

Optimized Cartesian coordinates of the neutral methanol clusters in the gas phase

Cartesian coordinates of the methanol dimer

Cartesian coordinates of : L2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	1.812250	-0.352486	0.425161
1	1.047286	-1.027091	0.834778
1	2.160524	0.304053	1.232942
1	2.656553	-0.953440	0.080979
8	1.334205	0.377511	-0.683231
1	0.537863	0.849693	-0.401559
6	-1.745308	-0.577528	-0.222720
1	-2.575534	-0.379934	-0.908872
1	-2.066532	-1.287119	0.547496
1	-0.917924	-1.010578	-0.787820
8	-1.246382	0.622831	0.353257
1	-1.946475	1.081759	0.827205

Cartesian coordinates of the methanol Trimer

Cartesian coordinates of : BL3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-2.645100	-0.507422	-0.032877
1	-2.253328	-1.346524	0.557643
1	-2.785543	-0.841086	-1.068931
1	-3.618880	-0.228098	0.373341
8	-1.815847	0.632070	0.050540
1	-0.951456	0.446612	-0.343628
6	0.676674	-1.776922	0.230901
1	0.022880	-1.920740	-0.641524
1	0.185009	-1.078716	0.925404
1	0.787096	-2.738559	0.736059
8	1.966305	-1.342366	-0.136995
1	1.866310	-0.515906	-0.629100
6	1.068286	1.766540	0.602738
1	0.133183	2.175788	0.995503
1	1.840324	2.540099	0.563114
1	1.411876	0.958189	1.250587
8	0.861703	1.182873	-0.687809
1	0.666093	1.875138	-1.328921

Cartesian coordinates of : L3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.446891	-0.929978	-0.101690
1	-1.021677	-0.144698	-0.492859
8	0.081426	1.306576	-0.705058
1	0.957028	0.884244	-0.750508
8	2.321952	-0.199958	-0.149926
1	3.232970	-0.288787	-0.446055
6	-2.826960	-0.682416	0.047911

1	-3.320561	-0.507386	-0.916625
1	-3.273607	-1.567702	0.505787
1	-3.022903	0.178170	0.702306
6	-0.007427	1.970347	0.545056
1	0.092018	1.266710	1.381170
1	0.757687	2.748525	0.639638
1	-0.991756	2.440321	0.595344
6	1.820821	-1.465786	0.282328
1	1.895289	-2.213865	-0.513082
1	2.358986	-1.814308	1.169587
1	0.766032	-1.327217	0.526921

Cartesian coordinates of : CY3_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	2.033943	1.874016	-0.127189
1	1.863761	2.011995	-1.201742
1	3.075689	1.573389	0.032226
1	1.868767	2.827148	0.378395
8	1.134354	0.935970	0.431019
1	1.231641	0.070006	-0.010406
6	0.510900	-2.483977	0.366312
1	-0.118616	-3.339375	0.097815
1	0.141886	-2.045854	1.301160
1	1.532506	-2.836902	0.517404
8	0.545523	-1.522066	-0.676373
1	-0.345138	-1.140207	-0.762059
6	-2.707511	0.912648	0.019332
1	-2.704668	1.791798	-0.635819
1	-2.945761	1.228715	1.041504
1	-3.486288	0.228667	-0.322213
8	-1.479671	0.215665	-0.035167
1	-0.739420	0.777947	0.257176

Cartesian coordinates of : CY3_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	2.000772	-1.760571	0.234019
1	2.332803	-1.142761	1.077602
1	2.820667	-1.849774	-0.487650
1	1.758645	-2.757061	0.607231
8	0.834149	-1.238827	-0.371775
1	0.995643	-0.328935	-0.685969
6	1.011802	2.127541	0.439871
1	0.886836	1.495489	1.328381
1	0.513748	3.087089	0.616978
1	2.075885	2.312684	0.280162
8	0.511467	1.490943	-0.723712
1	-0.413616	1.239648	-0.549274
6	-2.834052	-0.546478	0.013596
1	-3.138799	-1.295241	0.753577
1	-2.879801	-0.992299	-0.986716
1	-3.535542	0.288319	0.057276
8	-1.546908	-0.032452	0.299079
1	-0.877264	-0.737424	0.234746

Cartesian coordinates of the methanol tetramer

Cartesian coordinates of : P4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.452365	0.944141	-0.777472
1	-0.574393	0.820326	-1.169368
8	1.355283	0.359301	-0.814171
1	1.183940	0.537689	0.135518
8	0.101371	0.443422	1.576110
1	-0.589267	0.028082	1.028269
6	-2.401295	0.159703	-1.481968
1	-2.164678	-0.907273	-1.410479
1	-3.372048	0.339757	-1.016039
1	-2.465682	0.456738	-2.535734
6	2.617045	0.860343	-1.218913
1	2.671340	1.947983	-1.099702
1	3.431850	0.395094	-0.653533
1	2.741532	0.618259	-2.275393
6	-0.399004	1.676390	2.074345
1	-0.804579	2.290697	1.264286
1	-1.179816	1.507640	2.823872
1	0.434284	2.195443	2.552063
6	0.349974	-2.643147	0.814023
1	-0.440029	-3.160894	1.361116
1	0.999105	-3.394546	0.348662
1	0.932705	-2.045263	1.525316
8	-0.280514	-1.823540	-0.155169
1	0.405217	-1.336062	-0.638162

Cartesian coordinates of : BC4_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	3.532026	-0.442261	-0.781302
1	4.342425	0.201246	-0.422226
1	3.273249	-0.157401	-1.807246
1	3.882593	-1.475347	-0.780493
8	2.407083	-0.377917	0.078040
1	2.031244	0.520301	0.079212
6	-2.769816	0.300422	-0.574424
1	-2.175596	0.851343	-1.318007
1	-2.369338	0.521431	0.428903
1	-3.796226	0.671306	-0.614097
8	-2.805519	-1.081016	-0.836806
1	-1.892105	-1.402859	-0.817406
6	-0.449180	-1.463380	1.467313
1	-0.021999	-0.672994	2.096904
1	-0.045627	-2.429890	1.784171
1	-1.535129	-1.477685	1.587048
8	-0.183419	-1.220348	0.091698
1	0.785213	-1.210629	-0.042910
6	-0.275547	2.595024	0.521788
1	-0.594658	2.358005	1.544003
1	-1.154198	2.872955	-0.072098
1	0.403987	3.447856	0.556377
8	0.428430	1.519205	-0.069588
1	-0.131334	0.724131	-0.109132

Cartesian coordinates of : CY4_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	0.557719	3.531130	1.037335
6	-0.180544	2.737313	1.195279
1	0.078717	2.185839	2.106478
1	-1.161838	3.196613	1.329182
8	-0.255070	1.879815	0.070440
1	0.598423	1.397045	-0.028149
1	2.185847	-0.078716	-2.106479
6	2.737318	0.180545	-1.195277
1	3.531134	-0.557719	-1.037331
1	3.196619	1.161838	-1.329178
8	1.879816	0.255070	-0.070441
1	1.397046	-0.598423	0.028146
1	-0.557718	-3.531130	1.037335
6	0.180544	-2.737313	1.195279
1	-0.078718	-2.185838	2.106478
1	1.161839	-3.196613	1.329183
8	0.255071	-1.879816	0.070439
1	-0.598423	-1.397046	-0.028150
1	-2.185848	0.078719	-2.106479
6	-2.737318	-0.180544	-1.195277
1	-3.531134	0.557720	-1.037329
1	-3.196620	-1.161837	-1.329178
8	-1.879815	-0.255071	-0.070442
1	-1.397045	0.598423	0.028146

Cartesian coordinates of : L4_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.590431	1.709709	-0.490415
1	1.101339	0.884815	-0.593140
8	1.820914	-0.729029	-0.224553
1	1.026169	-1.134130	0.186790
8	-0.477777	-1.393915	1.013470
1	-1.264133	-1.323216	0.442823
6	1.288999	2.544284	0.407952
1	2.238184	2.896531	-0.015454
1	0.659881	3.414054	0.612191
1	1.501040	2.034845	1.357657
6	2.519439	-1.681000	-0.999851
1	2.879456	-2.512254	-0.382564
1	1.897907	-2.083199	-1.809351
1	3.382338	-1.179232	-1.442106
6	-0.562358	-0.358473	1.984840
1	-0.625453	0.626235	1.506597
1	-1.427255	-0.506826	2.639844
1	0.348607	-0.402788	2.585729
8	-2.695460	-0.624425	-0.427046
1	-3.502053	-1.058378	-0.720973
6	-2.427477	0.524370	-1.233443
1	-2.314715	0.248461	-2.286983
1	-3.227767	1.264486	-1.131907
1	-1.490025	0.956797	-0.877793

Cartesian coordinates of : CY4_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-2.663452	1.465281	0.195615
1	-2.770472	2.551415	0.098997
1	-2.610605	1.207608	1.260289
1	-3.546737	0.991211	-0.237747
8	-1.531536	0.997409	-0.513522
1	-0.709093	1.352026	-0.103221
6	1.747319	2.304616	-0.275216
1	1.865978	1.781281	-1.232164
1	2.730304	2.418782	0.195351
1	1.337436	3.297549	-0.469117
8	0.847040	1.624434	0.581839
1	1.172927	0.704198	0.699523
6	2.663456	-1.465302	-0.195691
1	2.610617	-1.207606	-1.260360
1	2.770457	-2.551440	-0.099094
1	3.546746	-0.991255	0.237686
8	1.531544	-0.997427	0.513452
1	0.709099	-1.352043	0.103158
6	-1.747295	-2.304555	0.275354
1	-2.730319	-2.418763	-0.195121
1	-1.865875	-1.781124	1.232261
1	-1.337402	-3.297471	0.469322
8	-0.847081	-1.624463	-0.581840
1	-1.172957	-0.704228	-0.699564

Cartesian coordinates of : CY4_4-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-0.065238	2.384102	0.804013
8	0.095900	1.738507	-0.443593
8	-1.939634	-0.023314	-0.795298
6	-3.072066	-0.171650	0.039661
8	1.970422	-0.207746	-0.830256
6	3.052179	-0.083421	0.071775
8	-0.070549	-1.934182	-0.291764
6	0.041253	-1.763631	1.109783
1	-0.358164	1.679216	1.593597
1	-0.816213	3.180258	0.745695
1	0.892823	2.832454	1.075644
1	-0.721802	1.234441	-0.646824
1	-2.788818	-0.289316	1.094056
1	-3.678722	-1.031953	-0.263265
1	-3.677400	0.731344	-0.059870
1	-1.380205	-0.828830	-0.742348
1	0.045646	-0.698368	1.383467
1	0.953126	-2.231220	1.498235
1	-0.821703	-2.245657	1.574682
1	0.718442	-1.504740	-0.682906
1	2.706635	0.071872	1.102990
1	3.712638	0.744825	-0.209250
1	3.626058	-1.011522	0.033564
1	1.401776	0.588669	-0.761565

Cartesian coordinates of : CY4_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-3.190249	0.023554	-0.658426
8	-1.978508	0.118498	0.068622
8	-0.211143	-1.906609	-0.136381
6	0.258538	-2.198150	1.168428
8	0.060312	1.856540	-0.220422
6	0.354492	2.321398	1.084562
8	1.672633	-0.166293	-1.018575
6	2.970371	-0.062377	-0.466442
1	-3.824970	-0.777432	-0.264039
1	-3.009001	-0.155866	-1.724269
1	-3.718180	0.972435	-0.547172
1	-1.455561	-0.709759	-0.032221
1	0.574553	-1.287568	1.694243
1	1.097769	-2.902163	1.139260
1	-0.562209	-2.655073	1.724317
1	0.504764	-1.423103	-0.602870
1	2.939532	0.108550	0.617814
1	3.539002	0.747459	-0.937373
1	3.489537	-1.004171	-0.655313
1	1.166121	0.655012	-0.825391
1	0.427194	1.494249	1.802433
1	-0.407443	3.025275	1.436232
1	1.314953	2.839980	1.044525
1	-0.781321	1.348548	-0.184868

Cartesian coordinates of : BC4_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.326990	-0.950682	-1.052609
6	-2.689646	-1.001462	-0.658916
1	-2.836687	-0.561803	0.335861
1	-3.334050	-0.486649	-1.379758
1	-2.977257	-2.053257	-0.622723
1	-1.044983	-0.020841	-1.033630
8	2.268541	0.668125	-0.702485
6	1.876290	-0.278625	-1.673756
1	1.245031	-1.073862	-1.250871
1	1.329578	0.183444	-2.505974
1	2.784089	-0.736688	-2.071967
1	1.475049	1.147072	-0.417292
8	-0.032040	-0.981549	1.407958
6	1.273112	-1.444734	1.741363
1	1.310493	-2.538860	1.739339
1	2.025062	-1.039297	1.055577
1	1.486680	-1.092396	2.751708
1	-0.317410	-1.344659	0.550187
8	-0.335613	1.387914	0.184521
6	-0.869979	2.589514	0.716172
1	-1.865749	2.426810	1.143172
1	-0.213635	3.011483	1.484488
1	-0.951564	3.302938	-0.105055
1	-0.244492	0.697940	0.878678

Cartesian coordinates of : BL4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.811234	-0.293706	0.926805
6	3.054823	-0.255468	0.259710
1	3.447556	-1.261129	0.065529
1	2.990499	0.280695	-0.697889
1	3.760209	0.271661	0.905859
1	1.175645	-0.749706	0.346634
8	-0.735271	1.555671	-1.176161
6	0.170412	2.322896	-0.371590
1	0.836957	2.919329	-1.001224
1	-0.380910	2.975432	0.312343
1	0.758228	1.605576	0.206393
1	-1.274143	2.141588	-1.718535
8	0.091862	-1.129214	-1.086657
6	-0.932959	-2.112040	-1.152023
1	-1.821479	-1.798851	-0.592112
1	-1.206575	-2.325676	-2.191181
1	-0.530344	-3.022852	-0.705493
1	-0.244102	-0.275742	-1.402113
8	-2.231981	0.166202	0.900047
6	-1.301880	-0.337998	1.841623
1	-0.798861	-1.243180	1.475499
1	-0.529654	0.395655	2.101162
1	-1.861726	-0.593525	2.743493
1	-1.750420	0.584760	0.173038

Cartesian coordinates of : L4_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	3.183072	-0.826081	-0.375495
6	3.439145	0.422943	0.254360
1	4.000169	0.292631	1.185324
1	3.978375	1.105404	-0.410228
1	2.463772	0.856653	0.484852
1	4.007524	-1.246005	-0.639484
8	0.431426	-0.773805	-0.510506
6	0.196277	-1.278226	0.798601
1	0.208768	-2.373699	0.804873
1	0.950738	-0.911825	1.506360
1	-0.792526	-0.931102	1.110367
1	1.353501	-0.955005	-0.751926
8	-1.087619	1.486937	-0.683230
6	-0.391462	2.266326	0.268482
1	-0.132728	1.679630	1.161147
1	0.525913	2.694261	-0.155599
1	-1.046011	3.085901	0.571286
1	-0.537807	0.702419	-0.871602
8	-2.988108	-0.131371	0.589612
6	-3.123266	-1.140543	-0.389008
1	-3.779613	-0.828648	-1.211576
1	-2.151821	-1.435968	-0.811578
1	-3.569947	-2.012204	0.095274
1	-2.512641	0.609115	0.174840

Cartesian coordinates of the methanol pentamer

Cartesian coordinates of : BC5_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.559649	-0.363488	-1.723089
1	-0.391625	-0.272966	-1.554687
8	-1.870980	-0.106870	-0.340084
1	-1.398343	-0.697901	0.311501
8	1.700498	0.199321	1.099085
1	1.219798	0.825235	0.520434
6	1.005994	0.717180	-2.522605
1	0.802984	1.683120	-2.045080
1	2.086814	0.604974	-2.640914
1	0.549903	0.700268	-3.520018
6	-3.265638	-0.354611	-0.329859
1	-3.486450	-1.384939	-0.630031
1	-3.694154	-0.171867	0.661664
1	-3.731974	0.324953	-1.045456
6	2.843911	-0.309147	0.429781
1	2.559830	-0.835995	-0.487496
1	3.545921	0.496583	0.186460
1	3.338588	-1.002182	1.113681
6	0.092190	-2.706761	0.522599
1	-0.773161	-3.359044	0.385619
1	0.506151	-2.440817	-0.456575
1	0.844245	-3.247719	1.107092
8	-0.348347	-1.548049	1.222055
1	0.422689	-0.936577	1.303727
6	-0.475383	2.484665	1.504411
1	0.395164	3.041883	1.854139
1	-1.341939	3.155110	1.489468
1	-0.665483	1.661730	2.204469
8	-0.176859	2.000473	0.203665
1	-0.907086	1.417101	-0.077005

Cartesian coordinates of : DC5-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	2.008917	-0.378285	0.164369
1	1.395530	0.235231	-0.283393
8	0.088155	0.955721	-1.346733
1	-0.761757	0.636365	-0.980269
8	-0.374300	-1.857996	0.785882
1	0.337752	-1.245428	1.054053
6	2.957332	-0.831873	-0.777673
1	3.623860	-0.023621	-1.104527
1	3.562734	-1.601593	-0.293394
1	2.478323	-1.268907	-1.664125
6	-0.055692	2.305921	-1.743684
1	-0.690542	2.395335	-2.632804
1	-0.481057	2.921852	-0.941033
1	0.937789	2.689213	-1.986159
6	0.042592	-2.555007	-0.376801
1	0.127180	-1.880739	-1.239320
1	1.008185	-3.044643	-0.216646
1	-0.711523	-3.316644	-0.586848
8	-0.035741	0.736265	1.840406
1	-0.881356	1.006891	1.456989
6	0.860022	1.829001	1.893279
1	1.025894	2.267567	0.900066
1	0.505963	2.610100	2.577317

1	1.812745	1.440091	2.253592
6	-3.384954	-0.351776	-0.279409
1	-3.896267	0.531009	-0.667944
1	-3.386562	-1.127480	-1.054169
1	-3.933376	-0.718543	0.594626
8	-2.066104	0.028238	0.069546
1	-1.556731	-0.755194	0.411967

Cartesian coordinates of : BL5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.363080	-1.324935	-1.227056
1	-0.115530	-0.488107	-1.345497
8	-0.928423	1.116462	-0.769348
1	-0.168783	1.275848	-0.145748
8	0.990636	1.211667	0.999023
1	1.913232	1.149979	0.689451
6	-0.532348	-2.272652	-0.675481
1	-1.271361	-2.607110	-1.415540
1	0.056644	-3.140261	-0.367263
1	-1.060541	-1.873643	0.200345
6	-1.313712	2.327482	-1.397971
1	-1.628047	3.073277	-0.659737
1	-0.496145	2.739496	-1.999349
1	-2.155685	2.107546	-2.057219
6	0.725902	0.071795	1.814209
1	1.014294	-0.850629	1.297077
1	1.262356	0.148028	2.765683
1	-0.348990	0.043769	2.008382
8	3.525472	0.529398	0.187698
1	4.388074	0.736910	0.559538
6	3.537963	-0.770514	-0.405342
1	4.236423	-0.806384	-1.247400
1	3.810940	-1.534659	0.330651
1	2.525499	-0.965018	-0.765281
6	-3.769472	-0.697549	0.458522
1	-4.325210	-1.232496	1.231638
1	-4.432270	0.061988	0.023141
1	-3.496833	-1.414948	-0.328438
8	-2.634895	-0.124244	1.068303
1	-2.125025	0.358256	0.392972

Cartesian coordinates of : BC5_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-4.312010	0.725019	-0.621449
6	-3.767931	-0.121300	-0.188041
1	-3.779662	-0.030198	0.904336
1	-4.278135	-1.044142	-0.470275
8	-2.446197	-0.187664	-0.691750
1	-1.934363	0.594721	-0.380482
1	0.562029	-1.033531	-1.633075
6	0.226000	-2.027093	-1.310690
1	-0.361115	-2.491186	-2.108916
1	1.099135	-2.651908	-1.108859
8	-0.530810	-1.950848	-0.107213
1	-1.348613	-1.432518	-0.298632
1	0.570488	2.396849	-0.937776

6	-0.254518	2.759598	-0.318566
1	0.117079	3.520180	0.376724
1	-1.020941	3.211680	-0.951016
8	-0.873418	1.691547	0.392233
1	-0.197410	1.152814	0.844660
1	1.630449	-1.577621	2.811636
6	1.058846	-0.646476	2.736981
1	0.115263	-0.761205	3.281135
1	1.634777	0.157989	3.197937
8	0.829157	-0.294840	1.382639
1	0.309752	-1.007688	0.914010
1	3.184713	-0.995893	-1.419362
6	3.410543	0.057624	-1.203737
1	4.237782	0.097616	-0.483679
1	3.739139	0.533203	-2.130068
8	2.275578	0.759373	-0.746537
1	1.959530	0.361169	0.082493

Cartesian coordinates of : L5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	2.720621	-0.360352	0.155437
1	2.087339	0.345530	0.380788
8	0.592768	1.388530	0.537779
1	0.183119	1.102813	-0.316900
8	-0.375671	0.416599	-1.740958
1	-0.746753	-0.437883	-1.420993
6	3.130792	-1.001653	1.341001
1	2.287651	-1.465166	1.874378
1	3.835611	-1.789154	1.064796
1	3.637111	-0.313077	2.029827
6	0.554221	2.798722	0.627957
1	1.084455	3.274340	-0.205808
1	-0.479090	3.169701	0.644548
1	1.040563	3.088765	1.561409
6	0.748295	0.145442	-2.574521
1	1.546712	-0.356339	-2.015506
1	0.454231	-0.465730	-3.433854
1	1.121208	1.104427	-2.940335
8	-1.198704	-1.812123	-0.489623
1	-2.023227	-1.586075	-0.022005
6	-0.154625	-1.958596	0.468600
1	0.781459	-2.081478	-0.080218
1	-0.061633	-1.063493	1.097606
1	-0.325140	-2.836052	1.101039
8	-3.252127	-0.526986	0.839739
1	-4.157949	-0.525011	0.513234
6	-2.701980	0.787357	0.735885
1	-2.608756	1.100894	-0.310125
1	-3.308821	1.510289	1.289974
1	-1.703396	0.749722	1.175615

Cartesian coordinates of : CY5_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-3.563871	-2.031122	-1.391265
6	-3.103904	-1.048107	-1.538709
1	-2.465726	-1.081527	-2.429301

1	-3.895217	-0.314086	-1.702219
8	-2.377815	-0.650799	-0.390396
1	-1.632037	-1.275940	-0.217770
1	-1.672397	1.197204	2.122111
6	-1.672979	2.040187	1.421112
1	-2.690612	2.437784	1.344839
1	-1.018669	2.822842	1.811660
8	-1.180689	1.657978	0.148835
1	-1.676984	0.861039	-0.157879
1	0.344344	-0.440660	1.580360
6	-0.032197	-1.470459	1.646656
1	0.675435	-2.073075	2.227668
1	-0.993671	-1.462786	2.166172
8	-0.239861	-2.028702	0.358627
1	0.570388	-1.840414	-0.168754
1	1.725438	3.473354	-0.402791
6	1.893661	2.524760	-0.924674
1	1.390995	2.559910	-1.897780
1	2.966779	2.402746	-1.086872
8	1.444814	1.429801	-0.146030
1	0.466282	1.506926	-0.019720
1	3.108572	-1.058152	1.082165
6	3.187250	-1.438412	0.055959
1	4.097168	-1.034006	-0.402035
1	3.269558	-2.527062	0.088243
8	2.041272	-1.111275	-0.708828
1	1.861469	-0.146818	-0.606566

Cartesian coordinates of : CY5_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-1.187419	2.986510	1.486756
6	-1.661282	2.046984	1.181809
1	-1.455975	1.285895	1.945872
1	-2.740669	2.205424	1.124867
8	-1.213884	1.641344	-0.097690
1	-0.227612	1.575738	-0.084925
1	-4.186511	-0.184145	-1.157903
6	-3.513257	-0.869284	-0.630420
1	-3.632572	-0.721224	0.451423
1	-3.799631	-1.894161	-0.873917
8	-2.172614	-0.685047	-1.040294
1	-1.873595	0.217393	-0.781177
1	2.112460	2.282828	-1.743641
6	2.159278	2.453552	-0.662534
1	3.208446	2.481017	-0.348270
1	1.703448	3.420575	-0.439341
8	1.441498	1.460898	0.051460
1	1.778842	0.566565	-0.206247
1	-1.305549	-1.397879	1.642168
6	-0.255692	-1.476314	1.337238
1	0.194965	-0.473618	1.367744
1	0.266383	-2.121181	2.048301
8	-0.143245	-2.057660	0.048184
1	-0.881504	-1.696461	-0.493189
1	3.327171	-2.652343	-0.067369
6	3.168777	-1.606495	0.214967
1	2.866398	-1.562107	1.269085
1	4.110194	-1.066026	0.098394
8	2.210294	-0.991866	-0.628891
1	1.359389	-1.484810	-0.547153

Cartesian coordinates of : CY5_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-0.745036	-1.531630	2.133681
6	0.012313	-1.131084	1.449634
1	-0.280027	-0.117993	1.140172
1	0.965325	-1.075656	1.982826
8	0.190668	-1.978599	0.328094
1	-0.631560	-1.911237	-0.206323
1	3.750811	-2.188631	-0.547613
6	3.503844	-1.166540	-0.241560
1	3.484026	-1.119498	0.855093
1	4.284866	-0.496136	-0.605869
8	2.277206	-0.746606	-0.807034
1	1.545055	-1.326953	-0.493578
1	-4.165996	-0.935070	-0.462791
6	-3.270811	-1.331336	0.030024
1	-3.121032	-0.796065	0.977867
1	-3.434011	-2.388496	0.249118
8	-2.136949	-1.232189	-0.810417
1	-1.929309	-0.279711	-0.930897
1	2.776961	2.457482	0.578310
6	1.718683	2.191477	0.682291
1	1.614688	1.466659	1.500708
1	1.160764	3.094137	0.941915
8	1.196165	1.689256	-0.531915
1	1.651795	0.839755	-0.737052
1	-1.797094	3.253989	0.135191
6	-2.012392	2.190825	0.292216
1	-1.618616	1.890644	1.273699
1	-3.096323	2.055616	0.297290
8	-1.479784	1.400962	-0.752144
1	-0.503554	1.526148	-0.770048

Cartesian coordinates of : P5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-0.618461	3.114815	-0.701405
1	-1.542206	3.474104	-0.234620
1	-0.741250	3.116004	-1.789766
1	0.192974	3.795631	-0.438384
8	-0.270600	1.825731	-0.226651
1	-0.963347	1.163880	-0.472363
6	0.756924	-2.708475	-0.990074
1	1.538761	-3.323073	-0.530784
1	1.204835	-2.054754	-1.743021
1	0.023612	-3.369571	-1.456477
8	0.072043	-1.949358	-0.002534
1	0.670955	-1.269799	0.363780
6	-0.520231	-0.253600	2.547115
1	-1.426322	-0.282872	1.928425
1	-0.683906	0.425106	3.392531
1	-0.332307	-1.258014	2.930232
8	0.611750	0.128643	1.786038
1	0.393922	0.942444	1.301373
6	-3.118272	-0.654397	-0.502910
1	-3.216313	-0.950747	0.548652
1	-3.437288	-1.489622	-1.136189

1	-3.778985	0.194628	-0.690416
8	-1.797800	-0.256336	-0.814939
1	-1.155718	-0.971244	-0.570356
6	3.079013	0.522768	-0.198114
1	2.867760	0.609175	0.874382
1	3.493528	1.469267	-0.567218
1	3.829596	-0.257346	-0.343453
8	1.926898	0.136767	-0.925049
1	1.249544	0.826559	-0.828921

Cartesian coordinates of the methanol hexamer

Cartesian coordinates of : BC6_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-0.852583	1.445697	2.457404
1	-1.812562	0.980481	2.210639
1	-0.961658	2.535334	2.478102
1	-0.527322	1.109556	3.443856
8	0.143748	1.058663	1.517853
1	-0.150399	1.316080	0.601925
6	1.310362	-1.180265	-2.254645
1	1.396231	-2.205510	-2.631882
1	2.140168	-0.964723	-1.573754
1	1.354831	-0.491689	-3.101833
8	0.061159	-0.988603	-1.602616
1	0.134350	-1.327602	-0.685390
6	1.387218	-2.317137	1.493488
1	1.404141	-2.398076	2.585448
1	2.300835	-1.825827	1.144156
1	1.325234	-3.321597	1.070614
8	0.237073	-1.600321	1.057733
1	0.298834	-0.655247	1.333059
6	-3.050023	-1.252221	-0.618386
1	-3.818077	-0.532989	-0.913210
1	-2.390325	-1.437752	-1.474315
1	-3.549612	-2.185926	-0.333214
8	-2.340187	-0.684690	0.469182
1	-1.664124	-1.310596	0.768373
6	-1.841682	1.998943	-1.212994
1	-1.862970	3.081198	-1.068010
1	-2.160165	1.778760	-2.237620
1	-2.530006	1.519646	-0.508368
8	-0.507706	1.563695	-0.992974
1	-0.394792	0.636425	-1.311406
6	2.880118	1.481479	-0.615162
1	1.966537	1.814343	-1.123129
1	3.375617	2.348265	-0.161033
1	3.560129	1.048765	-1.352978
8	2.604938	0.475552	0.345332
1	1.972445	0.835330	0.985656

Cartesian coordinates of : BC6_6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	3.938372	-0.511265	-0.454397

1	3.354964	-0.597827	0.315639
8	1.775104	-0.447313	1.363421
1	1.192953	-1.130614	0.935546
8	0.247416	-1.956065	-0.143048
1	-0.629652	-1.528882	-0.184104
6	3.707460	0.760673	-1.018072
1	3.940134	1.571557	-0.312971
1	4.366863	0.863371	-1.882528
1	2.668006	0.880781	-1.356884
6	1.735795	-0.573601	2.778677
1	0.722270	-0.413772	3.161843
1	2.089121	-1.560388	3.092788
1	2.397109	0.186769	3.197135
6	0.879466	-1.752993	-1.406701
1	0.419631	-2.384369	-2.173807
1	0.815243	-0.699923	-1.708264
1	1.932797	-2.018965	-1.300426
8	-1.772938	-0.107136	-0.494477
1	-1.084235	0.575160	-0.318738
6	-2.275462	0.073960	-1.814299
1	-2.987634	0.905933	-1.847484
1	-1.460736	0.260943	-2.522169
1	-2.791113	-0.844298	-2.102604
6	0.640284	2.798073	0.030213
1	-0.060104	3.316922	-0.626094
1	0.478805	3.140604	1.057779
1	1.661810	3.045632	-0.279113
8	0.396510	1.407021	-0.098863
1	0.982807	0.894933	0.497119
6	-5.044295	-0.434051	0.507926
1	-6.050735	-0.134033	0.807033
1	-5.057788	-0.643409	-0.571473
1	-4.789122	-1.360561	1.038931
8	-4.171509	0.624247	0.833163
1	-3.274525	0.366145	0.569975

Cartesian coordinates of : BL6_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.243565	1.451165	-0.961910
1	1.198477	0.511948	-0.711136
8	0.446029	-1.203857	-0.416218
1	-0.405501	-0.923285	-0.028743
8	-0.877359	0.380966	1.496143
1	-1.645388	0.932225	1.289918
6	2.468465	2.017800	-0.540385
1	3.285595	1.774248	-1.232714
1	2.343041	3.103811	-0.530709
1	2.748598	1.677595	0.463572
6	0.207341	-1.944006	-1.602856
1	-0.407939	-2.826258	-1.401850
1	-0.296663	-1.328827	-2.355070
1	1.179401	-2.261178	-1.987121
6	0.153415	1.198041	2.037371
1	0.330700	2.078244	1.409063
1	-0.089366	1.513011	3.059082
1	1.069347	0.603295	2.056207
8	-2.887834	1.491615	-0.109238
1	-3.752999	1.903657	-0.202700
6	-2.032228	1.892463	-1.191240
1	-2.361565	1.438033	-2.130548
1	-2.016930	2.981566	-1.287951

1	-1.023783	1.550085	-0.950689
6	3.653431	-1.078754	-0.026445
1	4.570418	-0.517756	0.169297
1	3.908715	-2.143613	-0.106244
1	3.244785	-0.744145	-0.991493
8	2.760229	-0.828357	1.036805
1	1.896030	-1.184751	0.773332
6	-2.645933	-2.155098	0.735318
1	-2.182857	-3.118603	0.509535
1	-2.196270	-1.752606	1.649903
1	-3.719175	-2.317710	0.889960
8	-2.402136	-1.304974	-0.374675
1	-2.763561	-0.424127	-0.190739

