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Optimized Cartesian coordinates of the neutral methanol clusters in the solvent phase (methanol)

Cartesian coordinates of the methanol dimer

Cartesian coordinates of : MeOH_2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-1.961335	0.458928	0.281305
1	-1.408558	1.404294	0.215090
1	-1.998322	0.148079	1.332327
1	-2.982402	0.631828	-0.064564
8	-1.390216	-0.542009	-0.542881
1	-0.472786	-0.674183	-0.245055
6	1.979561	0.479102	-0.264890
1	2.321975	0.065150	-1.217649
1	2.840134	0.816085	0.319518
1	1.328188	1.331735	-0.461551
8	1.205274	-0.470458	0.465234
1	1.741950	-1.251437	0.644573

Cartesian coordinates of the methanol trimer

Cartesian coordinates of : MeOH_2_1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-2.638731	-0.496866	-0.178000
1	-2.203300	-1.476236	0.055440
1	-2.774595	-0.420937	-1.262884
1	-3.618632	-0.433847	0.298841
8	-1.849639	0.564774	0.329989
1	-1.010624	0.611436	-0.157445
6	0.738869	-1.922376	0.248755
1	0.113765	-2.111834	-0.633117
1	0.176111	-1.291998	0.949982
1	0.951889	-2.876820	0.733882
8	1.977707	-1.332737	-0.107122
1	1.772295	-0.456558	-0.471072
6	1.100472	1.983224	0.449813
1	0.400950	2.819090	0.530325
1	2.120497	2.358815	0.340201
1	1.035895	1.372188	1.351254
8	0.750072	1.130046	-0.646156
1	0.806962	1.626154	-1.472505

Cartesian coordinates of : MeOH_3.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.825351	1.665369	-0.711457
1	0.924312	0.710960	-0.889931
8	0.826731	-1.103144	-0.680937
1	-0.076559	-1.200773	-0.319518
8	-1.648745	-0.859421	0.450444

1	-2.263896	-1.549901	0.724052
6	0.735588	1.812026	0.695536
1	1.700861	1.629957	1.184888
1	0.428668	2.838497	0.907240
1	-0.009114	1.128801	1.125936
6	1.754758	-1.557097	0.296391
1	1.579881	-1.077381	1.266292
1	1.699688	-2.643584	0.420021
1	2.755334	-1.292917	-0.050421
6	-2.357324	0.165309	-0.248730
1	-2.902294	-0.243622	-1.104058
1	-3.053221	0.681191	0.418661
1	-1.608484	0.874908	-0.606737

 Cartesian coordinates of : MeOH_3r_UUN.log

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	1.109103	-2.079770	0.433001
8	0.442070	-1.522729	-0.693349
8	-1.476659	0.184148	0.410431
6	-2.818982	0.390171	-0.009353
8	0.891735	1.222663	-0.580415
6	1.842753	1.782380	0.315935
1	0.997515	-1.441912	1.318327
1	2.175117	-2.227914	0.232190
1	0.651714	-3.048401	0.639390
1	0.826805	-0.641964	-0.863041
1	1.889900	1.219140	1.254563
1	1.610150	2.828779	0.538081
1	2.817509	1.735212	-0.171500
1	0.014241	1.196630	-0.154944
1	-3.466493	-0.429372	0.318110
1	-2.887713	0.490110	-1.097692
1	-3.164623	1.316289	0.451680
1	-1.118523	-0.625945	0.003998

 Cartesian coordinates of the methanol tetramer

Cartesian coordinates of : MeOH_3_112.log

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-3.122806	0.651189	-0.315377
1	-2.344370	0.439581	0.234141
8	-0.940615	-0.297833	1.110218
1	-0.227415	0.365074	1.149461
8	1.245597	1.362774	0.688634
1	1.507753	2.051997	1.312614
6	-3.857485	-0.547609	-0.488212
1	-4.123130	-1.003923	0.473246
1	-4.779275	-0.301451	-1.019381
1	-3.302286	-1.283732	-1.083611
6	-0.479171	-1.379441	0.305871
1	-0.502970	-1.119288	-0.760457
1	0.539850	-1.669791	0.582126
1	-1.148365	-2.225431	0.472658
6	0.960194	1.954209	-0.585628

1	0.150717	2.683078	-0.501241
1	1.851762	2.430532	-0.999864
1	0.645581	1.143038	-1.243962
6	3.071633	-0.945388	-0.982342
1	3.740396	-1.769604	-1.236671
1	2.078302	-1.167987	-1.393554
1	3.451609	-0.031126	-1.453866
8	3.043252	-0.836027	0.430731
1	2.487397	-0.072408	0.656575

Cartesian coordinates of : MeOH_3_11.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	3.360366	-0.505694	-0.946976
1	4.206833	0.177943	-0.831401
1	2.904169	-0.352971	-1.930454
1	3.723915	-1.531691	-0.880823
8	2.411538	-0.325308	0.098215
1	2.029003	0.568980	0.046921
6	-2.772783	0.230890	-0.686765
1	-2.131894	0.834515	-1.343096
1	-2.530719	0.465073	0.359878
1	-3.811709	0.513429	-0.866472
8	-2.647414	-1.153168	-0.956381
1	-1.737860	-1.404526	-0.725383
6	-0.397869	-1.379008	1.665165
1	0.049774	-0.564802	2.246025
1	0.005583	-2.334835	2.010974
1	-1.478961	-1.373802	1.818397
8	-0.165665	-1.198285	0.270428
1	0.801179	-1.163255	0.114746
6	-0.268963	2.610828	0.557750
1	-0.440747	2.364050	1.610930
1	-1.226580	2.855717	0.084785
1	0.382051	3.483920	0.501329
8	0.385351	1.549980	-0.125206
1	-0.139028	0.734407	-0.047835

Cartesian coordinates of : MeOH_3_12.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	0.891973	-0.029958	2.057435
6	0.118911	-0.701238	1.669761
1	0.269337	-1.703676	2.080702
1	-0.859854	-0.331684	1.981801
8	0.135555	-0.728133	0.242937
1	1.032991	-1.006175	-0.045743
1	2.947807	0.600263	-1.469270
6	3.229252	0.233160	-0.478489
1	4.314853	0.275989	-0.361370
1	2.763038	0.863757	0.280486
8	2.747253	-1.094797	-0.262960
1	3.107199	-1.683072	-0.937740
1	-2.558274	0.366248	-0.875671
6	-3.022474	-0.491354	-0.373114
1	-3.075041	-0.281877	0.703605
1	-4.041324	-0.606576	-0.748549
8	-2.323812	-1.695702	-0.639394

1	-1.391406	-1.541685	-0.407499
1	0.024584	2.476321	1.202351
6	-0.747202	2.511333	0.423134
1	-1.670855	2.072702	0.823177
1	-0.941947	3.557094	0.177523
8	-0.326612	1.859848	-0.762518
1	-0.143083	0.931192	-0.533511

Cartesian coordinates of : MeOH_4b.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-2.205889	-1.296945	-0.269233
1	-1.693166	-0.569304	-0.672141
8	-0.797011	0.948934	-1.023650
1	0.160805	0.994401	-0.810782
8	1.803817	1.138273	-0.225059
1	2.190387	0.243207	-0.310219
6	-2.473183	-0.921166	1.068858
1	-3.174073	-0.078399	1.124737
1	-2.921310	-1.777755	1.576739
1	-1.555443	-0.643236	1.605270
6	-1.438668	2.079689	-0.449168
1	-1.355707	2.075671	0.644400
1	-1.017568	3.013285	-0.837017
1	-2.495763	2.034001	-0.719089
6	1.758006	1.464803	1.160522
1	1.100435	0.780110	1.710471
1	2.757128	1.434311	1.604895
1	1.363579	2.478621	1.246920
8	2.332236	-1.531970	-0.173219
1	2.864101	-2.018606	-0.814280
6	0.967890	-1.944095	-0.274540
1	0.565366	-1.749748	-1.273410
1	0.856813	-3.004191	-0.031967
1	0.404927	-1.354082	0.450722

Cartesian coordinates of : MeOH_4r.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-2.487387	1.646927	0.142481
1	-2.505413	2.741409	0.139646
1	-2.460235	1.292119	1.178686
1	-3.399083	1.279490	-0.331741
8	-1.382909	1.152775	-0.605151
1	-0.544855	1.400852	-0.151193
6	1.990456	2.114884	-0.176527
1	2.023854	1.678703	-1.181475
1	2.981486	2.035727	0.281677
1	1.724950	3.169847	-0.259960
8	1.003155	1.482782	0.630080
1	1.222088	0.524963	0.694550
6	2.477906	-1.617576	-0.310143
1	2.375142	-1.213368	-1.323291
1	2.530692	-2.709535	-0.364412
1	3.405098	-1.242267	0.126433
8	1.406600	-1.199345	0.527076
1	0.551195	-1.451192	0.109266
6	-1.967691	-2.058679	0.369171

1	-2.996231	-1.972303	0.004347
1	-1.884188	-1.541464	1.332137
1	-1.733702	-3.114220	0.515694
8	-1.043545	-1.537765	-0.579656
1	-1.236897	-0.579683	-0.699036

Cartesian coordinates of : MeOH_N4_4r.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	0.347433	-0.340061	-0.048951
8	0.028286	-0.056686	1.308415
8	2.168446	0.101171	2.953709
6	1.857209	0.965635	4.040392
8	1.824847	-2.512479	3.557682
6	2.728314	-3.330419	2.823545
8	-0.672846	-2.359169	2.536779
6	-1.634062	-2.264735	3.581213
1	-0.554857	-0.568488	-0.624814
1	1.044874	-1.181886	-0.126924
1	0.819125	0.548517	-0.471318
1	-0.353767	-0.868826	1.715151
1	-1.369562	-1.478350	4.297036
1	-1.729409	-3.216232	4.113731
1	-2.594722	-2.018420	3.126357
1	0.210879	-2.538370	2.934292
1	3.751596	-3.215498	3.194442
1	2.705224	-3.090123	1.754637
1	2.419646	-4.368247	2.957976
1	2.060312	-1.567216	3.409418
1	0.901787	0.694597	4.504124
1	1.812251	2.008647	3.711818
1	2.650396	0.863989	4.782675
1	1.436832	0.152327	2.295590

Cartesian coordinates of : MeOH_4r_UUUU.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-0.032853	2.199924	0.899631
8	0.030833	1.896550	-0.489262
8	-1.920168	0.039006	-0.813672
6	-2.905304	-0.028952	0.210401
8	-0.030827	-1.896564	-0.489255
6	0.032848	-2.199875	0.899653
8	1.920172	-0.039019	-0.813674
6	2.905303	0.028926	0.210405
1	-0.066065	1.286242	1.506253
1	-0.911968	2.810342	1.130245
1	0.865632	2.762046	1.160247
1	-0.746713	1.332774	-0.702090
1	-2.447912	-0.082407	1.205233
1	-3.558661	-0.895969	0.070370
1	-3.507656	0.878858	0.149820
1	-1.337891	-0.751581	-0.756944
1	0.066019	-1.286164	1.506233
1	0.911979	-2.810252	1.130308
1	-0.865623	-2.762015	1.160279
1	0.746713	-1.332787	-0.702095
1	2.447905	0.082395	1.205234

1	3.558675	0.895931	0.070375
1	3.507640	-0.878893	0.149832
1	1.337895	0.751568	-0.756939

Cartesian coordinates of : MeOH_UUUD.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-3.135603	-0.028581	-0.680831
8	-2.000061	0.013921	0.174445
8	-0.043117	1.839784	-0.212581
6	0.349160	2.350683	1.055889
8	-0.125479	-1.926021	-0.136900
6	0.369244	-2.138582	1.180940
8	1.626945	-0.097116	-1.113960
6	2.883230	-0.038979	-0.449498
1	-3.776040	-0.882754	-0.439836
1	-2.840860	-0.086287	-1.734064
1	-3.701712	0.890607	-0.523106
1	-1.446130	-0.785987	0.029400
1	0.527439	-1.187137	1.703656
1	1.310802	-2.696941	1.163306
1	-0.376042	-2.719219	1.726693
1	0.538902	-1.378067	-0.612014
1	2.759327	0.029941	0.637615
1	3.472457	0.815963	-0.796555
1	3.424760	-0.957127	-0.683196
1	1.093741	0.691018	-0.861184
1	0.513135	1.543361	1.779040
1	-0.404769	3.037364	1.453554
1	1.284757	2.895973	0.919286
1	-0.842255	1.277502	-0.089629

Cartesian coordinates of : N4_12.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-2.763254	-0.260153	-0.963009
8	-1.382151	-0.451295	-1.255749
8	-0.419355	-1.429221	1.187541
6	0.844885	-2.074773	1.317926
8	-0.030057	1.202885	0.590396
6	-0.470441	2.382981	1.256465
8	2.463240	0.600486	-0.502597
6	1.931672	-0.012902	-1.663486
1	-2.919072	-0.057798	0.103420
1	-3.182590	0.563298	-1.549218
1	-3.282018	-1.182634	-1.226419
1	-0.905300	0.345226	-0.964829
1	1.260905	-0.847057	-1.415379
1	1.379946	0.702349	-2.286170
1	2.767364	-0.406510	-2.245253
1	1.710292	0.960989	-0.001764
1	0.811958	-3.091497	0.915426
1	1.635860	-1.507267	0.812992
1	1.072468	-2.124639	2.383490
1	-0.706089	-1.446398	0.255844
1	-1.550522	2.354147	1.428535
1	0.047454	2.511734	2.211137
1	-0.236048	3.227135	0.607482

1 -0.215196 0.405160 1.126599

 Cartesian coordinates of : N4_20.log

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	3.147818	0.267056	0.361706
8	2.014314	-0.239422	1.043932
8	0.398911	-1.114379	-1.014890
6	-0.406601	-2.285638	-0.925454
8	-0.970185	1.283842	-1.216255
6	-0.099158	2.173822	-0.506199
8	-2.556820	-0.104122	0.686630
6	-1.595012	-0.137036	1.728691
1	3.701814	-0.527306	-0.152665
1	2.870250	1.032319	-0.374908
1	3.806490	0.725097	1.102311
1	1.421244	-0.634443	0.375605
1	0.621657	2.633685	-1.186410
1	-0.674433	2.948974	0.006639
1	0.434447	1.567524	0.229702
1	-1.372868	1.744910	-1.962643
1	-1.286081	-2.114159	-0.295667
1	-0.730282	-2.613866	-1.918263
1	0.208432	-3.068491	-0.478987
1	-0.146476	-0.360420	-1.302991
1	-0.644479	-0.570187	1.391436
1	-1.399562	0.863662	2.133539
1	-1.997113	-0.762023	2.528330
1	-2.185086	0.418150	-0.042844

 Cartesian coordinates of : N4_25.log

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	3.453597	0.494311	-0.014826
8	3.144042	-0.872405	-0.289065
8	0.426417	-0.951763	-0.333063
6	0.132455	-1.325989	1.009588
8	-0.908132	1.367083	-0.583976
6	-0.260276	2.221414	0.348878
8	-3.144476	0.064229	0.394405
6	-3.189415	-0.998020	-0.542689
1	4.492063	0.602238	0.308444
1	3.271124	1.125536	-0.889381
1	2.794102	0.808966	0.795708
1	3.704209	-1.192083	-1.006529
1	0.180701	-2.412605	1.132708
1	0.826142	-0.853896	1.714109
1	-0.883079	-0.987090	1.233010
1	1.393840	-1.017045	-0.466249
1	-0.075386	1.707035	1.300096
1	0.691997	2.590883	-0.046798
1	-0.916569	3.073509	0.533995
1	-0.366242	0.550698	-0.662166
1	-3.532890	-0.656575	-1.527019
1	-2.207832	-1.475339	-0.662372
1	-3.894442	-1.743930	-0.169917
1	-2.438720	0.672254	0.100253

Cartesian coordinates of the methanol pentamer

Cartesian coordinates of : MeOH_3_11_12.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.745056	-1.090763	-1.912714
1	-0.088980	-1.153517	-1.414496
8	-1.449257	-0.835744	-0.202565
1	-0.924308	-1.002884	0.622617
8	1.437228	1.245194	0.993959
1	0.690385	1.569427	0.445354
6	0.695398	0.085869	-2.702959
1	0.533791	0.981848	-2.089764
1	1.657398	0.183515	-3.210721
1	-0.095046	0.032832	-3.461064
6	-2.744915	-1.420227	-0.110836
1	-2.674885	-2.501807	0.036690
1	-3.315118	-0.977242	0.711483
1	-3.262698	-1.222469	-1.050008
6	2.567742	0.984778	0.164042
1	2.358127	0.175030	-0.544033
1	2.863794	1.883970	-0.385623
1	3.389098	0.686993	0.818213
6	1.195276	-2.133037	1.419074
1	0.680501	-3.079116	1.594385
1	1.478830	-2.068090	0.362242
1	2.095409	-2.100250	2.040713
8	0.297281	-1.082301	1.772777
1	0.752872	-0.222588	1.614242
6	-1.710298	2.397117	0.831672
1	-1.328217	3.396514	1.044280
1	-2.764373	2.472404	0.547308
1	-1.625290	1.784521	1.737051
8	-0.931585	1.856055	-0.232300
1	-1.230302	0.934375	-0.378083

