	3.158071	1.114483	-0.519764
1	1.496276	1.163653	-0.484793
1	2.286199	0.738123	-1.856211
7	5.206935	1.229822	0.292469
1	5.177688	0.213592	0.402166
1	5.358163	1.641842	1.207471
1	6.013081	1.463850	-0.277725
7	-2.306056	-0.649461	-0.844173
1	-2.286195	-0.738123	-1.856213
1	-3.158070	-1.114482	-0.519768
1	-1.496276	-1.163647	-0.484792
7	-4.149689	1.696411	0.209029
1	-3.785590	2.188513	1.018710
1	-4.414275	2.397626	-0.475383
1	-3.389749	1.135452	-0.184092
7	4.149687	-1.696413	0.209028
1	3.785589	-2.188516	1.018709
1	3.389747	-1.135452	-0.184091
1	4.414270	-2.397627	-0.475385
7	-5.206933	-1.229825	0.292469
1	-6.013080	-1.463854	-0.277723
1	-5.358158	-1.641846	1.207471
1	-5.177687	-0.213595	0.402167
7	-0.437707	1.664692	0.317386
1	-0.793380	2.592221	0.106632
1	-1.086799	0.984859	-0.086348
1	-0.476579	1.554442	1.326358

Cartesian coordinates of : AM8_24

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.992572	-0.243789	0.837232
1	-2.874095	-0.686295	1.743132
1	-2.300013	-0.649369	0.202762
1	-3.926092	-0.479141	0.500353
7	-0.473199	-0.605356	-0.989713
1	-0.379753	-0.856899	-1.968974
1	0.298668	-1.042784	-0.480301
1	-0.343590	0.402473	-0.920344
7	-1.415342	2.337573	0.287137
1	-2.058083	1.582605	0.559167
1	-1.561889	3.111057	0.929298
1	-1.707389	2.666202	-0.628959
7	-5.973144	-0.776133	-0.338640
1	-5.905234	-1.161447	-1.274866
1	-6.626851	-1.350603	0.182846
1	-6.373582	0.152999	-0.416206
7	4.539153	-0.384328	0.674320
1	4.502634	0.480558	1.205357
1	5.495555	-0.721465	0.713968
1	4.316577	-0.142888	-0.296385
7	1.552923	1.310299	0.744175
1	0.605768	1.689751	0.656533
1	1.476951	0.317426	0.960943
1	1.992937	1.764730	1.538291
7	2.979566	0.395480	-1.830252
1	2.384077	-0.392232	-2.069452
1	2.481903	0.926026	-1.106802
1	3.063509	0.975581	-2.658690
7	1.916836	-2.008035	0.650797
1	2.840062	-1.580371	0.788855
1	2.051989	-2.814199	0.046720
1	1.606393	-2.371693	1.547359

Cartesian coordinates of : AM8_25-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.624617	2.952683	0.151138
1	3.412956	2.311934	0.026063
1	2.633644	3.614166	-0.618533
1	2.783139	3.482600	1.002008
7	4.341166	0.368456	-0.235623
1	4.866299	-0.075462	0.510837
1	3.381126	0.010311	-0.207322
1	4.762437	0.077938	-1.112028
7	-0.905209	-1.312637	2.218687
1	-1.572445	-2.007497	2.541599
1	-0.607580	-0.794911	3.040670
1	-1.411565	-0.658556	1.606241
7	-2.014213	0.638399	0.125961
1	-1.440898	1.475769	0.180849
1	-1.695032	0.116420	-0.692859
1	-2.977730	0.934968	-0.031512
7	0.796741	-2.895037	0.051926
1	0.317925	-2.517171	0.874037
1	1.077508	-3.848935	0.253173
1	1.637258	-2.334603	-0.069307
7	-0.855081	-1.417132	-2.081604
1	-0.292340	-1.342514	-2.924185
1	-0.388480	-2.088719	-1.460155
1	-1.743797	-1.822163	-2.361074
7	1.262342	0.097875	-0.025007
1	0.615818	-0.068302	-0.795088
1	1.389825	1.108248	0.068558

1	0.778400	-0.234728	0.807744
7	-5.120347	1.537631	-0.205924
1	-5.303551	2.400075	0.296381
1	-5.452413	1.660650	-1.156790
1	-5.680611	0.808813	0.223812

Cartesian coordinates of : AM8_26

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-4.515564	1.176821	-0.512081
1	-5.053274	1.141266	0.348834
1	-4.361969	0.207896	-0.813392
1	-5.102781	1.627734	-1.206900
7	-3.680935	-1.741941	-1.139043
1	-3.208421	-1.937346	-2.016076
1	-4.248326	-2.554719	-0.920392
1	-2.963177	-1.647000	-0.409359
7	-1.660777	-0.982785	1.054615
1	-1.621105	0.020275	0.868274
1	-1.998590	-1.091239	2.006547
1	-0.700646	-1.333206	1.038632
7	-1.598850	2.112995	-0.003966
1	-1.558376	3.085301	0.288372
1	-2.584166	1.892588	-0.194700
1	-1.102385	2.055360	-0.889164
7	1.363251	-2.092851	0.770772
1	2.002527	-2.434416	1.482730
1	1.036923	-2.909014	0.260750
1	1.912726	-1.519282	0.117760
7	2.825091	0.067190	-0.870400
1	2.460533	0.321356	-1.783115
1	3.835900	0.202848	-0.896445
1	2.424847	0.713061	-0.185758
7	1.086524	1.110264	1.508057
1	1.011458	0.102050	1.638423
1	0.170893	1.432500	1.191277
1	1.260530	1.527201	2.417039
7	6.056117	0.354170	-0.814003
1	6.514118	0.921857	-1.519212
1	6.308397	0.730824	0.093869
1	6.440363	-0.582936	-0.875648

Cartesian coordinates of : AM8_27

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.261650	2.412168	-0.755983
1	1.834072	3.250122	-0.791710
1	1.129254	2.105062	-1.715056
1	1.807980	1.683787	-0.276632
7	-1.261723	-2.411758	0.756619
1	-1.808032	-1.683524	0.277018
1	-1.129273	-2.104300	1.715571
1	-1.834180	-3.249673	0.792678
7	-2.793670	-0.137759	-0.675520
1	-2.540838	-0.096975	-1.658301
1	-2.439775	0.719226	-0.240265
1	-3.812216	-0.117225	-0.623238
7	-1.489078	2.409259	0.719344
1	-1.908518	3.333080	0.680956
1	-0.583541	2.461503	0.238543
1	-1.297952	2.212544	1.697149
7	1.488909	-2.409281	-0.718889
1	1.908299	-3.333121	-0.680397
1	1.297695	-2.212711	-1.696705

1	0.583416	-2.461400	-0.237992
7	2.793858	0.137877	0.675431
1	2.541495	0.097059	1.658331
1	3.812380	0.117377	0.622673
1	2.439799	-0.719117	0.240328
7	5.984126	0.030493	0.063981
1	6.125371	0.796344	-0.586377
1	6.061215	-0.836267	-0.458009
1	6.741461	0.053467	0.738426
7	-5.984094	-0.030960	-0.064983
1	-6.124886	-0.796962	0.585294
1	-6.741448	-0.054271	-0.739394
1	-6.061634	0.835698	0.457110

Cartesian coordinates of ammonia nanomer: (NH₃)₉

Cartesian coordinates of : AM9_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.145520	0.940525	-0.726905
1	-4.016899	1.235678	-0.294523
1	-3.282025	1.035290	-1.730301
1	-2.427228	1.627576	-0.458710
7	2.892620	-1.309894	-1.115717
1	2.124181	-0.884845	-1.637171
1	3.656385	-1.506120	-1.753786
1	3.206490	-0.605293	-0.452469
7	0.148215	0.022869	-1.247505
1	0.501212	0.104893	-0.292760
1	-0.542952	-0.726445	-1.222861
1	-0.365109	0.885833	-1.414581
7	-2.342546	-2.132498	-0.669935
1	-2.692106	-2.610585	-1.495186
1	-2.718625	-1.179063	-0.676889
1	-2.741404	-2.605097	0.136671
7	-1.178680	-0.146588	1.820986
1	-1.837798	-0.023531	1.052232
1	-1.718983	-0.339545	2.659203
1	-0.629958	-0.982798	1.605049
7	-0.852422	2.681956	0.388809
1	-0.735747	1.986485	1.127775
1	-1.097022	3.563282	0.830428
1	0.065330	2.804493	-0.049841
7	2.041257	2.309422	-0.757827
1	1.962054	1.752587	-1.604742
1	2.218265	1.656702	0.009861
1	2.847207	2.917928	-0.855965
7	0.615821	-2.546352	0.599659
1	0.706230	-3.449088	1.056203
1	1.425260	-2.432210	-0.017977
1	-0.220437	-2.583748	0.013358
7	1.936363	0.215455	1.645558
1	1.104774	0.615955	2.078141
1	2.691833	0.269381	2.322478
1	1.711316	-0.771977	1.506503

Cartesian coordinates of : AM9_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.098187	0.004583	-1.315994
1	0.485745	-0.829445	-1.367739
1	-0.478752	0.012078	-0.369434
1	0.533080	0.804143	-1.363484

7	-1.846393	-0.002459	1.619954
1	-2.426557	-0.004003	2.453633
1	-1.245293	0.822864	1.667315
1	-1.240763	-0.824592	1.667197
7	-0.049595	-2.581232	0.758108
1	-0.898670	-2.611815	0.183468
1	0.744136	-2.648382	0.117852
1	-0.043967	-3.420292	1.331107
7	-2.534520	-1.832795	-0.921481
1	-3.396205	-2.188216	-1.321445
1	-2.041353	-1.302035	-1.637209
1	-2.766438	-1.169879	-0.182362
7	1.685719	-0.002395	1.571272
1	1.075544	0.817561	1.506549
1	1.077594	-0.823579	1.501249
1	2.084887	-0.005338	2.505813
7	2.657689	1.840582	-0.804326
1	3.324289	2.557260	-0.532811
1	3.015087	1.418152	-1.655873
1	2.646277	1.128685	-0.070490
7	-2.540701	1.842887	-0.915818
1	-2.029920	1.318882	-1.624417
1	-3.397595	2.193807	-1.329720
1	-2.781003	1.175353	-0.183775
7	-0.049567	2.574869	0.750486
1	-0.906574	2.612960	0.188054
1	-0.024366	3.417249	1.318065
1	0.734348	2.628330	0.097295
7	2.640091	-1.847703	-0.817695
1	3.370181	-2.510417	-0.574451
1	2.621751	-1.122135	-0.097694
1	2.912781	-1.421547	-1.698230

Cartesian coordinates of : AM9_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.974654	-0.900144	-1.300204
1	-3.706876	-1.592561	-1.415959
1	-2.805034	-0.767671	-0.300614
1	-2.116630	-1.269183	-1.699822
7	-1.876603	-0.185191	1.671412
1	-1.465635	-1.116341	1.587062
1	-2.256915	-0.105681	2.610032
1	-1.104353	0.481545	1.599896
7	0.308646	2.166398	0.990576
1	-0.469950	2.352977	0.354570
1	0.342557	2.927024	1.662949
1	1.171339	2.201754	0.438416
7	-2.495522	2.000350	-0.574031
1	-2.755636	1.560321	0.308216
1	-2.893931	1.392417	-1.290078
1	-2.955145	2.903601	-0.632553
7	2.949534	1.722777	-0.701315
1	3.032850	2.281374	-1.545591
1	3.740609	1.962668	-0.110753
1	3.060559	0.738818	-0.966585
7	2.819436	-1.366271	-1.009483
1	2.048436	-1.754897	-1.545139
1	2.510174	-1.294675	-0.032778
1	3.592761	-2.021340	-1.060268
7	-0.424945	-2.653160	0.379095
1	-0.258698	-1.881559	-0.277804
1	-1.210654	-3.195920	0.032489
1	0.391290	-3.258273	0.361968
7	1.595768	-0.715284	1.753990
1	0.824780	-1.373896	1.852267
1	1.181305	0.213577	1.647360
1	2.115128	-0.716191	2.626515

7	0.039070	-0.027395	-1.242693
1	0.270714	0.110123	-2.223805
1	0.849898	0.300380	-0.718013
1	-0.718047	0.627041	-1.033405

Cartesian coordinates of : AM9_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.259040	-0.011895	-0.006340
1	3.611068	-0.910226	0.313321
1	4.060663	0.607902	-0.079841
1	2.649220	0.355624	0.729391
7	-1.681639	0.212419	-1.874446
1	-2.179905	0.184359	-2.759166
1	-1.951810	-0.620786	-1.347058
1	-2.015828	1.032471	-1.359890
7	1.001491	-1.521412	-1.659497
1	0.268600	-0.846073	-1.890704
1	1.248313	-2.007477	-2.516711
1	1.823773	-0.989930	-1.366457
7	-1.703384	-2.588196	-0.332933
1	-1.482933	-2.716065	0.652051
1	-0.803496	-2.588207	-0.815710
1	-2.231848	-3.398183	-0.641446
7	0.997369	1.944697	-1.338462
1	1.140711	2.648392	-2.056710
1	0.206490	1.366761	-1.634933
1	1.819157	1.341199	-1.335000
7	1.010554	1.371821	1.727205
1	0.997944	1.857055	0.825968
1	1.241940	2.054670	2.442715
1	0.048352	1.072154	1.895036
7	-1.871770	-0.137452	1.813038
1	-1.144181	-0.838569	1.975679
1	-2.522422	-0.174779	2.592258
1	-2.372143	-0.464441	0.988062
7	0.750887	-1.817986	1.562680
1	1.168244	-0.930181	1.842219
1	1.283082	-2.568389	1.991811
1	0.865913	-1.891134	0.549239
7	-1.856100	2.584499	0.088565
1	-1.833296	1.911588	0.856140
1	-2.348264	3.413271	0.404766
1	-0.892478	2.843530	-0.113701

Cartesian coordinates of : AM9_5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.396000	3.249617	-0.151880
1	0.552681	3.730622	-1.033248
1	0.390858	3.964738	0.569927
1	-0.546833	2.847103	-0.191536
7	-0.660161	-0.062130	1.517360
1	-0.986758	0.798954	1.077017
1	-1.139457	-0.127153	2.411367
1	-1.018986	-0.817694	0.931606
7	0.539867	0.191200	-1.438924
1	0.849089	1.036382	-0.956959
1	0.850583	-0.592705	-0.863928
1	1.067916	0.134877	-2.305632
7	-2.187496	1.630275	-0.755414
1	-2.888842	1.038270	-0.300975
1	-2.672716	2.186732	-1.453435
1	-1.538811	1.011779	-1.247642

7	2.279058	1.078507	1.275882
1	1.433980	0.585952	1.575105
1	2.798883	1.338784	2.108618
1	1.942630	1.936922	0.836803
7	1.305782	-2.443947	0.491991
1	2.203122	-2.182939	0.071796
1	1.118179	-1.765714	1.229187
1	1.423003	-3.350609	0.934343
7	3.723877	-0.876579	-0.637772
1	3.345133	-0.125807	-0.046979
1	4.683870	-1.044614	-0.352964
1	3.753809	-0.539165	-1.594784
7	-3.886347	-0.660589	0.572295
1	-4.789645	-0.985807	0.242437
1	-3.896117	-0.728108	1.585068
1	-3.169187	-1.300371	0.218612
7	-1.503074	-2.147334	-0.871072
1	-0.589782	-2.475823	-0.540210
1	-1.298774	-1.387469	-1.518625
1	-1.930370	-2.900285	-1.402233

Cartesian coordinates of : AM9_6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.035612	-2.151585	-1.470471
1	-1.670437	-1.359372	-1.558995
1	-1.546905	-2.999918	-1.688514
1	-0.731947	-2.191530	-0.496129
7	2.194647	0.728057	1.235244
1	2.745523	0.979593	2.050876
1	2.672473	-0.050963	0.774794
1	2.194691	1.537283	0.606861
7	1.157544	2.964695	-0.673042
1	0.992962	2.318504	-1.444206
1	1.326936	3.887711	-1.058518
1	0.291924	2.996012	-0.136557
7	-0.031112	-1.567803	1.539832
1	0.125211	-2.183542	2.333096
1	0.606783	-0.774756	1.643177
1	-0.985935	-1.211850	1.619994
7	-0.884270	1.760007	1.491651
1	-1.525814	0.993723	1.695452
1	0.063425	1.377450	1.532660
1	-0.967350	2.432663	2.248409
7	2.648937	-2.143008	-0.052666
1	2.713355	-2.309765	-1.052437
1	3.145322	-2.901025	0.406308
1	1.662143	-2.222165	0.199401
7	0.979372	0.073678	-1.738841
1	1.976347	0.096574	-1.938054
1	0.607144	-0.812967	-2.083713
1	0.899744	0.017723	-0.722190
7	-3.012332	-0.667197	0.974436
1	-3.232908	-1.641512	0.786092
1	-2.813069	-0.220987	0.073325
1	-3.856458	-0.243231	1.348648
7	-1.933048	1.053816	-1.399544
1	-2.540848	1.608803	-1.994334
1	-1.058654	0.900500	-1.904488
1	-1.682542	1.622427	-0.587151

Cartesian coordinates of : AM9_7

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
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7	3.000502	-1.694948	-0.017674
1	2.666706	-0.949318	-0.637315
1	3.930154	-1.437003	0.299829
1	3.102890	-2.539138	-0.573217
7	-0.762187	-1.576243	-1.888343
1	-0.469999	-2.315616	-2.520690
1	-1.778662	-1.544351	-1.913023
1	-0.505817	-1.859346	-0.935924
7	1.601531	0.559689	-1.724888
1	1.271256	1.495525	-1.470286
1	0.779182	-0.027106	-1.889759
1	2.092719	0.645413	-2.610121
7	-2.111493	1.215573	-1.128218
1	-2.654424	0.451104	-0.716703
1	-1.418271	0.759159	-1.720095
1	-2.730186	1.742264	-1.737941
7	0.062134	-2.027412	1.088271
1	1.068959	-1.952768	0.924086
1	-0.261732	-1.144329	1.486222
1	-0.076343	-2.741977	1.796935
7	1.951995	0.914748	1.504478
1	2.678809	1.571300	1.774591
1	2.229820	-0.000122	1.852516
1	1.969951	0.843390	0.485250
7	0.355240	3.053794	-0.327276
1	0.614339	2.849855	0.635032
1	0.313088	4.062204	-0.432175
1	-0.583888	2.676758	-0.469453
7	-1.157143	0.885401	1.943109
1	-1.586147	1.428562	2.686211
1	-0.144748	1.026764	1.997474
1	-1.464525	1.280233	1.053076
7	-2.978081	-1.305126	0.554031
1	-2.369644	-2.110274	0.424445
1	-3.872328	-1.641387	0.896758
1	-2.538637	-0.748131	1.289844

Cartesian coordinates of : AM9_8

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.315756	0.589631	1.843106
1	-1.804821	0.474376	2.725957
1	-1.339302	-0.311386	1.365434
1	-1.858973	1.238173	1.266109
7	-0.376336	0.093195	-1.683773
1	-0.570707	0.139613	-2.680104
1	-1.198395	-0.319021	-1.243724
1	0.406970	-0.554778	-1.559434
7	2.203709	-1.722303	-1.159709
1	2.148673	-2.208516	-0.267921
1	2.703558	-2.321517	-1.809437
1	2.781816	-0.894579	-0.988079
7	1.568701	-0.644884	1.738860
1	2.133836	-0.786301	2.570768
1	0.820836	0.009388	1.978129
1	2.157812	-0.174081	1.052838
7	3.616107	1.015906	-0.323455
1	4.004060	1.353551	-1.199789
1	2.801994	1.604391	-0.100517
1	4.322901	1.177656	0.388008
7	0.889843	2.279180	0.173341
1	0.370597	2.075528	1.026577
1	0.698289	3.247733	-0.065927
1	0.461556	1.686847	-0.545547
7	-2.647835	2.020062	-0.567649
1	-1.752594	2.083411	-1.046504
1	-3.039213	1.108835	-0.809896
1	-3.256804	2.746281	-0.929183

7	-0.603432	-2.444157	0.412872
1	0.157274	-1.968473	0.913204
1	-0.245854	-2.613179	-0.525517
1	-0.732855	-3.351550	0.851816
7	-3.317119	-1.084354	-0.396018
1	-2.527479	-1.639190	-0.051163
1	-3.883497	-1.683708	-0.988670
1	-3.884850	-0.835432	0.409551

Cartesian coordinates of : AM9_9

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.328523	0.713165	1.118279
1	-1.394984	0.920949	1.480007
1	-2.474948	-0.295652	1.210713
1	-3.000783	1.168544	1.729082
7	-1.602264	-0.717905	-1.654967
1	-2.076878	-0.030758	-1.068433
1	-2.101972	-0.786456	-2.535987
1	-0.665076	-0.352068	-1.847210
7	1.162531	0.749709	-1.562667
1	1.854004	0.978087	-2.271704
1	0.625959	1.598481	-1.377486
1	1.688619	0.531189	-0.716292
7	-1.271306	2.739264	-1.058068
1	-1.614975	3.681393	-0.896266
1	-1.800741	2.103872	-0.453347
1	-1.505653	2.503072	-2.018725
7	3.259660	0.214730	1.055977
1	4.162478	0.612886	1.295843
1	2.960869	-0.358114	1.841726
1	3.396455	-0.438868	0.279088
7	2.614443	-1.959059	-0.998337
1	2.096402	-1.634709	-1.810879
1	1.924199	-2.070443	-0.250384
1	3.002462	-2.870047	-1.219817
7	0.643912	1.949127	1.450421
1	1.602124	1.639660	1.266908
1	0.312173	2.453529	0.628423
1	0.678410	2.607749	2.222694
7	-2.708406	-2.458199	0.688198
1	-2.315511	-2.196943	-0.220015
1	-2.229167	-3.295432	1.005804
1	-3.680925	-2.712886	0.545317
7	0.317248	-1.299462	0.976702
1	-0.285783	-1.687952	1.697811
1	-0.255568	-1.260742	0.132712
1	0.487749	-0.327921	1.241640

Cartesian coordinates of : AM9_10

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.607033	0.108641	1.751908
1	2.048642	0.342416	2.636238
1	1.836362	0.850836	1.088983
1	0.594671	0.135550	1.897836
7	2.218205	1.830408	-0.985258
1	2.934695	2.518857	-1.194721
1	2.641838	0.902248	-1.076463
1	1.517678	1.883752	-1.722903
7	0.469063	-2.752082	0.379904
1	0.506470	-3.529731	1.031242
1	-0.501456	-2.625581	0.093844
1	0.770948	-1.913488	0.877875

7	2.985571	-1.279664	-0.722523
1	3.945041	-1.552816	-0.910794
1	2.394723	-2.100420	-0.859054
1	2.897584	-1.062562	0.271105
7	-0.399672	2.762078	0.712636
1	-0.432425	3.716899	1.056347
1	0.526917	2.613884	0.307564
1	-0.477278	2.140616	1.515295
7	-1.558754	-0.069909	1.753685
1	-2.070232	0.400995	1.004624
1	-2.124384	-0.015330	2.595843
1	-1.514749	-1.050397	1.481419
7	-2.591380	1.323035	-1.010909
1	-2.021211	1.053794	-1.812349
1	-3.422832	1.791211	-1.358160
1	-2.023586	2.016771	-0.512346
7	-0.008554	-0.076544	-1.371252
1	-0.619784	-0.873056	-1.204067
1	-0.063273	0.491227	-0.525859
1	0.939058	-0.452302	-1.399457
7	-2.630232	-1.878886	-0.641487
1	-2.728105	-2.264859	-1.576790
1	-2.841037	-0.878226	-0.699923
1	-3.353240	-2.309826	-0.072263

Cartesian coordinates of : AM9_11

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.946668	2.085376	-1.326171
1	1.046381	2.703501	-2.125814
1	1.053080	1.124676	-1.659026
1	1.723231	2.275855	-0.687698
7	0.291419	-0.971035	-1.925221
1	0.374780	-1.440932	-2.822175
1	-0.610301	-0.486415	-1.913888
1	0.234068	-1.700064	-1.215185
7	-2.007552	-1.608988	0.345134
1	-1.513500	-0.896116	0.886955
1	-2.302892	-1.128521	-0.504527
1	-2.849995	-1.859835	0.854293
7	-0.040475	0.680159	1.323415
1	0.231873	1.217819	2.142826
1	0.023617	1.316761	0.524688
1	0.706835	-0.002180	1.176397
7	0.431094	-3.463284	0.443974
1	-0.493982	-3.019392	0.395340
1	0.436026	-4.247798	-0.201131
1	0.533751	-3.851659	1.377092
7	2.534430	-1.075890	0.239930
1	2.283853	-0.760189	-0.697315
1	3.515486	-1.340600	0.224932
1	1.992853	-1.933925	0.382306
7	3.087604	1.941934	0.977785
1	4.093873	2.054660	0.904066
1	2.808273	2.339038	1.869154
1	2.883811	0.939646	0.998081
7	-2.107532	1.057363	-1.549293
1	-1.274411	1.636960	-1.423556
1	-2.705716	1.228935	-0.737602
1	-2.596770	1.405659	-2.368481
7	-3.174641	1.396014	1.383862
1	-3.293527	2.303056	1.823527
1	-2.219660	1.079049	1.558817
1	-3.808139	0.750461	1.844022

Cartesian coordinates of : AM9_12

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	4.110781	-0.126938	-0.237634
1	4.938151	0.025723	-0.805685
1	4.416478	-0.176291	0.729399
1	3.505305	0.692798	-0.331106
7	1.831908	2.009633	-0.787711
1	1.049480	2.423090	-0.268021
1	1.408635	1.346198	-1.436587
1	2.259056	2.748544	-1.338393
7	-0.685500	2.478849	1.027687
1	-1.602988	2.292044	0.612964
1	-0.794047	3.246690	1.683041
1	-0.419430	1.651744	1.561230
7	1.702412	-2.042816	-0.865949
1	1.110357	-1.376670	-1.365912
1	1.806703	-2.865236	-1.452507
1	2.625827	-1.610464	-0.773064
7	-0.820048	-2.378274	1.078196
1	-0.868882	-3.186942	1.690842
1	-0.626802	-1.565969	1.661946
1	0.011099	-2.489015	0.490225
7	-3.418146	1.605495	-0.390299
1	-4.223173	1.890374	0.159958
1	-3.587715	1.929171	-1.338435
1	-3.412893	0.580740	-0.416159
7	1.303531	-0.034992	1.595743
1	1.739693	0.741956	1.096789
1	1.690396	-0.056228	2.534815
1	1.606332	-0.885756	1.118061
7	-0.554658	0.089101	-1.080328
1	-0.960272	1.015298	-1.201541
1	-1.340460	-0.557558	-1.121197
1	-0.237757	0.063771	-0.109136
7	-3.428620	-1.597038	-0.398090
1	-4.250750	-1.798158	0.164197
1	-2.611651	-1.956440	0.111957
1	-3.522320	-2.144543	-1.248987

Cartesian coordinates of : AM9_13-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.437025	0.167545	-1.773195
1	-2.751800	0.799152	-1.031960
1	-1.581278	0.582499	-2.140190
1	-3.129293	0.173031	-2.515699
7	0.000025	-1.858864	-0.928802
1	-0.000051	-2.668463	-1.544334
1	0.817212	-1.302785	-1.187835
1	-0.817056	-1.302632	-1.187845
7	-2.725470	1.498824	1.038131
1	-1.784365	1.736437	1.343675
1	-2.866044	0.524549	1.309740
1	-3.380397	2.074920	1.556727
7	-2.578972	-1.707951	0.808352
1	-3.373981	-2.268258	1.098595
1	-1.773808	-2.325234	0.718855
1	-2.757920	-1.350533	-0.131988
7	2.725322	1.498946	1.038134
1	2.865919	0.524667	1.309718
1	3.380199	2.075051	1.556784
1	1.784191	1.736509	1.343636
7	-0.000046	0.075503	1.706889
1	0.818196	-0.499040	1.498211
1	-0.000027	0.228732	2.712396
1	-0.818282	-0.499063	1.498242

7	2.579060	-1.707893	0.808445
1	3.374062	-2.268185	1.098736
1	2.758037	-1.350505	-0.131900
1	1.773902	-2.325181	0.718946
7	0.000009	1.861181	-0.965980
1	0.819572	2.459407	-0.892477
1	-0.000148	1.267034	-0.131352
1	-0.819384	2.459656	-0.892629
7	2.437102	0.167514	-1.773157
1	3.129320	0.173024	-2.515707
1	2.751885	0.799163	-1.031962
1	1.581309	0.582416	-2.140107

Cartesian coordinates of : AM9_14

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.126754	1.971259	-0.604372
1	1.366432	2.472629	-0.139709
1	2.551283	1.338477	0.071711
1	2.832689	2.652848	-0.864270
7	-1.378544	-1.109125	-1.853993
1	-1.758693	-1.236586	-2.787396
1	-1.485163	-1.990734	-1.356547
1	-0.368632	-0.980423	-1.949048
7	-0.476769	3.456263	0.483183
1	-0.760095	3.837978	1.381085
1	-1.248145	2.869523	0.140726
1	-0.389484	4.245204	-0.151275
7	-2.660964	1.410810	-0.308918
1	-2.884778	0.956783	0.574050
1	-2.230591	0.685295	-0.890157
1	-3.537643	1.679476	-0.745673
7	1.828799	-0.854590	-1.663055
1	1.784523	0.161807	-1.779911
1	2.501226	-0.975763	-0.901520
1	2.244251	-1.246370	-2.503559
7	-2.651135	-1.519011	1.149972
1	-3.159398	-1.317334	0.293151
1	-1.872752	-2.131197	0.894734
1	-3.271643	-2.035019	1.765567
7	0.174150	-2.739899	0.411790
1	0.430348	-2.259209	1.271456
1	0.670057	-2.251965	-0.338141
1	0.535168	-3.687493	0.461302
7	0.076600	0.225597	1.084330
1	-0.829824	-0.143473	1.377684
1	0.042154	1.234093	1.228746
1	0.101493	0.107979	0.070176
7	2.975795	-0.766662	1.293636
1	2.004582	-0.480162	1.466628
1	3.573748	-0.273292	1.949820
1	3.056094	-1.755573	1.512366

Cartesian coordinates of : AM9_15

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.503446	1.644392	1.027264
1	2.889156	2.289055	1.709814
1	3.242959	1.406627	0.369714
1	1.779269	2.136707	0.493949
7	-2.727814	-1.788778	0.665749
1	-3.467378	-2.417302	0.961460
1	-1.910064	-2.348135	0.406532
1	-2.449410	-1.228163	1.467897

7	2.666982	-1.603316	0.928126
1	3.322362	-1.494430	0.157535
1	3.110921	-2.177199	1.638224
1	2.542977	-0.665136	1.312937
7	0.026365	-2.553055	-0.631751
1	0.192822	-3.343826	-1.246207
1	0.894986	-2.357453	-0.125822
1	-0.192557	-1.743540	-1.212244
7	-1.791498	0.016024	-1.655489
1	-2.165571	0.935658	-1.424012
1	-2.316085	-0.646127	-1.072949
1	-2.025922	-0.171403	-2.626201
7	0.048893	2.486988	-0.755590
1	-0.084369	1.707428	-1.398618
1	0.119362	3.333895	-1.312358
1	-0.825732	2.543331	-0.228940
7	-2.720287	1.758744	0.811701
1	-2.027945	1.220627	1.339968
1	-3.126916	2.452964	1.431017
1	-3.461458	1.106309	0.566383
7	-0.296514	-0.030879	1.274831
1	0.520128	0.565873	1.406883
1	0.006652	-0.977471	1.493790
1	-0.503034	-0.030241	0.274065
7	2.305256	0.034469	-1.568196
1	1.643190	0.057522	-0.793138
1	2.057515	-0.770828	-2.136651
1	2.130341	0.863138	-2.129547

Cartesian coordinates of : AM9_16

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.863987	1.841583	0.173140
1	3.946283	0.844277	0.388273
1	4.401634	2.030006	-0.666703
1	4.294288	2.364034	0.929187
7	-1.537803	1.561626	1.574078
1	-1.524568	2.009301	2.484809
1	-2.102698	0.715519	1.652383
1	-0.585789	1.271021	1.350476
7	-0.516996	-1.740806	0.983628
1	-0.059403	-2.255068	1.730872
1	-1.467275	-1.531176	1.292807
1	-0.028718	-0.847474	0.875967
7	-1.582103	2.518453	-1.338143
1	-1.029890	3.363010	-1.456012
1	-2.468994	2.680289	-1.806339
1	-1.770906	2.406729	-0.335439
7	-3.620059	-0.819220	1.023105
1	-4.343543	-0.138108	1.234959
1	-4.046307	-1.736687	1.116071
1	-3.355133	-0.700909	0.038907
7	1.316255	-2.347059	-1.446508
1	0.922218	-1.961459	-2.300353
1	1.647636	-3.280145	-1.671891
1	0.557698	-2.433522	-0.764750
7	0.951118	0.744606	-0.280423
1	1.323495	-0.016727	-0.848267
1	1.741591	1.372276	-0.108729
1	0.276565	1.245184	-0.860453
7	-2.009981	-0.604913	-1.578326
1	-1.652257	0.348966	-1.649111
1	-1.338597	-1.164571	-1.055288
1	-2.082451	-0.986880	-2.515543
7	3.145055	-1.090877	0.890097
1	2.741246	-1.538128	0.064531
1	2.368190	-0.691295	1.411042
1	3.569377	-1.812209	1.464063

 Cartesian coordinates of : AM9_17

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.370922	-1.047123	1.032861
1	-2.952500	-1.556649	1.691274
1	-2.102345	-1.686478	0.280230
1	-2.953738	-0.340638	0.588749
7	-0.844275	-2.590059	-1.238937
1	-1.105546	-3.492405	-1.624079
1	-0.251770	-2.750754	-0.420400
1	-0.233397	-2.126053	-1.911687
7	1.627622	-0.875691	-1.439908
1	1.125405	-0.264057	-0.793080
1	1.874096	-1.695836	-0.889665
1	2.494650	-0.397468	-1.669231
7	0.031362	1.082301	0.710477
1	0.816818	0.978886	1.351667
1	-0.641734	0.344723	0.935066
1	-0.460428	1.952274	0.920551
7	2.325696	2.199374	-1.090487
1	2.457635	3.194148	-0.934743
1	2.342058	2.054980	-2.095936
1	1.390784	1.952343	-0.757660
7	3.127362	0.235303	1.297943
1	3.725421	-0.536312	1.014193
1	3.621363	0.726342	2.037817
1	3.064112	0.869940	0.496229
7	-1.998013	0.498675	-1.589717
1	-1.932036	-0.518982	-1.635403
1	-2.163034	0.829860	-2.535596
1	-1.069415	0.816550	-1.310618
7	-2.667908	2.517536	0.778072
1	-2.955739	1.992389	1.598534
1	-2.708443	1.890470	-0.028758
1	-3.345187	3.259928	0.638555
7	0.735687	-2.014512	1.482145
1	-0.178455	-1.612039	1.690889
1	1.421546	-1.257762	1.537376
1	0.953591	-2.668035	2.228575

 Cartesian coordinates of : AM9_18

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.949811	2.650066	0.124922
1	1.201602	2.649580	1.110089
1	1.201552	3.559362	-0.250603
1	1.553791	1.946661	-0.314055
7	2.383430	0.010107	-0.539450
1	1.894988	-0.152540	0.345475
1	3.366585	-0.238081	-0.431698
1	1.970719	-0.614145	-1.226524
7	0.332295	-0.150884	1.867349
1	-0.006265	-1.091441	1.664882
1	-0.429787	0.487958	1.631289
1	0.474338	-0.091153	2.871291
7	-2.031727	1.796573	0.688893
1	-2.576648	2.471217	1.217444
1	-2.575482	1.543358	-0.137122
1	-1.179298	2.266750	0.369997
7	-2.867987	-1.307186	1.059638
1	-2.046327	-1.889263	0.891304
1	-3.335845	-1.671869	1.883386
1	-2.526747	-0.370732	1.282510

7	-0.124450	-2.654583	0.020059
1	-0.442383	-3.496354	-0.450879
1	-0.228385	-1.866400	-0.631536
1	0.868989	-2.771942	0.201035
7	-3.791396	0.079481	-1.484890
1	-4.680852	0.557716	-1.375684
1	-3.852948	-0.454283	-2.347024
1	-3.693905	-0.584363	-0.707304
7	5.586120	-0.431885	-0.274452
1	5.902322	-0.459393	0.689298
1	6.060233	-1.176951	-0.773916
1	5.892325	0.449686	-0.673236
7	-0.564479	-0.005577	-1.484124
1	-1.568011	0.173896	-1.541925
1	-0.157193	0.294711	-2.365725
1	-0.188695	0.625230	-0.776382

Cartesian coordinates of : AM9_19

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.903192	1.767146	0.888328
1	4.258525	0.967655	0.359185
1	4.237219	2.615376	0.442646
1	4.312775	1.736173	1.816371
7	0.659258	-2.805877	0.193317
1	1.028886	-3.280690	1.011775
1	0.970416	-3.330845	-0.618569
1	1.085514	-1.874531	0.151509
7	-4.081023	-0.231702	0.077086
1	-3.360371	-0.582183	-0.567616
1	-4.622331	-1.027956	0.400814
1	-4.716325	0.355292	-0.455809
7	-2.038011	2.079184	0.883043
1	-2.276475	2.908656	1.417011
1	-2.867885	1.487249	0.821980
1	-1.359537	1.544295	1.421626
7	3.964492	-0.906324	-0.719510
1	2.978913	-0.748195	-0.495636
1	4.236024	-1.801563	-0.325843
1	4.050137	-0.982277	-1.727957
7	-0.661773	1.926480	-1.859343
1	0.080468	2.613680	-1.955870
1	-1.298884	2.074664	-2.636767
1	-1.170804	2.138840	-0.991762
7	1.187060	0.241168	0.241015
1	0.741808	0.668937	-0.571276
1	1.863599	0.915138	0.607921
1	0.446372	0.112666	0.933812
7	-1.581902	-1.114741	-1.470509
1	-1.012365	-1.726357	-0.885834
1	-1.636694	-1.549648	-2.386882
1	-1.074833	-0.234912	-1.587269
7	-1.361320	-0.886083	1.808152
1	-2.258257	-0.645770	1.386260
1	-1.534032	-1.097947	2.786133
1	-1.031661	-1.740512	1.359002

Cartesian coordinates of : AM9_20

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.109220	0.438655	1.743366
1	-2.098206	-0.537808	1.444164
1	-2.857048	0.873741	1.206081
1	-2.382520	0.461946	2.721146

7	-1.960846	0.692255	-1.651381
1	-2.904320	0.676771	-1.260914
1	-2.048720	0.888986	-2.643998
1	-1.469528	1.486082	-1.226802
7	-0.376030	2.701382	0.152901
1	-0.749729	2.126295	0.908654
1	0.627402	2.522442	0.098022
1	-0.508611	3.676242	0.402143
7	-1.803943	-2.079268	-0.197385
1	-0.855039	-2.205001	0.151035
1	-1.742250	-1.334522	-0.900034
1	-2.064176	-2.940941	-0.668183
7	2.586958	-2.687889	0.049597
1	1.832677	-1.995452	0.129591
1	2.420246	-3.240430	-0.785473
1	2.526691	-3.317981	0.843076
7	2.875747	2.125653	-0.206801
1	3.537184	1.341644	-0.148447
1	2.905800	2.473846	-1.160996
1	3.234996	2.866893	0.387875
7	4.706372	-0.391242	0.013969
1	4.087971	-1.210025	0.010748
1	5.375364	-0.515382	-0.740174
1	5.236733	-0.420934	0.879831
7	0.676333	-0.288349	0.196506
1	1.448533	0.380000	0.177732
1	0.110648	-0.076891	-0.626726
1	0.086643	-0.013447	0.982010
7	-4.545005	-0.456885	-0.114470
1	-3.834998	-1.165705	0.078450
1	-5.131001	-0.799883	-0.869784
1	-5.137307	-0.380676	0.706864

 Cartesian coordinates of : AM9_21

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.416645	-0.561874	1.898249
1	-0.435534	-1.077839	1.670857
1	0.569788	-0.670727	2.896623
1	0.198512	0.421611	1.735326
7	0.429012	2.401076	0.358269
1	0.882964	3.066158	0.978442
1	0.033880	2.945978	-0.404176
1	1.166862	1.804050	-0.039719
7	-2.371721	-1.735443	0.646985
1	-2.450520	-1.696643	-0.367144
1	-2.513439	-0.772257	0.976172
1	-3.137344	-2.303032	0.997206
7	-2.495999	1.307118	1.234398
1	-3.066938	1.486741	0.405064
1	-1.597767	1.774436	1.104648
1	-2.954734	1.732562	2.033568
7	2.398943	0.183650	-0.447065
1	2.028343	-0.247920	0.401664
1	2.123226	-0.424878	-1.213256
1	3.418298	0.186134	-0.401333
7	-3.817251	0.811283	-1.523869
1	-4.135353	1.225243	-2.394104
1	-2.886842	0.410242	-1.679656
1	-4.452112	0.049872	-1.303577
7	-0.826747	-0.074665	-1.424319
1	-0.266934	0.488104	-2.060669
1	-0.355527	-0.980984	-1.352408
1	-0.717280	0.361067	-0.507755
7	5.639660	0.363672	-0.372531
1	5.867783	1.285071	-0.731406
1	6.119973	-0.318237	-0.950425
1	6.024556	0.295519	0.563901

7	0.486358	-2.730088	-0.387574
1	1.125053	-2.324491	0.292714
1	0.811843	-3.663164	-0.617195
1	-0.413063	-2.805728	0.088832

Cartesian coordinates of : AM9_22

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-5.333626	-0.372811	-0.010106
1	-5.636126	-0.149239	0.932402
1	-5.899226	0.173683	-0.651363
1	-5.546447	-1.351577	-0.173806
7	0.679940	-0.141118	-1.485218
1	0.428223	-0.718801	-0.683261
1	0.265381	0.773937	-1.315465
1	1.688277	-0.021394	-1.421740
7	3.091396	-0.472436	0.728976
1	2.994569	-1.273255	0.097044
1	3.879147	-0.662235	1.341284
1	2.249460	-0.451105	1.306494
7	-0.271753	-2.285257	1.002659
1	-0.616834	-3.127354	1.452469
1	0.206818	-1.723551	1.704393
1	-1.076775	-1.726804	0.711325
7	0.299819	0.667883	1.789724
1	-0.562608	0.479048	1.274642
1	0.833961	1.329154	1.226050
1	0.045798	1.137590	2.653697
7	-0.657424	2.867850	-0.518092
1	-1.083121	3.283152	0.305873
1	0.353977	2.843567	-0.355360
1	-0.832337	3.499886	-1.293717
7	-2.127384	-0.024004	-0.348828
1	-1.861967	0.952032	-0.498095
1	-3.142189	-0.070041	-0.248571
1	-1.881154	-0.508831	-1.209811
7	2.468353	2.417804	-0.145414
1	3.011202	3.073857	0.409728
1	2.721244	2.590638	-1.115460
1	2.809317	1.473048	0.083572
7	2.042947	-2.782149	-1.121260
1	2.371810	-3.723123	-1.310245
1	1.685527	-2.394427	-1.990772
1	1.248200	-2.838189	-0.478394

Cartesian coordinates of : AM9_23

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.392275	-2.422338	-1.735244
1	-0.544411	-3.398313	-1.971123
1	0.318225	-2.379877	-0.999671
1	-0.014445	-1.971297	-2.562924
7	1.095711	-1.860470	0.982064
1	1.383673	-0.957435	1.367185
1	1.626314	-2.578815	1.466164
1	0.108139	-1.986034	1.230454
7	-2.059629	-2.116128	0.977612
1	-1.927896	-2.208576	-0.030013
1	-2.671949	-2.865888	1.283425
1	-2.547784	-1.234154	1.136711
7	-0.704479	0.568674	-0.276703
1	0.093784	0.507405	0.355668
1	-0.739912	-0.318501	-0.779695
1	-1.534603	0.569001	0.318278

7	-3.715583	0.785851	0.984141
1	-4.593131	0.318789	0.774849
1	-3.832957	1.241207	1.884448
1	-3.586646	1.521371	0.281250
7	-2.685246	2.722755	-1.250850
1	-2.469708	3.706387	-1.123734
1	-3.032018	2.614129	-2.198674
1	-1.813178	2.192619	-1.171506
7	1.823491	1.187647	1.746214
1	2.784172	1.238038	1.390790
1	1.866251	1.234621	2.760225
1	1.356078	2.036566	1.437836
7	4.474445	1.199825	0.144895
1	3.854796	0.815085	-0.575739
1	4.899131	2.047703	-0.216290
1	5.223073	0.533564	0.304953
7	2.187604	-0.060374	-1.508156
1	1.392562	0.572262	-1.572305
1	1.935594	-0.778925	-0.826334
1	2.298567	-0.509019	-2.412032

Cartesian coordinates of : AM9_24

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	4.474433	-1.199864	-0.144967
1	3.854804	-0.815117	0.575680
1	4.899134	-2.047735	0.216215
1	5.223054	-0.533603	-0.305057
7	-0.392172	2.422404	1.735221
1	-0.544217	3.398396	1.971089
1	-0.014369	1.971341	2.562902
1	0.318314	2.379873	0.999639
7	-2.685279	-2.722803	1.250781
1	-1.813181	-2.192711	1.171496
1	-3.032099	-2.614164	2.198587
1	-2.469784	-3.706447	1.123677
7	-2.059585	2.116175	-0.977615
1	-2.671916	2.865937	-1.283401
1	-2.547763	1.234203	-1.136659
1	-1.927781	2.208646	0.029999
7	2.187630	0.060326	1.508144
1	1.935635	0.778910	0.826352
1	2.298601	0.508930	2.412040
1	1.392574	-0.572296	1.572262
7	1.823396	-1.187707	-1.746143
1	1.355984	-2.036591	-1.437665
1	1.866065	-1.234750	-2.760155
1	2.784106	-1.238100	-1.390799
7	1.095753	1.860439	-0.982086
1	1.383669	0.957359	-1.367137
1	1.626432	2.578715	-1.466202
1	0.108202	1.986053	-1.230531
7	-0.704523	-0.568628	0.276783
1	-0.739966	0.318540	0.779787
1	0.093712	-0.507324	-0.355620
1	-1.534670	-0.568973	-0.318166
7	-3.715612	-0.785768	-0.984098
1	-3.832976	-1.241076	-1.884431
1	-4.593159	-0.318711	-0.774792
1	-3.586683	-1.521328	-0.281248

Cartesian coordinates of : AM9_25

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
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7	1.220917	1.416402	-1.884024
1	1.889407	1.248264	-1.119989
1	1.217980	2.414162	-2.075766
1	1.588398	0.959567	-2.713812
7	-1.630439	0.021291	-1.628483
1	-2.180152	0.438937	-0.876857
1	-2.152918	0.175126	-2.486725
1	-0.762823	0.561292	-1.708436
7	-3.383457	2.037055	0.314457
1	-3.619032	2.509629	-0.553014
1	-2.403679	2.247052	0.536707
1	-3.966003	2.444745	1.039618
7	-0.452548	1.674042	1.017377
1	0.159127	2.118094	1.695663
1	0.129779	1.435680	0.215149
1	-0.767981	0.789632	1.420771
7	-2.454168	-2.862974	-0.663513
1	-3.233717	-3.196806	-1.221359
1	-1.738530	-3.582341	-0.684257
1	-2.073744	-2.025740	-1.115106
7	0.462050	-1.484676	0.377063
1	0.699800	-2.472165	0.362541
1	0.106772	-1.241550	-0.547033
1	-0.336528	-1.373066	1.004395
7	-2.434644	-0.774772	1.649223
1	-2.796496	-0.926872	2.585887
1	-2.629946	-1.615052	1.098718
1	-2.978142	-0.016266	1.232805
7	2.774229	0.620916	0.620303
1	2.090596	-0.136111	0.724262
1	2.749383	1.175866	1.470281
1	3.706483	0.210496	0.556657
7	5.759085	-0.625272	0.276319
1	6.271747	-0.035104	-0.370611
1	5.686533	-1.547388	-0.140997
1	6.316501	-0.714163	1.119458