Cartesian coordinates of : BL6_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.772518	-2.024313	0.049077
1	1.139371	-1.831175	-0.660445
8	-0.307045	-0.798518	-1.324539
1	0.078318	0.029611	-0.966238
8	0.677306	1.291207	0.113293
1	1.581651	1.616422	-0.061693
6	1.092743	-2.759277	1.052448
1	0.897723	-3.790429	0.733171
1	1.740560	-2.788845	1.932066
1	0.140030	-2.291227	1.330197
6	-1.077671	-0.518130	-2.489854
1	-1.815924	0.262792	-2.281776
1	-0.433237	-0.209519	-3.319946
1	-1.588839	-1.441543	-2.768715
6	0.643457	0.760888	1.442567
1	1.425825	0.006563	1.571708
1	0.770198	1.563408	2.176038
1	-0.333889	0.289912	1.579060
8	3.353577	1.703972	-0.042463
1	3.949001	2.432862	-0.241461
6	4.000711	0.450491	-0.276473
1	4.331584	0.367295	-1.316550
1	4.857320	0.327014	0.393314
1	3.267681	-0.332962	-0.071956
6	-3.417068	-1.052737	0.344119
1	-4.086225	-0.958134	1.203015
1	-3.558437	-0.183549	-0.311056
1	-3.690350	-1.964375	-0.203841
8	-2.093785	-1.116254	0.837634
1	-1.487952	-1.083862	0.076250
6	-2.668314	2.145469	0.758107
1	-3.734270	2.264124	0.549140
1	-2.541617	1.328431	1.480506
1	-2.300586	3.081340	1.197622
8	-2.025554	1.854264	-0.468599
1	-1.067210	1.862763	-0.319116

Cartesian coordinates of : BC6_7

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	3.240376	-1.263477	0.034886

1	3.078559	-0.333330	-0.212096
8	2.582717	1.402583	-0.322518
1	1.807677	1.425716	-0.913772
8	0.080724	1.047452	-1.328289
1	-0.077397	0.122353	-1.048881
6	4.622636	-1.443975	0.247981
1	5.004384	-0.792198	1.045377
1	4.778475	-2.481959	0.550889
1	5.206369	-1.258497	-0.662664
6	2.121843	1.683187	0.986408
1	1.727008	2.703034	1.061982
1	1.344651	0.972580	1.300253
1	2.972161	1.583788	1.664392
6	-1.008528	1.481996	-2.123144
1	-1.065528	0.923804	-3.064031
1	-1.957684	1.371174	-1.583987
1	-0.850266	2.538062	-2.351726
8	-0.610338	-1.272886	-0.120820
1	-1.565474	-1.447110	-0.238204
6	0.131996	-2.484709	0.008959
1	-0.190343	-3.037410	0.897615
1	0.002378	-3.114801	-0.877058
1	1.184968	-2.216839	0.108289
6	-4.412928	-1.552374	0.375561
1	-5.315186	-0.932187	0.338510
1	-4.206244	-1.821898	1.417836
1	-4.596292	-2.464499	-0.194635
8	-3.311139	-0.892780	-0.222560
1	-3.084534	-0.091214	0.284878
6	-1.483912	2.326933	1.226935
1	-0.923036	2.651465	0.343909
1	-0.890194	2.527876	2.126152
1	-2.417181	2.888836	1.292722
8	-1.826572	0.953700	1.139003
1	-1.040068	0.420164	0.940441

 Cartesian coordinates of : P6

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	2.478124	-1.110280	0.678387
1	1.624178	-1.045102	1.139878
8	-0.016862	-0.424951	1.684352
1	-0.037747	0.492218	1.353571
8	-0.035687	1.893493	0.161411
1	0.252040	1.370172	-0.634301
6	3.030729	0.185030	0.623952
1	3.086136	0.651956	1.616372
1	4.044978	0.098767	0.226435
1	2.455036	0.846765	-0.040273
6	-0.882166	-0.568716	2.801162
1	-0.557395	0.054124	3.642155
1	-1.911393	-0.313537	2.527518
1	-0.840117	-1.615406	3.108624
6	0.595746	3.161530	0.194863
1	1.677640	3.062173	0.341870
1	0.408124	3.719826	-0.728215
1	0.178705	3.719988	1.034618
8	0.406164	0.254973	-1.842159
1	-0.169136	-0.498415	-1.565214
6	1.598151	-0.257185	-2.424597
1	2.128679	-0.911628	-1.724169
1	1.370028	-0.802702	-3.346613

1	2.235531	0.593657	-2.676187
6	-0.407017	-2.792582	-0.350552
1	-0.891862	-3.268229	0.508247
1	0.615315	-2.510117	-0.078421
1	-0.374216	-3.509780	-1.173251
8	-1.155713	-1.671679	-0.802283
1	-1.400477	-1.104193	-0.047747
6	-3.203847	0.601074	-0.972933
1	-2.545840	0.613043	-1.849930
1	-3.860502	1.478232	-0.997119
1	-3.815791	-0.301112	-1.014093
8	-2.457385	0.549614	0.234271
1	-1.810635	1.275035	0.233040

Cartesian coordinates of : DC6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-2.579296	0.569604	-0.481492
1	-2.324794	1.026423	0.346424
8	-1.329657	1.454534	1.769109
1	-0.572938	1.593471	1.163443
8	0.373144	1.322045	-0.336236
1	1.336417	1.127377	-0.363282
6	-3.944481	0.208651	-0.423336
1	-4.591483	1.090174	-0.345702
1	-4.188912	-0.317883	-1.348497
1	-4.154430	-0.459251	0.422798
6	-1.157961	0.190652	2.388156
1	-1.003154	-0.602516	1.642822
1	-0.309089	0.196147	3.082286
1	-2.066148	-0.024846	2.955555
6	0.051990	2.084770	-1.494968
1	0.504754	3.081385	-1.450127
1	0.399582	1.573331	-2.398904
1	-1.034528	2.176037	-1.536596
8	2.941871	0.601734	-0.718051
1	2.771877	-0.366949	-0.682894
6	4.098643	0.914471	0.034837
1	4.225576	1.998373	0.013171
1	4.002572	0.593836	1.080036
1	4.990270	0.449501	-0.399539
8	2.001824	-1.857239	-0.213752
1	1.105316	-1.758404	-0.602043
6	1.852903	-1.735188	1.189475
1	1.609719	-0.702323	1.478307
1	1.063554	-2.396230	1.564955
1	2.799964	-2.020151	1.653533
6	-1.666952	-2.280365	-0.959297
1	-1.274363	-3.293365	-1.068699
1	-2.275810	-2.230082	-0.048052
1	-2.302049	-2.051600	-1.822198
8	-0.561800	-1.402027	-0.889803
1	-0.885439	-0.489618	-0.784200

Cartesian coordinates of : BC6_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-0.540521	0.180533	-1.504823

6	0.137319	-0.150841	-2.304928
1	-0.220913	-1.113311	-2.694123
1	0.097609	0.581522	-3.114875
8	1.477663	-0.229669	-1.864242
1	1.507515	-0.901248	-1.163469
1	3.142433	0.738995	-0.320022
6	3.170359	0.857885	0.768846
1	3.918493	0.180676	1.196128
1	3.456550	1.883529	1.011356
8	1.891371	0.628345	1.345305
1	1.584453	-0.267627	1.098008
1	1.206680	2.116351	-1.322993
6	0.561777	2.829801	-0.798228
1	1.136498	3.725209	-0.535603
1	-0.257282	3.123751	-1.459844
8	-0.004712	2.241928	0.365056
1	0.685248	1.693078	0.808918
1	0.979353	-3.867347	0.398844
6	1.324513	-3.019279	1.000264
1	0.916481	-3.107528	2.012484
1	2.414641	-3.049816	1.053804
8	0.949705	-1.786868	0.405168
1	-0.048334	-1.712768	0.397141
1	-3.476197	2.550844	0.823648
6	-3.190606	1.554078	1.175840
1	-2.767690	1.638819	2.183011
1	-4.085104	0.929135	1.219616
8	-2.277147	0.945343	0.278830
1	-1.428380	1.464658	0.274411
1	-2.507181	-1.478402	-1.506883
6	-2.330018	-2.195810	-0.698235
1	-3.290367	-2.602359	-0.363504
1	-1.717611	-3.015955	-1.084183
8	-1.640173	-1.587912	0.381137
1	-1.920078	-0.635091	0.441566

Cartesian coordinates of : L6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	2.967024	0.795367	-0.794459
1	2.398512	0.752851	-0.003395
8	1.356568	0.084048	1.350433
1	0.919226	-0.709078	0.950993
8	0.185520	-1.874993	0.009270
1	-0.758596	-1.625093	-0.136336
6	4.034818	-0.101250	-0.584777
1	3.678202	-1.116338	-0.355980
1	4.622537	-0.142573	-1.504641
1	4.693885	0.226388	0.230483
6	1.920074	-0.250532	2.603466
1	1.146663	-0.541233	3.324663
1	2.646361	-1.068001	2.516151
1	2.434950	0.633965	2.984672
6	0.831197	-1.963660	-1.254974
1	0.096746	-2.113620	-2.053143
1	1.409059	-1.053452	-1.464982
1	1.512236	-2.819009	-1.240287
8	-2.303759	-1.133021	-0.531153
1	-2.479310	-0.215672	-0.206356
6	-3.391440	-1.971240	-0.181557
1	-3.146609	-2.985851	-0.501854
1	-3.564048	-1.977278	0.901102

1	-4.309190	-1.653629	-0.687610
8	-2.644141	1.318984	0.448114
1	-2.213327	1.921390	-0.188939
6	-1.961655	1.411593	1.694874
1	-0.893769	1.183594	1.591479
1	-2.081300	2.409252	2.128956
1	-2.417796	0.681382	2.366989
8	-0.930727	2.486015	-1.307723
1	-1.035285	2.956081	-2.140858
6	-0.104127	1.333711	-1.501154
1	-0.595709	0.599014	-2.148991
1	0.876916	1.604299	-1.899748
1	0.042561	0.889686	-0.513497

Cartesian coordinates of : CY6_7

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-2.454578	-2.926885	1.402405
6	-2.810672	-2.565415	0.430965
1	-2.697427	-3.364807	-0.309288
1	-3.870766	-2.315961	0.515938
8	-2.120875	-1.396934	0.025089
1	-1.160365	-1.612148	-0.087466
1	-4.506392	1.111429	1.182406
6	-3.677262	1.489617	0.573410
1	-3.831233	1.180141	-0.468098
1	-3.681341	2.580967	0.621306
8	-2.431132	1.035002	1.069650
1	-2.330869	0.084927	0.825445
1	-1.667435	2.272300	-2.015691
6	-0.904409	1.581746	-1.637506
1	-1.331708	0.572877	-1.575860
1	-0.066023	1.570994	-2.338933
8	-0.415473	2.009808	-0.376316
1	-1.089590	1.759108	0.299175
1	1.667414	-2.272304	-2.015691
6	0.904389	-1.581758	-1.637490
1	1.331679	-0.572885	-1.575850
1	0.065990	-1.571012	-2.338902
8	0.415481	-2.009828	-0.376292
1	1.089602	-1.759113	0.299190
1	2.454533	2.926891	1.402401
6	2.810662	2.565426	0.430973
1	2.697434	3.364817	-0.309283
1	3.870755	2.315980	0.515980
8	2.120888	1.396939	0.025073
1	1.160377	1.612142	-0.087496
1	4.506406	-1.111396	1.182362
6	3.677266	-1.489614	0.573398
1	3.831214	-1.180177	-0.468125
1	3.681353	-2.580962	0.621337
8	2.431143	-1.034989	1.069646
1	2.330877	-0.084917	0.825427

Cartesian coordinates of : CY6_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	2.757030	1.336568	-2.064972

6	3.028393	1.856271	-1.139191
1	4.077388	1.641881	-0.905957
1	2.917790	2.932046	-1.294021
8	2.183505	1.482581	-0.065989
1	2.212529	0.497303	0.031589
1	0.610091	4.347360	0.917040
6	-0.097705	3.542074	1.143398
1	0.216933	3.041519	2.066016
1	-1.086396	3.979685	1.299980
8	-0.191862	2.630942	0.063409
1	0.676583	2.164612	-0.033797
1	-2.538598	1.710434	-2.067839
6	-3.121649	1.691331	-1.140236
1	-3.456673	2.708997	-0.910358
1	-4.000377	1.059713	-1.289860
8	-2.374121	1.148781	-0.066908
1	-1.534841	1.666330	0.028121
1	3.456673	-2.708998	0.910357
6	3.121649	-1.691331	1.140236
1	2.538598	-1.710435	2.067838
1	4.000378	-1.059713	1.289859
8	2.374121	-1.148781	0.066907
1	1.534841	-1.666330	-0.028121
1	-4.077388	-1.641881	0.905958
6	-3.028393	-1.856271	1.139191
1	-2.757029	-1.336568	2.064972
1	-2.917790	-2.932046	1.294021
8	-2.183505	-1.482581	0.065990
1	-2.212529	-0.497303	-0.031589
1	-0.216934	-3.041519	-2.066017
6	0.097705	-3.542074	-1.143399
1	-0.610091	-4.347360	-0.917040
1	1.086396	-3.979684	-1.299981
8	0.191862	-2.630942	-0.063409
1	-0.676583	-2.164612	0.033797

 Cartesian coordinates of : CY6_4

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	0.122004	0.087798	1.406482
6	0.303947	-0.908208	1.830585
1	0.915714	-0.804655	2.731879
1	-0.656215	-1.353453	2.104070
8	0.926644	-1.775124	0.891982
1	1.797315	-1.376553	0.667607
1	-1.941292	-3.417213	0.295062
6	-1.682130	-3.223660	-0.753532
1	-1.086204	-4.061391	-1.131055
1	-2.602965	-3.160646	-1.337729
8	-0.989069	-1.997658	-0.901785
1	-0.191470	-1.996303	-0.314113
1	-2.970736	-0.840909	1.286173
6	-3.370086	-0.196983	0.492890
1	-4.143646	-0.745092	-0.056967
1	-3.827554	0.680315	0.955918
8	-2.346461	0.251312	-0.377314
1	-1.835209	-0.537983	-0.676698
1	4.921750	0.543467	-0.009232
6	4.261381	-0.309786	-0.198707
1	4.093332	-0.396568	-1.279358
1	4.756209	-1.217666	0.151404
8	3.044615	-0.180170	0.511381

1	2.558770	0.616985	0.194134
1	-2.475988	3.609613	0.517203
6	-1.463325	3.472348	0.121317
1	-1.505262	3.494304	-0.974631
1	-0.839723	4.299339	0.465938
8	-0.887111	2.268046	0.596994
1	-1.423336	1.510468	0.261068
1	0.055088	1.505220	-2.078343
6	0.879752	0.949014	-1.618905
1	0.497957	-0.016539	-1.263056
1	1.644242	0.765069	-2.376888
8	1.478369	1.697009	-0.569343
1	0.744089	2.008724	0.003929

Cartesian coordinates of : CY6_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-0.059720	-0.041448	1.144064
6	-0.115492	-1.019881	1.642408
1	0.780786	-1.154701	2.258066
1	-0.993134	-1.036959	2.293846
8	-0.246848	-2.077910	0.706865
1	0.626297	-2.170172	0.258834
1	-3.541839	-1.875602	0.834306
6	-3.474669	-1.951893	-0.258596
1	-3.500550	-3.009837	-0.540805
1	-4.340721	-1.452600	-0.699042
8	-2.309644	-1.320364	-0.755610
1	-1.515366	-1.694218	-0.297254
1	-2.637330	0.815473	1.451327
6	-2.881103	1.545147	0.668933
1	-3.956992	1.502816	0.464335
1	-2.633911	2.543984	1.036203
8	-2.129473	1.312367	-0.508390
1	-2.203045	0.351004	-0.729973
1	3.895590	-2.137347	-1.452156
6	2.822160	-2.353893	-1.418599
1	2.343762	-1.919056	-2.304146
1	2.685020	-3.436770	-1.441938
8	2.243241	-1.870504	-0.221148
1	2.364497	-0.891573	-0.162722
1	-0.281373	4.200423	-0.747964
6	0.416738	3.425313	-1.083568
1	0.216033	3.196682	-2.136006
1	1.435192	3.810672	-0.995596
8	0.319444	2.268092	-0.272541
1	-0.580039	1.868291	-0.383613
1	2.113441	1.180914	2.060889
6	2.932002	1.167142	1.331428
1	3.384419	2.164390	1.289725
1	3.688211	0.451699	1.662655
8	2.478533	0.760671	0.052575
1	1.670929	1.283503	-0.169079

Cartesian coordinates of : CY6_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	2.466004	-0.087970	2.224487

6	3.097788	-0.435301	1.398702
1	4.043584	0.117641	1.417220
1	3.309470	-1.497946	1.539082
8	2.443026	-0.280104	0.150329
1	2.022668	0.613351	0.135524
1	2.114269	-3.208596	-1.746478
6	1.074464	-2.879488	-1.642562
1	0.855786	-2.147914	-2.431661
1	0.420046	-3.742943	-1.776886
8	0.832413	-2.347631	-0.354836
1	1.436064	-1.582244	-0.196726
1	-0.081094	0.062277	1.244610
6	-0.622648	-0.699321	1.821575
1	0.096572	-1.276705	2.413312
1	-1.314644	-0.196547	2.500860
8	-1.384651	-1.552539	0.980401
1	-0.743173	-2.021216	0.406607
1	1.388191	4.154078	0.142897
6	1.880532	3.235196	-0.192102
1	1.888882	3.214663	-1.288365
1	2.911723	3.239359	0.167480
8	1.238221	2.090727	0.344078
1	0.338080	2.010846	-0.058932
1	-3.952819	0.676314	1.630945
6	-4.202011	0.429452	0.591484
1	-4.864890	-0.442670	0.583021
1	-4.733187	1.274820	0.150057
8	-3.042089	0.196664	-0.183867
1	-2.529265	-0.553206	0.197739
1	-1.101301	0.434629	-2.753197
6	-0.466296	0.566780	-1.871280
1	-0.421979	-0.376848	-1.312564
1	0.545195	0.827135	-2.196702
8	-0.944995	1.627336	-1.055064
1	-1.800551	1.330165	-0.675571

Cartesian coordinates of : CY6_6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-4.059121	-1.079280	0.891530
6	-2.975263	-1.200335	0.999968
1	-2.592510	-0.412847	1.661446
1	-2.776160	-2.169768	1.462674
8	-2.331456	-1.176740	-0.260703
1	-2.363651	-0.249344	-0.601939
1	-0.334900	-3.406385	-1.892418
6	-0.033619	-3.552140	-0.849432
1	-0.744380	-4.230076	-0.363742
1	0.957261	-4.011954	-0.831112
8	0.048039	-2.319462	-0.155174
1	-0.823153	-1.853455	-0.220796
1	2.976740	-2.404112	1.157201
6	2.918036	-1.324518	0.980190
1	2.324845	-0.870065	1.784317
1	3.929122	-0.911417	1.009823
8	2.371157	-1.046730	-0.295411
1	1.482286	-1.474899	-0.343070
1	-3.360090	3.227198	-0.733496
6	-3.383689	2.219017	-0.306346
1	-3.307802	2.295436	0.786067
1	-4.339696	1.755512	-0.559990
8	-2.353864	1.412620	-0.846649

1	-1.477572	1.765979	-0.556732
1	4.360007	1.764474	-0.747785
6	3.446194	2.137596	-0.271898
1	3.494081	1.926197	0.805035
1	3.397510	3.219173	-0.411269
8	2.294127	1.571139	-0.866652
1	2.332245	0.591452	-0.758573
1	0.987751	1.355762	1.876544
6	0.054192	1.208244	1.320496
1	0.015981	0.170029	0.961368
1	-0.783651	1.377588	2.001952
8	-0.055640	2.138527	0.257245
1	0.770845	2.062791	-0.276151

Cartesian coordinates of : BC6_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.969679	-0.391974	-0.684136
6	-3.202995	-0.426264	-1.385421
1	-3.939074	0.235389	-0.915637
1	-3.070837	-0.130877	-2.431475
1	-3.581079	-1.449841	-1.351717
1	-1.612409	0.545534	-0.670511
8	1.555125	1.798855	-0.026369
6	2.334655	2.689831	-0.809154
1	3.373771	2.704146	-0.463920
1	2.312009	2.415726	-1.869394
1	1.913250	3.690543	-0.693634
1	1.865434	0.874933	-0.195353
8	2.350372	-0.673152	-0.623947
6	3.096719	-1.412162	0.327640
1	2.474652	-1.715567	1.179353
1	3.540092	-2.303764	-0.129113
1	3.900795	-0.770595	0.693723
1	1.565542	-1.208183	-0.887380
8	0.111669	-2.117140	-1.028962
6	-0.127493	-3.158126	-0.090953
1	-0.406871	-2.759528	0.891660
1	-0.920506	-3.826152	-0.444869
1	0.794364	-3.736831	0.001682
1	-0.663977	-1.516966	-1.031825
8	-1.413535	-0.720169	2.070862
6	-0.089775	-0.235613	1.975635
1	0.387455	-0.532206	1.031036
1	-0.036996	0.858403	2.052042
1	0.483611	-0.662331	2.803430
1	-1.822737	-0.652750	1.193122
8	-1.035444	1.998949	-0.423961
6	-1.650359	2.622052	0.696492
1	-1.995102	1.876016	1.424120
1	-0.950610	3.301947	1.192504
1	-2.507601	3.198456	0.340696
1	-0.055765	1.923237	-0.271857

Cartesian coordinates of : BC6_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.928610	-2.207976	0.270174

6	1.049353	-2.002015	1.671121
1	0.453033	-1.140626	1.999076
1	0.725869	-2.890443	2.222159
1	2.103056	-1.813181	1.892834
1	-0.044698	-2.210241	0.066164
8	-0.636107	0.854943	-1.644416
6	-0.509879	2.246557	-1.867652
1	-0.102853	2.759484	-0.987407
1	0.124204	2.463631	-2.736822
1	-1.509969	2.637244	-2.072602
1	0.251821	0.482558	-1.510511
8	-1.665408	-1.890801	0.101750
6	-2.429437	-1.831961	-1.095420
1	-3.496581	-1.729736	-0.865649
1	-2.106388	-0.998695	-1.727704
1	-2.282038	-2.774521	-1.626997
1	-1.710017	-1.017201	0.558676
8	0.891488	1.551745	0.964381
6	1.572006	1.737183	2.192419
1	1.975245	0.794018	2.579591
1	2.388990	2.459824	2.087710
1	0.849085	2.125940	2.912153
1	1.451609	1.058666	0.332830
8	-1.630806	0.526992	1.294875
6	-2.654729	1.344316	0.750388
1	-2.508491	2.394816	1.026708
1	-2.683810	1.260274	-0.342034
1	-3.604263	1.003630	1.169086
1	-0.758841	0.900931	1.047763
8	1.915013	-0.138086	-0.895191
6	3.045665	-0.352578	-1.722093
1	3.883326	-0.764273	-1.148622
1	2.807461	-1.034540	-2.545097
1	3.345293	0.610833	-2.139462
1	1.588764	-1.001927	-0.497006

Cartesian coordinates of : CY6_5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-2.370519	-1.280094	-0.352110
6	-2.633172	-2.340328	0.547362
1	-2.881698	-3.261306	0.008992
1	-1.777143	-2.532651	1.206692
1	-3.488307	-2.052538	1.162347
1	-1.525832	-1.447809	-0.833409
8	-2.371536	1.273696	0.442529
6	-2.972707	2.091788	-0.542236
1	-2.413251	2.067865	-1.486205
1	-4.005516	1.783005	-0.735982
1	-2.980079	3.116704	-0.166104
1	-2.427725	0.328453	0.166096
8	2.370484	1.280103	0.352096
6	2.633079	2.340378	-0.547344
1	1.777040	2.532671	-1.206672
1	2.881550	3.261355	-0.008947
1	3.488232	2.052657	-1.162335
1	1.525808	1.447780	0.833427
8	0.035760	1.302118	1.631170
6	-0.025938	-0.083113	1.935275
1	-0.955073	-0.325613	2.463113
1	0.039880	-0.697865	1.025236
1	0.821192	-0.318121	2.584180

1	-0.808121	1.525142	1.181010
8	2.371551	-1.273693	-0.442536
6	2.972852	-2.091753	0.542176
1	4.005760	-1.783107	0.735614
1	2.413645	-2.067625	1.486287
1	2.979967	-3.116717	0.166170
1	2.427743	-0.328444	-0.166123
8	-0.035770	-1.302168	-1.631132
6	0.025911	0.083062	-1.935247
1	-0.039862	0.697817	-1.025207
1	0.955018	0.325561	-2.463134
1	-0.821254	0.318064	-2.584108
1	0.808119	-1.525182	-1.180984

Cartesian coordinates of : BC6_5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.957487	-0.968480	0.038103
6	-2.847800	-2.053915	-0.172157
1	-3.498670	-1.866171	-1.032315
1	-2.299054	-2.987649	-0.333826
1	-3.466245	-2.155574	0.721152
1	-1.338548	-0.890462	-0.734508
8	0.122726	-0.890208	1.845408
6	-0.010605	-0.000758	2.949873
1	-0.545271	0.908558	2.658504
1	-0.534427	-0.493716	3.775661
1	0.996563	0.261103	3.281398
1	-0.720166	-0.955167	1.353206
8	1.906685	1.716096	-0.813524
6	1.588772	2.261993	0.453144
1	0.733365	1.751533	0.916170
1	2.445506	2.223563	1.138947
1	1.318396	3.309353	0.301545
1	2.183465	0.798822	-0.663372
8	-0.122842	-0.890889	-1.845129
6	0.010606	-0.001811	-2.949880
1	0.545372	0.907538	-2.658801
1	0.534381	-0.495097	-3.775502
1	-0.996527	0.260060	-3.281502
1	0.720037	-0.955782	-1.352894
8	-1.906525	1.716526	0.812945
6	-1.588531	2.261984	-0.453892
1	-0.733190	1.751264	-0.916753
1	-2.445266	2.223454	-1.139687
1	-1.318013	3.309355	-0.302621
1	-2.183438	0.799245	0.663080
8	1.957346	-0.968672	-0.037806
6	2.847652	-2.054029	0.172887
1	3.498569	-1.865917	1.032928
1	2.298897	-2.987682	0.334997
1	3.466049	-2.156093	-0.720408
1	1.338425	-0.890317	0.734785

Cartesian coordinates of the methanol heptamer

Cartesian coordinates of : BC7_8

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.514871	3.641780	0.025812
1	-1.602230	2.730599	-0.293793
8	-1.631496	0.840618	-0.084568
1	-1.050888	0.125616	-0.422323
8	-0.144824	-1.334120	-0.783435
1	0.819837	-1.187096	-0.794325
6	-0.259502	3.756504	0.652745
1	0.572031	3.625029	-0.054086
1	-0.191974	4.761267	1.075385
1	-0.137538	3.031771	1.472262
6	-1.849675	0.624616	1.305605
1	-2.446970	-0.281976	1.467445
1	-0.900134	0.533028	1.846868
1	-2.397376	1.490023	1.684850
6	-0.578717	-2.077431	-1.926400
1	-0.275155	-1.575938	-2.849838
1	-0.161469	-3.088467	-1.905210
1	-1.667254	-2.119072	-1.876375
8	2.302394	-0.548909	0.214405
1	1.977647	-1.001517	1.014147
6	2.003137	0.841064	0.323265
1	0.920653	1.009321	0.374767
1	2.478462	1.279664	1.206756
1	2.398368	1.322199	-0.574023
6	5.395479	0.329991	-0.861525
1	6.077886	0.835669	-1.547615
1	4.980440	1.080699	-0.173807
1	5.971401	-0.397379	-0.274833
8	4.393664	-0.287889	-1.638802
1	3.745443	-0.676299	-1.033635
6	-4.912571	-0.764966	-1.338054
1	-5.348083	-1.743395	-1.549448
1	-5.443981	-0.327668	-0.483563
1	-5.061946	-0.121962	-2.213802
8	-3.541552	-0.966574	-1.059178
1	-3.114436	-0.117807	-0.862370
6	-0.116170	-2.176191	3.076903
1	0.593315	-2.009886	3.888363
1	-1.044639	-1.639948	3.305805
1	-0.326860	-3.248373	3.007483
8	0.482438	-1.686774	1.889770
1	-0.090034	-1.828709	1.117632

Cartesian coordinates of : BC7_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	0.976828	-1.950641	-0.890213
1	1.381385	-1.000220	-1.265207
1	-0.079818	-2.022996	-1.167896
1	1.520940	-2.776205	-1.354858
8	1.148611	-2.054877	0.520387
1	0.380135	-1.625613	0.943578
6	-1.825975	-0.373267	2.346195
1	-2.810685	0.052477	2.132878
1	-1.278350	0.322471	2.986693
1	-1.939902	-1.329958	2.859006
8	-1.111568	-0.629051	1.139808
1	-0.849966	0.205320	0.688982
6	-0.518679	1.097171	-1.872635
1	-1.207044	0.248805	-1.938836

1	0.367435	0.894300	-2.482069
1	-1.013604	1.994526	-2.260048
8	-0.144075	1.297753	-0.509482
1	0.844627	1.385338	-0.455202
6	3.116324	2.620302	-0.161718
1	4.152959	2.627692	-0.515065
1	3.105546	2.768862	0.923553
1	2.580551	3.444836	-0.636396
8	2.467452	1.413232	-0.526770
1	2.875851	0.653506	-0.035629
6	4.413775	-1.433510	0.139964
1	4.117877	-1.705716	-0.880977
1	4.638999	-2.345244	0.702327
1	5.315374	-0.819853	0.091974
8	3.407434	-0.673544	0.788768
1	2.592238	-1.227108	0.859652
6	-3.245619	1.848548	0.087078
1	-4.169044	1.743209	0.662617
1	-3.443149	2.527755	-0.752698
1	-2.971217	0.864198	-0.321526
8	-2.257927	2.358164	0.960031
1	-1.412240	2.342958	0.485950
6	-3.868791	-1.952976	-0.831735
1	-4.330919	-2.156794	-1.799547
1	-3.927547	-2.863627	-0.222394
1	-4.444239	-1.159207	-0.335049
8	-2.532792	-1.563460	-1.071821
1	-2.100452	-1.363207	-0.222795

Cartesian coordinates of : BC7_5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-0.546841	0.154065	2.396093
1	-0.278973	1.212923	2.312001
1	-0.279031	-0.218692	3.391653
1	-1.626907	0.058252	2.254448
8	0.087698	-0.612456	1.378808
1	1.033403	-0.391985	1.342797
6	1.314456	-2.687523	-0.874959
1	0.517348	-3.042132	-1.536075
1	0.903685	-2.547700	0.132590
1	2.107833	-3.436793	-0.842115
8	1.881459	-1.479893	-1.372806
1	1.146803	-0.882894	-1.639405
6	-1.199651	0.565430	-2.489333
1	-1.217908	1.627073	-2.760705
1	-2.146761	0.285296	-2.017757
1	-1.073964	-0.027150	-3.397242
8	-0.103082	0.275394	-1.637514
1	0.007293	0.943429	-0.930369
6	-2.765660	1.779819	0.339290
1	-3.063758	2.173718	-0.642772
1	-1.676015	1.627024	0.343107
1	-2.998372	2.537010	1.093029
8	-3.471790	0.606012	0.673897
1	-3.070743	-0.142393	0.196539
6	-2.186744	-2.555042	0.608347
1	-2.188227	-2.194173	1.643727
1	-1.450640	-3.363104	0.518209
1	-3.175188	-2.952870	0.370497
8	-1.918394	-1.509039	-0.309343
1	-1.061617	-1.110018	-0.067954

6	1.170166	3.259994	-0.562150
1	0.246583	3.820461	-0.722063
1	1.872688	3.896190	-0.013522
1	1.601374	3.002603	-1.537200
8	0.833746	2.099350	0.180733
1	1.634695	1.563713	0.342728
6	4.003793	-0.064577	1.062821
1	4.118797	0.608793	1.914074
1	4.190377	-1.090298	1.398477
1	4.740443	0.202076	0.297901
8	2.681319	0.078754	0.570477
1	2.522020	-0.536320	-0.199262