Cartesian coordinates of : MeOH_4_13.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-0.664492	2.003540	0.656237
1	-0.630861	1.040032	0.805732
8	-0.666836	-0.769930	0.711282
1	0.180447	-1.147900	0.357602
8	1.559660	-1.667640	-0.380849
1	2.328996	-1.172177	-0.027092
6	-0.666209	2.215035	-0.745436
1	-0.891142	3.268518	-0.924547
1	0.312668	1.992413	-1.191187
1	-1.425441	1.601805	-1.246829
6	-1.044665	-1.459294	1.899720
1	-1.284037	-2.505424	1.685263
1	-0.247984	-1.415204	2.648270
1	-1.932917	-0.966559	2.299776
6	1.437235	-1.361993	-1.767828
1	1.324519	-0.283550	-1.928270
1	2.308035	-1.720384	-2.324121
1	0.544968	-1.868748	-2.139025

8	3.452500	0.050349	0.498894
1	4.373457	0.056541	0.212544
6	2.890762	1.354854	0.348628
1	3.376242	2.067377	1.020772
1	2.977372	1.706551	-0.683874
1	1.834161	1.279906	0.616077
6	-3.657474	0.170998	-0.156893
1	-4.495232	0.555053	-0.742767
1	-4.058790	-0.439539	0.661983
1	-3.111894	1.021092	0.273133
8	-2.834213	-0.591382	-1.023843
1	-2.013417	-0.786893	-0.536371

Cartesian coordinates of : MeOH_5b.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-2.833426	-0.625314	-0.132978
1	-2.150206	0.054922	-0.298362
8	-0.806674	1.179228	-0.623591
1	-0.283832	1.169196	0.212010
8	0.452474	0.857776	1.729615
1	0.924886	0.014892	1.538972
6	-2.921900	-1.445212	-1.282850
1	-2.004502	-2.027512	-1.442755
1	-3.748022	-2.143785	-1.133896
1	-3.122907	-0.858693	-2.187651
6	-1.069203	2.522934	-1.001745
1	-1.593162	3.067776	-0.208822
1	-0.140602	3.050960	-1.245688
1	-1.702829	2.499699	-1.889987
6	-0.627378	0.577559	2.616831
1	-1.356536	-0.098672	2.153785
1	-0.264291	0.134689	3.549118
1	-1.120598	1.524244	2.844120
8	1.447281	-1.500304	0.887455
1	2.219006	-1.305803	0.317631
6	0.377230	-1.902833	0.034322
1	-0.519859	-2.005393	0.649609
1	0.181886	-1.147846	-0.737399
1	0.596373	-2.863000	-0.442945
8	3.175898	-0.555490	-0.990943
1	4.137060	-0.552249	-0.908837
6	2.703534	0.789617	-1.093201
1	2.944147	1.363308	-0.192663
1	3.127918	1.286266	-1.969725
1	1.617963	0.737448	-1.203127

Cartesian coordinates of : MeOH_5r_UUUUD.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-1.751783	2.049081	1.043103
8	-1.212120	1.699879	-0.225567
8	1.423578	1.436832	0.116913
6	2.211939	2.465000	-0.470784
8	2.160929	-1.006077	-0.703401
6	3.160945	-1.541262	0.156950
8	-0.174567	-2.111235	0.045017
6	-0.234561	-1.555122	1.354476

8	-2.142799	-0.668296	-1.065983
6	-3.436136	-0.859301	-0.506743
1	-1.292520	2.966442	1.424817
1	-1.606878	1.246163	1.775898
1	-2.822519	2.219226	0.915164
1	-0.231419	1.610662	-0.135165
1	-4.161176	-0.169451	-0.950818
1	-3.428466	-0.717190	0.580477
1	-3.745899	-1.882772	-0.724182
1	-1.825221	0.236488	-0.828370
1	2.144006	2.444460	-1.563570
1	3.261119	2.370055	-0.173467
1	1.829961	3.422102	-0.111185
1	1.734542	0.559275	-0.214203
1	-1.257093	-1.579156	1.745573
1	0.126812	-0.517455	1.363438
1	0.403511	-2.155833	2.005525
1	-0.897401	-1.687411	-0.475517
1	3.327655	-2.602891	-0.048722
1	2.887487	-1.417872	1.211489
1	4.086558	-0.995288	-0.032217
1	1.324356	-1.508749	-0.562817

Cartesian coordinates of : MeOH_5r_UUUUU.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	0.027272	-1.203073	1.448353
8	0.129538	-2.030393	0.294716
8	2.221029	-0.821440	-0.885908
6	3.414788	-1.114301	-0.169690
8	1.239025	1.654255	-0.564708
6	1.767804	2.149200	0.659039
8	-2.136436	-1.128606	-0.848339
6	-3.256623	-1.269402	0.016895
8	-1.439603	1.474593	-0.733455
6	-1.970989	2.175150	0.383885
1	-0.761820	-1.556765	2.120053
1	-0.179744	-0.162163	1.166721
1	0.981965	-1.242331	1.977703
1	-0.686910	-1.870370	-0.232097
1	3.697042	-2.164546	-0.291025
1	3.306835	-0.893115	0.898648
1	4.208203	-0.486860	-0.579038
1	1.485252	-1.377613	-0.537864
1	-4.147725	-0.801735	-0.414538
1	-3.061138	-0.824686	1.000245
1	-3.446651	-2.336233	0.146444
1	-1.901717	-0.172117	-0.892193
1	2.848115	2.310145	0.581906
1	1.567965	1.462339	1.490161
1	1.284919	3.105155	0.869764
1	1.636670	0.768262	-0.742981
1	-1.726943	3.241124	0.330748
1	-1.593304	1.769671	1.330768
1	-3.056605	2.062797	0.363493
1	-0.456346	1.556321	-0.716253

Cartesian coordinates of : MeOH_N5_4r_1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-3.899681	0.382948	-0.227168
8	-2.647006	0.227290	0.429357
8	-0.562410	1.786050	-0.241717
6	0.091498	2.210440	0.951433
8	0.850227	-0.264913	-1.124205
6	1.569452	-0.129557	-2.346590
8	-1.108213	-1.932744	-0.166032
6	-0.463754	-2.207338	1.075537
8	2.582195	-0.592120	1.040922
6	3.534705	0.401032	0.702276
1	-4.610248	-0.381845	0.100643
1	-3.789534	0.329815	-1.315375
1	-4.291126	1.365275	0.040709
1	-2.247327	-0.637258	0.186798
1	0.553382	1.363347	1.474396
1	-0.610649	2.709895	1.625005
1	0.872101	2.918635	0.668070
1	-1.389236	1.305889	0.004052
1	-0.127823	-1.283096	1.561476
1	0.397396	-2.867890	0.933933
1	-1.190246	-2.703025	1.720837
1	-0.450235	-1.486800	-0.735195
1	2.256990	0.720970	-2.301845
1	0.886016	0.000707	-3.190758
1	2.146141	-1.044076	-2.492870
1	0.357952	0.571742	-0.913758
1	3.057958	1.370761	0.509566
1	4.121227	0.117698	-0.180629
1	4.215408	0.513800	1.548375
1	1.930186	-0.618184	0.317043

Cartesian coordinates of : MeOH_N5_5r.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-0.870268	-0.479030	-2.329258
8	-1.413749	-1.352681	-1.343670
8	0.792548	-2.147495	-0.012199
6	0.433791	-1.920903	1.346877
8	-2.089453	0.541800	0.438044
6	-2.801162	0.189281	1.616903
8	0.287191	1.765384	0.390422
6	0.101871	2.924583	-0.413442
8	2.227795	0.093305	-0.373687
6	3.308055	0.239437	0.540321
1	-0.422232	-1.044380	-3.152272
1	-0.109441	0.182317	-1.894663
1	-1.686184	0.131474	-2.720483
1	-0.652982	-1.802541	-0.909370
1	-2.290145	-0.605020	2.171984
1	-3.817360	-0.137753	1.376338
1	-2.856860	1.078500	2.246556
1	-1.982968	-0.242299	-0.149138
1	0.141682	-0.874960	1.508992
1	1.261276	-2.168397	2.019783
1	-0.416635	-2.564447	1.582003
1	1.423118	-1.431490	-0.259170
1	-0.537145	3.653596	0.094456
1	-0.343126	2.671228	-1.382313
1	1.082850	3.372342	-0.582325
1	-0.584927	1.315130	0.496166

1	2.974017	0.112315	1.576552
1	3.779879	1.221769	0.435597
1	4.045640	-0.531431	0.310879
1	1.523167	0.741339	-0.129254

Cartesian coordinates of the methanol hexamer

Cartesian coordinates of : MeOH_4_12_13.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.824953	2.275735	-0.222490
1	1.278128	1.817129	0.439177
8	-0.046677	0.711576	1.106031
1	0.245895	-0.141729	0.714543
8	0.629860	-1.399213	-0.411442
1	1.542355	-1.742564	-0.276053
6	0.941341	2.962629	-1.093663
1	0.362336	3.728236	-0.563520
1	1.545278	3.451563	-1.860480
1	0.241089	2.275609	-1.585778
6	-0.578289	0.486169	2.411345
1	-1.371804	-0.266849	2.373743
1	0.206807	0.161973	3.100965
1	-0.992643	1.432081	2.763071
6	0.582472	-0.709236	-1.663630
1	1.351589	0.070604	-1.702032
1	0.717959	-1.406501	-2.494643
1	-0.403373	-0.242230	-1.738985
8	3.247077	-1.813183	-0.094408
1	3.630965	-2.585734	0.337622
6	3.612329	-0.630192	0.623135
1	3.225223	-0.655775	1.646523
1	4.698261	-0.509694	0.643061
1	3.166489	0.213239	0.091609
6	-3.347278	1.055303	0.196322
1	-4.220505	1.060772	-0.460249
1	-3.296376	0.086980	0.708224
1	-3.469897	1.850427	0.942505
8	-2.199677	1.270308	-0.610829
1	-1.415726	1.149469	-0.044528
6	-2.722233	-2.101207	-0.758952
1	-3.763157	-2.287882	-0.485324
1	-2.672505	-1.161708	-1.323312
1	-2.378364	-2.924798	-1.395926
8	-1.971209	-2.021019	0.443056
1	-1.032685	-1.947045	0.203101

Cartesian coordinates of : MeOH_4r_11_12.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-4.213358	-1.545196	-0.543689
6	-3.665288	-0.698809	-0.118675
1	-4.339852	0.156151	-0.046325
1	-3.320876	-0.963442	0.887528
8	-2.579866	-0.322097	-0.957727
1	-1.937366	-1.066784	-1.020305
1	1.331214	-1.778520	-1.966458

6	0.403818	-1.235837	-1.756100
1	0.629934	-0.383028	-1.099987
1	-0.008806	-0.861595	-2.694890
8	-0.566247	-2.094673	-1.163919
1	-0.223003	-2.324945	-0.272566
1	-2.068975	1.416283	1.791736
6	-1.997507	2.254334	1.087799
1	-3.005307	2.612647	0.854981
1	-1.436623	3.061882	1.561540
8	-1.304271	1.880440	-0.096785
1	-1.756709	1.095604	-0.487837
1	-0.596861	-0.329884	1.084023
6	-0.303804	-1.062297	1.851021
1	0.191511	-0.534115	2.672356
1	-1.202233	-1.548893	2.235713
8	0.539826	-2.069085	1.303255
1	1.402418	-1.633347	1.117605
1	4.475765	0.099402	0.083004
6	3.649905	-0.601152	-0.080039
1	3.264539	-0.466254	-1.097511
1	4.027697	-1.620294	0.018670
8	2.627535	-0.416940	0.889989
1	2.163434	0.429497	0.691497
1	1.460071	3.398387	-1.234363
6	1.853372	2.389085	-1.077669
1	1.589655	1.765312	-1.940340
1	2.941109	2.443595	-1.002156
8	1.359944	1.834095	0.135420
1	0.374271	1.811675	0.087896

Cartesian coordinates of : MeOH_5_11b.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.167720	1.175547	-1.366425
1	0.184010	1.256314	-1.306498
8	-1.466295	1.493785	-1.001775
1	-1.811290	0.760982	-0.434659
8	-2.313006	-0.472451	0.599806
1	-1.586371	-1.139252	0.582697
6	1.746420	2.346286	-0.795143
1	1.402731	2.497274	0.234854
1	2.829399	2.208779	-0.784423
1	1.506430	3.229765	-1.394594
6	-1.785018	2.733153	-0.379348
1	-2.868941	2.861348	-0.297186
1	-1.339801	2.804675	0.620157
1	-1.382526	3.533317	-1.003272
6	-3.517859	-1.094794	0.165890
1	-3.457164	-1.390754	-0.887623
1	-3.743371	-1.975604	0.774737
1	-4.324982	-0.369790	0.282067
8	-0.333220	-2.274173	0.256475
1	0.534712	-1.816348	0.305286
6	-0.518111	-2.665680	-1.101435
1	-1.445266	-3.238698	-1.158878
1	-0.597673	-1.791166	-1.759155
1	0.307678	-3.297471	-1.442845
8	1.708623	0.669907	2.294466
1	2.107334	0.073712	1.638213
6	0.306409	0.584656	2.112555
1	0.022375	0.759840	1.064843
1	-0.087511	-0.392872	2.418903

1	-0.160722	1.355365	2.729785
6	3.093766	-1.578013	-0.606966
1	3.360366	-2.420819	0.032249
1	2.817356	-1.954960	-1.596841
1	3.959362	-0.915228	-0.702016
8	2.000800	-0.898479	0.003537
1	1.703242	-0.145155	-0.577803

Cartesian coordinates of : MeOH_6b.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-2.550321	1.658598	-0.671517
1	-2.475981	0.740483	-0.996116
8	-2.127178	-1.044938	-1.024579
1	-1.380235	-1.165091	-0.398324
8	-0.205323	-1.381973	0.850902
1	0.770084	-1.363121	0.705465
6	-2.188309	1.628883	0.697447
1	-1.254700	1.072150	0.855036
1	-2.037773	2.657964	1.031762
1	-2.971381	1.171568	1.317096
6	-3.251957	-1.738483	-0.499899
1	-3.009062	-2.785851	-0.292419
1	-3.618770	-1.268768	0.421317
1	-4.044518	-1.703441	-1.249242
6	-0.511639	-1.290495	2.233231
1	-0.090988	-2.134083	2.789862
1	-0.139471	-0.354340	2.667112
1	-1.599127	-1.309740	2.333747
8	2.414772	-1.214863	0.294165
1	2.421000	-0.481134	-0.362765
6	2.910936	-2.395907	-0.327858
1	2.848003	-3.204347	0.402074
1	2.313448	-2.664295	-1.206262
1	3.955415	-2.269995	-0.628124
8	2.000143	0.717449	-1.538237
1	2.009230	1.596483	-1.113895
6	0.641742	0.426622	-1.863908
1	-0.026637	0.699464	-1.039395
1	0.331717	0.962025	-2.766589
1	0.562859	-0.648536	-2.042609
8	1.384828	2.746446	0.163966
1	1.730126	3.631054	0.332326
6	1.418615	1.982542	1.367813
1	2.434086	1.912043	1.768824
1	0.749959	2.406510	2.122945
1	1.071019	0.978265	1.109628

Cartesian coordinates of : MeOH_6r_DUUDUU.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	2.745036	-2.532362	-0.645489
8	2.100269	-1.437257	-0.008208
8	-0.433334	-2.090256	0.468973
6	-0.890025	-1.635110	1.737861
8	2.357778	1.001608	-1.030088
6	3.631094	1.460340	-0.592575
8	-2.357782	-1.001609	-1.030091

6	-3.631095	-1.460344	-0.592571
8	-2.100268	1.437257	-0.008211
6	-2.745029	2.532367	-0.645491
8	0.433332	2.090256	0.468975
6	0.890023	1.635111	1.737864
1	2.266906	-2.777361	-1.599922
1	2.737243	-3.418103	-0.002312
1	3.780977	-2.244531	-0.834243
1	1.151958	-1.670262	0.151303
1	4.437229	0.956075	-1.135453
1	3.766833	1.293544	0.482482
1	3.688637	2.531795	-0.792742
1	2.255825	0.061075	-0.740439
1	1.701947	2.268473	2.110864
1	1.241658	0.597915	1.680672
1	0.053208	1.686546	2.438061
1	1.090654	1.787378	-0.202463
1	-1.701953	-2.268468	2.110859
1	-1.241655	-0.597912	1.680668
1	-0.053212	-1.686548	2.438060
1	-1.090654	-1.787377	-0.202464
1	-2.266898	2.777363	-1.599924
1	-2.737231	3.418107	-0.002313
1	-3.780972	2.244541	-0.834244
1	-1.151956	1.670259	0.151303
1	-4.437234	-0.956081	-1.135444
1	-3.766828	-1.293549	0.482487
1	-3.688637	-2.531799	-0.792739
1	-2.255833	-0.061074	-0.740447