Cartesian coordinates of : AM9_26

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	4.728031	-1.500473	-0.707130
1	4.645345	-1.916793	-1.628736
1	5.412057	-0.753312	-0.767108
1	5.099922	-2.207606	-0.081874
7	-0.594003	-1.979875	-0.314063
1	-0.424249	-2.899650	-0.709597
1	-1.379759	-1.575151	-0.821298
1	0.223204	-1.396933	-0.515466
7	-0.952119	1.681537	1.398041
1	-1.767702	1.069613	1.279502
1	-0.231898	1.078269	1.798725
1	-1.198059	2.362366	2.111872
7	0.128346	-1.051975	2.572570
1	-0.230065	-1.497458	1.721661
1	0.679043	-1.740160	3.076798
1	-0.669368	-0.818155	3.157201
7	-0.613243	1.093086	-1.728026
1	-0.882060	1.538974	-0.848999
1	0.262598	0.612696	-1.512422
1	-0.395134	1.830095	-2.392348
7	1.502897	3.110627	-0.053425
1	1.325245	3.591170	-0.929604
1	0.604308	2.787751	0.313191
1	1.878536	3.795998	0.594345
7	1.886251	-0.042722	-0.044885
1	2.072982	0.959123	-0.123388
1	2.768676	-0.537570	-0.179397
1	1.584855	-0.201745	0.917219

7	-3.080143	-0.625219	1.046106
1	-2.485921	-1.428242	1.239582
1	-3.954680	-0.756590	1.544650
1	-3.279501	-0.670604	0.043882
7	-3.081396	-0.647440	-2.146206
1	-2.976973	-1.361712	-2.860639
1	-2.258463	-0.031471	-2.187304
1	-3.895290	-0.095728	-2.401324

Cartesian coordinates of : AM9_27

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	5.183035	-0.323098	-1.028864
1	5.621908	-0.080494	-0.146451
1	5.600514	-1.188538	-1.354233
1	5.418144	0.401996	-1.698476
7	1.328062	2.493257	1.671481
1	2.016654	3.237115	1.609999
1	1.091807	2.395292	2.653918
1	1.776841	1.622909	1.359701
7	-3.594485	-1.059256	0.682347
1	-2.712618	-0.810653	1.152770
1	-4.359234	-0.789332	1.294354
1	-3.627656	-2.072379	0.609733
7	-1.154200	-1.223645	-1.428488
1	-1.223848	-1.454801	-2.414967
1	-2.102834	-1.150438	-1.063788
1	-0.752575	-0.284811	-1.360467
7	-3.418908	1.437568	-1.288580
1	-3.569889	0.604691	-0.713569
1	-4.144319	2.109224	-1.057156
1	-3.564279	1.165432	-2.256265
7	0.549300	-2.849767	0.582744
1	1.310560	-3.370564	0.157495
1	-0.028307	-3.523004	1.077730
1	-0.017096	-2.445253	-0.173591
7	2.176439	-0.039635	0.157706
1	1.855882	-0.928581	0.539039
1	3.044758	-0.208787	-0.349673
1	1.465748	0.263537	-0.508132
7	-0.823425	-0.213756	1.645450
1	-0.542917	0.389078	0.871538
1	-0.635231	0.309834	2.495189
1	-0.180658	-1.006326	1.627886
7	-0.319098	1.819210	-0.928102
1	-1.335775	1.933692	-0.979141
1	0.075849	2.291838	-1.736294
1	0.031543	2.303173	-0.097005

Cartesian coordinates of : AM9_28

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.194506	-1.296946	0.977107
1	-0.893778	-1.752877	1.562245
1	0.653428	-1.862636	0.984063
1	-0.569879	-1.326008	0.027103
7	1.479351	-1.177939	-1.780861
1	1.923954	-1.548323	-2.615554
1	0.483315	-1.391324	-1.846471
1	1.849666	-1.702439	-0.985029
7	2.965828	-2.192352	0.947365
1	3.038742	-1.191855	1.153826
1	2.880748	-2.687628	1.830250
1	3.846025	-2.486349	0.534232

7	2.252002	0.725124	0.691841
1	2.248549	1.738009	0.770049
1	1.319542	0.390802	0.946421
1	2.346981	0.504585	-0.298438
7	-1.745766	-0.736856	-1.844092
1	-2.107131	-1.065487	-2.734606
1	-2.543307	-0.538114	-1.243548
1	-1.298160	0.169904	-1.996141
7	-3.223045	-1.822261	1.176862
1	-3.130620	-0.834806	0.934350
1	-4.179586	-1.994138	1.467228
1	-3.051335	-2.368071	0.337440
7	0.160277	1.797787	-1.709691
1	0.498539	2.389255	-0.948671
1	0.277705	2.321694	-2.572182
1	0.778591	0.984350	-1.757883
7	-2.058681	1.100083	0.597811
1	-1.632402	1.558166	-0.208491
1	-2.422757	1.808765	1.226205
1	-1.312319	0.580887	1.064312
7	0.409006	3.517004	1.006600
1	1.037061	3.991886	1.647968
1	-0.021277	2.744813	1.509113
1	-0.331559	4.171429	0.771607

Cartesian coordinates of : AM9_29

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.989351	0.041216	-0.441480
1	1.503106	-0.728309	0.026974
1	1.892555	-0.128126	-1.439404
1	2.981978	-0.025078	-0.213201
7	0.276237	2.250011	0.980802
1	0.853525	2.908666	1.494874
1	-0.169654	2.763043	0.224309
1	0.902315	1.569476	0.533199
7	0.220590	-2.237671	0.983233
1	-0.468049	-2.774782	0.462237
1	-0.304726	-1.537296	1.517413
1	0.658006	-2.868227	1.648302
7	-1.425804	0.033236	2.433503
1	-2.378343	0.195310	2.116459
1	-0.860765	0.792868	2.038065
1	-1.418818	0.135975	3.443766
7	5.135978	-0.068559	0.379401
1	5.558499	0.849379	0.287527
1	5.182607	-0.330745	1.358624
1	5.709203	-0.724500	-0.140850
7	-2.813351	-1.573138	-0.049597
1	-2.871396	-0.549368	-0.070560
1	-3.735891	-1.939740	-0.263230
1	-2.599217	-1.826425	0.911606
7	-2.740725	1.585894	-0.092097
1	-3.534934	2.110924	-0.445704
1	-2.000620	1.626383	-0.802042
1	-2.382896	2.085281	0.718313
7	-0.417310	-1.583269	-2.111252
1	-0.533252	-2.190483	-2.916579
1	-1.257567	-1.664449	-1.530183
1	0.345843	-1.954923	-1.550683
7	-0.347941	1.546896	-2.132543
1	0.574921	1.748530	-1.755007
1	-0.400740	1.966645	-3.055684
1	-0.384864	0.527664	-2.248327

Cartesian coordinates of : AM9_30

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	5.183946	-1.068707	-0.574299
1	5.352431	-2.061871	-0.696628
1	5.565434	-0.592655	-1.385196
1	5.714006	-0.766191	0.236553
7	-1.278136	0.680610	1.268231
1	-0.522138	1.311226	1.536674
1	-0.930919	0.125013	0.485246
1	-1.416307	0.026074	2.034009
7	-0.828823	-2.509714	1.006258
1	-0.131699	-2.150834	1.652583
1	-0.690267	-3.513037	0.938645
1	-0.650514	-2.094780	0.085244
7	2.116721	-0.299406	0.138497
1	3.060960	-0.558884	-0.149499
1	1.541415	-1.136429	0.093888
1	1.726763	0.345329	-0.551294
7	-0.629554	-0.981865	-1.699968
1	0.140159	-0.357229	-1.932053
1	-1.470261	-0.402279	-1.748137
1	-0.699385	-1.677169	-2.437330
7	-2.903399	1.240607	-1.261716
1	-3.485618	1.943439	-1.705602
1	-3.466369	0.399755	-1.119793
1	-2.670989	1.551232	-0.317231
7	0.297209	1.967864	-1.213747
1	-0.696070	1.805363	-1.392075
1	0.593536	2.718573	-1.830060
1	0.385391	2.307856	-0.255311
7	-3.708852	-1.170785	0.496758
1	-4.524610	-1.707634	0.774120
1	-3.660301	-0.350944	1.097303
1	-2.881297	-1.730479	0.714186
7	1.506402	2.177326	1.833559
1	2.189848	2.873929	1.551319
1	1.846543	1.261907	1.516331
1	1.491663	2.179210	2.849092

Cartesian coordinates of : AM9_31-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-4.559587	1.301013	0.053209
1	-4.986292	1.375908	0.971541
1	-4.331036	0.313917	-0.101838
1	-5.268477	1.566643	-0.623335
7	-3.369867	-1.546661	-0.360973
1	-3.197775	-1.795761	-1.330077
1	-3.683833	-2.386609	0.114692
1	-2.478263	-1.257971	0.053584
7	-0.714088	-0.382185	0.834874
1	-1.011826	0.575081	0.622798
1	-0.542715	-0.421796	1.836118
1	0.186582	-0.517276	0.369228
7	-1.696356	2.511647	-0.181685
1	-1.647911	3.432361	0.245786
1	-2.671474	2.197029	-0.111042
1	-1.494490	2.642126	-1.169667
7	1.790694	-1.116515	-0.979769
1	1.627464	-2.110653	-0.817904
1	1.288797	-0.880273	-1.832512
1	2.779573	-0.929754	-1.164115
7	4.290667	0.660294	-0.949475
1	5.260694	0.801018	-1.210323
1	4.223991	0.673753	0.068979
1	3.755184	1.455487	-1.292417

7	1.584202	2.086192	-0.301284
1	1.655481	1.073264	-0.387403
1	0.617484	2.287386	-0.051400
1	2.170991	2.353590	0.484274
7	2.921000	0.027705	1.839019
1	2.249814	0.578138	2.366174
1	2.407382	-0.454928	1.100716
1	3.302998	-0.671732	2.467878
7	-0.095683	-3.442689	-0.073683
1	-0.592119	-2.608937	0.240601
1	0.015957	-4.057430	0.726388
1	-0.693050	-3.924185	-0.738361

Cartesian coordinates of : AM9_32

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-4.012696	-1.481698	1.341210
1	-4.522661	-0.652993	1.018121
1	-4.504765	-2.299662	0.995293
1	-4.076034	-1.507271	2.354182
7	-5.286802	1.139884	0.191486
1	-5.516895	1.889554	0.836290
1	-4.451024	1.422867	-0.331229
1	-6.056098	1.071790	-0.467494
7	4.578320	1.792876	1.495200
1	4.502523	1.479276	2.457657
1	5.291859	2.514012	1.464891
1	3.693016	2.222600	1.243068
7	1.649793	-0.034151	1.309817
1	1.522080	0.646819	2.051581
1	2.599250	-0.395478	1.365524
1	1.575279	0.441240	0.408439
7	4.059409	-0.384618	-0.751060
1	4.516431	0.219066	-0.066584
1	4.731536	-0.585322	-1.485113
1	3.298698	0.155931	-1.164947
7	1.676309	-2.433523	-0.653836
1	1.707853	-3.440068	-0.778704
1	2.635435	-2.080766	-0.615115
1	1.272322	-2.240961	0.260540
7	-1.217612	-0.813574	0.039780
1	-0.918119	-1.556287	-0.588050
1	-2.063492	-1.131966	0.522758
1	-0.470491	-0.709655	0.726633
7	-2.571307	1.663734	-1.252985
1	-2.097277	0.860446	-0.822201
1	-2.032443	2.497776	-1.041309
1	-2.544384	1.537438	-2.260121
7	1.055940	0.402026	-1.747214
1	1.153741	-0.618037	-1.738701
1	1.134897	0.721911	-2.707901
1	0.099279	0.581038	-1.444289

Cartesian coordinates of : AM9_33

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.110354	-0.234617	0.215931
1	-4.124094	-0.330279	0.165509
1	-2.732607	-1.052490	0.689844
1	-2.725672	-0.255858	-0.729440
7	-0.315743	-1.374806	0.570945
1	-0.515827	-1.297215	-0.424761
1	0.667591	-1.623469	0.663751
1	-0.426909	-0.432662	0.940813

7	-1.222377	1.998626	1.013546
1	-1.996167	1.337584	0.840044
1	-1.152561	2.113412	2.021541
1	-1.509796	2.901872	0.645758
7	-0.932701	0.513288	-1.965386
1	-0.000596	0.160565	-2.194497
1	-1.255774	1.069500	-2.751280
1	-0.809954	1.143002	-1.172566
7	2.983894	-1.883486	0.952643
1	3.152390	-2.795859	0.537884
1	3.805460	-1.298269	0.769018
1	2.928453	-2.032993	1.956521
7	1.948441	1.272621	0.828980
1	0.976204	1.543665	0.657260
1	1.949601	0.260394	0.961729
1	2.199799	1.686851	1.723231
7	4.860687	0.428018	0.086966
1	5.112201	0.341615	-0.892943
1	4.020910	1.008565	0.140756
1	5.618506	0.921782	0.547783
7	2.093156	-0.284368	-1.853403
1	2.230690	-0.975549	-1.117555
1	2.312799	0.616125	-1.431964
1	2.765064	-0.470387	-2.590875
7	-6.352826	-0.547300	0.110746
1	-6.651421	-1.125799	-0.667500
1	-6.814037	0.352002	0.021602
1	-6.689497	-0.981943	0.963556

Cartesian coordinates of : AM9_34

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.022195	-0.226675	1.083378
1	0.422270	-0.578968	1.948602
1	-0.066874	-1.027011	0.459125
1	-0.915580	0.117151	1.302144
7	0.935676	-2.830694	-0.740070
1	1.415276	-3.309178	-1.497516
1	0.227443	-3.474105	-0.397485
1	1.622153	-2.695698	0.011464
7	3.112209	-2.054814	1.335781
1	3.209022	-1.160306	0.838269
1	2.957261	-1.848542	2.317836
1	3.999103	-2.545681	1.277194
7	2.730131	0.458084	-0.336466
1	3.153261	1.382482	-0.419950
1	1.817922	0.547023	0.117544
1	2.555343	0.109780	-1.274997
7	-2.797171	1.075848	1.946794
1	-3.467354	1.368960	1.227254
1	-3.338131	0.707182	2.723875
1	-2.336491	1.914994	2.287877
7	-4.760126	1.475608	-0.444579
1	-4.423231	0.537492	-0.686442
1	-4.518974	2.097597	-1.209680
1	-5.773038	1.447686	-0.389304
7	-0.441974	-0.239090	-1.979422
1	-0.115328	0.528202	-1.397706
1	-0.257557	-0.001068	-2.948188
1	0.112190	-1.061677	-1.729269
7	-3.100151	-1.076948	-0.519329
1	-2.312405	-0.820210	-1.122213
1	-2.829899	-0.842820	0.434310
1	-3.215063	-2.083879	-0.573445
7	4.164163	3.366517	-0.387273
1	4.833812	3.299558	0.372280
1	3.517429	4.115277	-0.162065
1	4.672786	3.640919	-1.221207

 Cartesian coordinates of : AM9_35

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.756399	0.170759	0.451648
1	-3.839962	-0.231613	1.380791
1	-3.588871	-0.608535	-0.190190
1	-4.659094	0.584904	0.217687
7	-2.665774	-2.285676	-1.213869
1	-2.268864	-2.173579	-2.141302
1	-2.996199	-3.242767	-1.144217
1	-1.910500	-2.156498	-0.529790
7	-0.651053	-1.451096	0.969892
1	-0.760454	-0.439803	0.886607
1	-0.944088	-1.698818	1.910633
1	0.348498	-1.655292	0.906152
7	-1.130818	1.740449	0.292240
1	-1.205706	2.687624	0.652233
1	-2.070378	1.320007	0.330531
1	-0.876565	1.820883	-0.688467
7	2.483261	-2.103275	0.519893
1	3.172510	-2.420854	1.195301
1	2.246211	-2.909199	-0.051982
1	2.947453	-1.418108	-0.090411
7	3.633888	0.329169	-0.985311
1	3.233906	0.578719	-1.884336
1	4.614390	0.610167	-0.997452
1	3.147130	0.872855	-0.268207
7	1.797931	0.997455	1.447772
1	1.850763	-0.018323	1.514517
1	0.841194	1.225059	1.168731
1	1.939260	1.373461	2.380098
7	6.781560	1.104389	-0.802196
1	7.205604	1.722042	-1.486236
1	6.892821	1.533970	0.110398
1	7.308416	0.237272	-0.800914
7	-6.524227	1.450501	-0.653371
1	-7.357915	1.581602	-0.090395
1	-6.757927	0.810903	-1.405849
1	-6.290210	2.345199	-1.070821

Cartesian coordinates of ammonia decamer: (NH3)10

Cartesian coordinates of : AM10_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.097545	2.171213	-0.107042
1	2.238258	1.393651	0.546624
1	2.809871	2.868519	0.090841
1	2.312148	1.774128	-1.020793
7	-2.569830	-1.916855	-1.251441
1	-1.690256	-1.417163	-1.430998
1	-3.078942	-1.991056	-2.126796
1	-2.334528	-2.861337	-0.959422
7	-0.113973	-0.097194	-1.116740
1	-0.090668	-0.205643	-0.102119
1	-0.430322	0.858644	-1.281284
1	0.859991	-0.144449	-1.421903
7	-0.775423	3.140979	-1.049716
1	-0.709641	3.696987	-1.897134
1	0.177875	2.971152	-0.713656
1	-1.239900	3.716301	-0.352194

7	-0.487716	1.387290	1.880425
1	0.163479	1.875090	1.264673
1	-0.601572	1.955145	2.714878
1	-1.393358	1.349128	1.397699
7	3.053131	-0.700520	-1.341660
1	3.448280	-0.317301	-0.486054
1	3.815911	-0.922782	-1.973255
1	2.599729	-1.574029	-1.067317
7	0.883534	-2.843012	-0.321547
1	0.480893	-2.596427	-1.223205
1	0.172297	-2.601754	0.379681
1	1.013915	-3.849920	-0.304263
7	-2.934999	1.000678	0.022305
1	-3.871649	1.373028	0.142559
1	-3.025410	0.055315	-0.352601
1	-2.456768	1.574614	-0.672596
7	-1.274982	-1.710523	1.620628
1	-1.000758	-0.793936	1.977389
1	-1.596390	-2.260444	2.411718
1	-2.077970	-1.552705	1.012081
7	2.092902	-0.462609	1.648803
1	1.214740	-0.090427	2.015304
1	2.646039	-0.776072	2.440937
1	1.853386	-1.292386	1.103096

Cartesian coordinates of : AM10_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.287833	-1.828430	1.783265
1	0.217473	-2.492947	2.548256
1	-0.519548	-1.203556	1.845278
1	0.192759	-2.354786	0.912774
7	-2.492422	1.559456	-1.291163
1	-3.275925	2.069875	-1.686778
1	-1.794561	2.244544	-0.984411
1	-2.046656	1.041919	-2.046468
7	1.440757	1.162965	1.782925
1	2.050717	1.433862	2.548625
1	1.945190	1.343432	0.912996
1	1.302696	0.151382	1.844763
7	0.049878	3.179065	-0.146429
1	0.946764	2.951959	-0.579039
1	0.158220	2.921434	0.833697
1	-0.071510	4.186023	-0.196089
7	-1.725655	0.664188	1.783879
1	-2.264237	1.056984	2.550289
1	-2.135524	1.010521	0.914489
1	-0.780545	1.050583	1.844351
7	-2.779327	-1.547052	-0.145831
1	-2.612106	-1.328180	0.835385
1	-3.591556	-2.154134	-0.199447
1	-3.028534	-0.654920	-0.576163
7	-0.105002	-2.934700	-1.293916
1	-1.047162	-2.674916	-0.985212
1	0.119283	-2.285311	-2.045651
1	-0.155415	-3.866181	-1.694793
7	2.596171	1.376663	-1.292961
1	2.840988	0.430094	-0.985485
1	1.923901	1.248441	-2.047058
1	3.429409	1.799457	-1.690305
7	-0.000755	0.000483	-1.033232
1	-0.799805	-0.496410	-0.642337
1	-0.032241	0.942417	-0.646043
1	0.830105	-0.441720	-0.642990
7	2.728762	-1.633127	-0.146484
1	2.081807	-2.294816	-0.578704
1	2.453524	-1.598827	0.834220
1	3.660804	-2.032804	-0.198507

 Cartesian coordinates of : AM10_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.210464	-0.348613	1.543381
1	3.051984	-0.239933	2.101872
1	1.473842	0.207220	1.982477
1	2.400982	0.078011	0.635962
7	0.052589	-0.277297	-1.002966
1	-0.811107	-0.194366	-1.541635
1	0.602616	0.555918	-1.209123
1	-0.217309	-0.180603	-0.023909
7	-0.650903	0.721219	2.363211
1	-0.794720	-0.288707	2.313699
1	-0.909291	1.017930	3.299681
1	-1.314256	1.148973	1.711744
7	-0.197321	-2.335528	1.285436
1	-0.209267	-3.225519	1.774656
1	0.722021	-1.907366	1.434512
1	-0.249104	-2.533691	0.288210
7	-2.125883	1.955296	-0.207872
1	-2.754909	2.752914	-0.225867
1	-1.169395	2.318629	-0.272108
1	-2.296146	1.414943	-1.057494
7	-3.097885	-1.031173	0.589531
1	-2.950515	-0.024364	0.672339
1	-3.879767	-1.282060	1.186327
1	-2.266346	-1.489782	0.964735
7	2.630712	-1.984595	-1.100059
1	1.659333	-1.670923	-1.191157
1	2.756283	-2.834259	-1.639875
1	2.768634	-2.206858	-0.117580
7	0.910796	2.678872	0.293011
1	1.713699	2.236817	-0.159087
1	0.722520	2.167654	1.155500
1	1.184869	3.622794	0.547788
7	3.129938	1.021319	-1.411530
1	3.181571	-0.002995	-1.467030
1	4.071545	1.366058	-1.246978
1	2.857093	1.356894	-2.331694
7	-2.859966	-0.418967	-2.389263
1	-3.707212	-0.015941	-2.778194
1	-3.106199	-0.878753	-1.505759
1	-2.549245	-1.132372	-3.042172

 Cartesian coordinates of : AM10_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.312548	-1.508385	-1.753940
1	-1.471681	-2.185758	-1.001259
1	-1.639378	-1.929746	-2.618627
1	-0.300456	-1.381978	-1.837450
7	1.653528	-0.426489	-1.819343
1	2.199779	-0.605368	-2.656910
1	2.310765	-0.351367	-1.042082
1	1.216126	0.489278	-1.928958
7	-1.584174	-2.853156	1.012326
1	-2.111178	-2.034352	1.312387
1	-0.597374	-2.699826	1.225257
1	-1.903729	-3.651254	1.550851
7	1.589947	-2.541768	0.615103
1	2.387443	-1.908164	0.692133
1	1.243693	-2.425327	-0.336209
1	1.935197	-3.492911	0.701458

7	-0.821297	1.669712	-1.730256
1	-1.180804	0.715314	-1.821869
1	-1.340985	2.109807	-0.968035
1	-1.071482	2.162970	-2.582778
7	-3.070445	-0.005119	0.463180
1	-2.971233	1.008934	0.427989
1	-2.699971	-0.378799	-0.413958
1	-4.063838	-0.213851	0.490897
7	-0.032705	0.184081	1.123205
1	-0.999728	-0.107577	1.276820
1	0.083635	0.176164	0.108110
1	0.555183	-0.579723	1.455677
7	-1.666412	2.830104	1.119901
1	-1.006696	2.108276	1.419444
1	-1.140633	3.689148	0.985888
1	-2.314534	2.994405	1.884706
7	3.487146	0.069411	0.846063
1	3.350846	0.044025	1.853387
1	3.105578	0.965718	0.523201
1	4.490030	0.081423	0.685566
7	1.717675	2.491808	0.132836
1	1.080026	2.414276	-0.660944
1	1.935324	3.472367	0.276713
1	1.195068	2.142505	0.935070

Cartesian coordinates of : AM10_5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.451320	2.319491	-0.890604
1	-0.546068	2.705875	-0.619636
1	-1.225734	1.613768	-1.591492
1	-1.976853	3.054309	-1.354790
7	-1.033598	1.126239	2.051671
1	-1.455346	1.589607	2.851096
1	-1.386359	0.166095	2.028448
1	-1.392968	1.580281	1.209421
7	1.496904	2.298102	0.458591
1	2.294312	1.659612	0.440323
1	0.845181	1.948890	1.164456
1	1.840518	3.198213	0.780352
7	1.387893	-2.211043	-0.713752
1	1.738169	-3.157945	-0.826225
1	0.418666	-2.207079	-1.041569
1	1.355378	-2.012952	0.289263
7	-1.542336	-1.483752	-1.823379
1	-0.965397	-0.700815	-2.137275
1	-1.766746	-2.043812	-2.640483
1	-2.418562	-1.089752	-1.468131
7	1.562131	-0.758678	2.106137
1	0.849410	-0.031591	2.204035
1	1.898543	-0.978913	3.038912
1	2.339689	-0.341223	1.594181
7	-1.413395	-1.915284	1.385384
1	-1.394759	-1.948699	0.363034
1	-1.853774	-2.772570	1.705763
1	-0.442153	-1.934821	1.696663
7	3.610451	0.004872	-0.318410
1	3.004790	-0.754236	-0.643456
1	3.814050	0.588843	-1.125311
1	4.491834	-0.406680	-0.025062
7	0.850463	0.584203	-2.211517
1	1.279476	-0.304995	-1.953584
1	1.086419	1.256001	-1.478143
1	1.278097	0.902982	-3.075440
7	-3.588345	0.006794	-0.060456
1	-3.214623	-0.481101	0.752074
1	-4.564894	0.217016	0.116609
1	-3.082221	0.889088	-0.139678

Cartesian coordinates of : AM10_6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.388368	1.482206	1.902227
1	-0.513862	1.004690	1.956966
1	1.086712	0.736609	1.840094
1	0.533249	1.956964	2.788824
7	-2.869108	1.513763	-0.488192
1	-2.633061	1.189742	0.449643
1	-3.751161	2.013155	-0.425349
1	-2.147313	2.191946	-0.747229
7	-1.921195	-0.757639	1.707512
1	-1.188210	-1.442401	1.893241
1	-2.439259	-1.138602	0.909280
1	-2.544783	-0.757873	2.509884
7	-2.801074	-1.516810	-1.197014
1	-1.928626	-1.674558	-1.695600
1	-2.971860	-0.506045	-1.225736
1	-3.541694	-1.979305	-1.714531
7	-0.228804	3.189248	-0.701687
1	0.010862	2.723581	0.179792
1	0.492679	2.950041	-1.376310
1	-0.187535	4.192865	-0.554139
7	-0.166977	-2.902982	0.349053
1	-0.012298	-2.144207	-0.319186
1	0.463340	-3.663911	0.114005
1	-1.119094	-3.227968	0.198094
7	-0.075753	-0.064890	-0.972055
1	-0.615155	0.495505	-1.630091
1	0.795670	0.445470	-0.813190
1	-0.596750	-0.001076	-0.095196
7	2.225595	-1.157492	1.360668
1	2.571381	-1.442907	0.438794
1	1.368109	-1.693196	1.502729
1	2.895260	-1.479040	2.053883
7	2.737730	1.534857	-0.276109
1	2.229169	2.290866	0.176422
1	3.685254	1.860325	-0.443481
1	2.778136	0.776279	0.407266
7	2.655210	-1.338151	-1.720029
1	3.168763	-1.783666	-2.473020
1	2.845209	-0.337209	-1.748524
1	1.658920	-1.430842	-1.907954

Cartesian coordinates of : AM10_7

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.137052	1.817556	-0.208588
1	2.123502	1.957169	-0.280313
1	3.543065	2.671162	0.163054
1	3.489148	1.708467	-1.156108
7	1.325816	-0.445928	-2.068692
1	1.201384	0.423912	-1.550718
1	1.559570	-0.202721	-3.027029
1	2.137557	-0.917914	-1.659002
7	-0.029551	1.899661	-0.242990
1	-0.278180	1.537514	0.680607
1	-0.661923	1.436392	-0.901690
1	-0.274763	2.886434	-0.245363
7	-1.818489	-0.010163	-2.136261
1	-2.409521	-0.716948	-1.688846
1	-0.888782	-0.420411	-2.246316
1	-2.186990	0.154961	-3.068347

7	3.610460	-1.368880	-0.173861
1	3.858438	-0.393687	-0.010127
1	3.029980	-1.642387	0.615919
1	4.456448	-1.928501	-0.158167
7	1.802501	-0.095562	2.075625
1	0.904128	0.344998	2.278832
1	2.331830	-0.131980	2.941568
1	2.309173	0.516526	1.435002
7	-3.456982	1.488551	0.172461
1	-2.886300	1.164199	-0.612469
1	-4.428469	1.325744	-0.076795
1	-3.335329	2.494521	0.244568
7	-1.340817	0.315488	2.183123
1	-2.180061	0.726135	1.767193
1	-1.174437	-0.568350	1.698395
1	-1.552336	0.095680	3.152140
7	-3.208255	-1.709174	0.018041
1	-3.504966	-0.946106	0.622018
1	-2.241724	-1.931830	0.269642
1	-3.785521	-2.516816	0.227937
7	-0.040468	-2.011181	0.357750
1	0.126557	-3.014009	0.363799
1	0.664187	-1.588327	0.968762
1	0.185454	-1.686392	-0.584400

Cartesian coordinates of : AM10_8

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.971255	-1.215290	0.383173
1	3.918224	-1.501180	0.611985
1	2.688884	-0.505119	1.059479
1	3.003370	-0.767037	-0.533655
7	2.157156	2.143924	-0.123606
1	2.687015	3.005415	-0.035335
1	2.647868	1.550135	-0.793054
1	2.172043	1.668266	0.780044
7	1.024567	0.427544	2.305599
1	0.693129	-0.527625	2.166222
1	1.151481	0.555831	3.305436
1	0.262690	1.047393	2.014060
7	0.327838	-2.603255	1.067507
1	0.427797	-3.324651	1.776295
1	1.271225	-2.370071	0.730885
1	-0.177574	-3.026825	0.292556
7	-0.968633	2.453783	0.848894
1	-1.274818	3.325046	1.271915
1	-0.081035	2.637762	0.377278
1	-1.650863	2.207084	0.126104
7	-2.228033	-0.658300	1.459022
1	-1.873845	0.296690	1.379821
1	-2.811613	-0.694743	2.289538
1	-1.421275	-1.262122	1.625137
7	-0.045868	-0.029890	-0.937480
1	0.503435	0.789853	-0.675251
1	-1.009386	0.297029	-1.012483
1	-0.013305	-0.654430	-0.132485
7	2.536748	-0.014410	-2.563341
1	1.566223	-0.236086	-2.320693
1	2.921325	-0.800837	-3.078400
1	2.513937	0.772720	-3.205480
7	-3.247988	1.231079	-1.018020
1	-3.780903	1.888162	-1.579737
1	-3.803393	1.010740	-0.194904
1	-3.181643	0.351685	-1.537592
7	-2.556525	-1.710474	-1.513818
1	-2.995635	-2.599176	-1.726411
1	-2.553818	-1.570367	-0.499929
1	-1.593154	-1.736529	-1.836862

Cartesian coordinates of : AM10_9

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.137908	-2.250615	-0.156299
1	-1.913869	-1.963015	0.795185
1	-2.681060	-3.107125	-0.098730
1	-1.235610	-2.490042	-0.570951
7	2.863022	1.532306	-1.513769
1	3.367471	1.285921	-2.360412
1	2.802474	2.546573	-1.497220
1	1.905567	1.161805	-1.596213
7	-0.022093	-1.017280	1.943251
1	0.170390	-1.491843	2.820715
1	0.525709	-0.149513	1.931676
1	0.340822	-1.607381	1.194144
7	1.513651	1.693792	1.451791
1	0.727262	2.241538	1.084099
1	2.212845	1.656551	0.710027
1	1.918812	2.219915	2.220546
7	0.167835	0.205665	-1.127557
1	0.004307	0.532140	-0.176064
1	-0.725416	0.307452	-1.615143
1	0.340444	-0.795504	-1.048483
7	-2.726028	0.590385	1.388629
1	-3.189106	0.859615	2.251605
1	-3.330384	-0.075479	0.913974
1	-1.875759	0.078055	1.641890
7	-1.030252	2.857847	0.031863
1	-1.408238	3.798234	0.088608
1	-1.725295	2.213978	0.421481
1	-0.928472	2.630060	-0.954272
7	-2.866197	0.368146	-1.833135
1	-3.187786	1.036217	-1.138260
1	-2.814385	-0.545874	-1.375105
1	-3.556124	0.324733	-2.575437
7	1.085934	-2.925469	-0.709303
1	1.212058	-3.082430	-1.705883
1	1.137990	-3.837947	-0.264721
1	1.892565	-2.375800	-0.382627
7	3.149972	-0.963157	0.449389
1	2.690011	-0.582949	1.274181
1	3.255973	-0.173555	-0.192664
1	4.081258	-1.255668	0.730030

Cartesian coordinates of : AM10_10

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.715493	2.654902	-0.836722
1	-0.999994	3.402595	-1.462495
1	0.104258	2.976489	-0.312385
1	-1.470112	2.520140	-0.163785
7	1.842086	2.664411	0.893697
1	2.281084	3.232278	1.610819
1	2.579540	2.250126	0.328890
1	1.352564	1.884503	1.337798
7	0.166983	0.107037	0.923582
1	-0.263181	0.529745	0.099743
1	0.977112	-0.400385	0.570978
1	-0.496667	-0.600115	1.241464
7	-2.631905	0.151693	-1.327524
1	-3.396592	0.209579	-1.993515
1	-1.836305	0.642510	-1.736224
1	-2.886187	0.701193	-0.504000

7	1.519353	-2.797858	0.849792
1	1.869952	-3.750812	0.840088
1	0.997941	-2.681715	1.714755
1	0.860826	-2.695826	0.067982
7	-0.280928	-2.118028	-1.591419
1	-0.308202	-2.776505	-2.365069
1	0.367650	-1.365356	-1.852474
1	-1.197660	-1.671907	-1.546721
7	-2.480546	1.230194	1.663321
1	-1.534290	1.470262	1.954648
1	-2.553028	0.220982	1.802940
1	-3.126173	1.680183	2.304753
7	-2.253990	-1.995224	0.986324
1	-1.546321	-2.645407	0.649140
1	-2.570598	-1.488353	0.156572
1	-3.029597	-2.547025	1.340066
7	1.439377	0.465986	-1.997551
1	0.807060	1.225929	-1.742220
1	1.912900	0.736321	-2.853850
1	2.148047	0.374879	-1.265937
7	3.416881	-0.334337	0.407521
1	3.455967	0.111273	1.320536
1	4.375874	-0.498637	0.116004
1	2.971396	-1.248381	0.544349

Cartesian coordinates of : AM10_11

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.373542	1.443876	-1.662771
1	0.802409	1.834086	-2.497572
1	0.472570	0.426224	-1.724227
1	-0.625066	1.669922	-1.703883
7	0.760970	-1.720630	-1.420373
1	0.824955	-2.288730	-2.260860
1	1.702541	-1.666507	-1.019702
1	0.179133	-2.236912	-0.758306
7	2.961818	1.760883	0.218725
1	3.450779	2.648364	0.270326
1	2.580657	1.545450	1.138048
1	2.153227	1.873593	-0.396207
7	3.658957	-1.196775	-0.217891
1	4.149217	-1.512493	0.614380
1	3.602571	-0.172165	-0.165674
1	4.256976	-1.430027	-1.005595
7	-2.374705	-1.209002	-1.325013
1	-2.140508	-2.072172	-0.833869
1	-1.490557	-0.879850	-1.712059
1	-2.978617	-1.447997	-2.105949
7	-2.631487	1.962799	-1.022411
1	-2.920924	0.985377	-1.023116
1	-3.429552	2.532812	-1.281918
1	-2.366580	2.200092	-0.067469
7	-2.207557	-0.201733	1.696926
1	-3.023861	-0.169878	2.300713
1	-1.792006	0.733349	1.702304
1	-2.537342	-0.366457	0.743871
7	-1.042788	-3.022087	0.984292
1	-1.342351	-2.158813	1.447774
1	-0.143316	-3.286095	1.377256
1	-1.697286	-3.754468	1.244331
7	-0.467606	2.457733	1.309874
1	-0.492012	3.444387	1.549074
1	-0.073061	2.374682	0.370251
1	0.203724	2.002719	1.926324
7	0.990022	-0.185564	1.451736
1	0.157447	-0.542572	1.917031
1	1.665652	-0.941841	1.367726
1	0.703019	0.029417	0.495349

 Cartesian coordinates of : AM10_12

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.631311	-0.450579	-2.118850
1	3.134067	-0.115594	-1.294027
1	3.292820	-0.950348	-2.705365
1	2.330017	0.366754	-2.642936
7	-2.649768	0.359616	1.473459
1	-3.294581	0.356554	2.258440
1	-1.696772	0.309039	1.850914
1	-2.706454	1.279709	1.028762
7	1.472502	-2.219965	0.351520
1	0.462352	-2.405255	0.386192
1	1.939668	-3.103507	0.536100
1	1.697429	-1.952101	-0.607738
7	0.415473	0.307704	2.071093
1	0.799388	1.110857	1.568609
1	0.861043	-0.536031	1.707310
1	0.671972	0.396637	3.049416
7	-1.648556	-2.533696	0.384445
1	-1.944449	-2.459457	-0.586700
1	-2.053650	-1.723071	0.856751
1	-2.079667	-3.366630	0.773815
7	-0.401512	0.074693	-1.183565
1	0.393852	-0.434439	-1.568507
1	-1.252056	-0.300761	-1.606494
1	-0.458462	-0.174354	-0.194735
7	1.591365	2.252564	-0.135568
1	2.496400	1.787167	-0.171839
1	0.942770	1.721013	-0.720318
1	1.694806	3.178041	-0.539558
7	3.637535	0.030991	0.852016
1	4.548939	-0.376617	1.039206
1	3.452258	0.697107	1.597582
1	2.938088	-0.712297	0.938569
7	-1.695932	2.757750	-0.228356
1	-0.949039	3.018519	0.411645
1	-1.923956	3.575899	-0.783649
1	-1.300420	2.044572	-0.843607
7	-3.451383	-0.569762	-1.443573
1	-3.344990	-0.346445	-0.449488
1	-4.214800	-1.233242	-1.534494
1	-3.743829	0.283067	-1.912201

 Cartesian coordinates of : AM10_13

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.245658	-3.146401	0.159040
1	-0.298856	-2.647211	1.044378
1	-0.212772	-4.138422	0.374248
1	0.650899	-2.891291	-0.268659
7	-0.090416	2.909217	-1.368940
1	0.164821	2.570569	-2.293340
1	-1.003877	2.500937	-1.141001
1	-0.218958	3.913696	-1.450566
7	-2.855519	-1.701458	-0.972410
1	-2.835284	-1.746558	-1.988163
1	-3.674783	-2.229055	-0.683629
1	-2.033411	-2.218255	-0.640595
7	-2.746941	1.445745	-0.382065
1	-2.531326	1.454838	0.614576
1	-2.975582	0.470279	-0.597121
1	-3.587100	1.998733	-0.522314

7	2.695896	1.227682	-0.926169
1	2.837676	0.830211	0.004361
1	2.069335	2.025884	-0.820311
1	3.590080	1.579333	-1.253884
7	2.530326	-2.014137	-0.968540
1	2.504041	-1.110465	-1.442584
1	3.164644	-2.613175	-1.488131
1	2.957205	-1.813472	-0.065176
7	-0.064620	-0.215565	-0.840960
1	-0.060894	-1.124134	-1.295945
1	-0.898120	0.288636	-1.134882
1	0.756249	0.296788	-1.162240
7	-1.537902	-0.220407	1.916110
1	-0.959575	-0.303864	1.072816
1	-0.995324	-0.552162	2.708410
1	-2.337254	-0.836741	1.798822
7	0.412214	2.212062	1.768370
1	0.464799	3.114058	2.231095
1	-0.473078	1.776406	2.023391
1	0.376379	2.387016	0.762899
7	1.989374	-0.441622	1.644612
1	1.257258	-0.720517	0.989782
1	1.681532	0.462967	2.012270
1	2.014010	-1.110840	2.408168

Cartesian coordinates of : AM10_14

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.591625	0.070860	1.788870
1	-1.108176	0.829471	1.299298
1	-2.588989	0.265518	1.705204
1	-1.346438	0.130693	2.772542
7	1.822067	0.508465	-1.700011
1	1.938328	0.408860	-2.703655
1	2.748608	0.465259	-1.279084
1	1.289277	-0.297627	-1.361164
7	-4.070384	1.252282	0.259668
1	-3.822735	2.127323	0.713130
1	-3.380049	1.073677	-0.476774
1	-4.967560	1.401875	-0.192633
7	3.258816	-1.977238	0.074901
1	3.814257	-2.617088	0.635279
1	3.198333	-2.378176	-0.857447
1	3.790671	-1.107194	-0.014497
7	-0.331559	2.180328	-0.238409
1	-1.166079	1.941834	-0.773524
1	0.463189	1.891274	-0.818973
1	-0.297383	3.190109	-0.138222
7	-3.452421	-1.903627	0.138200
1	-2.663611	-1.849929	0.780227
1	-4.051431	-1.115282	0.381557
1	-3.960200	-2.761235	0.328166
7	0.066143	-1.689954	-0.260408
1	-0.507791	-2.456693	-0.600697
1	-0.442075	-1.247250	0.510240
1	0.936194	-2.076364	0.104987
7	-2.049655	0.042220	-1.810555
1	-1.090925	-0.204617	-1.559768
1	-2.606182	-0.773568	-1.541589
1	-2.086185	0.129643	-2.821882
7	4.468271	0.986611	0.144262
1	5.326093	0.927309	0.684771
1	3.686940	1.109886	0.799219
1	4.536848	1.828241	-0.420701
7	1.848740	0.542302	1.596801
1	1.549015	0.501301	2.565964
1	1.927435	-0.416834	1.259227
1	1.101874	0.993845	1.067559

 Cartesian coordinates of : AM10_15

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.709379	-0.962711	-0.696556
1	4.525690	-1.239914	-0.158010
1	3.726163	0.061447	-0.768559
1	3.844528	-1.334910	-1.632870
7	3.087745	2.060940	-0.460622
1	2.354978	2.418522	-1.066668
1	3.688502	2.842612	-0.218438
1	2.635162	1.722179	0.394302
7	1.936169	0.286291	1.791201
1	2.372469	-0.467616	1.260762
1	2.358157	0.281401	2.715634
1	0.957149	0.014093	1.908012
7	0.970909	-2.641011	0.067683
1	1.005093	-3.655220	0.081599
1	0.435882	-2.349441	-0.746938
1	1.918712	-2.291999	-0.078611
7	-2.768100	1.615100	-1.341458
1	-3.030114	2.335857	-2.005319
1	-2.686018	0.726340	-1.838443
1	-1.850067	1.846565	-0.963993
7	-0.500287	2.082081	0.852590
1	0.413219	2.293274	1.247015
1	-1.134448	2.832247	1.111348
1	-0.816956	1.225846	1.317068
7	-1.010511	-0.897076	1.861092
1	-1.961711	-0.841300	1.487272
1	-1.087118	-1.294812	2.793301
1	-0.472783	-1.563715	1.299649
7	0.569635	0.073703	-1.364198
1	0.212644	0.785457	-0.721911
1	1.490708	-0.194398	-1.019974
1	0.708919	0.527271	-2.263395
7	-2.185859	-1.398393	-1.586159
1	-1.219549	-1.069833	-1.514778
1	-2.186218	-2.324872	-1.999610
1	-2.561560	-1.470698	-0.643034
7	-3.939770	-0.199077	0.838611
1	-3.709814	0.576010	0.206156
1	-4.330474	0.197623	1.688358
1	-4.686313	-0.726949	0.394784

 Cartesian coordinates of : AM10_16

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.387501	-0.277950	-1.569653
1	2.157899	0.715004	-1.433368
1	2.853764	-0.589960	-0.720403
1	3.067165	-0.331806	-2.322808
7	-2.593181	-0.110171	-1.398790
1	-3.210055	-0.075387	-2.205448
1	-3.085613	-0.614959	-0.664546
1	-1.795406	-0.702931	-1.653413
7	1.653179	2.574666	-0.686080
1	1.948051	2.377623	0.269188
1	0.636870	2.710449	-0.680106
1	2.079940	3.451169	-0.969150
7	-1.476708	2.741986	-0.513948
1	-1.658687	2.723206	0.486524
1	-1.858812	1.870582	-0.893840
1	-2.000630	3.516286	-0.909671

7	-0.144139	-2.051892	-1.843504
1	0.683779	-1.442218	-1.813942
1	-0.052228	-2.711079	-1.074735
1	-0.093761	-2.590940	-2.703334
7	3.067752	0.752898	1.675152
1	3.881848	1.067755	1.154566
1	3.246307	0.950823	2.655065
1	3.011928	-0.263257	1.568305
7	-2.118173	-2.176392	0.930885
1	-1.243121	-1.650987	0.845006
1	-2.232704	-2.722436	0.081859
1	-2.022296	-2.827729	1.703769
7	0.026112	0.077198	0.715277
1	0.867202	0.548400	1.053542
1	-0.038850	0.297212	-0.278176
1	-0.776201	0.530157	1.159312
7	2.128634	-2.183499	0.933137
1	1.256388	-1.652191	0.844920
1	2.012678	-2.866028	1.675768
1	2.271932	-2.695351	0.067311
7	-2.939687	0.794122	1.718111
1	-2.949184	-0.223009	1.620293
1	-3.391134	1.173755	0.890177
1	-3.506090	1.041070	2.523233

Cartesian coordinates of : AM10_17

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.222152	-0.226660	-1.299677
1	-3.211206	0.704799	-0.876107
1	-4.123325	-0.356052	-1.749384
1	-2.515052	-0.191213	-2.030655
7	2.171616	-2.237827	-1.624111
1	1.988047	-2.291686	-0.621560
1	2.988691	-2.806742	-1.823837
1	1.382619	-2.674900	-2.092787
7	0.994452	-2.091791	1.437169
1	0.382778	-2.642557	0.832324
1	0.359270	-1.393325	1.833988
1	1.291531	-2.697281	2.197541
7	-1.467292	-0.050449	1.875410
1	-2.078304	0.074501	2.677677
1	-2.054525	0.049099	1.046495
1	-0.809709	0.737045	1.868790
7	3.006292	0.143853	0.288613
1	2.512207	-0.593484	0.800197
1	3.939495	0.224313	0.682042
1	3.107297	-0.219403	-0.658779
7	-0.010745	0.005239	-0.933165
1	0.764531	-0.350135	-1.493222
1	-0.567844	-0.815899	-0.688075
1	0.417820	0.308369	-0.057302
7	0.794494	2.129548	1.646006
1	0.764409	2.774290	0.853710
1	1.645080	1.585348	1.494588
1	0.929209	2.677717	2.490584
7	-2.023352	2.396313	-0.275804
1	-1.243925	1.838408	-0.633606
1	-1.775940	2.644412	0.678455
1	-2.042332	3.261501	-0.807893
7	-1.827758	-2.654528	0.117937
1	-1.816489	-2.343476	1.087971
1	-2.242673	-3.580828	0.088596
1	-2.459871	-2.010594	-0.367136
7	1.508059	2.683845	-1.260233
1	2.003251	3.255205	-1.936571
1	0.826185	2.117299	-1.759009
1	2.173487	2.032470	-0.842049