Cartesian coordinates of : BC7_7

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-3.640645	-0.952112	-0.031143
1	-3.212487	-0.089879	0.116092
8	-2.237126	1.445489	-0.004166
1	-1.593047	1.687048	0.682903
8	0.156830	1.687021	1.391759
1	0.309780	0.704993	1.318130
6	-4.991962	-0.736513	-0.372683
1	-5.095469	-0.118875	-1.275166
1	-5.441428	-1.711875	-0.571471
1	-5.551640	-0.258301	0.441529
6	-1.539407	1.383374	-1.237271
1	-1.209200	2.375529	-1.564023
1	-0.661609	0.725934	-1.167927
1	-2.225104	0.970177	-1.980642
6	0.539273	2.153566	2.678941
1	-0.067367	1.687674	3.461867
1	1.596888	1.947451	2.875023
1	0.377294	3.232470	2.703020
8	0.515211	-0.861801	0.892459
1	0.977992	-0.807535	0.018650
6	-0.719067	-1.572667	0.726323
1	-1.157130	-1.386175	-0.258460
1	-0.554348	-2.646764	0.860556
1	-1.423487	-1.222785	1.482552
6	2.305750	-3.315686	0.138928
1	2.770148	-4.292843	-0.007969
1	1.360549	-3.299457	-0.426581
1	2.967092	-2.543378	-0.274816
8	2.092789	-3.154151	1.524186
1	1.676442	-2.289820	1.654194
6	1.307758	-0.905708	-2.688676
1	1.373130	-1.993956	-2.629471
1	0.275867	-0.626791	-2.934347
1	1.974071	-0.557207	-3.484006
8	1.704326	-0.387461	-1.429816
1	1.693948	0.596057	-1.427993
6	2.869920	2.772304	-0.522879
1	3.502952	2.784431	-1.411379
1	2.782537	3.795097	-0.141513
1	3.343204	2.140360	0.238056
8	1.601788	2.261295	-0.908127
1	1.031455	2.220159	-0.114124

Cartesian coordinates of : BC7_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-2.643606	1.432607	0.915093
1	-2.590048	0.591114	0.423070
8	-2.366100	-1.022971	-0.334977
1	-1.561531	-1.091807	-0.884503
8	0.115980	-1.190940	-1.513912
1	0.405329	-0.220885	-1.549351
6	-3.650512	2.235867	0.343200
1	-4.622399	1.726714	0.320740
1	-3.747076	3.134121	0.957221
1	-3.398434	2.545668	-0.681731
6	-2.286282	-2.005913	0.685136
1	-2.468668	-3.009248	0.281032
1	-1.308592	-1.987281	1.182996
1	-3.059496	-1.780691	1.422813
6	0.387523	-1.804058	-2.766772
1	-0.103697	-1.262336	-3.581505
1	1.464837	-1.839325	-2.960392
1	-0.002091	-2.824001	-2.736670
8	1.397660	0.252981	2.064038
1	1.525306	-0.680573	1.812798
6	0.030460	0.573644	1.818927
1	-0.271682	0.277314	0.805725
1	-0.631333	0.088541	2.543251
1	-0.088116	1.654160	1.910977
6	3.805880	2.086683	0.175195
1	4.002563	2.751615	-0.667945
1	4.238230	2.529645	1.078504
1	4.288494	1.121349	-0.017326
8	2.402093	1.952387	0.300804
1	2.177554	1.324234	1.031778
6	-0.400177	2.114696	-1.541628
1	-1.189729	1.655893	-2.144046
1	-0.758119	2.203718	-0.510207
1	-0.179751	3.106695	-1.947841
8	0.747931	1.275659	-1.629210
1	1.423609	1.564630	-0.960703
6	1.210604	-3.567742	0.879969
1	1.613390	-3.844305	1.855777
1	0.179431	-3.936966	0.810936
1	1.814908	-4.051950	0.103727
8	1.267104	-2.159216	0.775594
1	0.893635	-1.869157	-0.082720

Cartesian coordinates of : BL7_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.452245	0.521155	2.289134
1	-2.341654	0.530524	1.893440
8	-3.599564	0.646610	0.526734
1	-3.098540	0.472115	-0.295912
8	-2.128460	0.023335	-1.697965
1	-1.853429	-0.905974	-1.644483
6	-0.621056	1.271696	1.428318
1	-1.031010	2.271880	1.229039
1	0.346820	1.392010	1.922478
1	-0.454739	0.757673	0.469678
6	-4.366635	1.825260	0.365808
1	-3.730355	2.704335	0.202112

1	-5.068710	1.733444	-0.470562
1	-4.936584	1.976223	1.284278
6	-1.099130	0.813563	-2.278092
1	-0.117018	0.552146	-1.871498
1	-1.084819	0.698781	-3.366941
1	-1.314894	1.857250	-2.037544
8	-1.554723	-2.556756	-0.753012
1	-1.878104	-3.390629	-1.110846
6	-2.175749	-2.284912	0.515764
1	-3.240963	-2.072764	0.391092
1	-2.028548	-3.122040	1.203301
1	-1.685843	-1.398415	0.924798
6	1.279924	-1.491251	1.015732
1	2.204823	-0.934688	1.186903
1	0.517632	-1.178411	1.739380
1	1.497783	-2.556758	1.142558
8	0.856776	-1.214804	-0.320086
1	0.167520	-1.842910	-0.585163
6	2.304662	1.708657	-0.618612
1	3.008582	2.496048	-0.896943
1	1.285856	2.074492	-0.799449
1	2.419540	1.496265	0.453118
8	2.605566	0.571981	-1.408113
1	1.957311	-0.127276	-1.196189
6	5.558979	0.475200	0.591311
1	6.067820	0.206979	1.519642
1	6.280198	0.396405	-0.232226
1	5.230975	1.521409	0.669320
8	4.472674	-0.409715	0.430561
1	3.994189	-0.171829	-0.382784

Cartesian coordinates of : BC7_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	1.086222	3.514731	1.895513
6	0.052822	3.189770	1.735797
1	-0.386433	2.908841	2.699046
1	-0.518000	4.019550	1.315096
8	-0.002625	2.109414	0.814609
1	0.439934	1.307900	1.219665
1	-0.552884	-0.645219	-2.395338
6	0.215219	-0.859681	-1.645230
1	1.198063	-0.728804	-2.102081
1	0.118041	-0.140342	-0.820111
8	0.115303	-2.200884	-1.181572
1	-0.802198	-2.308404	-0.864208
1	-4.395628	-1.618430	0.274378
6	-3.419682	-2.062936	0.498126
1	-3.159227	-1.835256	1.540453
1	-3.495906	-3.146283	0.387131
8	-2.428408	-1.604411	-0.399651
1	-2.383248	-0.621604	-0.361424
1	-1.206791	1.706652	-2.011196
6	-2.229462	1.680109	-1.616924
1	-2.635540	2.697175	-1.592025
1	-2.848747	1.071641	-2.280031
8	-2.272166	1.087475	-0.324340
1	-1.546664	1.474384	0.206468
6	2.570661	1.514234	-1.108831
1	3.174351	1.156556	-1.946968
1	3.146158	2.279726	-0.571720
1	2.391966	0.668941	-0.425998

8	1.367511	2.029154	-1.636394
1	0.807164	2.265614	-0.878802
6	-0.286197	-0.776118	2.240153
1	-0.084172	-1.536063	3.001125
1	-0.689096	-1.256820	1.340052
1	-1.031755	-0.075625	2.627079
8	0.892392	-0.034092	1.946009
1	1.509766	-0.645847	1.480330
6	3.334857	-2.156021	-0.044848
1	3.374915	-1.604472	-0.992643
1	3.542356	-3.213434	-0.240082
1	4.106881	-1.764543	0.620628
8	2.084578	-1.994214	0.599553
1	1.358484	-2.246226	-0.019495

Cartesian coordinates of : BC7_6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-1.292980	0.125393	2.084717
6	-0.239062	0.084610	1.798988
1	-0.138358	0.412928	0.756423
1	0.324753	0.768301	2.435634
8	0.299175	-1.228181	1.980747
1	-0.260962	-1.832852	1.463162
1	-1.055573	-3.969645	-1.062456
6	-1.789094	-3.183486	-0.857324
1	-2.240514	-2.857618	-1.801371
1	-2.571213	-3.589758	-0.213494
8	-1.191562	-2.090080	-0.175378
1	-0.445418	-1.713938	-0.719762
1	0.740371	0.561689	-3.005138
6	0.192051	0.331059	-2.085809
1	0.276901	1.171374	-1.390216
1	-0.860846	0.165309	-2.325720
8	0.693825	-0.871340	-1.500314
1	1.470620	-0.705307	-0.933666
1	3.423230	-2.761652	0.606113
6	3.658585	-1.714553	0.824728
1	4.027299	-1.634953	1.852437
1	4.443354	-1.382080	0.142512
8	2.529136	-0.881339	0.620676
1	1.786925	-1.131747	1.230069
6	3.081122	1.827307	-1.186929
1	2.704900	2.603997	-1.857044
1	4.109904	2.082667	-0.903490
1	3.097077	0.874941	-1.737701
8	2.222665	1.775252	-0.067356
1	2.452508	0.983196	0.444977
6	-0.898996	3.333966	0.334128
1	-1.168640	3.745767	-0.648286
1	0.083594	2.848472	0.260485
1	-0.817724	4.165845	1.037672
8	-1.895181	2.461277	0.829926
1	-2.049990	1.741871	0.194499
6	-3.992304	0.128781	0.185688
1	-3.820613	0.138693	1.268935
1	-4.581436	-0.756610	-0.080664
1	-4.559563	1.022402	-0.078881
8	-2.770860	0.172034	-0.536046
1	-2.249010	-0.623762	-0.318606

Cartesian coordinates of : DC7

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-2.790752	-2.941273	0.015453
6	-2.796496	-2.008369	-0.559323
1	-2.125851	-2.120280	-1.421590
1	-3.809240	-1.820587	-0.921339
8	-2.421262	-0.913356	0.251399
1	-1.506339	-1.058224	0.557150
1	-2.006919	2.223365	1.367680
6	-2.668271	2.476666	0.532307
1	-3.710964	2.410558	0.861723
1	-2.472062	3.501000	0.206912
8	-2.436595	1.619279	-0.574208
1	-2.494994	0.682023	-0.265234
1	0.083989	0.632968	3.524262
6	0.122438	-0.129997	2.737326
1	1.127241	-0.568904	2.705395
1	-0.592973	-0.919314	2.976525
8	-0.250590	0.405075	1.476872
1	0.424695	1.038949	1.184691
1	-0.922505	-0.102152	-2.685621
6	-0.051516	0.173890	-2.080900
1	-0.025233	-0.454374	-1.179596
1	0.851778	0.000739	-2.671519
8	-0.095340	1.555142	-1.745664
1	-0.978687	1.713660	-1.310807
1	1.940339	3.831318	0.181451
6	2.544383	2.929570	0.034468
1	3.103160	3.024055	-0.903010
1	3.253474	2.844477	0.860334
8	1.733755	1.767742	0.032333
1	1.055497	1.795687	-0.712288
6	0.392235	-3.319236	-0.386556
1	-0.450809	-4.006504	-0.488625
1	0.629692	-2.911488	-1.380520
1	1.258004	-3.887261	-0.023684
8	0.018845	-2.304329	0.519983
1	0.781020	-1.699808	0.617879
6	3.293847	-1.315257	-0.578720
1	3.481207	-2.374225	-0.389210
1	2.881241	-1.207838	-1.590303
1	4.248977	-0.780031	-0.526747
8	2.389612	-0.853982	0.407180
1	2.239895	0.105289	0.275866

Cartesian coordinates of : BL7_1-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	2.494795	-2.393403	0.277720
1	2.839406	-1.482931	0.355041
8	3.515614	0.164400	0.503827
1	2.905030	0.917890	0.356859
8	1.772446	2.242025	0.415580
1	0.875885	1.940550	0.651492
6	3.306740	-3.088621	-0.640921
1	4.353209	-3.138450	-0.311623
1	2.923015	-4.108472	-0.719745
1	3.281353	-2.632016	-1.640834

6	4.164625	0.356538	1.748367
1	4.822211	1.232549	1.722116
1	3.442880	0.479565	2.565159
1	4.768829	-0.531423	1.946954
6	1.704094	3.199523	-0.632675
1	1.147511	2.809513	-1.492408
1	1.238887	4.127445	-0.283089
1	2.729573	3.417193	-0.937706
8	-0.478242	0.735630	0.800560
1	-1.454283	0.658473	0.735045
6	0.042762	-0.517022	1.243125
1	1.119733	-0.397794	1.380123
1	-0.408318	-0.812029	2.195371
1	-0.118126	-1.305115	0.499102
8	-3.013074	0.081456	0.253568
1	-3.804716	-0.161607	0.760762
6	-2.936071	-0.745462	-0.901340
1	-2.863406	-1.804158	-0.627738
1	-3.811668	-0.600529	-1.545103
1	-2.040023	-0.456382	-1.455938
8	-5.588167	-0.577164	0.991773
1	-6.067452	-1.316157	1.379156
6	-6.387273	0.077524	0.013384
1	-6.671626	-0.604846	-0.794287
1	-7.284977	0.514704	0.461211
1	-5.773053	0.879180	-0.400147
6	1.419317	-0.017848	-2.088776
1	1.529225	-0.351893	-3.123065
1	2.221585	0.701251	-1.871124
1	1.537113	-0.882294	-1.423260
8	0.136390	0.571238	-1.968460
1	-0.041053	0.726549	-1.025867

Cartesian coordinates of : BL7_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	5.950131	-0.818138	-0.134233
1	5.160570	-0.803068	-0.699451
8	3.442494	-0.225084	-1.193441
1	2.571248	-0.632077	-1.056537
8	1.003540	-0.756495	-0.044170
1	0.056966	-1.016943	-0.165665
6	5.506913	-0.749198	1.198219
1	4.933732	-1.640282	1.493026
1	6.388889	-0.684005	1.839856
1	4.884132	0.139724	1.382721
6	3.335660	1.153725	-0.884806
1	2.719828	1.686682	-1.617521
1	2.903478	1.311828	0.113608
1	4.346523	1.567949	-0.896526
6	1.428067	-1.052594	1.278455
1	0.817823	-0.524312	2.020306
1	1.385356	-2.128827	1.475691
1	2.466180	-0.722291	1.370462
8	-1.590394	-1.028443	-0.490511
1	-2.048407	-0.352843	0.062650
6	-1.776041	-0.642894	-1.847886
1	-1.302748	-1.399435	-2.476370
1	-2.844101	-0.597871	-2.095183
1	-1.320101	0.334333	-2.045631
8	-3.111921	0.821358	0.717352
1	-3.973113	0.396431	0.875464

6	-3.305142	1.944639	-0.138863
1	-3.989533	1.698955	-0.958978
1	-3.708395	2.793657	0.423567
1	-2.329154	2.210692	-0.550232
8	-5.361590	-0.744400	0.533912
1	-6.262144	-0.796974	0.868898
6	-4.902514	-2.038446	0.146781
1	-4.969508	-2.749014	0.976431
1	-5.471152	-2.416049	-0.708731
1	-3.853763	-1.929364	-0.137215
6	-0.125980	2.243209	1.005054
1	-0.549543	3.249952	1.042353
1	-0.793813	1.569054	1.558279
1	0.855185	2.268552	1.497929
8	-0.019397	1.874530	-0.357056
1	0.456889	1.028281	-0.389747

Cartesian coordinates of : BC7_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	0.427341	-2.361012	-1.754637
6	0.938898	-2.818997	-0.901940
1	0.812144	-3.905329	-0.946568
1	2.002899	-2.576893	-0.965458
8	0.439554	-2.308510	0.329353
1	-0.551177	-2.263808	0.282569
1	3.312720	-1.504502	1.701941
6	2.694020	-0.653692	2.011197
1	2.132905	-0.928711	2.909890
1	3.345649	0.191699	2.244567
8	1.820713	-0.259691	0.963057
1	1.202608	-1.028513	0.749452
1	1.924067	1.889899	-1.178378
6	1.677352	2.667311	-0.446039
1	2.600757	3.029061	0.021287
1	1.199243	3.502167	-0.963104
8	0.770883	2.188439	0.536300
1	1.086835	1.309969	0.837453
1	-4.013398	-3.044934	0.427716
6	-3.039594	-2.876455	0.900719
1	-3.189469	-2.325638	1.836087
1	-2.590158	-3.845114	1.129605
8	-2.164717	-2.187413	0.025950
1	-2.530835	-1.283190	-0.150033
1	-1.910219	4.332018	0.698508
6	-2.331236	3.342540	0.908067
1	-2.109402	3.073912	1.946919
1	-3.415048	3.389335	0.780488
8	-1.830246	2.375685	0.002078
1	-0.861284	2.266357	0.156919
1	-3.086084	0.566139	-2.435430
6	-3.843042	0.361351	-1.670284
1	-4.565109	1.185189	-1.654209
1	-4.368858	-0.559637	-1.932194
8	-3.255602	0.177512	-0.393915
1	-2.705790	0.972265	-0.183152
6	4.635863	0.291912	-1.009366
1	5.316864	0.166309	-1.853659
1	4.483948	1.368752	-0.849660
1	5.117247	-0.128073	-0.115278
8	3.433897	-0.373025	-1.327678
1	2.822171	-0.275514	-0.576925

Cartesian coordinates of : CY7_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.361520	2.242534	-0.867500
1	2.015512	1.537837	-0.637338
8	3.125076	0.416398	-0.078421
1	2.753687	-0.454400	0.211420
8	2.077295	-1.847362	0.823147
1	1.153426	-1.924099	0.476742
6	1.275134	2.386755	-2.271657
1	0.830091	1.502043	-2.745877
1	0.639785	3.249616	-2.481068
1	2.262458	2.564154	-2.711404
6	3.837862	0.977804	1.012753
1	3.212382	1.034240	1.911554
1	4.735023	0.391108	1.238298
1	4.140056	1.988339	0.730265
6	2.781880	-3.034300	0.496723
1	2.394468	-3.887177	1.063616
1	2.715690	-3.256833	-0.574508
1	3.830665	-2.884685	0.762295
8	-0.196423	-1.888545	-0.489380
1	-1.135558	-1.876505	-0.179893
6	-0.039765	-0.853695	-1.445766
1	1.032996	-0.671023	-1.573418
1	-0.462704	-1.144398	-2.414902
1	-0.509615	0.080239	-1.110576
8	-2.774252	-1.600562	0.049459
1	-2.956277	-0.638203	0.190730
6	-3.526854	-2.039751	-1.068649
1	-4.593140	-2.102437	-0.824938
1	-3.397538	-1.369565	-1.926971
1	-3.172125	-3.036208	-1.341603
8	-3.146721	1.013152	0.249706
1	-2.247367	1.417380	0.324637
6	-3.963662	1.540969	1.280950
1	-3.511805	1.390088	2.268597
1	-4.140937	2.611013	1.130785
1	-4.921961	1.018454	1.249120
8	-0.709316	1.857293	0.777985
1	-0.023544	2.155037	0.137686
6	-0.129038	0.857291	1.602450
1	0.665745	0.318279	1.073646
1	0.285364	1.298576	2.515396
1	-0.905548	0.135434	1.876920

Cartesian coordinates of : CY7_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-4.652947	-1.791330	-0.535771
6	-3.762946	-2.088284	0.031025
1	-3.877849	-1.755288	1.069675
1	-3.690560	-3.178709	0.014849
8	-2.585492	-1.566980	-0.556069
1	-2.598187	-0.581807	-0.466493
1	-1.524347	-3.567397	1.957878
6	-0.711695	-2.871630	1.717309

1	-0.978009	-1.872459	2.082391
1	0.193873	-3.203065	2.230725
8	-0.446027	-2.860549	0.326392
1	-1.186165	-2.380836	-0.119395
1	1.889295	-3.027297	-2.193052
6	2.484632	-3.156960	-1.282110
1	2.413946	-4.200328	-0.956044
1	3.528663	-2.930855	-1.511488
8	2.066182	-2.275675	-0.256480
1	1.113537	-2.446708	-0.050598
1	-0.492572	4.452889	1.430226
6	-0.982748	3.479721	1.547586
1	-0.532991	2.957471	2.399566
1	-2.042660	3.644388	1.755434
8	-0.887527	2.716196	0.359919
1	0.066281	2.522159	0.182023
1	4.917738	-0.618665	0.404666
6	4.119024	0.030257	0.781532
1	3.747409	-0.377467	1.728241
1	4.533873	1.024401	0.965097
8	3.079851	0.162691	-0.171073
1	2.631303	-0.713431	-0.267555
1	2.202988	2.730640	-1.990450
6	2.269790	3.218213	-1.011578
1	3.320462	3.447684	-0.800278
1	1.707247	4.154384	-1.045142
8	1.710478	2.412481	0.009706
1	2.151101	1.526663	-0.012272
1	-2.802754	1.890590	-2.151583
6	-3.492821	1.704853	-1.321041
1	-3.922839	2.658804	-0.996172
1	-4.300437	1.058484	-1.672944
8	-2.847265	1.047057	-0.245370
1	-2.076424	1.598290	0.035925

 Cartesian coordinates of : CY7_2

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-0.889282	4.447066	-0.846180
6	-1.306976	3.734773	-0.126393
1	-0.869021	3.927880	0.860283
1	-2.386344	3.887133	-0.068148
8	-1.079327	2.398103	-0.543129
1	-0.102018	2.248042	-0.577254
1	0.084140	1.157689	1.856670
6	-0.603793	0.302828	1.866024
1	-0.140277	-0.520540	1.303221
1	-0.754785	-0.018557	2.899094
8	-1.865622	0.661919	1.325272
1	-1.698125	1.284089	0.577445
1	-4.178981	-0.722236	-0.923305
6	-4.160222	-1.527785	-0.178349
1	-4.951584	-1.350103	0.557768
1	-4.358786	-2.474933	-0.683219
8	-2.895279	-1.630222	0.449450
1	-2.648726	-0.760577	0.846568
1	3.687024	-0.663968	2.390032
6	2.821103	-0.033215	2.160768
1	1.954554	-0.409299	2.718470
1	3.034723	0.987296	2.487148
8	2.569045	-0.003858	0.768206
1	2.218461	-0.888211	0.481980

1	0.102820	-0.053827	-0.995040
6	-0.608017	-0.655321	-1.579720
1	-1.571495	-0.135668	-1.581358
1	-0.244821	-0.728975	-2.608579
8	-0.728464	-1.964857	-1.042003
1	-1.540400	-1.992284	-0.479418
1	2.300488	-2.725181	-1.839515
6	2.393922	-3.104748	-0.814978
1	2.104008	-4.160400	-0.798359
1	3.437400	-3.021296	-0.503284
8	1.606770	-2.349851	0.090705
1	0.679384	-2.301727	-0.259815
1	2.092683	1.015751	-2.245832
6	2.206190	2.002011	-1.778530
1	3.273138	2.223994	-1.672866
1	1.751617	2.752387	-2.429267
8	1.550032	2.058747	-0.523509
1	1.903719	1.325349	0.039900

Cartesian coordinates of : CY7_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-1.855116	3.734765	-1.892273
6	-2.429286	3.000755	-1.316855
1	-2.671141	3.428077	-0.336094
1	-3.359582	2.792011	-1.850010
8	-1.718167	1.782201	-1.193570
1	-0.914992	1.919462	-0.630487
1	-4.691181	0.899908	0.380747
6	-3.829049	0.424162	0.861946
1	-3.256255	1.188490	1.402767
1	-4.193029	-0.312701	1.581615
8	-3.023833	-0.251074	-0.088712
1	-2.546142	0.434641	-0.617380
1	-2.306727	-3.556650	-0.427067
6	-2.148581	-3.410473	0.648426
1	-3.117317	-3.450669	1.158691
1	-1.521211	-4.220447	1.025179
8	-1.481938	-2.187188	0.914443
1	-2.040332	-1.451255	0.566852
1	4.646110	1.845114	1.219589
6	3.560148	1.906387	1.351021
1	3.257612	1.201222	2.134759
1	3.303312	2.919824	1.667094
8	2.884286	1.647127	0.131886
1	2.991601	0.688466	-0.076485
1	0.102754	-0.042801	-1.189863
6	0.115958	-1.065284	-1.586484
1	-0.907801	-1.354718	-1.850080
1	0.729205	-1.082740	-2.490042
8	0.680004	-1.981629	-0.657016
1	0.007679	-2.123392	0.048612
1	3.689377	-1.651651	-2.003247
6	4.014955	-1.649784	-0.956303
1	4.176829	-2.683280	-0.631866
1	4.960943	-1.108587	-0.885451
8	3.076916	-0.996231	-0.120542
1	2.193055	-1.426916	-0.230181
1	0.295207	1.166349	2.459545
6	0.112017	0.843215	1.428607
1	0.788344	0.013381	1.188410
1	-0.916398	0.477300	1.351447

```
8      0.275886      1.923860      0.521460
1      1.233000      1.966396      0.279466
```

Cartesian coordinates of the methanol octamer

Cartesian coordinates of : BL8_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	0.436719	2.302831	2.593685
1	1.412933	2.782826	2.722787
1	0.552132	1.216564	2.680956
1	-0.232121	2.653903	3.380250
8	-0.147319	2.667465	1.350944
1	0.375851	2.307940	0.613551
6	0.288414	-0.074457	-0.464528
1	-0.289859	-0.795658	-1.050954
1	-0.087979	-0.069579	0.565147
1	1.331883	-0.393814	-0.463949
8	0.235382	1.237100	-1.041662
1	-0.691152	1.516172	-1.126140
6	-3.152615	3.221832	-0.479219
1	-2.559890	4.111389	-0.712878
1	-3.844559	3.449031	0.337389
1	-3.728045	2.936386	-1.361394
8	-2.310673	2.124272	-0.146291
1	-1.717574	2.364329	0.598295
6	1.233079	-3.295391	-0.290213
1	0.394222	-3.278024	-0.998618
1	1.458734	-4.342328	-0.047932
1	2.104702	-2.846149	-0.774932
8	0.935064	-2.547717	0.875257
1	-0.016703	-2.639820	1.046692
6	-2.840079	-3.533216	1.061779
1	-3.494448	-3.760712	0.211510
1	-3.453463	-3.158335	1.889431
1	-2.350104	-4.455706	1.379717
8	-1.828531	-2.612606	0.703849
1	-2.244532	-1.791010	0.374878
6	-3.075046	-0.574006	-1.835665
1	-2.219347	-0.031769	-2.257812
1	-3.998267	-0.181967	-2.276971
1	-2.978521	-1.629215	-2.101516
8	-3.105346	-0.486946	-0.421404
1	-2.938539	0.438228	-0.162279
6	3.932516	-1.223330	0.285256
1	2.995282	-1.118353	0.850935
1	4.674487	-0.509368	0.667599
1	4.311220	-2.232742	0.464586
8	3.734736	-1.085175	-1.108060
1	3.563930	-0.150594	-1.309931
6	2.984445	2.118526	0.064010
1	2.484320	1.415395	0.748347
1	2.522066	3.109838	0.158733
1	4.031327	2.196485	0.363572
8	2.956619	1.653803	-1.270822
1	2.027950	1.628352	-1.554184

Cartesian coordinates of : Ca8

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-0.723285	-0.855868	2.268363
1	-0.267640	-1.851344	2.188027
1	-1.805399	-0.946639	2.101725
1	-0.552342	-0.475549	3.277899
8	-0.139724	0.059168	1.365275
1	-0.428539	-0.146744	0.461341
6	-0.118877	0.993414	-2.456889
1	0.570633	0.924462	-3.306713
1	-0.192839	2.039268	-2.134105
1	-1.108578	0.660410	-2.775259
8	0.285268	0.146177	-1.395850
1	1.140315	0.439488	-1.030066
6	3.861002	0.721001	0.100909
1	4.214519	0.019694	-0.665054
1	4.397623	0.526627	1.036217
1	4.091115	1.737934	-0.226598
8	2.461117	0.631763	0.285301
1	2.238328	-0.263154	0.636328
6	-3.716221	-0.814781	-0.419799
1	-4.368452	-0.136123	-0.982714
1	-3.928278	-0.697593	0.652481
1	-3.956388	-1.840864	-0.709671
8	-2.353599	-0.582557	-0.711181
1	-2.179637	0.385328	-0.626832
6	-2.678368	2.206850	1.060978
1	-2.522112	3.220886	1.443108
1	-2.299690	1.488136	1.798415
1	-3.749466	2.048615	0.912540
8	-2.037195	2.033473	-0.193586
1	-1.087913	2.251022	-0.057499
6	1.489027	3.379129	-0.174092
1	1.875290	2.802112	-1.024596
1	2.327642	3.639544	0.481676
1	1.033386	4.299018	-0.546531
8	0.491824	2.668540	0.530465
1	0.868157	1.841125	0.880435
6	-1.350945	-3.388226	-0.075749
1	-1.933250	-3.796747	-0.910012
1	-2.029621	-2.875527	0.615803
1	-0.864878	-4.213546	0.449674
8	-0.334230	-2.522279	-0.540369
1	-0.746405	-1.734100	-0.937856
6	2.857162	-2.622934	-0.288437
1	2.599376	-3.679848	-0.415661
1	3.888443	-2.554139	0.066249
1	2.775850	-2.124019	-1.263076
8	2.024445	-2.005414	0.678562
1	1.100534	-2.130213	0.369681

Cartesian coordinates of : DC8_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	3.587318	-0.010905	1.125562
1	3.195238	-0.771725	0.640108
8	-2.475551	-2.063625	0.147998
1	-3.091197	-1.326408	-0.090405
8	-3.852285	0.143622	-0.422897
1	-3.153825	0.517043	-1.004053
6	4.980062	0.032539	0.876465

1	5.196829	0.154707	-0.192696
1	5.387892	0.890686	1.413775
1	5.475894	-0.874565	1.239343
6	-2.959828	-2.742318	1.293707
1	-3.023823	-2.074533	2.162210
1	-3.946122	-3.178792	1.104078
1	-2.260646	-3.549058	1.523234
6	-3.860275	0.902209	0.780570
1	-2.843319	1.047380	1.167441
1	-4.327541	1.880446	0.621427
1	-4.455569	0.353355	1.514226
8	-1.521016	0.833075	-1.629482
1	-1.008162	0.871233	-0.796352
6	-1.091906	-0.247432	-2.440153
1	-1.589156	-0.143528	-3.406641
1	-0.007629	-0.219474	-2.599809
1	-1.361210	-1.218010	-2.005372
8	-0.690665	2.031429	0.707497
1	0.286858	2.027605	0.786599
6	-1.085327	3.310388	0.242082
1	-0.836380	4.093342	0.966955
1	-0.620333	3.551257	-0.721737
1	-2.168715	3.291366	0.101058
8	-0.064867	-0.945510	0.316692
1	-0.928540	-1.415436	0.210681
6	0.116107	-0.676378	1.704517
1	-0.689184	-0.038780	2.081581
1	0.164701	-1.606975	2.282497
1	1.064704	-0.145053	1.820268
8	2.329423	-1.947778	-0.288930
1	1.385986	-1.687489	-0.166570
6	2.606058	-2.119064	-1.665781
1	1.910275	-2.830329	-2.124438
1	2.554858	-1.168681	-2.213959
1	3.618399	-2.518487	-1.755453
6	1.881770	1.523341	-1.014750
1	1.217760	2.185905	-1.576664
1	2.859083	1.499199	-1.512245
1	1.448514	0.514934	-1.012237
8	1.990607	2.029857	0.306314
1	2.600695	1.427843	0.781183

Cartesian coordinates of : BDC8

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-0.432810	-1.877476	-0.055606
1	0.290809	-1.331759	0.308848
8	-4.045700	0.236083	1.473262
1	-3.706816	0.971021	0.940215
8	2.191902	-1.310377	0.751639
1	2.523896	-0.390595	0.733440
6	0.113977	-3.100373	-0.511052
1	0.544517	-3.668543	0.320393
1	-0.698407	-3.682034	-0.952022
1	0.886769	-2.935935	-1.272427
6	-2.935307	-0.370500	2.100853
1	-2.215293	-0.781059	1.376719
1	-2.407890	0.329876	2.764167
1	-3.312891	-1.194842	2.710118
6	3.250542	-2.124492	0.285938
1	3.472921	-1.934021	-0.773564
1	4.164501	-1.965236	0.870827