Cartesian coordinates of : MeOH_6r_UUUNDD.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	0.273516	-0.927683	1.908852
8	1.070058	-1.707871	1.022761
8	-0.708694	-2.048410	-0.935983
6	-1.410133	-3.269882	-0.730703
8	3.053039	0.061190	0.606666
6	4.001017	-0.223458	-0.416130
8	1.369858	1.867973	-0.464045
6	0.892676	1.088010	-1.556545
8	-2.275852	0.097647	-0.498435
6	-3.325399	-0.403926	0.321790
8	-1.060152	2.181112	0.650405
6	-1.683637	3.355578	0.143250
1	0.003590	0.037550	1.461193
1	0.796962	-0.748852	2.853115
1	-0.641324	-1.487872	2.114790
1	1.882445	-1.183951	0.830300
1	-1.755955	-3.362822	0.305313
1	-0.779011	-4.129499	-0.976162
1	-2.277695	-3.269719	-1.393117
1	0.039292	-1.997060	-0.293560
1	-2.931999	-0.874375	1.230077
1	-3.935995	-1.130356	-0.223986
1	-3.955502	0.439979	0.608775
1	-1.677133	-0.653793	-0.724086
1	4.597486	0.662377	-0.655071
1	3.509078	-0.581411	-1.328195
1	4.664906	-1.005437	-0.044704
1	2.499493	0.822634	0.315460
1	-2.746197	3.379226	0.405654

1	-1.583220	3.422184	-0.946462
1	-1.189782	4.217035	0.595495
1	-1.508703	1.396610	0.249168
1	-0.019415	1.521935	-1.979719
1	0.681982	0.055224	-1.247558
1	1.667013	1.075002	-2.325911
1	0.585394	2.070443	0.095168

Cartesian coordinates of : MeOH_6r_UUUDUD.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-0.479722	-1.446313	1.462730
8	-1.023673	-2.209500	0.391013
8	-2.597968	-0.340341	-0.712881
6	-3.889424	-0.339137	-0.113916
8	-1.192819	1.833620	-0.025353
6	-1.753717	2.206827	1.228091
8	1.476102	1.815492	0.011326
6	1.870772	2.535409	-1.150469
8	2.736960	-0.518038	0.295644
6	3.124276	-0.676500	1.652756
8	1.130632	-2.061706	-1.204019
6	0.683600	-0.987417	-2.024100
1	-0.048127	-0.502034	1.099481
1	0.295297	-2.009607	1.992658
1	-1.291191	-1.221165	2.157695
1	-0.280962	-2.379143	-0.232348
1	-3.822726	-0.350559	0.980036
1	-4.475386	-1.201203	-0.446807
1	-4.398400	0.574503	-0.426290
1	-2.090284	-1.119697	-0.384673
1	-1.733903	1.372215	1.938319
1	-2.785877	2.551471	1.107713
1	-1.154251	3.025045	1.631355
1	-1.688418	1.048186	-0.361350
1	1.516140	-0.544992	-2.581150
1	0.201723	-0.202184	-1.423803
1	-0.046538	-1.385486	-2.730770
1	1.797537	-1.678873	-0.589400
1	1.562186	3.583441	-1.083674
1	1.443282	2.093079	-2.057338
1	2.959428	2.491185	-1.216550
1	0.489493	1.779130	0.030427
1	2.296529	-0.449686	2.334264
1	3.972220	-0.027815	1.896663
1	3.423355	-1.716151	1.798546
1	2.290290	0.356902	0.190593

Cartesian coordinates of : MeOH_6r_UUUUDD.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-3.077555	-0.025900	-1.449351
8	-2.351989	-0.020166	-0.225506
8	-0.823484	2.186973	-0.358940
6	-1.506407	3.308980	0.190977
8	1.138537	1.468079	1.300666
6	0.406558	0.438860	1.959018
8	-1.084693	-2.329675	0.264777

6	-1.401653	-2.797958	1.567314
8	3.061707	-0.119777	0.283796
6	3.859895	0.385854	-0.780586
8	1.277074	-1.752933	-0.910565
6	0.657997	-0.829839	-1.801318
1	-2.405593	0.063962	-2.310155
1	-3.804441	0.792327	-1.476245
1	-3.612267	-0.975164	-1.516585
1	-1.773785	0.779685	-0.219338
1	-2.468224	-3.029856	1.652765
1	-1.135487	-2.062222	2.335774
1	-0.828425	-3.709649	1.742876
1	-1.575455	-1.490181	0.092747
1	0.350947	0.087211	-1.279492
1	-0.221057	-1.277882	-2.276221
1	1.383434	-0.570862	-2.574806
1	0.558664	-2.112872	-0.346193
1	-0.920996	4.224337	0.062601
1	-1.717865	3.163232	1.256232
1	-2.451406	3.416365	-0.344494
1	0.000587	2.031672	0.160775
1	3.255664	0.953903	-1.497748
1	4.371236	-0.425965	-1.307075
1	4.608554	1.050863	-0.347528
1	2.469140	-0.819131	-0.076648
1	0.950166	0.064823	2.832422
1	0.202220	-0.397118	1.277356
1	-0.545759	0.861307	2.289534
1	1.939908	1.041225	0.919293

Cartesian coordinates of : MeOH_6r_UUUUUU.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	3.047554	1.222264	0.830336
8	2.359418	1.125967	-0.411320
8	-0.020114	2.262340	-0.078673
6	0.069296	3.589404	-0.580639
8	-2.371247	1.072864	-0.440549
6	-3.001846	1.322234	0.810075
8	2.284865	-1.502197	-0.878177
6	3.338778	-2.204409	-0.230312
8	0.014670	-2.145865	0.352217
6	-0.040874	-1.169757	1.385973
8	-2.278096	-1.564521	-0.882689
6	-3.405379	-2.105907	-0.204396
1	4.090371	0.905498	0.726196
1	2.562637	0.614487	1.603277
1	3.027311	2.267923	1.143422
1	2.328901	0.172090	-0.669467
1	0.282025	3.596682	-1.654810
1	0.847579	4.153681	-0.056346
1	-0.892682	4.076446	-0.408703
1	0.838497	1.799241	-0.243505
1	-3.047801	2.396207	1.017251
1	-2.472651	0.823994	1.631144
1	-4.019752	0.931149	0.756295
1	-1.467970	1.471745	-0.403509
1	3.297256	-3.273308	-0.461743
1	3.299212	-2.071714	0.857292
1	4.283745	-1.801224	-0.599139
1	1.421710	-1.815551	-0.511941
1	-4.339001	-1.723328	-0.629293

1	-3.378356	-1.873286	0.867004
1	-3.380722	-3.189648	-0.328805
1	-2.305213	-0.580171	-0.796183
1	-0.935603	-1.303253	2.003798
1	-0.036914	-0.150104	0.977471
1	0.840448	-1.300670	2.017798
1	-0.804171	-2.038578	-0.190196

Cartesian coordinates of : MeOH_N6_12.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-3.256476	-0.223613	-1.258939
8	-2.001169	-0.246427	-0.585950
8	-0.826414	2.079946	-0.544242
6	-1.426198	2.856543	0.488141
8	1.713507	1.642985	0.044464
6	2.585938	2.508573	-0.673746
8	2.264271	-0.874812	-0.667289
6	2.951324	-1.665065	0.296124
8	-0.094941	-2.115303	-1.077221
6	-0.340567	-3.155454	-0.135266
8	-1.470444	-0.648087	2.123422
6	-0.133944	-0.196898	1.985302
1	-3.916613	0.532370	-0.822464
1	-3.124835	-0.017350	-2.325358
1	-3.715603	-1.206197	-1.140662
1	-1.565108	0.650408	-0.650838
1	3.625773	2.350679	-0.371341
1	2.497796	2.355629	-1.754602
1	2.302251	3.535710	-0.437486
1	1.935138	0.707186	-0.186448
1	2.323365	-1.860610	1.173452
1	3.270147	-2.618594	-0.136566
1	3.834739	-1.108579	0.613749
1	1.421365	-1.330180	-0.901453
1	-0.425115	-2.758952	0.883325
1	-1.258345	-3.697578	-0.384689
1	0.501065	-3.849034	-0.181550
1	-0.816399	-1.451949	-1.000638
1	0.304061	-0.521535	1.031365
1	-0.059410	0.896462	2.039200
1	0.454619	-0.624364	2.800911
1	-1.899418	-0.537965	1.256580
1	-1.812778	2.215642	1.290551
1	-0.704808	3.561332	0.911903
1	-2.256380	3.417367	0.054683
1	0.125561	1.909172	-0.316799

Cartesian coordinates of : MeOH_N6_180.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-1.022345	2.662943	0.669434
8	-0.608404	2.344027	-0.656115
8	-1.557123	-0.066365	-1.036043
6	-2.841882	-0.134864	-1.647299
8	1.968958	1.799748	-0.280562
6	2.574518	1.094893	-1.362912
8	1.595645	-0.079000	1.600964

6	2.366722	-1.236421	1.286408
8	-0.973838	-0.877802	1.482559
6	-1.959212	-0.586293	2.465282
8	0.555260	-1.797022	-1.624319
6	0.134217	-2.991401	-0.984376
1	-0.618494	1.942735	1.392212
1	-0.698865	3.670273	0.947783
1	-2.113240	2.619537	0.699698
1	0.374164	2.221388	-0.631419
1	-0.111066	-2.817205	0.070466
1	-0.737772	-3.432146	-1.483173
1	0.960108	-3.704313	-1.038831
1	-0.167503	-1.148475	-1.543848
1	3.620272	0.861582	-1.135768
1	2.036030	0.165389	-1.579531
1	2.543698	1.743163	-2.240622
1	1.869083	1.166426	0.470768
1	-2.276914	0.461021	2.417383
1	-2.834430	-1.232256	2.343650
1	-1.514889	-0.774459	3.443733
1	-1.308747	-0.638044	0.590914
1	2.194651	-2.029613	2.021453
1	2.124772	-1.607174	0.284042
1	3.419843	-0.950008	1.320661
1	0.644627	-0.334983	1.607770
1	-3.579356	0.430643	-1.069052
1	-2.807391	0.252522	-2.669507
1	-3.139509	-1.184178	-1.674602
1	-1.235173	0.876345	-0.995268

Cartesian coordinates of : MeOH_N6_6.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-2.612650	-2.331007	0.542610
8	-2.354464	-1.292780	-0.393244
8	0.008338	-1.298815	-1.661596
6	0.037248	0.096124	-1.942684
8	-2.407680	1.258053	0.458632
6	-2.883107	2.116145	-0.568914
8	-0.008333	1.298815	1.661593
6	-0.037255	-0.096124	1.942679
8	2.354471	1.292778	0.393240
6	2.612660	2.331011	-0.542607
8	2.407675	-1.258058	-0.458631
6	2.883098	-2.116144	0.568921
1	-2.857970	-3.266824	0.030632
1	-1.753759	-2.498607	1.202060
1	-3.466896	-2.026376	1.149797
1	-1.494733	-1.457315	-0.844392
1	-2.209680	2.119816	-1.433639
1	-3.883894	1.818181	-0.897158
1	-2.934046	3.126824	-0.160762
1	-2.433925	0.323087	0.145312
1	1.753774	2.498610	-1.202063
1	2.857971	3.266827	-0.030622
1	3.466913	2.026387	-1.149788
1	1.494747	1.457323	0.844393
1	-0.963639	-0.372933	2.457160
1	0.050524	-0.690255	1.021312
1	0.810011	-0.323569	2.593025
1	-0.844018	1.499828	1.183065
1	3.883893	-1.818192	0.897152

1	2.209679	-2.119796	1.433652
1	2.934018	-3.126828	0.160778
1	2.433911	-0.323092	-0.145310
1	-0.050522	0.690258	-1.021319
1	0.963623	0.372937	-2.457179
1	-0.810027	0.323563	-2.593020
1	0.844024	-1.499823	-1.183066

Cartesian coordinates of : MeOH_N6_6r.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-2.857042	-2.360289	-0.847360
8	-1.995351	-1.746765	0.102538
8	0.513063	-2.597627	-0.098546
6	0.616010	-3.653824	0.847493
8	2.504898	-0.852075	0.102169
6	3.467543	-1.292610	-0.846751
8	1.995350	1.746763	-0.102541
6	2.857045	2.360288	0.847354
8	-0.513063	2.597628	0.098546
6	-0.616018	3.653824	-0.847493
8	-2.504897	0.852074	-0.102166
6	-3.467538	1.292612	0.846757
1	-2.651514	-2.003314	-1.862330
1	-3.907095	-2.166150	-0.605170
1	-2.682270	-3.437423	-0.810465
1	-2.129620	-0.767078	0.057664
1	-0.071945	-4.468871	0.599832
1	0.404461	-3.302463	1.863189
1	1.638353	-4.035559	0.812565
1	-0.404333	-2.228402	-0.055075
1	3.056334	-1.293857	-1.862014
1	3.824095	-2.298907	-0.603517
1	4.313130	-0.602853	-0.809927
1	1.724691	-1.459814	0.059646
1	-3.824086	2.298911	0.603527
1	-3.056327	1.293854	1.862019
1	-4.313128	0.602859	0.809934
1	-1.724687	1.459810	-0.059642
1	3.907096	2.166144	0.605162
1	2.651518	2.003316	1.862326
1	2.682277	3.437421	0.810456
1	2.129616	0.767076	-0.057666
1	-0.404471	3.302464	-1.863189
1	0.071934	4.468875	-0.599835
1	-1.638363	4.035554	-0.812562
1	0.404334	2.228408	0.055072

Cartesian coordinates of : MeOH_N6_81.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-2.125960	-1.168436	-2.200690
8	-1.282117	-0.820070	-1.105265
8	0.413022	1.139083	-1.633547
6	0.084758	2.493225	-1.331977
8	2.400135	-0.039099	-0.129611
6	3.682143	-0.388441	-0.643470

8	0.765051	-2.141487	0.108725
6	0.260072	-2.603151	1.358316
8	-2.670983	-0.234486	1.246073
6	-3.142231	1.055623	0.898486
8	1.402678	1.782507	1.721673
6	0.262813	0.957184	1.888269
1	-2.812571	-0.349509	-2.435869
1	-1.533352	-1.412574	-3.087021
1	-2.704653	-2.044673	-1.905860
1	-0.722014	-0.036312	-1.345179
1	-0.532281	-1.944687	1.730846
1	-0.130469	-3.621139	1.265005
1	1.085337	-2.603156	2.072695
1	0.007653	-1.856328	-0.442807
1	-0.103915	0.570320	0.926117
1	0.470627	0.104700	2.546818
1	-0.530316	1.559090	2.337329
1	2.033487	1.273315	1.185497
1	0.059508	2.662586	-0.250741
1	0.808785	3.175833	-1.786866
1	-0.901675	2.689713	-1.755511
1	1.232820	0.872055	-1.167457
1	-2.323588	1.713452	0.577053
1	-3.890828	1.012923	0.097675
1	-3.606022	1.492647	1.785229
1	-2.185664	-0.572549	0.471735
1	4.249048	-0.971339	0.088212
1	3.588537	-0.962076	-1.570629
1	4.218005	0.538423	-0.851388
1	1.871675	-0.858336	0.037129

Cartesian coordinates of the methanol heptamer

Cartesian coordinates of : MeOH_4r_11_22.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	1.155697	3.537284	1.666833
6	0.124734	3.192788	1.541173
1	-0.315705	2.996574	2.523360
1	-0.452890	3.971088	1.040299
8	0.079192	2.025666	0.721714
1	0.517553	1.267524	1.195330
1	-0.566780	-0.470236	-2.423806
6	0.174575	-0.760787	-1.671715
1	1.172013	-0.678646	-2.108091
1	0.109338	-0.067541	-0.820921
8	-0.020543	-2.108817	-1.257122
1	-0.941307	-2.158588	-0.923944
1	-4.421555	-1.650353	0.414346
6	-3.406944	-2.051537	0.504769
1	-3.028002	-1.836453	1.511105
1	-3.443150	-3.133497	0.368639
8	-2.555334	-1.517197	-0.498188
1	-2.496090	-0.540182	-0.386780
1	-1.395467	1.827319	-1.954045
6	-2.367273	1.859831	-1.448119
1	-2.656903	2.904469	-1.296141
1	-3.111177	1.373765	-2.082190
8	-2.324755	1.159337	-0.209239
1	-1.517793	1.455455	0.263954

6	2.777230	1.400185	-0.856213
1	3.550030	1.149340	-1.586132
1	3.215763	2.051259	-0.089813
1	2.443130	0.470482	-0.373742
8	1.718957	2.040369	-1.547085
1	1.016390	2.194266	-0.891285
6	-0.314855	-0.773380	2.191460
1	-0.188700	-1.625137	2.866261
1	-0.748765	-1.122389	1.245577
1	-0.997990	-0.054435	2.649981
8	0.929009	-0.111439	1.969877
1	1.501299	-0.741478	1.475268
6	3.221052	-2.311348	-0.119934
1	3.262074	-1.747832	-1.059170
1	3.395896	-3.370906	-0.331368
1	4.009736	-1.947536	0.540760
8	1.978662	-2.124509	0.545084
1	1.240736	-2.295404	-0.083143