 Cartesian coordinates of : AM10_18

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.829649	-3.411821	-0.219364
1	-0.945940	-4.102055	0.516366
1	-1.017333	-3.880574	-1.100606
1	0.156893	-3.128090	-0.226696
7	-0.191618	2.770494	-0.410684
1	-0.239533	3.778833	-0.299221
1	-1.085082	2.461084	-0.799631
1	-0.144056	2.360975	0.519608
7	-3.455145	-1.319783	0.052148
1	-4.326825	-1.837428	0.103674
1	-3.333109	-0.825493	0.938314
1	-2.699183	-2.001731	-0.032457
7	-3.066299	1.401209	-1.352943
1	-3.877709	2.005034	-1.253317
1	-3.344459	0.460494	-1.041848
1	-2.874168	1.339577	-2.349428
7	2.058810	0.837969	-1.691654
1	2.973792	0.905620	-1.240551
1	1.489947	1.636457	-1.397642
1	2.205816	0.927816	-2.692461
7	2.017595	-2.059307	-0.183776
1	2.045050	-1.302564	-0.871766
1	2.841414	-2.635780	-0.327844
1	2.122165	-1.600345	0.719889
7	1.847555	0.690863	1.739953
1	0.980614	0.371044	1.293295
1	1.667953	0.814339	2.731872
1	2.051817	1.609205	1.352108
7	-0.471119	-0.211380	-0.080817
1	-0.668310	-1.211066	-0.066037
1	-1.304306	0.242519	-0.451888
1	0.269941	-0.064611	-0.769193
7	4.534454	0.271129	0.170907
1	3.786741	0.154398	0.857905
1	5.306797	0.752277	0.620435
1	4.865817	-0.651043	-0.093569
7	-2.477731	0.984759	1.925721
1	-2.638817	1.615837	1.143171
1	-1.545091	0.597852	1.789214
1	-2.488794	1.528491	2.781866

 Cartesian coordinates of : AM10_19

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.232696	2.057254	0.156876
1	-2.045587	1.670295	0.640235
1	-1.269599	3.064598	0.290763
1	-0.399028	1.732958	0.651272
7	1.514990	1.236728	1.803829
1	2.402060	0.946236	1.385806
1	1.085337	0.368336	2.120634
1	1.718472	1.796515	2.626629
7	3.597664	0.182027	-0.370209
1	3.276257	1.054276	-0.795553
1	3.238083	-0.559720	-0.968778
1	4.610981	0.161136	-0.428775
7	-1.543118	-1.399901	0.870228
1	-0.573852	-1.312245	1.183223
1	-1.951563	-2.150900	1.421094
1	-2.048036	-0.550188	1.124159

7	0.293206	-3.325687	-0.894565
1	0.151019	-4.172433	-1.434384
1	0.733407	-2.623930	-1.489188
1	-0.617266	-2.944387	-0.641304
7	1.681873	2.728441	-1.014296
1	2.107820	3.646620	-1.093860
1	0.750422	2.787128	-1.420505
1	1.541262	2.520675	-0.024340
7	0.839989	-0.364299	-1.323483
1	0.905760	-0.368914	-0.305141
1	1.192403	0.547106	-1.612648
1	-0.158078	-0.355659	-1.524806
7	1.605491	-1.845661	1.459255
1	1.865495	-2.297307	2.331363
1	1.348690	-2.581945	0.793390
1	2.441968	-1.385740	1.098567
7	-4.038587	0.662312	0.918985
1	-4.599617	1.503698	1.014786
1	-4.555464	-0.084084	1.374771
1	-3.978890	0.436625	-0.079068
7	-2.721148	-0.018750	-1.718761
1	-2.126736	0.788826	-1.525595
1	-2.708310	-0.214805	-2.713406
1	-2.321056	-0.810030	-1.214356

Cartesian coordinates of : AM10_20

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.243929	-0.819167	0.118113
1	-2.801578	-0.447817	-0.729933
1	-3.007762	-1.807574	0.157263
1	-4.249215	-0.760471	-0.016950
7	-2.067158	1.417507	2.035016
1	-2.795382	1.905407	2.547513
1	-1.477828	0.952644	2.720387
1	-2.515563	0.686590	1.473926
7	-1.840488	0.403576	-2.427152
1	-1.079565	-0.038275	-2.936275
1	-1.433027	1.166031	-1.870331
1	-2.453968	0.826007	-3.117904
7	-0.723178	2.626034	-0.567830
1	0.275826	2.572987	-0.384499
1	-1.179372	2.358847	0.309676
1	-0.952181	3.597206	-0.756315
7	2.461039	-1.685299	0.750774
1	1.667671	-1.672568	1.389235
1	2.069041	-1.561151	-0.182225
1	2.869780	-2.613996	0.788376
7	1.397610	0.190262	-1.636514
1	1.179074	0.582890	-0.715953
1	2.413458	0.260903	-1.718731
1	1.003765	0.833509	-2.318768
7	1.148968	1.047350	1.420138
1	2.036958	0.777582	1.835887
1	0.509875	0.261453	1.570652
1	0.778180	1.834691	1.945256
7	-0.524812	-2.276834	-1.247836
1	-0.196834	-3.153301	-1.642218
1	0.161320	-1.550271	-1.480264
1	-1.381339	-2.021797	-1.733512
7	-0.634575	-1.620906	1.789224
1	-1.583131	-1.276853	1.922148
1	-0.519201	-2.417397	2.410080
1	-0.601928	-1.968127	0.822500
7	4.128352	0.751207	-0.298697
1	3.792217	-0.030319	0.267964
1	3.639935	1.584935	0.015059
1	5.117973	0.882126	-0.118688

Cartesian coordinates of : AM10_21

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.020332	-2.105415	1.456252
1	-0.778265	-2.161301	0.818087
1	0.837943	-2.495861	0.978147
1	-0.185352	-2.721562	2.238160
7	-0.260666	2.794263	1.735637
1	-0.130723	3.377146	2.556761
1	-0.216806	3.404887	0.924836
1	0.530171	2.148445	1.677189
7	-2.756657	-1.692212	-0.130309
1	-3.044088	-1.258949	-1.010355
1	-2.919293	-1.019566	0.623841
1	-3.359392	-2.493526	0.028700
7	-2.071574	0.225946	2.283443
1	-2.448569	0.127353	3.221259
1	-1.745857	1.188430	2.182332
1	-1.241639	-0.366187	2.218284
7	1.916616	0.431439	1.243904
1	1.329581	-0.343018	1.572942
1	2.312950	0.120597	0.354959
1	2.688228	0.527914	1.898158
7	-2.811789	0.053089	-2.814431
1	-3.459805	0.808288	-3.013742
1	-1.936169	0.466517	-2.495439
1	-2.629957	-0.427163	-3.689800
7	-0.693330	0.605583	-0.619569
1	-1.452707	1.129116	-0.183166
1	0.071533	0.668337	0.053324
1	-1.006709	-0.366663	-0.571786
7	2.113100	-0.287815	-1.957057
1	2.398569	0.692930	-1.993460
1	2.396449	-0.721170	-2.831396
1	1.093605	-0.259399	-1.949067
7	2.733248	-2.706385	-0.000023
1	2.657969	-1.921447	-0.652137
1	2.941944	-3.542471	-0.536562
1	3.530317	-2.532134	0.604315
7	1.715416	2.624491	-1.204324
1	1.776492	3.625516	-1.354271
1	1.891441	2.429585	-0.221218
1	0.765264	2.314473	-1.403566

Cartesian coordinates of : AM10_22

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.635465	-2.301884	-0.503008
1	-3.180350	-3.103907	-0.201552
1	-1.866365	-2.657032	-1.064394
1	-2.230490	-1.856463	0.329099
7	0.989061	-1.750046	0.035162
1	0.667338	-2.696909	0.213469
1	0.316528	-1.303540	-0.593863
1	1.888191	-1.803831	-0.453955
7	-4.168390	0.468185	-0.452230
1	-4.785475	0.621665	-1.244850
1	-4.763930	0.417296	0.369857
1	-3.750661	-0.459798	-0.570283
7	-0.934330	0.009297	-1.803585
1	-1.091910	0.980047	-1.527609
1	-1.846172	-0.441188	-1.848017
1	-0.542284	0.010765	-2.740288

7	1.175175	-0.540207	2.908423
1	2.056295	-0.054438	3.049401
1	1.222826	-1.008439	1.995112
1	1.117906	-1.258082	3.624425
7	-1.636686	-0.212578	1.479795
1	-0.885212	-0.189920	2.171425
1	-2.370404	0.419440	1.787918
1	-1.246237	0.185673	0.625888
7	4.132417	1.610532	-0.531135
1	4.253118	2.286447	-1.279177
1	3.190028	1.738215	-0.145292
1	4.799409	1.854986	0.194360
7	-1.886735	2.615876	-0.297117
1	-1.691124	2.846435	0.673396
1	-2.121931	3.485158	-0.766745
1	-2.719176	2.015346	-0.309968
7	3.826854	-1.426438	-1.295573
1	3.927244	-1.536111	-2.300031
1	4.575758	-1.961634	-0.866629
1	3.993083	-0.438362	-1.076102
7	1.211746	1.507898	0.493969
1	0.944569	1.573696	1.474137
1	1.156713	0.512814	0.274488
1	0.467197	1.957225	-0.037118

Cartesian coordinates of : AM10_23

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.204798	-0.581418	-2.163110
1	1.102047	-0.945930	-1.841312
1	0.230541	-0.570972	-3.178411
1	0.146120	0.388905	-1.846941
7	-0.116886	2.304920	-0.661231
1	-0.489275	3.163667	-1.055243
1	0.455639	2.567217	0.141543
1	-0.909900	1.750231	-0.318334
7	3.087542	-1.613468	-0.658536
1	3.350369	-1.828135	0.300285
1	3.145672	-0.592956	-0.755988
1	3.802273	-2.020002	-1.255112
7	2.880248	1.513215	-0.900716
1	2.804292	2.021803	-0.017328
1	2.028890	1.746105	-1.411791
1	3.667225	1.900169	-1.412952
7	-2.214670	0.069115	-0.066266
1	-1.804353	-0.439744	-0.849429
1	-2.288369	-0.589859	0.712326
1	-3.158351	0.353995	-0.329747
7	1.917998	2.472651	2.039419
1	1.259084	3.067436	2.533492
1	1.572115	1.509106	2.096429
1	2.791986	2.519077	2.555129
7	0.797466	-0.180597	1.105139
1	-0.175335	0.053670	0.898025
1	0.843335	-1.196649	1.045925
1	1.336633	0.158388	0.308497
7	-1.482551	-1.998540	2.220778
1	-0.853404	-1.454504	2.804995
1	-0.907507	-2.525136	1.558088
1	-1.962060	-2.660326	2.822047
7	0.200854	-3.083083	-0.247326
1	-0.315351	-2.480982	-0.889981
1	-0.001004	-4.047054	-0.494820
1	1.184205	-2.905324	-0.458894
7	-5.272720	1.041148	-0.633094
1	-5.885059	0.316776	-0.272604
1	-5.581341	1.265185	-1.573196
1	-5.403675	1.868244	-0.060103

Cartesian coordinates of : AM10_24

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.501457	1.688830	-0.037892
1	-0.419257	2.028220	-0.325096
1	1.200262	2.367287	-0.330207
1	0.697441	0.832623	-0.556723
7	-1.809413	-0.570294	-0.387043
1	-1.846746	0.388356	-0.731103
1	-1.381758	-1.141606	-1.119618
1	-1.160291	-0.560340	0.398434
7	-2.542444	2.653006	-0.666541
1	-2.506889	3.499561	-0.105641
1	-3.334543	2.097076	-0.325114
1	-2.766652	2.942117	-1.614385
7	-4.604815	0.494829	0.275361
1	-4.917889	0.425130	1.238382
1	-3.833821	-0.166951	0.142783
1	-5.378104	0.197267	-0.311017
7	0.310267	-0.292349	2.357730
1	0.314120	0.516929	1.727466
1	-0.235555	-0.043289	3.177519
1	1.274358	-0.411710	2.661596
7	2.108085	-1.165497	-0.200633
1	2.751599	-1.939249	-0.349492
1	2.499402	-0.591956	0.552325
1	1.248960	-1.585916	0.156654
7	0.025064	-2.431355	-2.164587
1	0.054118	-3.082774	-2.941162
1	0.057724	-2.954560	-1.288924
1	0.860957	-1.853485	-2.193648
7	-0.477578	-3.013448	0.929716
1	-0.275651	-2.251006	1.583054
1	-1.455764	-2.916265	0.665979
1	-0.379431	-3.890793	1.430835
7	3.268518	1.368170	-1.650559
1	4.183542	1.174681	-2.046349
1	2.737042	1.857147	-2.364755
1	2.807440	0.471293	-1.476869
7	3.165569	1.236296	1.522971
1	3.423371	1.542133	0.582119
1	3.875892	1.561989	2.170449
1	2.293145	1.710777	1.742843

Cartesian coordinates of : AM10_25

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.648529	2.671004	0.171886
1	0.653742	3.686801	0.158244
1	1.581399	2.366310	0.460921
1	0.557072	2.355500	-0.792525
7	3.075770	-1.598647	0.433565
1	3.666055	-2.311006	0.851993
1	2.165674	-1.626857	0.902045
1	2.898868	-1.876367	-0.529030
7	-1.750293	1.201183	1.565573
1	-1.926370	1.434232	2.538647
1	-2.594207	1.437736	1.039030
1	-0.991295	1.808357	1.234103
7	0.199288	-1.481587	1.811660
1	-0.603750	-2.095545	1.667679
1	-0.195479	-0.539422	1.776373
1	0.532607	-1.627125	2.760745

7	3.566361	1.417186	0.770202
1	4.410052	1.743652	0.308088
1	3.546434	0.392214	0.697973
1	3.666107	1.649053	1.754463
7	1.826159	0.579541	-2.004310
1	2.326680	0.850643	-1.158301
1	2.421653	0.806289	-2.794601
1	1.711199	-0.435623	-1.974031
7	-1.286715	0.352373	-1.469747
1	-1.096116	0.338732	-0.465881
1	-0.370936	0.469256	-1.911319
1	-1.781476	1.228241	-1.627476
7	-2.528670	-1.856700	0.547718
1	-2.355196	-1.678717	-0.439237
1	-3.447567	-2.276215	0.641504
1	-2.529762	-0.945875	1.009564
7	0.524472	-2.187729	-1.408986
1	0.391701	-2.025892	-0.408837
1	0.531849	-3.194180	-1.545934
1	-0.308544	-1.824845	-1.868919
7	-4.217155	0.881513	-0.450006
1	-3.633314	0.266433	-1.014290
1	-4.741396	1.479736	-1.081143
1	-4.889905	0.297523	0.037264

Cartesian coordinates of : AM10_26

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.436235	-3.014290	0.512308
1	2.160952	-2.509134	-0.004290
1	1.471502	-2.675233	1.469767
1	1.682751	-3.998880	0.525435
7	-2.684485	0.261238	-0.275709
1	-3.697855	0.278234	-0.386668
1	-2.341976	1.218151	-0.283990
1	-2.450611	-0.125826	0.637586
7	2.974553	-0.989025	-1.345455
1	3.473326	-0.096202	-1.300648
1	2.013208	-0.780868	-1.625504
1	3.396183	-1.537704	-2.089206
7	-0.216123	-1.168410	-1.514826
1	-0.348934	-1.662984	-2.392618
1	-1.133255	-0.807814	-1.231190
1	0.084873	-1.861259	-0.825798
7	-0.854199	-1.123115	1.999437
1	-0.952052	-1.912930	1.364552
1	0.118725	-0.808089	1.902507
1	-0.968414	-1.487463	2.941129
7	3.736103	1.981338	-0.807480
1	4.106266	2.685230	-1.438250
1	2.716183	2.084896	-0.776163
1	4.100110	2.186513	0.117706
7	-1.007226	2.046150	1.847651
1	-0.350303	2.372478	2.550318
1	-1.100236	1.034019	1.959179
1	-1.907877	2.461833	2.065640
7	0.591422	1.870156	-0.862617
1	0.355970	2.489453	-1.633144
1	0.364899	0.918430	-1.166521
1	-0.035435	2.097700	-0.086324
7	1.947234	0.104195	1.443127
1	2.492865	-0.426168	0.761321
1	2.596437	0.442069	2.147890
1	1.603415	0.917112	0.930893
7	-5.799312	0.003180	-1.058436
1	-6.314125	0.809329	-1.396797
1	-6.416082	-0.518782	-0.444779
1	-5.589920	-0.586039	-1.858044

Cartesian coordinates of : AM10_27

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.462693	1.195175	1.640652
1	0.072546	0.354818	1.869099
1	0.224285	1.875888	1.314675
1	-0.864202	1.552149	2.502597
7	-0.848067	-2.525479	0.441866
1	-0.343256	-2.007082	1.160674
1	-1.344253	-3.279809	0.906953
1	-1.550716	-1.883228	0.060211
7	1.832362	-0.984921	1.684140
1	2.449015	-0.221657	1.408170
1	2.027417	-1.744623	1.022146
1	2.137374	-1.295254	2.602529
7	2.001624	-2.918680	-0.737364
1	2.058243	-2.262915	-1.512793
1	1.003101	-3.036467	-0.536471
1	2.375866	-3.809306	-1.047833
7	-2.554337	-0.061994	-0.446580
1	-1.985486	0.427316	0.248939
1	-2.330189	0.345930	-1.349836
1	-3.540389	0.117303	-0.258000
7	3.546467	0.154769	-0.729700
1	2.643557	-0.018524	-1.188329
1	4.199352	0.489609	-1.432148
1	3.887099	-0.750896	-0.415166
7	0.598251	-0.230855	-1.347826
1	-0.040128	-0.937971	-1.706864
1	0.212592	0.679952	-1.608710
1	0.497016	-0.286094	-0.333075
7	2.228802	2.716481	0.568247
1	2.645125	3.507646	0.083895
1	2.707927	1.877581	0.223322
1	2.482926	2.821201	1.547238
7	-0.533688	2.689491	-1.203177
1	-1.272136	2.469149	-0.539655
1	-0.790344	3.540617	-1.692146
1	0.306578	2.873055	-0.653756
7	-5.752109	-0.120923	0.012343
1	-6.062852	-0.088858	0.977594
1	-5.774185	-1.090876	-0.286015
1	-6.428171	0.389908	-0.545453

Cartesian coordinates of : AM10_28

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.991877	1.326635	1.137992
1	3.452267	0.608147	0.570499
1	3.657286	1.657905	1.829438
1	2.240401	0.849174	1.634269
7	-2.599436	0.406035	-0.832643
1	-3.604777	0.434505	-0.654497
1	-2.134381	1.005312	-0.142282
1	-2.450008	0.830065	-1.744169
7	1.590452	3.115198	-0.921728
1	1.484569	4.084682	-0.637748
1	2.098837	3.124667	-1.801412
1	2.180597	2.642431	-0.224164
7	-0.647137	1.841036	1.129056
1	-0.727874	2.492209	1.903930
1	-0.064424	2.283662	0.416987
1	-0.131254	1.026600	1.463815

7	-1.794323	-2.272771	0.481592
1	-2.078748	-3.073899	-0.076128
1	-2.038987	-1.432648	-0.059766
1	-2.395383	-2.272798	1.301826
7	0.874772	-1.051358	1.833231
1	-0.004509	-1.482083	1.534836
1	0.962824	-1.203930	2.834248
1	1.603827	-1.606284	1.383249
7	1.238923	-2.951303	-0.629956
1	1.117648	-2.176770	-1.284181
1	1.365181	-3.802823	-1.168070
1	0.357640	-3.030044	-0.123255
7	0.671306	0.032865	-1.222047
1	0.951136	-0.040178	-0.242432
1	-0.322693	-0.197872	-1.230451
1	0.730413	1.028978	-1.437080
7	3.646420	-0.938208	-0.886444
1	2.913787	-0.575704	-1.496291
1	3.306914	-1.843394	-0.565152
1	4.482597	-1.091073	-1.440398
7	-5.770347	0.511111	-0.147821
1	-5.863693	1.092746	0.678627
1	-6.172189	-0.395397	0.067551
1	-6.334550	0.929137	-0.880429

Cartesian coordinates of : AM10_29

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.843644	2.851842	0.036840
1	-1.691057	2.068283	0.682724
1	-1.309840	3.648034	0.372345
1	-2.824844	3.111252	0.084763
7	-4.313954	0.302918	0.511874
1	-3.895287	0.919755	1.201845
1	-5.257503	0.629690	0.331272
1	-3.767990	0.395341	-0.349945
7	-1.438224	0.125133	1.507332
1	-0.465778	-0.132976	1.694148
1	-1.729121	-0.414432	0.691719
1	-1.991470	-0.235752	2.280787
7	-3.024107	-2.373748	-0.339907
1	-3.134050	-1.903191	-1.236127
1	-3.612118	-1.842662	0.304051
1	-3.413144	-3.307663	-0.423772
7	-2.161871	0.364098	-1.835416
1	-1.905990	1.295803	-1.500028
1	-1.368141	-0.251967	-1.646887
1	-2.266859	0.424018	-2.843952
7	1.005432	1.329321	-0.586599
1	0.886236	1.357878	0.424157
1	0.391032	2.049781	-0.958987
1	0.600614	0.433965	-0.866294
7	6.528534	0.340726	-0.298252
1	6.853666	0.302929	0.662235
1	7.204385	-0.155009	-0.870129
1	6.538005	1.313507	-0.587518
7	3.426306	-0.567034	-0.450354
1	4.421269	-0.340945	-0.423424
1	3.291929	-1.251292	-1.188728
1	2.909332	0.271762	-0.723734
7	0.035214	-1.745360	-0.641894
1	0.550681	-1.568422	0.220118
1	0.576396	-2.411383	-1.184717
1	-0.852298	-2.190817	-0.390529
7	1.671171	-0.649331	2.049720
1	2.378158	-0.718494	1.304136
1	1.751765	-1.481567	2.627521
1	1.938038	0.134623	2.639543

Cartesian coordinates of : AM10_30

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	5.142723	0.622204	-0.322323
1	5.004195	-0.391196	-0.316962
1	5.626539	0.868125	-1.180026
1	5.760954	0.859813	0.446641
7	0.081773	-1.892329	0.625531
1	-0.568579	-1.418248	1.251556
1	0.589275	-2.584634	1.167798
1	0.756613	-1.198811	0.296710
7	-4.305774	0.740979	-0.767586
1	-3.409491	0.675208	-1.255367
1	-4.720279	-0.187086	-0.776852
1	-4.915061	1.356131	-1.296361
7	-0.070436	1.365453	2.069359
1	0.600101	0.744359	2.516262
1	-0.302607	2.077202	2.757136
1	-0.920418	0.813141	1.909319
7	3.696630	-2.126521	-0.178604
1	3.527928	-2.835922	-0.884549
1	2.942157	-1.438993	-0.235169
1	3.637013	-2.583909	0.725633
7	0.015334	3.123935	-0.662307
1	0.937241	3.521931	-0.813079
1	-0.650468	3.890248	-0.668279
1	0.008874	2.703615	0.269120
7	1.994564	0.541817	-0.315318
1	1.635948	0.858992	-1.212524
1	2.970723	0.845505	-0.253004
1	1.452208	1.042873	0.388207
7	-1.267137	0.327417	-1.344097
1	-0.598134	-0.350237	-1.702287
1	-0.847596	1.254047	-1.445301
1	-1.320585	0.155296	-0.339545
7	-2.686022	-0.348787	1.584268
1	-3.042673	-0.550782	2.514569
1	-2.859722	-1.178073	1.005813
1	-3.294559	0.366469	1.177400
7	-2.681448	-2.348937	-0.799668
1	-2.680413	-1.638156	-1.528123
1	-3.058628	-3.205335	-1.191611
1	-1.702001	-2.508186	-0.551915

Cartesian coordinates of : AM10_31

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.383526	1.279784	1.257419
1	3.306817	0.262320	1.266633
1	4.279703	1.493863	0.826903
1	3.416341	1.605138	2.218378
7	-1.122766	-1.931307	0.991009
1	-1.062893	-2.218332	1.963535
1	-0.707723	-2.674607	0.436670
1	-0.548938	-1.088739	0.869215
7	-5.551442	-0.365143	-1.159077
1	-4.585180	-0.315428	-1.496986
1	-5.975755	-1.207415	-1.533485
1	-6.063424	0.424652	-1.538077
7	-2.331580	2.256255	0.574182
1	-1.996584	2.871458	1.310384
1	-2.973979	2.806900	0.010993
1	-2.883056	1.508182	1.018426

7	5.582890	-0.520584	-0.231387
1	6.212854	-0.343614	0.545242
1	4.780184	-1.041306	0.128926
1	6.079157	-1.126094	-0.878460
7	3.133578	0.754212	-1.798789
1	2.808482	1.456364	-1.137022
1	4.110300	0.575487	-1.559578
1	3.102069	1.160671	-2.728168
7	0.415509	0.639886	0.188364
1	0.632795	0.489157	-0.794730
1	1.215156	1.137874	0.581659
1	-0.402102	1.253242	0.230506
7	-2.471193	-0.234954	-1.460576
1	-2.219575	-0.943787	-0.771571
1	-1.875405	-0.372822	-2.271242
1	-2.217859	0.658975	-1.040451
7	-3.856347	-0.229148	1.486181
1	-4.594748	-0.318104	0.783627
1	-4.269859	-0.415195	2.394331
1	-3.166267	-0.958652	1.304871
7	2.623587	-1.596808	0.155696
1	2.611698	-1.094874	-0.736914
1	1.743934	-1.356635	0.610887
1	2.603512	-2.594030	-0.035656

Cartesian coordinates of : AM10_32

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.694029	1.312493	1.805242
1	1.368511	0.550015	1.943646
1	1.142373	2.002339	1.205796
1	0.539625	1.752763	2.707494
7	-1.425048	-2.351482	-0.837036
1	-2.186820	-3.001515	-0.665313
1	-1.406507	-2.174791	-1.841482
1	-1.683624	-1.456583	-0.405621
7	2.796839	-0.947525	1.648957
1	3.283679	-0.470350	0.892080
1	2.307266	-1.756486	1.252630
1	3.496262	-1.299505	2.295122
7	1.134900	-3.415407	0.585913
1	1.579804	-4.100878	-0.017455
1	0.284315	-3.092065	0.108588
1	0.839681	-3.911602	1.421887
7	-1.979408	0.585895	0.220636
1	-1.193320	0.809607	0.838171
1	-1.920900	1.220724	-0.571325
1	-2.847189	0.792015	0.717073
7	3.457474	1.642148	-0.253274
1	3.751716	1.915250	0.680596
1	4.227062	1.851661	-0.881762
1	2.671789	2.244523	-0.512487
7	-1.374597	-0.253232	-3.107644
1	-0.600619	-0.040939	-2.474498
1	-2.237319	0.022359	-2.648762
1	-1.270348	0.305073	-3.948076
7	0.966709	-0.291102	-0.993402
1	1.917605	0.037048	-0.816833
1	0.509899	-0.347274	-0.082847
1	1.031420	-1.253417	-1.317701
7	0.591026	2.770493	-1.014586
1	0.467691	1.776888	-1.228033
1	0.480595	3.293309	-1.878041
1	-0.167168	3.044985	-0.395862
7	-4.752473	0.813793	1.862504
1	-5.412232	1.584118	1.835998
1	-4.504653	0.655957	2.833933
1	-5.234754	-0.015757	1.531911

Cartesian coordinates of : AM10_33

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.105263	3.005263	-0.142833
1	2.058418	2.657939	-0.016258
1	1.163252	4.012308	-0.258176
1	0.573399	2.824115	0.712397
7	-0.409549	-2.838062	0.644097
1	-1.133924	-3.549125	0.655136
1	-0.135712	-2.672111	-0.328174
1	0.413137	-3.220940	1.109467
7	-0.439882	1.358816	-2.214829
1	-1.405568	1.677212	-2.198149
1	-0.097682	1.533764	-3.156126
1	0.086614	1.981530	-1.584166
7	0.932569	-1.517535	-1.890831
1	1.753693	-1.162078	-1.405729
1	0.337547	-0.702276	-2.062139
1	1.236691	-1.868619	-2.793929
7	-2.143195	-0.132910	0.181977
1	-3.136241	-0.260984	-0.015182
1	-1.786780	-1.000283	0.585164
1	-1.658208	-0.020650	-0.707052
7	-1.049901	2.124404	2.033717
1	-1.487280	1.414418	1.430177
1	-1.669309	2.929726	2.054335
1	-1.039734	1.748603	2.977975
7	-5.365895	-0.448909	-0.146046
1	-5.691228	-0.036923	0.722537
1	-5.832635	0.033026	-0.907237
1	-5.674269	-1.415498	-0.161734
7	1.049783	-0.028133	0.791450
1	0.431353	-0.821162	0.980341
1	0.922123	0.618579	1.568765
1	0.628244	0.457860	-0.002196
7	2.665904	-2.801952	0.803661
1	2.574998	-3.108736	-0.160359
1	3.635975	-2.911996	1.078466
1	2.428399	-1.810321	0.837304
7	3.766873	1.262593	0.057989
1	4.139462	0.986714	-0.844793
1	3.054128	0.583279	0.332677
1	4.527347	1.217611	0.728188

Cartesian coordinates of : AM10_34

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.857583	-1.436047	1.833053
1	1.759480	-2.085091	2.606551
1	2.025176	-1.970561	0.982286
1	0.981015	-0.926627	1.727077
7	0.603441	-1.239109	-1.357313
1	0.429908	-1.219843	-2.358073
1	-0.161364	-1.760080	-0.926705
1	1.461549	-1.776284	-1.211931
7	3.555005	-2.336488	-0.753021
1	3.714446	-1.322915	-0.709942
1	4.108212	-2.759191	-0.012953
1	3.930295	-2.679937	-1.631973
7	3.073790	0.596712	-0.208802
1	3.350720	1.577413	-0.214812
1	2.930278	0.293746	0.754266
1	2.176420	0.499395	-0.680668

7	-5.621898	0.556118	-0.534518
1	-4.857748	0.052313	-0.995414
1	-6.196179	-0.121067	-0.042783
1	-6.204346	0.972739	-1.253827
7	-2.794451	-0.318338	-1.337101
1	-2.379480	-1.123993	-0.868613
1	-2.580867	0.494948	-0.759609
1	-2.305675	-0.198941	-2.219092
7	-0.351017	0.679707	0.967253
1	0.346838	1.332707	1.313937
1	-1.230765	1.190481	0.870805
1	-0.046608	0.379565	0.037779
7	-1.475887	-2.220392	0.888285
1	-1.200674	-1.305791	1.256630
1	-2.369502	-2.472988	1.299701
1	-0.792981	-2.896246	1.219666
7	4.406475	3.541277	-0.311606
1	5.171392	3.267016	-0.919660
1	4.804655	3.800622	0.584898
1	3.977694	4.370370	-0.708988
7	-3.271272	2.100918	0.822038
1	-3.223576	3.057377	0.482527
1	-3.334631	2.155930	1.834901
1	-4.156070	1.704423	0.486145

Cartesian coordinates of : AM10_35

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.510456	2.229475	-1.573103
1	-0.492927	2.338839	-1.635977
1	-1.714509	1.310520	-1.958985
1	-1.936155	2.920949	-2.182665
7	-1.641407	2.210703	1.562744
1	-2.235843	2.929049	1.964767
1	-2.071691	1.309905	1.758224
1	-1.665576	2.317115	0.542264
7	1.644391	2.223861	-1.549003
1	2.073893	1.324838	-1.754105
1	1.668357	2.319448	-0.527463
1	2.239612	2.945882	-1.943204
7	1.513175	2.212526	1.587410
1	1.717019	1.290678	1.966428
1	0.495636	2.321731	1.650682
1	1.938791	2.899317	2.202304
7	-4.244708	-3.175549	-0.074311
1	-3.700756	-4.008937	-0.272115
1	-4.666113	-3.293745	0.841080
1	-4.994987	-3.129675	-0.755738
7	2.240046	-0.604718	-0.024307
1	1.561353	-0.666550	0.739780
1	2.871299	-1.403463	0.043908
1	2.786943	0.234214	0.151946
7	-0.033093	-0.556363	2.250058
1	-0.140506	-1.335166	2.892912
1	-0.783056	-0.624353	1.551641
1	-0.210749	0.296544	2.774909
7	0.031331	-0.534774	-2.259812
1	0.135391	-1.309066	-2.908638
1	0.781568	-0.610655	-1.562488
1	0.211314	0.321518	-2.778304
7	-2.241740	-0.602617	0.013317
1	-2.790343	0.236590	-0.156179
1	-2.871388	-1.402071	-0.061153
1	-1.562753	-0.656956	-0.751093
7	4.242934	-3.178563	0.065788
1	4.431186	-3.471628	-0.887182
1	3.786228	-3.950247	0.540618
1	5.135446	-3.022503	0.522367

 Cartesian coordinates of all the proposed isomers of ammonia clusters (NH₃)_n=2-10 at MP2/6-31++G(d,p) level of theory

Cartesian coordinates of ammonia dimer: (NH₃)₂

Cartesian coordinates of : NH3_N2_2.log

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7.0	-1.672416	0.000000	-0.099941
1.0	-0.689906	-0.000002	0.160913
1.0	-2.108960	-0.816367	0.309707
1.0	-2.108959	0.816366	0.309706
7.0	1.558958	0.000000	0.035708
1.0	1.526855	0.000098	-0.977305
1.0	2.087558	-0.815243	0.323227
1.0	2.087622	0.815145	0.323385

Cartesian coordinates of ammonia trimer: (NH₃)₃

Cartesian coordinates of : NH3_N3_2.log

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.727259	1.677926	-0.000011
1	-1.073226	2.174029	0.813451
1	-1.144814	0.747171	-0.000070
1	-1.073274	2.174162	-0.813372
7	1.816773	-0.209147	0.000020
1	2.419656	-0.157526	0.813285
1	1.219490	0.617841	0.000086
1	2.419273	-0.157650	-0.813537
7	-1.089508	-1.468777	-0.000003
1	-1.346166	-2.016554	-0.813392
1	-1.346314	-2.016415	0.813432
1	-0.074668	-1.365074	0.000079

Cartesian coordinates of ammonia tetramer: (NH₃)₄

Cartesian coordinates of : CY4

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.134740	-0.618723	-0.151696
1	2.805893	-0.922624	0.545324
1	2.549015	-0.822702	-1.054751
1	1.305745	-1.209996	-0.056885
7	-0.618721	-2.134731	0.151697
1	-1.210002	-1.305742	0.056889
1	-0.822690	-2.549011	1.054752
1	-0.922617	-2.805886	-0.545325
7	-2.134741	0.618716	-0.151696
1	-2.549021	0.822692	-1.054750
1	-1.305747	1.209989	-0.056890
1	-2.805891	0.922622	0.545326
7	0.618722	2.134739	0.151696
1	0.922627	2.805887	-0.545329
1	1.209990	1.305741	0.056888
1	0.822705	2.549018	1.054749

Cartesian coordinates of : P4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.540719	-1.476443	1.149284
1	-1.406509	-1.975887	1.322649
1	0.175604	-1.951239	1.688557
1	-0.304517	-1.587434	0.160923
7	0.360852	-0.769719	-1.712072
1	1.271592	-0.495550	-1.353536
1	-0.218096	0.065716	-1.678320
1	0.472403	-1.039906	-2.682217
7	1.785119	0.858567	0.598655
1	2.443538	1.156136	1.308760
1	1.023180	0.370880	1.059965
1	1.392712	1.689186	0.170686
7	-1.538968	1.349978	-0.111810
1	-1.490417	2.207915	0.425936
1	-1.320551	0.578498	0.515810
1	-2.502937	1.245008	-0.407615

Cartesian coordinates of : BC4_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.890320	1.581699	0.332849
1	2.464085	2.166181	-0.264573
1	1.622201	2.151504	1.127214
1	1.041660	1.341784	-0.183886
7	-0.441691	0.064164	-1.098729
1	-1.369220	-0.031511	-0.690399
1	0.123241	-0.727395	-0.795480
1	-0.549283	-0.005683	-2.104415
7	-3.330840	-0.062771	0.442178
1	-3.932424	0.718558	0.208667
1	-3.058247	0.046709	1.412054
1	-3.892759	-0.903796	0.380352
7	1.976961	-1.595148	0.262485
1	2.753866	-1.992265	-0.253335
1	1.947880	-2.068094	1.158430
1	2.185754	-0.611602	0.433887

Cartesian coordinates of ammonia pentamer: (NH3)5

Cartesian coordinates of : MP2_AM5_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.148530	-0.781362	0.964641
1	1.839127	-0.554926	1.903526
1	3.020593	-1.289640	1.062369
1	1.460839	-1.423309	0.563333
7	-0.076250	-2.496942	-0.458428
1	-0.901442	-1.903219	-0.343140
1	-0.329824	-3.427812	-0.145345
1	0.104595	-2.569729	-1.453879
7	-2.533337	-0.548740	-0.020680
1	-3.159642	-0.434650	-0.810541
1	-2.116913	0.366886	0.166431
1	-3.119714	-0.776587	0.775216
7	1.588532	1.612729	-0.996322
1	2.359049	2.265974	-1.085638

1	1.439083	1.214307	-1.916893
1	1.896249	0.853954	-0.383662
7	-1.105717	2.226533	0.511881
1	-0.861578	2.392600	1.482406
1	-1.554625	3.074350	0.182212
1	-0.228101	2.126277	-0.004035

Cartesian coordinates of : MP2_AM5_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.695861	-2.082414	0.623687
1	-1.349458	-1.303387	0.511691
1	-0.646568	-2.294974	1.614717
1	-1.107452	-2.896768	0.179967
7	-2.327672	0.546283	0.107120
1	-2.730764	0.627561	-0.820182
1	-1.527573	1.181638	0.150901
1	-3.027442	0.893148	0.754353
7	0.339132	2.224858	0.387285
1	0.961515	1.469942	0.687205
1	0.261446	2.878168	1.159892
1	0.822723	2.721976	-0.353680
7	0.689731	-0.365669	-1.944432
1	0.309274	-1.006834	-1.253222
1	0.505775	-0.746423	-2.865152
1	0.168461	0.499557	-1.859133
7	2.092005	-0.330166	0.822992
1	1.400711	-1.074589	0.874670
1	2.888799	-0.597665	1.389391
1	2.389201	-0.301601	-0.147985

Cartesian coordinates of : MP2_AM5_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.304684	2.045427	-0.255844
1	-1.127535	1.434740	-0.264253
1	-0.203775	2.418204	-1.194754
1	-0.523807	2.840729	0.335788
7	1.000550	0.086921	1.992895
1	0.330578	0.132002	2.752570
1	0.717433	0.771597	1.293736
1	1.893510	0.382144	2.371301
7	1.987606	-0.071293	-1.404516
1	2.668136	-0.411399	-0.734893
1	1.409198	0.616552	-0.928735
1	2.496839	0.406299	-2.139017
7	-2.559960	-0.114417	-0.263497
1	-3.212218	-0.245656	0.502118
1	-1.878512	-0.878405	-0.223929
1	-3.095340	-0.227989	-1.117608
7	-0.142009	-2.052515	-0.122060
1	0.423045	-1.772454	-0.920522
1	-0.098081	-3.063142	-0.052713
1	0.330017	-1.662086	0.692065

Cartesian coordinates of : MP2_AM5_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.528176	-1.543265	0.658146
1	2.711174	-0.548183	0.536114

1	3.332998	-2.054262	0.314054
1	2.464885	-1.730164	1.652335
7	2.228033	1.473655	-0.277421
1	1.980440	2.289188	0.271172
1	1.364235	1.040416	-0.600468
1	2.731626	1.809449	-1.090742
7	-0.078874	-0.657157	-1.009356
1	-0.998164	-1.017397	-0.750013
1	0.623585	-1.202112	-0.508001
1	0.041296	-0.863735	-1.996102
7	-1.618708	1.700250	0.549000
1	-1.166616	1.916346	1.429983
1	-1.784197	2.580234	0.074405
1	-0.968927	1.152918	-0.013469
7	-3.086279	-1.059098	0.070715
1	-3.309083	-1.610190	0.891641
1	-3.910464	-1.063544	-0.519165
1	-2.919215	-0.099661	0.370667

Cartesian coordinates of : MP2_AM5_5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.490174	1.351105	1.438209
1	-0.715442	1.988720	2.193292
1	0.178478	0.678381	1.798216
1	-1.333479	0.831600	1.201334
7	-2.662375	-0.292348	-0.272864
1	-1.893546	-0.150413	-0.926902
1	-3.427047	0.309782	-0.557469
1	-2.987793	-1.246429	-0.381467
7	0.090906	0.677457	-1.612518
1	1.083874	0.448282	-1.608374
1	-0.037440	1.318281	-0.829876
1	-0.093247	1.189585	-2.468944
7	2.809300	0.094086	-0.104747
1	2.830804	0.989109	0.370580
1	3.738472	-0.304941	-0.040554
1	2.169076	-0.514508	0.401206
7	0.309097	-1.783614	0.524718
1	0.556236	-2.740039	0.294953
1	0.069240	-1.305588	-0.340840
1	-0.535455	-1.818621	1.085263

Cartesian coordinates of : MP2_AM5_6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.827999	-1.231549	0.334487
1	1.870675	-1.540470	0.154406
1	3.039329	-1.440879	1.303964
1	3.447989	-1.805836	-0.225893
7	-0.222756	-1.721462	-0.302470
1	-0.812888	-2.368666	0.208605
1	-0.405997	-1.879194	-1.287491
1	-0.541356	-0.777341	-0.082006
7	2.113332	1.761208	-0.353822
1	2.323104	1.948346	-1.328498
1	2.479715	0.831207	-0.138742
1	2.650725	2.430560	0.186601
7	-0.931573	1.341636	0.351690
1	-1.075905	1.660849	1.304612
1	-1.526281	1.921690	-0.232255
1	0.039239	1.562504	0.112462
7	-3.840990	-0.068195	-0.059471
1	-4.310773	-0.318963	0.801519

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1    -2.851426    0.044316    0.135970
1    -3.948233   -0.839577   -0.706147
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Cartesian coordinates of ammonia hexamer: (NH₃)₆

Cartesian coordinates of : MP2_AM6_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.440792	-1.095558	1.488676
1	-1.519084	-0.087761	1.353300
1	-0.586741	-1.251086	2.013827
1	-2.211433	-1.393318	2.077153
7	1.440792	1.095555	-1.488680
1	1.519087	0.087758	-1.353303
1	2.211429	1.393314	-2.077164
1	0.586737	1.251081	-2.013825
7	1.440798	-1.837019	-0.204354
1	0.586741	-2.369581	-0.076529
1	1.519031	-1.215880	0.600741
1	2.211440	-2.495532	-0.167925
7	-1.440681	-0.741528	-1.693160
1	-1.518983	-1.128188	-0.752695
1	-0.586597	-1.118516	-2.090397
1	-2.211285	-1.102329	-2.245289
7	1.440684	0.741533	1.693166
1	2.211288	1.102334	2.245296
1	0.586600	1.118520	2.090402
1	1.518988	1.128194	0.752701
7	-1.440802	1.837017	0.204352
1	-0.586747	2.369584	0.076527
1	-2.211447	2.495526	0.167923
1	-1.519031	1.215878	-0.600743

Cartesian coordinates of : MP2_AM6_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.604489	-0.012173	2.052063
1	-0.684751	-0.150091	3.053107
1	0.365836	0.207486	1.846950
1	-0.825510	-0.893265	1.589190
7	-2.404279	1.128626	-0.248908
1	-2.545947	2.130089	-0.328901
1	-1.905557	0.953217	0.626192
1	-3.326545	0.716718	-0.151967
7	1.953334	-1.534851	-0.209514
1	1.947964	-2.200686	0.556404
1	2.021435	-0.605303	0.205158
1	2.812105	-1.695836	-0.725402
7	-1.213243	-2.045925	-0.268723
1	-0.234603	-2.015823	-0.547384
1	-1.693292	-1.294945	-0.754398
1	-1.607360	-2.923008	-0.588799
7	0.312385	0.866601	-1.928297
1	0.651877	-0.089536	-1.886221
1	0.272922	1.135124	-2.905177
1	-0.642142	0.868001	-1.568780
7	1.915155	1.599688	0.621652
1	1.422616	1.616884	-0.275041
1	2.835776	2.000911	0.477086
1	1.423147	2.226300	1.250079

Cartesian coordinates of : MP2_AM6_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.400343	2.118960	-0.340143
1	1.697075	2.904965	0.228798
1	1.539663	2.400020	-1.305185
1	2.037351	1.340927	-0.152695
7	0.343110	-2.213198	-0.384504
1	-0.097695	-1.477961	-0.947345
1	-0.398188	-2.652173	0.152437
1	0.678798	-2.923922	-1.026877
7	-0.987466	0.244440	-1.743953
1	-1.132062	0.488659	-2.717457
1	-0.445481	0.992377	-1.318704
1	-1.899711	0.239303	-1.287608
7	-0.457825	0.305293	1.685869
1	-0.266253	0.600842	2.637126
1	-0.026871	0.986646	1.063063
1	0.046031	-0.563060	1.533724
7	2.948206	-0.531780	0.345813
1	3.243923	-0.635141	1.310603
1	3.710163	-0.880357	-0.225904
1	2.150071	-1.153648	0.203156
7	-3.329382	0.091793	0.384191
1	-3.807214	-0.774695	0.603919
1	-3.952662	0.846931	0.646438
1	-2.495835	0.151726	0.971599

Cartesian coordinates of : MP2_AM6_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.352710	-1.247749	-0.094691
1	1.918231	-1.647371	0.730730
1	3.054644	-1.903556	-0.418311
1	1.619775	-1.185998	-0.797810
7	-0.153423	0.028071	-1.718861
1	0.350167	0.793940	-1.276347
1	-1.144784	0.204232	-1.545484
1	-0.006913	0.111648	-2.719713
7	-0.615720	0.824313	1.632351
1	0.154543	1.270364	1.137757
1	-0.436014	-0.177602	1.626619
1	-0.579359	1.138048	2.595947
7	2.112782	1.852582	0.074744
1	2.463479	0.893212	0.094192
1	2.491665	2.340542	0.879275
1	2.500892	2.307847	-0.744565
7	-2.950369	0.759172	-0.445542
1	-3.334126	1.662282	-0.701503
1	-2.339271	0.897339	0.363108
1	-3.732713	0.185001	-0.151622
7	-0.767169	-2.193145	0.566287
1	-0.439916	-3.137952	0.396955
1	-0.624525	-1.661413	-0.291067
1	-1.767450	-2.253280	0.721828