1	2.950227	-3.168529	0.396392
8	3.426216	1.112139	0.374821
1	2.915181	1.454424	-0.389591
6	4.818875	1.184678	0.133647
1	5.326948	0.791976	1.016628
1	5.112525	0.584579	-0.736511
1	5.141585	2.219848	-0.021395
8	1.423724	1.627376	-1.330512
1	0.930612	1.506637	-0.490113
6	1.144391	0.481819	-2.124644
1	1.528624	-0.432897	-1.651179
1	0.066095	0.363196	-2.287202
1	1.633867	0.620836	-3.090486
8	0.099274	0.812167	0.861327
1	-0.834750	1.080156	0.722269
6	0.469420	0.892303	2.232031
1	0.006174	1.758259	2.716267
1	0.178936	-0.021851	2.761651
1	1.555103	1.001468	2.276513
8	-2.255257	1.634401	-0.174263
1	-2.284223	0.848853	-0.790324
6	-1.946346	2.813391	-0.907168
1	-0.973562	2.727457	-1.405838
1	-2.719459	3.023198	-1.653439
1	-1.907460	3.643578	-0.199402
6	-3.424753	-1.304231	-1.475027
1	-4.152569	-0.782250	-2.099109
1	-3.292287	-2.318165	-1.867269
1	-3.805858	-1.344242	-0.448977
8	-2.201216	-0.577205	-1.545898
1	-1.511683	-1.065845	-1.031231

Cartesian coordinates of : BC8_11

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-2.859930	0.983107	-0.283119
1	-2.077951	1.504631	-0.538346
8	2.337662	1.076680	1.392445
1	1.848592	0.250166	1.230424
8	2.062298	-1.632094	0.636039
1	1.140121	-1.903305	0.450023
6	-3.852703	1.838952	0.249509
1	-4.216826	2.548384	-0.502299
1	-4.687962	1.212775	0.570011
1	-3.484333	2.397537	1.119232
6	3.706519	0.744117	1.428483
1	3.924665	0.002563	2.206519
1	4.053466	0.337801	0.466034
1	4.266920	1.657316	1.644269
6	2.929290	-2.632708	0.150517
1	2.731466	-3.604175	0.617964
1	2.846616	-2.750647	-0.939597
1	3.952904	-2.331672	0.389694
8	-0.255913	-2.634341	-0.464278
1	-1.048678	-2.388215	0.059697
6	-0.290347	-1.841785	-1.630227
1	0.617802	-2.055691	-2.205018
1	-1.160298	-2.078781	-2.255852
1	-0.314722	-0.769602	-1.384509
8	-0.262461	-0.052196	0.985048
1	-0.251671	0.738835	0.418127
6	-0.712708	0.327584	2.274895

1	-0.007222	1.017887	2.753260
1	-1.707637	0.791550	2.227182
1	-0.786391	-0.582101	2.873356
8	-0.392711	2.180791	-0.714117
1	0.176236	1.905213	-1.465201
6	0.232295	3.243242	0.009339
1	1.135590	2.883813	0.513751
1	0.468705	4.076954	-0.658918
1	-0.484701	3.586838	0.758375
8	1.324712	1.217003	-2.581307
1	0.995245	0.502474	-3.137631
6	2.427790	0.743147	-1.798524
1	2.138702	-0.096373	-1.155230
1	3.263878	0.461299	-2.446344
1	2.729620	1.571043	-1.155293
6	-3.797774	-2.019514	-0.086565
1	-3.863841	-3.109518	-0.090941
1	-4.670421	-1.620466	0.445011
1	-3.817759	-1.654748	-1.120166
8	-2.593331	-1.665260	0.565711
1	-2.446886	-0.709516	0.436483

Cartesian coordinates of : BL8_6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.901831	1.315445	-1.465580
1	0.844304	0.403881	-1.114075
8	-3.013177	-0.395415	2.008173
1	-3.425478	-0.191133	1.158048
8	4.469721	-0.650290	1.125901
1	3.648156	-0.770499	1.629937
6	0.735796	1.258060	-2.870673
1	-0.078682	0.577855	-3.151601
1	0.488737	2.262283	-3.221736
1	1.658149	0.931483	-3.365567
6	-1.688425	0.107114	1.982638
1	-1.047451	-0.473634	1.300057
1	-1.650366	1.162468	1.684590
1	-1.274899	0.004147	2.988052
6	4.155035	-0.882525	-0.224376
1	3.860899	-1.926628	-0.407308
1	3.344512	-0.225679	-0.581683
1	5.048546	-0.670460	-0.816304
8	1.735301	-0.593452	1.737242
1	1.373415	-0.978294	0.920930
6	1.639200	0.820837	1.642118
1	1.875104	1.228300	2.627378
1	2.353017	1.228795	0.913676
1	0.628087	1.141134	1.361790
8	0.573662	-1.298113	-0.755352
1	-0.364694	-1.600400	-0.617184
6	1.172181	-2.145397	-1.731477
1	1.523255	-3.077113	-1.275841
1	0.458459	-2.378863	-2.527643
1	2.028366	-1.619252	-2.160636
8	-1.833163	-2.264216	-0.496866
1	-2.603883	-1.676485	-0.580672
6	-1.973728	-3.136344	0.626880
1	-2.307777	-2.584010	1.509139
1	-2.678606	-3.940643	0.395887
1	-0.990515	-3.572549	0.816135
8	-3.522645	-0.063380	-0.818352

1	-4.391707	0.143556	-1.178486
6	-2.579724	0.952867	-1.193138
1	-2.589607	1.111594	-2.275499
1	-2.768190	1.890508	-0.666120
1	-1.593495	0.590079	-0.893837
6	0.048242	3.971581	0.744982
1	-0.644673	4.525964	1.381356
1	0.837999	3.548921	1.380900
1	0.508727	4.673531	0.038704
8	-0.690830	2.966224	0.083403
1	-0.086770	2.449562	-0.482652

Cartesian coordinates of : BC8_12

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-0.348064	-1.730458	1.786077
1	-1.304553	-1.874818	1.792438
8	1.617726	-1.281099	-2.402132
1	1.568214	-1.948914	-1.696756
8	2.806904	1.202840	1.203153
1	2.063926	1.642421	0.749092
6	-0.127247	-0.350867	1.510020
1	-0.561687	0.284280	2.291694
1	0.950231	-0.179597	1.488411
1	-0.546361	-0.070175	0.535344
6	1.401520	-0.030610	-1.789606
1	0.327835	0.187909	-1.667597
1	1.866286	0.026433	-0.797003
1	1.834377	0.747434	-2.425293
6	4.001544	1.427129	0.485775
1	3.976814	0.964163	-0.510690
1	4.216084	2.496813	0.369291
1	4.816318	0.973231	1.054898
8	0.534924	2.421005	0.183799
1	-0.203565	2.026621	-0.323998
6	-0.020136	3.284406	1.158627
1	0.783159	3.579214	1.837430
1	-0.445416	4.184690	0.699408
1	-0.803381	2.782274	1.740705
8	-1.758670	1.598348	-1.047817
1	-1.998015	0.647122	-1.128755
6	-1.848363	2.205809	-2.328378
1	-1.168988	1.728205	-3.044521
1	-2.871483	2.159440	-2.715489
1	-1.559459	3.253134	-2.217697
8	-2.425839	-1.009341	-1.179222
1	-2.789524	-1.311398	-0.331545
6	-1.430404	-1.931741	-1.625316
1	-0.633364	-2.045183	-0.882391
1	-1.877790	-2.907711	-1.837855
1	-0.991144	-1.533560	-2.540740
8	-3.194537	-1.237425	1.514145
1	-3.840782	-1.780428	1.979148
6	-3.480553	0.149873	1.740325
1	-4.527245	0.371622	1.515367
1	-3.251756	0.427546	2.773240
1	-2.845389	0.721259	1.060704
6	2.885724	-2.271790	0.603956
1	3.626136	-2.330178	-0.197573
1	2.872825	-1.247020	0.996217
1	3.177910	-2.964813	1.400882
8	1.632151	-2.637553	0.041464

1 0.930522 -2.513810 0.705486

Cartesian coordinates of : BL8_5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.966700	0.361663	0.057755
1	1.220711	-0.479768	-0.352318
8	0.193134	3.272743	1.057162
1	-0.301194	2.968153	0.271005
8	-4.566209	-0.175955	-0.852827
1	-3.599560	-0.267070	-0.812988
6	1.313190	0.272750	1.431525
1	2.391158	0.099427	1.561231
1	1.038419	1.224660	1.890695
1	0.764195	-0.539414	1.927702
6	1.501999	3.576462	0.633652
1	1.963021	2.724680	0.113939
1	1.526683	4.446879	-0.035376
1	2.095758	3.812066	1.522114
6	-5.113747	-1.195219	-0.049719
1	-4.927833	-2.195084	-0.465397
1	-4.718031	-1.168888	0.976321
1	-6.193870	-1.038437	-0.003532
8	-1.941267	-0.351392	-0.002282
1	-1.241646	-1.030156	0.034954
6	-2.034280	0.295541	1.259711
1	-3.031276	0.740351	1.327187
1	-1.913771	-0.420708	2.082228
1	-1.282020	1.087590	1.359510
8	-0.252219	-2.494340	0.391094
1	0.713361	-2.558922	0.298611
6	-0.725729	-3.273799	1.474610
1	-0.500045	-4.336087	1.332822
1	-0.302460	-2.938720	2.429540
1	-1.810306	-3.149504	1.508825
8	2.304400	-2.095036	-0.518709
1	3.152123	-1.723267	-0.207692
6	2.430094	-2.457211	-1.889511
1	2.755866	-1.602785	-2.492427
1	3.138950	-3.281401	-2.015030
1	1.444658	-2.778731	-2.230841
8	4.518993	-0.590110	-0.025953
1	5.426613	-0.699955	0.274218
6	4.271906	0.770064	-0.387831
1	4.447592	1.440322	0.459601
1	4.895851	1.070047	-1.235043
1	3.218084	0.834392	-0.667170
6	-2.299134	2.237421	-1.547252
1	-2.436906	3.247815	-1.936753
1	-2.568926	1.517808	-2.327651
1	-2.972112	2.091496	-0.694529
8	-0.935282	2.114935	-1.177527
1	-0.764876	1.207097	-0.874572

Cartesian coordinates of : BC8_10

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-3.816705	2.177769	-0.863154

6	-2.771994	2.471794	-0.994715
1	-2.510250	2.402800	-2.056142
1	-2.629311	3.500232	-0.659212
8	-1.924505	1.646628	-0.202640
1	-2.121761	0.695382	-0.344117
1	1.166355	0.506129	1.832208
6	0.710844	1.470323	1.582716
1	-0.295155	1.511954	2.009974
1	1.308916	2.283096	2.007310
8	0.643930	1.615122	0.163050
1	-0.310453	1.742836	-0.088521
1	-0.449048	-1.274310	1.146218
6	-1.545546	-1.297522	1.164429
1	-1.875539	-2.269660	1.547578
1	-1.910818	-0.512688	1.832768
8	-2.087916	-1.056555	-0.131920
1	-1.506268	-1.526175	-0.781708
1	3.133709	0.870227	-2.087602
6	2.509061	0.003190	-2.320612
1	1.829309	0.255398	-3.141061
1	3.137601	-0.834478	-2.627293
8	1.774090	-0.413670	-1.169640
1	1.331526	0.362308	-0.743886
1	0.595495	-3.395672	0.017035
6	0.148216	-3.520910	-0.975061
1	0.850806	-4.048423	-1.629129
1	-0.762744	-4.117585	-0.892807
8	-0.217353	-2.265651	-1.538766
1	0.538780	-1.646175	-1.477612
6	3.057898	-1.668101	2.126880
1	3.296319	-0.628903	2.393881
1	3.954015	-2.135157	1.700959
1	2.789689	-2.204307	3.039070
8	1.952374	-1.747895	1.249668
1	2.173408	-1.341742	0.394350
6	-4.771506	0.396316	1.098885
1	-3.906424	1.023382	1.361036
1	-4.829519	-0.441425	1.806267
1	-5.677787	0.996336	1.207143
8	-4.713507	-0.044589	-0.241678
1	-3.950166	-0.636084	-0.329462
6	3.856262	1.814026	0.411898
1	3.502085	0.776206	0.315576
1	3.752838	2.122064	1.461358
1	4.916987	1.839232	0.152519
8	3.183652	2.684997	-0.470324
1	2.228581	2.585635	-0.332074

Cartesian coordinates of : BC8_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	1.742670	-4.582037	0.740060
6	2.130009	-3.560095	0.665117
1	2.077096	-3.087971	1.654623
1	3.176469	-3.604946	0.356854
8	1.421808	-2.817249	-0.307641
1	0.465028	-2.762057	-0.059662
1	0.073503	-0.265906	-0.539670
6	0.629516	0.026218	-1.440971
1	0.095250	-0.359363	-2.316389
1	0.651358	1.119629	-1.493040
8	1.968831	-0.441670	-1.405695

1	1.945384	-1.369411	-1.078496
1	-2.033601	-1.425143	-1.290282
6	-1.872603	-2.474105	-1.014102
1	-2.839379	-2.985215	-0.938203
1	-1.279142	-2.963547	-1.791450
8	-1.157062	-2.577516	0.213220
1	-1.445473	-1.833339	0.786374
1	-1.066624	3.916505	1.454359
6	-1.595583	2.963087	1.549808
1	-1.562052	2.637694	2.595764
1	-2.638088	3.105369	1.255295
8	-1.031780	1.980051	0.693275
1	-0.079856	1.810006	0.965944
1	-3.753974	-0.117597	0.103904
6	-3.571589	-0.395948	1.147181
1	-4.097781	0.297453	1.813422
1	-3.951924	-1.404149	1.327828
8	-2.177517	-0.410169	1.433364
1	-1.780438	0.430487	1.125204
6	-2.251044	1.606524	-2.794865
1	-1.227343	1.729461	-3.173080
1	-2.729773	2.592682	-2.748982
1	-2.805770	0.987643	-3.503259
8	-2.277313	0.948541	-1.545673
1	-1.781542	1.466168	-0.887029
6	1.254868	0.036389	2.050461
1	1.953947	-0.110569	2.879886
1	1.501011	-0.663020	1.241311
1	0.239030	-0.171711	2.399415
8	1.295464	1.384778	1.595900
1	2.116037	1.506002	1.056549
6	3.971218	2.301364	-0.791061
1	3.228756	2.780910	-1.441035
1	4.783943	1.908689	-1.411376
1	4.381564	3.052637	-0.113624
8	3.393669	1.277358	-0.003401
1	2.984158	0.591053	-0.587413

 Cartesian coordinates of : BC8_5

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	1.743300	-2.910749	-2.439769
6	1.058466	-2.517752	-1.681982
1	0.411361	-1.759042	-2.135432
1	0.427107	-3.329236	-1.313701
8	1.783527	-1.993815	-0.576142
1	2.262814	-1.166343	-0.846161
1	1.325772	-2.999300	2.672989
6	0.313593	-2.881707	2.273655
1	0.040601	-3.785883	1.717567
1	-0.382703	-2.754092	3.104789
8	0.222921	-1.730723	1.444480
1	0.886729	-1.813725	0.690948
1	4.708457	0.290316	-0.079558
6	4.387720	0.304958	-1.128132
1	4.790544	1.199681	-1.615201
1	4.791999	-0.576592	-1.629505
8	2.975378	0.260791	-1.240015
1	2.593520	0.987192	-0.687748
1	-1.755832	1.199788	2.587129
6	-1.113956	1.250554	1.701997
1	-1.496556	0.562363	0.942281

1	-1.155653	2.261835	1.293370
8	0.239942	0.949261	2.035786
1	0.337589	-0.022240	2.027378
1	3.400731	2.448231	1.907277
6	2.839593	2.982315	1.131245
1	2.268187	3.790811	1.599427
1	3.546206	3.421465	0.423460
8	1.987610	2.111409	0.409233
1	1.339352	1.692432	1.029688
6	-4.618260	1.887484	-0.879546
1	-5.001874	0.908629	-1.201009
1	-4.558852	2.541486	-1.758758
1	-5.332524	2.321283	-0.175966
8	-3.378619	1.776798	-0.217081
1	-2.726068	1.394503	-0.835689
6	-0.172306	0.828183	-1.483799
1	0.483566	0.646325	-2.342800
1	0.231057	0.286497	-0.615764
1	-0.158086	1.895885	-1.250256
8	-1.507841	0.433715	-1.760811
1	-1.633955	-0.479939	-1.434668
6	-3.195440	-1.693957	0.207571
1	-3.376339	-0.654682	0.510387
1	-3.360735	-2.360523	1.061182
1	-3.903551	-1.959352	-0.580073
8	-1.887432	-1.863548	-0.328099
1	-1.226514	-1.788599	0.389341

Cartesian coordinates of : BL8_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-3.964511	-1.339704	-1.812232
1	-3.771539	-1.494310	-0.876891
8	4.306112	-1.001894	-0.377669
1	3.583430	-0.621593	-0.910674
8	2.109790	0.269656	-1.504411
1	1.731068	0.455626	-0.619026
6	-4.681332	-0.126327	-1.916078
1	-4.097106	0.730833	-1.554002
1	-4.906238	0.027392	-2.973255
1	-5.633532	-0.162557	-1.368537
6	4.623655	-2.282439	-0.875019
1	3.762938	-2.965439	-0.836137
1	4.988519	-2.243778	-1.909469
1	5.416612	-2.694025	-0.246701
6	2.413151	1.510537	-2.114004
1	1.500713	2.067398	-2.364229
1	3.045539	2.134003	-1.469134
1	2.954438	1.304672	-3.039127
8	1.437040	0.895306	1.049674
1	0.791824	1.628635	1.228710
6	2.677660	1.117209	1.718709
1	3.383028	0.361023	1.364646
1	3.073373	2.111693	1.484812
1	2.554274	1.025043	2.802508
8	-0.467328	2.689586	1.294456
1	-1.190157	2.113166	0.950243
6	-0.339339	3.815174	0.441757
1	-0.071434	3.518822	-0.580744
1	-1.268773	4.392362	0.410867
1	0.453832	4.448563	0.843691
8	-2.097353	1.013564	0.031401

1	-2.682202	0.360247	0.453038
6	-1.248277	0.348340	-0.906632
1	-0.713914	-0.483816	-0.434948
1	-1.824708	-0.021845	-1.759899
1	-0.516699	1.082093	-1.255285
8	-3.629378	-1.103755	1.056597
1	-4.512655	-1.003525	1.428724
6	-2.841061	-1.964539	1.895427
1	-2.821221	-1.586896	2.921405
1	-3.242370	-2.981622	1.880099
1	-1.823984	-1.959378	1.500302
6	1.356133	-2.308669	0.604392
1	1.138766	-3.379154	0.608663
1	1.323745	-1.948659	-0.434561
1	2.369938	-2.149228	0.991884
8	0.380939	-1.671072	1.412317
1	0.638461	-0.734965	1.470658

Cartesian coordinates of : BC8_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-4.430192	-0.601284	0.403593
1	-3.585042	-0.991795	0.673600
8	0.484718	-0.399877	-1.387535
1	1.151021	-1.035471	-1.078668
8	2.729805	-1.541141	-0.155470
1	2.879167	-0.585126	0.088787
6	-4.695346	0.536548	1.199423
1	-3.898120	1.285551	1.111282
1	-5.632088	0.969787	0.841484
1	-4.822831	0.274283	2.257731
6	1.105506	0.441821	-2.341476
1	0.474752	1.326570	-2.465088
1	2.095408	0.776931	-2.006777
1	1.205619	-0.056245	-3.314533
6	3.900606	-2.076777	-0.748501
1	4.219445	-1.473023	-1.605573
1	4.721497	-2.131153	-0.025012
1	3.671444	-3.086385	-1.094153
8	2.983741	1.001274	0.371529
1	2.121528	1.458455	0.185318
6	3.419468	1.398740	1.661598
1	4.141227	0.661140	2.021946
1	3.908893	2.377925	1.621915
1	2.579768	1.447624	2.363632
8	0.668545	2.212245	0.188333
1	-0.163978	1.687197	0.052253
6	0.435843	3.551705	-0.197650
1	0.313107	3.642179	-1.285059
1	-0.457006	3.950929	0.296167
1	1.299637	4.148331	0.104748
8	-1.692564	1.052833	-0.091861
1	-1.606984	0.084079	0.043314
6	-2.319368	1.230179	-1.355267
1	-1.769141	0.697470	-2.140513
1	-3.351600	0.863442	-1.322405
1	-2.321662	2.300239	-1.579497
8	-1.848529	-1.679201	0.191632
1	-0.995476	-2.013851	0.546149
6	-2.115898	-2.270826	-1.076847
1	-1.350833	-1.979851	-1.803501
1	-2.162018	-3.361626	-0.993288

1	-3.091326	-1.901421	-1.402276
6	0.588209	-0.897178	2.047255
1	-0.336135	-0.784642	2.618004
1	1.436878	-0.859984	2.739808
1	0.666615	-0.069993	1.330268
8	0.529022	-2.153425	1.383042
1	1.347759	-2.238233	0.862618

Cartesian coordinates of : BC8_9

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-2.969376	-2.145395	0.167938
1	-3.024474	-1.428301	0.821142
8	2.255376	1.736563	-0.707655
1	3.001272	1.103813	-0.718197
8	4.192950	-0.025992	-0.031899
1	3.530520	-0.666419	0.314798
6	-1.593803	-2.300591	-0.154290
1	-1.021779	-2.711067	0.687585
1	-1.533741	-3.002798	-0.989805
1	-1.144498	-1.344043	-0.454314
6	2.279299	2.383202	0.560852
1	1.869828	1.732105	1.342513
1	3.299331	2.674808	0.827251
1	1.663564	3.283158	0.484380
6	5.342275	-0.701944	-0.498975
1	5.832160	-1.258216	0.308080
1	5.104774	-1.396813	-1.314619
1	6.039056	0.049060	-0.876012
8	2.098337	-1.591307	0.505598
1	1.387925	-1.105469	0.982054
6	1.655962	-1.901669	-0.805050
1	2.538638	-2.073410	-1.427489
1	1.048527	-2.814536	-0.810835
1	1.075372	-1.080996	-1.243499
8	0.164641	-0.134049	1.707104
1	-0.458842	0.266797	1.071995
6	-0.530377	-0.570003	2.860233
1	-1.026417	0.268480	3.360460
1	-1.283794	-1.328894	2.617700
1	0.206059	-1.004063	3.539321
8	-2.547596	0.502232	0.995861
1	-2.606089	0.550363	0.018898
6	-3.428588	1.459468	1.558458
1	-3.100965	2.481773	1.335007
1	-4.452076	1.324955	1.191163
1	-3.420589	1.318726	2.641353
8	-3.223844	0.014255	-1.615512
1	-3.399870	-0.878974	-1.269865
6	-2.480582	-0.080331	-2.821931
1	-1.511120	-0.562496	-2.657566
1	-3.046201	-0.620155	-3.589047
1	-2.298779	0.937199	-3.172597
6	-0.892356	2.291181	-0.872508
1	-1.932333	2.205389	-1.204172
1	-0.880923	2.765002	0.119395
1	-0.353490	2.934243	-1.577671
8	-0.328078	0.992758	-0.829121
1	0.648681	1.112390	-0.856645

Cartesian coordinates of : DC8_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.983337	-0.612296	-1.584637
1	1.354511	-1.079622	-0.811395
8	2.451765	-1.397145	0.627817
1	2.454955	-0.464612	0.941716
8	2.323254	1.253350	1.121677
1	1.621038	1.561913	0.496760
6	2.070089	0.009986	-2.244977
1	2.742386	-0.728476	-2.700131
1	1.661805	0.646930	-3.033590
1	2.645451	0.646079	-1.558837
6	3.781928	-1.788952	0.344985
1	4.278149	-1.081342	-0.332550
1	4.375202	-1.877172	1.262496
1	3.746383	-2.766800	-0.140157
6	3.451598	2.101132	1.016268
1	3.860396	2.109756	-0.002330
1	3.203097	3.128601	1.304719
1	4.217341	1.725674	1.698504
8	0.419587	2.002397	-0.595664
1	0.018510	1.171294	-0.919536
6	-0.607224	2.808464	-0.037022
1	-0.144518	3.737682	0.301478
1	-1.371321	3.043795	-0.785412
1	-1.090212	2.316984	0.815613
8	-1.736476	0.311752	-1.280787
1	-1.551986	-0.618692	-1.000616
6	-1.782436	0.384213	-2.696664
1	-0.859544	-0.018223	-3.126887
1	-2.641646	-0.166956	-3.094464
1	-1.880381	1.437164	-2.972696
8	-1.560900	-2.096153	-0.137338
1	-1.664887	-1.804569	0.794803
6	-0.506018	-3.045590	-0.209602
1	0.364713	-2.722862	0.374229
1	-0.841280	-4.024124	0.151692
1	-0.212020	-3.133051	-1.257401
8	-1.546340	-0.759708	2.219141
1	-2.193019	-0.081082	1.934763
6	-0.242536	-0.222125	2.038337
1	-0.026700	-0.056575	0.971939
1	-0.114104	0.722212	2.577644
1	0.476734	-0.947338	2.423891
6	-4.450295	0.091084	0.721075
1	-4.923644	0.002361	1.700624
1	-5.161161	0.555926	0.029084
1	-4.196604	-0.911850	0.355727
8	-3.288348	0.893740	0.877240
1	-2.805315	0.880210	0.026330

Cartesian coordinates of : BC8_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.536990	-1.492567	1.658216
1	-2.213765	-1.370332	0.969404
8	2.616349	0.875524	-0.280977
1	2.241925	0.055630	0.099027
8	1.840471	-1.737330	0.354992

1	0.955175	-1.695045	-0.064881
6	-1.055639	-2.828211	1.634009
1	-0.820245	-3.154347	0.613707
1	-0.136804	-2.853889	2.223267
1	-1.784617	-3.516082	2.076604
6	3.748012	0.539837	-1.055208
1	4.554895	0.140175	-0.429085
1	3.506630	-0.199590	-1.830489
1	4.102044	1.450312	-1.542972
6	2.532463	-2.830534	-0.216802
1	2.078056	-3.786216	0.072521
1	2.549732	-2.771638	-1.312852
1	3.559613	-2.806323	0.153904
8	-0.256733	-1.671241	-1.360502
1	-1.184075	-1.462772	-1.128071
6	0.205963	-0.626264	-2.205433
1	1.281829	-0.762993	-2.343343
1	-0.282396	-0.665284	-3.185570
1	0.040643	0.357067	-1.751776
8	-2.704451	-0.664643	-0.681238
1	-2.389241	0.287508	-0.578290
6	-3.837536	-0.695053	-1.534131
1	-4.670814	-0.132408	-1.099523
1	-3.600603	-0.275573	-2.517970
1	-4.141385	-1.736350	-1.657106
8	-1.953818	1.767839	-0.360562
1	-1.005518	2.008170	-0.524617
6	-2.348874	2.244065	0.918106
1	-1.666595	1.885735	1.695610
1	-2.381950	3.339093	0.929137
1	-3.354454	1.864195	1.116948
8	0.562434	2.626102	-0.775258
1	1.226450	1.913221	-0.654691
6	0.771219	3.557608	0.273001
1	0.550693	3.106126	1.248710
1	1.803561	3.923844	0.273620
1	0.099317	4.403169	0.105752
6	1.076243	0.524699	2.412655
1	1.850663	1.287540	2.295844
1	0.458139	0.774100	3.285582
1	1.566593	-0.442293	2.579653
8	0.309203	0.510939	1.221469
1	-0.356312	-0.198606	1.315653

Cartesian coordinates of : BL8_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-0.507103	-1.984664	1.256912
1	0.089319	-1.250403	1.498078
8	4.580410	1.570101	0.457511
1	4.547205	0.602448	0.556028
8	3.735272	-1.101651	0.427693
1	2.898212	-0.880531	0.875697
6	0.172350	-2.762186	0.285429
1	1.098598	-3.182945	0.695492
1	-0.484847	-3.586123	-0.001032
1	0.411642	-2.167172	-0.606148
6	3.770579	1.901812	-0.643618
1	4.147274	1.472661	-1.583487
1	2.730397	1.565674	-0.508203
1	3.767076	2.990219	-0.741732
6	3.433430	-1.507616	-0.896149

1	3.166334	-2.570910	-0.934637
1	2.606136	-0.921013	-1.318269
1	4.326795	-1.353795	-1.506694
8	1.338238	0.030426	1.235395
1	1.060801	0.298434	0.325267
6	1.568861	1.180890	2.047257
1	2.538159	1.634137	1.812804
1	0.769642	1.917434	1.909584
1	1.568779	0.852927	3.088312
8	0.402015	0.364208	-1.222633
1	-0.572328	0.175238	-1.235814
6	0.722469	1.161830	-2.350980
1	0.052647	0.929890	-3.184802
1	0.644325	2.230199	-2.117965
1	1.750344	0.942298	-2.653337
8	-2.148128	-0.161523	-1.523684
1	-2.810857	0.220397	-0.914284
6	-2.433754	-1.537414	-1.712997
1	-2.420729	-2.080888	-0.762333
1	-3.409427	-1.669578	-2.192491
1	-1.660389	-1.945738	-2.368028
8	-4.221259	1.381407	-0.473790
1	-4.514262	1.981240	-1.167260
6	-5.296657	1.106466	0.418901
1	-5.614029	2.014450	0.943495
1	-6.152706	0.674885	-0.110946
1	-4.914810	0.380087	1.136122
6	-2.069175	0.711731	1.661021
1	-2.775818	1.536223	1.783519
1	-1.523977	0.569266	2.603907
1	-1.348801	0.992883	0.877827
8	-2.805675	-0.439401	1.303209
1	-2.169482	-1.176195	1.263243

Cartesian coordinates of : BL8_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.251056	0.478179	2.316903
1	1.941312	0.280700	1.651482
8	2.916892	1.945163	-1.300512
1	3.076023	1.175446	-0.728568
8	2.912979	-0.352161	0.313745
1	2.300784	-0.879561	-0.279268
6	0.607803	-0.743429	2.636683
1	1.291875	-1.431212	3.148662
1	-0.219841	-0.514053	3.312220
1	0.204831	-1.243258	1.744216
6	2.688405	3.070445	-0.475860
1	1.834354	2.923063	0.199801
1	3.571970	3.324417	0.123958
1	2.463610	3.915743	-1.129849
6	4.054652	-1.139141	0.618980
1	3.775257	-2.038860	1.178729
1	4.580931	-1.435874	-0.294163
1	4.724572	-0.534760	1.233442
8	1.401013	-1.664915	-1.315295
1	0.551495	-2.026888	-0.970740
6	1.143256	-0.923566	-2.503589
1	1.814231	-0.059966	-2.531800
1	1.314474	-1.549191	-3.385373
1	0.109384	-0.560814	-2.517763
8	-0.962229	-2.469635	-0.402162

1	-1.710775	-1.829517	-0.321927
6	-1.484566	-3.773439	-0.587418
1	-2.118095	-4.065647	0.257380
1	-2.069007	-3.843589	-1.511494
1	-0.641706	-4.464629	-0.650043
8	-3.049174	-0.906462	0.053273
1	-3.273146	-0.113202	-0.468953
6	-2.984377	-0.524838	1.424037
1	-2.271705	0.294483	1.574134
1	-3.973643	-0.227242	1.789336
1	-2.652334	-1.399979	1.988252
8	-3.739942	1.519574	-1.084196
1	-4.532961	1.612907	-1.621721
6	-3.569352	2.679260	-0.263387
1	-3.463435	3.576366	-0.881023
1	-4.415048	2.801680	0.421548
1	-2.652748	2.532275	0.310672
6	-0.365206	1.079273	-0.305647
1	-1.168803	1.266058	-1.026143
1	0.591886	1.343975	-0.774591
1	-0.354635	0.003852	-0.074638
8	-0.630854	1.854006	0.849852
1	0.029280	1.589891	1.518579

Cartesian coordinates of : BC8_8

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-3.136352	0.589641	-1.893948
6	-3.481002	-0.031869	-1.060547
1	-4.494785	0.274533	-0.782217
1	-3.492311	-1.078805	-1.373577
8	-2.604315	0.078651	0.055274
1	-2.411869	1.036766	0.231247
1	-1.167913	-2.187508	2.052441
6	-0.312363	-1.761522	1.518409
1	-0.026838	-0.814763	1.989853
1	0.536026	-2.445820	1.577204
8	-0.632627	-1.565476	0.140325
1	-1.372760	-0.885951	0.076287
1	1.134082	-1.813063	-2.879089
6	1.868038	-1.936838	-2.076753
1	1.834178	-2.970447	-1.714702
1	2.864260	-1.732181	-2.473902
8	1.625538	-1.022928	-1.015055
1	0.714048	-1.191343	-0.638362
1	-2.446577	4.306156	1.595401
6	-2.407324	3.214252	1.674901
1	-1.679420	2.939422	2.446455
1	-3.392703	2.849756	1.972473
8	-2.086711	2.627448	0.425367
1	-1.164396	2.887134	0.178837
1	4.265915	1.164557	-0.257683
6	3.338968	1.461697	0.246406
1	3.097924	0.726670	1.022951
1	3.494365	2.436142	0.714377
8	2.279130	1.597927	-0.689953
1	2.002774	0.702121	-0.970828
1	0.527828	4.099302	-2.049190
6	0.590606	4.449648	-1.013047
1	1.562545	4.930298	-0.857315
1	-0.196256	5.187642	-0.842568
8	0.396021	3.389787	-0.092600