Cartesian coordinates of : MeOH_5r_11_12.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	-1.673693	-3.616298	0.210544
6	-2.040814	-2.742112	-0.336676
1	-1.439451	-2.613958	-1.244362
1	-3.081031	-2.910593	-0.620856
8	-2.002727	-1.580787	0.478717
1	-1.074824	-1.400386	0.724717
1	-2.348633	1.772710	1.145068
6	-3.185119	1.646391	0.450007
1	-4.066536	1.308733	1.004987
1	-3.414158	2.604408	-0.020690
8	-2.854410	0.724682	-0.583419
1	-2.579751	-0.131899	-0.172168
1	0.317530	0.912482	3.501295
6	0.426962	0.079874	2.796828
1	1.492607	-0.090241	2.604003
1	0.005459	-0.819771	3.250289
8	-0.286019	0.320689	1.592777
1	0.122725	1.070707	1.123473
1	-0.765900	-0.603407	-2.724958
6	-0.114888	0.028161	-2.110840
1	0.035575	-0.451556	-1.133280
1	0.850303	0.127838	-2.612415
8	-0.666516	1.333744	-1.960955
1	-1.534011	1.218531	-1.495811
1	0.316733	4.083832	0.344566
6	1.240276	3.539200	0.125665
1	1.725036	3.983341	-0.748644
1	1.910627	3.618732	0.982530
8	0.975464	2.157288	-0.087083
1	0.355740	2.021703	-0.851707
6	1.341519	-3.000181	-0.453431
1	0.777669	-3.934892	-0.480296
1	1.265503	-2.519913	-1.438861
1	2.394343	-3.233803	-0.256700
8	0.789232	-2.186755	0.567572
1	1.314959	-1.362792	0.599576
6	3.558963	-0.294396	-0.693196
1	4.103923	-1.191636	-0.394687
1	3.116921	-0.464333	-1.681894
1	4.264929	0.539926	-0.756002

8	2.561983	-0.050523	0.289842
1	2.109967	0.794208	0.092534

Cartesian coordinates of : MeOH_6_13.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-3.156334	0.477391	-2.090061
1	-3.012977	0.887048	-1.212848
8	-2.826623	1.672631	0.357997
1	-2.280608	1.203745	1.029956
8	-1.130806	0.534334	2.104211
1	-0.394520	0.145277	1.586178
6	-4.422810	-0.153357	-2.070601
1	-5.233688	0.564812	-1.896996
1	-4.579436	-0.622583	-3.044308
1	-4.479281	-0.933265	-1.299590
6	-2.284919	2.976357	0.189433
1	-2.370261	3.560799	1.111309
1	-1.231277	2.935252	-0.111152
1	-2.854699	3.474615	-0.597241
6	-1.563999	-0.393913	3.093808
1	-1.776124	-1.373289	2.651861
1	-0.807732	-0.507340	3.877024
1	-2.476207	0.005023	3.540523
8	0.587293	-0.552472	0.314929
1	1.572744	-0.656251	0.362666
6	0.264876	0.088541	-0.918925
1	-0.784233	0.393321	-0.875076
1	0.890493	0.973546	-1.072423
1	0.394544	-0.599550	-1.761447
8	3.201297	-0.823162	0.154565
1	3.742360	-0.009214	0.230493
6	3.491717	-1.427829	-1.102576
1	3.384085	-0.709026	-1.922187
1	4.506067	-1.838813	-1.111980
1	2.780300	-2.242768	-1.249736
8	4.895256	1.303075	0.071879
1	4.610041	2.097550	-0.395274
6	6.167672	0.887079	-0.425470
1	6.122017	0.667703	-1.496196
1	6.927243	1.650177	-0.237641
1	6.434482	-0.021511	0.115591
6	-2.301175	-2.066459	-0.055748
1	-3.164607	-2.722543	0.076155
1	-2.524987	-1.098705	0.418114
1	-2.149879	-1.892441	-1.128395
8	-1.184953	-2.700553	0.544541
1	-0.433075	-2.084017	0.488610

Cartesian coordinates of : MeOH_7.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.439788	-2.264116	0.805971
1	2.066521	-1.526204	0.604642
8	3.138182	-0.342155	0.076888
1	2.703624	0.497222	-0.215367
8	2.011805	1.906302	-0.807123
1	1.096282	1.971360	-0.439787

6	1.294754	-2.410232	2.211424
1	0.831632	-1.525636	2.664005
1	0.650805	-3.272537	2.391594
1	2.263867	-2.588112	2.687840
6	3.873340	-0.858824	-1.027597
1	3.214918	-1.075623	-1.876631
1	4.647056	-0.152651	-1.344996
1	4.351564	-1.785614	-0.705978
6	2.762486	3.022859	-0.340424
1	2.367591	3.957444	-0.750020
1	2.753534	3.077070	0.753928
1	3.792159	2.895711	-0.679717
8	-0.264281	1.917077	0.534190
1	-1.189363	1.869355	0.187881
6	-0.088868	0.854021	1.461508
1	0.981774	0.765748	1.672674
1	-0.614998	1.057121	2.400521
1	-0.441865	-0.100375	1.049872
8	-2.806030	1.555161	-0.164758
1	-2.916803	0.571169	-0.182035
6	-3.645157	2.078322	0.858723
1	-4.698595	1.873750	0.642681
1	-3.391923	1.654584	1.837320
1	-3.496405	3.158901	0.892942
8	-3.049311	-1.089788	-0.110529
1	-2.149917	-1.470189	-0.266261
6	-3.931320	-1.603859	-1.102258
1	-3.563609	-1.388971	-2.111885
1	-4.058156	-2.684878	-0.989218
1	-4.900182	-1.119146	-0.969190
8	-0.636000	-1.911849	-0.818619
1	0.069636	-2.161210	-0.174262
6	-0.112979	-0.887698	-1.656626
1	0.598609	-0.256117	-1.111231
1	0.387852	-1.315668	-2.530917
1	-0.942366	-0.259082	-1.995061

Cartesian coordinates of : MeOH_7r_1.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-3.819908	-1.966552	-0.268199
8	-2.592416	-1.415201	-0.728208
8	-2.787057	1.146640	-0.040293
6	-3.653539	1.847156	-0.923868
8	-0.732965	2.816841	0.163036
6	-0.861783	3.691791	1.275633
8	1.875330	2.319120	0.107120
6	2.524693	3.198937	-0.801221
8	3.091552	-0.006434	-0.322382
6	4.245635	-0.107929	0.501974
8	1.970482	-2.396296	-0.028055
6	2.412159	-3.342869	-0.991623
8	-0.624032	-2.874764	0.309042
6	-1.017576	-2.967692	1.672115
1	-4.665590	-1.581183	-0.847463
1	-3.982570	-1.747251	0.793049
1	-3.770760	-3.049646	-0.400426
1	-2.578927	-0.454242	-0.495009
1	-1.913797	-3.588251	1.779849
1	-1.214323	-1.977397	2.097657
1	-0.200332	-3.433065	2.226727
1	-1.288878	-2.314190	-0.160308

1	1.892087	-3.213777	-1.946881
1	2.257183	-4.366098	-0.634401
1	3.481059	-3.184815	-1.149519
1	0.996857	-2.508110	0.100372
1	-0.257850	4.594503	1.135531
1	-0.561419	3.200794	2.207430
1	-1.911857	3.981471	1.352862
1	0.211616	2.533562	0.099451
1	4.905796	-0.909375	0.154293
1	3.975165	-0.294537	1.546820
1	4.784491	0.839892	0.441341
1	2.588170	-0.854076	-0.249805
1	2.402057	2.865602	-1.837229
1	3.592998	3.278625	-0.574127
1	2.069722	4.185803	-0.692872
1	2.245086	1.411372	-0.021147
1	-3.202324	1.966534	-1.914779
1	-3.904443	2.834891	-0.523468
1	-4.572656	1.265997	-1.022259
1	-1.961804	1.680661	0.063371

Cartesian coordinates of : MeOH_7r_2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	1.294767	-2.410201	2.211458
8	1.439777	-2.264116	0.806000
8	3.138147	-0.342158	0.076847
6	3.873334	-0.858838	-1.027613
8	2.011806	1.906311	-0.807157
6	2.762502	3.022827	-0.340384
8	-0.264271	1.917083	0.534155
6	-0.088848	0.854045	1.461491
8	-2.806018	1.555191	-0.164791
6	-3.645115	2.078347	0.858718
8	-3.049325	-1.089757	-0.110520
6	-3.931351	-1.603865	-1.102214
8	-0.636026	-1.911864	-0.818581
6	-0.112978	-0.887774	-1.656646
1	2.066504	-1.526207	0.604642
1	2.703597	0.497219	-0.215426
1	1.096280	1.971364	-0.439824
1	0.831738	-1.525558	2.664042
1	0.650742	-3.272444	2.391656
1	2.263875	-2.588166	2.687852
1	3.214942	-1.075606	-1.876677
1	4.647088	-0.152687	-1.344971
1	4.351516	-1.785647	-0.705984
1	2.367598	3.957448	-0.749890
1	2.753577	3.076946	0.753974
1	3.792166	2.895706	-0.679713
1	-1.189355	1.869355	0.187847
1	0.981801	0.765745	1.672613
1	-0.614930	1.057185	2.400524
1	-0.441891	-0.100351	1.049895
1	-2.916797	0.571199	-0.182068
1	-4.698558	1.873765	0.642712
1	-3.391844	1.654614	1.837308
1	-3.496371	3.158928	0.892930
1	-2.149934	-1.470167	-0.266247
1	-3.563644	-1.389042	-2.111856
1	-4.058208	-2.684876	-0.989113
1	-4.900203	-1.119126	-0.969167

1	0.069612	-2.161219	-0.174226
1	0.598503	-0.256079	-1.111243
1	0.387984	-1.315810	-2.530831
1	-0.942373	-0.259263	-1.995248

Cartesian coordinates of : MeOH_7r_UUDDUD.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
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6	-1.228565	3.741105	-0.238583
8	-1.045693	2.395053	-0.664280
8	1.578303	1.984508	-0.553236
6	2.236891	1.820548	-1.803303
8	2.524069	-0.036005	0.887520
6	2.708462	0.017744	2.294783
8	1.632866	-2.434488	0.168689
6	2.435101	-2.881687	-0.919925
8	-0.744100	-2.047175	-0.957738
6	-0.567507	-0.761976	-1.544568
8	-2.909156	-1.591847	0.523212
6	-4.117929	-1.542023	-0.225266
8	-1.925699	0.774695	1.261008
6	-0.684467	0.428433	1.863099
1	-0.743183	4.438211	-0.928883
1	-0.827241	3.897416	0.769426
1	-2.300535	3.944818	-0.227099
1	-0.074112	2.207921	-0.666229
1	0.011929	1.275186	1.839076
1	-0.214321	-0.423903	1.351600
1	-0.872922	0.154861	2.903162
1	-1.721461	1.342347	0.477781
1	-4.047684	-0.825680	-1.051704
1	-4.962819	-1.268619	0.414299
1	-4.294591	-2.536965	-0.636676
1	-2.679663	-0.683714	0.836029
1	3.546471	-0.615228	2.603992
1	1.806611	-0.301539	2.829882
1	2.929172	1.052257	2.564887
1	2.185587	-0.931167	0.634372
1	0.094544	-0.135184	-0.930003
1	-1.526013	-0.245547	-1.658235
1	-0.115513	-0.889348	-2.531059
1	-1.540679	-2.006506	-0.374317
1	2.346903	-2.208535	-1.780692
1	2.150490	-3.893274	-1.224611
1	3.473928	-2.891869	-0.585647
1	0.698756	-2.381116	-0.149555
1	2.066524	0.818944	-2.215161
1	3.313866	1.986727	-1.701538
1	1.828611	2.559664	-2.495176
1	1.890702	1.269048	0.053264

Cartesian coordinates of : MeOH_7r_UUUUDD.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
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6	-2.516228	-3.006864	1.102640
8	-1.722948	-1.830441	1.212931
8	0.297706	-1.959773	-0.499004
6	0.055644	-0.925127	-1.444692

8	2.892026	-1.583084	-0.065621
6	3.608280	-1.976392	-1.230852
8	-2.989361	0.292943	0.189159
6	-3.933927	-0.285304	-0.704317
8	3.095812	1.066019	-0.003718
6	4.024316	1.607750	0.928132
8	0.698293	2.016697	0.646958
6	0.166674	1.094559	1.592978
8	-1.440708	2.144613	-0.949360
6	-2.123488	3.368906	-0.699936
1	-2.014634	-3.861603	1.566994
1	-2.733570	-3.244327	0.055073
1	-3.456753	-2.824513	1.625940
1	-0.906961	-1.944046	0.666952
1	-4.714260	-0.822217	-0.155311
1	-3.450732	-0.975232	-1.406348
1	-4.396579	0.524512	-1.271512
1	-2.510465	-0.440574	0.647017
1	-2.248253	3.542479	0.375213
1	-3.107606	3.372567	-1.179258
1	-1.523431	4.177232	-1.120895
1	-1.986236	1.414689	-0.566138
1	4.676995	-1.765921	-1.122164
1	3.231722	-1.461657	-2.122394
1	3.472322	-3.051548	-1.359956
1	2.978632	-0.601342	0.026626
1	0.097215	0.083772	1.171459
1	-0.827934	1.409362	1.927829
1	0.838217	1.070816	2.453295
1	0.013151	2.132439	-0.054169
1	3.693975	1.446863	1.960197
1	4.166240	2.679705	0.759281
1	4.978604	1.098849	0.780650
1	2.210176	1.474614	0.157118
1	0.366440	-1.229419	-2.449562
1	0.582747	-0.002448	-1.170811
1	-1.018570	-0.718057	-1.455278
1	1.255369	-1.925963	-0.254323

Cartesian coordinates of the methanol octamer

Cartesian coordinates of : MeOH_5_21_14.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-3.599722	-0.081136	-1.181102
1	-3.154493	-0.828035	-0.717507
8	2.520482	-2.111330	-0.072674
1	3.122637	-1.369978	0.171259
8	3.867563	0.151458	0.518296
1	3.135472	0.521344	1.060273
6	-4.920608	0.041802	-0.667165
1	-4.914515	0.213243	0.415885
1	-5.389231	0.897905	-1.155192
1	-5.511407	-0.854275	-0.882843
6	2.958614	-2.691205	-1.297265
1	2.967932	-1.953635	-2.107994
1	3.959423	-3.120496	-1.190334
1	2.258741	-3.488198	-1.553942
6	3.872132	0.862368	-0.718794
1	2.856452	0.949819	-1.125059

1	4.293866	1.864755	-0.590694
1	4.498260	0.307227	-1.420148
8	1.508054	0.891977	1.629521
1	1.005577	0.905346	0.788988
6	1.061222	-0.166071	2.467063
1	1.562880	-0.050943	3.429424
1	-0.021064	-0.117385	2.626336
1	1.314817	-1.147791	2.050113
8	0.666988	2.033767	-0.755697
1	-0.308557	2.008473	-0.839045
6	1.037616	3.336247	-0.329587
1	0.797773	4.088791	-1.088604
1	0.545034	3.608650	0.611733
1	2.117449	3.334968	-0.165246
8	0.119047	-0.934340	-0.294168
1	0.968502	-1.420328	-0.161377
6	-0.043496	-0.716260	-1.693773
1	0.794503	-0.139759	-2.096029
1	-0.137843	-1.665836	-2.232853
1	-0.960727	-0.137986	-1.834556
8	-2.287433	-1.993747	0.213960
1	-1.348826	-1.697783	0.164730
6	-2.686223	-2.112474	1.573646
1	-2.026287	-2.794915	2.118231
1	-2.689995	-1.139134	2.078947
1	-3.699707	-2.517141	1.586710
6	-1.915836	1.527494	0.945652
1	-1.279202	2.227988	1.492195
1	-2.890654	1.476505	1.443432
1	-1.443502	0.537378	0.962442
8	-2.043165	2.000403	-0.391090
1	-2.618338	1.353392	-0.854315

Cartesian coordinates of : MeOH_5_21_15.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-3.599724	-0.081134	-1.181101
1	-3.154493	-0.828033	-0.717508
8	2.520481	-2.111329	-0.072675
1	3.122636	-1.369978	0.171259
8	3.867562	0.151458	0.518297
1	3.135472	0.521344	1.060275
6	-4.920610	0.041801	-0.667162
1	-4.914516	0.213243	0.415887
1	-5.389235	0.897903	-1.155190
1	-5.511407	-0.854278	-0.882839
6	2.958616	-2.691203	-1.297266
1	2.967935	-1.953632	-2.107994
1	3.959424	-3.120495	-1.190334
1	2.258742	-3.488195	-1.553945
6	3.872134	0.862368	-0.718792
1	2.856454	0.949821	-1.125057
1	4.293868	1.864755	-0.590692
1	4.498261	0.307227	-1.420146
8	1.508052	0.891975	1.629522
1	1.005576	0.905343	0.788989
6	1.061221	-0.166075	2.467063
1	1.562877	-0.050947	3.429424
1	-0.021066	-0.117390	2.626335
1	1.314816	-1.147794	2.050112
8	0.666990	2.033767	-0.755697
1	-0.308555	2.008473	-0.839047