Cartesian coordinates of : MP2_AM6_5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.278215	-1.613878	1.312605

1	1.129377	-1.577335	0.750492
1	0.462777	-2.225342	2.100452
1	0.119711	-0.679896	1.683687
7	-1.271512	1.220172	-1.588054
1	-0.628340	1.160252	-2.371292
1	-2.069901	1.752841	-1.918493
1	-1.597875	0.267141	-1.399924
7	1.550862	1.821448	-0.010542
1	0.655706	1.860377	-0.492980
1	1.998900	2.725316	-0.113475
1	1.328381	1.702892	0.972793
7	2.747679	-1.032235	-0.633137
1	2.498542	-0.045859	-0.543178
1	2.647440	-1.293609	-1.607411
1	3.730378	-1.127855	-0.403173
7	-2.041263	-1.694881	-0.746279
1	-1.889372	-2.411891	-1.448034
1	-2.929427	-1.913858	-0.307254
1	-1.311617	-1.808406	-0.034764
7	-1.200656	1.229508	1.711888
1	-1.256974	1.297414	0.697665
1	-1.358612	2.157762	2.088140
1	-1.972364	0.649111	2.021384

Cartesian coordinates of : MP2_AM6_6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.794529	-0.938451	-0.443028
1	3.691192	-0.837992	0.020931
1	2.909610	-1.673526	-1.132579
1	2.116179	-1.259968	0.252763
7	0.412015	-1.088857	1.509994
1	0.485194	-0.073895	1.542039
1	0.350601	-1.426216	2.464210
1	-0.467142	-1.319849	1.050960
7	-2.033280	1.630051	0.072820
1	-1.376286	1.379470	-0.665821
1	-1.481800	1.930062	0.869548
1	-2.579194	2.426286	-0.236066
7	1.429687	1.867184	0.593611
1	0.888649	2.350817	-0.114803
1	1.982072	1.166251	0.104103
1	2.073477	2.543327	0.990082
7	-2.525190	-1.442445	0.088937
1	-2.633013	-0.430573	0.183181
1	-3.004538	-1.882935	0.866833
1	-3.020367	-1.726676	-0.749663
7	-0.089487	-0.034487	-1.791529
1	0.892850	-0.129684	-1.544602
1	-0.162632	-0.193466	-2.790783
1	-0.582768	-0.792402	-1.325965

Cartesian coordinates of : MP2_AM6_7

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.053788	-0.242752	1.980746
1	0.567010	-1.044748	1.948982
1	-0.047192	0.091869	2.938685
1	0.381283	0.475484	1.404695
7	0.236456	-2.047479	-1.018068
1	0.366084	-3.000873	-1.337040
1	-0.467050	-2.066046	-0.287783
1	1.108921	-1.735166	-0.593690
7	-2.952904	-0.130189	0.630126

1	-3.570451	0.444869	1.192062
1	-2.085309	-0.257480	1.152282
1	-3.399949	-1.035732	0.540190
7	-1.070154	0.748808	-1.808470
1	-0.628879	-0.163422	-1.919904
1	-1.425913	1.032113	-2.714928
1	-1.871720	0.598970	-1.195958
7	0.973828	2.169881	-0.026972
1	0.280988	1.810925	-0.696536
1	1.671295	2.680392	-0.559900
1	0.504428	2.864118	0.546489
7	2.796471	-0.504658	0.122025
1	3.417325	-0.477401	-0.679519
1	3.386640	-0.559955	0.944935
1	2.303122	0.386805	0.161230

Cartesian coordinates of : MP2_AM6_8

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.120089	-1.313572	-1.025284
1	0.119682	-1.831143	-1.898234
1	0.101276	-0.328349	-1.270147
1	-0.768227	-1.514476	-0.560728
7	-2.691088	-1.590529	0.422202
1	-2.968031	-0.642459	0.160037
1	-2.748644	-1.658038	1.432423
1	-3.385703	-2.229513	0.051235
7	-0.120093	1.313568	1.025278
1	0.768225	1.514475	0.560729
1	-0.101280	0.328342	1.270133
1	-0.119690	1.831132	1.898232
7	2.896343	-1.418825	0.442047
1	1.969427	-1.541667	0.027422
1	2.813563	-1.587448	1.438628
1	3.498128	-2.147719	0.074781
7	-2.896343	1.418823	-0.442058
1	-2.813561	1.587439	-1.438640
1	-1.969427	1.541666	-0.027433
1	-3.498127	2.147722	-0.074798
7	2.691091	1.590536	-0.422184
1	2.748652	1.658057	-1.432404
1	2.968032	0.642463	-0.160030
1	3.385706	2.229514	-0.051207

Cartesian coordinates of : MP2_AM6_9

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.322395	1.215330	0.014541
1	-3.206081	1.349375	0.493333
1	-2.157339	0.212358	-0.050451
1	-2.438947	1.566087	-0.929988
7	0.658543	2.129980	-0.715936
1	1.355141	1.550368	-0.258098
1	-0.213228	2.033512	-0.201482
1	0.960628	3.094589	-0.646395
7	-0.285372	-0.262205	2.144995
1	-0.814431	-0.836432	1.492021
1	-0.663087	0.675260	2.049377
1	-0.503578	-0.579357	3.083391
7	2.572763	-0.345125	0.845112
1	3.211108	0.315024	1.276259
1	3.001057	-1.259551	0.943077
1	1.709403	-0.346738	1.393523
7	0.921009	-0.748490	-1.946987

1	0.685457	0.222905	-2.137930
1	1.340557	-1.130978	-2.787501
1	1.646617	-0.702733	-1.232995
7	-1.500007	-1.928939	-0.410891
1	-1.239328	-2.808199	0.024624
1	-0.710688	-1.634156	-0.996769
1	-2.275046	-2.145191	-1.029832

Cartesian coordinates of : MP2_AM6_10

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.109825	-0.702344	1.673402
1	-0.127428	-1.058683	2.623220
1	0.811726	-0.917807	1.292911
1	-0.785374	-1.242925	1.140684
7	1.799874	1.722224	-0.572681
1	2.070902	2.488931	-1.177574
1	1.334405	2.122049	0.234309
1	1.121056	1.142634	-1.068153
7	2.868092	-1.009749	0.420181
1	3.470493	-1.030965	1.236088
1	2.800122	-0.039995	0.105009
1	3.349865	-1.533462	-0.302845
7	0.109841	-0.702473	-1.673322
1	0.127499	-1.058920	-2.623098
1	-0.811726	-0.917902	-1.292849
1	0.785370	-1.242981	-1.140505
7	-2.868094	-1.009773	-0.420170
1	-3.470430	-1.030948	-1.236127
1	-2.800147	-0.040030	-0.104957
1	-3.349930	-1.533517	0.302792
7	-1.799889	1.722237	0.572591
1	-1.121095	1.142689	1.068145
1	-2.070909	2.489027	1.177383
1	-1.334393	2.121951	-0.234438

Cartesian coordinates of : MP2_AM6_11

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.168428	-0.073207	1.959775
1	0.403777	-0.515918	2.840986
1	0.275102	-0.766020	1.221392
1	-0.817047	0.164023	1.996862
7	1.181470	1.802799	-0.368428
1	2.005780	1.301973	-0.695436
1	1.050004	1.498228	0.595782
1	1.421515	2.788710	-0.354735
7	3.238249	-0.624378	-0.201827
1	3.483848	-0.446280	0.765297
1	3.926263	-1.268764	-0.573851
1	2.333476	-1.091251	-0.212956
7	0.249322	-1.401129	-0.987781
1	0.515827	-2.015391	-1.750344
1	0.302008	-0.447704	-1.336701
1	-0.732157	-1.589283	-0.776884
7	-2.756608	-1.379553	-0.040988
1	-3.565670	-1.637540	-0.594798
1	-2.660650	-0.363300	-0.077531
7	-1.992956	1.671912	-0.415710
1	-2.186110	2.393089	0.271953
1	-2.428673	1.981913	-1.278374
1	-0.982649	1.684375	-0.571699
1	-2.959978	-1.645967	0.915753

Cartesian coordinates of : MP2_AM6_12

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.130512	-2.522886	-0.758428
1	-1.637846	-3.401183	-0.761054
1	-1.053465	-2.233149	-1.727387
1	-1.718408	-1.833615	-0.283065
7	1.130482	2.522944	0.758286
1	1.718421	1.833653	0.283005
1	1.053438	2.233300	1.727273
1	1.637771	3.401268	0.760831
7	2.750308	0.282416	-0.758269
1	2.461049	0.204287	-1.727284
1	2.447236	-0.571360	-0.282977
1	3.764603	0.282190	-0.760706
7	1.619650	-2.240501	0.758355
1	2.126586	-3.119030	0.760910
1	0.728760	-2.404950	0.283006
1	1.407278	-2.028979	1.727335
7	-1.619736	2.240471	-0.758364
1	-2.126701	3.118981	-0.760911
1	-1.407421	2.028921	-1.727350
1	-0.728821	2.404955	-0.283073
7	-2.750195	-0.282451	0.758414
1	-2.460770	-0.204337	1.727380
1	-3.764490	-0.282226	0.761023
1	-2.447200	0.571327	0.283080

Cartesian coordinates of : MP2_AM6_13

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.077617	-2.089352	0.135043
1	-2.766605	-1.335651	0.103789
1	-2.047220	-2.431768	1.089266
1	-2.434746	-2.851148	-0.431302
7	0.608243	-0.656627	-0.835769
1	0.663728	-0.783119	-1.842103
1	-0.216777	-1.179235	-0.530887
1	1.426720	-1.122819	-0.442413
7	-0.989164	1.826217	0.437782
1	-0.738167	1.864171	1.419783
1	-0.703051	2.709128	0.029266
1	-0.423646	1.091909	0.009319
7	3.485487	-1.356367	0.480832
1	3.562397	-0.343572	0.398729
1	4.286841	-1.770570	0.018794
1	3.555160	-1.597155	1.462894
7	-3.829252	0.535275	-0.026649
1	-4.199150	0.774979	-0.939782
1	-2.983206	1.089032	0.120404
1	-4.518920	0.834865	0.653443
7	2.790056	1.654395	-0.202860
1	2.552692	2.395490	0.446473
1	1.930751	1.161463	-0.439958
1	3.138928	2.099210	-1.044374

Cartesian coordinates of : MP2_AM6_14

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.892584	0.614757	-0.291027

1	-3.752783	0.545720	0.242365
1	-3.141343	1.048389	-1.174003
1	-2.271416	1.261311	0.199299
7	-0.441643	2.200052	0.822077
1	0.005946	1.779815	0.008184
1	0.023640	1.828060	1.643023
1	-0.263658	3.197914	0.804792
7	0.306054	0.298884	-1.621286
1	0.431409	0.482394	-2.611546
1	-0.677316	0.081350	-1.481869
1	0.819326	-0.557150	-1.397888
7	-1.458026	-2.096106	0.734128
1	-1.917876	-2.933846	0.394009
1	-1.918304	-1.300054	0.292523
1	-1.657047	-2.039295	1.727168
7	2.900932	0.910641	0.431964
1	3.005169	1.844645	0.810576
1	2.139611	0.930464	-0.240989
1	3.750567	0.697011	-0.078034
7	1.648620	-1.995789	-0.067118
1	0.708346	-2.134720	0.303673
1	2.147014	-1.369134	0.558602
1	2.125247	-2.889954	-0.061048

Cartesian coordinates of : MP2_AM6_15

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.174862	-1.746266	-0.958659
1	3.039288	-2.277514	-0.962061
1	1.599183	-2.138406	-1.696513
1	1.698342	-1.949043	-0.076776
7	0.398586	-2.064357	1.615343
1	0.664952	-1.598348	2.475590
1	-0.110284	-2.900062	1.881273
1	-0.245893	-1.446109	1.113212
7	2.552913	1.407263	-0.889350
1	2.382982	1.771552	-1.820875
1	2.444990	0.391321	-0.940353
1	3.529693	1.591183	-0.686096
7	0.378126	2.431299	1.178089
1	1.148616	2.169818	0.559637
1	0.679383	2.274454	2.133264
1	0.226003	3.428636	1.078753
7	-1.091946	-0.051095	-0.199426
1	-2.068611	0.012567	-0.478391
1	-0.538056	-0.107901	-1.047646
1	-0.831720	0.824430	0.254456
7	-4.340081	0.014570	-0.714254
1	-4.818962	-0.114570	-1.597836
1	-4.688679	0.874184	-0.306374
1	-4.618452	-0.746091	-0.105473

Cartesian coordinates of : MP2_AM6_16

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.062451	1.194749	0.317558
1	3.700249	1.413374	-0.440497
1	3.387601	1.719287	1.122748
1	2.148337	1.576461	0.061775
7	0.159887	2.284257	-0.348380
1	-0.427512	1.573856	0.099610
1	-0.173204	2.379334	-1.302167
1	-0.035426	3.169384	0.107790
7	0.418701	-1.257304	-1.579045

1	1.122866	-1.645276	-0.949402
1	0.780714	-0.370151	-1.912099
1	0.346531	-1.870532	-2.383132
7	2.527864	-1.900904	0.665334
1	2.781782	-0.910857	0.646154
1	3.384621	-2.441818	0.631128
1	2.095901	-2.093537	1.562092
7	-1.429916	-0.152278	0.754813
1	-1.146512	-0.577052	1.630840
1	-1.004788	-0.694657	0.002404
1	-2.440800	-0.249203	0.686164
7	-4.666041	-0.226738	0.217124
1	-5.229155	0.388805	0.792235
1	-5.144469	-1.118863	0.172452
1	-4.657356	0.158964	-0.719918

Cartesian coordinates of : MP2_AM6_17

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.163232	-0.658890	1.968250
1	1.042203	-1.024605	2.317266
1	-0.325429	-0.262650	2.763702
1	0.379431	0.105211	1.330528
7	0.565384	1.717854	-0.243042
1	-0.458360	1.775807	-0.278261
1	0.902203	1.827277	-1.195563
1	0.885533	2.544343	0.253913
7	-2.548359	1.599407	-0.271519
1	-3.106441	2.018492	0.464727
1	-2.622491	0.582564	-0.172662
1	-2.996400	1.850654	-1.146468
7	-2.253446	-1.478198	-0.005728
1	-2.928880	-2.216656	0.156418
1	-1.563226	-1.512191	0.742694
1	-1.746207	-1.701490	-0.858342
7	3.496287	0.282534	-0.108322
1	4.071055	0.582685	0.669657
1	3.546301	-0.727394	-0.157550
1	2.534990	0.543876	0.086555
7	0.541012	-1.480664	-1.476618
1	1.225885	-1.384319	-2.217533
1	0.838274	-2.243785	-0.879669
1	0.572786	-0.632117	-0.920565

Cartesian coordinates of : MP2_AM6_18

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.130920	-0.364794	2.150849
1	1.692830	-0.799802	2.873210
1	1.638560	0.445425	1.813862
1	1.063371	-1.013066	1.369354
7	-1.361915	-0.034404	0.250158
1	-2.355242	-0.155133	0.066499
1	-1.222245	-0.010382	1.255910
1	-0.872094	-0.866259	-0.066086
7	-4.589333	-0.055321	-0.403527
1	-5.196353	-0.224310	0.390102
1	-4.934147	-0.622105	-1.169480
1	-4.702674	0.915418	-0.671163
7	1.116033	-2.133252	-0.678035
1	1.612140	-3.001618	-0.507623
1	1.808497	-1.420997	-0.921041
1	0.540694	-2.290090	-1.498891
7	0.702065	2.245597	-0.173547

1	0.493054	2.915481	-0.906677
1	0.660125	2.761953	0.699288
1	-0.066660	1.567575	-0.149180
7	3.038543	0.316913	-1.067412
1	3.807813	0.331569	-0.406412
1	2.359840	1.019729	-0.764505
1	3.418306	0.623439	-1.956569

Cartesian coordinates of : MP2_AM6_19

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.861546	-0.578901	-0.389076
1	-2.168704	-1.332007	-0.339632
1	-3.092069	-0.457534	-1.370344
1	-3.708198	-0.915484	0.058385
7	-1.162634	0.888562	1.977867
1	-1.074889	0.203494	2.719994
1	-1.770418	0.493093	1.262211
1	-1.637707	1.692298	2.372939
7	-1.115386	2.123163	-1.247565
1	-0.668663	2.594648	-0.469739
1	-1.727868	1.413647	-0.855300
1	-1.691026	2.802424	-1.731088
7	1.143734	0.035045	-0.160108
1	0.700289	0.470120	0.646190
1	2.149811	0.165771	-0.081472
1	0.824125	0.566504	-0.965339
7	-0.473389	-2.587171	-0.229905
1	-0.274334	-3.148108	-1.051345
1	-0.272212	-3.173153	0.573220
1	0.191580	-1.805407	-0.218980
7	4.440211	0.142426	-0.018131
1	4.876955	0.684403	-0.754525
1	4.668730	-0.831156	-0.181135
1	4.877667	0.414585	0.854382

Cartesian coordinates of : MP2_AM6_20

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	4.375533	0.419113	-0.105415
1	4.907013	-0.442589	-0.149935
1	4.487834	0.796167	0.828484
1	4.809899	1.070566	-0.748778
7	1.118161	0.046596	-0.154249
1	0.860741	-0.917128	-0.355307
1	2.128960	0.131983	-0.238268
1	0.701527	0.612898	-0.885935
7	-0.561303	-2.760853	0.018720
1	-0.063111	-3.404390	0.623439
1	-1.260815	-3.304680	-0.474043
1	-1.050956	-2.091342	0.611123
7	-1.999589	-0.108145	-1.535647
1	-2.144484	-0.373229	-0.564291
1	-1.381547	-0.805641	-1.936353
1	-2.889471	-0.181316	-2.016473
7	-1.627917	2.598898	0.117751
1	-1.631535	1.919431	-0.640625
1	-0.661884	2.796743	0.352417
1	-2.040814	3.457576	-0.226768
7	-1.436796	-0.148063	1.681231
1	-0.458753	0.022874	1.442331
1	-1.485607	-0.368545	2.670485
1	-1.903625	0.747792	1.551763

Cartesian coordinates of : MP2_AM6_21

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.411036	-3.544774	-0.616421
1	0.535431	-3.857179	-0.432536
1	-0.665959	-3.879250	-1.538337
1	-1.017792	-4.006609	0.051027
7	0.059422	-0.414109	0.281390
1	0.983615	-0.480503	0.706354
1	-0.185458	-1.351326	-0.034016
1	-0.602296	-0.160143	1.014103
7	3.213490	0.030038	1.062792
1	3.463554	0.502416	1.923982
1	3.036906	0.741395	0.354455
1	4.024793	-0.503969	0.773391
7	-2.529431	0.874524	1.798243
1	-3.375535	0.393858	2.081393
1	-2.640789	1.160612	0.826361
1	-2.462795	1.712417	2.364591
7	-2.104158	1.259172	-1.332972
1	-2.598544	0.682971	-2.004880
1	-1.265019	0.754821	-1.046721
1	-1.811641	2.096698	-1.823425
7	1.792783	1.855832	-1.104335
1	1.076553	1.181196	-0.833437
1	1.912076	1.803320	-2.109435
1	1.445405	2.784500	-0.893744

Cartesian coordinates of : MP2_AM6_22

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.185666	-0.035661	0.940157
1	-2.487759	0.029237	1.906317
1	-3.019582	0.054826	0.363761
1	-1.589254	0.773294	0.760387
7	0.019782	2.228696	0.369755
1	0.798152	1.587759	0.550122
1	0.140309	3.033564	0.974924
1	0.118943	2.567175	-0.581086
7	2.185719	0.035795	0.940233
1	3.019642	-0.054740	0.363855
1	1.589312	-0.773176	0.760521
1	2.487797	-0.029017	1.906403
7	-0.019714	-2.228612	0.369945
1	-0.118839	-2.567180	-0.580867
1	-0.798090	-1.587657	0.550224
1	-0.140266	-3.033423	0.975185
7	-4.668703	0.036832	-1.223804
1	-5.042861	0.936727	-1.500887
1	-5.455610	-0.581976	-1.067400
1	-4.145698	-0.330861	-2.009855
7	4.668599	-0.037028	-1.223873
1	5.043411	-0.936855	-1.500294
1	5.455051	0.582504	-1.068047
1	4.145219	0.329646	-2.010150

Cartesian coordinates of : MP2_AM6_23

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.120032	1.651460	0.327865

1	-1.699965	2.347283	-0.128400
1	-1.274520	1.757040	1.324874
1	-1.479542	0.734284	0.062160
7	-1.917075	-1.353344	-0.466523
1	-0.947063	-1.562609	-0.216761
1	-2.038553	-1.631863	-1.435091
1	-2.512257	-1.966206	0.082211
7	1.120031	-1.651459	0.327868
1	1.274517	-1.757039	1.324878
1	1.479541	-0.734283	0.062163
1	1.699965	-2.347282	-0.128396
7	1.917076	1.353345	-0.466520
1	2.512257	1.966206	0.082215
1	0.947063	1.562610	-0.216760
1	2.038555	1.631864	-1.435087
7	-4.784037	0.062600	0.169691
1	-4.836219	0.818746	0.840687
1	-5.308665	0.340477	-0.650341
1	-3.812081	-0.057715	-0.096587
7	4.784038	-0.062602	0.169688
1	4.836219	-0.818747	0.840686
1	5.308663	-0.340481	-0.650344
1	3.812080	0.057714	-0.096587

Cartesian coordinates of ammonia heptamer: (NH3)7

Cartesian coordinates of : MP2_AM7_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.821503	-1.251282	-0.226265
1	2.736331	-0.303126	0.148803
1	3.299757	-1.190100	-1.119058
1	3.436030	-1.772125	0.390698
7	0.000005	-1.341010	1.613079
1	0.000007	-2.022729	2.364789
1	0.815345	-1.535319	1.035487
1	-0.815334	-1.535323	1.035488
7	-0.000002	-0.982290	-1.845757
1	-0.821273	-1.286201	-1.325920
1	0.821272	-1.286200	-1.325921
1	-0.000002	-1.490641	-2.723794
7	-1.827794	1.355673	1.101098
1	-1.238191	0.771442	1.688035
1	-2.223550	2.085028	1.683658
1	-1.209703	1.802785	0.427119
7	-0.000010	2.133193	-1.499358
1	-0.811861	2.550783	-1.942808
1	0.811834	2.550789	-1.942814
1	-0.000007	1.136262	-1.736344
7	-2.821501	-1.251285	-0.226263
1	-3.436018	-1.772137	0.390702
1	-3.299765	-1.190095	-1.119049
1	-2.736328	-0.303132	0.148814
7	1.827797	1.355681	1.101085
1	1.209700	1.802789	0.427109
1	1.238201	0.771452	1.688030
1	2.223557	2.085040	1.683638

Cartesian coordinates of : MP2_AM7_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.489115	0.029494	-2.078444
1	-0.043773	0.809958	-1.689465

1	0.458158	0.114245	-3.089276
1	1.453186	0.183746	-1.799136
7	2.374318	1.524615	0.193279
1	1.597521	1.360743	0.836154
1	3.125397	1.963727	0.714830
1	2.061292	2.198722	-0.496971
7	0.079424	0.236460	1.908837
1	0.599083	-0.602764	1.656600
1	-0.833045	0.171819	1.465894
1	-0.076180	0.213657	2.911057
7	-1.025340	-2.260197	-0.512089
1	-1.297802	-3.061439	-1.071275
1	-0.379117	-2.596372	0.194559
1	-0.498358	-1.621362	-1.112307
7	-3.031258	-0.125833	0.499082
1	-3.777954	0.024663	-0.171683
1	-3.481617	-0.382006	1.371663
1	-2.492718	-0.936639	0.179153
7	-1.118511	2.274851	-0.463434
1	-1.804131	1.617693	-0.090342
1	-1.624047	3.086016	-0.803675
1	-0.562053	2.582368	0.327265
7	2.234180	-1.694252	0.456099
1	2.027129	-2.165734	-0.417703
1	3.068475	-2.127925	0.836656
1	2.467061	-0.729075	0.224696

Cartesian coordinates of : MP2_AM7_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.352090	0.418144	1.879527
1	-1.233477	0.623385	1.412744
1	-0.544914	0.410487	2.875777
1	-0.091185	-0.531436	1.619466
7	1.265364	-2.290210	0.980775
1	1.749607	-1.765376	0.247300
1	1.331605	-3.275907	0.749041
1	1.785850	-2.165822	1.842993
7	2.306986	-0.429437	-1.302554
1	3.150096	-0.513192	-1.860087
1	2.321889	0.484485	-0.852041
1	1.521433	-0.409539	-1.945138
7	1.908894	2.136816	0.609877
1	2.795871	2.035126	1.092392
1	1.196926	1.647961	1.161699
1	1.686689	3.126745	0.628521
7	-1.400450	-1.692013	-0.912882
1	-0.996941	-0.924564	-1.446725
1	-0.699633	-1.980534	-0.234135
1	-1.554563	-2.471224	-1.542797
7	-0.538983	1.333823	-1.543269
1	0.295885	1.637197	-1.048559
1	-1.313106	1.403294	-0.886781
1	-0.709308	2.006257	-2.283503
7	-3.218933	0.503003	0.272620
1	-2.854688	-0.387482	-0.075363
1	-3.789000	0.312337	1.089692
1	-3.844558	0.876915	-0.433166

Cartesian coordinates of : MP2_AM7_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.286791	-1.527582	0.585002
1	2.298151	-1.070010	1.490208

1	2.885040	-2.343692	0.655037
1	1.330843	-1.848319	0.436477
7	-3.349395	-0.269617	0.025110
1	-2.740025	0.537245	-0.116121
1	-3.661121	-0.266405	0.989696
1	-4.174104	-0.143159	-0.550861
7	-1.096347	1.802836	-0.798370
1	-0.877478	1.198413	-1.585533
1	-0.201093	1.988203	-0.344182
1	-1.420274	2.684714	-1.182793
7	1.751979	1.902960	0.743790
1	2.071757	2.688357	1.300406
1	2.578477	1.416529	0.413040
1	1.256291	1.259151	1.361483
7	-0.699571	-1.915905	-0.558757
1	-0.765057	-2.862202	-0.920153
1	-0.251211	-1.347637	-1.276425
1	-1.655716	-1.574221	-0.450982
7	-0.345821	-0.017912	2.074927
1	-0.480068	-0.757313	1.386189
1	-0.565245	-0.404954	2.986627
1	-1.044610	0.689333	1.870908
7	1.450334	0.000100	-2.101713
1	1.537598	1.005964	-2.001422
1	1.938438	-0.414980	-1.307918
1	1.953607	-0.259175	-2.943601

Cartesian coordinates of : MP2_AM7_5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.354345	0.754120	-0.370482
1	-4.085020	0.420246	-0.989294
1	-3.797608	1.383638	0.289276
1	-2.994996	-0.047951	0.152423
7	-1.616574	-1.414847	1.032127
1	-1.049612	-0.739644	1.540832
1	-1.032016	-1.787753	0.287697
1	-1.835688	-2.179045	1.661159
7	-0.119084	1.333363	1.645327
1	-0.889833	1.920618	1.945524
1	-0.123538	1.327562	0.627278
1	0.736854	1.793885	1.935427
7	-0.414992	0.693902	-1.584186
1	-0.373800	0.916856	-2.574198
1	-1.382302	0.858300	-1.297834
1	-0.252787	-0.309389	-1.501739
7	2.300566	-0.852799	1.085642
1	3.106528	-1.141426	1.629569
1	1.546569	-0.664856	1.739276
1	2.525953	0.040496	0.646743
7	2.419739	1.819868	-0.648262
1	1.495731	1.564189	-1.001196
1	3.078504	1.738324	-1.415101
1	2.389560	2.802323	-0.398164
7	0.745988	-2.365754	-1.140850
1	0.604168	-3.348697	-0.932256
1	1.390538	-1.989132	-0.439775
1	1.213704	-2.333513	-2.040861

Cartesian coordinates of : MP2_AM7_6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.066076	-1.296751	-0.094386
1	3.227529	-2.054240	0.560587

1	3.804380	-1.355682	-0.787424
1	2.179039	-1.482248	-0.572015
7	-1.668848	-2.010595	1.132667
1	-1.450741	-1.105886	1.556537
1	-1.037167	-2.698716	1.528523
1	-2.601428	-2.267810	1.438744
7	-1.184913	1.021569	1.749025
1	-1.849128	1.134411	0.984011
1	-0.272972	1.320555	1.415202
1	-1.458091	1.649817	2.496445
7	2.086414	1.438671	1.068718
1	2.792819	2.163894	0.991845
1	2.504487	0.570599	0.720254
1	1.933453	1.303637	2.063464
7	0.259591	-1.451717	-1.422269
1	0.059741	-1.948694	-2.283730
1	0.120535	-0.459961	-1.605462
1	-0.450332	-1.728965	-0.745820
7	-2.768458	0.442091	-0.901978
1	-1.980302	0.702458	-1.487622
1	-2.644695	-0.535917	-0.657366
1	-3.613860	0.521495	-1.455232
7	0.167652	1.828470	-1.514849
1	0.774083	2.143856	-2.265125
1	0.745929	1.740610	-0.677518
1	-0.485879	2.584620	-1.336789

 Cartesian coordinates of : MP2_AM7_7

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.314353	1.038790	-1.828254
1	-0.409020	1.640314	-2.638709
1	0.312721	1.497234	-1.171998
1	-1.228032	0.974279	-1.389442
7	-2.833078	1.447248	0.384651
1	-1.996525	1.259969	0.943527
1	-3.633156	1.455069	1.008217
1	-2.750189	2.385680	0.008757
7	-0.149581	0.435025	1.592220
1	0.584795	0.963053	1.123144
1	-0.094936	-0.508755	1.218701
1	0.105062	0.382109	2.573009
7	0.443428	-1.906923	-0.952517
1	0.686219	-2.668932	-1.577675
1	0.354036	-1.063215	-1.519872
1	-0.497897	-2.097714	-0.607363
7	-2.555278	-1.768064	0.179576
1	-2.685293	-1.873737	1.180049
1	-3.281584	-2.316643	-0.267833
1	-2.734581	-0.788495	-0.035016
7	2.340835	1.846911	-0.032775
1	2.735017	0.925669	0.177304
1	2.791096	2.520620	0.578181
1	2.628003	2.083908	-0.977018
7	3.068795	-1.129544	0.587037
1	3.833583	-1.619690	0.135155
1	2.198212	-1.473379	0.170777
1	3.077090	-1.421455	1.558541

 Cartesian coordinates of : MP2_AM7_8

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.347664	-1.571135	1.050781
1	0.688845	-2.361971	1.587187

1	0.771472	-0.737411	1.448364
1	0.729146	-1.658544	0.109500
7	3.417815	0.529416	0.244428
1	2.622756	0.811166	0.818876
1	3.863161	1.379996	-0.083304
1	4.084825	0.076391	0.860156
7	0.754631	1.635652	1.682527
1	0.012225	1.385781	2.327811
1	0.350624	1.627518	0.739580
1	1.012149	2.592113	1.903091
7	-0.265555	1.174510	-1.190483
1	-1.285274	1.200090	-1.249208
1	0.021534	0.204588	-1.286713
1	0.095106	1.667898	-2.000352
7	1.919276	-1.382003	-1.767006
1	1.764875	-0.980204	-2.685370
1	2.429130	-2.246369	-1.914898
1	2.525401	-0.748172	-1.241496
7	-3.414245	1.048433	-0.965350
1	-3.324887	0.260460	-0.319987
1	-4.047865	0.769326	-1.706028
1	-3.864055	1.808435	-0.467316
7	-2.813137	-1.419085	0.916864
1	-3.156955	-1.400960	1.871234
1	-1.791712	-1.461772	0.967013
1	-3.125641	-2.298864	0.519532

 Cartesian coordinates of : MP2_AM7_9

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.754629	-1.635660	-1.682519
1	1.012147	-2.592122	-1.903079
1	0.012223	-1.385792	-2.327803
1	0.350624	-1.627522	-0.739571
7	-0.265555	-1.174504	1.190489
1	0.021533	-0.204582	1.286715
1	0.095104	-1.667888	2.000362
1	-1.285274	-1.200085	1.249213
7	0.347664	1.571131	-1.050786
1	0.688845	2.361964	-1.587196
1	0.771471	0.737404	-1.448366
1	0.729148	1.658544	-0.109507
7	-2.813137	1.419087	-0.916865
1	-3.125638	2.298864	-0.519528
1	-1.791712	1.461771	-0.967016
1	-3.156956	1.400967	-1.871235
7	-3.414248	-1.048432	0.965348
1	-3.324889	-0.260460	0.319984
1	-4.047872	-0.769325	1.706023
1	-3.864053	-1.808436	0.467314
7	3.417816	-0.529417	-0.244428
1	3.863163	-1.379996	0.083307
1	4.084825	-0.076395	-0.860160
1	2.622756	-0.811170	-0.818874
7	1.919279	1.382010	1.767000
1	1.764877	0.980213	2.685365
1	2.429135	2.246375	1.914889
1	2.525403	0.748177	1.241492

 Cartesian coordinates of : MP2_AM7_10

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.775661	2.301139	0.419385
1	2.250969	3.062509	-0.055565

1	1.817532	2.522858	1.409550
1	0.786027	2.360874	0.152994
7	-1.158193	2.171100	-0.565137
1	-0.935372	1.422026	-1.216538
1	-1.630577	2.902232	-1.085470
1	-1.828133	1.796860	0.107743
7	0.623458	-0.188509	-1.838421
1	0.654955	-1.006977	-1.235546
1	1.235983	0.502451	-1.415896
1	1.023061	-0.449260	-2.733159
7	3.169813	-0.566174	0.658485
1	3.789589	-0.517556	1.460161
1	2.763398	0.363410	0.533028
1	3.758116	-0.746241	-0.148233
7	-2.149332	-1.644794	-0.707951
1	-1.893627	-1.013167	-1.460541
1	-2.731508	-2.372632	-1.107770
1	-1.277521	-2.075861	-0.406141
7	0.703326	-2.522452	0.619428
1	1.539622	-1.940887	0.719298
1	1.017258	-3.485341	0.552548
1	0.185887	-2.447872	1.489590
7	-3.079854	0.518420	1.393683
1	-2.754465	0.312815	2.331486
1	-4.087108	0.619542	1.448709
1	-2.878240	-0.290896	0.803448

Cartesian coordinates of : MP2_AM7_11

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.776806	1.999339	-0.637833
1	2.274552	2.868224	-0.479022
1	2.212774	1.542407	-1.431040
1	1.917570	1.398477	0.170198
7	-1.097677	1.718848	0.804445
1	-1.894968	1.384026	0.260685
1	-0.412668	2.087547	0.147232
1	-1.434985	2.503163	1.353373
7	-3.530819	0.376878	-0.815766
1	-3.525847	0.271581	-1.824135
1	-4.491693	0.556434	-0.546415
1	-3.250638	-0.515234	-0.405445
7	1.199707	-0.162862	1.812531
1	0.915415	-1.127263	1.669127
1	1.402730	-0.063876	2.802423
1	0.372166	0.408824	1.614419
7	-1.979899	-1.845973	0.680174
1	-1.177515	-1.702117	0.065053
1	-2.013121	-2.823954	0.943463
1	-1.825604	-1.303023	1.522339
7	0.219608	-0.978244	-1.420142
1	0.017222	0.015344	-1.360241
1	1.232295	-1.072384	-1.351570
1	-0.049095	-1.277572	-2.351757
7	3.291903	-1.087538	-0.462261
1	4.118967	-0.526169	-0.631166
1	2.843439	-0.735687	0.382289
1	3.611607	-2.031888	-0.277843

Cartesian coordinates of : MP2_AM7_12

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.408616	1.741963	0.022034
1	-3.731701	0.774649	0.001318

1	-3.799279	2.181975	0.847486
1	-3.805347	2.218975	-0.779624
7	-3.504299	-1.432885	-0.055501
1	-3.705894	-1.970445	-0.890930
1	-2.503594	-1.230479	-0.044388
1	-3.712839	-2.030501	0.736239
7	2.138058	0.438991	-2.141215
1	3.071475	0.248634	-2.490758
1	1.656876	0.942646	-2.879045
1	2.233668	1.076755	-1.347212
7	2.095702	2.114965	0.516829
1	1.240082	2.658648	0.556139
1	1.976606	1.319005	1.145134
1	2.829732	2.700083	0.901076
7	1.482271	-2.238294	-0.487268
1	1.682713	-1.502943	-1.165473
1	1.818775	-3.115571	-0.868081
1	0.471040	-2.301731	-0.424421
7	1.892254	-0.640004	2.151349
1	1.235916	-1.002036	2.835547
1	1.899019	-1.293574	1.363504
1	2.807090	-0.680448	2.588779
7	-0.709146	0.012371	-0.015511
1	-0.111143	0.101341	0.800552
1	-1.364933	0.793196	-0.007544
1	-0.091839	0.132069	-0.813314

Cartesian coordinates of : MP2_AM7_13

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.201946	1.988294	-0.388903
1	1.328952	2.850572	-0.905831
1	0.286780	2.011926	0.052807
1	1.185099	1.219409	-1.052154
7	-2.194825	0.860833	-1.566083
1	-1.902715	1.179070	-0.641458
1	-3.131810	1.212885	-1.731775
1	-1.593196	1.303076	-2.252569
7	-1.315790	0.922680	1.479948
1	-1.530629	1.539093	2.257352
1	-0.447773	0.440983	1.715214
1	-2.044643	0.209337	1.451964
7	1.728888	-0.196096	1.818089
1	1.953935	-0.149348	2.806453
1	1.895220	0.724481	1.414257
1	2.417936	-0.805605	1.380877
7	0.318909	-1.152486	-0.997826
1	0.415955	-1.062538	0.011567
1	0.298533	-2.143776	-1.213751
1	-0.586748	-0.770209	-1.258007
7	3.489863	-0.960737	-0.699244
1	3.889818	-0.029724	-0.728121
1	2.558640	-0.911186	-1.106975
1	4.060075	-1.555259	-1.289297
7	-3.145948	-1.479881	0.439949
1	-2.615963	-2.337869	0.542979
1	-2.893427	-1.065535	-0.453843
1	-4.125340	-1.738033	0.398804

Cartesian coordinates of : MP2_AM7_14

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.275288	-0.884927	-1.325226
1	-0.491202	-1.504267	-1.112913

1	-1.464847	-0.974726	-2.317942
1	-2.095005	-1.224335	-0.822772
7	-3.733666	-0.864391	0.739401
1	-3.485579	0.121662	0.662857
1	-3.531187	-1.164282	1.686356
1	-4.736813	-0.942254	0.616052
7	-2.442381	1.892534	-0.209054
1	-1.934090	1.196397	-0.753928
1	-1.748591	2.499596	0.213903
1	-2.980696	2.462460	-0.852321
7	0.238215	0.650663	1.100062
1	0.954546	0.014187	1.434319
1	-0.218609	0.191139	0.314274
1	-0.454037	0.742182	1.835708
7	1.284484	-2.545616	-0.348761
1	2.008859	-1.910417	-0.009333
1	1.019585	-3.141364	0.428535
1	1.718126	-3.150465	-1.038154
7	3.552231	-0.460532	0.580180
1	3.308052	0.435593	0.152463
1	3.830312	-0.263126	1.536092
1	4.386209	-0.797460	0.110314
7	2.338760	2.218554	-0.568096
1	1.532262	1.970018	0.006600
1	2.613658	3.166120	-0.334914
1	2.032559	2.229351	-1.534736

Cartesian coordinates of : MP2_AM7_15

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.285793	0.551316	0.975574
1	3.387709	1.107709	1.817967
1	4.204215	0.169616	0.774703
1	2.681795	-0.239255	1.209549
7	0.705398	-1.606389	-1.615478
1	1.456843	-1.197710	-2.160082
1	0.149665	-0.839106	-1.238210
1	0.121349	-2.126441	-2.260778
7	-0.584324	0.659142	0.189528
1	-0.027301	1.333628	-0.336558
1	-0.007668	0.382916	0.979035
1	-1.400920	1.137441	0.570075
7	1.410545	-1.989029	1.414020
1	0.521673	-2.005848	1.902805
1	1.916988	-2.815793	1.712607
1	1.206607	-2.091728	0.418312
7	1.776039	2.187366	-1.287361
1	2.370951	1.697178	-0.616491
1	1.929889	3.182573	-1.169074
1	2.095560	1.953416	-2.220655
7	-3.048920	-1.127400	-0.759023
1	-3.000481	-2.112720	-0.526707
1	-2.132013	-0.715123	-0.587516
1	-3.241312	-1.064300	-1.752181
7	-3.597151	1.378736	1.109715
1	-3.970920	1.221464	2.038635
1	-3.741985	0.529705	0.564844
1	-4.152309	2.116186	0.690897

Cartesian coordinates of : MP2_AM7_16

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.540873	-1.471989	0.723212
1	-3.406599	-1.969042	0.540008

1	-2.416994	-1.472673	1.730574
1	-2.693671	-0.499061	0.445165
7	2.665498	1.601717	-0.360467
1	3.587123	2.002601	-0.223343
1	2.699641	0.638687	-0.022270
1	2.516890	1.550901	-1.363443
7	0.054336	-3.109200	-0.360365
1	-0.059301	-4.107797	-0.223275
1	0.084625	-2.955052	-1.363335
1	-0.796739	-2.657261	-0.022146
7	2.545287	-1.464396	0.723146
1	3.408587	-1.965632	0.539894
1	1.779073	-2.083185	0.445188
1	2.484023	-1.356726	1.730508
7	-0.004413	2.936346	0.723315
1	-0.002018	3.934686	0.540509
1	0.914580	2.582325	0.445169
1	-0.066980	2.829002	1.730633
7	-2.719839	1.507556	-0.360523
1	-1.902925	2.018658	-0.022301
1	-3.527834	2.105280	-0.223504
1	-2.601450	1.404190	-1.363483
7	-0.000005	-0.000023	-1.212811
1	-0.810115	-0.464584	-0.816295
1	0.002728	0.933894	-0.816437
1	0.807425	-0.469286	-0.816365

Cartesian coordinates of : MP2_AM7_17

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.223343	1.794266	-1.411613
1	0.242870	2.518939	-1.946644
1	-0.920298	1.375940	-2.018767
1	0.459428	1.063610	-1.205361
7	1.530089	-0.464907	-0.034884
1	1.093654	-0.002003	0.760492
1	2.540903	-0.400524	0.072515
1	1.282324	-1.446395	0.034158
7	-0.409912	1.457643	1.770315
1	-0.097735	2.223106	2.358084
1	-1.361777	1.239057	2.045358
1	-0.455809	1.798588	0.810115
7	-3.148846	0.528115	-0.079835
1	-2.682497	-0.004885	-0.814098
1	-2.815269	1.483111	-0.157382
1	-4.141961	0.540980	-0.285483
7	-1.233878	-1.447998	-1.715156
1	-1.206236	-1.826331	-0.767896
1	-1.474376	-2.202584	-2.348847
1	-0.285123	-1.160799	-1.933128
7	4.790401	-0.167042	0.045463
1	5.306776	-1.035073	-0.038460
1	5.167838	0.328293	0.845045
1	4.997604	0.386561	-0.777729
7	-1.440039	-1.727070	1.441508
1	-2.169186	-1.043796	1.241295
1	-1.820755	-2.420583	2.075874
1	-0.711678	-1.226272	1.940277

Cartesian coordinates of : MP2_AM7_18

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.696841	0.484997	-0.931839
1	2.709595	0.650896	0.074037

1	3.653485	0.488534	-1.267012
1	2.318901	-0.445788	-1.083186
7	1.180894	-2.103070	1.320709
1	1.093724	-2.072902	0.305000
1	0.669452	-2.918920	1.640085
1	2.158897	-2.272815	1.531200
7	0.451653	-1.766302	-1.823511
1	0.057991	-2.631460	-2.178538
1	0.747188	-1.230020	-2.632742
1	-0.302215	-1.242398	-1.366589
7	-1.383263	-0.165512	0.061664
1	-2.388775	-0.063761	0.183735
1	-1.008385	-0.575104	0.911521
1	-0.980471	0.766871	-0.017464
7	-4.658960	0.078063	0.202697
1	-5.144475	-0.365537	0.973726
1	-4.972493	1.041085	0.166772
1	-4.970431	-0.373580	-0.649302
7	0.293707	2.504338	-0.763477
1	0.658776	3.396222	-0.445972
1	-0.255181	2.697201	-1.594549
1	1.095759	1.936126	-1.044066
7	1.574536	1.007498	1.950519
1	1.661175	1.340350	2.903753
1	0.851702	1.555248	1.493675
1	1.257922	0.039676	1.978582

Cartesian coordinates of : MP2_AM7_19

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.445489	-2.156046	-0.177567
1	1.197803	-2.683282	-0.608238
1	0.108115	-2.714505	0.599877
1	0.856602	-1.309983	0.220477
7	1.588073	0.739493	0.563126
1	2.587470	0.649074	0.385832
1	1.470927	1.532560	1.185416
1	1.129557	0.975700	-0.318180
7	4.784686	0.281015	0.005360
1	5.402713	0.828492	0.593206
1	5.015496	0.499969	-0.956966
1	5.015605	-0.694138	0.156604
7	-2.714603	-1.503704	-0.185809
1	-2.887129	-0.597612	-0.611137
1	-3.434510	-2.140446	-0.507122
1	-1.818294	-1.837132	-0.531972
7	-1.303774	0.232330	2.039894
1	-1.335888	0.154918	3.050025
1	-0.334449	0.127544	1.750519
1	-1.833154	-0.542636	1.643247
7	-2.688377	1.856397	-0.239833
1	-2.249440	1.548295	0.631065
1	-3.687383	1.908283	-0.070082
1	-2.378248	2.804678	-0.424061
7	-0.274872	0.586349	-1.975299
1	-0.283005	0.737315	-2.977692
1	-0.234140	-0.415696	-1.812996
1	-1.165011	0.917776	-1.606924

Cartesian coordinates of : MP2_AM7_20

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.654747	-1.517640	2.050655
1	0.597785	-2.508226	2.264740

1	0.999125	-1.067329	2.892597
1	1.375747	-1.405697	1.330097
7	2.530002	-0.917916	-0.358621
1	2.831232	0.053966	-0.282562
1	1.817822	-0.961225	-1.085370
1	3.327646	-1.452957	-0.684302
7	2.842657	2.268841	0.025934
1	3.162298	2.679033	0.896033
1	1.823942	2.207072	0.062948
1	3.090724	2.915535	-0.714185
7	-0.080577	1.193676	0.060154
1	-1.074682	1.402612	0.063760
1	0.062414	0.551383	0.835418
1	0.078903	0.626425	-0.769175
7	-3.462791	1.748109	0.069228
1	-3.109723	2.699099	0.078349
1	-3.963567	1.627330	-0.804403
1	-4.145440	1.682055	0.816336
7	-0.190003	-1.379148	-2.174242
1	-0.654086	-0.986723	-2.986772
1	-0.901395	-1.517451	-1.452272
1	0.140179	-2.297768	-2.451630
7	-2.118621	-1.430848	0.325255
1	-1.339840	-1.415911	0.983917
1	-2.809295	-2.081891	0.682401
1	-2.537689	-0.504845	0.335526