1	1.061083	2.684623	-0.275108
6	-3.427662	-3.263518	0.348846
1	-3.479458	-2.242529	0.753526
1	-3.047658	-3.935479	1.130202
1	-4.438287	-3.583913	0.085898
8	-2.644465	-3.324626	-0.826040
1	-1.782076	-2.930991	-0.622562
6	4.366074	-2.121987	1.044904
1	4.903295	-1.190570	0.817723
1	4.532410	-2.830826	0.222821
1	4.792751	-2.547964	1.955080
8	2.993628	-1.897787	1.282770
1	2.584569	-1.555745	0.468854

Cartesian coordinates of : BC8_7

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	0.280491	0.158525	-0.484519
6	-0.417801	0.427551	-1.287436
1	0.156941	0.704954	-2.175654
1	-1.042470	-0.438649	-1.518722
8	-1.274548	1.495259	-0.879483
1	-0.693000	2.259061	-0.671082
1	-4.229804	1.481889	1.180294
6	-3.432226	1.079986	1.814833
1	-2.930052	1.907219	2.327976
1	-3.876179	0.420237	2.562401
8	-2.513477	0.316782	1.049728
1	-2.077608	0.888575	0.349553
1	-0.900594	-2.318891	-0.115146
6	-0.995678	-2.585774	0.941912
1	-2.020690	-2.911668	1.140477
1	-0.311817	-3.407313	1.167197
8	-0.641197	-1.494672	1.794801
1	-1.294328	-0.774387	1.657754
1	1.921941	4.865601	-0.116124
6	0.960781	4.450326	0.207370
1	0.928519	4.442476	1.303225
1	0.162297	5.096604	-0.162496
8	0.755117	3.159081	-0.330462
1	1.472045	2.549531	-0.036769
1	2.396370	-2.829248	2.080410
6	2.641981	-1.762765	2.138669
1	2.522558	-1.424461	3.172700
1	3.683341	-1.624180	1.839272
8	1.828259	-1.004973	1.254874
1	0.864235	-1.114417	1.516493
1	2.644246	0.345566	-1.476434
6	3.312991	0.974249	-0.876774
1	4.226984	0.413916	-0.646180
1	3.584484	1.861703	-1.451925
8	2.679124	1.416042	0.317219
1	2.352359	0.625409	0.793003
6	-3.879817	-0.506425	-1.928067
1	-3.258551	0.395546	-2.009870
1	-4.899788	-0.209502	-1.648582
1	-3.921810	-0.991540	-2.905533
8	-3.335191	-1.439648	-1.014939
1	-3.183824	-0.975075	-0.176583
6	2.611915	-2.670464	-1.875942
1	2.736402	-3.591913	-1.291847
1	3.559900	-2.113786	-1.858384

1	2.397015	-2.947449	-2.909798
8	1.532251	-1.890190	-1.411569
1	1.694818	-1.645894	-0.483848

Cartesian coordinates of : BC8_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	0.001207	-0.056536	-1.415037
6	0.824395	-0.720574	-1.711014
1	0.604306	-1.145811	-2.695974
1	1.744150	-0.131705	-1.770524
8	1.035540	-1.748551	-0.750034
1	0.196088	-2.242189	-0.666175
1	2.694219	-1.540192	2.705227
6	2.059430	-0.663664	2.533644
1	1.032693	-0.891626	2.837355
1	2.440192	0.166266	3.133401
8	2.097029	-0.264625	1.173343
1	1.635083	-0.935301	0.610674
1	2.224187	2.125056	-0.811732
6	1.806306	2.656557	0.049220
1	2.574893	2.727170	0.825771
1	1.513553	3.665356	-0.249588
8	0.643525	2.007646	0.554433
1	0.901154	1.105337	0.838751
1	-3.204911	-3.650162	-0.029613
6	-2.212221	-3.285872	0.258640
1	-2.306826	-2.587631	1.100011
1	-1.609691	-4.136679	0.580734
8	-1.548674	-2.686126	-0.842222
1	-2.042842	-1.885232	-1.094658
1	-1.455252	4.093511	-1.170866
6	-2.085395	3.273012	-0.810658
1	-2.319964	3.445286	0.247433
1	-3.015503	3.274411	-1.383785
8	-1.450103	2.022800	-1.007035
1	-0.631563	1.982370	-0.436416
1	-4.719406	0.338093	-1.159603
6	-4.082046	0.031839	-0.322715
1	-4.102107	0.811971	0.448195
1	-4.485247	-0.889304	0.105059
8	-2.757448	-0.225710	-0.755049
1	-2.304385	0.636919	-0.961284
6	4.372019	-0.964660	-1.230366
1	3.528884	-1.667648	-1.262180
1	5.148943	-1.375119	-0.572087
1	4.790096	-0.871716	-2.235281
8	3.963674	0.325872	-0.819203
1	3.486110	0.229140	0.021818
6	-1.539239	0.531602	2.158845
1	-2.441466	0.064934	2.576882
1	-1.821904	1.437354	1.606700
1	-0.884393	0.828306	2.981696
8	-0.815661	-0.370023	1.342048
1	-1.372841	-0.564352	0.571284

Cartesian coordinates of : BC8_6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
----	---	---	---

```

-----
8   -1.900791    2.340491   -0.431199
1   -0.937347    2.442689   -0.296948
8    0.705937    2.472595    0.373367
1    1.512430    2.247062   -0.138461
8    3.021069    1.497540   -0.609715
1    2.999630    0.559839   -0.309435
6   -2.558989    3.400243    0.227840
1   -2.282544    4.376667   -0.187987
1   -3.634405    3.258821    0.092545
1   -2.344996    3.408788    1.306288
6    0.736473    1.700844    1.558396
1    0.610989    0.627304    1.352183
1    1.676504    1.845711    2.103758
1   -0.090394    2.030242    2.192851
6    4.216100    2.110780   -0.160097
1    4.298080    2.084731    0.933349
1    5.097317    1.624967   -0.593786
1    4.197276    3.152418   -0.485669
8    2.860541   -1.080273    0.112447
1    2.000182   -1.328802    0.507868
6    3.064419   -1.882517   -1.043924
1    4.044732   -1.627224   -1.450436
1    3.058866   -2.947679   -0.787204
1    2.301896   -1.692714   -1.808622
8    0.471895   -2.164330    0.844416
1   -0.417431   -1.785094    1.102121
6    0.655692   -3.399639    1.523554
1    0.624833   -3.259159    2.608600
1   -0.111919   -4.124150    1.233292
1    1.637813   -3.791111    1.248370
8   -1.952410   -1.385650    1.344768
1   -2.428323   -1.505196    0.484135
6   -2.359391   -0.152207    1.924963
1   -2.235004    0.680094    1.220506
1   -3.405378   -0.208069    2.246038
1   -1.736433    0.021295    2.805637
8   -2.973321   -1.554701   -1.110258
1   -2.113770   -1.628227   -1.571760
6   -3.645294   -0.374990   -1.547022
1   -3.062922    0.527914   -1.328065
1   -3.859584   -0.427743   -2.619631
1   -4.594273   -0.330033   -1.008268
6   -0.120486   -0.104691   -1.435844
1   -0.553727    0.495671   -2.238238
1   -0.640906    0.145478   -0.502094
1    0.941860    0.151111   -1.340530
8   -0.299909   -1.477234   -1.776626
1    0.051716   -2.000051   -1.035207
-----

```

Cartesian coordinates of : L8

Atomic number (AN) and Cartesian coordinates

```

-----
AN      X          Y          Z
-----
8      1.808001    2.085275   -1.352122
1      2.054971    2.098072   -0.407840
8      2.013779    1.943906    1.392691
1      1.922628    0.968675    1.491611
8      1.495859   -0.676782    1.587501
1      1.793023   -1.165519    0.771790
6      2.876860    2.573563   -2.130940
1      3.769170    1.936470   -2.052931
1      2.550052    2.579078   -3.173539
-----

```


1	3.156301	3.597568	-1.852587
6	0.773931	2.530895	1.727767
1	0.024929	2.355730	0.940644
1	0.394689	2.143895	2.684281
1	0.925604	3.607994	1.825697
6	1.830889	-1.431632	2.737665
1	1.283682	-2.382047	2.758041
1	2.905245	-1.640648	2.784242
1	1.548500	-0.847584	3.616966
8	2.239091	-1.956443	-0.576609
1	1.428456	-2.357077	-0.970209
6	2.917391	-1.153021	-1.534868
1	3.807909	-0.749527	-1.047003
1	3.231554	-1.756895	-2.392148
1	2.296058	-0.314949	-1.871140
8	-0.170735	-2.986666	-1.124735
1	-0.766019	-2.266411	-1.420219
6	-0.490453	-3.243819	0.233637
1	-0.387653	-2.335321	0.843116
1	-1.510973	-3.629836	0.333681
1	0.208559	-3.999563	0.600021
8	-1.531015	-0.700316	-1.347267
1	-2.406506	-0.274413	-1.416922
6	-0.527719	0.307247	-1.305712
1	-0.122816	0.515855	-2.300227
1	-0.922447	1.241474	-0.891114
1	0.288179	-0.039362	-0.661403
8	-3.725487	0.874098	-0.980859
1	-3.377509	1.202374	-0.131041
6	-5.068557	0.458965	-0.806809
1	-5.155845	-0.319298	-0.038757
1	-5.712580	1.302141	-0.534426
1	-5.411867	0.052166	-1.759349
6	-1.877471	0.041944	1.795384
1	-2.396480	-0.741985	1.241191
1	-0.826237	0.043950	1.487110
1	-1.949464	-0.161369	2.869577
8	-2.532129	1.269525	1.470069
1	-2.031257	2.010719	1.826789

Cartesian coordinates of : CY8_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	2.559880	1.240493	2.156978
6	3.392344	0.555564	1.957720
1	4.328203	1.123642	1.946052
1	3.437531	-0.185496	2.759162
8	3.208984	-0.139704	0.733558
1	2.966812	0.520343	0.045579
1	3.030553	-3.565365	1.449086
6	2.366886	-3.407453	0.592081
1	2.971938	-3.357717	-0.321048
1	1.684719	-4.256658	0.517373
8	1.585517	-2.237315	0.763188
1	2.186898	-1.451048	0.780789
1	1.407550	-1.752423	-2.538409
6	0.657557	-1.084830	-2.098051
1	1.168031	-0.244754	-1.607825
1	0.024408	-0.693401	-2.898774
8	-0.174805	-1.786455	-1.189131
1	0.376078	-2.017496	-0.402678
1	0.564180	0.210481	0.826456

6	-0.120718	0.071136	1.675319
1	-0.816183	-0.737164	1.425101
1	0.465332	-0.231404	2.548238
8	-0.811195	1.284797	1.941388
1	-1.769829	1.105497	1.831255
1	-3.281970	-2.981796	-0.299559
6	-3.503914	-2.237751	-1.073069
1	-3.336873	-2.685711	-2.058273
1	-4.554680	-1.950600	-0.992832
8	-2.721513	-1.066829	-0.909313
1	-1.768092	-1.309639	-0.997417
1	-5.307948	0.590957	0.881614
6	-4.414612	1.217704	0.986883
1	-4.298310	1.822638	0.079195
1	-4.560388	1.886856	1.837134
8	-3.266932	0.432298	1.244093
1	-3.077223	-0.134621	0.459663
1	2.534298	3.297636	-2.302583
6	2.623559	2.212098	-2.187158
1	1.960967	1.722055	-2.913646
1	3.653098	1.920565	-2.404770
8	2.326859	1.814597	-0.863300
1	1.435883	2.162791	-0.600732
1	-2.047501	2.229423	-0.968156
6	-1.016449	1.885231	-1.103184
1	-0.979621	0.807313	-0.901731
1	-0.720774	2.062760	-2.140497
8	-0.122533	2.603611	-0.265319
1	-0.339951	2.341662	0.660681

Cartesian coordinates of : CY8_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	0.687135	-0.126842	-1.557465
6	-0.074693	-0.355067	-2.317345
1	-0.284299	0.556483	-2.890645
1	0.332866	-1.105657	-2.998348
8	-1.259582	-0.878869	-1.746225
1	-1.724521	-0.154584	-1.262200
1	-3.949082	-2.671437	-0.379477
6	-3.281752	-2.284230	0.398247
1	-3.353585	-1.190114	0.426520
1	-3.595166	-2.691145	1.361673
8	-1.942855	-2.707354	0.171687
1	-1.614287	-2.239174	-0.622381
1	-1.268763	0.034700	1.824658
6	-0.277536	-0.366252	1.582449
1	-0.097663	-0.221211	0.507486
1	0.478557	0.194094	2.139383
8	-0.166680	-1.732871	1.950381
1	-0.846680	-2.222122	1.433312
1	1.945260	2.077818	-2.029880
6	1.978620	2.796926	-1.203694
1	2.970762	3.261963	-1.176285
1	1.232042	3.575275	-1.381176
8	1.677505	2.170664	0.031512
1	2.125561	1.286764	0.049879
1	0.579329	-2.553474	-0.866132
6	1.451207	-3.088235	-0.469452
1	1.142152	-4.092181	-0.162042
1	2.202287	-3.171306	-1.258051
8	2.039116	-2.383167	0.615695

1	1.323933	-2.222262	1.277916
1	4.908017	-0.777060	-0.541938
6	4.359488	-0.025977	0.036599
1	4.568951	-0.172748	1.101870
1	4.711091	0.966364	-0.256536
8	2.970030	-0.093721	-0.234167
1	2.612562	-0.959762	0.103200
1	-2.755339	2.559689	-1.826814
6	-3.347110	1.889034	-1.192907
1	-4.012717	2.490517	-0.564198
1	-3.955638	1.245270	-1.831817
8	-2.516854	1.055138	-0.402772
1	-1.891272	1.623057	0.113772
1	-0.225012	4.017605	2.237333
6	-0.836542	3.115621	2.128351
1	-0.496952	2.365168	2.852293
1	-1.875796	3.367991	2.349742
8	-0.782898	2.624802	0.802093
1	0.153919	2.420429	0.547234

Cartesian coordinates of : CY8_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-0.661146	-0.049278	-1.053131
6	0.313764	-0.100140	-1.553698
1	0.240186	0.383926	-2.531927
1	1.034393	0.455432	-0.940958
8	0.739205	-1.448283	-1.704533
1	0.047073	-2.028894	-1.308231
1	3.649047	-3.497289	-0.850129
6	3.249547	-2.983822	0.030832
1	2.360386	-3.520200	0.385079
1	4.005681	-2.998432	0.818030
8	2.954056	-1.628226	-0.262697
1	2.193709	-1.603817	-0.896622
1	0.426516	-0.854336	2.763909
6	0.673013	-0.500019	1.758064
1	0.462458	-1.300607	1.039715
1	0.023866	0.351129	1.514121
8	2.036095	-0.104966	1.702037
1	2.495546	-0.683887	1.046080
1	-2.537170	1.216705	-1.922204
6	-3.159753	1.479080	-1.058041
1	-3.579059	2.479476	-1.213999
1	-3.982641	0.763719	-0.984611
8	-2.420986	1.419356	0.149671
1	-1.574212	1.920045	0.024515
1	3.327660	1.101772	-0.666491
6	3.147262	2.150644	-0.401406
1	4.075974	2.586429	-0.019050
1	2.846007	2.693373	-1.302059
8	2.107732	2.267076	0.560018
1	2.123700	1.454794	1.127319
1	0.254224	4.729081	-0.994548
6	-0.432471	4.194591	-0.328929
1	-0.275545	4.539803	0.698642
1	-1.457956	4.428084	-0.625900
8	-0.253820	2.792182	-0.437683
1	0.634022	2.556001	-0.055595
1	-2.661754	-1.836600	-1.886012
6	-2.351565	-2.825524	-1.524233
1	-3.220395	-3.335858	-1.096145

1	-1.979113	-3.407600	-2.369227
8	-1.302714	-2.723027	-0.574112
1	-1.634599	-2.179068	0.175737
1	-3.771712	-0.731446	2.681231
6	-2.724643	-1.021607	2.539350
1	-2.087380	-0.343514	3.119368
1	-2.587636	-2.037665	2.915441
8	-2.372236	-1.014335	1.169363
1	-2.379708	-0.088726	0.819501

Cartesian coordinates of : CY8_5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-3.042815	-3.266200	0.538643
6	-2.335089	-3.087533	1.358652
1	-2.894894	-2.951543	2.290265
1	-1.693367	-3.964814	1.461581
8	-1.506485	-1.968434	1.098091
1	-2.067191	-1.151042	1.116181
1	-1.335651	-0.122369	-1.449062
6	-1.070892	-1.032994	-2.001329
1	-1.989966	-1.549154	-2.304272
1	-0.521347	-0.748104	-2.901759
8	-0.240305	-1.890844	-1.236176
1	-0.651200	-1.997960	-0.343813
1	2.751521	-3.009721	-2.643233
6	3.005223	-2.724292	-1.616487
1	2.725686	-3.542814	-0.942017
1	4.084090	-2.569463	-1.552486
8	2.370912	-1.510695	-1.253973
1	1.389529	-1.642050	-1.271086
1	1.460178	0.829716	-1.485044
6	1.131733	1.855722	-1.690539
1	2.002219	2.455259	-1.981741
1	0.426033	1.841567	-2.525185
8	0.472409	2.431528	-0.574471
1	1.056965	2.317306	0.218212
1	2.404282	-2.448665	2.024794
6	1.990582	-1.433739	1.998896
1	0.962317	-1.471806	1.621230
1	1.975073	-1.039407	3.016915
8	2.811638	-0.576577	1.216842
1	2.752357	-0.876544	0.279607
1	3.988975	2.342383	0.261235
6	3.441549	2.714146	1.136186
1	4.090228	2.643381	2.015920
1	3.187202	3.763714	0.971773
8	2.234471	2.000780	1.336493
1	2.437162	1.031024	1.351514
1	-3.919532	-0.614860	-0.852564
6	-4.248690	-0.258347	0.131983
1	-4.929946	0.587605	-0.011215
1	-4.794333	-1.060017	0.635498
8	-3.150958	0.104224	0.950399
1	-2.705530	0.882029	0.527133
1	-2.390267	4.037944	-1.107766
6	-2.674257	3.385195	-0.275461
1	-2.359262	3.850035	0.665526
1	-3.761780	3.280075	-0.268308
8	-2.111344	2.094299	-0.431670
1	-1.120403	2.181306	-0.452165

Cartesian coordinates of : CY8_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	3.032354	3.096095	-1.038434
8	2.243716	1.928042	-0.891876
8	-0.366955	2.327465	-1.182677
6	-0.799287	1.084079	-1.720242
8	2.112607	0.621561	1.456109
6	0.789626	1.046754	1.762130
8	1.762043	-1.983310	1.305855
6	2.902272	-2.777389	1.581734
8	0.680230	-2.169019	-1.114434
6	1.621907	-1.484212	-1.927486
8	-1.938093	-1.819491	-1.351585
6	-2.570698	-3.084416	-1.436937
8	-1.988434	2.204811	0.977811
6	-3.242921	2.850342	0.841959
8	-2.406741	-0.436951	0.894215
6	-1.839402	-1.314595	1.855004
1	2.801408	3.838323	-0.264837
1	2.882916	3.550405	-2.023708
1	4.080333	2.805646	-0.942723
1	1.288554	2.161459	-1.008030
1	0.060143	0.605150	1.069679
1	0.700424	2.136550	1.717272
1	0.556211	0.714043	2.775721
1	2.346292	1.042156	0.598013
1	3.243827	-2.629523	2.611684
1	3.728099	-2.550100	0.896660
1	2.619090	-3.824061	1.453903
1	1.992215	-1.022068	1.393891
1	-0.824860	-1.624855	1.574234
1	-2.465437	-2.204539	1.988426
1	-1.788390	-0.779876	2.806442
1	-2.328458	-0.868450	0.010851
1	2.534754	-2.078665	-2.049647
1	1.882433	-0.502534	-1.512627
1	1.168912	-1.337271	-2.910853
1	1.026379	-2.183777	-0.189361
1	-2.274472	-3.739968	-0.608901
1	-2.332380	-3.580511	-2.383938
1	-3.649396	-2.921833	-1.388617
1	-0.958711	-1.951133	-1.318800
1	-1.892010	1.027724	-1.764288
1	-0.430994	0.240019	-1.121716
1	-0.399257	0.998239	-2.732818
1	-0.870246	2.459277	-0.348095
1	-3.898175	2.620490	1.688948
1	-3.748066	2.558464	-0.087068
1	-3.062847	3.926815	0.819796
1	-2.138393	1.229600	0.996794

Cartesian coordinates of the methanol nonamer

Cartesian coordinates of : BC9_14

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
----	---	---	---

```
-----  
6      1.347008      3.257602      -2.162763  
8      0.784409      2.569104      -1.056604  
8     -1.654898      1.689265      -0.293425  
6     -1.389598      1.824690      1.103946  
8     -2.617064     -0.607220     -1.063325  
6     -3.490480     -0.443689     -2.169876  
8     -0.643731     -2.292331     -0.304931  
6     -0.889276     -2.111892      1.090998  
8      1.826850     -1.966056     -1.068771  
6      2.135448     -2.809090     -2.167941  
8      2.302355      0.586217     -0.312377  
6      2.267050      0.282437      1.083447  
1      1.325598      2.640454     -3.067598  
1      2.382025      3.550967     -1.954900  
1      0.753055      4.156945     -2.334978  
1      1.354767      1.783563     -0.822565  
1     -1.502432      2.867690      1.416366  
1     -0.372681      1.493335      1.344199  
1     -2.107905      1.200099      1.640228  
1     -0.886710      2.060619     -0.773288  
1     -2.940417     -0.148173     -3.069985  
1     -4.255805      0.310502     -1.955345  
1     -3.980599     -1.401294     -2.354384  
1     -2.218062      0.273974     -0.816154  
1      3.213889     -0.164000      1.403188  
1      1.453659     -0.415933      1.312187  
1      2.100187      1.217923      1.622611  
1      2.234139     -0.262337     -0.795443  
1     -1.741243     -2.719285      1.412428  
1     -1.100461     -1.060674      1.319291  
1      0.009038     -2.423479      1.629186  
1     -1.347107     -1.812386     -0.787613  
1      1.604401     -2.493031     -3.072457  
1      1.875790     -3.850342     -1.946738  
1      3.209860     -2.744094     -2.348736  
1      0.863693     -2.067170     -0.826072  
6      2.925451      3.765698      1.097566  
1      3.509678      3.820658      2.018572  
1      3.076782      4.698699      0.538289  
1      3.303890      2.926525      0.495533  
8      1.572158      3.582941      1.462249  
1      1.073226      3.425961      0.645298  
6     -4.723315      0.638243      1.097182  
1     -5.063680      1.111512      2.020639  
1     -5.606550      0.305740      0.535516  
1     -4.185512      1.389014      0.499712  
8     -3.888309     -0.444088      1.456426  
1     -3.504194     -0.794515      0.637484  
6      1.817363     -4.404047      1.105599  
1      1.584451     -4.932266      2.032601  
1      2.549742     -5.000237      0.544923  
1      0.895876     -4.323825      0.510373  
8      2.328694     -3.133934      1.456379  
1      2.432464     -2.628834      0.634637
```

Cartesian coordinates of : BDC9_2

```
-----  
Atomic number (AN) and Cartesian coordinates
```

```
AN      X      Y      Z  
-----  
6     -1.616752     -0.879632     -2.076908  
1     -0.902410     -0.263920     -2.637798  
1     -2.629846     -0.495774     -2.240102  
1     -1.563123     -1.907787     -2.445831
```

8	-1.287228	-0.913195	-0.700348
1	-1.509519	-0.069404	-0.269689
6	-2.347209	-0.411898	2.364975
1	-2.204220	-0.364204	3.449547
1	-2.159351	-1.436147	2.023612
1	-3.379373	-0.141381	2.131000
8	-1.494194	0.510268	1.695898
1	-0.555083	0.198188	1.805001
6	2.053631	0.394262	1.999912
1	2.168616	0.951570	1.060498
1	2.968305	-0.173129	2.196897
1	1.877149	1.097716	2.816683
8	0.926269	-0.471475	1.932892
1	1.070430	-1.075869	1.178114
6	1.242439	-2.717929	-1.134897
1	1.279789	-2.606797	-2.224031
1	0.228731	-2.990856	-0.827540
1	1.930642	-3.512004	-0.839956
8	1.673705	-1.524055	-0.491329
1	1.223554	-0.737358	-0.865665
6	4.915349	-0.236774	-0.227800
1	4.449824	0.693006	0.135037
1	4.841231	-0.257582	-1.324228
1	5.973843	-0.210603	0.040780
8	4.350487	-1.380018	0.365817
1	3.434565	-1.467408	0.051493
6	1.846244	1.924689	-1.678992
1	1.906683	2.807523	-1.028989
1	1.594389	2.249020	-2.695714
1	2.825404	1.441216	-1.699466
8	0.914651	0.982029	-1.186037
1	0.007740	1.357054	-1.208071
6	-3.464171	-3.337463	0.067633
1	-3.705800	-3.115121	-0.981359
1	-3.980751	-2.603959	0.703409
1	-3.854062	-4.329477	0.305222
8	-2.073974	-3.355443	0.299807
1	-1.725781	-2.479503	0.055595
6	-2.192389	2.611041	-2.285348
1	-1.772371	3.612027	-2.435179
1	-3.278176	2.691827	-2.169293
1	-1.978966	2.005404	-3.169387
8	-1.607562	1.964115	-1.167964
1	-1.725159	2.504034	-0.345511
6	-0.174839	3.396483	1.331642
1	0.428817	2.575609	0.918987
1	0.102099	3.550791	2.379999
1	0.038189	4.311489	0.774542
8	-1.563193	3.124612	1.203113
1	-1.711516	2.240434	1.605283

Cartesian coordinates of : DC9

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.049863	2.370002	-0.063313
1	-0.868757	2.029898	-0.177760
8	-3.420736	-0.727762	0.275677
1	-2.750102	-1.449017	0.304567
8	1.057135	0.258471	1.381123
1	0.931805	1.026070	0.785539
6	-0.022577	3.706775	0.386936
1	-0.382971	3.769881	1.422698

1	0.983356	4.132765	0.344804
1	-0.680276	4.306751	-0.253443
6	-4.524873	-1.143892	-0.507249
1	-4.201358	-1.598596	-1.451175
1	-5.146680	-1.862990	0.037594
1	-5.127186	-0.260655	-0.733674
6	-0.139861	0.137470	2.131432
1	-0.333571	1.044868	2.716872
1	-1.001088	-0.055287	1.476852
1	-0.015346	-0.699952	2.821911
8	-2.570864	1.767600	-0.181867
1	-2.750851	0.800982	-0.129394
6	-3.196660	2.362777	0.941731
1	-3.157004	3.447161	0.813956
1	-4.245130	2.055127	1.018152
1	-2.685657	2.094661	1.876015
8	-0.348801	-0.264395	-1.020034
1	0.531431	0.161963	-1.115600
6	-1.029766	-0.187490	-2.261053
1	-1.238921	0.854880	-2.527832
1	-0.453540	-0.663303	-3.063789
1	-1.979972	-0.716420	-2.146513
8	2.208583	0.675599	-1.351138
1	2.921916	0.217406	-0.851374
6	2.585109	2.027997	-1.541812
1	2.742529	2.536287	-0.581881
1	3.499159	2.096715	-2.142646
1	1.768456	2.531382	-2.060462
8	4.049997	-0.617911	0.180491
1	3.433380	-1.338849	0.415989
6	4.375334	0.120206	1.351212
1	3.470496	0.481012	1.852140
1	4.962778	-0.488660	2.047051
1	4.984353	0.971060	1.038225
6	1.699923	-2.551962	-1.100362
1	2.366068	-3.408439	-1.224523
1	0.681024	-2.856618	-1.370942
1	2.016831	-1.750828	-1.777790
8	1.784779	-2.157821	0.262395
1	1.358690	-1.290638	0.425909
6	-0.951331	-3.426705	0.997964
1	-1.772795	-4.101130	1.246352
1	-0.120909	-4.003979	0.580882
1	-0.604074	-2.928612	1.909188
8	-1.451330	-2.494359	0.051873
1	-0.776884	-1.831350	-0.200352

Cartesian coordinates of : BDC9_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.804325	1.825740	-0.092524
1	2.555416	1.221088	-0.229729
8	-3.712198	1.991765	0.026911
1	-4.141176	1.109265	0.061678
8	4.987465	-0.376969	1.367903
1	4.519647	-0.597725	0.547323
6	1.324023	2.175319	-1.382946
1	1.047383	1.280892	-1.956112
1	0.429375	2.783456	-1.248451
1	2.075389	2.751583	-1.936688
6	-4.155408	2.778993	1.116423
1	-5.227554	2.992640	1.041086

1	-3.957095	2.289360	2.077212
1	-3.610246	3.724237	1.085381
6	4.936222	1.025359	1.514359
1	5.358521	1.547990	0.644979
1	3.911550	1.392223	1.672343
1	5.530932	1.287051	2.392113
8	3.416271	-0.299362	-0.960604
1	2.577098	-0.814137	-1.056165
6	4.038533	-0.136531	-2.225988
1	4.925510	0.483324	-2.080184
1	4.349274	-1.100767	-2.641751
1	3.368791	0.363231	-2.935155
8	0.987591	-1.370074	-1.009990
1	0.650325	-0.977019	-0.172094
6	0.601851	-2.735444	-1.089829
1	1.111174	-3.339062	-0.328683
1	-0.481998	-2.833629	-0.968206
1	0.889721	-3.101914	-2.077072
8	0.436935	-0.100645	1.326961
1	0.610519	0.746390	0.865072
6	1.528971	-0.368936	2.196703
1	2.464565	-0.527836	1.645677
1	1.672375	0.448103	2.911103
1	1.292065	-1.280889	2.749729
8	-1.302306	0.871100	-0.542206
1	-2.030509	1.441093	-0.217470
6	-1.644482	0.478497	-1.862442
1	-2.645882	0.029897	-1.894086
1	-1.619751	1.333388	-2.549343
1	-0.908504	-0.263450	-2.181430
6	-1.534224	-2.204945	1.758234
1	-2.222826	-3.030419	1.950656
1	-0.526820	-2.613237	1.609663
1	-1.515356	-1.536669	2.624751
8	-1.986771	-1.535624	0.594832
1	-1.488363	-0.701604	0.467037
6	-5.166719	-1.362900	-0.772314
1	-6.059064	-0.808821	-1.069794
1	-4.546558	-1.533478	-1.660844
1	-5.476930	-2.332108	-0.365681
8	-4.485215	-0.594704	0.201254
1	-3.622375	-1.018748	0.409629

Cartesian coordinates of : BL9

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.541497	-0.200977	-1.331300
1	-2.153856	-0.518755	-0.641787
8	4.464816	1.275717	-0.486402
1	3.597519	1.603517	-0.784684
8	-3.943797	0.327995	0.320346
1	-3.255214	0.911748	0.689600
6	-2.222146	0.701781	-2.181058
1	-2.399697	1.661675	-1.679768
1	-1.589761	0.871637	-3.057242
1	-3.182099	0.292138	-2.516732
6	4.626752	1.710930	0.844461
1	4.623141	2.804973	0.924815
1	3.839078	1.316128	1.505380
1	5.591378	1.340404	1.201324
6	-5.005929	1.126677	-0.155387
1	-5.539786	1.625614	0.663418