6	1.037618	3.336246	-0.329586
1	0.797774	4.088792	-1.088601
1	0.545035	3.608648	0.611735
1	2.117450	3.334967	-0.165243
8	0.119046	-0.934340	-0.294170
1	0.968501	-1.420328	-0.161379
6	-0.043497	-0.716258	-1.693774
1	0.794503	-0.139755	-2.096030
1	-0.137842	-1.665833	-2.232856
1	-0.960728	-0.137984	-1.834557
8	-2.287434	-1.993745	0.213958
1	-1.348826	-1.697782	0.164727
6	-2.686222	-2.112475	1.573645
1	-2.026284	-2.794915	2.118228
1	-2.689994	-1.139135	2.078946
1	-3.699704	-2.517143	1.586710
6	-1.915835	1.527494	0.945651
1	-1.279199	2.227986	1.492195
1	-2.890653	1.476507	1.443432
1	-1.443503	0.537376	0.962442
8	-2.043165	2.000403	-0.391090
1	-2.618340	1.353393	-0.854315

Cartesian coordinates of : MeOH_5r_21_12.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
1	1.750022	4.617843	-0.583485
6	2.065025	3.569734	-0.553757
1	1.883018	3.115588	-1.534638
1	3.135093	3.530134	-0.343008
8	1.391532	2.866142	0.479953
1	0.426602	2.810439	0.268649
1	0.100147	0.274565	0.548303
6	0.680817	-0.089804	1.406761
1	0.151425	0.182220	2.326057
1	0.743258	-1.180566	1.343491
8	2.003408	0.434150	1.395610
1	1.941873	1.372553	1.099860
1	-1.980417	1.298404	1.438187
6	-1.896600	2.375881	1.253966
1	-2.897346	2.821339	1.241369
1	-1.319364	2.831463	2.062652
8	-1.216571	2.636137	0.026693
1	-1.500321	1.948125	-0.618530
1	-1.149023	-3.779525	-1.373597
6	-1.661701	-2.835708	-1.579095
1	-1.648782	-2.641046	-2.656121
1	-2.697640	-2.913338	-1.242956
8	-1.054777	-1.763703	-0.861278
1	-0.099288	-1.666377	-1.134590
1	-3.684602	0.081691	-0.068783
6	-3.586739	0.502469	-1.075404
1	-4.122437	-0.129566	-1.791176
1	-4.026928	1.501745	-1.091419
8	-2.214153	0.630669	-1.442778
1	-1.770800	-0.230216	-1.280356
6	-1.994068	-2.141401	2.565707
1	-0.943105	-2.185125	2.878794
1	-2.295649	-3.132722	2.206966
1	-2.602059	-1.888592	3.436502
8	-2.209824	-1.141047	1.585376
1	-1.733861	-1.395659	0.773624

6	1.323893	0.112399	-2.098822
1	2.096125	0.329644	-2.843117
1	1.479311	0.752429	-1.221234
1	0.344278	0.336173	-2.529019
8	1.340629	-1.266439	-1.739040
1	2.133123	-1.419480	-1.167997
6	3.749224	-2.413214	0.700103
1	2.862837	-2.840686	1.182817
1	4.488850	-2.164123	1.467186
1	4.176874	-3.158043	0.027356
8	3.417145	-1.268400	-0.075980
1	3.020572	-0.581516	0.513005

Cartesian coordinates of : MeOH_6_12_15.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.758765	1.041713	1.592009
1	-1.788425	1.041717	0.617211
8	2.764904	-2.102798	-1.777982
1	2.718096	-2.025636	-0.810631
8	2.236113	-1.096996	0.768838
1	2.475467	-0.142976	0.645263
6	-0.435019	1.316879	2.020678
1	-0.116281	2.316982	1.702201
1	-0.425944	1.275808	3.111528
1	0.274080	0.577888	1.626461
6	2.666743	-0.784502	-2.292480
1	1.768463	-0.268713	-1.926250
1	3.542161	-0.178968	-2.028227
1	2.605275	-0.857267	-3.380389
6	2.436681	-1.490936	2.122503
1	3.485203	-1.373665	2.411400
1	1.806654	-0.905310	2.800767
1	2.160581	-2.542986	2.204510
8	2.565307	1.480569	0.227948
1	1.695205	1.635413	-0.206542
6	2.768099	2.412498	1.283700
1	3.837906	2.447768	1.495786
1	2.432191	3.412371	0.992921
1	2.239135	2.108626	2.194900
8	0.214716	1.638199	-1.093620
1	-0.318357	0.825021	-0.997000
6	-0.611231	2.774288	-1.297336
1	-1.224674	2.656861	-2.195421
1	-1.269906	2.956395	-0.438612
1	0.047903	3.634978	-1.422696
8	-2.510243	0.528192	-1.056216
1	-2.651168	-0.340709	-0.631788
6	-3.775143	1.164972	-1.196402
1	-4.415617	0.622112	-1.898510
1	-4.286620	1.245667	-0.230537
1	-3.595833	2.168775	-1.585994
8	-3.066398	-1.351530	0.908600
1	-2.535043	-0.725110	1.432918
6	-2.648448	-2.677574	1.200423
1	-1.564745	-2.783103	1.084401
1	-2.934505	-2.966538	2.217409
1	-3.148176	-3.342564	0.493572
6	-0.523243	-1.996579	-1.299272
1	-1.602185	-2.089382	-1.450990
1	-0.051766	-1.725726	-2.250954
1	-0.132229	-2.967055	-0.976754

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8 -0.305621 -0.998142 -0.311080
1 0.582405 -1.118602 0.081193
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Cartesian coordinates of : MeOH_6_13_14.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-0.695263	-0.491188	1.558615
1	-1.486174	-0.190483	1.077259
8	-3.681465	-1.085649	-1.465805
1	-3.299025	-0.274205	-1.084612
8	-2.617102	0.924909	0.099604
1	-1.842151	1.481926	-0.171701
6	-0.422393	0.463850	2.567835
1	-1.162848	0.427265	3.376306
1	0.561194	0.233304	2.988027
1	-0.389749	1.485035	2.164739
6	-4.035408	-1.922179	-0.379566
1	-3.188727	-2.087864	0.299792
1	-4.869259	-1.507258	0.200703
1	-4.344129	-2.887529	-0.786197
6	-3.551724	1.715715	0.826775
1	-3.090844	2.140661	1.724768
1	-3.948008	2.525153	0.206341
1	-4.374096	1.064025	1.127085
8	-0.397265	2.232048	-0.445186
1	0.338439	1.762834	0.009934
6	-0.007907	2.441500	-1.799158
1	-0.791185	3.026148	-2.283347
1	0.933495	2.998121	-1.848510
1	0.108368	1.491156	-2.333102
8	1.842702	1.066375	0.480049
1	1.822836	0.150155	0.862004
6	2.726169	1.882768	1.244829
1	2.339012	2.030564	2.258165
1	3.721534	1.430990	1.297025
1	2.797453	2.850357	0.745641
8	2.090914	-1.490110	1.116779
1	1.498640	-1.799972	0.397544
6	1.815935	-2.196272	2.319907
1	0.757028	-2.120915	2.583719
1	2.096174	-3.250226	2.222624
1	2.419765	-1.745721	3.110191
8	0.836373	-1.903424	-1.272580
1	1.442337	-1.261090	-1.697450
6	-0.500828	-1.461713	-1.475929
1	-0.644964	-0.440735	-1.100411
1	-0.773877	-1.501427	-2.535592
1	-1.160931	-2.128160	-0.918865
6	3.900196	-0.472233	-1.710795
1	4.140640	-1.161260	-2.521741
1	4.660990	0.314098	-1.676754
1	3.900172	-1.019677	-0.761134
8	2.611343	0.076285	-1.982138
1	2.361742	0.622143	-1.210541

Cartesian coordinates of : MeOH_8.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
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8	-3.259823	-0.765522	-1.768650
1	-2.714379	-1.125032	-1.039447
8	-1.906698	-1.779170	0.390794
1	-1.470585	-1.137153	0.994411
8	-0.523282	-0.015809	1.883848
1	-0.833209	0.910661	1.729632
6	-4.600659	-0.720116	-1.317459
1	-4.717764	-0.050992	-0.454689
1	-5.216426	-0.337906	-2.134398
1	-4.971355	-1.714205	-1.039092
6	-1.012598	-2.861685	0.171190
1	-0.044010	-2.516094	-0.208576
1	-0.848900	-3.430314	1.093904
1	-1.465725	-3.521972	-0.571145
6	-0.100659	-0.180649	3.229108
1	0.842289	0.348666	3.409762
1	-0.856396	0.180869	3.933595
1	0.056077	-1.247749	3.401646
8	-1.487033	2.356229	1.180439
1	-0.804773	2.657148	0.534597
6	-2.677356	1.988503	0.489638
1	-3.421618	1.718362	1.241329
1	-3.061983	2.823485	-0.104112
1	-2.510710	1.127648	-0.170250
8	0.666462	2.938371	-0.300948
1	0.729880	2.391194	-1.117849
6	1.657532	2.446855	0.595462
1	1.610455	1.351977	0.675607
1	2.660989	2.742163	0.272144
1	1.462841	2.876199	1.580959
8	0.898618	1.024614	-2.159053
1	1.787168	0.628962	-2.009340
6	-0.059389	0.112320	-1.629613
1	-1.054537	0.470282	-1.900573
1	0.074737	-0.890330	-2.051950
1	0.009766	0.049099	-0.533271
8	3.174972	-0.296682	-1.583834
1	2.946354	-1.128275	-1.118365
6	4.254365	0.317414	-0.890576
1	4.022498	0.450565	0.172256
1	5.168859	-0.276551	-0.986460
1	4.422005	1.298150	-1.339119
6	2.191359	-1.888291	1.288184
1	1.476154	-1.079329	1.118387
1	1.711381	-2.658217	1.900079
1	3.068436	-1.497094	1.813367
8	2.543465	-2.408145	0.005114
1	3.173444	-3.131424	0.109685

Cartesian coordinates of : MeOH_8r_DDDUDDU.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	3.464573	-0.338989	-1.951967
8	3.182482	0.211157	-0.670126
8	1.515219	2.288460	-0.727184
6	2.290511	3.447147	-0.441997
8	-0.157013	1.729259	1.284738
6	0.723372	0.923833	2.057376
8	-2.726162	1.048374	0.998546
6	-3.455664	2.270475	1.025740
8	2.398523	-1.959899	0.686596
6	2.677797	-2.258658	2.047320

8	-0.136105	-2.654729	0.161292
6	-1.011866	-2.005488	1.076748
8	-0.900580	-1.217499	-1.964159
6	-0.165342	-0.034596	-1.667837
8	-3.300871	-0.357829	-1.192063
6	-4.407766	-1.209808	-0.930975
1	2.664910	-1.013143	-2.278667
1	4.412412	-0.886103	-1.941396
1	3.540131	0.487898	-2.661219
1	2.928482	-0.530733	-0.073302
1	3.065386	3.594930	-1.200953
1	2.763913	3.377638	0.544022
1	1.619660	4.307763	-0.451530
1	2.118181	1.504326	-0.723816
1	1.558820	1.516786	2.445833
1	1.123853	0.091157	1.463793
1	0.157561	0.515886	2.897952
1	0.340840	2.011425	0.480389
1	0.509401	-0.211567	-0.817973
1	-0.835522	0.792115	-1.408797
1	0.436421	0.259047	-2.532479
1	-1.848403	-1.026094	-1.768998
1	-3.134937	2.942919	0.222788
1	-3.333885	2.775667	1.988819
1	-4.511206	2.030455	0.884629
1	-1.766585	1.257806	1.100257
1	-5.299567	-0.625558	-0.681618
1	-4.195697	-1.904254	-0.110556
1	-4.607121	-1.785511	-1.836238
1	-3.089901	0.158433	-0.375217
1	2.556843	-3.328290	2.245398
1	2.026314	-1.693918	2.725278
1	3.713894	-1.978674	2.244035
1	1.481897	-2.253532	0.465786
1	-2.028113	-2.405421	0.998436
1	-1.043417	-0.923225	0.897139
1	-0.638396	-2.185784	2.087310
1	-0.383796	-2.334293	-0.736664

Cartesian coordinates of : MeOH_8r_DDDUUUU.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	0.207930	-0.234487	2.317643
8	1.401499	-0.757366	1.753433
8	2.518733	1.187819	0.326044
6	3.279425	2.099546	1.109382
8	0.597325	2.619312	-0.772184
6	0.664249	3.111154	-2.102359
8	-1.897558	2.096294	-0.090737
6	-2.209975	2.763756	1.126189
8	-2.992333	-0.281016	0.313218
6	-4.378260	-0.267802	-0.008725
8	-1.914251	-2.533613	-0.606022
6	-1.277064	-3.137584	0.516117
8	0.282989	-1.768596	-1.943556
6	0.311267	-0.389299	-1.591148
8	2.057201	-2.641490	-0.107157
6	3.369342	-2.154112	-0.384646
1	-0.531348	0.021432	1.544835
1	0.416259	0.660023	2.915221
1	-0.223198	-0.997940	2.968273
1	1.842792	-0.034349	1.239834

1	4.064945	-2.435295	0.412575
1	3.368148	-1.063628	-0.495891
1	3.699611	-2.612010	-1.318438
1	1.714296	-2.133241	0.658007
1	1.266304	0.072971	-1.865137
1	0.152811	-0.251160	-0.512722
1	-0.496003	0.112283	-2.130647
1	0.966799	-2.215211	-1.392777
1	-1.810622	2.222979	1.991270
1	-3.292590	2.877430	1.243065
1	-1.754580	3.755288	1.089248
1	-2.244709	1.171945	-0.031549
1	-0.513587	-2.474164	0.941433
1	-0.809783	-4.087153	0.237794
1	-2.041333	-3.322942	1.272744
1	-1.205991	-2.320545	-1.256889
1	-4.890383	-1.124433	0.440564
1	-4.536388	-0.281073	-1.092250
1	-4.806660	0.650056	0.398693
1	-2.587976	-1.102180	-0.061353
1	2.656091	2.594962	1.862116
1	3.748900	2.859619	0.476827
1	4.061542	1.531539	1.616527
1	1.800535	1.693307	-0.132341
1	0.087730	4.035957	-2.206872
1	0.292552	2.374188	-2.822987
1	1.711750	3.322249	-2.326355
1	-0.336238	2.381309	-0.541840

Cartesian coordinates of : MeOH_8r_UDDDUDDD.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	0.006789	-0.298655	-1.549028
8	-1.198321	-1.026866	-1.764645
8	-0.975696	-3.286930	-0.367053
6	-2.271152	-3.683681	0.070113
8	0.429980	-2.122351	1.556707
6	-0.304253	-0.913883	1.727351
8	2.805902	-1.454930	0.566324
6	3.156751	-2.421153	-0.417655
8	2.650679	0.993425	-0.456475
6	3.943154	1.570363	-0.309319
8	0.771118	2.723671	0.252985
6	0.611754	3.494770	-0.932027
8	-1.591415	1.955986	1.181092
6	-1.696612	2.135939	2.584687
8	-2.973694	0.547341	-0.590820
6	-3.367117	1.559785	-1.512460
1	-0.193508	0.637026	-1.013118
1	0.482707	-0.066488	-2.505676
1	0.702128	-0.893793	-0.944055
1	-1.937993	-0.511025	-1.356740
1	-2.854935	-4.093616	-0.759759
1	-2.817715	-2.841996	0.511840
1	-2.144029	-4.457473	0.828768
1	-1.078038	-2.520411	-0.983461
1	-0.726389	-0.867820	2.735619
1	-1.118675	-0.841908	0.997925
1	0.359279	-0.052772	1.580018
1	-0.043300	-2.673813	0.885574
1	0.402765	2.856096	-1.798082
1	1.508293	4.089418	-1.135204

1	-0.232448	4.170425	-0.780496
1	1.456077	2.030964	0.078306
1	2.331075	-2.598307	-1.117163
1	3.438877	-3.369553	0.049819
1	4.011597	-2.034225	-0.975387
1	1.967972	-1.745487	1.005277
1	4.691051	0.998465	-0.867807
1	4.240146	1.619999	0.743537
1	3.904042	2.584121	-0.713111
1	2.667912	0.083665	-0.067059
1	-2.499632	2.122567	-1.876974
1	-4.075515	2.253498	-1.049768
1	-3.851601	1.069961	-2.358635
1	-2.508517	0.993659	0.156507
1	-1.746039	3.199023	2.842961
1	-0.848375	1.681722	3.108641
1	-2.615345	1.648944	2.917043
1	-0.696173	2.233448	0.865761