Cartesian coordinates of : MP2_AM7_21

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.844179	-0.486188	0.672289
1	4.545808	0.164302	1.008214
1	3.407953	-0.074568	-0.156565
1	4.338339	-1.322231	0.380956
7	0.626854	-2.194911	-0.738043
1	0.624846	-1.694679	0.150790
1	1.439827	-2.801121	-0.744880
1	-0.189207	-2.796598	-0.752187
7	0.862171	-0.095823	1.667408
1	0.745340	0.828329	1.257408
1	1.856746	-0.316217	1.593759
1	0.644939	-0.014964	2.655360
7	-1.847308	0.053122	-0.254352
1	-1.519890	-0.381920	-1.110687
1	-1.266123	-0.323559	0.489457
1	-2.808767	-0.244318	-0.101624
7	1.926635	0.622489	-1.530325
1	2.085426	0.955515	-2.474748
1	1.366268	-0.226009	-1.589683
1	1.366191	1.323464	-1.049575
7	-0.216987	2.666192	-0.031566
1	-0.260429	3.322605	-0.803704
1	-0.956286	1.971213	-0.163976
1	-0.431737	3.194986	0.807104
7	-5.024659	-0.555813	0.196900
1	-5.507309	-1.133442	-0.481722
1	-5.300257	-0.882833	1.115727
1	-5.377880	0.388570	0.094403

Cartesian coordinates of : MP2_AM7_22

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.682641	-0.690673	1.995436
1	-2.231034	-0.004281	1.468985

1	-1.042670	-0.179952	2.594642
1	-2.316384	-1.186587	2.613436
7	0.575140	-0.361384	-0.383223
1	-0.017899	-0.473860	-1.200460
1	0.018432	-0.700121	0.399379
1	1.367125	-0.995594	-0.497160
7	-2.282284	-2.104310	-0.913907
1	-1.596052	-2.706283	-1.355144
1	-3.143262	-2.636558	-0.852446
1	-1.961803	-1.923374	0.034859
7	3.463472	-1.747521	-0.428992
1	3.749608	-2.457859	0.235147
1	3.697494	-0.836856	-0.035233
1	4.025613	-1.881043	-1.261859
7	3.178578	1.210952	0.670175
1	3.145323	1.445605	1.655745
1	2.233257	0.980937	0.368416
1	3.466540	2.048161	0.176590
7	-0.320056	2.689823	-0.758477
1	-0.036853	3.339787	-0.034178
1	-0.008581	3.075003	-1.642858
1	0.174976	1.812313	-0.605227
7	-2.996650	1.001789	-0.226443
1	-3.901813	1.412660	-0.425460
1	-2.285423	1.684842	-0.486133
1	-2.885508	0.192331	-0.833022

Cartesian coordinates of : MP2_AM7_23

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.191116	-0.744386	1.474947
1	2.935807	-0.951310	2.132224
1	2.463273	-1.116164	0.565483
1	1.376351	-1.282349	1.765763
7	-0.597407	-2.234794	1.043520
1	-0.651671	-1.433799	0.419681
1	-1.520832	-2.393791	1.429214
1	-0.348929	-3.049315	0.494087
7	-0.339033	0.755154	-0.109458
1	0.062154	1.416025	-0.767951
1	0.391633	0.573153	0.575546
1	-1.107925	1.228766	0.367725
7	-3.234123	1.615659	0.898091
1	-3.479560	0.904057	0.210797
1	-3.574345	1.308318	1.802244
1	-3.742907	2.461164	0.666048
7	-2.976101	-0.560340	-1.410372
1	-3.074777	-1.566947	-1.342839
1	-3.156520	-0.310883	-2.376413
1	-2.006823	-0.327155	-1.200623
7	2.172725	-0.782762	-1.692450
1	2.537104	-1.062020	-2.596084
1	1.160094	-0.805051	-1.751131
1	2.435400	0.187626	-1.528964
7	2.849632	1.948765	-0.130371
1	3.839175	2.164970	-0.079633
1	2.353964	2.804011	0.095797
1	2.641673	1.269628	0.601683

Cartesian coordinates of : MP2_AM7_24

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.087542	2.651607	-0.504638
1	-1.198895	2.621915	-1.512119

1	-1.480970	3.534017	-0.196514
1	-1.653865	1.898173	-0.104563
7	-2.306170	0.099549	0.795912
1	-1.526546	-0.461094	0.450016
1	-3.172318	-0.369732	0.538821
1	-2.255877	0.092280	1.808980
7	0.225559	-1.171896	-0.704119
1	1.064326	-1.640465	-0.355185
1	0.535473	-0.308462	-1.139100
1	-0.150942	-1.754366	-1.444866
7	2.991437	-2.300792	0.375112
1	3.109104	-2.359286	1.380570
1	3.445272	-3.117989	-0.017758
1	3.499958	-1.475528	0.051594
7	4.004675	0.497902	-0.627080
1	3.909007	0.667513	-1.622430
1	4.835288	0.997408	-0.328629
1	3.200431	0.926843	-0.161558
7	-5.157902	-1.169392	-0.236433
1	-5.947170	-0.961088	0.364081
1	-5.299187	-0.665684	-1.104301
1	-5.197671	-2.159031	-0.450790
7	1.453537	1.415478	0.950153
1	1.659535	1.921168	1.805492
1	1.047908	0.526037	1.225257
1	0.711970	1.930174	0.470661

Cartesian coordinates of : MP2_AM7_25

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.821748	-1.586400	-1.158822
1	-2.511387	-1.030917	-0.652670
1	-2.326153	-2.189640	-1.799696
1	-1.297217	-0.920346	-1.720211
7	-0.544575	1.560711	1.642654
1	0.257872	1.177156	1.126760
1	-0.571935	1.074191	2.533610
1	-0.327016	2.528794	1.858229
7	1.540337	0.189811	-0.128351
1	1.111840	0.276573	-1.044890
1	1.378779	-0.768813	0.180890
1	2.543667	0.317979	-0.239595
7	0.403491	-2.679565	0.775128
1	0.747117	-3.585688	0.476581
1	-0.381997	-2.430138	0.168589
1	0.040691	-2.801122	1.714137
7	-1.015685	1.479655	-1.747896
1	-1.962986	1.600308	-2.088462
1	-0.491170	2.305976	-2.012949
1	-1.058604	1.462785	-0.732723
7	4.831336	0.446002	-0.142385
1	5.059512	-0.447315	0.278074
1	5.130020	1.170119	0.500283
1	5.392084	0.537216	-0.981392
7	-3.429782	0.514912	0.689837
1	-2.559732	0.931907	1.024128
1	-3.866596	0.042684	1.473807
1	-4.050410	1.272408	0.426351

Cartesian coordinates of : MP2_AM7_26

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.133946	-0.692089	-1.205511
1	-3.977547	-0.139001	-1.107284

1	-2.940105	-1.134218	-0.308305
1	-3.337532	-1.423946	-1.876646
7	-0.000002	-0.000023	-0.814547
1	0.441334	0.839661	-1.191383
1	-0.947852	-0.037663	-1.191395
1	0.506526	-0.802069	-1.191378
7	0.967608	3.060083	-1.205498
1	1.868381	3.514151	-1.107275
1	0.487786	3.113272	-0.308295
1	0.435577	3.602289	-1.876645
7	2.166392	-2.367999	-1.205481
1	2.109291	-3.375129	-1.107264
1	2.452363	-1.979048	-0.308280
1	2.901952	-2.178310	-1.876638
7	2.217814	-0.576836	1.427533
1	1.916051	-0.889815	2.343126
1	1.399232	-0.248725	0.917946
1	2.834390	0.215340	1.569083
7	-0.609341	2.209109	1.427501
1	-0.484228	1.336123	0.917938
1	-1.603672	2.347054	1.569000
1	-0.187458	2.104265	2.343115
7	-1.608523	-1.632246	1.427506
1	-1.230833	-2.562342	1.568988
1	-1.728636	-1.214472	2.343129
1	-0.915047	-1.087410	0.917939

Cartesian coordinates of : MP2_AM7_27

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.511455	0.322513	0.243157
1	3.373325	-0.678970	0.102804
1	4.027001	0.441536	1.108904
1	4.118983	0.649872	-0.500465
7	1.426464	2.930432	-0.381375
1	2.063228	2.162468	-0.191382
1	0.490186	2.545342	-0.450036
1	1.669840	3.323284	-1.282610
7	2.259926	-2.575290	-0.098867
1	1.409494	-2.054895	0.107319
1	2.332673	-3.334342	0.569072
1	2.150644	-2.996854	-1.014213
7	-1.719851	-2.121659	-0.780686
1	-0.957979	-1.618744	-0.325361
1	-1.574539	-3.112915	-0.625233
1	-1.635382	-1.965242	-1.779052
7	-1.829728	2.050047	-0.210451
1	-2.587115	1.418147	0.060200
1	-1.854626	2.846145	0.418848
1	-2.061254	2.405004	-1.132639
7	-3.898615	-0.229192	0.496901
1	-3.322276	-0.971190	0.095710
1	-4.059089	-0.460392	1.471247
1	-4.803829	-0.263154	0.040922
7	0.281819	-0.200807	0.791914
1	-0.346613	0.521470	0.436280
1	0.118776	-0.245820	1.793619
1	1.228265	0.156931	0.671908

Cartesian coordinates of : MP2_AM7_28

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.478364	-2.314964	0.484042
1	0.359359	-3.303972	0.290600

1	0.173316	-2.169708	1.441017
1	1.481411	-2.116927	0.457481
7	-1.895184	-0.064006	-0.250575
1	-2.864566	-0.307510	-0.061235
1	-1.308335	-0.853958	0.005275
1	-1.784366	0.038852	-1.254461
7	-5.084870	-0.393732	0.501728
1	-5.196185	0.564618	0.811432
1	-5.347858	-0.994589	1.274062
1	-5.753659	-0.552863	-0.242675
7	0.775337	-0.042376	-2.033021
1	1.365543	-0.368545	-2.789629
1	0.622327	-0.821468	-1.397400
1	1.303439	0.646964	-1.508381
7	-0.172854	2.542158	-0.149584
1	-0.156934	2.701126	-1.151915
1	-0.594992	3.365349	0.267136
1	-0.814491	1.757886	-0.002739
7	2.502061	1.566362	1.170542
1	3.168546	2.331266	1.194748
1	2.273085	1.357151	2.136968
1	1.646884	1.930565	0.740410
7	3.434165	-1.294902	0.192983
1	3.708783	-1.314726	-0.783009
1	4.254426	-1.552857	0.730830
1	3.205125	-0.326438	0.428682

 Cartesian coordinates of : MP2_AM7_29

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.454585	-1.546537	-0.007731
1	-1.914920	-2.286160	0.511337
1	-1.490868	-1.813060	-0.985654
1	-2.017796	-0.703550	0.098427
7	-2.887108	1.325213	0.299499
1	-3.539956	1.767107	-0.340277
1	-1.947322	1.640180	0.044987
1	-3.087011	1.703607	1.219897
7	1.453810	-0.593015	0.908616
1	1.512254	-0.671064	1.919541
1	2.184947	-1.196043	0.529249
1	0.552789	-0.996272	0.642532
7	3.882790	1.345795	-0.003967
1	3.705074	2.044341	-0.716476
1	4.329531	1.821595	0.771735
1	2.983097	0.992953	0.317994
7	-5.330987	-0.742954	-0.328079
1	-5.133536	-1.599553	-0.830112
1	-4.448338	-0.347374	-0.019304
1	-5.876329	-0.984229	0.490100
7	4.146773	-1.779482	-0.425799
1	4.898703	-2.254599	0.060195
1	4.156765	-2.115549	-1.382002
1	4.360963	-0.783236	-0.440324
7	0.099131	1.968226	-0.475289
1	0.519814	2.839999	-0.172527
1	0.606970	1.209204	-0.018943
1	0.276398	1.890975	-1.471122

 Cartesian coordinates of : MP2_AM7_30

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-5.234147	0.214636	-0.362163
1	-5.769258	0.883758	-0.902798

1	-5.372695	0.433098	0.617320
1	-5.634333	-0.700398	-0.532227
7	-1.922907	0.172371	-0.228551
1	-1.446465	0.574697	-1.031399
1	-2.923192	0.191099	-0.411527
1	-1.628032	-0.802710	-0.184303
7	0.911646	1.192520	-1.476282
1	0.872812	1.407215	-0.483454
1	1.489163	1.885631	-1.936779
1	1.364584	0.290719	-1.569873
7	2.020754	-0.886202	1.146156
1	2.875357	-0.654194	0.643282
1	2.301705	-1.263385	2.045085
1	1.529877	-0.012296	1.326682
7	-0.319412	-2.638838	-0.093055
1	0.499370	-2.139939	0.261297
1	-0.075718	-3.035489	-0.993866
1	-0.493691	-3.419231	0.530489
7	4.488378	0.252684	-0.658161
1	5.405596	0.406099	-0.254887
1	4.630444	-0.131477	-1.585352
1	4.051029	1.160321	-0.769934
7	-0.028703	1.649617	1.647697
1	-0.808655	1.180229	1.170171
1	-0.073248	1.400359	2.630554
1	-0.203913	2.648386	1.602041

Cartesian coordinates of ammonia octamer: (NH₃)₈

Cartesian coordinates of : MP2_AM8_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.109504	1.726363	1.261954
1	-3.067935	1.462392	1.466698
1	-2.040322	2.717953	1.467270
1	-1.966549	1.609821	0.253791
7	-1.726176	-2.108774	-1.263200
1	-2.717715	-2.039302	-1.468666
1	-1.462345	-3.067145	-1.468405
1	-1.609804	-1.966380	-0.254937
7	1.125441	1.375173	1.703012
1	1.494154	1.825752	2.533881
1	1.376005	0.390004	1.761470
1	0.110179	1.426298	1.761222
7	2.108586	-1.726831	1.262704
1	2.039121	-2.718481	1.467634
1	3.066912	-1.463068	1.468204
1	1.966354	-1.609927	0.254480
7	1.727100	2.109242	-1.261454
1	2.718791	2.039848	-1.466211
1	1.609979	1.966501	-0.253327
1	1.463409	3.067680	-1.466528
7	-1.374845	1.126394	-1.702733
1	-0.389667	1.376983	-1.760941
1	-1.825319	1.495521	-2.533475
1	-1.425962	0.111162	-1.761451
7	1.376054	-1.125773	-1.702266
1	1.427226	-0.110523	-1.760647
1	1.827031	-1.494655	-2.532845
1	0.390907	-1.376324	-1.761153
7	-1.126643	-1.375777	1.701985
1	-1.377238	-0.390629	1.760664
1	-1.495891	-1.826680	2.532440
1	-0.111418	-1.426924	1.760821

Cartesian coordinates of : MP2_AM8_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.148330	-2.084689	0.010668
1	1.283427	-1.568777	-0.856539
1	1.520234	-3.017432	-0.134688
1	0.144280	-2.184349	0.144848
7	-2.140586	2.187831	0.095339
1	-3.059207	1.973050	-0.278554
1	-1.940402	1.512889	0.839789
1	-2.211700	3.105988	0.521314
7	2.140591	-0.095341	2.187823
1	2.211711	-0.521316	3.105980
1	3.059210	0.278552	1.973037
1	1.940404	-0.839790	1.512882
7	-1.148332	0.010671	2.084686
1	-1.520238	-0.134685	3.017429
1	-0.144283	0.144847	2.184347
1	-1.283432	-0.856536	1.568774
7	-1.148335	-0.010668	-2.084684
1	-0.144287	-0.144849	-2.184350
1	-1.283428	0.856536	-1.568764
1	-1.520244	0.134698	-3.017424
7	-2.140593	-2.187825	-0.095338
1	-1.940408	-1.512885	-0.839788
1	-3.059212	-1.973041	0.278557
1	-2.211711	-3.105983	-0.521312
7	2.140588	0.095336	-2.187825
1	1.940403	0.839786	-1.512884
1	3.059207	-0.278559	-1.973040
1	2.211708	0.521311	-3.105982
7	1.148337	2.084685	-0.010671
1	1.520246	3.017426	0.134685
1	0.144288	2.184350	-0.144849
1	1.283434	1.568773	0.856537

Cartesian coordinates of : MP2_AM8_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.726205	-0.252264	-1.539242
1	3.251620	-0.573062	-2.345672
1	3.197492	0.576754	-1.192659
1	1.807392	0.042959	-1.868701
7	-2.610078	1.636695	-0.372078
1	-1.705056	1.942343	-0.013281
1	-3.143318	1.294033	0.420294
1	-3.094770	2.458011	-0.718401
7	0.502423	2.205780	0.098057
1	0.495761	1.732423	-0.802961
1	1.279859	1.816497	0.633694
1	0.714379	3.183731	-0.071419
7	2.513884	0.341319	1.696447
1	3.202512	0.372289	2.439794
1	2.864602	-0.280701	0.974892
1	1.664266	-0.076438	2.070104
7	-0.421150	0.018111	-2.185714
1	-0.609148	-0.178762	-3.163463
1	-1.250203	0.475693	-1.808618
1	-0.335504	-0.875762	-1.704228
7	0.566555	-2.209660	-0.050200
1	0.756246	-3.185483	0.153650
1	0.385807	-1.742575	0.836879
1	1.423772	-1.808121	-0.426719
7	-0.644833	-0.143185	2.194329
1	-0.542288	0.761956	1.740743

1	-0.867232	0.028281	3.169438
1	-1.452653	-0.603218	1.773132
7	-2.634772	-1.614962	0.203407
1	-3.358700	-2.324144	0.178208
1	-2.898353	-0.879176	-0.444324
1	-1.774118	-2.030357	-0.145429

Cartesian coordinates of : MP2_AM8_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.585607	-1.399213	0.527472
1	2.130242	-1.484784	1.430090
1	3.472018	-1.888211	0.595251
1	2.789418	-0.407156	0.399913
7	-2.526985	1.897739	0.755969
1	-2.925289	2.695244	0.271202
1	-2.819629	1.051859	0.258870
1	-2.958550	1.879350	1.674276
7	0.441885	-1.509829	-1.845906
1	0.814672	-1.936376	-2.688049
1	-0.309901	-2.108758	-1.520551
1	1.173709	-1.556082	-1.134024
7	-2.841945	-0.758171	-0.808469
1	-2.242232	-1.344383	-0.225233
1	-2.344568	-0.601361	-1.678763
1	-3.674723	-1.292143	-1.031906
7	0.041492	1.629202	-1.479343
1	-0.232212	2.131833	-2.316738
1	-0.694118	1.770512	-0.792058
1	0.065510	0.633727	-1.707437
7	2.848102	1.709533	-0.191866
1	1.962813	1.835515	-0.693383
1	3.583350	1.644159	-0.888529
1	3.026921	2.560416	0.331481
7	0.273180	0.669373	1.840622
1	1.066384	0.909292	1.251962
1	-0.523318	1.202214	1.491375
1	0.484218	1.026004	2.767361
7	-0.831037	-2.226009	1.175183
1	-0.058443	-2.838846	0.936731
1	-0.427848	-1.333501	1.471316
1	-1.290521	-2.636894	1.981214

Cartesian coordinates of : MP2_AM8_5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.727891	1.042596	-1.919913
1	0.755717	1.354736	-2.884506
1	-0.047505	1.513519	-1.458752
1	0.498907	0.050706	-1.920833
7	-2.744515	0.058998	-1.492392
1	-3.722413	0.083854	-1.223106
1	-2.708089	0.320639	-2.471889
1	-2.270251	0.789987	-0.961783
7	-1.191784	1.980157	0.578399
1	-0.211561	1.999257	0.857919
1	-1.586736	2.880561	0.830798
1	-1.653735	1.274073	1.153786
7	2.088651	1.890905	0.789811
1	2.471789	2.830321	0.797423
1	1.903460	1.636497	-0.181251
1	2.818180	1.272001	1.127245
7	-2.293407	-0.722350	1.776832
1	-2.819665	-1.075005	2.568443

1	-2.667197	-1.162490	0.942694
1	-1.327409	-1.032400	1.875652
7	0.919077	-0.995371	1.942061
1	1.674154	-1.154199	1.273085
1	1.204422	-1.419668	2.819268
1	0.899898	0.010371	2.090609
7	-0.312542	-1.954473	-1.016434
1	-0.151703	-1.907871	-0.012688
1	-0.450748	-2.930256	-1.258837
1	-1.192947	-1.471406	-1.200248
7	2.815273	-1.284399	-0.625613
1	1.929493	-1.571160	-1.038565
1	3.080247	-0.423181	-1.091683
1	3.513182	-1.981330	-0.862032

Cartesian coordinates of : MP2_AM8_6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.712345	-0.060334	-0.356416
1	-4.046132	0.098376	-1.301306
1	-3.215210	0.783757	-0.059603
1	-4.538341	-0.146955	0.226395
7	-1.789390	2.220548	0.526715
1	-1.101623	1.629430	1.000479
1	-2.048066	2.968377	1.161271
1	-1.320923	2.651153	-0.263197
7	-0.219983	0.099480	-1.713459
1	-1.092797	0.048326	-1.195978
1	-0.459992	0.012295	-2.695805
1	0.326629	-0.726525	-1.461573
7	-1.615015	-2.259840	0.559367
1	-1.150440	-2.635096	-0.261315
1	-2.063864	-3.040641	1.026866
1	-2.356328	-1.641192	0.223790
7	3.712336	-0.060363	0.356455
1	4.046118	0.098353	1.301345
1	3.215217	0.783733	0.059628
1	4.538335	-0.147004	-0.226349
7	1.789420	2.220536	-0.526718
1	1.101648	1.629427	-1.000487
1	1.320951	2.651152	0.263186
1	2.048114	2.968358	-1.161275
7	1.614993	-2.259836	-0.559388
1	2.356308	-1.641208	-0.223781
1	2.063841	-3.040652	-1.026863
1	1.150366	-2.635074	0.261273
7	0.219987	0.099464	1.713444
1	0.459986	0.012267	2.695791
1	1.092806	0.048310	1.195972
1	-0.326627	-0.726537	1.461546

Cartesian coordinates of : MP2_AM8_7

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.153829	0.144893	1.672652
1	-0.639435	0.030999	2.556332
1	0.187378	-0.774248	1.396656
1	-0.855663	0.422462	0.991974
7	1.727353	-2.393103	0.871899
1	1.880075	-3.351191	0.574723
1	2.108431	-2.321083	1.809603
1	2.281295	-1.784670	0.262888
7	2.918072	-0.282044	-1.084360
1	2.185397	-0.239661	-1.785678

1	2.843211	0.578952	-0.543716
1	3.806244	-0.264178	-1.573648
7	0.066658	1.500382	-1.538776
1	0.093794	2.108100	-2.350858
1	0.848435	1.764209	-0.945287
1	-0.789642	1.715478	-1.026228
7	2.223093	2.051868	1.017750
1	1.457974	1.485715	1.396178
1	3.020857	1.943447	1.635462
1	1.944251	3.025512	1.079844
7	-2.731560	1.804027	0.035842
1	-3.093890	0.856717	0.173443
1	-3.304073	2.241462	-0.678887
1	-2.900714	2.322523	0.891656
7	-0.697118	-1.602645	-1.300295
1	-0.405131	-0.657216	-1.550646
1	-0.639420	-2.172075	-2.137772
1	-0.009559	-1.962840	-0.642886
7	-3.361556	-1.241322	0.287598
1	-2.529614	-1.464462	-0.267451
1	-3.266860	-1.721214	1.176392
1	-4.161143	-1.657127	-0.178266

Cartesian coordinates of : MP2_AM8_8

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.361598	-1.241210	-0.287671
1	-4.161234	-1.656998	0.178122
1	-2.529709	-1.464328	0.267467
1	-3.266809	-1.721125	-1.176442
7	-0.697246	-1.602554	1.300336
1	-0.009717	-1.962799	0.642922
1	-0.639554	-2.171970	2.137825
1	-0.405197	-0.657138	1.550667
7	0.066769	1.500416	1.538795
1	-0.789511	1.715508	1.026213
1	0.093909	2.108189	2.350836
1	0.848572	1.764176	0.945310
7	-2.731462	1.804081	-0.035847
1	-3.303920	2.241487	0.678945
1	-3.093845	0.856798	-0.173504
1	-2.900627	2.322657	-0.891609
7	-0.153775	0.144941	-1.672617
1	0.187382	-0.774210	-1.396597
1	-0.855662	0.422532	-0.992003
1	-0.639307	0.031056	-2.556340
7	2.223232	2.051818	-1.017759
1	3.020974	1.943392	-1.635497
1	1.944409	3.025470	-1.079820
1	1.458085	1.485690	-1.396168
7	2.918032	-0.282175	1.084288
1	3.806220	-0.264372	1.573549
1	2.843219	0.578828	0.543647
1	2.185383	-0.239731	1.785630
7	1.727156	-2.393257	-0.871837
1	2.108264	-2.321376	-1.809540
1	1.879768	-3.351331	-0.574559
1	2.281149	-1.784821	-0.262875

Cartesian coordinates of : MP2_AM8_9

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.616126	2.949532	-0.150895
1	1.449404	2.385423	-0.340657

1	0.420155	3.497166	-0.982496
1	0.859388	3.615518	0.575291
7	1.557476	-0.646449	1.947576
1	1.960411	-0.488656	2.865474
1	1.321861	-1.632217	1.895795
1	0.668600	-0.146501	1.912333
7	2.826149	0.816406	-0.558629
1	3.831005	0.950738	-0.530302
1	2.622849	0.241197	-1.369517
1	2.554935	0.273913	0.263894
7	1.443706	-2.302207	-1.161630
1	0.735444	-2.433616	-0.438452
1	2.332258	-2.170687	-0.690855
1	1.511239	-3.166702	-1.688126
7	-1.261761	0.959932	1.596021
1	-0.753751	1.665325	1.060403
1	-2.141544	0.805647	1.100810
1	-1.499938	1.378888	2.489912
7	-0.587226	0.164006	-1.796964
1	0.095067	-0.591396	-1.730460
1	-0.509142	0.542778	-2.735677
1	-0.270830	0.894279	-1.163281
7	-1.109796	-2.196776	0.683576
1	-1.166671	-1.254431	1.068721
1	-1.591743	-2.815086	1.327829
1	-1.654023	-2.180388	-0.172940
7	-3.491880	0.267727	-0.558405
1	-4.035013	0.997456	-1.006400
1	-2.643174	0.125863	-1.109873
1	-4.046344	-0.579709	-0.605973

Cartesian coordinates of : MP2_AM8_10

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.399591	-0.169183	-1.862516
1	-2.805505	0.042510	-0.952340
1	-1.873567	0.648908	-2.149748
1	-3.157353	-0.287575	-2.525841
7	3.145467	1.050970	0.508506
1	4.127698	1.083971	0.256767
1	2.961770	1.879245	1.065070
1	2.596723	1.129447	-0.351837
7	-2.958210	-0.115546	1.295000
1	-2.578413	0.506112	2.000813
1	-2.264638	-0.847909	1.145059
1	-3.785854	-0.545829	1.693489
7	-0.802110	-2.178982	0.061140
1	0.205955	-2.224519	-0.097982
1	-1.226254	-1.747107	-0.760294
1	-1.135278	-3.136999	0.102550
7	1.112873	0.927349	-1.859867
1	0.748019	-0.014206	-1.965293
1	0.400115	1.461614	-1.357973
1	1.192744	1.317916	-2.792877
7	-0.905464	2.307304	0.122578
1	-0.777446	3.279465	0.383372
1	-1.904571	2.128489	0.129049
1	-0.504109	1.727657	0.863232
7	0.399065	0.141079	2.024334
1	1.376359	0.185009	1.746009
1	0.381609	-0.013105	3.027043
1	0.001542	-0.687282	1.584067
7	2.375635	-1.983151	-0.297145
1	2.925906	-2.747799	0.079305
1	2.652898	-1.135963	0.195119
1	2.667992	-1.860936	-1.260967

Cartesian coordinates of : MP2_AM8_11

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.864454	0.063927	-1.969268
1	-1.252105	0.231521	-2.891690
1	-1.063076	0.882442	-1.397787
1	-1.390350	-0.696091	-1.546850
7	-1.553971	-1.934512	0.637692
1	-1.390778	-1.344278	1.449141
1	-0.623809	-2.119365	0.259825
1	-1.916198	-2.818987	0.979934
7	0.864468	-0.063919	1.969271
1	1.390363	0.696095	1.546843
1	1.063100	-0.882443	1.397806
1	1.252115	-0.231493	2.891698
7	1.375647	-1.904382	-0.741506
1	2.298549	-1.513545	-0.548365
1	0.895351	-1.253776	-1.361805
1	1.523770	-2.764940	-1.258826
7	-3.909789	0.130201	-0.055004
1	-4.217505	0.191151	-1.018967
1	-4.729437	-0.080332	0.503393
1	-3.268163	-0.658785	0.020212
7	-1.375652	1.904377	0.741496
1	-2.298563	1.513557	0.548364
1	-1.523753	2.764929	1.258832
1	-0.895358	1.253755	1.361780
7	3.909774	-0.130203	0.055021
1	4.217474	-0.191157	1.018989
1	3.268174	0.658803	-0.020209
1	4.729437	0.080301	-0.503364
7	1.553975	1.934515	-0.637703
1	0.623817	2.119376	-0.259829
1	1.390771	1.344254	-1.449131
1	1.916192	2.818981	-0.979979

Cartesian coordinates of : MP2_AM8_12-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.892881	1.676732	0.332882
1	-3.329407	2.585531	0.226692
1	-2.116498	1.617085	-0.326087
1	-2.489620	1.641009	1.263184
7	-0.529520	0.765108	-1.610382
1	0.477162	0.915715	-1.688005
1	-0.912454	0.793846	-2.549627
1	-0.663862	-0.179325	-1.257809
7	-0.789669	-1.583127	0.755034
1	-1.775593	-1.581047	0.487008
1	-0.679470	-2.329368	1.434631
1	-0.599648	-0.708123	1.243119
7	-3.833359	-1.258504	-0.186770
1	-4.105486	-1.417370	-1.150427
1	-3.752764	-0.250080	-0.045161
1	-4.595857	-1.594404	0.390934
7	0.361373	1.362856	1.508610
1	0.096536	1.613460	0.560332
1	0.294292	2.199443	2.077815
1	1.338719	1.082535	1.486060
7	3.141393	-0.380059	1.410092
1	4.146339	-0.454026	1.529490
1	2.853773	-1.085463	0.725850
1	2.726843	-0.636551	2.300362
7	2.599388	1.364129	-1.292357
1	2.619191	2.370741	-1.166244

1	3.375679	1.135012	-1.904184
1	2.801390	0.945220	-0.385490
7	1.869147	-2.005370	-0.892132
1	1.893633	-1.370697	-1.683409
1	0.933255	-1.941918	-0.483527
1	1.982745	-2.943577	-1.260345

Cartesian coordinates of : MP2_AM8_13

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.818915	1.866513	-0.953377
1	3.373497	2.714206	-0.910817
1	2.588277	1.716250	-1.929145
1	1.948627	2.034284	-0.443247
7	-1.969850	-1.613232	-1.216555
1	-2.476685	-2.355742	-1.686150
1	-1.012769	-1.939389	-1.081055
1	-2.383169	-1.499333	-0.295495
7	3.020899	-0.729940	0.838802
1	3.881922	-0.935452	1.333240
1	2.319431	-0.486075	1.531658
1	3.178506	0.103541	0.270671
7	1.181263	-2.381969	-1.027967
1	1.399615	-3.372455	-1.073466
1	1.906887	-1.941782	-0.452880
1	1.301632	-2.020361	-1.969156
7	-2.000701	1.481419	-1.551265
1	-2.732127	1.845558	-2.152963
1	-1.966987	0.466733	-1.681602
1	-1.126135	1.860846	-1.899507
7	0.221380	2.033353	0.828240
1	-0.664491	2.094698	0.334012
1	0.219597	2.752988	1.543228
1	0.230930	1.128856	1.300125
7	-3.032757	0.336263	1.298364
1	-2.844033	0.908596	2.114668
1	-2.769272	0.883722	0.479273
1	-4.038084	0.203660	1.264586
7	-0.143999	-1.014822	1.799933
1	-0.005331	-1.624460	2.599114
1	0.149611	-1.532662	0.975130
1	-1.145505	-0.849319	1.716561

Cartesian coordinates of : MP2_AM8_14

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.071136	0.349755	1.800043
1	-0.291196	0.335461	2.747678
1	-0.294595	-0.472874	1.328417
1	-0.329711	1.165094	1.334434
7	-0.335104	-2.250932	-0.211009
1	-0.757091	-2.955683	-0.807641
1	0.522570	-2.657194	0.149447
1	-0.061628	-1.472293	-0.815716
7	0.587598	0.372460	-1.691679
1	0.446039	1.058363	-0.954943
1	1.577144	0.113598	-1.683861
1	0.414492	0.851275	-2.569969
7	-1.276332	2.739747	0.128144
1	-1.883385	2.144564	-0.442547
1	-1.871242	3.260103	0.764483
1	-0.852477	3.425965	-0.487553
7	-3.179065	-1.442638	1.060823
1	-2.238028	-1.780829	0.862854

1	-3.140010	-0.888652	1.908708
1	-3.766118	-2.245579	1.256375
7	3.567833	-0.585556	-1.327684
1	3.580966	-0.330851	-0.337133
1	3.726740	-1.584892	-1.393910
1	4.361703	-0.136861	-1.771331
7	3.215956	0.384479	1.639022
1	3.587350	-0.127618	2.432150
1	3.521422	1.345359	1.752669
1	2.195744	0.382184	1.727417
7	-2.688141	0.464610	-1.441970
1	-3.315039	0.437296	-2.238569
1	-3.076458	-0.143429	-0.720829
1	-1.804366	0.054005	-1.730466

Cartesian coordinates of : MP2_AM8_15

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.257369	-0.282809	-1.700993
1	0.018804	-0.305723	-2.687651
1	1.212680	0.062912	-1.636048
1	-0.340498	0.427506	-1.275591
7	0.642439	0.125632	1.997320
1	0.810352	0.151747	2.998157
1	0.952108	1.021515	1.616199
1	1.266713	-0.578123	1.612369
7	1.740466	-2.501100	0.013305
1	1.072633	-2.014348	-0.585481
1	2.170823	-3.239220	-0.534029
1	1.213049	-2.957927	0.749342
7	-1.750257	-1.651222	0.584286
1	-1.188252	-1.123683	1.250968
1	-1.812435	-2.606219	0.919840
1	-1.209413	-1.656953	-0.276026
7	-4.231231	-0.028795	-0.461587
1	-4.550609	-0.407568	-1.345789
1	-3.568167	-0.690274	-0.053674
1	-5.039632	0.026129	0.147343
7	3.448106	0.126616	-0.563301
1	3.829374	0.614544	0.241022
1	3.067564	-0.755406	-0.219448
1	4.233748	-0.096886	-1.165362
7	1.433978	2.560980	0.130260
1	0.518983	2.500241	-0.308801
1	1.734921	3.528281	0.093919
1	2.082391	2.008720	-0.424568
7	-1.650525	1.757118	0.002846
1	-1.826839	2.719674	0.273267
1	-2.555755	1.352895	-0.240845
1	-1.324947	1.273215	0.835930

Cartesian coordinates of : MP2_AM8_16

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.299851	-2.008019	0.095873
1	-2.942073	-1.399435	-0.643734
1	-3.132278	-2.968578	-0.182012
1	-4.305802	-1.888067	0.138379
7	2.293546	0.379870	-1.732846
1	1.778003	1.186452	-2.068885
1	2.826512	0.026386	-2.520406
1	1.612787	-0.334183	-1.469318
7	-1.403563	2.887465	-0.090724
1	-0.462295	2.719187	0.271918

1	-1.324367	3.520036	-0.879976
1	-1.921756	3.389293	0.622920
7	-1.453389	-0.051907	1.749516
1	-2.088733	-0.795425	1.453878
1	-1.641567	0.128679	2.730496
1	-1.734090	0.778013	1.232865
7	-1.687168	0.020120	-1.661081
1	-0.804806	-0.413837	-1.400148
1	-1.722459	0.933365	-1.210150
1	-1.668726	0.174158	-2.663157
7	3.663825	-1.222676	0.714265
1	3.768729	-0.787247	1.623562
1	4.545565	-1.673296	0.497347
1	3.513574	-0.484219	0.030513
7	0.607389	-1.735637	-0.117625
1	1.542170	-1.876946	0.265557
1	0.215675	-2.654772	-0.296950
1	0.040907	-1.315635	0.619124
7	1.222334	1.666256	1.075174
1	1.854188	1.308293	0.364320
1	1.790517	1.993191	1.848910
1	0.658463	0.886277	1.407085

Cartesian coordinates of : MP2_AM8_17

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	4.157011	-0.173614	0.807689
1	5.101061	-0.185752	0.436934
1	4.246636	-0.098426	1.815274
1	3.709522	0.684310	0.477948
7	0.212033	0.267444	0.979283
1	-0.766569	0.237846	0.709437
1	0.230926	0.182827	1.990530
1	0.652127	-0.568759	0.597728
7	1.991216	-2.157154	-0.348509
1	2.753217	-1.600826	0.048813
1	2.014299	-3.064110	0.106834
1	2.229556	-2.321351	-1.321585
7	2.347215	2.159901	-0.277920
1	1.544901	1.674369	0.130682
1	2.310271	3.131866	0.007804
1	2.245507	2.142898	-1.286616
7	-3.038163	1.519734	1.040119
1	-3.989778	1.871529	1.021669
1	-2.529002	2.112413	1.687790
1	-2.634044	1.675470	0.112169
7	-1.110528	-1.536684	-1.532629
1	-0.195355	-1.786886	-1.165070
1	-1.795852	-1.741831	-0.803969
1	-1.299023	-2.158308	-2.311678
7	-1.456758	1.585139	-1.640457
1	-0.553489	1.988427	-1.415071
1	-1.315208	0.577386	-1.753510
1	-1.730301	1.959792	-2.542553
7	-3.130144	-1.663422	0.937761
1	-3.135276	-0.655562	1.104225
1	-2.804042	-2.112865	1.786429
1	-4.093254	-1.953862	0.808426

Cartesian coordinates of : MP2_AM8_18

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.514251	-2.212048	1.396078
1	-2.228500	-2.909797	1.211960

1	-1.237873	-2.336816	2.365092
1	-1.976977	-1.298095	1.338076
7	2.428439	2.266496	-0.534298
1	3.238990	2.871901	-0.607884
1	2.769363	1.325119	-0.334255
1	2.006454	2.232526	-1.456833
7	1.110145	-3.021857	-0.354489
1	1.303334	-4.013877	-0.266732
1	0.844148	-2.862336	-1.321023
1	0.283128	-2.822191	0.210767
7	3.300889	-0.785068	0.208267
1	4.192524	-1.044922	-0.201181
1	2.671248	-1.580841	0.076390
1	3.457398	-0.699137	1.207501
7	-0.135641	2.785249	1.269441
1	-0.514197	3.714607	1.118791
1	0.760859	2.742274	0.779412
1	0.062746	2.709734	2.261734
7	-2.724057	0.639674	0.932553
1	-2.003035	1.347382	1.065520
1	-3.561393	0.978035	1.394447
1	-2.923460	0.608306	-0.067794
7	-2.591518	0.332831	-2.276116
1	-1.607467	0.216517	-2.027794
1	-2.888521	-0.503671	-2.766059
1	-2.658427	1.099782	-2.935865
7	0.045786	0.024686	-0.664465
1	-0.398144	-0.691758	-0.096537
1	-0.069711	0.890783	-0.144261
1	1.038976	-0.183278	-0.642280

Cartesian coordinates of : MP2_AM8_19

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.447357	0.972953	0.402825
1	-3.417728	-0.034543	0.572306
1	-3.656938	1.416724	1.290986
1	-4.247004	1.147922	-0.196796
7	-2.904734	-2.123370	0.898232
1	-3.012443	-2.775835	0.129535
1	-1.920231	-1.851282	0.941765
1	-3.128323	-2.631163	1.746933
7	-0.869210	1.960576	-1.324980
1	-0.504489	1.117777	-1.765972
1	-1.711662	1.698277	-0.812044
1	-1.156828	2.589452	-2.067292
7	0.709585	-0.702210	-2.499931
1	0.213052	-1.280528	-3.169992
1	1.353902	-0.128574	-3.034622
1	1.275659	-1.328924	-1.922369
7	1.448635	2.742243	0.667872
1	0.696455	2.516270	0.009172
1	1.012318	3.210313	1.456041
1	2.029468	3.441672	0.216113
7	3.107527	0.145210	1.401709
1	4.021698	0.238000	0.970111
1	2.585365	0.996346	1.172236
1	3.267724	0.156509	2.404047
7	-0.228829	-0.585226	0.751450
1	0.676933	-0.490955	1.201575
1	-0.744213	0.261513	0.973547
1	-0.035926	-0.526811	-0.246049
7	2.143185	-2.421272	-0.296890
1	2.850381	-3.145203	-0.359917
1	2.501188	-1.689796	0.318407
1	1.340025	-2.829483	0.170269

Cartesian coordinates of : MP2_AM8_20

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.751051	1.993306	0.639809
1	3.510961	2.528635	1.045156
1	2.572377	1.194761	1.251452
1	1.928402	2.586664	0.666209
7	2.188162	-0.762732	2.149623
1	1.489402	-0.987901	2.850500
1	3.079843	-1.049086	2.541015
1	2.005724	-1.365065	1.341491
7	1.430603	-2.275568	-0.497741
1	1.714057	-1.525492	-1.126658
1	1.742246	-3.150712	-0.904624
1	0.412668	-2.288798	-0.487271
7	2.585336	0.383071	-2.036420
1	3.451338	-0.066529	-2.314840
1	2.798013	0.992958	-1.243313
1	2.307942	0.975298	-2.812195
7	-1.931724	-2.239722	-0.397851
1	-2.692007	-1.615736	-0.112036
1	-2.132783	-2.528668	-1.350051
1	-2.008184	-3.073284	0.176538
7	-4.146587	-0.176767	0.499328
1	-3.769181	0.737102	0.236851
1	-4.310442	-0.151848	1.500342
1	-5.059848	-0.257248	0.064754
7	-0.205258	0.606696	-0.041980
1	0.523579	0.510633	-0.744812
1	-0.745958	-0.255283	-0.092347
1	0.286584	0.569820	0.845930
7	-2.665072	2.484032	-0.326193
1	-1.764215	2.001336	-0.264037
1	-2.759669	2.838768	-1.271546
1	-2.626430	3.293468	0.283477

Cartesian coordinates of : MP2_AM8_21

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.764991	-2.877020	1.134141
1	0.228697	-2.710609	0.954943
1	-0.860729	-3.094069	2.120960
1	-1.021459	-3.721321	0.632734
7	-0.067112	0.200883	-2.448783
1	0.315035	-0.445170	-3.132583
1	-0.364486	1.020603	-2.968883
1	-0.916550	-0.235218	-2.074060
7	2.323920	-2.291516	0.493101
1	2.987965	-2.461275	1.241888
1	2.486311	-1.335353	0.165454
1	2.594976	-2.907724	-0.266728
7	2.692761	0.643294	-0.702406
1	2.557560	1.502462	-0.170393
1	1.908630	0.580711	-1.351109
1	3.536594	0.767007	-1.251870
7	-2.529682	-0.988857	-0.953399
1	-2.134178	-1.597495	-0.238643
1	-2.905831	-0.167467	-0.479827
1	-3.312847	-1.481671	-1.368671
7	-0.128856	0.382510	0.924301
1	0.794365	0.250506	1.327311
1	-0.640746	-0.465857	1.155755
1	0.017336	0.326506	-0.082246
7	1.387686	3.162805	0.907527
1	1.087137	3.890228	0.268555

1	1.605099	3.614069	1.788951
1	0.596520	2.542891	1.066436
7	-2.937688	1.766732	0.659468
1	-1.978225	1.567319	0.941234
1	-2.933144	2.628298	0.125260
1	-3.480296	1.940817	1.497884

Cartesian coordinates of : MP2_AM8_22

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	5.190212	-0.472086	0.442827
1	5.716351	-1.241855	0.045656
1	5.761425	0.359780	0.349081
1	5.087163	-0.658106	1.433708
7	-0.203249	0.028888	1.757416
1	0.531491	-0.362406	1.167945
1	-1.070784	-0.438695	1.508938
1	0.003375	-0.223933	2.717944
7	-0.704037	-2.250324	-1.011013
1	0.211955	-2.228949	-0.573347
1	-0.693807	-3.004065	-1.689824
1	-0.796543	-1.367637	-1.519990
7	2.057535	-0.325537	-0.492038
1	3.056094	-0.322323	-0.290878
1	1.939584	-0.716462	-1.420784
1	1.744929	0.642333	-0.543880
7	-1.055497	0.680111	-2.109636
1	-0.213860	1.217385	-1.922240
1	-1.750009	1.005049	-1.434874
1	-1.378544	0.947132	-3.033716
7	-2.902658	1.476539	0.389206
1	-3.797373	1.950498	0.452124
1	-3.047438	0.504149	0.662081
1	-2.299771	1.882255	1.097259
7	0.563546	2.561416	0.050118
1	-0.228147	3.083319	-0.309864
1	1.172922	3.227724	0.512055
1	0.209883	1.914394	0.756835
7	-3.063393	-1.697034	0.911945
1	-3.950981	-1.859020	0.447101
1	-3.059810	-2.293409	1.733000
1	-2.325311	-2.030976	0.283894

Cartesian coordinates of : MP2_AM8_23

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.602745	-2.136085	-1.714523
1	1.122646	-1.659914	-2.443909
1	-0.093079	-1.477836	-1.355866
1	0.106348	-2.900366	-2.160326
7	-1.237996	-0.325132	0.056485
1	-2.251591	-0.378584	0.145015
1	-0.967843	0.625856	0.294923
1	-0.831920	-0.923448	0.772201
7	0.957331	-2.439441	1.470813
1	1.003898	-2.490083	0.452859
1	1.902718	-2.280109	1.803460
1	0.680105	-3.354983	1.808643
7	2.778069	0.088108	-0.608698
1	3.785071	0.188198	-0.678003
1	2.504037	0.354822	0.339154
1	2.565565	-0.898877	-0.715850
7	0.436760	1.630386	-2.088162
1	-0.285202	0.917134	-2.096017

1	0.592728	1.925687	-3.045361
1	1.291276	1.183748	-1.748972
7	1.398098	0.742069	2.160501
1	0.718212	1.420025	1.818298
1	0.931347	-0.155970	2.251731
1	1.680410	1.035039	3.089369
7	-0.274106	3.001910	0.588882
1	-0.034775	2.749663	-0.374091
1	-1.189504	3.439111	0.573067
1	0.381421	3.717362	0.885940
7	-4.511918	-0.492240	0.137894
1	-4.886052	-1.207720	0.750547
1	-4.831990	-0.702174	-0.800494
1	-4.936695	0.386400	0.411332

Cartesian coordinates of : MP2_AM8_24

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.314407	-0.614481	1.976373
1	-0.443170	-0.572633	1.289324
1	0.848887	-1.448238	1.752318
1	-0.106947	-0.771515	2.886165
7	0.939140	-2.646584	-0.580338
1	1.146630	-3.464519	-1.143287
1	0.848083	-1.845017	-1.208139
1	0.030503	-2.800151	-0.156444
7	-1.795729	-0.373704	-0.379226
1	-2.806560	-0.376042	-0.254930
1	-1.513877	0.568710	-0.643897
1	-1.591046	-0.959221	-1.182240
7	-0.647739	2.668397	-0.792406
1	-0.421274	3.343505	-1.515308
1	-1.451752	3.039181	-0.296516
1	0.136407	2.642992	-0.133687
7	1.209793	0.133633	-1.984482
1	1.467633	0.400779	-2.928469
1	2.050020	0.173674	-1.410721
1	0.569350	0.844211	-1.638819
7	3.411685	-0.745124	0.253716
1	3.388536	-0.458156	1.226245
1	2.713108	-1.480003	0.143442
1	4.321774	-1.161862	0.089235
7	1.713908	2.091339	1.126492
1	2.547606	1.808231	0.621425
1	1.315474	1.240178	1.530114
1	2.014948	2.688041	1.889473
7	-5.004892	-0.490790	0.332430
1	-5.572621	0.322129	0.122910
1	-4.987920	-0.595820	1.340252
1	-5.487803	-1.297267	-0.046367