6	-0.710393	0.508452	-2.250619
1	-1.785585	0.466766	-2.045678
1	-0.556333	0.515859	-3.335187
1	-0.248782	-0.390849	-1.823862
8	2.356059	1.153472	-1.119840
1	2.396435	0.158152	-0.905826
6	3.352791	1.458413	-2.085377
1	4.354651	1.282704	-1.679167
1	3.222339	0.850552	-2.986779
1	3.258940	2.513330	-2.350673
8	2.588361	-1.289605	-0.556046
1	1.796923	-1.889427	-0.458613
6	3.487224	-1.512310	0.524211
1	2.937614	-1.712074	1.448104
1	4.159107	-2.346001	0.293931
1	4.083702	-0.605467	0.664153
8	0.576105	-2.920586	-0.226621
1	-0.330881	-2.564615	-0.369549
6	0.601666	-3.615997	1.015226
1	0.638895	-2.916060	1.857261
1	-0.274734	-4.265989	1.105944
1	1.499553	-4.238864	1.025843
6	1.366256	2.813325	1.855553
1	1.129242	2.765049	2.920585
1	1.826824	3.785616	1.645323
1	0.431302	2.723248	1.288797
8	2.261639	1.748935	1.572659
1	2.397269	1.693492	0.608360
6	-0.267965	-0.273468	1.500186
1	-0.931497	-1.143489	1.539222
1	-0.792979	0.582160	1.948370
1	-0.074397	-0.039737	0.440372
8	0.915548	-0.599347	2.192729
1	1.519253	0.161870	2.104384

Cartesian coordinates of : BC9_12

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	3.277960	-1.558513	2.229335
6	3.901030	-1.629631	1.327939
1	4.811183	-1.039127	1.475909
1	4.180216	-2.675464	1.180823
8	3.203224	-1.195452	0.174416
1	3.065407	-0.214743	0.244041
1	2.609523	-4.272589	-1.037689
6	1.898301	-3.613314	-1.547538
1	2.427486	-3.046075	-2.320538
1	1.129451	-4.227317	-2.022981
8	1.256252	-2.751476	-0.622744
1	1.927421	-2.102441	-0.280711
1	-1.238394	-3.807941	0.156896
6	-1.927698	-3.130377	-0.356167
1	-2.652400	-3.720636	-0.923820
1	-2.458365	-2.530917	0.394441
8	-1.211879	-2.287988	-1.254192
1	-0.239680	-2.354763	-1.044656
1	1.371516	4.432486	-2.586284
6	1.981870	3.546546	-2.378776
1	1.885742	2.843616	-3.214580
1	3.026567	3.853376	-2.298710
8	1.612686	2.950815	-1.150514
1	0.661402	2.695709	-1.168308

1	-4.158274	-0.820844	-1.567983
6	-3.453787	-0.071392	-1.948956
1	-3.180596	-0.328227	-2.976981
1	-3.939634	0.907328	-1.945126
8	-2.301248	0.005695	-1.120452
1	-1.791053	-0.865271	-1.202454
1	-1.189401	1.977945	1.049361
6	-1.425888	2.748134	0.304321
1	-2.505511	2.942499	0.306076
1	-0.906048	3.669512	0.576394
8	-0.985448	2.376792	-0.995344
1	-1.362959	1.496643	-1.195760
1	1.249005	1.804101	1.745357
6	2.343521	1.826485	1.786681
1	2.680591	2.838461	2.035172
1	2.665713	1.144365	2.577787
8	2.929908	1.390505	0.567498
1	2.554307	1.937153	-0.159110
6	-4.162555	0.605173	1.845555
1	-4.541736	0.275033	2.814316
1	-3.859017	1.656312	1.929493
1	-4.973166	0.526536	1.111112
8	-3.071434	-0.229977	1.505514
1	-2.802448	-0.058220	0.579318
6	0.074169	-0.615030	1.434681
1	1.146984	-0.718968	1.614069
1	-0.356512	-1.621374	1.357582
1	-0.054765	-0.102111	0.465477
8	-0.480598	0.119678	2.504525
1	-1.446005	0.036170	2.426633

Cartesian coordinates of : L9

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.560183	-1.283954	-0.685760
1	-0.289782	-1.586118	-0.293093
8	-1.654415	-2.346643	0.384156
1	-2.506395	-1.844140	0.354599
8	-3.851686	-0.865619	0.404339
1	-3.636169	-0.080773	-0.165700
6	0.729924	-1.937730	-1.927254
1	0.243710	-1.381731	-2.742240
1	1.802552	-1.995783	-2.139410
1	0.318762	-2.953945	-1.905465
6	-1.393955	-2.714099	1.726759
1	-1.585055	-1.881215	2.414800
1	-2.008337	-3.569927	2.028836
1	-0.339958	-2.996181	1.800344
6	-5.065357	-1.440428	-0.048295
1	-5.909443	-0.765882	0.130699
1	-5.022328	-1.680308	-1.117364
1	-5.230082	-2.362944	0.512668
8	-3.099433	0.993241	-1.277580
1	-2.822552	1.868540	-0.905556
6	-1.975051	0.415580	-1.925539
1	-2.156823	-0.660090	-2.023777
1	-1.840006	0.841951	-2.925981
1	-1.056392	0.552693	-1.340718
8	-2.118129	3.135914	-0.074243
1	-1.254229	2.757507	0.221256
6	-2.877755	3.421020	1.088993
1	-3.169015	2.501601	1.614941

1	-2.315311	4.060417	1.777305
1	-3.781388	3.948654	0.777514
8	-0.050092	1.851721	0.958843
1	0.804885	1.654041	0.511478
6	-0.567408	0.663840	1.536389
1	-1.438191	0.302788	0.971061
1	0.190640	-0.126526	1.542329
1	-0.878971	0.872130	2.565113
8	2.242520	1.172279	-0.193869
1	3.119266	1.438151	0.140358
6	2.313627	1.061334	-1.607415
1	2.662324	1.994875	-2.061541
1	2.983654	0.242257	-1.894556
1	1.306786	0.835232	-1.963549
6	5.700691	0.624653	0.507816
1	5.091447	-0.247114	0.264294
1	6.590170	0.652994	-0.129916
1	6.002557	0.563877	1.558460
8	4.876996	1.768372	0.276417
1	5.322197	2.569192	0.569490
6	2.938412	-2.820547	0.601188
1	3.884316	-3.367566	0.617946
1	2.500989	-2.856361	1.608093
1	2.253318	-3.326162	-0.091712
8	3.215782	-1.498827	0.196733
1	2.370278	-1.027746	0.090859

Cartesian coordinates of : BC9_13

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-4.753543	-0.635335	1.762607
6	-5.104175	-0.289024	0.784014
1	-5.820854	-1.016666	0.386373
1	-5.612232	0.670009	0.911648
8	-4.028198	-0.091470	-0.114104
1	-3.531151	-0.939761	-0.201580
1	-4.784960	2.885694	-1.270330
6	-3.694847	2.873540	-1.382246
1	-3.435251	2.277383	-2.263933
1	-3.346035	3.897823	-1.534864
8	-3.069705	2.373404	-0.214165
1	-3.321473	1.424903	-0.108451
1	-1.456255	4.001960	2.149466
6	-1.029651	4.447761	1.244129
1	-1.738019	5.180937	0.842067
1	-0.103077	4.963455	1.507378
8	-0.715938	3.461981	0.277668
1	-1.536114	2.951816	0.067995
6	2.802467	-2.735136	-0.390164
1	2.787417	-2.108872	-1.290264
1	2.596113	-3.768904	-0.676531
8	1.809655	-2.336464	0.539102
1	1.949798	-1.383026	0.724094
1	2.514276	4.170273	-0.611862
6	2.363253	3.098575	-0.779709
1	1.768379	2.958401	-1.688002
1	3.333189	2.614074	-0.918506
8	1.728681	2.501623	0.344892
1	0.779511	2.783003	0.368338
1	3.143002	0.791923	2.699207
6	3.636241	0.393807	1.807077
1	4.419790	1.091904	1.488589

1	4.094151	-0.567724	2.054532
8	2.700915	0.176646	0.759737
1	2.207023	1.038039	0.599495
1	-3.398503	-4.298713	-1.274308
6	-3.338626	-3.220921	-1.463756
1	-2.623446	-3.042206	-2.274211
1	-4.322791	-2.864906	-1.777876
8	-2.979757	-2.517046	-0.288644
1	-2.063560	-2.779421	-0.034478
1	-0.395337	-4.057225	2.242332
6	-0.548102	-4.494355	1.249479
1	0.242149	-5.229415	1.059172
1	-1.513452	-5.005896	1.234785
8	-0.571744	-3.500041	0.241309
1	0.261644	-2.978340	0.296285
6	5.546352	-0.469577	-1.261346
1	6.386959	-0.071226	-1.833655
1	5.861606	-0.568423	-0.212934
1	5.311786	-1.469969	-1.650455
8	4.466872	0.424811	-1.409662
1	3.773651	0.197826	-0.766051
1	3.801882	-2.688984	0.059997

Cartesian coordinates of : CY9_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	4.079953	1.832535	-1.112674
6	4.042419	1.505160	-0.067107
1	4.294320	2.351874	0.574959
1	4.786791	0.716058	0.090764
8	2.743851	1.058297	0.289471
1	2.474192	0.365386	-0.363891
1	-1.456167	-3.513520	-1.272958
6	-0.419456	-3.315545	-1.571440
1	-0.404685	-3.077867	-2.637547
1	0.175852	-4.220047	-1.401541
8	0.107185	-2.205544	-0.870113
1	0.170443	-2.400472	0.108041
1	2.019735	-2.148534	2.987578
6	1.814227	-2.238613	1.916257
1	2.399945	-3.070119	1.516848
1	2.120742	-1.308435	1.417019
8	0.442060	-2.527378	1.687719
1	-0.095132	-1.805954	2.111352
1	-0.300205	0.129529	0.546426
6	-0.323002	0.552255	1.563487
1	-0.923472	1.468654	1.545605
1	0.699204	0.802963	1.857931
8	-0.836924	-0.382592	2.503526
1	-1.796732	-0.489319	2.300567
1	-3.631700	0.310400	-2.154260
6	-4.144956	1.037715	-1.510866
1	-5.098163	0.609771	-1.191457
1	-4.344759	1.945033	-2.091286
8	-3.389347	1.330442	-0.350798
1	-2.522233	1.708879	-0.636733
6	3.285097	-1.706770	-1.642469
8	2.213695	-0.782519	-1.554344
1	4.150879	-1.180699	-2.050921
1	3.034254	-2.536118	-2.312599
1	3.549588	-2.113865	-0.658007
1	1.385904	-1.289109	-1.354474

6	0.945380	3.851665	1.301574
1	0.732478	3.262664	2.201959
1	1.903665	4.367808	1.431172
1	0.161577	4.602011	1.181305
8	0.953491	3.045754	0.138474
1	1.620298	2.325559	0.227742
6	-0.456837	1.132986	-2.077828
1	-0.433149	2.600703	-0.774413
1	0.633273	1.218686	-2.014602
1	-0.747600	0.152096	-1.677130
1	-0.749217	1.187728	-3.130413
8	-1.096211	2.184425	-1.367245
6	-2.930826	-1.701906	0.459539
1	-2.499885	-2.545657	1.007715
1	-3.830853	-2.049338	-0.062526
1	-2.194086	-1.356512	-0.278414
8	-3.243644	-0.682722	1.394382
1	-3.390588	0.140244	0.873405

Cartesian coordinates of : CY9_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-4.383778	0.379019	-1.840023
1	-4.607178	1.339719	-2.310562
1	-5.321830	-0.166924	-1.689848
1	-3.739582	-0.199394	-2.511604
8	-3.744643	0.641133	-0.604172
1	-3.486044	-0.219997	-0.199084
6	-4.019159	-2.240709	1.451774
1	-4.918609	-1.625285	1.529500
1	-3.434957	-2.130906	2.372318
1	-4.318866	-3.289836	1.346572
8	-3.292798	-1.802134	0.319696
1	-2.467338	-2.338054	0.245422
6	-1.499997	-4.554993	-0.704567
1	-1.059848	-5.497862	-0.360254
1	-1.079318	-4.304965	-1.684776
1	-2.579679	-4.688783	-0.808404
8	-1.281906	-3.518266	0.234603
1	-0.312660	-3.343266	0.282278
6	1.986337	-4.174193	1.271927
1	2.882935	-4.683775	0.900772
1	1.271448	-4.926085	1.615544
1	2.265597	-3.540024	2.120726
8	1.364463	-3.424831	0.245395
1	1.987057	-2.718164	-0.047917
6	3.995111	-2.121423	-1.636911
1	3.592599	-1.592053	-2.507697
1	3.868452	-3.196221	-1.789030
1	5.065573	-1.901453	-1.552551
8	3.307861	-1.769803	-0.450912
1	3.388241	-0.794897	-0.316980
6	4.862956	1.053766	0.741427
1	5.479559	1.913551	0.454864
1	5.500126	0.167244	0.791773
1	4.436198	1.238876	1.733381
8	3.854210	0.806768	-0.220620
1	3.220153	1.562714	-0.205431
6	2.803212	4.093936	-0.846510
1	2.206880	4.110775	-1.765799
1	3.853382	3.952826	-1.114097
1	2.695541	5.056631	-0.334828

8	2.425479	3.023797	-0.001054
1	1.469953	3.120200	0.226484
6	-0.459057	3.404725	1.993775
1	0.440386	3.568215	2.591791
1	-0.856684	2.408464	2.219881
1	-1.205799	4.157708	2.273566
8	-0.101350	3.523715	0.629792
1	-0.879301	3.257366	0.083933
6	-3.398302	3.809715	-0.086977
1	-2.941643	4.796324	0.026136
1	-3.802781	3.491250	0.881123
1	-4.222633	3.887658	-0.805320
8	-2.398245	2.921887	-0.550556
1	-2.777825	2.011242	-0.572750

Cartesian coordinates of : CY9_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-2.392874	0.726598	-1.804109
1	-2.673167	0.600904	-0.857264
6	-3.490122	1.197153	-2.564793
1	-3.145378	1.357328	-3.588355
1	-3.876732	2.145154	-2.171939
1	-4.302127	0.461877	-2.578802
8	1.614387	0.937460	1.879157
1	1.317166	1.805394	1.518504
6	0.498331	0.058027	1.861708
1	0.867741	-0.965625	1.969325
1	-0.055572	0.129236	0.914204
1	-0.187793	0.266582	2.688202
8	-0.373843	-2.656740	-0.213450
1	0.559357	-2.371141	-0.372227
6	-1.087432	-2.625789	-1.443308
1	-1.853469	-3.405219	-1.413447
1	-0.413762	-2.829054	-2.282714
1	-1.570194	-1.653628	-1.604081
8	-1.875432	-1.684163	1.718003
1	-1.241912	-2.034445	1.039603
6	-2.752607	-2.729855	2.100087
1	-3.459108	-2.324910	2.827334
1	-2.199805	-3.552813	2.565070
1	-3.315498	-3.116861	1.242068
8	0.570752	3.053711	0.628005
1	0.294166	2.640521	-0.231567
6	1.273689	4.254095	0.365033
1	1.607082	4.664050	1.320549
1	0.626856	4.989995	-0.124987
1	2.151430	4.077845	-0.268967
8	2.123173	-2.073309	-0.872738
1	2.631052	-1.379232	-0.380903
6	2.887170	-3.268335	-0.883862
1	2.251296	-4.068495	-1.270071
1	3.220995	-3.538838	0.123779
1	3.761436	-3.168050	-1.536595
8	-3.034514	0.475749	0.721385
1	-2.604125	-0.324684	1.116190
6	-2.682546	1.633277	1.467281
1	-3.404390	2.417240	1.226578
1	-1.676120	1.991193	1.218674
1	-2.733598	1.431260	2.542446
8	0.017461	1.792004	-1.603173
1	-0.915988	1.515526	-1.767041

6	0.838914	0.634167	-1.667991
1	1.623963	0.716559	-0.908407
1	1.306608	0.538715	-2.653505
1	0.260287	-0.271989	-1.463563
8	3.499258	-0.312289	0.539923
1	2.866269	0.192447	1.115130
6	4.383984	0.597572	-0.086248
1	4.960177	0.048131	-0.834103
1	5.078010	1.033261	0.640613
1	3.841617	1.407723	-0.591199

Cartesian coordinates of : BC9_5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.226291	-3.027434	-0.559417
1	-1.994465	-2.413892	-0.441304
6	-0.937389	-3.652665	0.684930
1	-0.370049	-4.562922	0.478558
1	-1.861151	-3.924242	1.205324
1	-0.339573	-2.997749	1.332585
8	3.385975	-1.792168	-0.311444
1	2.518095	-1.852051	-0.755925
6	3.391326	-2.656348	0.817712
1	4.357340	-2.538155	1.311211
1	3.283517	-3.701694	0.507972
1	2.596169	-2.396361	1.525653
8	0.823360	-0.675515	1.595573
1	0.978354	-0.934151	0.669816
6	-0.482559	-0.139201	1.664193
1	-0.695291	0.082272	2.713786
1	-1.243416	-0.846063	1.301483
1	-0.566583	0.789701	1.083874
8	-0.866025	2.624045	-0.816746
1	-0.001704	2.466763	-0.353996
6	-1.086356	4.019940	-0.914029
1	-2.053017	4.173152	-1.399564
1	-0.308862	4.498509	-1.518522
1	-1.109068	4.494086	0.075073
8	-2.991412	1.224644	-0.124413
1	-2.192610	1.700603	-0.464444
6	-3.353559	1.798435	1.118741
1	-4.022013	1.102482	1.632214
1	-3.878434	2.749905	0.974950
1	-2.473769	1.969306	1.751762
8	0.795763	-1.485023	-1.097378
1	0.049883	-2.141455	-1.009739
6	0.301838	-0.294904	-1.700384
1	0.971722	0.526810	-1.431463
1	-0.701835	-0.054845	-1.328220
1	0.266565	-0.390182	-2.790513
8	3.448167	0.886445	-0.224106
1	3.467196	-0.086049	-0.075655
6	3.952269	1.145541	-1.523609
1	3.798012	2.206301	-1.733774
1	3.427197	0.553348	-2.283032
1	5.023065	0.924375	-1.579912
8	-3.267124	-1.397314	-0.167323
1	-3.092841	-0.422871	-0.158397
6	-4.451262	-1.642318	-0.907888
1	-4.591531	-2.723732	-0.964562
1	-4.378493	-1.240887	-1.924514
1	-5.321268	-1.199481	-0.410733

8	1.389754	2.374158	0.485910
1	2.142611	1.782648	0.233961
6	1.380468	2.546845	1.893627
1	0.419768	2.992993	2.169974
1	2.183066	3.223002	2.207753
1	1.487423	1.583873	2.403320

Cartesian coordinates of : CY9_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	2.243739	-1.841198	-1.170257
1	2.396923	-0.868069	-1.223945
6	1.291763	-2.278189	-2.126503
1	1.357926	-3.366702	-2.182283
1	1.506973	-1.864895	-3.117372
1	0.267989	-2.001508	-1.840590
8	-0.690675	1.656802	1.784925
1	-1.253442	2.207121	1.194599
6	-1.240267	0.348989	1.801931
1	-0.541513	-0.308610	2.321679
1	-1.393263	-0.035943	0.785689
1	-2.196896	0.328968	2.336924
8	1.334127	-2.102157	1.298810
1	1.706195	-2.092046	0.381130
6	2.047489	-1.152672	2.072458
1	1.605690	-1.126523	3.071031
1	1.991030	-0.147472	1.635137
1	3.100861	-1.440360	2.166514
8	-1.234041	-2.678876	1.009700
1	-0.312961	-2.375464	1.200298
6	-1.244350	-4.097585	1.015913
1	-2.246330	-4.425312	0.730234
1	-1.016923	-4.485220	2.014127
1	-0.521438	-4.506820	0.300869
8	-2.116182	2.816354	-0.162000
1	-1.973689	2.104080	-0.832491
6	-3.463896	3.246238	-0.181310
1	-3.578645	4.018271	0.581846
1	-4.154708	2.424552	0.045385
1	-3.727519	3.674679	-1.154420
8	2.914743	0.741783	-0.978594
1	2.429554	1.268547	-0.296869
6	4.293630	0.755101	-0.645683
1	4.811207	0.090685	-1.340512
1	4.461756	0.397078	0.376914
1	4.711332	1.763329	-0.742833
8	-2.350831	-1.566227	-1.123181
1	-1.872949	-1.994101	-0.369524
6	-3.683007	-1.317818	-0.705149
1	-4.211604	-0.845983	-1.536423
1	-3.712952	-0.646113	0.162736
1	-4.196532	-2.250544	-0.447727
8	-1.380172	0.846831	-1.770379
1	-1.722804	-0.066310	-1.626741
6	0.024185	0.843371	-1.571664
1	0.346726	1.874120	-1.403046
1	0.551849	0.456346	-2.449873
1	0.305449	0.246541	-0.690407
8	1.770209	2.223178	0.911049
1	0.925778	1.912989	1.317443
6	1.577529	3.573138	0.512236
1	2.319594	3.809349	-0.255197

1	1.716689	4.251986	1.360192
1	0.574850	3.723998	0.093546

Cartesian coordinates of : BC9_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-2.136655	-1.348099	0.700527
1	-2.493922	-0.509015	0.291293
6	-2.968839	-1.739693	1.783392
1	-2.477774	-2.568919	2.297618
1	-3.952340	-2.066279	1.428135
1	-3.098823	-0.914391	2.491403
8	0.869613	-0.950022	-1.913093
1	0.390267	-1.775598	-1.685140
6	0.101450	0.143509	-1.434302
1	0.662851	1.061433	-1.625625
1	-0.084200	0.069200	-0.352172
1	-0.860640	0.212392	-1.953618
8	0.355105	2.428173	1.116988
1	1.282323	2.175342	0.880152
6	-0.151131	1.491693	2.058663
1	-1.146063	1.155798	1.739593
1	-0.237717	1.957267	3.045594
1	0.495537	0.611198	2.136149
8	-1.428621	2.729758	-0.736457
1	-0.675066	2.641458	-0.087178
6	-1.961702	4.040375	-0.635791
1	-2.833014	4.100695	-1.292029
1	-1.227146	4.784713	-0.959501
1	-2.273964	4.268355	0.389801
8	-0.751650	-2.934024	-1.022348
1	-1.389294	-2.452666	-0.457471
6	-0.436539	-4.178274	-0.415027
1	0.399657	-4.612267	-0.967117
1	-1.286359	-4.867655	-0.474421
1	-0.145125	-4.044348	0.633363
8	2.803018	1.585849	0.653765
1	2.997197	0.875476	-0.009356
6	3.565761	1.366584	1.827235
1	3.285754	2.133344	2.553452
1	4.638117	1.453863	1.621667
1	3.363541	0.379347	2.260259
8	-3.136885	0.807368	-0.330932
1	-2.496269	1.561893	-0.459984
6	-3.859204	0.599380	-1.532918
1	-4.362009	-0.368350	-1.464045
1	-3.193941	0.587579	-2.404072
1	-4.616797	1.378333	-1.672221
8	0.324338	-1.924226	1.932638
1	-0.401985	-1.572379	1.390366
6	1.541997	-1.819494	1.224080
1	2.339219	-2.159838	1.888874
1	1.758529	-0.784466	0.924712
1	1.551357	-2.442641	0.320030
8	3.303744	-0.353307	-1.079376
1	2.435010	-0.719575	-1.380202
6	4.047099	0.040919	-2.221588
1	4.938871	0.567041	-1.874577
1	3.467091	0.713394	-2.864140
1	4.357712	-0.831483	-2.805762

Cartesian coordinates of : BC9_6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.234535	-0.492876	-2.167002
1	1.069760	-0.954700	-1.993105
6	-0.051919	0.326201	-1.050946
1	-1.131651	0.323434	-0.877162
1	0.268750	1.364908	-1.217867
1	0.433470	-0.038219	-0.136514
8	1.379859	2.187408	1.067547
1	1.997856	1.796704	0.403735
6	2.113292	2.764896	2.129793
1	1.400359	3.249707	2.801074
1	2.820270	3.518582	1.766089
1	2.666778	2.003342	2.693680
8	1.278772	-2.130372	1.199110
1	0.304882	-2.187415	1.025043
6	1.493844	-1.178138	2.231982
1	2.535146	-1.262798	2.551339
1	0.846123	-1.387759	3.090937
1	1.306538	-0.152377	1.887169
8	-1.340245	-2.178021	0.995482
1	-1.978411	-1.742477	0.372273
6	-2.041865	-2.623800	2.140426
1	-1.358733	-3.234101	2.736648
1	-2.906228	-3.234480	1.860244
1	-2.388035	-1.780031	2.751758
8	-3.243323	1.601295	-0.587644
1	-2.530463	1.950159	-0.005830
6	-3.114216	2.156391	-1.885095
1	-3.958660	1.804086	-2.481192
1	-2.182820	1.838710	-2.372037
1	-3.145308	3.250621	-1.850650
8	2.578313	-1.509799	-0.950726
1	2.094971	-1.808951	-0.124866
6	3.503400	-2.504959	-1.361431
1	4.015864	-2.139181	-2.253456
1	2.988681	-3.439180	-1.607742
1	4.246640	-2.699509	-0.581006
8	-3.190272	-1.111146	-0.546856
1	-3.289628	-0.133787	-0.487496
6	-3.051661	-1.464665	-1.919559
1	-2.985329	-2.553265	-1.970760
1	-2.139991	-1.039912	-2.355960
1	-3.928446	-1.140956	-2.490783
8	-1.318469	2.208985	1.200697
1	-0.361218	2.292850	1.007946
6	-1.480416	1.141081	2.121338
1	-2.537300	1.102545	2.397876
1	-0.886710	1.309029	3.028226
1	-1.193641	0.177332	1.679915
8	3.091101	1.138755	-0.690218
1	3.027734	0.160450	-0.734612
6	2.996357	1.657288	-2.010467
1	2.800981	2.729213	-1.932242
1	2.177790	1.185973	-2.567001
1	3.936916	1.511844	-2.553036

Cartesian coordinates of : BC9_2-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-0.519330	2.881856	0.165508
1	0.328580	2.610443	-0.307114
6	-0.673939	4.290829	0.097709
1	-1.652060	4.544564	0.512141
1	-0.625431	4.641719	-0.938500
1	0.099133	4.798416	0.683876
8	-1.325728	-1.204725	-1.750864
1	-1.694091	-0.393635	-1.338464
6	-2.388157	-2.118203	-1.983012
1	-1.950058	-3.034124	-2.388023
1	-3.092148	-1.714235	-2.719242
1	-2.914068	-2.342782	-1.049355
8	2.789205	-1.576568	0.380464
1	1.934343	-1.889102	-0.027765
6	3.803985	-2.506741	0.039876
1	4.756768	-2.115940	0.405214
1	3.871582	-2.646613	-1.044501
1	3.618978	-3.477125	0.513846
8	-0.811563	0.728279	1.894424
1	-0.841165	1.625271	1.518268
6	0.337120	0.094640	1.345953
1	0.426267	-0.892135	1.805050
1	1.249777	0.664132	1.554268
1	0.237614	-0.034883	0.259057
8	3.525965	0.912709	0.010885
1	3.237504	-0.031415	0.125194
6	4.148537	1.357821	1.201280
1	4.397594	2.413719	1.077009
1	5.074057	0.802570	1.391325
1	3.488015	1.249816	2.070495
8	-2.595658	-1.226171	1.070370
1	-2.043173	-0.448545	1.281605
6	-3.498822	-1.417431	2.137850
1	-4.026318	-2.358675	1.964240
1	-4.243561	-0.610384	2.192037
1	-2.982724	-1.478760	3.103869
8	0.636437	-2.584323	-0.664616
1	-0.023166	-2.003434	-1.120835
6	-0.067925	-3.365160	0.295131
1	0.611663	-3.582382	1.125645
1	-0.390575	-4.314162	-0.148615
1	-0.940366	-2.821238	0.674714
8	-2.350940	1.170052	-0.896882
1	-1.711057	1.851601	-0.605958
6	-3.561111	1.347007	-0.181380
1	-4.166193	0.449938	-0.323003
1	-4.110730	2.220121	-0.552350
1	-3.375643	1.466153	0.894175
8	1.512026	2.110316	-1.181424
1	2.318010	1.779141	-0.708338
6	1.111201	1.118349	-2.120080
1	0.033533	1.206247	-2.285624
1	1.319243	0.109088	-1.744603
1	1.631235	1.258560	-3.072598

Cartesian coordinates of : BC9_8

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	2.651456	-0.711101	1.160068
1	1.829253	-0.459408	1.639615

6	2.524357	-2.072615	0.766743
1	3.413636	-2.333781	0.187363
1	1.632817	-2.237926	0.148794
1	2.484370	-2.726814	1.645831
8	-0.302254	-3.057103	-0.975459
1	-1.167861	-2.617536	-0.862635
6	-0.316404	-4.271641	-0.258487
1	0.660902	-4.744228	-0.387220
1	-1.083978	-4.961148	-0.631515
1	-0.484139	-4.113526	0.816590
8	-1.022839	2.616887	-0.903574
1	-0.282356	2.107344	-1.358716
6	-1.710061	3.436530	-1.834342
1	-2.527295	3.933751	-1.307861
1	-2.126979	2.839553	-2.652949
1	-1.044896	4.199259	-2.251906
8	0.242004	-0.251149	2.299722
1	-0.185275	0.536768	1.909636
6	-0.582655	-1.397585	2.172085
1	-0.123993	-2.191510	2.767107
1	-0.654733	-1.729849	1.129642
1	-1.590344	-1.209186	2.557102
8	3.208693	0.906819	-0.874055
1	3.030704	0.341835	-0.079360
6	4.145283	0.240293	-1.703162
1	4.397160	0.908268	-2.528966
1	3.729594	-0.687842	-2.116701
1	5.061286	0.006427	-1.149810
8	0.074087	2.391842	1.612480
1	-0.248937	2.771334	0.778283
6	1.480919	2.570645	1.703624
1	1.831867	1.955470	2.535107
1	1.734918	3.616744	1.908321
1	1.991714	2.250375	0.787814
8	0.764348	1.085492	-1.900559
1	1.699229	1.185677	-1.596210
6	0.333006	-0.200801	-1.458772
1	-0.676363	-0.370091	-1.843291
1	0.307755	-0.257871	-0.361486
1	0.982866	-0.991639	-1.842406
8	-2.672453	-1.733515	-0.487609
1	-2.501674	-0.896932	-0.005119
6	-3.552368	-1.454235	-1.560738
1	-3.682487	-2.374672	-2.133124
1	-3.145772	-0.682864	-2.227716
1	-4.532340	-1.125963	-1.195906
8	-2.182725	0.679113	0.651736
1	-1.819508	1.367220	0.054286
6	-2.925492	1.303322	1.690364
1	-3.362389	0.511243	2.302537
1	-3.737468	1.917707	1.285099
1	-2.271326	1.922062	2.313874

Cartesian coordinates of : BC9_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	2.628289	1.081433	0.455444
1	1.834408	1.294910	1.036236
6	3.719173	1.910177	0.832352
1	4.564665	1.669978	0.184126
1	4.006974	1.730870	1.873018
1	3.468292	2.969134	0.707531

8	0.927223	-2.866797	0.607038
1	1.799143	-2.557240	0.279859
6	0.583226	-2.058232	1.724096
1	-0.475698	-2.214871	1.944846
1	0.734739	-0.992470	1.509178
1	1.172480	-2.332995	2.604805
8	-2.667490	-0.822401	0.356739
1	-2.119111	-1.497114	-0.117454
6	-3.203723	0.105395	-0.578755
1	-4.117541	0.525238	-0.150735
1	-3.461209	-0.399615	-1.516627
1	-2.501739	0.921032	-0.795830
8	-1.279172	2.657631	-1.990165
1	-0.384069	2.271499	-1.972044
6	-1.873777	2.351535	-3.232597
1	-2.889603	2.753794	-3.220607
1	-1.934179	1.267091	-3.404436
1	-1.331885	2.805470	-4.071443
8	3.168237	-1.525459	-0.122691
1	3.008560	-0.620347	0.217256
6	3.623385	-1.417652	-1.462853
1	3.639952	-2.421960	-1.890345
1	4.639009	-1.007327	-1.499903
1	2.959192	-0.785644	-2.065510
8	0.967480	1.052371	-1.779977
1	1.687271	1.233515	-1.149082
6	0.227166	-0.052100	-1.277558
1	-0.558347	-0.288570	-1.998838
1	-0.245085	0.182299	-0.311884
1	0.861867	-0.937010	-1.157426
8	0.560878	1.822566	1.769031
1	-0.135356	1.187323	2.082785
6	-0.095555	2.825571	0.999407
1	0.642350	3.292855	0.340899
1	-0.519714	3.595372	1.652947
1	-0.888076	2.400762	0.373579
8	-1.498622	0.339182	2.405741
1	-1.898209	-0.149113	1.637930
6	-2.508652	1.141617	2.995127
1	-2.053213	1.708555	3.810211
1	-3.311589	0.519602	3.404314
1	-2.935122	1.847235	2.270735
8	-1.259598	-2.695914	-0.875281
1	-0.374835	-2.787560	-0.441995
6	-1.945676	-3.933624	-0.759881
1	-2.960544	-3.787877	-1.135577
1	-1.999833	-4.264995	0.283579
1	-1.455135	-4.708859	-1.357164