Cartesian coordinates of : MeOH_8r_UUDDUDD.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	4.231523	-1.139249	-0.521741
8	2.840580	-1.022533	-0.801249
8	2.273418	1.596475	-0.797562
6	3.328107	2.283441	-0.131071
8	0.173716	2.667589	0.436117
6	-0.345141	3.675402	-0.425128
8	-2.061026	1.433187	1.234098
6	-2.009418	0.209724	1.956429
8	-3.508758	0.686789	-0.882113
6	-4.701710	-0.005351	-0.531980
8	-1.533893	-0.984394	-1.519239
6	-0.331786	-0.229336	-1.414057
8	1.321249	-1.738262	1.267392
6	1.446299	-0.577434	2.076590
8	-0.922183	-2.865116	0.304225
6	-0.389962	-4.005614	-0.363514
1	4.493367	-0.645735	0.421608
1	4.830234	-0.708001	-1.330301
1	4.465184	-2.201783	-0.439249
1	2.607425	-0.064512	-0.866465
1	1.026409	0.309475	1.581144
1	2.496921	-0.380322	2.316858
1	0.900228	-0.752268	3.004978
1	1.871237	-1.590860	0.459453
1	0.032205	-4.716596	0.353261
1	0.385511	-3.717818	-1.083346
1	-1.207970	-4.488135	-0.900486
1	-0.174612	-2.422258	0.769579
1	-1.555220	-0.591842	1.358167
1	-3.011862	-0.105177	2.264768
1	-1.403286	0.372542	2.849042
1	-2.634630	1.285993	0.443269
1	0.522075	-0.792658	-1.805519
1	-0.127576	0.046993	-0.370471
1	-0.454115	0.686248	-1.997783
1	-1.455963	-1.734013	-0.883944
1	-4.486984	-0.874593	0.100298
1	-5.237420	-0.338431	-1.426477
1	-5.338255	0.685418	0.023683
1	-2.849337	0.032305	-1.217250

1	3.409738	1.966786	0.915344
1	3.170194	3.366112	-0.164990
1	4.260607	2.048459	-0.647899
1	1.429824	1.872111	-0.364385
1	-0.922026	4.413578	0.140702
1	-0.981535	3.242259	-1.205310
1	0.500833	4.176852	-0.899795
1	-0.593505	2.160499	0.794998

Cartesian coordinates of the methanol nonamer

Cartesian coordinates of : MeOH_9r_Flat.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	4.659902	1.013439	-1.038975
8	3.650388	0.408947	-0.239989
8	2.627388	-1.740373	-1.446492
6	3.818301	-2.443990	-1.779562
8	2.399582	2.569669	0.675135
6	2.884484	2.983038	1.944512
8	-0.000280	3.717529	0.595922
6	0.126333	4.943999	-0.111512
8	-2.417190	2.926399	-0.201738
6	-3.438189	3.549661	0.565588
8	-3.569799	0.594926	-0.767735
6	-4.110805	0.562172	-2.080776
8	-3.141009	-1.987059	-0.280407
6	-4.309529	-2.527136	0.322943
8	-1.204168	-3.180773	1.130691
6	-1.552327	-4.558015	1.209435
8	1.284165	-3.337688	0.207602
6	2.237304	-3.493709	1.250777
1	5.378032	0.238411	-1.314523
1	5.184126	1.794657	-0.479082
1	4.239608	1.449005	-1.952144
1	3.066832	1.127476	0.099560
1	3.916521	2.637187	2.035255
1	2.294396	2.549759	2.758999
1	2.870669	4.074622	2.033668
1	1.466757	2.875181	0.581505
1	-0.647934	5.655890	0.193631
1	0.064681	4.789142	-1.193863
1	1.104232	5.367368	0.128157
1	-0.854030	3.299133	0.334592
1	-4.370955	3.615455	-0.004363
1	-3.103917	4.560557	0.808527
1	-3.625662	3.006500	1.497895
1	-2.711472	2.009463	-0.411293
1	-3.377529	0.195694	-2.806981
1	-4.393251	1.582360	-2.349637
1	-5.003248	-0.071523	-2.122254
1	-3.302012	-0.320572	-0.517106
1	-4.418555	-3.590922	0.085619
1	-5.172312	-1.989676	-0.076933
1	-4.291079	-2.401161	1.411036
1	-2.354858	-2.354677	0.189585
1	-1.703411	-4.989560	0.213152
1	-2.483279	-4.637258	1.774539
1	-0.776762	-5.128673	1.730446
1	-0.294438	-3.124438	0.750214

1	1.741204	-3.985454	2.090414
1	2.620181	-2.524054	1.587561
1	3.076940	-4.117020	0.924277
1	1.669758	-2.721606	-0.460930
1	3.542134	-3.467298	-2.043257
1	4.511743	-2.473520	-0.931118
1	4.319802	-1.983035	-2.637119
1	2.891619	-0.896774	-1.006515

Cartesian coordinates of : MeOH_N9_0.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	3.454263	1.803575	2.322350
8	2.449414	0.926895	1.825299
8	3.064205	0.376474	-0.685310
6	2.703591	1.533073	-1.432148
8	0.018720	1.891623	1.486256
6	-0.809902	0.739463	1.584562
8	-0.671415	3.082809	-0.763371
6	-1.755047	3.934928	-0.407665
8	1.914959	-1.804118	-1.666422
6	2.904485	-2.812668	-1.840146
8	0.378272	-2.734547	0.279386
6	1.157161	-2.560613	1.458960
8	-2.075455	-2.014222	0.984089
6	-2.848637	-3.195123	1.165786
8	-3.461951	-0.421359	-0.635739
6	-4.407403	0.411295	0.023624
8	-1.553429	0.869717	-1.962542
6	-0.447268	-0.022387	-1.898741
1	2.705505	0.639979	0.911153
1	3.145668	2.136352	3.314653
1	3.573714	2.680566	1.676296
1	4.414985	1.286221	2.405909
1	-1.260004	1.743975	-1.605686
1	-0.824649	-1.042393	-2.011700
1	0.072500	0.050864	-0.932595
1	0.270039	0.175451	-2.701277
1	-0.540060	-2.409275	0.452811
1	1.937859	-3.324535	1.470658
1	0.536666	-2.676969	2.353196
1	1.629561	-1.570133	1.481900
1	1.252092	-2.133837	-1.008768
1	3.629422	-2.445666	-2.568613
1	2.456815	-3.736046	-2.220113
1	3.425446	-3.025977	-0.899687
1	-0.300320	2.699808	0.071693
1	-2.188140	4.327762	-1.329022
1	-1.408824	4.772144	0.206067
1	-2.529207	3.385710	0.141645
1	-2.574701	-1.402886	0.387105
1	-2.279200	-3.869932	1.807947
1	-3.043358	-3.695118	0.210963
1	-3.801709	-2.965201	1.652652
1	2.606993	-0.419321	-1.059937
1	3.435163	2.314301	-1.215943
1	1.706497	1.896263	-1.152933
1	2.718607	1.324427	-2.506445
1	0.954030	1.615648	1.662518
1	-1.582190	0.792162	0.808361
1	-1.296385	0.687588	2.563902
1	-0.231752	-0.176977	1.428781

1	-2.830921	0.135536	-1.155457
1	-5.116449	-0.237646	0.540503
1	-4.953089	1.029671	-0.695572
1	-3.924620	1.062059	0.762376

Cartesian coordinates of : MeOH_N9_10.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-0.969129	-3.696622	0.633818
8	-1.289480	-3.040349	-0.590299
8	0.759890	-1.500693	-1.062441
6	0.331141	-0.313896	-1.723010
8	-3.280278	-1.389529	-0.048834
6	-4.527489	-1.660369	-0.677652
8	-2.977252	1.239333	-0.231218
6	-3.345597	1.873954	0.987039
8	-0.837471	2.635946	-0.970287
6	-1.126594	4.026597	-0.884301
8	1.415618	2.384267	0.413676
6	1.326791	2.663091	1.804573
8	3.525838	0.813965	-0.038934
6	4.154653	1.181853	-1.261464
8	3.354752	-1.861717	-0.383603
6	3.342651	-2.794721	0.693272
8	0.832367	-0.628527	1.605637
6	-0.473131	-0.077700	1.639469
1	-2.047154	-2.421069	-0.427485
1	-0.274160	-4.506860	0.405914
1	-1.867296	-4.118530	1.094133
1	-0.489999	-3.007648	1.340921
1	2.476660	-1.877574	-0.814557
1	4.286140	-2.688190	1.230281
1	3.261642	-3.820142	0.319206
1	2.516061	-2.593617	1.383968
1	0.978957	-0.946611	0.696562
1	-0.694651	0.195822	2.674110
1	-1.231834	-0.797956	1.302221
1	-0.542608	0.822940	1.015359
1	0.011011	2.463607	-0.494205
1	-2.069129	4.202973	-1.406407
1	-0.340957	4.618881	-1.363495
1	-1.234915	4.348828	0.157715
1	-2.169466	1.690990	-0.577572
1	-4.073204	1.235399	1.492945
1	-3.803287	2.850483	0.796778
1	-2.477848	2.008124	1.643781
1	-0.004884	-2.136694	-0.991816
1	1.045401	0.479912	-1.486570
1	-0.659402	-0.006945	-1.367253
1	0.296860	-0.456033	-2.807339
1	3.472358	-0.167365	-0.010917
1	4.127083	2.270724	-1.333733
1	3.628627	0.756382	-2.123523
1	5.197911	0.851685	-1.279714
1	-3.086446	-0.423573	-0.136256
1	-4.725556	-2.728919	-0.576827
1	-4.501615	-1.402459	-1.741454
1	-5.335436	-1.103934	-0.191911
1	2.150905	1.744664	0.258161
1	0.363054	3.145340	1.990575
1	2.126164	3.342698	2.118274
1	1.379346	1.739996	2.390087

Cartesian coordinates of : MeOH_N9_12.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-1.073256	2.434183	-1.996686
8	-2.125695	2.041249	-1.123879
8	-1.249270	2.162557	1.381240
6	-2.012631	1.218440	2.120375
8	1.383272	2.462343	1.091185
6	1.503376	3.880761	1.041140
8	2.452311	1.362607	-1.064557
6	3.787947	1.087330	-0.655651
8	-2.983184	-0.502380	-1.060704
6	-4.349059	-0.363505	-0.683799
8	-1.995408	-2.107965	0.843319
6	-2.144547	-3.475451	0.478245
8	0.578483	-1.940025	1.584907
6	1.192820	-0.664554	1.725641
8	2.151458	-2.970288	-0.324556
6	3.536015	-2.931199	-0.001023
8	1.328449	-0.922413	-1.835502
6	-0.066958	-0.828832	-1.587481
1	-2.333417	1.081522	-1.218750
1	-1.039712	3.524964	-2.001254
1	-1.253856	2.082388	-3.016902
1	-0.102155	2.053900	-1.653362
1	1.130666	-2.468234	0.961460
1	0.454399	0.026975	2.137345
1	1.531331	-0.277400	0.756395
1	2.048534	-0.712641	2.408222
1	-1.609238	2.193782	0.460513
1	-1.548398	1.101934	3.101744
1	-2.036244	0.241336	1.621500
1	-3.040002	1.571963	2.259557
1	0.435636	2.244095	1.260442
1	2.544927	4.118118	0.816287
1	1.237856	4.327508	2.003929
1	0.865420	4.305506	0.258244
1	1.948792	-2.243841	-0.961353
1	3.739522	-3.753347	0.686681
1	3.806999	-1.987899	0.488293
1	4.152598	-3.057946	-0.896380
1	-2.543342	-1.073488	-0.386178
1	-4.830119	0.292326	-1.411554
1	-4.443030	0.083521	0.312494
1	-4.857574	-1.332918	-0.691304
1	1.985444	1.785341	-0.299264
1	4.239619	0.426141	-1.398422
1	3.808479	0.589474	0.320808
1	4.375994	2.008769	-0.597559
1	1.745804	-0.051988	-1.620355
1	-0.459028	-1.839744	-1.445404
1	-0.590226	-0.368193	-2.432065
1	-0.275530	-0.246937	-0.676864
1	-1.063309	-1.974997	1.141107
1	-3.148632	-3.604382	0.069780
1	-2.030831	-4.126795	1.350375
1	-1.412940	-3.767356	-0.284400

Cartesian coordinates of : MeOH_N9_13.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	3.414159	1.537214	1.573715
8	2.242580	0.977232	0.980052
8	2.922943	-1.183526	-0.266443
6	3.467114	-0.705776	-1.494286
8	1.015529	-2.867209	-0.888600
6	1.494754	-4.201306	-0.747790
8	-0.839610	-2.479003	0.937302
6	-0.150798	-1.766688	1.957746
8	-3.096105	-1.181074	0.458408
6	-3.836799	-0.980920	1.656049
8	-3.121338	1.082015	-0.933962
6	-4.048164	0.970763	-2.009561
8	-0.676382	1.101128	-1.987169
6	-0.161386	-0.169270	-1.609730
8	1.318015	2.602982	-0.970254
6	1.168830	3.877277	-0.351987
8	-0.091288	1.735025	2.328114
6	-1.131691	1.641080	1.372566
1	2.474299	0.090052	0.574922
1	3.128431	2.476455	2.051596
1	4.175673	1.740535	0.813545
1	3.825263	0.862732	2.329669
1	-0.018368	1.778947	-1.712318
1	-0.984300	-0.889752	-1.626718
1	0.256644	-0.142469	-0.592624
1	0.614323	-0.509330	-2.303245
1	-1.662092	-1.984767	0.692836
1	0.517801	-2.464863	2.465746
1	-0.850791	-1.348087	2.688635
1	0.450757	-0.947102	1.541577
1	0.239363	-2.746357	-0.282004
1	2.398608	-4.295662	-1.352465
1	0.751859	-4.919858	-1.106341
1	1.740707	-4.426171	0.295744
1	1.714196	1.990099	-0.311402
1	0.506770	4.478349	-0.977481
1	2.135950	4.384029	-0.269651
1	0.726870	3.782991	0.646961
1	-3.094814	-0.339275	-0.063735
1	-3.799902	-1.909480	2.229187
1	-4.882037	-0.744204	1.433576
1	-3.406980	-0.174103	2.261036
1	2.174544	-1.808293	-0.470922
1	4.527249	-0.493388	-1.342546
1	2.963195	0.214760	-1.815609
1	3.363588	-1.459191	-2.280485
1	0.725039	1.385115	1.928106
1	-2.037605	2.055223	1.820667
1	-1.335192	0.599002	1.087389
1	-0.905165	2.209706	0.461479
1	-2.219134	1.220775	-1.311874
1	-5.025556	0.739975	-1.582082
1	-3.762825	0.167156	-2.697389
1	-4.117229	1.911656	-2.563687

Cartesian coordinates of : MeOH_N9_15.log-----
Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
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6	-0.047890	0.282566	-1.080171
8	0.225940	-0.624979	-2.132583
8	2.602216	-1.480029	-0.938363
6	3.605812	-2.395996	-1.366323
8	1.239486	-2.154781	1.188354
6	1.450747	-1.188846	2.213081
8	-1.386310	-2.303752	0.852543
6	-2.035521	-2.680727	2.059423
8	-3.271225	-1.016723	-0.543673
6	-3.217339	-1.335555	-1.931976
8	3.140744	1.139167	-0.629162
6	3.124583	1.621426	-1.968943
8	1.374962	2.303348	1.001458
6	2.063403	2.688027	2.181832
8	-1.280206	2.152489	1.248186
6	-1.448473	1.038286	2.115955
8	-3.231058	1.687139	-0.528748
6	-3.097269	2.250744	-1.827636
1	1.109169	-1.000214	-1.972647
1	-1.128030	0.303026	-0.909394
1	0.286691	1.301584	-1.321083
1	0.435306	-0.025528	-0.144402
1	2.001230	1.859627	0.380020
1	1.343406	3.176942	2.841557
1	2.870163	3.393087	1.956817
1	2.482625	1.818422	2.701377
1	0.273848	-2.192297	0.978755
1	2.475288	-1.302044	2.572137
1	0.761703	-1.351502	3.048758
1	1.316675	-0.165829	1.836453
1	-2.017240	-1.779201	0.302767
1	-1.340539	-3.299152	2.631429
1	-2.938796	-3.263172	1.853337
1	-2.303770	-1.803193	2.659757
1	-2.481293	1.979482	0.040582
1	-3.955011	1.926121	-2.419232
1	-2.178709	1.910482	-2.320889
1	-3.094144	3.344145	-1.782225
1	2.127813	-1.827743	-0.133419
1	4.114719	-1.952040	-2.223315
1	3.158927	-3.346897	-1.670417
1	4.335842	-2.575018	-0.571413
1	-3.312059	-0.036018	-0.459882
1	-3.174751	-2.422768	-2.019347
1	-2.323129	-0.910813	-2.403227
1	-4.112342	-0.974895	-2.448790
1	-0.321077	2.235420	1.042817
1	-2.494046	1.017154	2.432391
1	-0.813309	1.131073	3.004097
1	-1.213838	0.094202	1.606497
1	3.045034	0.160968	-0.659217
1	2.992902	2.704502	-1.932523
1	2.297512	1.182087	-2.538673
1	4.068514	1.395406	-2.475002

Cartesian coordinates of : MeOH_N9_16.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	0.674218	4.251287	-0.049405
8	0.434048	2.848851	-0.123297
8	-1.649067	2.078589	1.227465
6	-1.208447	1.015568	2.066753