Cartesian coordinates of : MP2_AM8_25

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.886593	-0.632459	-1.958389
1	0.938049	-1.129714	-2.840994
1	-0.092402	-0.568169	-1.690451
1	1.322311	-1.216741	-1.247620
7	-1.333418	-2.865053	-0.186588
1	-1.518484	-1.865728	-0.280486
1	-2.124974	-3.286662	0.286129
1	-1.295569	-3.265915	-1.116866
7	-1.518304	0.299872	0.065890
1	-1.021857	1.114411	-0.292585

1	-1.128949	0.139566	0.990910
1	-2.495984	0.561448	0.184892
7	1.143359	1.211969	2.007505
1	1.367254	1.602894	2.916366
1	0.524259	1.867736	1.541834
1	2.001263	1.186802	1.456604
7	1.466487	-1.874006	1.017814
1	1.174577	-1.045406	1.535405
1	1.957915	-2.478180	1.668762
1	0.620553	-2.370920	0.736724
7	3.469993	0.420054	-0.039166
1	3.319038	0.600296	-1.025974
1	3.020610	-0.472924	0.160563
1	4.468676	0.306307	0.096303
7	-4.709338	1.000526	0.246759
1	-5.101245	1.216594	1.156166
1	-5.226826	0.211642	-0.123462
1	-4.898652	1.793164	-0.355928
7	0.747679	2.408695	-1.113779
1	0.556176	3.064088	-1.863882
1	0.982717	1.509633	-1.535652
1	1.580188	2.738590	-0.637086

Cartesian coordinates of : MP2_AM8_26

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.195113	-0.247892	-1.927661
1	2.087758	-0.181240	-1.443226
1	1.389411	-0.524208	-2.884451
1	0.682189	-1.015909	-1.500052
7	-0.687609	-2.734321	-0.578813
1	-1.264621	-1.889665	-0.495295
1	-0.910760	-3.330261	0.211993
1	-0.990861	-3.234322	-1.408235
7	-1.918245	0.060735	-0.342725
1	-1.549926	0.538955	-1.157942
1	-1.345455	0.339405	0.454978
1	-2.868000	0.392345	-0.189778
7	0.253509	0.668483	1.954067
1	0.819264	1.421665	1.575705
1	0.794176	-0.193294	1.863908
1	0.129820	0.852561	2.943799
7	1.942339	-1.886580	1.104652
1	2.406629	-2.671917	1.547146
1	2.642569	-1.374535	0.576055
1	1.263492	-2.262059	0.444171
7	-5.085249	0.651041	0.268338
1	-5.209461	0.847817	1.254571
1	-5.392021	-0.301026	0.106431
1	-5.711951	1.262658	-0.241468
7	3.489260	0.873532	0.154252
1	3.610087	0.726154	1.151008
1	2.754040	1.572530	0.043442
1	4.352465	1.284215	-0.185789
7	0.882332	2.592570	-0.635332
1	-0.004692	2.771293	-0.176443
1	0.765183	1.753154	-1.206193
1	1.050508	3.372699	-1.261779

Cartesian coordinates of : MP2_AM8_27

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.429512	2.449821	-0.934339
1	1.152599	3.154515	-1.030763

1	-0.457929	2.940632	-0.955633
1	0.519316	2.039119	-0.006098
7	-0.462426	-2.654292	0.099677
1	-0.447917	-3.587742	-0.298203
1	0.501402	-2.412364	0.336106
1	-0.971190	-2.722579	0.975300
7	0.980057	-0.520770	-2.121580
1	0.226207	-1.102617	-1.767651
1	0.968692	-0.585252	-3.133456
1	0.766719	0.445481	-1.874731
7	2.584552	-1.698655	0.313633
1	3.177031	-0.976443	0.720200
1	2.357056	-1.374995	-0.628379
1	3.155572	-2.533107	0.225769
7	-2.037956	0.165291	-0.194335
1	-3.051869	0.176142	-0.101628
1	-1.737217	-0.796310	-0.340190
1	-1.803090	0.678188	-1.037600
7	0.488056	0.538349	1.646638
1	-0.444472	0.448682	1.236581
1	0.373962	0.642569	2.649717
1	0.973165	-0.342203	1.486697
7	-5.254270	0.375107	0.387121
1	-5.257164	0.909700	1.248113
1	-5.828020	0.876694	-0.280983
1	-5.719786	-0.504859	0.577099
7	3.487399	1.307255	0.786615
1	2.506603	1.355064	1.054098
1	3.987510	2.044034	1.269721
1	3.548359	1.492913	-0.208091

Cartesian coordinates of : MP2_AM8_28

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.122781	-2.182563	-0.574900
1	0.278034	-3.110067	-0.653861
1	-0.620848	-2.127853	0.309610
1	0.643011	-1.512224	-0.549960
7	1.634314	0.495121	-0.896689
1	2.431085	1.104849	-0.709579
1	0.820859	0.900017	-0.432384
1	1.457208	0.536189	-1.895417
7	4.446891	1.700939	0.096868
1	4.513329	0.736278	0.420027
1	4.539234	2.307973	0.903325
1	5.244006	1.885134	-0.501568
7	-2.129187	-0.103967	-1.735574
1	-1.538237	0.677387	-1.463519
1	-2.347253	0.006000	-2.720657
1	-1.540957	-0.935015	-1.642923
7	-3.988988	1.606833	0.218401
1	-4.222882	2.488530	-0.224439
1	-4.850971	1.236707	0.602895
1	-3.669924	0.966588	-0.507490
7	3.769288	-1.344666	0.621871
1	3.439199	-1.753619	1.488707
1	2.957580	-0.994812	0.113625
1	4.176973	-2.097027	0.078347
7	-2.678844	-1.441825	1.252106
1	-3.164700	-2.326344	1.353031
1	-3.129629	-0.779286	1.873664
1	-2.828524	-1.112180	0.301368
7	-0.857029	1.283898	0.996809
1	-0.404685	1.889496	1.674027
1	-1.833931	1.570620	0.942267
1	-0.863624	0.346267	1.388663

Cartesian coordinates of : MP2_AM8_29

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	5.025031	0.566249	0.268202
1	4.907579	0.989971	1.181100
1	5.466749	-0.335440	0.404229
1	5.673297	1.143244	-0.254672
7	-0.505394	1.485113	1.585317
1	-0.324960	2.153377	2.327765
1	-0.931498	0.661859	2.009490
1	0.399315	1.164980	1.227899
7	-1.688726	-0.882999	-1.591483
1	-2.443988	-0.375339	-1.126820
1	-1.029269	-0.159340	-1.874199
1	-2.078784	-1.280012	-2.440835
7	-0.464364	2.095901	-1.600523
1	0.217693	2.829378	-1.761553
1	-1.329247	2.397510	-2.036287
1	-0.625158	2.048512	-0.594530
7	-1.442508	-1.533606	1.711565
1	-1.653015	-1.491957	0.717358
1	-0.476242	-1.836532	1.781428
1	-2.017364	-2.260683	2.122738
7	0.649501	-2.856901	-0.599822
1	1.184947	-3.149413	-1.409926
1	0.310981	-3.701074	-0.151549
1	-0.164953	-2.339374	-0.932883
7	1.786515	0.170490	-0.080867
1	1.597104	-0.829806	-0.063165
1	2.793517	0.293192	-0.159882
1	1.357911	0.531860	-0.928029
7	-3.419778	0.961920	0.317999
1	-2.546954	1.361213	0.661212
1	-4.065850	1.724508	0.146316
1	-3.803753	0.416200	1.082075

Cartesian coordinates of : MP2_AM8_30

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.643923	2.283241	-0.839820
1	-3.336199	3.001133	-1.024970
1	-2.262707	2.014166	-1.740403
1	-1.886215	2.722886	-0.311229
7	3.484119	0.255048	0.839767
1	3.259217	-0.591637	0.311220
1	3.024339	0.175773	1.740376
1	4.481268	0.236974	1.024872
7	2.643920	-2.283237	-0.839820
1	2.262701	-2.014161	-1.740402
1	1.886213	-2.722885	-0.311229
1	3.336196	-3.001128	-1.024974
7	0.255029	-3.483906	0.839895
1	0.236947	-4.481031	1.025125
1	-0.591643	-3.259066	0.311300
1	0.175736	-3.024011	1.740443
7	2.283218	2.643893	-0.839844
1	3.001056	3.336216	-1.025028
1	2.014110	2.262676	-1.740418
1	2.722942	1.886203	-0.311293
7	-0.255030	3.483903	0.839896
1	-0.175737	3.024008	1.740444
1	-0.236947	4.481028	1.025127
1	0.591642	3.259063	0.311301
7	-2.283220	-2.643896	-0.839843
1	-3.001060	-3.336217	-1.025023

1	-2.014114	-2.262681	-1.740419
1	-2.722941	-1.886203	-0.311293
7	-3.484113	-0.255047	0.839769
1	-3.024328	-0.175770	1.740375
1	-4.481261	-0.236974	1.024878
1	-3.259215	0.591639	0.311220

Cartesian coordinates of : MP2_AM8_31

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.520834	-1.818968	0.052230
1	0.840978	-2.697225	-0.340822
1	0.607277	-1.900932	1.059430
1	1.169806	-1.092565	-0.250344
7	2.329143	0.696150	-0.851297
1	3.092475	1.154731	-0.352641
1	1.458373	1.154210	-0.573792
1	2.460043	0.904856	-1.836468
7	5.027200	1.339706	0.813707
1	5.096081	0.327538	0.715636
1	4.994462	1.556435	1.803304
1	5.881238	1.748195	0.451672
7	-2.329070	-0.696197	-0.851458
1	-2.459886	-0.904959	-1.836629
1	-3.092444	-1.154751	-0.352841
1	-1.458324	-1.154241	-0.573853
7	-4.388737	1.645244	-0.023517
1	-4.048551	2.391309	0.572285
1	-4.842743	2.084599	-0.816366
1	-3.580116	1.130093	-0.368702
7	4.388738	-1.645246	-0.023050
1	4.048502	-2.391277	0.572766
1	3.580147	-1.130114	-0.368332
1	4.842812	-2.084645	-0.815835
7	-5.027269	-1.339661	0.813352
1	-5.881276	-1.748171	0.451268
1	-4.994615	-1.556334	1.802964
1	-5.096142	-0.327498	0.715219
7	-0.520839	1.818971	0.052084
1	-0.840949	2.697206	-0.341043
1	-1.169785	1.092551	-0.250506
1	-0.607368	1.900991	1.059272

Cartesian coordinates of : MP2_AM8_32

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.361848	2.436614	0.462954
1	-0.190069	2.587903	1.450971
1	-0.348241	1.431022	0.293345
1	-1.306676	2.754128	0.274907
7	-0.204556	-0.705537	-0.113927
1	-0.145435	-1.274251	-0.952460
1	-0.840077	-1.184452	0.517043
1	0.727849	-0.690575	0.311271
7	2.670252	-0.167770	0.971044
1	2.788903	0.708891	0.461895
1	2.853699	0.028576	1.949216
1	3.396231	-0.810561	0.659793
7	2.525943	2.548484	-0.772957
1	3.027057	3.421029	-0.647351
1	1.555680	2.706277	-0.496683
1	2.529583	2.352456	-1.767908
7	4.805817	-2.357533	-0.226488
1	4.260655	-2.823991	-0.942126

1	5.611989	-1.944704	-0.681053
1	5.150218	-3.073442	0.402673
7	-3.602706	-2.285612	-0.646573
1	-3.411339	-1.819890	0.240076
1	-2.965117	-3.069183	-0.731456
1	-4.537287	-2.675016	-0.593551
7	-2.850041	0.771473	-1.332875
1	-3.027592	1.370786	-2.130802
1	-3.256478	-0.142403	-1.523673
1	-1.846647	0.623900	-1.266467
7	-3.084427	-0.124677	1.650920
1	-3.128335	0.467294	0.820464
1	-3.905268	0.068997	2.214844
1	-2.282353	0.179117	2.192350

Cartesian coordinates of : MP2_AM8_33

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.251205	-2.317274	-0.926336
1	-1.867049	-3.109348	-1.074759
1	-1.048476	-1.932578	-1.842669
1	-1.780082	-1.608264	-0.408359
7	1.251018	2.317036	0.926500
1	1.779976	1.608098	0.408507
1	1.048115	1.932201	1.842736
1	1.866846	3.109078	1.075158
7	2.675858	0.054783	-0.686258
1	2.363438	-0.000829	-1.649586
1	2.331134	-0.781515	-0.212407
1	3.692391	0.006446	-0.698589
7	1.331498	-2.406171	0.872703
1	1.735402	-3.334460	0.932859
1	0.488614	-2.474830	0.297350
1	1.034611	-2.158409	1.810250
7	-1.331417	2.405954	-0.872908
1	-1.735232	3.334268	-0.933284
1	-1.034416	2.158002	-1.810368
1	-0.488609	2.474642	-0.297446
7	-2.675822	-0.054809	0.686318
1	-2.363363	0.000876	1.649629
1	-3.692353	-0.006442	0.698683
1	-2.331099	0.781441	0.212384
7	-5.906271	-0.021010	0.127532
1	-5.745289	-0.168225	-0.862048
1	-6.424148	0.844169	0.226622
1	-6.505130	-0.770704	0.452917
7	5.906330	0.021465	-0.127546
1	5.745414	0.169361	0.861943
1	6.505130	0.770962	-0.453495
1	6.424245	-0.843757	-0.226070

Cartesian coordinates of ammonia nanomer: (NH3)9

Cartesian coordinates of : MP2_AM9_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.344079	-0.370997	-0.073309
1	3.608641	-1.289949	0.265858
1	4.205601	0.152843	-0.187342
1	2.804078	0.081804	0.664425
7	-1.665552	0.371678	-1.952271
1	-2.180308	0.448031	-2.824079

1	-2.051602	-0.427141	-1.449178
1	-1.882732	1.206272	-1.404525
7	0.819667	-1.729458	-1.601745
1	0.179638	-0.995416	-1.904975
1	1.015884	-2.310979	-2.410423
1	1.695815	-1.275890	-1.345841
7	-2.120112	-2.430731	-0.387225
1	-2.124701	-2.608573	0.611295
1	-1.147985	-2.486692	-0.683928
1	-2.627017	-3.190599	-0.828346
7	1.226140	1.853384	-1.424657
1	1.447484	2.550941	-2.127647
1	0.384941	1.368049	-1.735987
1	1.979033	1.170398	-1.433519
7	1.270593	1.311522	1.705338
1	1.255340	1.764708	0.790860
1	1.620832	1.987724	2.376470
1	0.297304	1.132048	1.945597
7	-1.860324	0.135932	1.973362
1	-1.211402	-0.653159	1.984673
1	-2.374956	0.119397	2.848253
1	-2.528828	-0.061389	1.234359
7	0.550574	-1.879799	1.667552
1	1.115142	-1.060889	1.878852
1	0.927708	-2.664768	2.187127
1	0.670326	-2.072268	0.674441
7	-1.650044	2.780968	0.065460
1	-1.663792	2.165396	0.875906
1	-2.139097	3.634720	0.308913
1	-0.680497	3.017891	-0.118783

Cartesian coordinates of : MP2_AM9_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.182819	1.071798	0.624113
1	-2.609276	0.566713	1.299111
1	-2.781121	1.999472	0.539896
1	-4.111082	1.181922	1.017749
7	0.512526	-3.014076	-0.549059
1	0.458954	-3.450762	0.365529
1	0.596616	-3.767664	-1.223616
1	-0.384632	-2.553795	-0.712784
7	-1.189618	-1.005545	1.978208
1	-1.572790	-1.552213	2.742493
1	-0.170013	-1.062859	2.038868
1	-1.459490	-1.457354	1.108282
7	1.936312	-1.039831	1.650378
1	2.296689	-0.122794	1.396422
1	1.904659	-1.591977	0.797186
1	2.618388	-1.468504	2.267029
7	-2.032883	-1.230428	-1.300936
1	-2.560377	-0.524182	-0.784795
1	-1.436388	-0.704594	-1.934428
1	-2.701151	-1.736533	-1.874062
7	0.029901	2.010542	1.214094
1	1.036147	1.878522	1.127855
1	-0.111807	2.756411	1.887846
1	-0.342510	1.161157	1.633198
7	1.671716	-0.221159	-1.902294
1	2.022907	-0.412715	-2.834568
1	0.812638	0.319351	-2.003651
1	1.427798	-1.117208	-1.485404
7	-0.809284	1.812553	-1.829171
1	-0.587455	1.984535	-0.845073
1	-1.820283	1.756239	-1.897188
1	-0.527041	2.633547	-2.354922
7	3.086397	1.641306	0.147113
1	3.020849	2.608397	-0.153294

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1      2.750163      1.053121      -0.621840
1      4.073872      1.447659      0.277036
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Cartesian coordinates of : MP2_AM9_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.235725	-1.082445	-0.529204
1	4.007069	-1.411081	0.044084
1	3.515719	-1.250564	-1.490875
1	2.444355	-1.706609	-0.338545
7	-2.872856	1.621336	-0.917445
1	-2.078162	1.112721	-1.312478
1	-3.135732	2.350716	-1.571590
1	-3.654519	0.976694	-0.867098
7	-0.181151	0.140477	-1.414158
1	-0.220101	-0.296329	-0.497567
1	0.585208	0.809588	-1.371202
1	0.109283	-0.596742	-2.048882
7	2.491139	2.015074	-0.823638
1	3.002561	2.398347	-1.611985
1	2.819054	1.057206	-0.681798
1	2.775276	2.548844	-0.008353
7	1.014589	0.155034	1.938972
1	1.774125	-0.014374	1.284873
1	1.424420	0.195004	2.866872
1	0.635732	1.081852	1.728978
7	0.791347	-2.781368	0.417049
1	0.596115	-2.165640	1.202976
1	0.960529	-3.708405	0.793687
1	-0.070583	-2.836212	-0.127895
7	-2.086795	-2.413323	-0.942326
1	-2.226410	-1.860448	-1.781138
1	-2.269324	-1.803612	-0.141968
1	-2.790107	-3.144000	-0.948262
7	-0.320847	2.743530	0.764825
1	-0.365328	3.696248	1.110325
1	-1.237440	2.519728	0.380987
1	0.343503	2.728885	-0.005168
7	-2.158951	-0.426198	1.513030
1	-1.188872	-0.361797	1.818641
1	-2.719939	-0.625560	2.334751
1	-2.421830	0.500724	1.188891

Cartesian coordinates of : MP2_AM9_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.791507	1.941545	-0.531260
1	1.783657	2.090063	-0.581636
1	3.226576	2.849261	-0.403182
1	3.083504	1.602994	-1.442242
7	0.252210	-0.328617	-1.923571
1	0.120677	0.548145	-1.421279
1	0.154595	-0.119758	-2.912287
1	1.219655	-0.618657	-1.775818
7	-0.308910	2.268839	0.157250
1	0.039048	1.797595	0.990673
1	-1.295121	2.025882	0.056449
1	-0.280751	3.266501	0.344967
7	-3.361937	1.420023	-0.474176
1	-3.302122	0.463300	-0.834457
1	-3.396610	2.044805	-1.273280
1	-4.254773	1.514307	-0.001001
7	3.085394	-1.293013	-0.780570
1	3.407055	-0.432119	-0.349044

1	2.547790	-1.801480	-0.083076
1	3.900938	-1.848072	-1.013960
7	1.472119	0.321615	2.035134
1	1.383957	-0.645891	1.727208
1	2.110581	0.780384	1.387423
1	1.925225	0.310562	2.943185
7	-1.730935	-0.449550	1.968742
1	-0.846238	-0.001310	2.199579
1	-2.213733	0.171530	1.324152
1	-2.285194	-0.481963	2.818025
7	0.420254	-2.447672	0.687438
1	-0.389541	-2.078885	1.185767
1	0.257303	-2.240343	-0.294538
1	0.410430	-3.456949	0.792125
7	-2.629848	-1.486876	-1.139766
1	-2.570852	-1.867391	-0.200712
1	-1.674512	-1.279254	-1.434156
1	-2.990533	-2.217321	-1.743429

Cartesian coordinates of : MP2_AM9_5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.978610	-0.075346	-1.788846
1	-0.985550	-0.203446	-1.983527
1	-2.282720	-0.869850	-1.224445
1	-2.466239	-0.132625	-2.677195
7	2.592941	1.723442	0.964902
1	3.014413	2.315096	1.672846
1	1.688335	1.405677	1.316679
1	2.396563	2.314068	0.163234
7	1.274833	0.086915	-2.066113
1	1.728494	0.156371	-2.971185
1	1.966769	-0.273828	-1.415042
1	1.043089	1.032271	-1.762448
7	3.535364	-1.170729	0.349676
1	3.809231	-1.628669	1.213056N_NH3_N9_33.log
1	3.386603	-0.181121	0.566587
1	4.338011	-1.230346	-0.268517
7	-0.261030	2.512844	-0.743113
1	-1.035843	2.002959	-1.161422
1	-0.221037	2.222668	0.229923
1	-0.482269	3.501970	-0.768320
7	0.594508	-2.413565	-0.112388
1	0.586661	-3.427301	-0.172263
1	0.370785	-2.057433	-1.037871
1	1.563774	-2.136844	0.052511
7	-0.128449	0.290235	1.803470
1	-1.120323	0.505623	1.697564
1	0.011567	0.052424	2.780787
1	0.050561	-0.559449	1.269942
7	-3.112772	1.154360	0.950945
1	-4.057354	0.810235	1.087874
1	-2.847451	0.927604	-0.007631
1	-3.159970	2.164894	1.025578
7	-2.522585	-2.110140	0.586726
1	-2.745779	-1.442979	1.317798
1	-1.517646	-2.274264	0.625521
1	-2.992086	-2.979812	0.813150

Cartesian coordinates of : MP2_AM9_6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.210755	-0.861829	1.144928
1	4.115408	-1.314829	1.212008

1	2.869052	-0.963401	0.185674
1	2.576132	-1.367886	1.752803
7	1.838804	-0.821364	-1.666154
1	1.201317	-1.606249	-1.556866
1	2.268156	-0.905008	-2.581626
1	1.263796	0.020102	-1.678599
7	-0.000066	1.933159	-1.282616
1	0.820705	2.133684	-0.708907
1	-0.000098	2.606144	-2.043010
1	-0.820789	2.133681	-0.708840
7	2.713383	2.144745	0.445646
1	3.343272	2.338816	-0.326220
1	3.007238	1.249909	0.841734
1	2.882981	2.860269	1.144794
7	-2.713420	2.144738	0.445806
1	-2.883048	2.860169	1.145042
1	-3.343287	2.338903	-0.326054
1	-3.007271	1.249846	0.841771
7	-3.210727	-0.861909	1.144840
1	-2.576086	-1.367936	1.752722
1	-2.869010	-0.963466	0.185590
1	-4.115359	-1.314951	1.211912
7	0.000011	-2.839807	0.001918
1	-0.000007	-1.998458	0.583810
1	0.814726	-3.391161	0.249563
1	-0.814810	-3.391077	0.249395
7	-1.838743	-0.821377	-1.666234
1	-1.201226	-1.606245	-1.557009
1	-1.263764	0.020110	-1.678637
1	-2.268112	-0.904981	-2.581702
7	0.000005	0.001374	1.416530
1	0.000073	0.187350	2.415364
1	-0.811491	0.486298	1.041364
1	0.811478	0.486261	1.041264

 Cartesian coordinates of : MP2_AM9_7

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.035885	2.166271	1.174505
1	-0.169494	2.539461	0.782015
1	-1.397108	2.865036	1.815938
1	-0.786693	1.344165	1.723004
7	-0.733402	-0.919490	2.140290
1	-0.945291	-1.365536	3.026658
1	-0.088809	-1.530633	1.646438
1	-1.598484	-0.880473	1.602560
7	1.775665	2.764575	-0.162571
1	1.738777	2.579472	-1.159256
1	2.186470	1.938560	0.267774
1	2.409782	3.543196	-0.021444
7	2.353879	-0.032342	1.415628
1	2.186560	-1.021747	1.233764
1	1.556749	0.270453	1.969521
1	3.174658	0.030511	2.009772
7	-3.271982	-0.007346	0.375711
1	-2.719276	0.837874	0.518729
1	-3.415457	-0.084236	-0.625664
1	-4.182958	0.141795	0.796699
7	-1.125471	1.145841	-1.969009
1	-0.124886	1.057103	-2.137604
1	-1.509170	1.742642	-2.694043
1	-1.231293	1.636231	-1.082768
7	-1.141568	-1.956039	-1.415403
1	-1.831523	-2.103086	-0.683622
1	-1.243779	-0.973439	-1.684788
1	-1.440933	-2.513760	-2.209752
7	1.782739	-0.134013	-1.860314
1	2.575976	-0.347211	-2.454877

1	2.118404	-0.059510	-0.902347
1	1.149184	-0.927151	-1.888549
7	1.349702	-2.910679	0.304974
1	2.183406	-3.037281	-0.259976
1	0.583715	-2.685588	-0.334674
1	1.145735	-3.814287	0.719809

Cartesian coordinates of : MP2_AM9_8

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.901538	2.227867	-0.770567
1	0.772264	3.023960	-1.385976
1	0.531395	1.402192	-1.245665
1	0.307192	2.380570	0.040148
7	-0.139440	-0.586345	-1.804809
1	-0.326303	-0.884235	-2.756973
1	0.668339	-1.118253	-1.477603
1	-0.938837	-0.878670	-1.249569
7	3.655595	0.975132	-0.180577
1	4.286544	1.077916	-0.968939
1	4.125978	1.392839	0.615772
1	2.824897	1.542298	-0.379490
7	2.516232	-1.982221	-0.582662
1	2.399039	-2.406513	0.331680
1	2.973812	-1.082051	-0.427095
1	3.168396	-2.568451	-1.093478
7	-2.720592	1.487430	-1.064884
1	-2.952130	0.500508	-0.944627
1	-1.903363	1.521732	-1.665419
1	-3.484154	1.927334	-1.567013
7	-1.448150	2.108014	1.719198
1	-1.975039	1.988006	0.849401
1	-1.586695	3.064428	2.029305
1	-1.886429	1.515659	2.417392
7	-3.219144	-1.549114	-0.227105
1	-2.404379	-1.955301	0.242412
1	-3.905412	-1.342415	0.491561
1	-3.622964	-2.277028	-0.807625
7	1.017970	-0.016270	1.865431
1	1.727396	0.164663	1.160705
1	0.346660	0.749471	1.806743
1	1.480939	0.068570	2.765016
7	-0.561096	-2.617331	1.017668
1	-0.036774	-1.808567	1.362811
1	-0.000257	-3.035048	0.282328
1	-0.610499	-3.293744	1.772350

Cartesian coordinates of : MP2_AM9_9

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.199793	-0.147473	1.601212
1	0.713210	-0.292480	2.465611
1	0.692045	-0.685536	0.889464
1	-0.711080	-0.589369	1.729765
7	4.344750	-0.518056	0.794404
1	5.269424	-0.474804	0.381147
1	4.472409	-0.549015	1.799539
1	3.852375	0.346916	0.563202
7	2.330345	1.765447	0.026727
1	1.819203	1.506194	-0.815939
1	1.667833	1.654147	0.788661
1	2.563717	2.749862	-0.044394
7	0.051374	0.760165	-2.117792
1	-0.047505	1.040935	-3.088292

1	-0.486630	1.420305	-1.559981
1	-0.423262	-0.135284	-2.014782
7	-2.920482	-1.007755	1.888410
1	-3.305836	-0.491890	1.093096
1	-3.490445	-1.837205	2.019101
1	-3.053031	-0.439936	2.718991
7	-3.402752	0.373025	-0.841579
1	-2.850557	-0.352024	-1.293255
1	-2.803395	1.191834	-0.769655
1	-4.175765	0.607323	-1.454261
7	1.924113	-1.675909	-0.894321
1	1.762011	-0.843173	-1.455567
1	2.167754	-2.426929	-1.532523
1	2.753174	-1.497447	-0.325487
7	-1.231539	-2.066527	-0.898079
1	-0.222124	-2.123768	-0.755486
1	-1.650857	-1.964759	0.022967
1	-1.532931	-2.964430	-1.263136
7	-1.239591	2.444716	0.396415
1	-0.745546	1.691064	0.879353
1	-2.016211	2.727114	0.985590
1	-0.610051	3.238931	0.348501

Cartesian coordinates of : MP2_AM9_10

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.367754	-1.735885	0.364635
1	-2.521297	-2.716561	0.573496
1	-1.703392	-1.377530	1.046080
1	-1.879986	-1.693313	-0.527849
7	1.287708	-2.062434	0.759490
1	2.243995	-1.723976	0.780787
1	1.244514	-2.898879	1.331079
1	0.699672	-1.351683	1.193971
7	-0.413810	0.530664	1.682052
1	-0.852575	0.944228	0.860097
1	-0.953575	0.839525	2.484601
1	0.511179	0.948155	1.770153
7	-1.850332	1.398954	-1.190563
1	-2.729174	1.323301	-0.675619
1	-1.653523	0.482574	-1.588599
1	-2.025522	2.032158	-1.964715
7	2.834486	1.034266	1.830732
1	3.498985	1.756090	2.090150
1	2.752975	0.418554	2.633472
1	3.252163	0.490040	1.074831
7	3.546342	-0.405803	-0.938887
1	2.809318	0.233272	-1.240569
1	3.295094	-1.328671	-1.277431
1	4.399495	-0.141469	-1.420304
7	-4.434583	0.604515	0.477158
1	-4.665586	0.841640	1.435306
1	-3.931100	-0.285178	0.483206
1	-5.312070	0.466497	-0.011457
7	-0.045486	-1.195763	-1.987508
1	0.403667	-1.691002	-1.215727
1	0.066056	-1.757989	-2.824847
1	0.489618	-0.341918	-2.122687
7	1.309915	1.844607	-1.042708
1	1.645282	1.896351	-0.083327
1	0.289926	1.823605	-0.993480
1	1.560467	2.720327	-1.491432

Cartesian coordinates of : MP2_AM9_11

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.558224	0.132316	1.428896
1	-3.288163	0.444182	2.356045
1	-3.042775	-0.730062	1.232247
1	-4.545469	-0.096414	1.477120
7	-1.637261	-2.067276	0.397200
1	-1.525033	-1.836975	-0.585035
1	-1.630110	-3.078566	0.473841
1	-0.814801	-1.704470	0.885994
7	0.717220	-0.549774	1.813431
1	0.279732	0.356681	1.642954
1	0.861300	-0.636864	2.814147
1	1.639087	-0.527288	1.386163
7	-0.936588	1.948771	0.714058
1	-0.986816	2.960557	0.767252
1	-1.886447	1.595548	0.799532
1	-0.604478	1.708403	-0.217804
7	1.815896	-2.058527	-1.045659
1	1.150176	-2.488149	-0.412256
1	2.218933	-2.803475	-1.603964
1	2.560222	-1.668421	-0.467533
7	3.983429	-0.361024	0.594766
1	3.575327	0.553346	0.380941
1	4.788591	-0.486426	-0.009940
1	4.342111	-0.325101	1.543170
7	0.275968	0.564139	-2.022162
1	0.525863	0.818573	-2.973124
1	-0.723643	0.357561	-2.035736
1	0.768299	-0.307094	-1.811673
7	-2.942919	0.218762	-1.772751
1	-3.163355	0.392587	-0.793553
1	-3.455819	-0.614456	-2.041726
1	-3.336151	0.984839	-2.309459
7	2.309954	2.161075	-0.097833
1	1.768223	2.452767	0.709369
1	1.642609	1.757652	-0.757396
1	2.690278	3.001837	-0.519212

Cartesian coordinates of : MP2_AM9_12

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.430766	-1.124964	-1.393679
1	-1.715103	-1.464153	-2.307973
1	-1.432393	-0.108120	-1.450759
1	-2.184798	-1.377789	-0.751437
7	-1.061521	2.167595	-1.904255
1	-1.101216	3.163380	-1.711365
1	-1.378884	2.055742	-2.861913
1	-0.075000	1.890545	-1.869585
7	1.846553	1.162143	-1.454665
1	1.876196	0.144830	-1.467637
1	2.643361	1.487063	-1.992332
1	1.996658	1.450929	-0.488723
7	1.563448	-2.155185	-1.470878
1	1.748477	-2.477390	-2.415610
1	0.580428	-1.871473	-1.433162
1	1.651164	-2.969291	-0.870242
7	1.632266	1.893533	1.674807
1	2.145418	2.004270	2.542994
1	1.051524	2.718921	1.572208
1	1.009728	1.093448	1.789372
7	0.102036	-0.912361	1.605246
1	-0.260605	-1.164262	0.688208
1	-0.387003	-1.489110	2.282421
1	1.086110	-1.183013	1.625451
7	3.207918	-1.010919	1.086808
1	3.298957	-0.000336	1.110932

1	3.004883	-1.273642	0.125185
1	4.104745	-1.408678	1.341558
7	-2.175738	1.323481	1.078897
1	-1.342227	0.875134	1.452322
1	-1.953289	1.626495	0.131804
1	-2.361573	2.151334	1.633873
7	-3.713816	-1.375486	0.801030
1	-4.676466	-1.332105	0.485382
1	-3.406302	-0.421701	1.004646
1	-3.715446	-1.895884	1.671209

Cartesian coordinates of : MP2_AM9_13

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.728851	0.943416	1.493101
1	3.303333	0.185318	1.140865
1	3.339431	1.580866	1.992279
1	2.345044	1.434259	0.683364
7	-3.463744	-0.274934	-1.084383
1	-3.098382	-0.936211	-0.390979
1	-3.456515	-0.745814	-1.983348
1	-4.440606	-0.109829	-0.863217
7	-2.035428	-1.987866	1.070551
1	-1.492994	-1.264292	1.547205
1	-1.349780	-2.623217	0.673337
1	-2.545275	-2.507156	1.777611
7	1.236959	-2.224733	0.565053
1	1.503405	-3.077055	1.046295
1	0.952403	-1.553404	1.273609
1	2.072586	-1.850520	0.118812
7	-2.115835	2.351672	0.108142
1	-2.237502	3.169210	-0.480931
1	-2.680771	2.513871	0.935812
1	-2.532383	1.559551	-0.386031
7	1.029137	2.099958	-0.903297
1	1.241140	2.868552	-1.531057
1	0.159664	2.333286	-0.426831
1	0.813253	1.287097	-1.477460
7	-0.125830	-0.775868	-1.874011
1	-0.360915	-1.283637	-2.721080
1	-0.980633	-0.321628	-1.562900
1	0.112428	-1.464932	-1.159122
7	3.131454	-0.628704	-1.498961
1	3.519189	0.304404	-1.412844
1	2.170655	-0.521382	-1.817963
1	3.650775	-1.101520	-2.230701
7	-0.302810	0.451785	2.187290
1	0.709427	0.586615	2.139671
1	-0.585708	0.723759	3.123924
1	-0.710554	1.130720	1.547286

Cartesian coordinates of : MP2_AM9_14

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.512525	-0.705245	1.892317
1	-0.604587	-0.935549	2.877063
1	-0.071145	-1.507259	1.436267
1	-1.456982	-0.650304	1.521069
7	0.816312	-3.065179	0.187324
1	1.168043	-3.951511	0.534664
1	1.615640	-2.542335	-0.174438
1	0.227994	-3.278470	-0.611400
7	0.043737	-0.196903	-1.508536
1	-0.222138	0.645327	-1.002062

1	0.932805	-0.509677	-1.127426
1	0.218171	0.076637	-2.470257
7	-1.098304	2.195091	0.495666
1	-1.147845	3.093386	0.966442
1	-0.721697	1.529432	1.167253
1	-2.061138	1.903383	0.313977
7	2.318180	0.918591	1.323025
1	1.398308	0.566357	1.581993
1	2.190323	1.749137	0.745585
1	2.782552	1.209588	2.176349
7	1.590519	3.159330	-0.870077
1	0.627820	2.882499	-0.677196
1	1.824592	2.851072	-1.806879
1	1.628172	4.172510	-0.874750
7	-2.471706	-1.897336	-0.704877
1	-2.195896	-2.607377	-0.035082
1	-2.917224	-2.380874	-1.477541
1	-1.616582	-1.459190	-1.057094
7	-3.916769	0.849008	-0.093545
1	-4.654727	0.798398	0.600343
1	-3.568566	-0.099859	-0.244326
1	-4.353189	1.151954	-0.957559
7	3.265294	-1.212589	-0.662444
1	4.044578	-1.785194	-0.354001
1	3.113447	-0.486802	0.046918
1	3.576109	-0.748646	-1.509887

Cartesian coordinates of : MP2_AM9_15

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.293677	2.354238	0.743724
1	1.428320	2.882631	0.752305
1	3.054787	3.012856	0.864381
1	2.375644	1.931745	-0.179169
7	-1.159784	-1.668213	1.544605
1	-1.593896	-2.229358	2.270275
1	-1.913256	-1.236535	1.015087
1	-0.687134	-2.306287	0.908694
7	-1.494913	1.679788	1.492762
1	-1.438715	2.428974	2.173324
1	-1.012869	1.982738	0.645949
1	-0.986443	0.884813	1.868281
7	-3.525263	0.088501	-0.153366
1	-3.875509	0.605141	-0.953720
1	-3.060882	0.759641	0.465626
1	-4.341956	-0.267038	0.333023
7	1.927507	-0.676400	1.648318
1	2.450663	-0.973627	2.466169
1	0.938797	-0.810869	1.858759
1	2.082350	0.329201	1.554094
7	2.183923	0.164982	-1.554115
1	2.399424	-0.326944	-0.690427
1	2.838881	-0.141439	-2.264959
1	1.252784	-0.135808	-1.833970
7	1.172572	-3.035028	-0.343841
1	1.318270	-3.946147	0.078808
1	1.661961	-3.051104	-1.232582
1	1.636331	-2.340535	0.244635
7	-0.966007	-1.020038	-1.848992
1	-1.263488	-1.393604	-2.745309
1	-1.815499	-0.832171	-1.315523
1	-0.473950	-1.772812	-1.369858
7	-0.415795	2.195890	-1.450932
1	-1.006319	2.784739	-2.029082
1	-0.621978	1.225030	-1.684328
1	0.542267	2.350723	-1.747625

Cartesian coordinates of : MP2_AM9_16

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.083021	0.653978	-2.082166
1	0.171073	0.898706	-3.063463
1	-0.716449	0.026494	-2.000705
1	-0.154538	1.507617	-1.580514
7	-2.731506	-0.994692	2.050487
1	-3.590790	-1.534160	2.058749
1	-2.514296	-0.791159	3.020324
1	-2.923203	-0.110380	1.574396
7	-2.863742	1.296578	-0.051841
1	-2.681597	0.521687	-0.686328
1	-2.046781	1.903577	-0.084880
1	-3.643919	1.823861	-0.428855
7	0.392156	-0.522640	1.135764
1	-0.528849	-0.876644	1.389811
1	0.560799	0.292076	1.718438
1	0.314386	-0.164849	0.187187
7	-1.988637	-1.688354	-1.149199
1	-1.118763	-2.187367	-1.343699
1	-2.152316	-1.769135	-0.147552
1	-2.734618	-2.197397	-1.612912
7	3.484716	-0.983730	1.499089
1	3.933788	-1.744316	1.001646
1	3.777090	-1.050602	2.467508
1	2.476212	-1.132191	1.465635
7	2.661557	1.584502	-0.260472
1	3.406957	2.100787	-0.715919
1	2.158157	1.077264	-0.985155
1	3.106312	0.886468	0.336212
7	1.055564	-2.426836	-1.396468
1	1.702909	-3.087379	-1.810714
1	1.243522	-2.382260	-0.400129
1	1.254699	-1.503542	-1.771474
7	-0.064767	3.045998	0.250778
1	0.893804	2.685399	0.235604
1	-0.375167	3.028295	1.217396
1	-0.016965	4.025518	-0.012415

Cartesian coordinates of : MP2_AM9_17

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.105235	-0.300084	-1.741480
1	1.587176	-0.197954	-2.628968
1	1.263894	0.552347	-1.209926
1	0.103046	-0.342277	-1.942641
7	1.111840	1.481035	1.016664
1	0.675390	0.584239	1.225180
1	0.931514	2.086034	1.811868
1	2.122443	1.329141	0.988084
7	4.204000	0.759301	0.721775
1	4.060885	-0.210889	0.435746
1	4.729120	1.220517	-0.013076
1	4.800463	0.751864	1.541934
7	3.231570	-2.090692	-0.226706
1	3.704228	-2.721566	-0.864895
1	2.447816	-1.671373	-0.730604
1	2.850435	-2.665429	0.516824
7	-0.377110	-1.481717	0.945940
1	0.136417	-1.449417	0.068197
1	0.018439	-2.238694	1.494536
1	-1.329852	-1.754443	0.710883
7	-3.677374	-1.726279	0.593298
1	-4.532893	-1.756910	0.049203

1	-3.564429	-0.775969	0.954472
1	-3.817019	-2.345845	1.384426
7	-2.049033	-0.291731	-1.885457
1	-2.471553	-0.941621	-1.226516
1	-2.167372	0.642005	-1.499755
1	-2.593713	-0.339579	-2.740046
7	-2.500199	0.984173	1.505959
1	-2.237399	1.593136	0.733228
1	-2.738710	1.575845	2.294195
1	-1.666856	0.454767	1.748920
7	-1.058679	2.669933	-0.932249
1	-0.240683	2.365057	-0.397812
1	-1.174185	3.665614	-0.772627
1	-0.828358	2.563815	-1.915039

Cartesian coordinates of : MP2_AM9_18

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-4.085507	0.193682	-0.554128
1	-3.306704	0.826757	-0.723057
1	-4.214756	-0.367790	-1.388045
1	-4.922874	0.753924	-0.441141
7	1.116121	0.093814	2.002285
1	1.603271	-0.553908	1.387821
1	0.123458	-0.128524	1.940257
1	1.409320	-0.115464	2.950900
7	2.063082	0.910852	-1.849624
1	1.793892	1.705320	-1.273534
1	2.458493	1.283858	-2.706074
1	1.202081	0.418680	-2.093874
7	-1.443232	1.910944	0.046794
1	-0.482783	2.235760	-0.048372
1	-1.987139	2.715703	0.341971
1	-1.456639	1.237890	0.811076
7	-0.715916	-0.559535	-1.913686
1	-1.153220	0.241423	-1.462960
1	-0.666808	-1.307800	-1.227160
1	-1.325569	-0.867872	-2.662910
7	0.259946	-2.965967	0.136709
1	0.247435	-3.628774	-0.632194
1	1.161221	-2.485876	0.103525
1	0.255808	-3.520196	0.987279
7	-1.937795	-0.945701	1.546091
1	-1.426136	-1.655652	1.024024
1	-2.778437	-0.725133	1.011819
1	-2.244357	-1.373866	2.413852
7	3.101214	-1.452054	-0.161600
1	3.490461	-2.156133	-0.781170
1	3.854156	-1.189858	0.467187
1	2.887548	-0.630588	-0.739301
7	1.643110	2.892007	0.699493
1	2.634347	3.062005	0.565657
1	1.544501	2.026420	1.237423
1	1.292264	3.653403	1.270662

Cartesian coordinates of : MP2_AM9_19

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.348179	0.105893	1.987703
1	1.671146	0.164363	2.948666
1	0.406578	0.498349	1.978555
1	1.935770	0.735467	1.440864
7	0.098106	1.768265	-0.743539
1	-0.157319	2.631280	-1.212897

1	1.070553	1.863305	-0.459013
1	-0.452100	1.728699	0.111944
7	-1.821005	0.957075	1.837048
1	-2.019160	-0.029356	1.974713
1	-2.133298	1.441021	2.672944
1	-2.421629	1.260414	1.065984
7	-0.745812	-1.376482	-0.305306
1	-0.285361	-2.025350	-0.936780
1	-0.152496	-1.338975	0.519526
1	-0.641783	-0.453412	-0.724314
7	-3.310922	1.416055	-0.867188
1	-2.561997	1.410895	-1.552176
1	-3.694815	0.469994	-0.831999
1	-4.034007	2.033380	-1.219883
7	-3.872669	-1.627913	-0.341118
1	-4.282035	-1.843873	0.561099
1	-4.184426	-2.349030	-0.982157
1	-2.856476	-1.703593	-0.254138
7	2.473489	-2.463433	0.429724
1	2.111244	-1.723817	1.034266
1	1.970493	-3.315021	0.655317
1	3.441411	-2.625555	0.686329
7	3.419682	1.658640	-0.021016
1	3.319013	0.995386	-0.794482
1	4.229734	1.379524	0.522794
1	3.644233	2.565124	-0.418170
7	2.370401	-0.410779	-2.030291
1	2.579987	-0.756280	-2.959976
1	1.444061	0.005319	-2.052589
1	2.336533	-1.209508	-1.396543

Cartesian coordinates of : MP2_AM9_20

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.238718	0.682334	1.805101
1	-2.194766	0.534615	2.807894
1	-2.102161	-0.221764	1.355728
1	-3.184968	0.978816	1.590483
7	-1.508445	-1.827707	-0.158249
1	-1.445346	-1.284246	-1.014961
1	-1.556213	-2.805890	-0.426576
1	-0.617774	-1.701861	0.335512
7	1.152357	-1.235537	1.370477
1	1.200398	-0.228846	1.525429
1	1.140096	-1.674540	2.285683
1	2.025620	-1.517991	0.922765
7	0.642712	1.921840	1.143148
1	0.791827	2.895613	1.383103
1	-0.326253	1.690053	1.359153
1	0.773441	1.826008	0.140121
7	3.898460	-1.785013	-0.196185
1	4.650911	-2.188784	0.350690
1	3.990103	-2.157652	-1.134787
1	4.051250	-0.775697	-0.243417
7	3.661553	1.324938	-0.226395
1	2.853852	1.313926	-0.846947
1	4.276814	2.075901	-0.518357
1	3.304425	1.562687	0.693591
7	-4.457563	-0.703904	-0.466507
1	-4.913683	-1.231758	-1.202514
1	-5.113734	-0.657488	0.305031
1	-3.645769	-1.236691	-0.155852
7	-2.073922	1.249983	-1.463313
1	-2.270919	1.977969	-2.142715
1	-1.812460	1.714569	-0.598532
1	-2.956831	0.777269	-1.269226
7	1.009663	0.382817	-1.771000
1	1.318047	0.190881	-2.718662

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1      0.002141      0.542203      -1.810412
1      1.159270      -0.465558      -1.231767

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Cartesian coordinates of : MP2_AM9_21