 Cartesian coordinates of : BC9_9

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.423215	-0.626487	2.189208
1	-1.867125	-0.898352	1.362020
6	-1.541091	0.787846	2.277656
1	-1.078063	1.099105	3.216239
1	-2.591837	1.099223	2.278229
1	-1.022606	1.285856	1.447832
8	1.074109	-1.538560	-1.586155
1	0.355273	-2.201441	-1.590945
6	0.527922	-0.321107	-1.114174
1	1.350248	0.389430	-0.993894

1	0.038809	-0.442806	-0.133768
1	-0.197554	0.096737	-1.822717
8	-0.121856	2.725203	-0.414425
1	0.581908	2.297589	0.149490
6	-0.434124	3.981474	0.167935
1	-1.260418	4.419158	-0.397265
1	0.425547	4.657566	0.118730
1	-0.740090	3.871252	1.215164
8	-2.332467	1.505001	-1.060258
1	-1.472062	1.920901	-0.773792
6	-2.532339	1.775178	-2.438663
1	-3.448989	1.270435	-2.751842
1	-1.698591	1.405481	-3.046711
1	-2.648160	2.850392	-2.610507
8	-1.176372	-2.990641	-1.060868
1	-1.833474	-2.276708	-0.954575
6	-0.921408	-3.525106	0.228223
1	-0.138924	-4.279384	0.125001
1	-1.815693	-4.000865	0.646695
1	-0.572031	-2.752126	0.925986
8	1.691980	1.805595	1.202294
1	1.530698	0.950284	1.670935
6	3.040070	1.826851	0.743299
1	3.122256	2.615322	-0.010212
1	3.323025	0.867912	0.292650
1	3.721625	2.059174	1.568552
8	-2.754371	-0.902022	-0.214810
1	-2.548893	0.009006	-0.580171
6	-4.154278	-0.991794	0.019530
1	-4.353837	-1.950433	0.502447
1	-4.713737	-0.945908	-0.920630
1	-4.492069	-0.184419	0.678169
8	1.304422	-0.575070	2.349009
1	0.352830	-0.803419	2.340868
6	2.068850	-1.642586	1.798820
1	3.100373	-1.301035	1.700771
1	1.710288	-1.921919	0.801362
1	2.039848	-2.517620	2.457536
8	3.711152	-1.083681	-0.929502
1	2.851959	-1.489462	-1.141363
6	4.163483	-0.407745	-2.083116
1	5.103123	0.088728	-1.828312
1	3.446683	0.355739	-2.418578
1	4.350100	-1.096168	-2.916398

Cartesian coordinates of : BC9_10

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-0.622270	-0.787839	1.468006
1	-0.655662	-0.674539	0.497419
6	0.587538	-0.226225	1.936172
1	0.594522	-0.312008	3.025394
1	0.675832	0.834182	1.662456
1	1.458274	-0.764974	1.535256
8	1.046406	-2.837255	-0.400711
1	0.285845	-2.333098	-0.748608
6	0.638800	-3.669835	0.678503
1	1.542563	-4.103348	1.111108
1	-0.000835	-4.482547	0.318163
1	0.106794	-3.090516	1.439573
8	0.944344	2.754655	-0.032797
1	1.719859	2.157139	0.097754

6	1.189811	3.580099	-1.156976
1	0.278506	4.146563	-1.361499
1	1.441879	2.986503	-2.044716
1	2.006452	4.283199	-0.959749
8	-0.636943	-0.896260	-1.316330
1	-1.561184	-0.616953	-1.537190
6	0.260728	0.043834	-1.897557
1	1.177147	0.058396	-1.297158
1	-0.177845	1.046447	-1.893285
1	0.507565	-0.240991	-2.926035
8	-2.862913	0.415048	-1.639058
1	-2.611581	0.989440	-0.885095
6	-4.265602	0.212140	-1.675835
1	-4.460855	-0.642402	-2.327709
1	-4.771564	1.090585	-2.092049
1	-4.654861	0.004306	-0.674879
8	3.228681	-1.332235	-0.307787
1	2.420592	-1.899772	-0.267247
6	3.914624	-1.613001	-1.517426
1	4.751190	-0.915417	-1.595618
1	3.260804	-1.480454	-2.387603
1	4.304524	-2.636015	-1.517504
8	-1.560069	1.820758	0.281522
1	-0.642373	2.140576	0.134284
6	-1.997515	2.233943	1.564460
1	-3.059502	1.994542	1.646261
1	-1.856082	3.311442	1.703585
1	-1.459007	1.698121	2.357747
8	-3.393008	-0.513643	1.325247
1	-2.471465	-0.340254	1.580623
6	-3.442088	-1.842920	0.852146
1	-4.492237	-2.101738	0.693736
1	-3.013114	-2.548933	1.573295
1	-2.910772	-1.955206	-0.105402
8	3.107482	1.247510	0.292932
1	3.117696	0.288752	0.052425
6	3.705327	1.407146	1.567713
1	3.645366	2.464735	1.833735
1	4.757857	1.105500	1.548679
1	3.182255	0.821754	2.334459

Cartesian coordinates of : BC9_11

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.454556	2.333878	-0.769445
1	0.565040	2.322315	-0.329809
6	1.760206	3.669395	-1.129220
1	2.734736	3.670123	-1.621778
1	1.810557	4.323355	-0.250128
1	1.013888	4.068223	-1.824676
8	-1.189908	-0.396907	1.494950
1	-1.067762	-1.004918	0.744657
6	-2.399739	-0.690040	2.163718
1	-2.498953	0.023227	2.985853
1	-2.398828	-1.703692	2.586167
1	-3.269584	-0.573614	1.505293
8	-3.069496	-1.511088	-1.149642
1	-2.122658	-1.749657	-1.224160
6	-3.779351	-2.582192	-0.553812
1	-4.770784	-2.214227	-0.281917
1	-3.278774	-2.942309	0.353522
1	-3.893383	-3.416860	-1.253800

8	3.596755	-1.381514	-0.496363
1	3.428640	-0.614167	0.101739
6	3.884070	-0.860350	-1.783001
1	3.788199	-1.672007	-2.507935
1	4.906771	-0.470024	-1.826556
1	3.184508	-0.059209	-2.053427
8	-0.874205	2.450616	0.452957
1	-1.578667	1.797865	0.237303
6	-0.882750	2.709602	1.845219
1	-0.063939	3.402020	2.059025
1	-0.735007	1.786784	2.415757
1	-1.825422	3.180427	2.146794
8	1.631042	-3.122836	-0.071360
1	2.398163	-2.558211	-0.335942
6	1.500125	-3.002834	1.338929
1	0.801733	-3.771387	1.677255
1	1.103755	-2.017955	1.622988
1	2.463927	-3.160652	1.833800
8	-0.415833	-1.714730	-0.863685
1	0.292432	-2.386752	-0.669344
6	0.231720	-0.508623	-1.263236
1	-0.519308	0.285922	-1.285038
1	0.678040	-0.610950	-2.258016
1	1.012690	-0.230272	-0.545031
8	2.964637	0.835239	0.842865
1	2.528408	1.439732	0.197269
6	2.118425	0.754429	1.980868
1	2.530335	-0.004981	2.649894
1	1.091679	0.471708	1.710326
1	2.095664	1.711317	2.516301
8	-3.010775	1.108892	-0.469747
1	-3.090175	0.144825	-0.629777
6	-3.370512	1.799454	-1.654052
1	-3.133703	2.854837	-1.503042
1	-4.442117	1.701737	-1.859885
1	-2.807444	1.431991	-2.520411

Cartesian coordinates of : BC9_7

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	3.158843	-0.189616	0.752859
1	2.600118	-0.974531	0.579997
6	3.243154	0.075618	2.142414
1	3.746511	1.037939	2.261874
1	3.837896	-0.693873	2.648121
1	2.247819	0.121914	2.595325
8	-2.371538	2.586754	-0.473215
1	-1.386503	2.612307	-0.474501
6	-2.851865	3.751154	0.175462
1	-3.935300	3.654674	0.273994
1	-2.629583	4.648835	-0.411012
1	-2.414842	3.864039	1.175390
8	-3.135237	-1.890075	-1.187920
1	-3.384960	-1.054495	-0.722168
6	-4.072730	-2.905883	-0.885892
1	-3.756003	-3.816140	-1.398627
1	-5.072995	-2.635147	-1.240405
1	-4.119506	-3.107560	0.191434
8	2.142631	-2.285570	-0.691586
1	1.188431	-2.301899	-0.885339
6	2.853706	-1.894459	-1.855244
1	3.907019	-1.817689	-1.577713

1	2.517414	-0.915488	-2.221998
1	2.750938	-2.636727	-2.654591
8	2.471610	1.565566	-1.110725
1	2.754447	0.957226	-0.384200
6	3.607748	1.995758	-1.835408
1	3.261740	2.617784	-2.663215
1	4.160520	1.142036	-2.245674
1	4.285783	2.588182	-1.210019
8	-3.529339	0.290174	0.279450
1	-3.177515	1.128093	-0.100635
6	-2.844734	0.054636	1.500288
1	-3.276039	-0.838766	1.957904
1	-2.974494	0.896595	2.190362
1	-1.771304	-0.116959	1.346596
8	-0.527014	-1.651523	-0.826613
1	-1.459559	-1.947886	-0.963068
6	-0.422909	-0.318820	-1.325571
1	0.601848	0.026255	-1.160499
1	-1.108581	0.353753	-0.797886
1	-0.644923	-0.285395	-2.397010
8	0.549741	-1.348981	1.718935
1	0.079515	-1.536963	0.885134
6	0.951601	-2.575108	2.302976
1	1.496697	-2.336817	3.220062
1	1.613482	-3.140319	1.634878
1	0.089996	-3.199628	2.569734
8	0.250906	2.694847	-0.041632
1	1.015071	2.459012	-0.606425
6	0.442249	2.051854	1.210448
1	-0.466843	2.198803	1.800646
1	1.287495	2.494248	1.751070
1	0.614067	0.973489	1.099186

Cartesian coordinates of the methanol decamer

Cartesian coordinates of : BC10_5

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-2.751361	-2.133256	0.072466
1	-2.023035	-2.102967	0.729849
6	-2.528797	-3.155427	-0.890713
1	-3.355430	-3.115149	-1.603311
1	-2.528727	-4.142832	-0.416344
1	-1.582505	-3.018697	-1.429072
8	2.121556	1.988841	-1.365894
1	1.428173	2.411590	-0.779373
6	2.933347	3.004446	-1.938422
1	3.719034	2.519011	-2.520771
1	3.397492	3.621210	-1.161548
1	2.345456	3.645856	-2.602281
8	-0.992727	-1.445039	1.983733
1	-0.023750	-1.293997	1.941195
6	-1.608428	-0.203392	2.282879
1	-2.681646	-0.382388	2.391986
1	-1.455752	0.528532	1.477092
1	-1.221612	0.214339	3.219946
8	-2.183118	2.509133	0.149961
1	-2.616553	1.675067	-0.164795
6	-2.959949	3.079647	1.187134
1	-2.516934	4.044738	1.444266
1	-2.964842	2.443299	2.082019

1	-3.992654	3.241798	0.862079
8	0.841130	-3.070591	-1.765684
1	0.840583	-2.154481	-2.088505
6	1.051800	-3.046054	-0.370819
1	1.740182	-3.854102	-0.100923
1	0.112798	-3.199342	0.182687
1	1.481273	-2.092018	-0.039573
8	0.709425	-0.313597	-2.030896
1	1.308019	0.441253	-2.155545
6	-0.147390	0.010187	-0.948592
1	-0.817331	-0.838118	-0.781422
1	-0.753195	0.895406	-1.171766
1	0.422672	0.184267	-0.024350
8	-3.409039	0.339813	-0.732498
1	-3.228505	-0.553280	-0.354879
6	-3.401636	0.224822	-2.146756
1	-3.393801	1.234136	-2.565008
1	-4.297870	-0.296262	-2.500525
1	-2.510685	-0.309076	-2.500826
8	3.204649	-0.018330	0.143618
1	2.879786	0.747908	-0.374463
6	3.818638	-0.951041	-0.735462
1	4.119004	-1.816736	-0.140833
1	4.713245	-0.519097	-1.197515
1	3.124837	-1.285810	-1.514821
8	0.425832	3.031245	0.301863
1	-0.531745	2.833986	0.160752
6	0.782974	2.631479	1.618521
1	1.793272	2.997380	1.814716
1	0.776457	1.540812	1.735466
1	0.101098	3.070996	2.354994
8	1.626478	-0.803620	2.181213
1	2.181637	-0.490341	1.431310
6	2.343650	-1.807728	2.880690
1	1.720430	-2.141807	3.712540
1	3.285117	-1.413836	3.278012
1	2.558160	-2.669667	2.235718

Cartesian coordinates of : BC10_7

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-3.475801	0.093560	0.016005
1	-2.938855	0.720298	0.540948
6	-3.985281	0.792899	-1.110667
1	-4.333522	0.051141	-1.832982
1	-3.208972	1.406595	-1.584774
1	-4.829644	1.430923	-0.826454
8	2.493556	-1.434046	1.653957
1	2.624123	-0.945367	0.808394
6	3.680787	-1.336472	2.421748
1	3.517778	-1.875794	3.356812
1	3.927300	-0.293252	2.653377
1	4.526683	-1.791167	1.895187
8	-1.873916	2.077072	0.967430
1	-1.175446	1.909561	1.675436
6	-2.455069	3.360463	1.162548
1	-3.098523	3.572803	0.305629
1	-1.681403	4.132990	1.223187
1	-3.057429	3.382114	2.075944
8	0.045824	-2.532372	-2.115006
1	-0.865367	-2.357901	-1.822376
6	0.751878	-3.000509	-0.986415

1	1.664173	-3.491591	-1.335228
1	0.167277	-3.729964	-0.410425
1	1.040702	-2.183368	-0.308655
8	-2.357289	-2.236231	-0.753620
1	-2.773029	-1.416749	-0.408633
6	-3.068748	-3.374160	-0.308691
1	-2.601483	-4.252453	-0.760112
1	-4.119472	-3.340081	-0.619016
1	-3.024546	-3.474963	0.783154
8	0.098134	-0.963258	2.791117
1	0.992042	-1.197005	2.447567
6	-0.851767	-1.296575	1.789746
1	-1.850198	-1.104280	2.192691
1	-0.782023	-2.350790	1.504992
1	-0.717548	-0.690874	0.880817
8	-0.550030	1.811939	-1.443015
1	-1.013146	1.920928	-0.586624
6	-0.422509	0.422495	-1.737102
1	-0.062877	0.327394	-2.763452
1	-1.385064	-0.092359	-1.654791
1	0.301252	-0.069455	-1.072598
8	0.092995	1.658522	2.550734
1	0.068530	0.717270	2.862173
6	1.167574	1.748203	1.620523
1	1.170478	2.753448	1.194773
1	1.046880	1.019326	0.807007
1	2.129581	1.567449	2.110985
8	2.989659	-0.102865	-0.619889
1	2.673116	0.810225	-0.806459
6	3.096175	-0.810942	-1.847566
1	3.574585	-1.769342	-1.634039
1	3.723242	-0.261767	-2.559198
1	2.112099	-1.004536	-2.292337
8	2.069430	2.333824	-1.334135
1	1.084446	2.297371	-1.360758
6	2.555835	2.741046	-2.602329
1	3.646353	2.691603	-2.570142
1	2.258793	3.770889	-2.826723
1	2.195387	2.082880	-3.402697

Cartesian coordinates of : CY10_1

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.139766	-1.054413	-2.114289
1	-0.503366	-1.658550	-1.666427
6	-0.479177	0.183419	-2.333695
1	-1.189404	0.862914	-2.809949
1	0.385197	0.057533	-2.994957
1	-0.141048	0.633067	-1.391720
8	1.248149	2.813428	-1.194580
1	0.523173	2.644719	-0.543484
6	1.506029	4.207931	-1.228171
1	2.350784	4.374943	-1.899302
1	1.761167	4.592985	-0.234402
1	0.638753	4.757543	-1.610702
8	0.771976	-2.568387	-1.017496
1	1.321993	-2.425513	-0.208749
6	1.578037	-3.185857	-2.005606
1	0.983705	-3.264059	-2.919099
1	1.882638	-4.191394	-1.695699
1	2.477024	-2.594247	-2.217640
8	-3.481776	-0.348076	1.723900

1	-3.475622	-0.605116	0.772744
6	-4.590277	0.503974	1.946821
1	-4.477485	0.953894	2.935458
1	-5.530701	-0.058992	1.926665
1	-4.639034	1.303366	1.197630
8	3.368183	1.244828	-0.735692
1	2.621123	1.864907	-0.910651
6	3.126404	0.049472	-1.460253
1	3.932203	-0.651330	-1.226892
1	3.120900	0.235796	-2.540624
1	2.171245	-0.412530	-1.173758
8	-0.755323	2.481261	0.501624
1	-0.749378	1.788825	1.207637
6	-2.022397	2.431823	-0.136589
1	-1.927226	2.904107	-1.118355
1	-2.771874	2.980148	0.445629
1	-2.364651	1.398187	-0.277721
8	-3.489837	-0.779789	-0.920693
1	-2.615803	-0.897281	-1.371533
6	-4.433091	-1.667430	-1.495859
1	-5.382882	-1.530115	-0.973956
1	-4.120431	-2.712065	-1.387638
1	-4.582125	-1.446700	-2.558140
8	3.095537	0.236589	1.702897
1	3.349346	0.703136	0.870952
6	2.228570	1.081958	2.444308
1	1.580086	0.462949	3.068583
1	1.588995	1.677823	1.780065
1	2.804308	1.759216	3.084095
8	-0.910391	0.355589	2.070915
1	-1.869337	0.153344	2.153552
6	-0.355440	-0.642833	1.225207
1	0.573857	-0.254162	0.793776
1	-1.040891	-0.896493	0.407441
1	-0.120130	-1.553506	1.787287
8	2.467638	-2.248986	0.999050
1	2.702640	-1.327392	1.273583
6	2.445863	-3.084365	2.141890
1	2.131939	-4.080722	1.822804
1	1.737454	-2.718650	2.895789
1	3.440603	-3.155500	2.594293

Cartesian coordinates of : BC10_13

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	3.165609	0.092026	-0.163976
1	2.846360	-0.209220	0.711271
6	3.272114	1.509832	-0.171002
1	3.544227	1.812670	-1.184858
1	4.058765	1.844466	0.514196
1	2.325309	1.994766	0.090582
8	0.128743	3.338288	0.041915
1	0.226015	2.677352	0.754588
6	-0.299374	4.556908	0.610535
1	-0.415831	5.278646	-0.201091
1	0.430575	4.955700	1.326478
1	-1.266435	4.452880	1.122011
8	-2.249118	-1.125841	-1.321091
1	-1.412951	-0.836475	-1.790106
6	-3.220959	-1.512285	-2.285614
1	-4.154397	-1.713647	-1.755725
1	-2.908388	-2.415923	-2.818733

1	-3.391752	-0.707217	-3.007806
8	-2.050317	-2.470696	1.043344
1	-2.110812	-2.081870	0.145883
6	-3.142433	-1.993249	1.818758
1	-2.923814	-2.206699	2.867487
1	-4.068044	-2.511853	1.544563
1	-3.287843	-0.914431	1.689954
8	2.084049	-0.650215	2.249736
1	1.473366	-1.420888	2.045131
6	2.891267	-0.948690	3.380890
1	3.594606	-0.125236	3.517752
1	3.453528	-1.874757	3.225574
1	2.279238	-1.044542	4.283352
8	2.322620	-1.131151	-2.398042
1	2.638864	-0.722073	-1.558869
6	3.191291	-0.743560	-3.449375
1	2.903720	-1.301392	-4.342281
1	4.232015	-0.981590	-3.205781
1	3.110137	0.329533	-3.664887
8	0.596994	-2.569892	1.403674
1	-0.382216	-2.548226	1.504849
6	0.862685	-2.438926	0.010788
1	1.928412	-2.611395	-0.150861
1	0.609661	-1.431065	-0.346782
1	0.293826	-3.174444	-0.566270
8	-3.609733	0.897289	0.094367
1	-3.059797	0.261406	-0.395501
6	-3.301934	2.203120	-0.352186
1	-3.969310	2.893005	0.169456
1	-3.469401	2.316332	-1.432111
1	-2.262063	2.484789	-0.131335
8	-0.163185	-0.151097	-2.495665
1	0.684772	-0.646601	-2.573216
6	0.114893	1.048948	-1.778675
1	-0.813824	1.609975	-1.671902
1	0.836716	1.674116	-2.314346
1	0.510676	0.835964	-0.775905
8	0.245647	1.376206	1.955223
1	1.011519	0.797723	2.127837
6	-0.902480	0.551834	1.819759
1	-1.787860	1.189957	1.838061
1	-0.969020	-0.171535	2.641637
1	-0.899441	-0.001119	0.868550

Cartesian coordinates of : BDC10

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.194994	-1.676357	1.296838
1	1.903220	-1.433355	0.643844
6	1.759213	-2.520149	2.285257
1	0.952590	-2.846168	2.946890
1	2.510912	-1.990665	2.882142
1	2.225037	-3.403601	1.832731
8	3.257184	1.289944	-1.157609
1	2.602034	1.667734	-0.531101
6	3.540033	2.187993	-2.210913
1	4.267578	1.709060	-2.868892
1	3.972587	3.121139	-1.833226
1	2.640764	2.423332	-2.794070
8	-0.659375	0.116520	2.305156
1	0.044828	-0.477644	1.985066
6	-1.898626	-0.416432	1.884271

1	-2.641110	0.387585	1.896429
1	-2.242397	-1.218225	2.553751
1	-1.834205	-0.800316	0.858513
8	-2.692259	-1.064960	-1.534147
1	-1.938619	-1.653031	-1.309322
6	-3.874495	-1.682119	-1.057669
1	-4.702488	-0.988155	-1.219457
1	-3.808970	-1.901220	0.016487
1	-4.082947	-2.611222	-1.599932
8	1.474228	1.786492	0.759405
1	0.604926	2.283500	0.805102
6	2.050105	1.643816	2.051031
1	2.853289	0.905362	1.976362
1	1.302863	1.293119	2.768998
1	2.476095	2.593401	2.394325
8	3.051803	-1.337559	-0.534905
1	3.225837	-0.420497	-0.835064
6	2.544942	-2.096450	-1.624597
1	2.285505	-3.087169	-1.242973
1	3.302174	-2.207992	-2.407817
1	1.639454	-1.641701	-2.040573
8	-0.724775	-2.741861	-0.652141
1	-0.123097	-2.045736	-0.330080
6	-0.897835	-3.707836	0.365435
1	-1.640667	-4.427459	0.014391
1	-1.253347	-3.252494	1.298417
1	0.039354	-4.239403	0.569260
8	-2.679032	1.452210	-0.568668
1	-2.524825	0.516254	-0.833307
6	-3.214608	2.149017	-1.678431
1	-3.368245	3.187141	-1.375487
1	-4.176902	1.723230	-1.984684
1	-2.531321	2.129804	-2.536350
8	0.067266	-0.102583	-0.720645
1	0.571119	0.384604	-0.041910
6	0.075458	0.660731	-1.912962
1	-0.711165	0.266122	-2.562683
1	1.042650	0.588136	-2.427979
1	-0.138257	1.718666	-1.708441
8	-0.862783	2.913112	0.715444
1	-1.460938	2.275387	0.253815
6	-1.421374	3.201664	1.991326
1	-0.887563	4.063313	2.399158
1	-1.309501	2.346317	2.666176
1	-2.481130	3.461776	1.895191

Cartesian coordinates of : BC10_3

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.677901	-1.152561	2.377894
1	1.260680	-1.488937	1.655254
6	1.427786	-0.980546	3.564416
1	0.729201	-0.754021	4.373013
1	2.134661	-0.145311	3.471226
1	1.984381	-1.887533	3.824422
8	-2.647525	-1.665970	-2.372841
1	-1.684502	-1.695938	-2.246243
6	-2.917401	-0.608016	-3.267215
1	-4.002993	-0.518804	-3.356179
1	-2.502260	-0.796729	-4.265116
1	-2.518797	0.349449	-2.900547
8	2.666668	-0.462518	-1.670319

1	2.667587	0.444248	-1.231574
6	3.836538	-0.615350	-2.460875
1	3.853551	-1.637400	-2.844833
1	4.738366	-0.445164	-1.863361
1	3.830266	0.079602	-3.306472
8	0.696970	3.403361	-0.371632
1	-0.035089	3.033147	0.184732
6	0.142320	4.080835	-1.483933
1	0.964247	4.510305	-2.060055
1	-0.518556	4.890537	-1.157532
1	-0.423350	3.398472	-2.131486
8	-3.170222	0.660207	1.035706
1	-2.771881	-0.175014	1.377200
6	-4.140566	0.344086	0.048546
1	-4.411812	1.271500	-0.461887
1	-5.041901	-0.074195	0.510742
1	-3.748687	-0.369741	-0.686888
8	-1.186212	2.413437	1.170999
1	-1.963342	1.844679	0.956303
6	-0.761341	2.076735	2.482791
1	0.089347	2.717583	2.730664
1	-0.444752	1.026972	2.539075
1	-1.561730	2.256508	3.208190
8	2.212872	-2.123829	0.436643
1	2.441974	-1.531036	-0.311424
6	1.759872	-3.366635	-0.083779
1	1.308721	-3.925007	0.739695
1	2.596816	-3.948383	-0.485453
1	1.005350	-3.215663	-0.863554
8	-0.049438	-0.958575	-1.764377
1	0.891053	-0.889300	-2.001916
6	-0.344258	0.074296	-0.833056
1	-1.425467	0.070462	-0.667923
1	-0.043343	1.057662	-1.213637
1	0.144787	-0.099863	0.135865
8	-1.950869	-1.600876	1.801685
1	-1.062271	-1.429899	2.171915
6	-1.803369	-2.557097	0.758926
1	-2.709734	-2.543315	0.149537
1	-1.663955	-3.562696	1.172672
1	-0.954282	-2.310833	0.109607
8	2.708615	1.717380	-0.332204
1	1.996986	2.395781	-0.467861
6	2.665076	1.323817	1.032981
1	3.314012	0.450776	1.153273
1	1.647741	1.044996	1.336212
1	3.030963	2.128899	1.679095

Cartesian coordinates of : BC10_4

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	2.844504	-1.997771	-0.849724
1	1.879028	-2.041044	-1.066524
6	3.581029	-2.302928	-2.023233
1	4.634695	-2.102356	-1.818425
1	3.259142	-1.684202	-2.868759
1	3.467683	-3.358528	-2.290610
8	-2.773260	1.436442	-0.785825
1	-1.923549	1.833789	-1.057365
6	-3.386871	0.810561	-1.898381
1	-4.386387	0.500812	-1.588301
1	-2.835024	-0.082981	-2.219130

1	-3.478224	1.499693	-2.746232
8	0.526398	-0.791116	2.814519
1	-0.010392	0.011673	2.716555
6	0.583238	-1.390909	1.535391
1	1.137794	-2.328523	1.626301
1	1.108438	-0.753831	0.809545
1	-0.417555	-1.601557	1.132056
8	-1.946012	-2.748369	-0.733849
1	-2.372107	-2.009994	-0.234162
6	-1.976589	-3.909644	0.077073
1	-1.484278	-4.715115	-0.471516
1	-3.008148	-4.211893	0.289281
1	-1.446166	-3.754590	1.025600
8	-0.374017	2.629156	-1.509159
1	0.416006	2.413938	-0.972498
6	0.006227	2.981018	-2.826715
1	-0.906873	3.181701	-3.390628
1	0.552245	2.167888	-3.320574
1	0.626320	3.884258	-2.834751
8	3.436282	0.263766	0.335181
1	3.221228	-0.584187	-0.140515
6	3.752993	-0.046335	1.691422
1	4.317179	0.794388	2.102634
1	4.377325	-0.943454	1.738885
1	2.847469	-0.206294	2.288968
8	0.351240	-1.776963	-1.652641
1	-0.459849	-2.258161	-1.357389
6	0.055670	-0.391144	-1.662951
1	1.001237	0.159481	-1.589587
1	-0.578006	-0.105582	-0.812366
1	-0.443993	-0.097336	-2.594416
8	1.535753	1.985672	0.301434
1	2.259375	1.282586	0.254792
6	1.984058	3.035429	1.149496
1	1.325635	3.895639	1.002888
1	3.009225	3.325927	0.898323
1	1.942244	2.730267	2.202159
8	-2.984453	-0.785942	0.743202
1	-2.685946	0.106913	0.468920
6	-2.987168	-0.915143	2.154747
1	-3.478862	-1.861055	2.394638
1	-3.556857	-0.103043	2.619960
1	-1.973051	-0.923745	2.566570
8	-0.851743	1.251867	1.493233
1	-0.012031	1.404933	1.015783
6	-1.464696	2.511369	1.732818
1	-2.506308	2.327203	2.003821
1	-1.453158	3.134905	0.831913
1	-0.970379	3.043910	2.555175

 Cartesian coordinates of : BC10_10

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-3.948147	-0.889976	0.135008
1	-3.224707	-1.455754	-0.218815
6	-5.171107	-1.261923	-0.474105
1	-5.946866	-0.593466	-0.094880
1	-5.443355	-2.293073	-0.222348
1	-5.125899	-1.163285	-1.565905
8	2.567761	0.004371	-2.074685
1	2.550146	0.854660	-1.539521
6	3.681311	0.032403	-2.956040

1	3.731671	-0.930919	-3.467649
1	4.615290	0.190714	-2.405424
1	3.568161	0.824414	-3.702654
8	-0.312863	1.014960	2.312352
1	0.253361	0.215580	2.323634
6	-1.682531	0.644596	2.382126
1	-2.279677	1.523478	2.130353
1	-1.944792	0.306636	3.390807
1	-1.929366	-0.148292	1.666195
8	0.554281	2.997357	0.695276
1	0.238548	2.316844	1.331861
6	-0.566168	3.712976	0.187903
1	-0.262135	4.192317	-0.746628
1	-0.873759	4.493599	0.892667
1	-1.413491	3.044924	-0.004241
8	-1.879663	-2.392878	-0.678447
1	-1.270222	-1.942145	-1.295037
6	-1.155321	-2.727107	0.497664
1	-1.859244	-2.754641	1.333822
1	-0.381875	-1.982436	0.719095
1	-0.686569	-3.712662	0.400204
8	-0.109946	-0.698630	-1.825163
1	0.754740	-0.647175	-2.263829
6	-0.138505	0.336103	-0.848118
1	-1.106494	0.300644	-0.342126
1	-0.035098	1.323511	-1.312483
1	0.656779	0.202879	-0.103422
8	-3.176409	1.679520	-0.449717
1	-3.518115	0.838110	-0.089519
6	-3.124544	1.541092	-1.853386
1	-2.574246	2.397461	-2.254809
1	-4.127050	1.537553	-2.301835
1	-2.598921	0.624598	-2.158589
8	2.527854	-1.839624	-0.066375
1	2.599612	-1.169019	-0.779906
6	2.153519	-3.080434	-0.645013
1	1.979554	-3.786167	0.170235
1	2.953796	-3.472689	-1.282423
1	1.232052	-2.983665	-1.231292
8	2.703676	2.021746	-0.475012
1	1.878087	2.495850	-0.200597
6	3.243667	1.451361	0.709954
1	4.000770	0.716274	0.420524
1	2.464902	0.940979	1.292083
1	3.711290	2.220268	1.332626
8	1.355786	-1.149296	2.255263
1	1.754454	-1.394848	1.389372
6	2.354665	-1.218279	3.258485
1	1.908878	-0.877191	4.194747
1	3.209823	-0.573400	3.020944
1	2.711404	-2.245599	3.389927

Cartesian coordinates of : CY10_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	4.363034	0.162417	-0.474357
1	3.827352	0.242072	0.345015
6	4.296129	-1.188582	-0.899034
1	5.028194	-1.323615	-1.697475
1	3.299566	-1.442253	-1.286656
1	4.538622	-1.874881	-0.079251
8	-3.260016	1.958384	0.051565