8	-3.642329	0.867616	-0.020719
6	-4.120596	1.316188	-1.282306
8	-2.800465	-1.615576	-0.361831
6	-3.794667	-2.580908	-0.038421
8	-0.599016	-2.603627	0.702048
6	0.100218	-3.314330	-0.319218
8	1.419829	-1.259529	1.775663
6	2.541569	-2.137205	1.780835
8	2.251571	1.203956	1.028519
6	3.477583	1.379260	0.331308
8	0.699293	0.826735	-1.986486
6	-0.285778	0.080530	-1.278835
8	2.573373	-1.112356	-1.293876
6	3.781430	-1.234239	-2.019480
1	-0.424934	2.621755	0.333500
1	1.649157	4.445464	-0.499390
1	0.687711	4.590027	0.991014
1	-0.090093	4.805335	-0.601780
1	1.699821	-0.395143	1.398260
1	2.195492	-3.112787	2.130800
1	3.314531	-1.774242	2.467033
1	2.956594	-2.235017	0.772873
1	-1.948712	-1.897224	0.060491
1	-4.732324	-2.260568	-0.496901
1	-3.937436	-2.658658	1.044526
1	-3.525506	-3.564429	-0.437040
1	0.756847	1.692350	-1.542081
1	-0.481368	-0.835777	-1.840023
1	-1.221422	0.643304	-1.182489
1	0.075805	-0.193495	-0.278537
1	-3.323737	-0.066376	-0.115532
1	-4.465918	2.344384	-1.163191
1	-4.958550	0.699292	-1.622352
1	-3.330710	1.294256	-2.042179
1	2.074322	-0.338828	-1.615993
1	4.315221	-2.102678	-1.625807
1	4.423102	-0.351907	-1.897952
1	3.602326	-1.392534	-3.089697
1	0.065369	-2.040982	1.169950
1	-0.613053	-3.562392	-1.110535
1	0.519619	-4.244610	0.079522
1	0.905551	-2.699621	-0.736785
1	1.598372	1.848519	0.680584
1	4.072249	0.473090	0.463457
1	4.030557	2.238051	0.726793
1	3.305726	1.524878	-0.741532
1	-2.442928	1.756758	0.730676
1	-0.144436	1.158506	2.275584
1	-1.339575	0.043685	1.575012
1	-1.758737	1.013440	3.012457

 Cartesian coordinates of : MeOH_N9_21.log

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-2.919451	1.346092	0.917976
8	-2.689107	-0.016438	1.274212
8	-3.015878	-1.636448	-0.853675
6	-4.018388	-1.052763	-1.678420
8	-0.572399	-1.285429	-1.918934
6	-0.431774	0.049639	-1.436554
8	1.604790	-2.307791	-0.876253
6	2.566576	-2.772666	-1.819462

8	-0.177753	0.103530	2.343918
6	0.241162	1.454924	2.195546
8	0.683181	-2.507437	1.736060
6	-0.683068	-2.803617	1.479740
8	2.202165	-0.122130	0.621854
6	3.307126	-0.461433	1.454704
8	2.081610	2.325988	-0.509848
6	2.974026	2.271024	-1.614520
8	-0.523526	3.063588	-0.995592
6	-0.804083	4.183503	-0.176718
1	-1.800968	-0.077896	1.691112
1	-3.890840	1.396686	0.421240
1	-2.146803	1.720209	0.234906
1	-2.952653	1.980738	1.810383
1	0.413839	2.811320	-0.867454
1	-1.852088	4.452570	-0.328596
1	-0.181945	5.047745	-0.438479
1	-0.658811	3.958051	0.888342
1	0.759447	-2.062648	-1.338632
1	3.490394	-2.976705	-1.276432
1	2.761154	-2.013069	-2.583172
1	2.224502	-3.693054	-2.300696
1	0.478403	-0.493355	1.936314
1	-0.424990	2.068784	2.806016
1	0.171095	1.780408	1.150573
1	1.269250	1.592679	2.544143
1	-2.918761	-1.086136	-0.039978
1	-4.153200	-1.699836	-2.546437
1	-3.721238	-0.055413	-2.024558
1	-4.970307	-0.976560	-1.143383
1	1.173856	-2.686657	0.915801
1	-1.258949	-2.489872	2.352892
1	-0.839743	-3.875400	1.317241
1	-1.050529	-2.256245	0.602150
1	-1.454702	-1.599640	-1.613487
1	0.495471	0.460103	-1.844854
1	-0.374296	0.074420	-0.338031
1	-1.264736	0.679134	-1.761081
1	2.118156	1.458875	-0.047924
1	2.883635	3.209768	-2.163656
1	2.726377	1.443251	-2.290027
1	4.009994	2.156724	-1.278108
1	2.027621	-0.869139	0.006945
1	3.509766	0.396602	2.098498
1	4.200246	-0.677317	0.859945
1	3.064946	-1.326830	2.080787

Cartesian coordinates of : MeOH_N9_25.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	3.656723	-2.015207	-0.776533
8	2.579026	-1.133417	-0.466010
8	0.496191	-1.802248	-1.863960
6	-0.163410	-2.806306	-1.096355
8	-1.568380	-0.264771	-2.427799
6	-2.615752	-1.102302	-2.906730
8	-2.646591	0.933082	-0.319589
6	-3.206519	-0.018742	0.580072
8	-1.152510	2.731105	0.957014
6	-1.826069	3.976828	0.800080
8	1.025495	2.859772	-0.577822
6	0.604466	2.099748	-1.705289

8	3.232778	1.446002	0.059488
6	3.696653	1.348101	1.402000
8	0.909699	-1.140094	1.734041
6	0.222451	0.005919	1.247912
8	-1.320269	-2.754101	2.035833
6	-1.855189	-2.287300	3.261699
1	1.815138	-1.310531	-1.084385
1	4.468882	-1.805730	-0.078660
1	4.011097	-1.851315	-1.798106
1	3.349301	-3.059128	-0.661419
1	1.879494	2.478625	-0.271507
1	-0.437898	2.354344	-1.913824
1	0.666142	1.022519	-1.504563
1	1.209518	2.333351	-2.586835
1	-2.063690	1.559710	0.176799
1	-4.116615	-0.416583	0.125939
1	-3.468418	0.456111	1.531354
1	-2.514065	-0.848682	0.774059
1	-0.447597	-2.335299	1.910262
1	-2.826760	-2.764985	3.403839
1	-2.005052	-1.199441	3.253279
1	-1.212522	-2.545020	4.111711
1	3.034995	0.538026	-0.257582
1	3.755446	2.358751	1.808829
1	4.691607	0.892983	1.438264
1	3.010133	0.756207	2.018979
1	1.629129	-1.332383	1.102329
1	-0.551726	0.268571	1.972456
1	-0.257388	-0.193489	0.278323
1	0.899853	0.860486	1.139206
1	-0.193131	-1.147348	-2.144085
1	0.589964	-3.333253	-0.504506
1	-0.666129	-3.526047	-1.750442
1	-0.897511	-2.365767	-0.411455
1	-1.913528	0.240013	-1.648647
1	-2.217541	-1.696109	-3.731827
1	-3.455112	-0.503830	-3.274252
1	-2.973320	-1.781142	-2.123579
1	-0.274698	2.798188	0.509837
1	-2.821820	3.871880	1.234291
1	-1.926726	4.243026	-0.258093
1	-1.293083	4.776221	1.323314

Cartesian coordinates of : MeOH_N9_45.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-1.709319	0.728575	2.240914
8	-1.471364	-0.674905	2.159645
8	1.211697	-0.511024	2.483608
6	2.039631	-1.519781	1.911507
8	1.591092	1.874049	1.296751
6	2.923684	1.834682	0.791703
8	-0.240050	2.746241	-0.403953
6	-0.644426	3.990310	0.159644
8	-2.438673	1.416144	-1.050775
6	-2.671254	1.706371	-2.425362
8	-2.634125	-1.068613	-0.285160
6	-4.025023	-1.348707	-0.123450
8	-0.890141	-3.014021	-1.066504
6	-0.656227	-3.555719	0.228838
8	1.194814	-1.371553	-1.595186
6	0.553952	-0.188197	-1.146846

8	3.864133	-1.042866	-1.012364
6	4.237490	-0.198405	-2.086429
1	-1.849210	-0.978243	1.307331
1	-1.388605	1.063214	3.229053
1	-2.772823	0.955453	2.114820
1	-1.136022	1.272930	1.479118
1	0.540067	-2.099620	-1.526198
1	1.287705	0.621682	-1.168453
1	0.183463	-0.290852	-0.113975
1	-0.284634	0.082816	-1.798407
1	0.447382	2.353658	0.192098
1	-1.402846	4.422992	-0.495646
1	0.202391	4.679993	0.225670
1	-1.075033	3.852637	1.158184
1	-1.599340	1.863072	-0.770637
1	-3.594038	1.204374	-2.720634
1	-1.851624	1.342386	-3.054907
1	-2.789163	2.783452	-2.577607
1	-1.596321	-2.341482	-0.974780
1	0.186204	-4.245360	0.154518
1	-1.533188	-4.100181	0.593218
1	-0.401627	-2.768702	0.950146
1	1.419840	1.033512	1.783116
1	3.018379	2.622048	0.039697
1	3.146954	0.866606	0.326653
1	3.646177	2.024077	1.592389
1	-2.531606	-0.135071	-0.627843
1	-4.116749	-2.362238	0.269989
1	-4.546500	-1.288189	-1.082810
1	-4.481133	-0.647915	0.583098
1	0.265517	-0.753873	2.379858
1	3.077353	-1.209615	2.045506
1	1.847270	-1.636936	0.838345
1	1.887991	-2.480679	2.413850
1	2.944441	-1.328408	-1.169039
1	5.268005	0.120772	-1.916996
1	3.603841	0.697389	-2.139811
1	4.187367	-0.718091	-3.050520

Cartesian coordinates of : MeOH_N9_52.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-0.612455	0.279052	-2.203769
8	0.317153	-0.324827	-1.318306
8	0.070344	-0.725262	1.375807
6	-0.744971	-0.095941	2.357370
8	2.568887	0.012716	1.627173
6	3.632732	-0.839313	2.031607
8	2.542697	1.719742	-0.485151
6	2.794911	1.799666	-1.877798
8	0.049895	2.469728	0.182026
6	0.025882	3.592859	1.048974
8	-2.456265	1.611364	0.143178
6	-3.190206	2.337702	-0.834647
8	-3.305732	-0.877691	-0.169256
6	-4.439137	-1.179469	0.636948
8	-1.431329	-2.705696	0.269169
6	-1.000878	-3.372303	-0.915457
8	2.960364	-1.213224	-1.115230
6	2.488843	-2.492475	-0.736020
1	0.035129	-0.219733	-0.389745
1	-0.299685	0.034937	-3.221138

1	-0.624825	1.369705	-2.086660
1	-1.625280	-0.110570	-2.041102
1	-0.701977	-2.171516	0.644416
1	-1.879382	-3.845173	-1.357469
1	-0.264115	-4.146392	-0.678344
1	-0.568028	-2.661505	-1.626727
1	-0.849267	2.062112	0.154768
1	1.036119	4.005922	1.085551
1	-0.273049	3.309706	2.064814
1	-0.657268	4.365618	0.679580
1	1.027892	-0.503999	1.534425
1	-1.784232	-0.359220	2.143696
1	-0.641950	0.992576	2.308539
1	-0.488886	-0.445085	3.362317
1	2.778418	0.443772	0.770965
1	3.260256	-1.473663	2.838234
1	4.477037	-0.251299	2.405445
1	3.966956	-1.467156	1.201304
1	-2.624145	-1.584050	-0.041242
1	-5.145079	-0.352328	0.541883
1	-4.162063	-1.288124	1.691445
1	-4.924544	-2.099462	0.297169
1	1.600453	1.939538	-0.314864
1	3.799581	1.413157	-2.058307
1	2.744935	2.836520	-2.229372
1	2.078549	1.196720	-2.449018
1	2.173051	-0.663894	-1.278239
1	3.356672	-3.112166	-0.497275
1	1.927185	-2.974547	-1.544679
1	1.844847	-2.437849	0.154468
1	-2.720135	0.659247	0.083210
1	-2.789867	3.353490	-0.868522
1	-4.251566	2.385419	-0.570365
1	-3.088183	1.885831	-1.827686

Cartesian coordinates of : MeOH_N9_6r.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-0.021151	-0.034642	0.095324
8	0.053095	0.086289	1.513830
8	2.520968	0.050096	2.381039
6	2.625574	0.800429	3.589635
8	-1.409995	-1.179439	3.380728
6	-1.301281	-0.160965	4.373412
8	-0.680565	-3.480925	4.390022
6	-1.336192	-4.582159	3.765746
8	1.920626	-3.215818	5.013603
6	1.721043	-2.317540	6.103502
8	3.646944	-2.198027	3.330578
6	4.360283	-3.201703	2.612150
8	-1.968823	-2.701938	6.749601
6	-3.259331	-2.669827	6.161800
8	5.068579	-1.299507	5.567403
6	5.353890	-2.604775	6.043769
8	-0.053053	2.757683	2.340697
6	0.933230	3.193854	1.419379
1	0.241398	-1.047079	-0.225615
1	0.647973	0.683561	-0.389307
1	-1.048240	0.179570	-0.203104
1	1.000226	-0.009529	1.808103
1	-2.028367	0.636528	4.190787

1	-0.293237	0.269599	4.385120
1	-1.503136	-0.616699	5.346376
1	-0.961382	-0.847258	2.572217
1	-0.966169	-4.731798	2.747119
1	-2.418797	-4.422292	3.737746
1	-1.123999	-5.473656	4.357387
1	-0.928058	-2.635823	3.924147
1	3.628577	1.225640	3.695259
1	2.409734	0.172107	4.461462
1	1.893077	1.610824	3.547157
1	2.955719	-0.817110	2.537533
1	1.437740	-2.864245	7.008416
1	0.940739	-1.584047	5.869364
1	2.661919	-1.790014	6.281074
1	1.031993	-3.476360	4.685352
1	3.708746	-3.705162	1.891766
1	4.781501	-3.942769	3.299033
1	5.173947	-2.711413	2.076099
1	2.949719	-2.625787	3.899334
1	1.305480	4.161197	1.762379
1	0.519831	3.316490	0.410721
1	1.777710	2.493275	1.369904
1	-0.258862	1.833567	2.115649
1	-3.908029	-2.080839	6.813114
1	-3.684732	-3.676088	6.062701
1	-3.239882	-2.197709	5.170258
1	-1.368927	-3.090043	6.088902
1	5.636321	-2.521862	7.095118
1	6.184855	-3.064085	5.494337
1	4.477436	-3.262532	5.969126
1	4.667819	-1.402957	4.686684

Cartesian coordinates of : MeOH_N9_78.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	1.754248	3.805003	-0.876722
8	1.369137	2.434986	-0.874251
8	-0.975726	2.493088	0.356063
6	-0.942297	2.746436	1.753532
8	2.947449	0.951024	0.671107
6	2.125765	0.893275	1.833699
8	3.682016	-1.387706	-0.378753
6	4.027300	-1.071808	-1.722228
8	1.687357	-3.108790	0.021254
6	1.449346	-2.966895	1.419565
8	-0.367809	-1.739851	-0.890892
6	0.243378	-0.526008	-1.321022
8	-3.051287	-1.587682	-1.074365
6	-3.746956	-2.647696	-0.430327
8	-3.111250	1.061044	-0.479268
6	-3.432832	1.625654	-1.743367
8	-1.180136	-0.364787	1.439802
6	-2.341869	-0.688186	2.182479
1	0.482646	2.372413	-0.435532
1	2.691079	3.888825	-1.430147
1	1.911624	4.176612	0.142819
1	0.996308	4.422293	-1.368960
1	-1.047901	-1.017480	0.730772
1	-2.448348	0.066470	2.965486
1	-2.261416	-1.673812	2.657362
1	-3.243681	-0.666006	1.558234
1	-2.106633	-1.824841	-1.161888

1	-4.730971	-2.272048	-0.144359
1	-3.221419	-2.981136	0.471461
1	-3.874307	-3.499126	-1.106126
1	3.438593	-0.543462	0.075005
1	4.133272	-2.008873	-2.271644
1	4.976785	-0.528521	-1.763380
1	3.248699	-0.467151	-2.201426
1	-1.662873	1.814779	0.165755
1	-0.146244	3.471341	1.940413
1	-0.735556	1.827960	2.310942
1	-1.891991	3.174462	2.093022
1	2.459017	-2.530850	-0.201700
1	0.640442	-3.647824	1.691374
1	1.143715	-1.942250	1.667807
1	2.342083	-3.227374	1.996273
1	0.351416	-2.382861	-0.661890
1	-0.520855	0.256508	-1.310720
1	0.646955	-0.623563	-2.333801
1	1.048421	-0.234369	-0.634932
1	2.461588	1.501286	0.008554
1	2.583076	0.189482	2.532746
1	1.110162	0.550681	1.593577
1	2.065764	1.876882	2.313445
1	-3.105282	0.084598	-0.574349
1	-3.394671	2.711689	-1.639557
1	-4.439842	1.335935	-2.061018
1	-2.714155	1.320072	-2.512856