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.285972	-0.010452	0.212858
1	4.287962	-0.117019	0.328552
1	3.081301	-0.105668	-0.781560
1	2.842464	-0.796661	0.685955
7	1.818487	-0.113680	-2.651911
1	1.727645	-0.920151	-3.259454
1	1.717862	0.709029	-3.235794
1	1.042688	-0.124352	-1.987183
7	-0.014317	-0.063940	-0.119887
1	0.258945	0.858128	0.209006
1	-0.980029	-0.210568	0.156770
1	0.543873	-0.731440	0.406402
7	1.598782	-2.520297	1.582368
1	0.764369	-2.875863	1.108499
1	2.312121	-3.238511	1.509718
1	1.372118	-2.438143	2.568139
7	1.806619	2.682389	0.743625
1	2.077358	3.284172	-0.028505
1	2.156568	3.130039	1.585426
1	2.344685	1.815109	0.632614
7	-2.731368	1.284943	-1.204677
1	-2.342104	1.973061	-0.556947
1	-1.955457	0.934597	-1.757762
1	-3.352673	1.775392	-1.838813
7	-1.363394	3.050373	1.049487
1	-0.350891	2.934789	0.976876
1	-1.548204	4.045499	1.117846
1	-1.648509	2.642037	1.933379
7	-0.925774	-3.120548	-0.183188
1	-1.248861	-4.037827	-0.471789
1	-0.577208	-2.654095	-1.014823
1	-1.745246	-2.589488	0.117541
7	-3.416111	-1.221997	0.552422
1	-4.242962	-1.733551	0.261773
1	-3.356525	-0.385819	-0.035144
1	-3.593562	-0.910227	1.501608

Cartesian coordinates of : MP2_AM9_22

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.709679	-1.910681	-0.656425
1	-2.356017	-2.341285	-1.308469
1	-1.215490	-1.169676	-1.148237
1	-2.261653	-1.470388	0.075151
7	-1.117005	1.716421	-0.239070
1	-0.762956	2.665287	-0.303572
1	-2.060664	1.715118	-0.624742
1	-0.535921	1.138277	-0.846507
7	0.894010	-0.327363	-1.805546
1	1.146128	-1.148326	-1.260262
1	0.951299	-0.595779	-2.783055
1	1.620021	0.374334	-1.652417
7	1.053786	-3.144163	0.156202
1	1.242073	-4.003145	-0.350741
1	0.082477	-2.886979	-0.038734
1	1.104436	-3.378136	1.142742
7	2.834649	2.122010	-1.070107
1	3.831052	2.296116	-0.989250

1	2.461903	2.873001	-1.641650
1	2.433983	2.213388	-0.132794
7	3.257803	-0.834145	0.760797
1	3.474254	-0.274705	-0.058135
1	4.130419	-1.225137	1.098229
1	2.669787	-1.608849	0.456855
7	-2.502414	-0.080710	1.906140
1	-1.899919	0.589756	1.423837
1	-3.009937	0.421704	2.626848
1	-1.903408	-0.744964	2.385249
7	-4.183769	0.881809	-0.714989
1	-3.913169	0.329535	0.095544
1	-4.376876	0.240157	-1.475446
1	-5.055037	1.350616	-0.493980
7	1.496666	1.638767	1.676223
1	0.531438	1.452206	1.417731
1	1.496931	1.998932	2.623651
1	2.006520	0.755330	1.669579

Cartesian coordinates of : MP2_AM9_23

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.112784	-1.138388	1.415754
1	3.796561	-0.692617	0.803058
1	3.616628	-1.662744	2.122114
1	2.602926	-0.398247	1.888123
7	0.103262	0.247294	1.827136
1	0.202732	-0.552675	1.209913
1	-0.771182	0.715375	1.594064
1	0.015996	-0.111686	2.771912
7	1.026629	-1.605380	-0.879224
1	1.757688	-1.625752	-0.163026
1	1.299609	-2.274274	-1.592807
1	1.070019	-0.684965	-1.308433
7	1.751249	1.906620	-0.383215
1	0.929121	1.757912	-0.967535
1	1.467988	1.601778	0.547176
1	1.904670	2.908875	-0.335267
7	-2.809477	1.679593	1.228599
1	-2.951278	2.659069	1.003076
1	-3.496434	1.138705	0.697628
1	-3.043084	1.580703	2.211413
7	-1.969743	-2.196329	-0.072922
1	-0.985433	-2.059113	-0.320929
1	-2.035849	-2.045294	0.929032
1	-2.173278	-3.178841	-0.228714
7	-4.418030	-0.261126	-0.631301
1	-4.520206	0.065373	-1.586028
1	-3.638973	-0.922489	-0.612309
1	-5.263011	-0.777538	-0.411784
7	-1.096415	0.935560	-1.574018
1	-1.525632	1.144110	-0.675119
1	-1.298140	-0.042200	-1.757140
1	-1.590352	1.478430	-2.274667
7	4.484680	0.433200	-0.918219
1	5.238372	1.109078	-0.973817
1	3.603084	0.950191	-0.870473
1	4.492889	-0.088464	-1.787582

Cartesian coordinates of : MP2_AM9_24

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.366264	2.917391	-0.109379
1	-0.075392	3.298629	0.720818

1	1.078383	3.581339	-0.394554
1	0.840836	2.058529	0.172560
7	1.614338	-0.005209	0.136300
1	1.442050	-0.922867	0.541909
1	2.621718	0.093686	0.018589
1	1.190258	-0.019192	-0.789120
7	0.165157	-2.645565	1.595069
1	-0.512629	-3.316249	1.247900
1	-0.354715	-1.811992	1.871308
1	0.568407	-3.045631	2.435711
7	-2.783835	2.071951	0.318553
1	-3.637744	2.617991	0.302986
1	-2.970416	1.180059	-0.135001
1	-2.092653	2.558927	-0.243660
7	-0.894023	0.320550	2.178390
1	-0.009194	0.489799	1.702194
1	-0.759900	0.531949	3.161918
1	-1.564607	0.997769	1.812560
7	-0.227520	-2.603523	-1.650336
1	0.023751	-3.298395	-2.344269
1	-0.033156	-1.683546	-2.039340
1	0.382611	-2.728753	-0.847931
7	-2.656038	-1.110281	-0.268872
1	-3.573727	-1.525199	-0.144874
1	-2.067220	-1.802453	-0.733785
1	-2.263191	-0.955227	0.657102
7	4.852078	0.440381	-0.018562
1	5.288257	-0.183634	0.650537
1	5.294952	0.274862	-0.915095
1	5.082507	1.387124	0.260261
7	-0.609237	0.579704	-2.215434
1	-1.457012	0.212627	-1.786560
1	-0.825356	0.785678	-3.185255
1	-0.407108	1.466380	-1.757012

Cartesian coordinates of : MP2_AM9_25

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	4.627335	1.282559	0.566052
1	4.753452	0.711418	1.393729
1	5.383454	1.061615	-0.071614
1	4.745937	2.249261	0.846366
7	-0.855712	0.739923	2.025171
1	-0.560292	1.128594	2.914681
1	-1.106399	-0.230445	2.191163
1	-0.037710	0.721086	1.414791
7	-1.384515	-0.449518	-1.662267
1	-1.054004	0.480626	-1.417825
1	-0.558238	-1.019545	-1.847689
1	-1.874631	-0.352340	-2.546267
7	-0.485628	2.925015	-1.116356
1	-0.544794	3.394279	-2.014024
1	-1.439949	2.723760	-0.809205
1	-0.103538	3.599788	-0.461611
7	-2.358881	-1.946942	0.947263
1	-2.158351	-1.462224	0.068028
1	-2.724009	-2.864406	0.713470
1	-3.112591	-1.444417	1.404438
7	1.076058	-2.528595	-1.889417
1	2.041783	-2.519008	-2.200159
1	1.075504	-2.709824	-0.882161
1	0.635818	-3.319374	-2.347787
7	1.523468	0.548599	-0.191998
1	1.503696	-0.202031	-0.876976
1	2.496430	0.828145	-0.078103
1	1.018012	1.330044	-0.609603
7	-3.106753	1.772105	0.103153
1	-2.479285	1.472156	0.853115

1	-3.928155	2.195708	0.519688
1	-3.407938	0.938264	-0.389341
7	0.846622	-2.366468	1.183233
1	1.248522	-2.818344	1.996971
1	-0.162674	-2.325290	1.318688
1	1.175994	-1.404238	1.163396

Cartesian coordinates of : MP2_AM9_26

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.769293	-2.171184	-0.207811
1	3.205329	-2.896946	0.352312
1	3.179238	-2.239838	-1.134098
1	3.072747	-1.274457	0.181718
7	-1.344677	2.378082	-1.447853
1	-1.828587	3.023988	-2.062769
1	-1.599229	1.436951	-1.743701
1	-1.743765	2.484810	-0.514483
7	-0.273205	-3.296772	-0.846795
1	-0.146547	-3.769904	-1.735693
1	-0.479727	-4.020946	-0.166614
1	0.633120	-2.902699	-0.591920
7	-2.334312	-0.827700	-1.436692
1	-2.867423	-0.696338	-0.581237
1	-1.797023	-1.687043	-1.318233
1	-2.998163	-0.982681	-2.187786
7	1.711107	2.806747	-0.851520
1	1.817920	3.742667	-0.472498
1	0.727540	2.715289	-1.130119
1	2.258345	2.781807	-1.706497
7	3.298676	0.682553	1.073881
1	2.862662	1.392256	0.483369
1	4.206422	1.038222	1.354181
1	2.734540	0.624053	1.915690
7	0.257303	0.008154	0.282083
1	0.930531	-0.743226	0.163153
1	-0.429669	-0.100023	-0.460830
1	0.756248	0.866269	0.064648
7	-2.198545	-1.368651	1.791479
1	-1.296792	-0.975271	1.523162
1	-2.207101	-1.466412	2.800692
1	-2.248767	-2.302207	1.399078
7	-2.014496	1.907587	1.614215
1	-2.685740	1.157652	1.749713
1	-2.050639	2.505803	2.431958
1	-1.103486	1.456512	1.589892

Cartesian coordinates of : MP2_AM9_27

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.027149	0.266870	-2.007259
1	-1.067639	0.192123	-3.018530
1	-1.680556	0.996445	-1.720986
1	-1.384242	-0.608030	-1.634239
7	-2.529184	2.508651	-0.377556
1	-3.465186	2.793814	-0.111356
1	-1.986079	3.355998	-0.503230
1	-2.121136	2.010593	0.410429
7	-0.726592	0.742429	1.711220
1	-0.209921	-0.106070	1.479766
1	-0.174957	1.497410	1.301794
1	-0.691212	0.850600	2.720213
7	1.049686	-1.395575	0.011616
1	1.957123	-1.722969	-0.313717

1	0.697851	-0.784696	-0.722112
1	0.412393	-2.192291	0.035796
7	1.077475	2.203667	-0.403340
1	1.951094	1.750056	-0.151225
1	1.315942	3.042608	-0.920898
1	0.573017	1.581582	-1.034054
7	2.979643	0.487094	1.639665
1	2.564402	1.247834	2.166349
1	3.620508	0.010659	2.265494
1	2.233767	-0.168237	1.400270
7	-3.275912	-0.773439	0.469310
1	-3.680841	-0.208761	-0.270202
1	-4.016082	-0.944787	1.141884
1	-2.568555	-0.197920	0.927905
7	-1.487021	-3.374524	0.048189
1	-1.750883	-3.946003	-0.746879
1	-2.171406	-2.621459	0.131465
1	-1.576089	-3.962363	0.869699
7	4.018818	-0.743323	-1.121198
1	5.007859	-0.959325	-1.167052
1	3.875239	-0.095062	-0.349691
1	3.777245	-0.264691	-1.981412

Cartesian coordinates of : MP2_AM9_28

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.355651	0.114133	0.346911
1	-1.966688	0.098669	1.283870
1	-1.866828	-0.606123	-0.184107
1	-3.335776	-0.151670	0.418045
7	-0.498369	-1.819766	-1.483627
1	-0.955646	-2.021019	-2.366726
1	0.049050	-2.639909	-1.244687
1	0.159113	-1.052783	-1.644296
7	1.412224	0.702840	-1.756623
1	0.732212	1.410595	-1.478038
1	2.138527	0.699028	-1.045507
1	1.848944	1.032927	-2.611570
7	-1.097543	2.590821	-0.969122
1	-1.327976	3.451937	-0.484169
1	-1.668032	1.840198	-0.564284
1	-1.394558	2.718449	-1.931152
7	3.855253	0.911275	0.673633
1	4.420528	0.603171	1.458317
1	4.339209	1.705592	0.267820
1	2.966695	1.253012	1.054616
7	0.967642	1.549652	1.560903
1	0.713754	2.062579	2.398355
1	0.709599	0.571197	1.704737
1	0.392051	1.910290	0.804515
7	2.930628	-1.969215	-0.381489
1	2.572343	-1.864467	-1.324874
1	3.669610	-2.663242	-0.418376
1	3.356536	-1.075717	-0.132599
7	0.489796	-1.584762	1.663814
1	1.299047	-1.824169	1.088326
1	-0.328600	-1.848865	1.124424
1	0.512887	-2.183167	2.483034
7	-5.585600	-0.483364	0.389759
1	-6.058376	-0.681064	1.264038
1	-5.844731	-1.214432	-0.262427
1	-5.961553	0.387677	0.033600

Cartesian coordinates of : MP2_AM9_29

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.679410	-0.181549	-1.965858
1	2.447841	0.509797	-2.671939
1	3.524057	-0.642126	-2.288642
1	2.911900	0.321460	-1.106104
7	3.193100	1.037819	0.913774
1	2.384021	0.662417	1.413274
1	3.274592	2.012604	1.185040
1	4.016345	0.572424	1.282486
7	0.371032	0.177301	1.980001
1	-0.003234	0.006741	1.041973
1	0.164508	1.150499	2.189232
1	-0.131157	-0.400597	2.645202
7	1.515845	-2.387631	0.266295
1	2.240015	-3.078034	0.434246
1	1.520637	-1.742864	1.051914
1	1.802851	-1.839095	-0.542220
7	-1.536949	-3.131653	-0.225136
1	-1.617191	-3.586854	-1.128943
1	-1.863532	-3.806548	0.459041
1	-0.538278	-2.987036	-0.050544
7	-3.186751	-0.458047	0.720844
1	-2.770566	-1.326630	0.384324
1	-4.018336	-0.702262	1.247839
1	-2.523512	-0.054358	1.374382
7	-0.445654	-0.101508	-1.004748
1	-1.061745	-0.905660	-1.064212
1	-0.939060	0.692214	-1.401373
1	0.380249	-0.295319	-1.564338
7	-2.805421	2.185863	-0.999002
1	-3.081994	1.316047	-0.538561
1	-3.250344	2.202931	-1.910732
1	-3.212711	2.948645	-0.467912
7	0.172938	2.888467	0.333428
1	-0.693366	2.693186	-0.164716
1	0.870534	2.247731	-0.030831
1	0.464625	3.827258	0.084927

Cartesian coordinates of : MP2_AM9_30

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.236256	-1.878608	2.393520
1	0.727499	-2.205194	1.554123
1	0.926372	-1.820034	3.135899
1	-0.404754	-2.619614	2.660334
7	-2.945847	0.200764	-0.913003
1	-3.878972	-0.002141	-1.256195
1	-2.751957	1.177034	-1.133077
1	-2.970977	0.133527	0.105444
7	1.526844	-2.591714	-0.350751
1	2.127888	-1.826007	-0.649264
1	0.668901	-2.537763	-0.902908
1	1.993825	-3.455578	-0.605279
7	-1.301787	-2.375247	-1.897695
1	-1.270410	-2.395882	-2.911688
1	-1.806773	-1.527365	-1.630988
1	-1.876921	-3.161040	-1.612294
7	-2.167821	0.315111	2.183278
1	-1.408569	-0.348384	2.336755
1	-1.736956	1.221881	2.035892
1	-2.701066	0.377556	3.043698
7	3.402179	0.114804	-1.026745
1	3.609391	0.373794	-1.985807
1	3.277046	0.981539	-0.501080
1	4.237397	-0.333694	-0.664693
7	-1.408820	3.054897	-1.068001
1	-0.737932	2.444745	-0.604234

1	-1.592326	3.846510	-0.462383
1	-0.971390	3.415937	-1.908070
7	0.202703	0.490167	-0.041525
1	0.997861	0.202146	-0.607942
1	0.246389	-0.100304	0.786890
1	-0.630799	0.176166	-0.534237
7	2.391471	2.611581	0.682112
1	1.485806	2.158640	0.562957
1	2.312206	3.563976	0.343551
1	2.582971	2.667263	1.676250

Cartesian coordinates of : MP2_AM9_31

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	4.955957	0.645127	0.376947
1	4.681473	-0.118404	-0.239825
1	5.537345	1.282246	-0.155496
1	5.538800	0.259923	1.111274
7	3.188049	-1.318044	-1.387484
1	3.090161	-1.087718	-2.369892
1	2.936985	-2.294705	-1.285267
1	2.512707	-0.759810	-0.864777
7	-3.177284	-1.867840	-0.028122
1	-3.043104	-2.223778	0.912094
1	-3.642455	-2.598104	-0.556513
1	-2.253738	-1.723063	-0.435653
7	-2.003718	0.618857	1.897789
1	-2.207069	0.888909	2.854928
1	-2.860983	0.231808	1.514763
1	-1.341382	-0.156454	1.939546
7	-3.377878	1.032568	-1.372823
1	-3.593288	0.171044	-0.872946
1	-3.437124	1.791628	-0.702779
1	-4.109847	1.184071	-2.058367
7	-0.636031	2.746214	-0.070595
1	-0.706786	3.716249	0.215595
1	-1.105076	2.658522	-0.965390
1	-1.150150	2.173751	0.600805
7	1.729710	0.777455	0.509856
1	1.205888	1.612866	0.243396
1	2.715595	1.022329	0.603898
1	1.398068	0.541867	1.440788
7	-0.023197	-1.934936	1.487300
1	0.963110	-1.869619	1.713879
1	-0.286259	-2.907359	1.606763
1	-0.118717	-1.705188	0.499712
7	-0.566889	-0.586036	-1.400425
1	0.185216	-0.065733	-0.949774
1	-1.320551	0.075283	-1.588292
1	-0.209853	-0.894121	-2.299569

Cartesian coordinates of : MP2_AM9_32

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	4.364471	-0.226244	0.157281
1	3.682873	0.492738	0.405497
1	5.082491	-0.214624	0.873848
1	4.810885	0.075928	-0.702261
7	-4.370688	-0.448976	0.683965
1	-5.044845	-0.794739	1.357671
1	-4.883239	-0.245630	-0.166664
1	-3.712143	-1.201840	0.483281
7	-1.864040	-2.392600	0.489709
1	-1.059285	-1.761177	0.503298

1	-1.582744	-3.197822	-0.061285
1	-1.983785	-2.732307	1.439026
7	-1.981701	0.115573	-1.947720
1	-2.513545	0.276508	-2.795739
1	-2.246984	-0.794450	-1.583869
1	-2.279328	0.798920	-1.257614
7	-1.786396	1.365613	1.143391
1	-1.673375	1.853249	2.025970
1	-2.696514	0.904720	1.168231
1	-1.076645	0.635904	1.102326
7	2.715876	-2.895728	-0.350619
1	3.348103	-2.117406	-0.155751
1	2.780219	-3.551954	0.419311
1	3.057088	-3.374563	-1.176403
7	0.572633	-0.527579	-0.118164
1	1.143442	-1.351428	-0.310706
1	1.225377	0.215248	0.116197
1	0.114120	-0.254488	-0.985179
7	-0.018400	2.837475	-1.014096
1	-0.231363	3.780026	-1.322335
1	-0.761180	2.537945	-0.380334
1	-0.079331	2.236867	-1.830169
7	2.360891	2.196928	0.924984
1	3.061065	2.931680	0.944516
1	1.932334	2.187566	1.845218
1	1.637789	2.493888	0.262815

Cartesian coordinates of : MP2_AM9_33

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.634523	0.322020	2.099221
1	-2.077923	0.843379	2.847453
1	-2.137963	-0.553089	2.003413
1	-1.760535	0.839396	1.229935
7	-1.613898	1.360898	-0.900942
1	-1.832276	0.435410	-1.262703
1	-0.593494	1.431559	-0.903856
1	-1.939377	2.033524	-1.588923
7	-3.126795	-1.705124	-1.014372
1	-3.785396	-1.002400	-0.674300
1	-3.320286	-2.563765	-0.509011
1	-3.360932	-1.889619	-1.984680
7	1.508779	0.427814	1.760421
1	1.527438	1.034394	0.943818
1	2.048181	0.887370	2.486815
1	0.538875	0.396494	2.076596
7	3.517134	-1.616460	0.435757
1	3.895273	-2.365050	1.005315
1	3.049099	-2.045103	-0.355434
1	2.801998	-1.129728	0.979043
7	-4.629054	0.852641	0.110443
1	-5.283643	1.429336	-0.406689
1	-4.915102	0.886047	1.082562
1	-3.711824	1.289267	0.046877
7	0.133736	-1.742941	-0.438222
1	-0.873555	-1.679005	-0.577277
1	0.366514	-2.730179	-0.417140
1	0.350824	-1.367544	0.480758
7	1.475613	1.001315	-1.494203
1	1.381947	1.240372	-2.476220
1	2.461325	1.124762	-1.258818
1	1.247611	0.011626	-1.401171
7	4.555060	1.150759	-0.570485
1	5.297342	1.144192	-1.261104
1	4.453589	0.200573	-0.209663
1	4.869917	1.741336	0.191075

Cartesian coordinates of : MP2_AM9_34

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.507596	-0.688693	1.817773
1	-0.406488	-1.145628	1.830140
1	0.888160	-0.750179	2.756923
1	0.323206	0.295195	1.636027
7	0.474979	2.398823	0.270702
1	0.863785	3.036213	0.959011
1	0.132205	2.980282	-0.488012
1	1.254081	1.844179	-0.097336
7	-2.387873	-1.672545	1.138776
1	-2.417875	-1.852979	0.140475
1	-2.597277	-0.679463	1.268301
1	-3.133788	-2.209947	1.566968
7	-2.596519	1.459103	1.250733
1	-3.157724	1.547807	0.404230
1	-1.662230	1.806108	1.045099
1	-2.999043	2.067852	1.954739
7	2.531602	0.217173	-0.559091
1	2.107383	-0.334836	0.183460
1	2.307511	-0.248378	-1.432022
1	3.543457	0.189080	-0.447859
7	-4.007624	0.745683	-1.480193
1	-4.319864	1.123175	-2.367720
1	-3.093403	0.313261	-1.627124
1	-4.660777	0.013879	-1.223561
7	-0.981133	-0.128917	-1.618238
1	-0.587338	0.265361	-2.467191
1	-0.531837	-1.035516	-1.481972
1	-0.663179	0.462186	-0.854415
7	5.774235	0.418570	-0.182701
1	5.948890	1.406442	-0.326839
1	6.375145	-0.089194	-0.821697
1	6.080625	0.192447	0.756574
7	0.476693	-2.780907	-0.615192
1	0.685832	-2.227737	0.214334
1	1.335310	-3.231023	-0.912857
1	-0.158455	-3.516624	-0.325661

Cartesian coordinates of : MP2_AM9_35

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.965244	2.687206	-0.262247
1	-1.479797	3.536729	-0.469131
1	0.022558	2.879212	-0.431415
1	-1.237915	1.988788	-0.949790
7	0.304121	-3.402026	-0.826174
1	0.478318	-4.316855	-0.425274
1	-0.557831	-3.041429	-0.416488
1	0.144649	-3.539827	-1.817768
7	-0.770614	0.754205	2.215644
1	-0.185601	1.168540	2.934402
1	-1.682253	0.607389	2.637382
1	-0.890796	1.458406	1.482292
7	-2.019836	-1.958381	0.832636
1	-2.770056	-1.282243	0.684282
1	-1.334275	-1.468717	1.404187
1	-2.404348	-2.708712	1.398056
7	1.436012	-0.498521	0.107299
1	2.364371	-0.481148	0.525870
1	1.260031	-1.461473	-0.178584
1	0.765044	-0.276751	0.841531
7	-1.167710	-0.181005	-1.815208
1	-0.206782	-0.063447	-1.495253

1	-1.131507	-0.369342	-2.811937
1	-1.496115	-1.027895	-1.357091
7	4.645949	-0.408635	0.674259
1	4.876122	-1.380219	0.500193
1	4.859841	0.110754	-0.169309
1	5.268151	-0.077190	1.402201
7	2.128380	2.408370	-0.907523
1	1.935125	1.416795	-0.753210
1	2.463184	2.523006	-1.857532
1	2.887624	2.671808	-0.289536
7	-3.702727	0.641269	0.012054
1	-3.470417	1.485523	0.524103
1	-4.640148	0.760063	-0.355431
1	-3.055491	0.590874	-0.771930

Cartesian coordinates of : MP2_AM9_36

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-4.713318	-1.373462	1.026193
1	-4.477504	-2.345529	1.189815
1	-5.234035	-1.050998	1.833798
1	-5.345437	-1.345525	0.234374
7	0.691419	-2.033072	0.597262
1	0.491460	-2.959398	0.961647
1	1.442855	-1.654466	1.172503
1	-0.137857	-1.456226	0.762160
7	1.579510	1.752339	0.668754
1	0.692632	2.209270	0.880247
1	2.312785	2.368204	1.005884
1	1.635210	0.906299	1.229873
7	-0.568040	-1.662416	-2.319409
1	-1.511102	-2.002469	-2.165013
1	-0.175266	-2.220271	-3.069857
1	-0.036477	-1.864898	-1.472146
7	-0.340024	1.482035	-1.959050
1	-0.415863	0.503508	-2.242648
1	0.519360	1.568475	-1.420013
1	-0.228707	2.028842	-2.806643
7	-1.259500	3.291509	0.471359
1	-2.202504	3.220143	0.837064
1	-1.103202	4.270843	0.258591
1	-1.228531	2.772075	-0.406828
7	-1.747228	-0.046772	0.681233
1	-1.612600	0.680492	1.376020
1	-2.711152	-0.366817	0.756862
1	-1.631868	0.403033	-0.223240
7	3.059508	-0.531954	-1.114594
1	2.313783	-1.214432	-1.004318
1	2.628423	0.379464	-0.982568
1	3.396686	-0.583865	-2.068815
7	3.459784	-0.842184	1.914613
1	3.880581	-0.058664	2.402038
1	3.695772	-0.760365	0.924222
1	3.907779	-1.678879	2.272459

Cartesian coordinates of : MP2_AM9_37

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.625877	2.362297	1.166296
1	-0.917142	3.281745	0.849697
1	-0.960874	2.267488	2.119836
1	0.398603	2.375406	1.211294
7	1.750705	-3.165534	-0.508123
1	1.973584	-4.145145	-0.647780

1	0.742226	-3.099958	-0.360001
1	1.946635	-2.693169	-1.384977
7	-2.528878	0.163733	-0.482178
1	-3.518834	0.354470	-0.337805
1	-2.331327	0.350185	-1.460286
1	-1.997866	0.852565	0.049925
7	-1.406321	-2.724398	0.093059
1	-2.006294	-3.415131	-0.346463
1	-1.847229	-1.810658	-0.054797
1	-1.439340	-2.907461	1.090975
7	3.133214	-1.135014	1.495531
1	4.145216	-1.207108	1.477079
1	2.765761	-1.912982	0.942655
1	2.847988	-1.290953	2.456775
7	2.495183	2.135119	0.986846
1	2.758544	1.168954	1.175618
1	3.163160	2.725870	1.470243
1	2.627134	2.286303	-0.013589
7	2.372379	2.044227	-2.239444
1	1.794194	1.239064	-1.990241
1	1.801756	2.675582	-2.790658
1	3.118103	1.717913	-2.843953
7	0.747754	-0.086898	-0.679864
1	0.245196	0.646571	-0.186321
1	0.112648	-0.877952	-0.710821
1	1.506535	-0.360470	-0.060689
7	-5.741899	0.469795	0.121418
1	-5.947171	1.062472	0.917482
1	-5.991106	-0.477984	0.379661
1	-6.363927	0.751089	-0.627636

Cartesian coordinates of : MP2_AM9_38

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-5.236828	1.641724	0.118310
1	-5.379421	2.643359	0.177024
1	-5.769249	1.310351	-0.677798
1	-5.646690	1.230182	0.948747
7	1.264629	0.748561	1.716522
1	0.661652	-0.018868	2.004661
1	0.988488	0.993766	0.768534
1	1.048672	1.539587	2.313347
7	3.386805	2.529562	-0.450774
1	3.542110	2.510282	0.550528
1	3.497404	3.487592	-0.761553
1	2.422728	2.253884	-0.612076
7	-2.192482	0.414470	0.079060
1	-3.108729	0.857045	0.038069
1	-1.498662	1.154752	0.060777
1	-2.066124	-0.127531	-0.775145
7	0.881875	0.743791	-1.561950
1	0.050482	0.892035	-2.125278
1	0.856856	-0.230419	-1.264829
1	1.681096	0.831496	-2.182502
7	0.986774	-2.238284	-0.190937
1	1.090189	-3.244663	-0.280560
1	1.934919	-1.859644	-0.123246
1	0.533053	-2.066821	0.705823
7	-1.420136	-1.702492	-2.228986
1	-0.618893	-1.940605	-1.641612
1	-1.088072	-1.647998	-3.185826
1	-2.073214	-2.477657	-2.193031
7	3.686419	-0.656393	0.270102
1	4.489558	-1.102427	0.699690
1	3.141088	-0.207403	1.005884
1	4.037385	0.094534	-0.317919
7	-1.112121	-1.524109	2.239699
1	-1.512271	-2.452841	2.154733

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1   -1.613012   -0.906081    1.592077
1   -1.315873   -1.213726    3.184153

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Cartesian coordinates of : MP2_AM9_39

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.711202	-0.627244	0.344470
1	-4.454669	-0.026390	-0.006317
1	-4.160088	-1.418779	0.793053
1	-3.201430	-0.994379	-0.459989
7	-0.025802	-2.085677	0.774487
1	0.985358	-1.976429	0.769074
1	-0.235944	-2.882388	1.366268
1	-0.414415	-1.262851	1.232159
7	-1.376704	0.710313	1.912553
1	-2.196648	0.308677	1.443588
1	-1.644746	0.889307	2.875272
1	-1.210616	1.617758	1.488359
7	-1.680181	-1.763964	-1.866607
1	-1.053921	-1.956592	-1.081094
1	-1.795890	-2.623580	-2.391693
1	-1.209806	-1.108492	-2.480826
7	5.026810	0.565032	-1.021284
1	5.739790	0.868950	-0.366850
1	5.472477	0.524152	-1.931507
1	4.318993	1.302101	-1.059582
7	1.906334	0.784044	1.608431
1	0.925227	0.599620	1.807832
1	2.305145	-0.074010	1.230899
1	2.361318	0.956504	2.498636
7	2.613630	2.575558	-0.844506
1	1.877168	2.492062	-1.536750
1	2.295894	2.096704	0.002870
1	2.699394	3.563039	-0.630355
7	3.180567	-1.790357	-0.019588
1	3.840252	-1.088424	-0.366025
1	2.698599	-2.166899	-0.829990
1	3.731335	-2.550778	0.365978
7	-5.866096	1.548676	-0.847413
1	-6.193227	1.308271	-1.775881
1	-5.274272	2.366362	-0.936710
1	-6.676770	1.821814	-0.304228

Cartesian coordinates of : MP2_AM9_40

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.798158	2.310632	-0.607125
1	-1.755846	3.210375	-0.140489
1	-2.354600	1.676755	-0.026328
1	-2.312023	2.459812	-1.469111
7	-3.100188	-0.106806	0.847471
1	-4.090642	-0.339734	0.881838
1	-2.682990	-0.457816	1.702672
1	-2.675469	-0.620432	0.074512
7	-1.363548	-0.919250	-1.696299
1	-1.196755	0.075358	-1.815964
1	-0.472590	-1.333974	-1.422170
1	-1.602548	-1.295373	-2.607423
7	2.881314	0.814739	-1.918716
1	2.345176	1.026156	-1.080921
1	2.704833	1.550453	-2.593098
1	3.864237	0.854006	-1.674334
7	3.698534	1.427563	1.531336
1	2.741459	1.395407	1.175482

1	3.670276	1.832495	2.460852
1	4.221924	2.075127	0.952629
7	1.631563	-1.966788	-1.015410
1	2.273704	-2.041929	-0.224195
1	1.597366	-2.881574	-1.453433
1	2.067456	-1.322488	-1.673326
7	3.719482	-1.768407	1.421182
1	3.855998	-0.758034	1.474146
1	3.447555	-2.083060	2.346321
1	4.623479	-2.186529	1.229540
7	0.763985	0.740791	0.587195
1	0.791155	-0.217839	0.242411
1	0.439317	0.686421	1.548214
1	0.025286	1.224375	0.074764
7	-6.344963	-0.621318	0.811486
1	-6.840931	-0.528596	1.690292
1	-6.632428	-1.499564	0.395617
1	-6.668542	0.122115	0.203665

Cartesian coordinates of ammonia decamer: (NH₃)₁₀

Cartesian coordinates of : MP2_AM10_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.778914	-2.506157	-0.000642
1	-2.069687	-1.718671	0.583928
1	-2.359012	-3.299981	0.253445
1	-2.037321	-2.244828	-0.948145
7	2.415177	2.202391	-1.309839
1	1.592098	1.635250	-1.530878
1	3.004932	2.234306	-2.134710
1	2.099685	3.151439	-1.139401
7	0.111923	0.137570	-1.299843
1	0.028263	0.218274	-0.289590
1	0.559805	-0.761841	-1.460194
1	-0.844879	0.053611	-1.639501
7	1.204743	-3.032575	-1.120175
1	1.108362	-3.569107	-1.976158
1	0.279927	-2.973566	-0.690891
1	1.786102	-3.583798	-0.496998
7	0.711768	-1.252445	2.022057
1	0.131552	-1.862712	1.451131
1	0.895901	-1.742526	2.891937
1	1.605709	-1.142871	1.536639
7	-3.149385	0.316852	-1.526676
1	-3.660922	-0.215395	-0.831145
1	-3.813486	0.604417	-2.237296
1	-2.812072	1.155192	-1.056225
7	-1.408727	2.739448	-0.219850
1	-1.003318	2.687397	-1.149813
1	-0.633031	2.606101	0.435828
1	-1.752755	3.686680	-0.097722
7	3.128881	-0.665898	0.103184
1	4.109165	-0.919022	0.166017
1	3.087039	0.287278	-0.252874
1	2.700049	-1.274945	-0.590224
7	1.020924	1.977144	1.625663
1	0.909782	1.020444	1.957988
1	1.263845	2.545617	2.430631
1	1.827993	1.975513	1.006682
7	-2.217132	0.116547	1.726306
1	-1.288235	-0.060156	2.104522
1	-2.836030	0.297176	2.509985
1	-2.154267	0.980583	1.191745

Cartesian coordinates of : MP2_AM10_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.853611	2.142494	-1.151853
1	1.733223	1.934683	-0.157296
1	2.768255	1.793590	-1.419139
1	1.886399	3.151981	-1.251270
7	-1.853574	2.141952	1.152737
1	-1.886365	3.151390	1.252651
1	-2.768218	1.792915	1.419848
1	-1.733183	1.934627	0.158077
7	1.160304	1.266940	1.799926
1	1.226970	0.251104	1.810645
1	0.173025	1.514109	1.721513
1	1.479517	1.595765	2.705379
7	-1.839737	-1.121650	1.881156
1	-2.625351	-0.871015	1.278568
1	-1.452964	-0.238016	2.201505
1	-2.226564	-1.587705	2.696178
7	-1.160278	1.267789	-1.799436
1	-0.172993	1.514909	-1.720939
1	-1.226962	0.251959	-1.810572
1	-1.479509	1.597000	-2.704743
7	1.839709	-1.120784	-1.881597
1	2.226582	-1.586508	-2.696786
1	1.452948	-0.237022	-2.201605
1	2.625294	-0.870399	-1.278865
7	1.231909	-2.007704	1.293582
1	1.323287	-2.073944	0.282361
1	1.508455	-2.903010	1.683716
1	0.237586	-1.891615	1.490348
7	-1.231926	-2.007057	-1.294428
1	-1.508473	-2.902170	-1.685004
1	-0.237603	-1.890872	-1.491137
1	-1.323304	-2.073796	-0.283240
7	-3.826334	-0.275264	-0.485983
1	-3.746295	0.686960	-0.797216
1	-4.755276	-0.597350	-0.734791
1	-3.149039	-0.807151	-1.029345
7	3.826315	-0.275526	0.485901
1	3.149104	-0.807721	1.029064
1	3.746153	0.686562	0.797521
1	4.755308	-0.597589	0.734547

Cartesian coordinates of : MP2_AM10_3-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.549524	-2.216868	1.024510
1	-1.280739	-1.378377	1.536226
1	-2.217166	-1.939213	0.306929
1	-2.034887	-2.828872	1.671410
7	2.546284	-1.082522	1.410365
1	2.985993	-1.619428	2.151737
1	3.294525	-0.613065	0.909753
1	2.144564	-1.758861	0.755205
7	-2.867311	1.467462	0.618980
1	-2.222555	2.109014	0.158511
1	-2.306326	0.938659	1.281924
1	-3.524455	2.024930	1.154123
7	-0.091049	0.492911	2.257394
1	-0.012436	1.401075	1.808913
1	0.789672	0.002738	2.080462
1	-0.142936	0.665110	3.256844
7	1.030270	-3.012646	-0.576501
1	0.164476	-2.911571	-0.039038
1	0.839473	-2.638207	-1.500716

1	1.203247	-4.005836	-0.692970
7	2.377370	2.180097	0.271711
1	3.102305	2.887373	0.201871
1	2.461780	1.768149	1.195391
1	2.613766	1.442793	-0.396018
7	2.760066	-0.145538	-1.877603
1	1.738648	-0.184621	-1.905935
1	3.085336	-1.091206	-1.705534
1	3.090386	0.115749	-2.800545
7	-0.429640	3.233634	-0.711061
1	0.501342	2.954873	-0.387915
1	-0.369096	3.363649	-1.716155
1	-0.618461	4.150549	-0.318498
7	-3.542980	-0.926736	-1.266716
1	-3.535459	-0.679549	-2.250704
1	-3.502278	-0.060465	-0.723611
1	-4.440566	-1.364707	-1.088618
7	-0.262191	-0.084973	-1.186316
1	-0.532003	0.889973	-1.082734
1	0.049281	-0.375880	-0.263439
1	-1.124505	-0.598530	-1.350215

Cartesian coordinates of : MP2_AM10_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.259961	-0.994227	1.583528
1	-1.745600	-0.140969	1.793112
1	-3.066372	-0.719185	1.022021
1	-2.621141	-1.353949	2.461322
7	1.740196	-2.795579	-1.157701
1	1.919178	-3.585522	-1.767041
1	2.498526	-2.132889	-1.279361
1	0.884753	-2.339665	-1.470710
7	0.176426	1.169837	2.084826
1	0.860560	1.779499	1.638276
1	0.560409	0.225170	2.066910
1	0.126190	1.452301	3.058843
7	0.819240	-2.030118	1.723071
1	0.984055	-2.625197	2.528998
1	1.156207	-2.534917	0.901438
1	-0.191134	-1.945038	1.617113
7	-1.179632	-1.355973	-1.475608
1	-1.401231	-1.617187	-0.514984
1	-1.554675	-0.414880	-1.570747
1	-1.737402	-1.954812	-2.077299
7	1.940170	3.045986	0.100682
1	2.868302	3.390186	-0.122106
1	1.628174	2.482162	-0.689473
1	1.336270	3.859161	0.155274
7	3.123632	-0.074973	0.431838
1	2.466609	-0.653756	0.954839
1	3.034493	0.870957	0.792005
1	4.057333	-0.396852	0.664699
7	-1.433394	1.850103	-0.690837
1	-0.588117	1.761295	-1.252652
1	-1.732649	2.817787	-0.760986
1	-1.138252	1.693359	0.273618
7	-4.268484	0.348133	-0.503608
1	-3.415285	0.858061	-0.733660
1	-4.977496	1.026774	-0.249190
1	-4.593230	-0.116193	-1.344172
7	1.332984	0.716561	-2.041685
1	1.723699	0.805261	-2.974467
1	0.643090	-0.031513	-2.077325
1	2.076500	0.382301	-1.425849

Cartesian coordinates of : MP2_AM10_5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.278186	-1.556543	0.925435
1	-2.609075	-1.019783	0.128498
1	-1.662732	-0.942021	1.463223
1	-3.087841	-1.764163	1.500280
7	-0.050267	0.257323	2.232423
1	0.736770	-0.304296	1.901622
1	0.101734	0.439604	3.219190
1	0.008463	1.151187	1.752774
7	0.222817	2.332697	-0.419069
1	0.161173	1.469993	-0.956145
1	0.156346	3.102911	-1.076696
1	1.158625	2.363369	-0.011135
7	-0.187490	-0.773963	-1.799275
1	-1.149376	-0.443577	-1.701459
1	-0.048054	-1.475906	-1.075542
1	-0.160133	-1.277183	-2.681934
7	3.073201	1.805937	0.881708
1	3.869763	2.355137	1.184635
1	2.841381	1.162263	1.630816
1	3.358153	1.237805	0.087625
7	2.826267	0.284723	-1.938883
1	3.282877	-0.324857	-2.609616
1	2.917681	1.229953	-2.297330
1	1.829366	0.059975	-1.949441
7	2.244991	-1.477841	0.845953
1	1.610750	-2.204010	0.512692
1	3.046522	-1.945691	1.256456
1	2.584431	-0.971682	0.031703
7	-0.088095	-3.583836	0.127304
1	-0.916581	-3.050992	0.411251
1	-0.353448	-4.160448	-0.664554
1	0.133840	-4.223340	0.883674
7	-3.147875	0.544772	-1.670120
1	-4.080104	0.156346	-1.771615
1	-2.993360	1.124771	-2.488713
1	-3.158168	1.165316	-0.855518
7	-2.650395	2.185872	0.903481
1	-1.687869	2.367212	0.613144
1	-2.603592	1.536624	1.681750
1	-3.042320	3.051499	1.257657

Cartesian coordinates of : MP2_AM10_6-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.355934	-0.993721	-1.503491
1	1.372611	-1.079643	-1.759195
1	2.595977	-0.004424	-1.580700
1	2.890709	-1.489610	-2.209689
7	-2.056551	-0.793520	1.881727
1	-2.408465	-0.981131	2.815552
1	-1.190068	-0.258078	1.981376
1	-1.773449	-1.689345	1.493260
7	-0.801306	-1.818899	-1.719816
1	-0.744374	-2.547768	-2.424239
1	-1.788061	-1.573064	-1.627015
1	-0.505965	-2.229536	-0.834915
7	-3.652222	-0.672723	-0.958680
1	-3.698324	0.290053	-1.273573
1	-3.388143	-0.655779	0.024275
1	-4.584346	-1.064152	-1.032826
7	0.827077	-2.400413	0.997914
1	1.533400	-2.139109	0.312099
1	0.764018	-1.623776	1.649222

1	1.170163	-3.204819	1.511687
7	-0.502221	1.440644	-1.462894
1	-0.558152	1.910136	-2.361804
1	-0.558571	0.439813	-1.653784
1	-1.343282	1.700794	-0.947387
7	3.513343	-0.100034	1.378209
1	3.249968	-0.524081	0.489153
1	4.363585	0.428360	1.213903
1	3.757313	-0.852077	2.013747
7	2.605353	2.122711	-1.074509
1	2.848334	2.286836	-0.103587
1	2.900714	2.937463	-1.600930
1	1.587646	2.061708	-1.127163
7	0.529748	1.014126	1.676520
1	0.318693	1.285958	0.717614
1	1.515139	0.745453	1.694879
1	0.449856	1.850556	2.246684
7	-2.807010	2.138915	0.683422
1	-2.369587	2.837597	1.274340
1	-2.692874	1.234142	1.137313
1	-3.799488	2.347923	0.672887

Cartesian coordinates of : MP2_AM10_7

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.205348	1.949186	2.048020
1	0.572998	2.609819	2.724684
1	0.249859	2.378243	1.122776
1	-0.777360	1.818910	2.264783
7	-1.084826	-0.040034	-2.438719
1	-1.408769	0.037887	-3.397812
1	-0.108315	-0.331632	-2.475614
1	-1.612862	-0.800224	-2.005987
7	3.006665	0.737379	0.637616
1	3.821081	1.289520	0.887387
1	3.224888	-0.235917	0.859745
1	2.256301	1.011592	1.269519
7	2.153513	-0.520546	-2.173739
1	2.599957	-1.428557	-2.254076
1	2.559711	-0.060697	-1.357301
1	2.439951	0.015336	-2.986967
7	0.657096	2.469249	-1.009892
1	0.853571	3.259461	-1.614981
1	0.088034	1.810891	-1.539118
1	1.540686	2.004913	-0.813109
7	-2.473015	1.688605	-0.033615
1	-1.950453	2.558155	0.007546
1	-3.418364	1.931511	-0.313615
1	-2.061048	1.159657	-0.803329
7	-2.744067	-0.700388	2.001480
1	-2.618893	0.180628	1.498964
1	-3.497140	-0.576418	2.669154
1	-1.901546	-0.884666	2.535748
7	0.223313	-1.018961	0.528182
1	0.644532	-0.759567	-0.359566
1	-0.744143	-1.242274	0.318723
1	0.217116	-0.174082	1.095781
7	-2.824400	-2.213955	-0.765220
1	-2.485982	-3.167923	-0.691382
1	-3.749059	-2.269935	-1.179525
1	-2.941119	-1.860564	0.186910
7	2.899681	-2.384666	1.252450
1	1.904990	-2.177374	1.134408
1	3.047017	-2.668585	2.214835
1	3.119209	-3.189201	0.675476

Cartesian coordinates of : MP2_AM10_8

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.212674	-1.852673	1.922468
1	0.127680	-2.525938	2.676914
1	-0.576263	-1.210786	1.992744
1	0.105925	-2.363467	1.049202
7	-2.574496	1.748951	-1.218137
1	-3.349584	2.386136	-1.371123
1	-1.765691	2.311608	-0.946988
1	-2.342018	1.347841	-2.122265
7	1.498124	1.110515	1.922470
1	2.123687	1.373539	2.676916
1	1.993859	1.273467	1.049204
1	1.336702	0.106332	1.992745
7	0.180066	3.161761	-0.218428
1	1.083316	2.822809	-0.547724
1	0.200765	3.028915	0.788731
1	0.153734	4.161163	-0.394372
7	-1.710797	0.742154	1.922471
1	-2.251365	1.152393	2.676917
1	-2.099784	1.089998	1.049205
1	-0.760438	1.104450	1.992747
7	-2.828199	-1.424936	-0.218428
1	-2.723501	-1.340587	0.788731
1	-3.680541	-1.947442	-0.394372
1	-2.986282	-0.473224	-0.547727
7	-0.227389	-3.104054	-1.218137
1	-1.119067	-2.684936	-0.946989
1	0.003744	-2.702165	-2.122265
1	-0.391664	-4.093892	-1.371125
7	2.801885	1.355104	-1.218136
1	2.884757	0.373329	-0.946988
1	2.338275	1.354328	-2.122265
1	3.741248	1.707758	-1.371121
7	0.000000	0.000000	-1.474831
1	-0.818779	-0.456189	-1.085177
1	0.014318	0.937180	-1.085179
1	0.804462	-0.480988	-1.085178
7	2.648132	-1.736823	-0.218430
1	1.902966	-2.349584	-0.547725
1	2.522736	-1.688326	0.788730
1	3.526805	-2.213719	-0.394375