1	-3.301143	0.995200	-0.162414
6	-3.911547	2.157989	1.296335
1	-4.026760	3.233931	1.444630
1	-3.325401	1.747474	2.128525
1	-4.902161	1.692977	1.296426
8	0.470527	-2.803027	-0.576910
1	0.681186	-2.020215	-1.138246
6	1.418325	-2.881214	0.479384
1	0.925088	-3.329074	1.348183
1	1.791713	-1.887240	0.753533
1	2.262781	-3.517185	0.190533
8	-3.550750	-0.649564	-0.327381
1	-2.915448	-1.328015	0.013824
6	-4.172730	-1.156176	-1.493883
1	-4.726032	-0.339690	-1.963026
1	-4.875872	-1.960875	-1.248969
1	-3.434091	-1.536232	-2.210533
8	2.612845	1.416788	-2.089003
1	3.393535	1.044402	-1.619483
6	2.080421	2.446595	-1.268135
1	1.205720	2.860846	-1.774387
1	2.815589	3.244106	-1.113312
1	1.754390	2.056909	-0.294347
8	0.763561	-0.499332	-1.854412
1	1.491333	0.147988	-2.018884
6	-0.486669	0.129346	-2.091272
1	-1.273594	-0.552211	-1.752232
1	-0.630868	0.331231	-3.158750
1	-0.575552	1.064568	-1.524787
8	-1.939031	-2.603141	0.413819
1	-1.032318	-2.666721	0.007410
6	-2.567948	-3.871285	0.361131
1	-3.580621	-3.759554	0.756340
1	-2.032499	-4.601820	0.977701
1	-2.627234	-4.249485	-0.666222
8	-0.765069	2.792275	0.199743
1	-1.714324	2.525981	0.091189
6	-0.638356	4.200445	0.171264
1	0.423480	4.442487	0.265886
1	-1.177467	4.673865	1.000664
1	-1.006990	4.611549	-0.775352
8	0.250445	0.974869	1.896316
1	-0.022152	1.752599	1.360090
6	-0.541167	-0.127130	1.468043
1	-0.358656	-0.962832	2.147674
1	-0.273885	-0.433787	0.449542
1	-1.609851	0.116200	1.502824
8	2.737101	0.112852	1.670289
1	1.836823	0.522705	1.723260
6	3.059047	-0.466834	2.919395
1	4.079268	-0.853125	2.857801
1	2.383120	-1.298433	3.159200
1	3.010949	0.271058	3.727377

Cartesian coordinates of : BC10_2

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-0.223414	1.449701	1.009875
1	0.146520	1.770336	0.162967
6	0.318703	0.153397	1.239422
1	-0.105065	-0.219505	2.176581
1	1.411554	0.187778	1.335649

1	0.040179	-0.537435	0.435932
8	1.924345	-2.372886	-0.139626
1	1.252542	-2.199294	-0.845515
6	1.255983	-2.972819	0.963581
1	1.660575	-2.552221	1.890865
1	1.425949	-4.055217	0.967059
1	0.177992	-2.774086	0.920997
8	3.229696	2.090576	0.163472
1	3.385884	1.116446	0.239641
6	3.065670	2.626006	1.469350
1	3.198403	3.708066	1.406286
1	3.819014	2.218919	2.151514
1	2.065609	2.412664	1.867656
8	1.076031	2.148183	-1.332165
1	1.923059	2.307141	-0.837919
6	1.250702	0.951249	-2.087948
1	0.284687	0.671479	-2.514360
1	1.601512	0.129686	-1.450596
1	1.967352	1.106398	-2.900368
8	-2.827696	0.686052	1.252420
1	-1.961432	1.066251	0.998465
6	-3.102282	1.098047	2.576735
1	-4.018417	0.598078	2.898981
1	-3.257119	2.182851	2.637120
1	-2.291683	0.823167	3.264595
8	-1.908049	-0.105558	-1.305938
1	-1.785242	0.866386	-1.388933
6	-3.247224	-0.423281	-1.667562
1	-3.349392	-1.509771	-1.619439
1	-3.472597	-0.081029	-2.683334
1	-3.947786	0.026573	-0.955792
8	-0.067393	-2.029567	-1.832394
1	-0.705108	-1.308166	-1.635949
6	-0.778796	-3.257042	-1.938992
1	-0.039948	-4.061894	-1.973107
1	-1.364391	-3.285067	-2.865091
1	-1.437217	-3.399208	-1.075941
8	3.645473	-0.503391	0.505870
1	2.971371	-1.184092	0.242245
6	4.941095	-0.999351	0.216265
1	5.661263	-0.213606	0.455378
1	5.042663	-1.260641	-0.842879
1	5.167119	-1.881805	0.824609
8	-2.126448	-2.069466	0.771341
1	-2.283121	-1.118972	0.631000
6	-2.478971	-2.362326	2.104868
1	-2.349437	-3.437089	2.255746
1	-3.523896	-2.103452	2.317383
1	-1.837279	-1.832410	2.824097
8	-1.627992	2.572205	-1.594913
1	-0.676654	2.773140	-1.634390
6	-2.262367	3.402655	-0.630252
1	-3.263347	2.999592	-0.465563
1	-2.343029	4.431462	-0.995841
1	-1.722591	3.392534	0.323901

Cartesian coordinates of : BC10_9

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.249050	-0.934753	-1.950116
1	1.188374	-1.170302	-1.932549
6	0.059020	0.164288	-1.077778

1	-0.156276	1.080690	-1.642370
1	0.936402	0.350219	-0.446677
1	-0.792997	-0.033693	-0.417079
8	-0.077112	2.569794	0.654991
1	-0.976703	2.348350	0.311169
6	-0.162496	2.993792	2.007370
1	0.759097	3.531845	2.246204
1	-0.255178	2.130475	2.675653
1	-1.010058	3.672313	2.151638
8	0.659810	-2.218490	0.679604
1	1.449433	-2.045461	0.118443
6	0.933723	-3.253307	1.613632
1	0.036600	-3.389841	2.220068
1	1.763841	-2.979844	2.274773
1	1.167487	-4.194538	1.104361
8	-3.456435	-0.334366	-0.536817
1	-2.807004	-1.079190	-0.505258
6	-4.544685	-0.641958	0.316316
1	-5.319169	0.110768	0.155110
1	-4.248993	-0.621481	1.372936
1	-4.957967	-1.629211	0.083512
8	2.255850	2.814049	-0.581530
1	1.357936	2.757125	-0.172496
6	2.132794	2.866043	-1.992223
1	3.044283	3.312404	-2.395337
1	1.279319	3.485550	-2.288745
1	2.007119	1.863692	-2.423077
8	-2.506786	2.133586	-0.317257
1	-2.854818	1.208867	-0.364831
6	-2.650183	2.736077	-1.592242
1	-2.068672	3.661551	-1.592043
1	-3.698602	2.979807	-1.796155
1	-2.276305	2.081416	-2.388386
8	-1.874060	-2.475742	-0.454999
1	-0.927886	-2.332703	-0.252339
6	-1.988082	-3.140245	-1.707860
1	-3.052340	-3.202320	-1.946175
1	-1.584833	-4.157190	-1.644721
1	-1.466283	-2.581822	-2.489509
8	3.403619	0.655063	0.413052
1	3.112283	1.500030	-0.016318
6	2.774054	0.591695	1.690405
1	2.730601	-0.457984	1.998110
1	1.750552	0.982289	1.652288
1	3.353057	1.150891	2.431988
8	-0.229781	-0.301947	2.522800
1	0.188795	-0.771613	1.782409
6	-1.623518	-0.300692	2.290957
1	-2.127403	-0.177058	3.253669
1	-1.960810	-1.243295	1.837167
1	-1.925739	0.527468	1.632287
8	2.779387	-1.491252	-0.845190
1	3.071839	-0.630088	-0.413076
6	3.909408	-2.309424	-1.102424
1	3.556560	-3.246281	-1.538858
1	4.455793	-2.531231	-0.178744
1	4.590127	-1.825751	-1.810268

 Cartesian coordinates of : BC10_11

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-0.082042	3.723406	0.141972

1	-0.032547	2.970696	0.766724
6	-0.985520	4.672613	0.664308
1	-1.022161	5.515516	-0.029862
1	-0.667479	5.045677	1.645958
1	-2.000834	4.261696	0.763357
8	-2.187328	-2.561592	1.004008
1	-2.678383	-1.817347	0.563909
6	-2.682359	-2.753672	2.315605
1	-2.117929	-3.570635	2.771003
1	-3.742210	-3.031186	2.299403
1	-2.561617	-1.854110	2.931980
8	0.320419	0.356960	-2.283981
1	0.674676	-0.550263	-2.229987
6	1.164275	1.185906	-1.494386
1	0.699983	2.170689	-1.407929
1	2.149341	1.295909	-1.965450
1	1.297999	0.772700	-0.485532
8	-3.553720	-0.621627	-0.119624
1	-3.042815	-0.088125	-0.786625
6	-4.734690	-1.098997	-0.743227
1	-5.266750	-1.724094	-0.022344
1	-4.505608	-1.698794	-1.631009
1	-5.386189	-0.267436	-1.032751
8	2.443196	0.809967	1.848878
1	2.848690	0.153023	1.245172
6	2.966019	2.089243	1.523036
1	2.486058	2.819788	2.177322
1	2.745987	2.365895	0.483506
1	4.048850	2.126797	1.687311
8	-0.162084	1.542554	1.774986
1	0.705871	1.095337	1.863367
6	-1.125920	0.675196	1.203733
1	-1.982436	1.281213	0.897239
1	-1.477293	-0.068669	1.928690
1	-0.739384	0.151623	0.317097
8	-2.323462	0.777384	-1.953201
1	-1.379133	0.564754	-2.128698
6	-2.466829	2.189697	-1.862388
1	-3.433120	2.394306	-1.392609
1	-2.459940	2.642291	-2.859832
1	-1.671395	2.638578	-1.255578
8	0.397961	-2.666154	0.615153
1	-0.590142	-2.640522	0.727434
6	1.029961	-2.219098	1.805576
1	2.101520	-2.133539	1.607290
1	0.878939	-2.937882	2.618167
1	0.654206	-1.238419	2.119585
8	1.611940	-1.932716	-1.506030
1	1.069929	-2.217105	-0.703656
6	2.055333	-3.096506	-2.192410
1	2.611124	-2.775993	-3.075917
1	1.206750	-3.709763	-2.510637
1	2.711950	-3.698242	-1.554230
8	3.598969	-0.817980	-0.018284
1	2.928372	-1.163100	-0.647343
6	4.689403	-0.253609	-0.725086
1	5.437965	0.047947	0.010193
1	4.386412	0.629253	-1.301342
1	5.143904	-0.984707	-1.402957

Cartesian coordinates of : BC10_8

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

```
-----  
8      2.872169      1.526109      0.779224  
1      2.181682      1.235001      1.410633  
6      2.480583      2.768670      0.212752  
1      3.205038      3.019375     -0.565573  
1      2.494368      3.562479      0.967796  
1      1.483837      2.719764     -0.240378  
8      -1.253589      2.223941      1.227325  
1      -0.467422      1.804117      1.631085  
6      -2.218184      1.191925      1.028605  
1      -3.154983      1.661682      0.721883  
1      -2.397977      0.628062      1.948263  
1      -1.902909      0.493556      0.244227  
8      -0.771640      3.116012     -1.234481  
1      -0.932997      2.902812     -0.283296  
6      -1.696366      4.098024     -1.666914  
1      -1.499422      4.298765     -2.721628  
1      -1.574356      5.029955     -1.104287  
1      -2.731790      3.751762     -1.562852  
8      3.749965     -0.536904     -0.701910  
1      3.471459      0.231227     -0.149970  
6      4.293318     -0.075963     -1.924639  
1      4.590342     -0.949376     -2.508398  
1      5.178350      0.545772     -1.750700  
1      3.559879      0.497651     -2.505175  
8      0.762544      0.704720      2.316592  
1      0.627821     -0.252552      2.020264  
6      0.773490      0.741355      3.739454  
1      0.993083      1.764654      4.049842  
1      1.541782      0.072802      4.139654  
1      -0.202405      0.449944      4.142477  
8      -0.558569      0.568735     -2.104546  
1      -0.719185      1.527359     -1.962820  
6      0.538176      0.196979     -1.286473  
1      0.686156     -0.882251     -1.381914  
1      0.355859      0.432681     -0.226895  
1      1.456678      0.706089     -1.599802  
8      -3.783542     -1.391295      0.694284  
1      -3.346346     -1.331392     -0.177326  
6      -5.178822     -1.335263      0.499025  
1      -5.654864     -1.405742      1.479864  
1      -5.541647     -2.166202     -0.120312  
1      -5.490842     -0.392292      0.029917  
8      0.456734     -1.740258      1.621862  
1      1.101835     -2.048744      0.936762  
6      -0.855945     -2.120117      1.215620  
1      -1.572471     -1.728432      1.938441  
1      -0.948758     -3.210569      1.183799  
1      -1.102482     -1.708219      0.230329  
8      2.094968     -2.570187     -0.296497  
1      2.704622     -1.830095     -0.536900  
6      2.868166     -3.715024      0.027532  
1      2.190630     -4.473074      0.425943  
1      3.626587     -3.484082      0.783540  
1      3.360545     -4.118807     -0.863579  
8      -2.531371     -1.226745     -1.756742  
1      -1.894102     -0.499122     -1.934426  
6      -2.039884     -2.418796     -2.341104  
1      -2.721113     -3.227876     -2.067125  
1      -1.036369     -2.669489     -1.971940  
1      -2.006662     -2.340934     -3.433460  
-----
```

Cartesian coordinates of : BC10_1

```
-----
```


Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-2.918937	-1.546859	-0.706790
1	-1.953841	-1.734824	-0.694715
6	-3.393299	-1.831506	-2.010779
1	-4.483435	-1.888891	-1.967592
1	-3.001176	-2.788610	-2.370300
1	-3.108249	-1.044627	-2.721566
8	3.471222	1.992440	-0.654016
1	2.618452	2.181261	-0.215136
6	3.306840	2.077502	-2.062687
1	4.279822	1.875833	-2.515248
1	2.987236	3.081769	-2.362095
1	2.581620	1.337242	-2.421140
8	-1.038314	-0.272723	1.085740
1	-0.159630	-0.701181	1.095740
6	-1.810041	-0.780174	2.155416
1	-2.737535	-0.202593	2.192202
1	-1.292958	-0.669209	3.118538
1	-2.071903	-1.835982	2.005698
8	-1.280575	2.606508	0.865541
1	-1.875956	1.842092	0.711665
6	-1.703125	3.663623	0.021683
1	-0.983169	4.478332	0.124395
1	-2.692327	4.027584	0.319759
1	-1.745191	3.344449	-1.025670
8	-0.391066	-2.487160	-1.042082
1	0.282870	-1.806218	-0.847975
6	-0.262571	-3.580390	-0.153212
1	-0.952915	-4.356423	-0.492409
1	-0.523191	-3.297116	0.874334
1	0.756957	-3.980409	-0.154512
8	0.915570	-0.066420	-1.210991
1	1.073608	0.474666	-0.410389
6	-0.191700	0.505984	-1.893508
1	-0.459643	-0.171826	-2.707945
1	0.069901	1.484000	-2.320665
1	-1.053211	0.622226	-1.225575
8	-3.279595	1.038785	-0.107387
1	-3.066218	0.088919	-0.272843
6	-4.670344	1.160469	0.100530
1	-4.891156	2.210789	0.305856
1	-5.007491	0.559447	0.954859
1	-5.236709	0.854885	-0.788213
8	3.627761	-0.600956	0.126979
1	3.657532	0.350893	-0.123192
6	3.820594	-1.382506	-1.045943
1	3.772857	-2.433549	-0.750529
1	4.805518	-1.188327	-1.484259
1	3.033361	-1.182790	-1.780701
8	1.178398	1.796077	0.797133
1	0.230130	2.121370	0.806431
6	1.567089	1.491787	2.129099
1	2.551525	1.015402	2.093939
1	0.853540	0.798757	2.588181
1	1.631862	2.402862	2.733230
8	1.411379	-1.547217	1.196357
1	2.210262	-1.114168	0.798889
6	1.787569	-2.165267	2.411165
1	0.923992	-2.719563	2.789500
1	2.086644	-1.425647	3.165192
1	2.615403	-2.867748	2.259810

Cartesian coordinates of : BC10_6

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-2.907680	-1.299075	0.375431
1	-2.449848	-0.682128	1.003817
6	-4.005148	-1.898464	1.043546
1	-4.465011	-2.613124	0.357615
1	-4.752089	-1.146892	1.322197
1	-3.683057	-2.431462	1.945298
8	3.125658	0.448731	-1.935351
1	3.114922	-0.401436	-1.446717
6	3.631233	1.428358	-1.039573
1	3.674484	2.378464	-1.575908
1	4.640306	1.169434	-0.700289
1	2.978853	1.553012	-0.165254
8	-1.403388	-2.884606	-1.119324
1	-1.969436	-2.316872	-0.541371
6	-1.672616	-2.565927	-2.471760
1	-0.967866	-3.119165	-3.095949
1	-1.549041	-1.492578	-2.667356
1	-2.691230	-2.859139	-2.750490
8	3.004399	-1.571981	-0.139498
1	2.190580	-2.124335	-0.036312
6	4.107323	-2.264827	0.414695
1	5.001436	-1.659618	0.248494
1	4.249797	-3.241231	-0.060844
1	3.980169	-2.410797	1.494545
8	-1.886815	0.446877	2.043190
1	-0.926845	0.529037	2.236954
6	-2.336652	1.727041	1.609231
1	-3.412929	1.654833	1.433236
1	-1.846968	2.032250	0.675860
1	-2.154343	2.480605	2.382807
8	0.672169	1.187673	2.318133
1	0.743041	1.835997	1.580254
6	1.932880	0.589978	2.566485
1	1.831315	-0.035078	3.456714
1	2.695438	1.352330	2.762850
1	2.263470	-0.038723	1.727431
8	0.838353	-3.019596	0.364394
1	0.132772	-3.084166	-0.316802
6	0.242511	-2.482002	1.534788
1	0.989726	-2.509568	2.331509
1	-0.624794	-3.076494	1.842191
1	-0.075493	-1.440813	1.387521
8	0.758364	2.908362	0.252215
1	0.623464	2.464291	-0.607036
6	0.054090	4.144276	0.296350
1	-0.035131	4.430813	1.346735
1	-0.941882	4.041911	-0.144563
1	0.611225	4.923569	-0.234706
8	0.527186	1.068187	-1.803913
1	1.445096	0.904690	-2.122503
6	0.244259	0.041310	-0.857314
1	-0.754574	0.227845	-0.446910
1	0.969591	0.054615	-0.034079
1	0.258374	-0.947075	-1.326952
8	-1.878350	2.427751	-1.715809
1	-1.095821	1.982818	-2.077484
6	-3.003477	1.581431	-1.864524
1	-3.870877	2.125725	-1.483552
1	-2.902862	0.648786	-1.291202
1	-3.189554	1.334031	-2.917034

Cartesian coordinates of : BC10_15

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	2.154788	4.514599	0.092337
8	1.509580	3.383839	-0.463350
8	2.763038	1.068225	-0.476639
6	2.658314	0.595813	-1.814726
8	2.732630	-0.806517	1.294382
6	3.446018	-0.381926	2.444892
8	0.692417	-2.533083	0.958572
6	1.166231	-3.099885	-0.263359
8	-1.857289	-2.237122	0.873017
6	-2.346009	-3.330319	1.638630
8	-1.054844	3.968944	-0.231146
6	-1.563941	4.579160	-1.404311
8	-3.134378	2.496516	0.517335
6	-3.998417	3.001978	1.518313
8	-3.511131	-0.143772	0.571894
6	-4.130179	-0.660247	-0.594613
8	-1.983134	-3.411073	-1.681482
6	-3.264550	-3.948158	-1.920713
1	1.898914	4.644362	1.149840
1	1.886606	5.427583	-0.451482
1	3.232620	4.360363	0.005002
1	0.532020	3.491340	-0.361618
1	3.165618	1.279297	-2.503506
1	1.609896	0.496728	-2.117764
1	3.139282	-0.384849	-1.860136
1	2.271991	1.924509	-0.400454
1	2.880581	0.369255	3.007057
1	4.419315	0.037888	2.166196
1	3.606943	-1.253283	3.082708
1	2.666257	-0.044536	0.646771
1	-3.401288	-0.832596	-1.395703
1	-4.863199	0.074138	-0.935334
1	-2.818096	-0.783392	0.839544
1	1.999598	-3.783115	-0.073105
1	1.498342	-2.319308	-0.956413
1	0.338774	-3.647167	-0.721066
1	1.349558	-1.871289	1.259510
1	-1.994869	-3.274872	2.673630
1	-2.025748	-4.283450	1.201412
1	-3.438130	-3.283277	1.632003
1	-0.856749	-2.236774	0.933910
1	-2.397518	5.249919	-1.168033
1	-1.902874	3.832606	-2.130783
1	-0.757883	5.165352	-1.852185
1	-1.746768	3.364800	0.126632
1	-3.727979	2.626121	2.511346
1	-5.040898	2.736974	1.309548
1	-3.906250	4.090585	1.518095
1	-3.181342	1.512535	0.519383
1	-3.160493	-4.723337	-2.682856
1	-3.696224	-4.408218	-1.020710
1	-3.967294	-3.191818	-2.296823
1	-2.011991	-2.854080	-0.885013
1	-4.651167	-1.600836	-0.377309
6	5.459784	-1.127749	-0.527852
1	6.065045	-1.234523	-1.430821
1	6.106132	-1.310749	0.341427
1	5.083371	-0.095932	-0.478666
8	4.406502	-2.066992	-0.607520

1 3.796539 -1.878282 0.123669

Cartesian coordinates of : BC10_14

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	1.501296	2.773000	0.618199
8	2.073304	2.290190	-0.591777
8	3.712808	0.345138	-0.242093
6	5.026507	0.737133	-0.612167
8	2.765089	-2.140578	-0.635451
6	3.418035	-2.873148	0.392879
8	0.146773	-2.392288	-0.557645
6	-0.299074	-2.957370	-1.784604
8	-1.589513	-1.254073	0.949775
6	-1.834211	-2.190653	1.990150
8	-0.078370	1.911426	-2.059633
6	-0.400595	0.578323	-1.686993
8	-1.876675	3.173035	-0.487815
6	-1.817673	4.478341	0.055895
8	-2.515387	1.275474	1.303421
6	-3.811570	0.916856	0.840817
8	-3.434274	-1.900114	-1.084176
6	-4.731140	-2.206547	-0.620680
1	0.459193	2.442313	0.715703
1	1.531422	3.867597	0.644424
1	2.074232	2.371677	1.458667
1	1.355306	2.227494	-1.272600
1	5.329328	1.640812	-0.073480
1	5.093797	0.921567	-1.689179
1	5.706982	-0.075452	-0.348859
1	3.070396	1.091894	-0.438289
1	3.407204	-2.326439	1.343321
1	4.453337	-3.096411	0.113174
1	2.879977	-3.815151	0.520110
1	3.113372	-1.221557	-0.632322
1	-3.796166	0.640181	-0.220764
1	-4.460341	1.784889	0.972946
1	-1.968943	0.465231	1.260634
1	0.034761	-3.996619	-1.873836
1	0.080940	-2.387089	-2.639761
1	-1.390861	-2.922043	-1.791446
1	1.129686	-2.265797	-0.572460
1	-0.965015	-2.282493	2.650377
1	-2.075880	-3.176205	1.575910
1	-2.683759	-1.830038	2.575769
1	-0.855963	-1.616520	0.369663
1	-1.248654	0.192078	-2.263631
1	-0.638859	0.510811	-0.616867
1	0.475079	-0.046851	-1.880442
1	-0.758546	2.498001	-1.664467
1	-1.050521	4.558094	0.835546
1	-2.784480	4.775078	0.477972
1	-1.566432	5.165339	-0.754420
1	-2.058201	2.520694	0.226171
1	-5.240354	-2.761984	-1.410772
1	-4.710494	-2.832336	0.281732
1	-5.317831	-1.302495	-0.406558
1	-2.900668	-1.549362	-0.350411
1	-4.217788	0.082701	1.425491
6	1.315926	-0.412142	1.775861
1	0.534241	-0.027502	2.438528
1	1.210195	-1.505752	1.714002

1	1.148859	0.000565	0.770185
8	2.571792	-0.036530	2.299947
1	3.192080	0.044892	1.557693

Cartesian coordinates of : BC10_17

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-4.009985	2.146478	-0.540761
8	-3.092949	1.787278	0.485709
8	-3.048903	-0.751300	0.780908
6	-3.895619	-0.960514	1.902971
8	-1.322745	-2.740436	0.323833
6	-2.193043	-3.460073	-0.532614
8	1.288647	-2.854219	-0.140934
6	1.810148	-3.600389	0.953512
8	2.953991	-1.023018	-0.806754
6	3.625555	-1.568498	-1.934248
8	-1.260397	3.675601	0.409730
6	-1.285380	4.606398	1.476794
8	1.297440	3.648263	-0.285020
6	1.591468	4.473412	-1.398628
8	3.036399	1.649225	-0.622922
6	4.207592	1.673357	0.174227
8	4.761771	-1.843243	1.181529
6	6.065529	-1.390667	0.893196
1	-3.491808	2.317362	-1.489900
1	-4.560672	3.052065	-0.264848
1	-4.713883	1.320291	-0.670053
1	-2.342345	2.432050	0.492242
1	-4.910355	-0.600363	1.695061
1	-3.508289	-0.448829	2.789354
1	-3.931641	-2.035106	2.101618
1	-2.939444	0.239566	0.654817
1	-2.488376	-2.861305	-1.402606
1	-3.095272	-3.777804	0.004531
1	-1.661570	-4.349121	-0.878495
1	-1.781783	-1.910512	0.576340
1	4.070851	1.117324	1.109533
1	4.427492	2.716311	0.412935
1	2.803828	0.708336	-0.771588
1	1.544169	-4.658291	0.858390
1	1.430779	-3.218409	1.906693
1	2.898177	-3.497901	0.944542
1	0.313859	-2.751854	-0.027936
1	2.923021	-1.782822	-2.745427
1	4.153276	-2.490571	-1.662470
1	4.353110	-0.830036	-2.281521
1	2.218976	-1.654344	-0.544530
1	-0.962807	5.598286	1.140677
1	-0.643895	4.285862	2.305004
1	-2.315445	4.675522	1.834152
1	-0.325841	3.556819	0.115151
1	1.473856	3.931043	-2.343065
1	2.612642	4.866088	-1.338203
1	0.891619	5.312267	-1.384851
1	1.868018	2.847825	-0.331755
1	6.766407	-2.056198	1.401695
1	6.285497	-1.419078	-0.183383
1	6.238964	-0.368837	1.257703
1	4.129229	-1.391290	0.596982
1	5.061284	1.250981	-0.370322
6	-5.630453	-2.341900	-1.068272

1	-6.605120	-2.263712	-1.554747
1	-5.794711	-2.580313	-0.007890
1	-5.083188	-3.174184	-1.531918
8	-4.967983	-1.109278	-1.239450
1	-4.185640	-1.083731	-0.661993

Cartesian coordinates of : BC10_16

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

6	-4.445782	0.383045	-1.539524
8	-3.377162	0.183504	-0.624314
8	-2.431348	-2.318358	-0.504783
6	-3.281333	-2.709267	0.559954
8	-0.043734	-3.501534	-0.514497
6	-0.228081	-4.550984	-1.447617
8	2.402997	-2.529979	-0.311212
6	2.893388	-3.097803	0.898298
8	3.377165	-0.183508	-0.624329
6	4.445786	-0.383057	-1.539535
8	-2.402991	2.529978	-0.311225
6	-2.893392	3.097804	0.898281
8	0.043746	3.501515	-0.514479
6	0.228058	4.550980	-1.447588
8	2.431372	2.318366	-0.504816
6	3.281376	2.709276	0.559906
8	4.857426	-0.411761	1.753879
6	5.922230	0.511687	1.783796
1	-4.081275	0.788593	-2.488385
1	-5.193096	1.066930	-1.119645
1	-4.914526	-0.587024	-1.725550
1	-2.886424	1.054016	-0.521554
1	-4.333971	-2.677580	0.252619
1	-3.146637	-2.068645	1.439726
1	-3.027271	-3.736723	0.830277
1	-2.603378	-1.368796	-0.680761
1	-0.507491	-4.166948	-2.434802
1	-1.000059	-5.249623	-1.105949
1	0.718496	-5.089542	-1.533190
1	-0.869899	-2.966810	-0.473106
1	3.146652	2.068694	1.439702
1	3.027363	3.736754	0.830190
1	2.603392	1.368802	-0.680788
1	3.070392	-4.171455	0.774286
1	2.187331	-2.942911	1.720383
1	3.834947	-2.602194	1.147764
1	1.467032	-2.817613	-0.445737
1	4.081276	-0.788584	-2.488405
1	5.193084	-1.066962	-1.119662
1	4.914550	0.587005	-1.725545
1	2.886428	-1.054020	-0.521558
1	-3.070361	4.171463	0.774276
1	-2.187358	2.942883	1.720379
1	-3.834972	2.602221	1.147720
1	-1.467019	2.817599	-0.445733
1	0.507454	4.166963	-2.434785
1	1.000031	5.249628	-1.105927
1	-0.718530	5.089525	-1.533134
1	0.869923	2.966806	-0.473105
1	6.682429	0.117235	2.461430
1	6.381787	0.646845	0.794446
1	5.607066	1.494952	2.159210
1	4.253052	-0.182202	1.027174

1	4.334013	2.677530	0.252572
6	-5.922255	-0.511690	1.783751
1	-6.682490	-0.117248	2.461349
1	-5.607081	-1.494942	2.159190
1	-6.381768	-0.646871	0.794384
8	-4.857472	0.411784	1.753866
1	-4.253062	0.182226	1.027190

Cartesian coordinates of : BC10_12

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.040634	1.094830	2.253866
1	0.635620	0.250789	2.548250
6	0.003021	2.064309	2.170083
1	0.412329	2.962716	1.703908
1	-0.374808	2.315023	3.168078
1	-0.823918	1.705914	1.544366
8	0.797345	-1.125383	-1.338725
1	1.751412	-1.062789	-1.577814
6	0.335551	0.216899	-1.138343
1	-0.748545	0.231962	-1.288363
1	0.803751	0.895084	-1.856811
1	0.560635	0.563116	-0.123380
8	-0.504478	3.035437	-0.831535
1	-1.280860	2.534828	-0.516061
6	-0.736191	3.412425	-2.171295
1	0.177037	3.881691	-2.547108
1	-1.557370	4.135112	-2.257942
1	-0.966441	2.546610	-2.807621
8	-2.710281	1.606488	-0.016102
1	-2.939403	0.662124	-0.180430
6	-3.534408	2.136472	1.003181
1	-3.223098	3.169600	1.177201
1	-3.428313	1.578785	1.942316
1	-4.590216	2.134573	0.708018
8	1.360470	-2.441761	1.025898
1	1.103640	-1.980410	0.200815
6	2.741821	-2.202049	1.258958
1	3.005936	-2.692870	2.197230
1	2.957758	-1.129796	1.343161
1	3.353100	-2.624450	0.453727
8	-0.347104	-1.209670	2.736371
1	0.295013	-1.818040	2.317038
6	-1.452988	-1.131084	1.849302
1	-2.138872	-0.369380	2.226164
1	-1.992374	-2.083234	1.790479
1	-1.135526	-0.840222	0.838321
8	-3.407494	-0.938933	-0.473597
1	-2.683484	-1.533469	-0.783551
6	-4.496088	-1.045219	-1.376952
1	-5.266109	-0.340857	-1.054746
1	-4.918491	-2.055704	-1.364536
1	-4.194808	-0.795581	-2.400306
8	3.317221	-0.378855	-1.475721
1	3.257077	0.265198	-0.722517
6	4.651178	-0.817966	-1.634572
1	4.662394	-1.592316	-2.404340
1	5.050023	-1.239733	-0.703717
1	5.301788	0.003501	-1.955372
8	-1.515699	-2.577134	-1.401495
1	-0.648142	-2.169657	-1.586397
6	-1.321951	-3.778718	-0.664730

1	-2.292378	-4.071724	-0.257453
1	-0.615471	-3.636449	0.160331
1	-0.958246	-4.578882	-1.317662
8	3.069456	1.373250	0.474297
1	2.400018	1.202849	1.173928
6	2.807422	2.659893	-0.080798
1	3.435741	2.767192	-0.968730
1	3.074806	3.446703	0.633141
1	1.754034	2.766265	-0.366673