Cartesian coordinates of : MP2_AM10_9-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.299126	2.762190	0.912476
1	1.883162	1.932319	1.047626
1	1.715548	3.296892	0.156608
1	1.399390	3.332151	1.746763
7	-1.532233	1.294599	1.650667
1	-2.021662	1.842551	2.350509
1	-2.157120	1.209646	0.852931
1	-0.723789	1.838824	1.352226
7	2.943991	0.111224	1.490237
1	3.482289	-0.447137	0.835600
1	2.098334	-0.426402	1.702613
1	3.492019	0.167115	2.342832
7	0.207812	-1.349698	1.930886
1	-0.069638	-1.821642	1.074237
1	-0.395537	-0.528426	2.004481
1	-0.025058	-1.969662	2.700013
7	-3.316868	0.948670	-1.210685
1	-3.710485	0.246747	-1.829449
1	-3.794723	1.819226	-1.419928

1	-2.337683	1.064185	-1.481346
7	2.182844	-2.528492	-0.662303
1	1.181658	-2.375862	-0.800839
1	2.434171	-3.386182	-1.142541
1	2.318567	-2.696965	0.328915
7	-0.841482	-1.735725	-1.236346
1	-1.017057	-2.195271	-2.124328
1	-0.726980	-0.743324	-1.433452
1	-1.689043	-1.835439	-0.675827
7	2.632210	0.362829	-1.903095
1	3.262469	0.378368	-2.698101
1	2.596430	-0.598841	-1.560316
1	3.067631	0.911123	-1.168283
7	-0.261044	1.594932	-1.758132
1	-0.104776	2.110175	-0.894013
1	-0.406615	2.285730	-2.489015
1	0.637533	1.147383	-1.961753
7	-3.297362	-1.537785	0.799087
1	-2.803821	-1.334655	1.661511
1	-4.144817	-2.038525	1.041823
1	-3.559347	-0.643309	0.390967

Cartesian coordinates of : MP2_AM10_10

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.524983	-1.649080	0.212491
1	-4.082430	-2.493980	0.277028
1	-3.972502	-0.948978	0.794563
1	-2.618179	-1.835515	0.637331
7	-1.955501	0.706683	2.082976
1	-1.607276	-0.244493	1.984291
1	-2.071913	0.892905	3.073200
1	-1.211922	1.307493	1.733715
7	0.009804	2.013691	-0.136950
1	0.597945	1.437773	-0.738687
1	-0.933016	1.992803	-0.524070
1	0.342015	2.968955	-0.227244
7	-1.566625	-0.658530	-2.126501
1	-1.731103	0.343824	-2.166278
1	-2.324962	-1.032004	-1.553444
1	-1.697464	-1.020157	-3.066332
7	1.662861	-0.195683	-1.938401
1	2.173804	-0.926447	-1.440790
1	0.687197	-0.486739	-1.998842
1	2.017489	-0.179419	-2.889908
7	3.263866	-2.000384	0.143617
1	2.779658	-1.412205	0.820943
1	4.258556	-1.884503	0.304662
1	3.044234	-2.966561	0.359358
7	3.811718	1.523155	-0.241804
1	3.819958	2.529525	-0.366994
1	4.686517	1.176061	-0.619808
1	3.064008	1.143281	-0.822365
7	1.849430	0.312281	1.902336
1	1.851523	0.412010	2.912501
1	1.096865	0.896609	1.539833
1	2.705634	0.737270	1.545703
7	-0.352436	-1.801911	0.737082
1	-0.078038	-2.779090	0.753865
1	0.432734	-1.269640	1.110302
1	-0.451682	-1.534341	-0.240339
7	-3.219579	1.754405	-0.619573
1	-3.711479	2.638289	-0.540350
1	-3.067597	1.397479	0.324818
1	-3.848457	1.107395	-1.083561

Cartesian coordinates of : MP2_AM10_11

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.058406	-1.541382	-1.847638
1	-0.845942	-0.894369	-1.831530
1	0.784755	-0.971114	-1.812416
1	-0.069262	-1.986992	-2.759919
7	-2.833619	-1.059789	0.647032
1	-2.791917	-0.793932	-0.334314
1	-3.799840	-1.287259	0.859926
1	-2.296239	-1.922866	0.750450
7	-2.211352	0.973293	-1.860041
1	-1.321080	1.412665	-2.079653
1	-2.559435	1.478679	-1.046228
1	-2.840788	1.165728	-2.632767
7	-2.672632	2.044048	1.205319
1	-1.894115	2.352366	1.778227
1	-2.698144	1.024543	1.260604
1	-3.516877	2.398319	1.642400
7	-0.721666	-3.374306	0.630419
1	-0.398065	-2.893112	-0.211339
1	0.010204	-3.310481	1.328912
1	-0.850489	-4.355822	0.412130
7	0.206435	2.545879	-0.504575
1	0.253253	1.815009	0.205665
1	0.973230	3.188031	-0.334163
1	-0.657524	3.052199	-0.339535
7	0.209088	0.028808	1.628163
1	0.151917	-0.022456	2.641626
1	0.875564	-0.689271	1.338160
1	-0.706416	-0.265841	1.291681
7	2.458373	0.645906	-1.656751
1	2.939559	1.057115	-0.856305
1	1.637969	1.231227	-1.801573
1	3.058338	0.756105	-2.468002
7	2.485160	-1.854638	0.382857
1	2.092685	-2.688430	-0.041400
1	3.432650	-2.085437	0.663375
1	2.545189	-1.153561	-0.355369
7	3.071549	1.557825	1.325902
1	3.166114	2.466950	1.765399
1	3.678019	0.923493	1.834448
1	2.116176	1.239006	1.476701

Cartesian coordinates of : MP2_AM10_12-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.558442	-2.142245	0.809889
1	-1.603791	-2.487903	0.696527
1	-2.968205	-2.630944	1.599361
1	-3.078313	-2.433173	-0.011889
7	-0.662620	-1.256595	-2.150681
1	-0.566525	-1.915468	-1.382559
1	-0.863278	-1.792496	-2.988794
1	-1.482987	-0.678904	-1.951470
7	0.541401	-2.843802	0.694035
1	0.660620	-2.424414	1.611317
1	1.253661	-2.417547	0.095766
1	0.779355	-3.826598	0.786190
7	2.443662	-1.264077	-1.279735
1	2.807249	-0.371197	-0.956920
1	1.597239	-1.069345	-1.812503
1	3.129146	-1.648816	-1.921163
7	-3.059018	0.522680	-1.040401
1	-3.089695	-0.071413	-0.215530
1	-2.788373	1.454060	-0.727993

1	-4.005484	0.595430	-1.398787
7	-0.746403	0.497891	1.848436
1	0.229979	0.195927	1.847113
1	-1.002278	0.617763	2.824032
1	-1.316544	-0.267322	1.492750
7	0.351877	1.674294	-1.140358
1	-0.285532	2.366078	-1.523009
1	-0.028658	1.436344	-0.226718
1	0.216351	0.839414	-1.707170
7	-2.046378	3.160111	0.609279
1	-1.368596	3.901748	0.470703
1	-1.577052	2.401436	1.105700
1	-2.768312	3.533600	1.215633
7	2.421558	-0.187581	1.911320
1	2.771789	-1.091957	1.611740
1	2.875503	0.021327	2.795099
1	2.777476	0.481630	1.227743
7	3.302762	1.919594	-0.381826
1	3.935916	1.979464	-1.172646
1	3.495176	2.731015	0.196641
1	2.345370	2.010374	-0.738878

Cartesian coordinates of : MP2_AM10_13

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.521268	-0.340147	-2.460664
1	0.431352	-0.190824	-2.122631
1	-0.694124	-1.337218	-2.384376
1	-0.531561	-0.112273	-3.449819
7	0.679180	3.111821	-0.708599
1	1.058163	2.620031	-1.512476
1	0.749374	4.103128	-0.915370
1	-0.318382	2.882918	-0.678555
7	2.473652	-0.136362	-1.206128
1	2.607109	-1.069492	-0.826121
1	2.723306	0.502927	-0.446868
1	3.175620	-0.016678	-1.930579
7	2.695220	1.780778	1.294405
1	2.180537	1.324050	2.040335
1	2.025049	2.367546	0.791684
1	3.378698	2.391728	1.728580
7	-2.230589	1.936681	-0.807117
1	-1.845742	1.136039	-1.307122
1	-2.663834	1.602109	0.052140
1	-2.963842	2.336463	-1.382597
7	2.189539	-1.838695	1.655228
1	1.467861	-1.121470	1.759818
1	2.153115	-2.440373	2.471561
1	3.085826	-1.363231	1.684051
7	-0.062019	0.174076	1.107412
1	-0.489435	1.066153	1.338421
1	-0.833327	-0.458645	0.907985
1	0.400931	0.326990	0.214858
7	0.468878	-3.149315	-0.701182
1	0.437272	-4.153822	-0.555108
1	1.084398	-2.768600	0.021195
1	0.942705	-3.010943	-1.588338
7	-2.419735	-1.888866	-0.033570
1	-2.700561	-1.322519	-0.828019
1	-3.100169	-2.636499	0.058601
1	-1.529725	-2.326124	-0.280787
7	-3.294375	0.497181	1.947128
1	-4.274975	0.440556	2.199228
1	-2.775363	0.586779	2.813855
1	-3.029654	-0.388768	1.518062

Cartesian coordinates of : MP2_AM10_14

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-3.171998	-0.983940	-1.361690
1	-3.923336	-1.037131	-2.040630
1	-2.360516	-0.604804	-1.839578
1	-3.439630	-0.300380	-0.651379
7	3.328072	-0.828369	-0.955312
1	2.781016	-0.266600	-1.605674
1	4.207304	-1.048825	-1.410322
1	3.541447	-0.234825	-0.160211
7	1.039043	0.552784	-2.755436
1	0.428494	0.289841	-1.975292
1	1.020783	-0.199578	-3.435890
1	0.636852	1.366671	-3.208173
7	-1.660446	-3.164457	0.297656
1	-1.432138	-4.002291	-0.227608
1	-2.284676	-2.603039	-0.287518
1	-2.198666	-3.467069	1.103069
7	2.244945	0.268927	2.275932
1	1.562976	0.601202	2.950901
1	3.136406	0.250032	2.761694
1	2.002735	-0.703902	2.060576
7	-3.532667	1.013226	1.091039
1	-3.308486	0.456001	1.908574
1	-4.389831	1.511693	1.304667
1	-2.793627	1.709110	0.982713
7	-1.213102	3.160973	0.468052
1	-1.594534	3.609206	-0.359539
1	-0.220710	2.989082	0.275739
1	-1.244668	3.857135	1.206648
7	1.524108	-2.509623	1.072003
1	1.925087	-3.389731	1.378019
1	2.023847	-2.225089	0.229238
1	0.553237	-2.695763	0.825094
7	1.810416	2.459557	-0.084083
1	2.063592	1.803158	0.655485
1	2.522075	3.182589	-0.102177
1	1.878587	1.957253	-0.965628
7	-0.349215	-0.053628	-0.082940
1	0.509815	-0.058488	0.458593
1	-0.850952	-0.899597	0.173301
1	-0.886570	0.746002	0.238767

Cartesian coordinates of : MP2_AM10_15-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.905646	1.192009	-1.694300
1	-1.279214	1.617874	-1.010352
1	-1.934925	1.798042	-2.507975
1	-2.830234	1.215434	-1.262514
7	-2.149354	-1.991592	-1.236790
1	-2.919042	-2.416833	-1.742706
1	-1.298264	-2.432066	-1.570327
1	-2.099690	-1.011245	-1.516084
7	-0.383551	1.820888	1.029798
1	0.527693	1.508368	1.359032
1	-1.050416	1.097260	1.293929
1	-0.619358	2.650628	1.564881
7	-2.005019	-0.982475	1.744459
1	-1.024707	-1.156781	1.954654
1	-2.185327	-1.490060	0.875612
1	-2.543686	-1.425420	2.482439
7	-4.230563	0.932007	0.430148
1	-5.008026	0.282143	0.391643
1	-3.494878	0.491518	0.981566

1	-4.554830	1.747622	0.937718
7	2.463636	0.349766	2.018069
1	1.728027	-0.350874	2.087870
1	3.194146	-0.094314	1.461839
1	2.833044	0.498200	2.951633
7	0.891653	-2.152584	0.843464
1	1.807725	-2.577457	0.946966
1	0.885490	-1.664387	-0.055156
1	0.221302	-2.911411	0.774069
7	2.463876	2.118421	-0.654815
1	3.119241	2.874827	-0.821648
1	2.540609	1.838983	0.322454
1	1.529853	2.503400	-0.760173
7	0.871756	-0.475823	-1.893445
1	-0.071717	-0.094251	-1.947015
1	1.121436	-0.768589	-2.833205
1	1.481411	0.305749	-1.659125
7	3.976613	-0.778735	-0.569444
1	3.634127	0.122120	-0.895580
1	3.408929	-1.486398	-1.022963
1	4.927476	-0.895253	-0.901480

Cartesian coordinates of : MP2_AM10_16

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.422114	-0.283401	-1.720107
1	2.201619	0.692742	-1.499567
1	2.953969	-0.648484	-0.935689
1	3.048037	-0.273836	-2.519359
7	-2.670319	-0.033020	-1.525292
1	-3.240095	0.010549	-2.364406
1	-3.220488	-0.517294	-0.822611
1	-1.877703	-0.644341	-1.734396
7	1.679684	2.570518	-0.692185
1	1.955763	2.400781	0.271029
1	0.666977	2.711176	-0.701104
1	2.106057	3.445190	-0.979408
7	-1.487839	2.774246	-0.563041
1	-1.682476	2.804272	0.432538
1	-1.914793	1.917462	-0.920462
1	-1.970298	3.558996	-0.987838
7	-0.196239	-1.991476	-2.044598
1	0.649300	-1.416815	-1.973375
1	-0.077423	-2.768491	-1.402593
1	-0.202601	-2.391367	-2.977959
7	3.169856	0.756983	1.749608
1	3.896601	1.136193	1.151523
1	3.492768	0.863996	2.705392
1	3.111370	-0.242653	1.554885
7	-2.189050	-2.216129	0.947868
1	-1.279957	-1.753712	0.963919
1	-2.270358	-2.692775	0.056546
1	-2.191985	-2.928275	1.670116
7	0.036185	0.034317	0.975530
1	0.871336	0.495799	1.332241
1	-0.032144	0.305446	-0.002255
1	-0.766799	0.462035	1.436050
7	2.231746	-2.215646	0.959000
1	1.334165	-1.729301	0.942963
1	2.208056	-2.889212	1.717148
1	2.315876	-2.743047	0.096949
7	-3.002123	0.745592	1.898010
1	-3.002262	-0.238399	1.631914
1	-3.529883	1.248550	1.193045
1	-3.510729	0.830928	2.771218

Cartesian coordinates of : MP2_AM10_17

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.793341	1.988419	0.795311
1	2.129534	1.570102	1.439190
1	3.313521	2.689830	1.311058
1	2.240349	2.469887	0.085331
7	-2.324355	-1.074320	-1.484003
1	-2.947318	-1.200166	-2.275397
1	-1.712084	-1.892116	-1.460445
1	-2.897734	-1.084439	-0.639500
7	3.837370	-0.815196	-0.197917
1	3.898218	-0.837465	-1.210714
1	4.763517	-1.047210	0.146078
1	3.649266	0.153318	0.072784
7	-0.130603	-3.413606	-1.348343
1	0.425033	-3.295787	-0.498365
1	0.515359	-3.365564	-2.129401
1	-0.498216	-4.359185	-1.338309
7	-2.111973	2.080518	-0.889262
1	-2.338249	2.053806	0.100581
1	-2.116405	1.105730	-1.196873
1	-2.888624	2.540038	-1.353976
7	0.775640	3.205185	-1.438858
1	-0.198514	2.918511	-1.299912
1	0.995962	3.047548	-2.417179
1	0.811274	4.209996	-1.299075
7	-1.143214	1.089009	2.201645
1	-0.883559	0.678026	3.092529
1	-0.539418	0.684084	1.479308
1	-0.912118	2.075382	2.264052
7	1.581733	-2.647580	1.205650
1	0.969766	-1.949788	1.615749
1	1.891063	-3.258272	1.953609
1	2.397559	-2.149601	0.847364
7	-3.777017	-0.543841	1.327748
1	-3.910822	-1.284064	2.007903
1	-4.629318	0.005723	1.326055
1	-3.025294	0.055845	1.669190
7	0.470952	0.049323	-0.240186
1	0.735109	0.936959	-0.657783
1	-0.300702	-0.319142	-0.792985
1	1.259732	-0.577358	-0.363363

Cartesian coordinates of : MP2_AM10_18-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.697795	-2.093771	-0.776752
1	1.155962	-1.331487	-1.175750
1	1.856158	-2.771198	-1.515178
1	2.609007	-1.712373	-0.516670
7	4.419902	-0.637260	0.112849
1	4.255161	0.338853	-0.140926
1	5.205131	-0.963626	-0.440557
1	4.731370	-0.644652	1.078492
7	3.391055	2.298234	-0.481176
1	2.594618	1.999055	0.084704
1	3.041933	2.527100	-1.405278
1	3.758320	3.155669	-0.083659
7	-0.424308	-2.635463	1.427617
1	-0.494377	-3.610503	1.702613
1	-0.143945	-2.128948	2.261535
1	0.352058	-2.559943	0.762130
7	-2.412688	-2.093038	-1.096185
1	-2.631986	-2.946612	-1.598590
1	-3.285632	-1.727932	-0.729704

1	-1.848926	-2.346239	-0.285412
7	-2.671344	-0.087158	1.553361
1	-2.017311	-0.862033	1.471404
1	-3.194863	-0.229477	2.410586
1	-2.134450	0.773287	1.658326
7	1.198737	0.701492	1.038378
1	0.617963	0.435511	0.242091
1	1.815680	-0.081624	1.229756
1	0.584389	0.814609	1.837467
7	-3.444263	1.506820	-1.050273
1	-3.408872	0.843650	-0.273957
1	-3.502503	0.970075	-1.909095
1	-4.310586	2.029037	-0.972257
7	-1.256869	2.743458	0.987611
1	-1.845752	2.630505	0.164406
1	-0.287463	2.706603	0.688539
1	-1.419245	3.672505	1.360201
7	-0.470663	0.300954	-1.710716
1	-1.069940	1.112720	-1.584494
1	-1.099942	-0.505497	-1.711797
1	-0.073428	0.383090	-2.641916

Cartesian coordinates of : MP2_AM10_19

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.723709	1.465202	2.107349
1	-1.160886	1.217337	2.914648
1	-2.063758	0.594776	1.700534
1	-2.529184	1.969177	2.463163
7	-2.152821	-1.224093	0.421893
1	-1.822956	-1.046758	-0.527008
1	-2.710224	-2.071956	0.399367
1	-1.314809	-1.425337	0.962981
7	0.912819	-0.750742	1.269690
1	0.575646	0.170120	0.999414
1	1.644330	-0.586681	1.954572
1	1.368714	-1.120555	0.436654
7	0.369822	2.461693	-0.126403
1	1.239148	2.555147	0.401369
1	-0.378447	2.331070	0.556435
1	0.203428	3.356525	-0.577008
7	0.998077	-2.269157	-1.549383
1	0.178136	-1.704101	-1.766109
1	1.273893	-2.744146	-2.402568
1	0.716050	-2.990283	-0.886249
7	0.317314	-3.932238	1.141650
1	-0.556799	-4.342336	1.449954
1	0.354955	-2.975465	1.485717
1	1.062844	-4.452555	1.590345
7	-1.008135	0.270454	-2.125707
1	-1.955983	0.646116	-2.129958
1	-0.665320	0.312820	-3.080336
1	-0.452960	0.930306	-1.579236
7	-3.707591	1.349679	-0.827427
1	-3.441346	2.222005	-0.384897
1	-4.717728	1.345168	-0.908952
1	-3.435023	0.593898	-0.203725
7	3.325482	2.100841	1.110809
1	4.037929	2.804684	0.949944
1	3.360231	1.443317	0.329557
1	3.597676	1.604348	1.951877
7	2.697026	0.520723	-1.520382
1	3.160286	0.731649	-2.397542
1	1.880557	1.122257	-1.443236
1	2.353608	-0.437074	-1.574333

Cartesian coordinates of : MP2_AM10_20

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.643733	-0.901419	0.466748
1	-0.832764	-1.370308	0.053323
1	-1.647921	-1.170490	1.446846
1	-2.479510	-1.315593	0.050710
7	-0.630565	1.643083	-1.333458
1	-1.415646	1.910760	-1.917939
1	-0.455826	2.413078	-0.696334
1	-0.932532	0.856022	-0.760014
7	0.858114	-2.333986	-0.920381
1	1.650458	-2.628124	-0.358722
1	1.208587	-1.609342	-1.550355
1	0.592568	-3.129639	-1.492011
7	1.846895	0.146052	-2.640762
1	2.691187	0.604080	-2.314506
1	1.060604	0.709050	-2.311232
1	1.856874	0.190307	-3.654274
7	-4.609442	-1.360457	-0.707149
1	-4.680965	-0.387251	-0.414005
1	-4.764677	-1.396765	-1.708210
1	-5.368158	-1.874064	-0.273560
7	3.723077	-0.791272	0.179560
1	3.407198	0.175685	0.078516
1	4.694149	-0.762536	0.472857
1	3.711930	-1.201411	-0.748439
7	2.573163	2.185878	0.013351
1	3.134043	2.921225	0.431477
1	1.793584	1.999151	0.649623
1	2.174517	2.573190	-0.835466
7	1.513533	-1.487155	2.372443
1	1.897557	-1.943035	3.193188
1	2.275531	-1.354191	1.704948
1	0.861348	-2.138209	1.948450
7	0.254022	1.377309	2.002733
1	-0.634254	1.104292	1.592527
1	0.043454	1.916610	2.836490
1	0.690108	0.501790	2.302350
7	-3.851461	1.451182	0.568996
1	-2.979035	0.925645	0.574900
1	-4.121836	1.619178	1.531748
1	-3.665802	2.356391	0.152551

Cartesian coordinates of : MP2_AM10_21-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-2.268223	-1.247311	-1.034045
1	-2.843988	-1.935853	-1.509282
1	-1.346491	-1.288910	-1.474900
1	-2.667874	-0.332049	-1.245811
7	0.703858	-1.454971	-2.303926
1	0.812725	-1.901484	-3.208975
1	1.204948	-2.026446	-1.622886
1	1.211660	-0.577206	-2.345922
7	2.114141	0.447990	0.083958
1	1.474577	0.572451	0.864895
1	2.231067	-0.554098	-0.033930
1	3.018846	0.830896	0.352809
7	-0.642018	1.481424	1.641400
1	-0.455883	2.268253	2.254704
1	-1.618690	1.222283	1.772509
1	-0.550528	1.816950	0.684732
7	5.026710	1.818069	0.694147
1	5.063670	2.580110	0.027055
1	5.177845	2.214976	1.614360

1	5.812875	1.209005	0.498753
7	-0.039639	1.941365	-1.628892
1	-0.417637	1.274819	-2.295117
1	0.307563	2.731736	-2.162727
1	0.766942	1.491457	-1.186582
7	-3.191370	1.815308	-0.938027
1	-3.804004	2.509949	-1.350188
1	-3.380963	1.788156	0.058853
1	-2.230761	2.131222	-1.056455
7	2.062182	-3.024386	0.156687
1	1.906195	-4.011796	-0.017130
1	1.298454	-2.687088	0.751615
1	2.923061	-2.959707	0.689585
7	-0.372084	-1.771388	1.581296
1	-1.066485	-1.789500	0.835093
1	-0.264072	-0.788204	1.826323
1	-0.777016	-2.237716	2.386552
7	-3.506353	-0.057270	1.720147
1	-4.502936	-0.000194	1.537952
1	-3.397788	-0.585929	2.578916
1	-3.095759	-0.607894	0.965978

Cartesian coordinates of : MP2_AM10_22

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.634542	0.825836	2.379259
1	-1.049546	-0.096153	2.265468
1	-0.827058	1.121869	3.330621
1	-1.149220	1.448542	1.760720
7	-1.483151	2.731517	-0.303877
1	-1.700550	3.698787	-0.084025
1	-1.752818	2.596451	-1.273912
1	-0.463408	2.637750	-0.260280
7	-2.057554	-2.081273	1.357232
1	-1.918825	-2.654192	0.529798
1	-2.676915	-1.315495	1.071080
1	-2.576166	-2.653166	2.016857
7	-3.702202	0.335783	0.255062
1	-3.795460	0.033630	-0.715563
1	-3.166372	1.201435	0.251359
1	-4.630885	0.558638	0.597024
7	1.512253	2.040177	0.276231
1	1.134678	1.580238	1.102874
1	2.010310	1.333426	-0.266984
1	2.195398	2.722998	0.586021
7	-3.206429	-0.928357	-2.631075
1	-3.227037	-0.524132	-3.560855
1	-2.237849	-0.909476	-2.303980
1	-3.482827	-1.898974	-2.730459
7	-0.538940	-0.403874	-1.103911
1	0.152270	0.234709	-1.487889
1	-0.000024	-1.049079	-0.531161
1	-1.077987	0.148500	-0.442631
7	2.815638	-0.524943	-1.151178
1	2.622306	-0.919641	-2.065551
1	2.357710	-1.120324	-0.462891
1	3.821533	-0.587732	-1.005506
7	1.182228	-1.794939	1.409872
1	1.366030	-0.926175	1.903060
1	1.729304	-2.523388	1.856770
1	0.198539	-2.002873	1.579002
7	5.995149	-0.198054	-0.536523
1	6.649330	-0.908733	-0.230040
1	5.891014	0.464901	0.222995
1	6.427367	0.294544	-1.309563

Cartesian coordinates of : MP2_AM10_23

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.584583	1.199815	1.718729
1	-0.046351	0.352415	1.894976
1	0.088836	1.904805	1.430398
1	-0.972540	1.501753	2.606468
7	-0.858170	-2.406409	0.327385
1	-0.400083	-2.016588	1.147351
1	-1.336185	-3.253194	0.618008
1	-1.577071	-1.736673	0.040554
7	1.762335	-1.074858	1.976164
1	2.295499	-0.248876	1.720441
1	2.012204	-1.786378	1.287335
1	2.117996	-1.386755	2.874485
7	2.116503	-3.018282	-0.530556
1	2.379983	-2.532721	-1.381374
1	1.098674	-2.963477	-0.467698
1	2.372750	-3.992784	-0.646722
7	-2.611580	0.040407	-0.476429
1	-2.059945	0.561300	0.205643
1	-2.384795	0.401851	-1.396134
1	-3.598948	0.217213	-0.307332
7	3.425208	0.260887	-0.647925
1	2.574049	0.004050	-1.157617
1	4.098850	0.593108	-1.330956
1	3.805267	-0.599759	-0.266449
7	0.665469	-0.358660	-1.984793
1	0.490163	-0.654243	-2.940043
1	0.291729	0.587278	-1.891482
1	0.105935	-0.964184	-1.388700
7	2.208226	2.798161	0.770158
1	2.707355	3.616230	0.435011
1	2.681326	1.976120	0.384321
1	2.346732	2.780881	1.775702
7	-0.274449	2.633611	-1.353753
1	-1.158991	2.623981	-0.857221
1	-0.282592	3.445524	-1.961860
1	0.452912	2.778796	-0.655138
7	-5.811022	-0.119304	0.137911
1	-6.385566	0.418448	0.776096
1	-5.612961	-1.009336	0.580099
1	-6.369795	-0.306367	-0.686390

Cartesian coordinates of : MP2_AM10_24-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.407535	-1.679490	1.703593
1	-1.624273	-0.692990	1.831692
1	-0.406633	-1.781541	1.856636
1	-1.882368	-2.197688	2.434833
7	1.654979	-0.733004	1.922023
1	2.668629	-0.745672	1.863162
1	1.421037	-0.330795	2.823862
1	1.334701	-0.089569	1.196613
7	0.740816	0.903743	-0.689118
1	0.066762	0.189149	-0.968239
1	0.349477	1.788898	-0.998821
1	1.587221	0.738155	-1.239487
7	-1.465426	-1.481114	-1.409260
1	-2.348154	-1.024966	-1.619512
1	-1.519018	-1.761817	-0.427362
1	-1.439206	-2.325494	-1.972439
7	3.577203	-0.004159	-1.603363
1	3.220842	-0.936330	-1.391989
1	4.270138	-0.090155	-2.337901

1	4.043016	0.353390	-0.774013
7	1.758568	-2.474429	-0.757755
1	1.829715	-3.467784	-0.948391
1	0.913853	-2.136384	-1.209515
1	1.614289	-2.361234	0.242201
7	-1.638736	1.603375	1.371022
1	-1.754857	2.316883	2.083954
1	-0.640771	1.429637	1.280750
1	-1.910881	2.013854	0.476476
7	-4.120041	-0.123887	0.141760
1	-5.045589	0.163560	0.441428
1	-3.443188	0.283585	0.784353
1	-4.069815	-1.130044	0.260845
7	-2.506248	1.940406	-1.685264
1	-2.992166	2.629975	-2.248199
1	-3.187702	1.247471	-1.378586
1	-1.849432	1.467282	-2.297011
7	3.531723	1.992277	0.912454
1	3.483026	2.251807	1.890988
1	2.587016	1.784437	0.600966
1	3.847200	2.808352	0.400054

Cartesian coordinates of : MP2_AM10_25

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.923361	2.817082	0.586865
1	1.597327	3.147238	-0.095332
1	1.340780	2.027802	1.084201
1	0.786832	3.570182	1.252815
7	1.766825	0.131261	2.011076
1	1.141235	0.011501	2.801599
1	2.689889	-0.148321	2.327020
1	1.482213	-0.549566	1.307219
7	0.569806	-1.837480	-0.311372
1	0.578711	-1.067232	-0.982794
1	0.599570	-2.695025	-0.855637
1	-0.348234	-1.832303	0.134855
7	0.884083	0.832969	-2.003813
1	1.859699	0.855601	-1.697810
1	0.412576	1.567884	-1.482923
1	0.872819	1.108179	-2.981047
7	-2.549044	-1.997211	0.497143
1	-2.638036	-3.007653	0.528111
1	-3.361167	-1.612622	0.975769
1	-2.638865	-1.703128	-0.475909
7	-2.364665	-0.100654	-2.028506
1	-2.486571	0.637210	-1.338773
1	-2.851659	0.176980	-2.873491
1	-1.371059	-0.123570	-2.242634
7	-1.883501	1.198691	0.886768
1	-1.021621	1.686007	0.644387
1	-1.673481	0.207962	0.986641
1	-2.153377	1.533169	1.806552
7	-4.895262	0.173202	0.660879
1	-4.062356	0.738594	0.511814
1	-5.610232	0.768884	1.061985
1	-5.227840	-0.131865	-0.246679
7	3.769787	0.899915	-0.610853
1	3.635674	1.458962	0.225312
1	4.655478	1.186353	-1.015093
1	3.879444	-0.065277	-0.295779
7	3.677600	-2.152756	0.304134
1	2.660967	-2.154594	0.211760
1	3.904215	-2.585820	1.192885
1	4.054147	-2.760667	-0.415273

Cartesian coordinates of : MP2_AM10_26

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.066217	0.133097	2.317751
1	0.807731	0.611123	2.115008
1	-0.104779	-0.000910	3.323084
1	0.014915	-0.788651	1.894642
7	-0.241440	-2.640979	0.432076
1	-0.578740	-3.367556	1.056142
1	0.086211	-3.115991	-0.403652
1	-1.051174	-2.068507	0.166066
7	2.822002	1.602772	1.086737
1	3.336790	1.949036	0.282526
1	2.953777	0.585151	1.103103
1	3.293599	1.978220	1.903997
7	2.939326	-1.513736	0.912561
1	3.271722	-1.602815	-0.048671
1	2.007284	-1.922168	0.942417
1	3.535892	-2.093808	1.493098
7	-2.343946	-0.427344	-0.010476
1	-1.982521	0.030369	0.822605
1	-2.151898	0.199186	-0.788592
1	-3.354887	-0.507019	0.076243
7	3.464692	-1.262449	-2.233608
1	3.312999	-1.972402	-2.941459
1	2.595400	-0.732973	-2.127365
1	4.171169	-0.633765	-2.599344
7	0.890349	0.138204	-1.218494
1	0.049259	0.520781	-1.644233
1	1.222726	0.852178	-0.576674
1	0.581052	-0.625739	-0.624818
7	-1.553497	2.153656	-2.029043
1	-1.092737	2.554084	-2.839261
1	-1.140701	2.572058	-1.191815
1	-2.524656	2.442927	-2.073761
7	-0.260409	2.966821	0.733814
1	-0.711673	2.273490	1.325323
1	-0.430775	3.878307	1.145593
1	0.736571	2.777373	0.820875
7	-5.543687	-1.132517	-0.036952
1	-5.995667	-0.794129	-0.878462
1	-6.190546	-0.988234	0.729610
1	-5.416537	-2.132290	-0.142784

Cartesian coordinates of : MP2_AM10_27-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	3.776951	0.063498	1.131550
1	3.326299	0.972475	1.208174
1	3.218219	-0.574683	1.688533
1	4.692502	0.127329	1.562099
7	2.563269	-0.876762	-1.653048
1	3.156695	-1.338209	-2.334610
1	1.939079	-1.583185	-1.268459
1	3.160642	-0.578817	-0.880463
7	1.939017	2.768538	0.843052
1	1.284552	3.373217	1.329147
1	1.512994	2.505657	-0.050948
1	2.745744	3.345671	0.626587
7	0.860473	1.743083	-1.919831
1	-0.086670	1.438414	-2.121197
1	1.443709	0.901000	-1.940767
1	1.146521	2.330848	-2.696519
7	-2.448263	-2.290664	1.225962
1	-3.301770	-2.535073	0.736113
1	-2.636456	-2.397194	2.216575

1	-2.266205	-1.302961	1.045815
7	-1.878302	0.649610	0.088094
1	-1.656059	0.130281	-0.762863
1	-2.830291	1.004566	0.007263
1	-1.264482	1.458504	0.094676
7	-0.834140	-1.262961	-2.233211
1	-1.463281	-1.922298	-2.679585
1	-0.331468	-1.768930	-1.502268
1	-0.142411	-1.001307	-2.928139
7	0.617583	0.005603	2.131114
1	0.471523	0.042586	3.134516
1	-0.297389	0.071308	1.688505
1	1.130261	0.845354	1.870562
7	0.577124	-2.625038	0.299309
1	1.154155	-3.440108	0.480493
1	-0.375859	-2.857529	0.579851
1	0.872626	-1.888376	0.940663
7	-4.974212	1.711118	0.048586
1	-5.473384	1.145650	0.725620
1	-5.456353	1.615673	-0.837851
1	-5.069937	2.677952	0.337451

Cartesian coordinates of : MP2_AM10_28

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.139360	3.458925	0.859745
1	-1.567942	3.402352	-0.061346
1	-1.317854	4.382014	1.237848
1	-0.137275	3.368949	0.724407
7	-1.581125	-1.996522	-1.366107
1	-0.705460	-2.500955	-1.449409
1	-1.917176	-1.803324	-2.302924
1	-1.377033	-1.109159	-0.909277
7	2.263679	-1.316597	-1.806473
1	1.770391	-1.771894	-1.034457
1	1.580059	-1.126426	-2.531980
1	2.910552	-1.994353	-2.197177
7	1.707229	0.352381	2.000579
1	1.639381	0.674462	2.960825
1	2.691148	0.168340	1.803634
1	1.468619	1.138711	1.399133
7	-2.415327	1.977660	-1.703483
1	-2.155126	1.262534	-1.026614
1	-2.091828	1.678581	-2.616394
1	-3.427965	2.011543	-1.743145
7	-3.514517	-2.139652	1.147369
1	-3.441908	-2.944001	1.760257
1	-4.500738	-2.011372	0.950182
1	-3.047595	-2.367170	0.269932
7	-1.434574	0.305285	0.901317
1	-2.195186	-0.289365	1.232376
1	-1.601662	1.258602	1.226114
1	-0.592542	0.001087	1.386011
7	0.850802	-2.439924	0.782538
1	-0.139084	-2.620478	0.920076
1	1.345333	-3.193580	1.249700
1	1.073343	-1.577945	1.286825
7	0.986330	1.629360	-0.840088
1	1.637846	0.959121	-1.238781
1	0.734429	2.292755	-1.564861
1	0.143995	1.115791	-0.592083
7	4.277308	0.252823	0.205057
1	4.317447	1.255282	0.056633
1	3.685562	-0.139822	-0.525601
1	5.215156	-0.106454	0.066916

Cartesian coordinates of : MP2_AM10_29

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.624849	2.951559	0.104750
1	1.501225	2.479635	-0.106553
1	0.853074	3.911666	0.339912
1	0.243143	2.516575	0.943397
7	0.209148	-2.679611	-0.432272
1	-0.449994	-3.296306	-0.895110
1	0.506707	-1.971203	-1.106659
1	1.034287	-3.229243	-0.206622
7	-1.356419	2.032436	-2.114266
1	-2.322945	2.212737	-1.863490
1	-1.195847	2.498985	-3.000798
1	-0.762888	2.482931	-1.411762
7	1.136499	-0.097794	-2.038270
1	1.765464	0.457797	-1.462445
1	0.265824	0.427797	-2.106247
1	1.535361	-0.114427	-2.971733
7	-2.043933	-0.357426	0.057666
1	-2.994238	-0.708489	-0.045487
1	-1.426245	-1.164305	0.113640
1	-1.800664	0.129081	-0.801700
7	-1.241491	1.553056	2.330054
1	-1.633014	0.923907	1.618157
1	-1.785221	2.410122	2.316396
1	-1.401719	1.127975	3.237590
7	-5.132966	-1.493454	0.067570
1	-5.571039	-1.017643	0.847704
1	-5.747785	-1.392181	-0.731636
1	-5.098314	-2.480201	0.296073
7	1.242007	-0.589692	1.786428
1	0.695145	-1.242838	1.224434
1	1.367899	-1.026205	2.695013
1	0.647327	0.223020	1.940452
7	3.309321	-2.526488	0.037799
1	3.369979	-2.206313	-0.921756
1	4.250557	-2.680417	0.378937
1	2.891333	-1.779034	0.584139
7	3.337891	1.139744	0.170489
1	4.093153	0.590735	-0.225841
1	2.803770	0.529935	0.793102
1	3.771325	1.859599	0.739268

Cartesian coordinates of : MP2_AM10_30-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	0.429529	1.402653	1.749421
1	1.374291	1.032350	1.863761
1	0.473335	2.116922	1.026146
1	0.185703	1.875112	2.614337
7	-1.766014	-2.876009	-0.499689
1	-2.580449	-3.447757	-0.692551
1	-1.162421	-2.913984	-1.315367
1	-2.072402	-1.907291	-0.386255
7	3.093441	-0.270245	1.398139
1	3.349537	0.111396	0.492613
1	2.441417	-1.038401	1.250028
1	3.930638	-0.650153	1.825443
7	0.378612	-1.976907	1.562550
1	0.526621	-2.444104	2.452057
1	-0.411647	-2.438077	1.107521
1	0.082674	-1.026636	1.777058
7	-2.148582	0.216849	-0.065699
1	-1.514969	0.561980	0.651845
1	-1.745057	0.485156	-0.957015

1	-3.042254	0.692284	0.038443
7	3.101099	2.319429	-0.596246
1	3.429609	2.446520	0.355518
1	3.709919	2.868281	-1.194066
1	2.171786	2.735399	-0.646145
7	1.404250	-3.164681	-1.334193
1	1.274364	-2.804355	-0.390210
1	2.395180	-3.121914	-1.545695
1	1.147649	-4.145694	-1.313912
7	0.828364	0.070324	-1.432457
1	1.769991	0.455903	-1.438091
1	0.627866	-0.163253	-0.463558
1	0.856491	-0.821157	-1.920982
7	-0.018691	3.027456	-1.159757
1	0.030285	2.067791	-1.507619
1	0.041142	3.651966	-1.957387
1	-0.941885	3.158076	-0.759223
7	-5.237153	1.155814	0.348351
1	-5.795674	1.417421	-0.455799
1	-5.550603	1.722707	1.127683
1	-5.455125	0.190733	0.568501

Cartesian coordinates of : MP2_AM10_31

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	2.831004	2.987909	0.072216
1	3.204070	2.147064	0.506997
1	3.252314	3.077013	-0.845491
1	3.141763	3.781951	0.620429
7	-0.594300	-1.739861	0.999619
1	-1.579115	-1.782054	1.253951
1	-0.069717	-2.140351	1.770202
1	-0.345353	-0.754324	0.940910
7	-3.905079	-1.677772	0.927771
1	-3.617301	-1.564186	-0.047035
1	-4.138855	-2.655143	1.067004
1	-4.763622	-1.153228	1.058733
7	-2.928708	2.015620	-1.452842
1	-2.728302	2.994882	-1.626844
1	-3.815317	1.817178	-1.904383
1	-3.058108	1.900186	-0.445080
7	4.838628	-1.531867	-0.383251
1	5.355617	-1.233895	-1.202903
1	4.579149	-0.696471	0.134116
1	5.482409	-2.060921	0.194173
7	1.728739	-1.499873	-1.204142
1	1.546628	-1.573468	-2.199381
1	2.649074	-1.902260	-1.034078
1	1.023852	-2.052352	-0.720842
7	0.107928	1.215053	-0.246468
1	0.635289	0.493777	-0.736912
1	0.738801	2.012031	-0.164260
1	-0.657521	1.488615	-0.858738
7	-2.313883	-1.143318	-1.698543
1	-1.496716	-1.469469	-1.189534
1	-2.272414	-1.533171	-2.633545
1	-2.251826	-0.130219	-1.781836
7	-2.592114	1.265214	1.552551
1	-2.884860	0.298346	1.670936
1	-2.700577	1.730331	2.446816
1	-1.600907	1.255555	1.319505
7	2.709446	0.109138	1.420766
1	2.302824	-0.301972	0.582227
1	1.971378	0.655520	1.853615
1	2.925717	-0.650671	2.057499

Cartesian coordinates of : MP2_AM10_32

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-0.825519	2.088721	-1.558963
1	-1.759184	2.265141	-1.188684
1	-0.678678	2.736463	-2.326237
1	-0.167504	2.342379	-0.828175
7	3.763594	-1.104743	1.360344
1	4.182891	-1.117007	0.431645
1	4.483249	-1.359489	2.027495
1	3.495253	-0.138018	1.536813
7	4.366173	-0.506635	-1.727869
1	4.823253	0.385036	-1.881879
1	3.357097	-0.354069	-1.752102
1	4.606661	-1.100503	-2.513487
7	1.174797	-0.474235	-1.613748
1	1.076131	-1.154999	-2.360422
1	0.446567	0.224576	-1.756525
1	0.957236	-0.957475	-0.743123
7	0.694651	-1.512584	1.479388
1	0.355375	-2.276799	2.056030
1	0.526912	-0.656123	2.000414
1	1.714821	-1.606420	1.437464
7	-0.952256	1.659832	1.842576
1	-1.432977	2.527270	1.626735
1	-1.059469	1.510043	2.840669
1	-1.458752	0.916083	1.361608
7	-2.055563	-0.694601	-0.050809
1	-2.740714	-1.430851	-0.217242
1	-1.208203	-1.140045	0.300904
1	-1.801590	-0.295952	-0.950825
7	-3.744471	1.988021	-0.166514
1	-4.145034	2.411180	0.663202
1	-3.394993	1.065429	0.090622
1	-4.505082	1.861077	-0.825070
7	2.153428	1.614994	0.847899
1	1.193858	1.686444	1.183988
1	2.133751	1.151558	-0.056112
1	2.506658	2.555164	0.710106
7	-4.281335	-3.059458	-0.375395
1	-4.445196	-3.411211	-1.311862
1	-5.182604	-2.798932	0.008352
1	-3.934225	-3.835133	0.177337

Cartesian coordinates of : MP2_AM10_33-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	1.933285	-0.361179	2.128606
1	1.748252	-1.237351	1.631291
1	2.757295	0.049815	1.700219
1	2.189695	-0.607328	3.079549
7	-2.439190	0.212157	-0.297995
1	-3.412399	0.135948	-0.007841
1	-2.411624	0.862640	-1.078918
1	-1.924455	0.666710	0.456730
7	1.482897	-2.841509	0.264703
1	2.110777	-2.507903	-0.461188
1	0.534873	-2.849199	-0.118428
1	1.731736	-3.805684	0.458902
7	-1.515231	-2.742387	-0.776710
1	-1.701693	-2.996735	-1.741135
1	-1.826338	-1.773290	-0.651835
1	-2.117956	-3.324290	-0.204258
7	-0.461130	1.685810	1.824368
1	0.293432	1.007610	1.960621
1	-0.036106	2.540203	1.479728

1	-0.839599	1.900403	2.741384
7	3.887139	-0.854599	-0.973695
1	4.310617	-1.446065	-0.266133
1	4.531469	-0.830511	-1.757043
1	3.840375	0.088456	-0.586840
7	-1.035611	2.872967	-1.589508
1	-0.241723	2.284706	-1.349575
1	-1.457738	3.189711	-0.724782
1	-0.690627	3.685772	-2.086244
7	0.792731	0.249316	-1.225052
1	1.621721	-0.335177	-1.317451
1	0.240622	-0.143705	-0.467053
1	0.234563	0.108488	-2.062059
7	2.992116	2.039342	0.106769
1	2.122358	1.719943	-0.322141
1	3.326180	2.837767	-0.422368
1	2.772900	2.373895	1.038721
7	-5.610794	-0.309452	0.469137
1	-6.240958	0.164010	-0.167787
1	-5.926516	-0.106425	1.410400
1	-5.722619	-1.305676	0.321177

Cartesian coordinates of : MP2_AM10_34

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
7	-1.460610	2.364842	-1.679376
1	-0.440855	2.434712	-1.705446
1	-1.695892	1.462717	-2.080146
1	-1.832683	3.073234	-2.303218
7	-1.711282	2.376970	1.479548
1	-2.312004	3.113255	1.835330
1	-2.155708	1.494364	1.710229
1	-1.714593	2.441834	0.458728
7	1.711230	2.376956	-1.479590
1	2.155651	1.494337	-1.710222
1	1.714543	2.441877	-0.458773
1	2.311949	3.113221	-1.835416
7	1.460562	2.364940	1.679329
1	1.695850	1.462815	2.080096
1	0.440807	2.434806	1.705413
1	1.832643	3.073333	2.303165
7	-4.191515	-3.329095	-0.063170
1	-4.006771	-4.002580	-0.797475
1	-4.015608	-3.790131	0.821902
1	-5.180545	-3.111033	-0.098290
7	2.249749	-0.665445	0.046163
1	1.561030	-0.672698	0.799742
1	2.824588	-1.501080	0.137174
1	2.857001	0.128429	0.220731
7	-0.105898	-0.627879	2.276584
1	-0.233777	-1.445605	2.863810
1	-0.845010	-0.642581	1.568105
1	-0.279305	0.181583	2.863400
7	0.105934	-0.627980	-2.276569
1	0.233843	-1.445730	-2.863757
1	0.845054	-0.642616	-1.568096
1	0.279298	0.181460	-2.863428
7	-2.249707	-0.665498	-0.046149
1	-2.856953	0.128378	-0.220728
1	-2.824551	-1.501131	-0.137152
1	-1.560986	-0.672763	-0.799727
7	4.191538	-3.329060	0.063227
1	4.015749	-3.790034	-0.821901
1	4.006667	-4.002589	0.797460
1	5.180568	-3.111027	0.098507