Cartesian coordinates of : MeOH_N9_93.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	3.240796	-0.110908	1.772798
8	3.181650	-0.207976	0.353155
8	2.456263	1.984656	-0.981490
6	3.442030	2.976370	-0.715198
8	0.130032	2.693572	0.131927
6	0.273543	2.039620	1.387899
8	-2.371642	2.515036	-0.750504
6	-3.024437	3.623338	-0.141607
8	-3.581214	0.250278	-0.014874
6	-3.034077	0.093204	1.290538
8	-2.966776	-2.067008	-1.191339
6	-3.398473	-3.048428	-0.252148
8	-0.384701	-1.662553	-0.896233
6	-0.218446	-0.296735	-1.270518
8	2.220722	-2.442566	-0.861139
6	2.736403	-2.225093	-2.172350
8	0.230485	-1.489846	1.811857
6	0.936869	-2.642448	2.243588
1	2.800778	-1.069670	0.074544
1	3.629886	0.880460	2.015036
1	3.920432	-0.864418	2.184602
1	2.247119	-0.230341	2.214951
1	-1.412411	2.556608	-0.516288
1	-4.095377	3.523306	-0.327487
1	-2.677354	4.567040	-0.573809
1	-2.854021	3.640997	0.940971
1	-3.265455	-1.181355	-0.868296
1	-3.220088	-4.031156	-0.690806
1	-4.466765	-2.942365	-0.041516
1	-2.837876	-2.971547	0.687868
1	1.245579	-2.398617	-0.907976

1	3.824839	-2.252036	-2.104354
1	2.429779	-1.247465	-2.563149
1	2.402868	-3.008077	-2.859455
1	2.716933	1.154153	-0.514676
1	3.187300	3.863871	-1.296606
1	4.435548	2.629936	-1.016156
1	3.461921	3.243852	0.347832
1	-3.168473	1.057630	-0.405570
1	-3.638764	-0.643367	1.823600
1	-3.064927	1.038859	1.841855
1	-1.995548	-0.263517	1.254248
1	-1.323850	-1.926533	-1.087558
1	0.776171	0.018541	-0.941707
1	-0.963606	0.338076	-0.777680
1	-0.295739	-0.171579	-2.355040
1	-0.061396	-1.631124	0.892200
1	1.278138	-2.456707	3.264311
1	1.812491	-2.841078	1.612619
1	0.295848	-3.532060	2.247266
1	0.932030	2.481810	-0.402168
1	-0.611345	2.269277	1.986412
1	1.160434	2.406048	1.917519
1	0.351100	0.950298	1.275584

Cartesian coordinates of the methanol decamer

Cartesian coordinates of : MeOH_N10_0.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-2.624227	-2.344409	0.089790
1	-1.885703	-2.238664	0.729027
6	-2.275381	-3.257664	-0.944668
1	-3.136789	-3.342914	-1.609168
1	-2.046664	-4.246335	-0.534026
1	-1.412716	-2.906926	-1.525862
8	1.937707	2.064486	-1.390525
1	1.226251	2.501431	-0.847881
6	2.763780	3.059461	-1.990912
1	3.570570	2.547412	-2.517337
1	3.194719	3.717620	-1.230288
1	2.192413	3.656415	-2.707176
8	-0.909461	-1.509851	1.989674
1	0.055493	-1.319490	1.965460
6	-1.581221	-0.283070	2.242856
1	-2.644841	-0.502809	2.367220
1	-1.464636	0.419219	1.405481
1	-1.208754	0.191149	3.157411
8	-2.419087	2.408886	0.137059
1	-2.781489	1.539033	-0.156657
6	-3.142986	2.859355	1.274772
1	-2.771376	3.853121	1.532317
1	-2.993585	2.193700	2.133415
1	-4.213003	2.927853	1.056555
8	1.258237	-2.968874	-1.793380
1	1.078250	-2.052206	-2.071469
6	1.325173	-2.978622	-0.379214
1	1.926585	-3.836549	-0.068511
1	0.329368	-3.071919	0.078078
1	1.789524	-2.063478	0.007854
8	0.651749	-0.287797	-2.068066

1	1.241806	0.480573	-2.167122
6	-0.163390	-0.030005	-0.934373
1	-0.802048	-0.901713	-0.770255
1	-0.802811	0.844876	-1.095739
1	0.445867	0.123975	-0.032891
8	-3.480708	0.100344	-0.719595
1	-3.211854	-0.768636	-0.345177
6	-3.463087	-0.010555	-2.138274
1	-3.625809	0.986348	-2.552444
1	-4.260007	-0.674273	-2.488382
1	-2.497616	-0.387703	-2.497010
8	3.171344	0.249408	0.211723
1	2.762527	0.969379	-0.317107
6	3.912780	-0.590825	-0.667405
1	4.306858	-1.421994	-0.078997
1	4.750526	-0.044187	-1.111727
1	3.276339	-0.993223	-1.464005
8	0.168978	3.098439	0.255015
1	-0.771316	2.823030	0.140850
6	0.604021	2.707678	1.553631
1	1.588579	3.149156	1.720471
1	0.687607	1.617206	1.643175
1	-0.084228	3.073699	2.322446
8	1.663200	-0.741285	2.218595
1	2.194049	-0.371308	1.476743
6	2.464460	-1.681497	2.924963
1	1.870783	-2.063303	3.757352
1	3.366690	-1.205975	3.321919
1	2.753688	-2.521885	2.282897

Cartesian coordinates of : MeOH_N10_100.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	3.512296	-0.143279	0.048873
1	2.928070	-0.745711	0.553782
6	4.047689	-0.882128	-1.045475
1	4.496027	-0.169492	-1.740309
1	3.261613	-1.439845	-1.568879
1	4.819171	-1.580169	-0.705260
8	-2.472121	1.559664	1.600950
1	-2.634586	1.014992	0.795748
6	-3.584797	1.413395	2.476060
1	-3.400154	2.034408	3.354113
1	-3.707457	0.373206	2.797639
1	-4.506956	1.749553	1.992019
8	1.827184	-2.069773	0.961933
1	1.164193	-1.895440	1.687496
6	2.431673	-3.348678	1.162567
1	3.051491	-3.563334	0.290254
1	1.666872	-4.125047	1.256720
1	3.059916	-3.342885	2.057283
8	0.077074	2.565723	-2.135712
1	0.960058	2.341488	-1.784282
6	-0.717097	2.956548	-1.032177
1	-1.628241	3.421917	-1.415715
1	-0.197684	3.683486	-0.394519
1	-1.006229	2.096604	-0.411243
8	2.472052	2.163872	-0.860964
1	2.848439	1.341625	-0.474660
6	3.136247	3.301202	-0.333872
1	2.666444	4.187579	-0.765609
1	4.198620	3.301304	-0.600463

1	3.042097	3.350480	0.757135
8	-0.091202	1.048219	2.723210
1	-0.974802	1.280593	2.345430
6	0.891673	1.289364	1.723591
1	1.873272	1.079037	2.156389
1	0.869005	2.329067	1.384003
1	0.746936	0.638555	0.848180
8	0.479434	-1.882129	-1.421606
1	0.947629	-1.987769	-0.565495
6	0.402223	-0.495625	-1.741755
1	0.098661	-0.408690	-2.786876
1	1.372111	-0.003081	-1.613949
1	-0.343199	0.021201	-1.120233
8	-0.144579	-1.604162	2.602191
1	-0.107304	-0.652615	2.866693
6	-1.203942	-1.721750	1.655814
1	-1.184038	-2.734810	1.249504
1	-1.074707	-1.006001	0.831623
1	-2.176568	-1.544709	2.126035
8	-3.064849	0.106916	-0.579780
1	-2.742672	-0.806761	-0.761885
6	-3.197899	0.795859	-1.817522
1	-3.607523	1.784993	-1.603173
1	-3.886071	0.268258	-2.486125
1	-2.227048	0.917922	-2.313934
8	-2.169286	-2.333032	-1.290000
1	-1.184687	-2.320244	-1.301614
6	-2.634787	-2.643732	-2.599634
1	-3.724174	-2.576825	-2.587978
1	-2.346542	-3.659610	-2.886247
1	-2.243903	-1.936104	-3.339933

Cartesian coordinates of : MeOH_N10_101.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.177694	-1.082875	-2.095539
1	-0.580411	-1.688518	-1.596834
6	-0.450851	0.100998	-2.398762
1	-1.125979	0.785616	-2.916299
1	0.400950	-0.117944	-3.051408
1	-0.085143	0.590399	-1.486324
8	1.485790	2.728048	-1.278289
1	0.720300	2.589632	-0.669263
6	1.936560	4.068709	-1.113045
1	2.782603	4.220922	-1.785295
1	2.262313	4.253970	-0.083510
1	1.145357	4.778993	-1.372674
8	0.552635	-2.697884	-0.834865
1	1.134723	-2.493784	-0.063650
6	1.316692	-3.434020	-1.781947
1	0.664310	-3.669394	-2.625055
1	1.684307	-4.368540	-1.346642
1	2.169376	-2.850407	-2.148195
8	-3.533913	-0.071529	1.667044
1	-3.534562	-0.326611	0.713113
6	-4.567002	0.883021	1.875848
1	-4.506214	1.220506	2.911765
1	-5.551990	0.435468	1.707653
1	-4.450261	1.748421	1.214189
8	3.449546	0.982226	-0.854379
1	2.732348	1.642961	-1.025605
6	3.094995	-0.234458	-1.500389

1	3.875937	-0.967567	-1.285456
1	3.024108	-0.100134	-2.585026
1	2.137848	-0.622766	-1.125396
8	-0.611200	2.564141	0.346558
1	-0.674028	1.903004	1.077925
6	-1.857214	2.561347	-0.340988
1	-1.696238	2.976318	-1.339001
1	-2.592696	3.178954	0.184858
1	-2.252739	1.542202	-0.443647
8	-3.555591	-0.629594	-0.951449
1	-2.680386	-0.799272	-1.376377
6	-4.455273	-1.667456	-1.324081
1	-5.403839	-1.482484	-0.816533
1	-4.077578	-2.649684	-1.021127
1	-4.627217	-1.664828	-2.404873
8	3.145068	0.189401	1.659472
1	3.395295	0.560670	0.778733
6	2.303869	1.130547	2.315862
1	1.649566	0.591592	3.004890
1	1.675982	1.669739	1.594967
1	2.899360	1.856754	2.878313
8	-0.949611	0.526522	2.013838
1	-1.925356	0.389243	2.061260
6	-0.431238	-0.539612	1.226512
1	0.530976	-0.225372	0.807320
1	-1.108717	-0.783042	0.399311
1	-0.270029	-1.438067	1.832000
8	2.319066	-2.310573	1.128021
1	2.614671	-1.394833	1.347060
6	2.160661	-3.051965	2.330027
1	1.725017	-4.018657	2.069729
1	1.491212	-2.540340	3.030874
1	3.126848	-3.218841	2.816729

Cartesian coordinates of : MeOH_N10_103.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-3.304966	0.050801	0.196700
1	-2.976649	-0.040009	-0.721913
6	-3.389995	1.434809	0.517493
1	-3.574668	1.516398	1.590563
1	-4.215351	1.910420	-0.021571
1	-2.456156	1.958044	0.281757
8	0.124696	3.455626	0.743677
1	-0.129523	2.819712	0.047892
6	0.788709	4.532658	0.106117
1	1.127827	5.222260	0.881981
1	0.123174	5.075248	-0.575977
1	1.665597	4.190743	-0.459642
8	2.211746	-1.451530	0.940299
1	1.384754	-1.232686	1.452304
6	3.101330	-2.180038	1.786567
1	3.987843	-2.427503	1.199745
1	2.634935	-3.104877	2.137693
1	3.400275	-1.572149	2.646078
8	1.957204	-2.274650	-1.633501
1	2.016615	-2.086945	-0.672079
6	3.043711	-1.620712	-2.279458
1	2.840287	-1.613197	-3.351799
1	3.981972	-2.156717	-2.100620
1	3.153513	-0.587854	-1.929027
8	-2.133779	0.001829	-2.277447

1	-1.586133	-0.822281	-2.365284
6	-2.863193	0.259921	-3.476582
1	-3.477968	1.143809	-3.302328
1	-3.511355	-0.584954	-3.723989
1	-2.181461	0.455347	-4.308959
8	-2.381283	-1.647888	2.077033
1	-2.723297	-1.054648	1.368562
6	-3.132519	-1.414525	3.263861
1	-2.807041	-2.140195	4.010597
1	-4.202814	-1.550476	3.081119
1	-2.960360	-0.404423	3.653837
8	-0.703490	-2.180031	-2.003810
1	0.274608	-2.142284	-2.097239
6	-0.972373	-2.309187	-0.610913
1	-2.033674	-2.534989	-0.490632
1	-0.747334	-1.374771	-0.077441
1	-0.384698	-3.119950	-0.168171
8	3.751086	0.777513	0.184434
1	3.174384	0.020176	0.393634
6	3.380325	1.851253	1.032828
1	4.093733	2.662738	0.873260
1	3.415050	1.561474	2.090948
1	2.372408	2.225140	0.805532
8	0.114081	-0.729336	2.332032
1	-0.730686	-1.237053	2.286368
6	-0.194173	0.614590	1.972039
1	0.732946	1.189142	1.972883
1	-0.889110	1.064371	2.689570
1	-0.637832	0.666729	0.968139
8	-0.239324	1.760785	-1.389186
1	-1.012331	1.248117	-1.701364
6	0.908254	0.931063	-1.501762
1	1.796705	1.559948	-1.406798
1	0.933842	0.424011	-2.473382
1	0.939746	0.170190	-0.707229

Cartesian coordinates of : MeOH_N10_104.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-1.048103	1.801411	1.154560
1	-1.790528	1.508067	0.569815
6	-1.546706	2.763698	2.075275
1	-0.707462	3.105150	2.685150
1	-2.306845	2.325909	2.731588
1	-1.975875	3.624129	1.550483
8	-3.412513	-1.331530	-1.003029
1	-2.720974	-1.651996	-0.387927
6	-3.591378	-2.226446	-2.090287
1	-4.318323	-1.777719	-2.768811
1	-3.978597	-3.190499	-1.745302
1	-2.655229	-2.391259	-2.634884
8	0.734594	0.106912	2.429880
1	0.053807	0.648936	1.987549
6	1.980850	0.393352	1.818909
1	2.618821	-0.493126	1.894181
1	2.489418	1.230235	2.316430
1	1.849256	0.626925	0.756196
8	2.690278	0.796323	-1.652420
1	1.977422	1.415504	-1.382600
6	3.922871	1.346547	-1.207407
1	4.717809	0.651770	-1.485542
1	3.932562	1.474628	-0.117480

1	4.117158	2.314606	-1.681006
8	-1.552490	-1.475513	0.924624
1	-0.731660	-2.021302	1.067945
6	-2.197340	-1.158400	2.152575
1	-2.984375	-0.432113	1.933176
1	-1.490065	-0.716738	2.860257
1	-2.651307	-2.050378	2.596636
8	-3.012579	1.318399	-0.580149
1	-3.182819	0.389033	-0.847246
6	-2.545197	2.055895	-1.706109
1	-2.419822	3.093493	-1.387980
1	-3.271336	2.022879	-2.524025
1	-1.578209	1.674207	-2.051625
8	0.915581	2.695649	-0.772413
1	0.231347	2.113765	-0.393681
6	1.264987	3.664811	0.203903
1	2.096719	4.249813	-0.192998
1	1.578327	3.191847	1.142052
1	0.424102	4.336680	0.409208
8	2.562769	-1.676186	-0.556289
1	2.449854	-0.756558	-0.890205
6	2.980469	-2.499705	-1.634777
1	3.174436	-3.497192	-1.235286
1	3.900910	-2.115601	-2.087291
1	2.206791	-2.573618	-2.407991
8	-0.050793	0.084366	-0.788485
1	-0.611063	-0.272497	-0.073401
6	-0.187396	-0.766294	-1.912067
1	0.633440	-0.543705	-2.599342
1	-1.141420	-0.598482	-2.429836
1	-0.123560	-1.824133	-1.623288
8	0.692689	-2.834764	0.958650
1	1.322006	-2.312385	0.402987
6	1.307889	-3.095667	2.215964
1	0.732445	-3.879878	2.712313
1	1.308384	-2.196007	2.840031
1	2.334697	-3.449663	2.076443

Cartesian coordinates of : MeOH_N10_10.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.952946	-2.745858	0.642727
1	1.678552	-2.333267	0.121385
6	1.425333	-3.254587	1.880795
1	0.583043	-3.736626	2.380802
1	1.801186	-2.451219	2.525861
1	2.218200	-3.993693	1.730335
8	-2.514110	1.632378	-2.569135
1	-1.561468	1.440138	-2.509146
6	-2.845407	2.476973	-1.482420
1	-3.920610	2.664939	-1.522103
1	-2.319448	3.438063	-1.537557
1	-2.614284	2.008602	-0.514074
8	2.687054	1.169023	-1.107197
1	2.628381	1.487200	-0.165647
6	3.806671	1.766900	-1.758340
1	3.868124	1.345700	-2.762844
1	4.732813	1.544412	-1.220099
1	3.679561	2.850516	-1.832100
8	0.070281	2.625928	2.062211
1	-0.619920	1.929033	2.163509
6	-0.301413	3.503095	1.003492

1	0.396076	4.342414	1.009713
1	-1.316460	3.885504	1.150077
1	-0.245074	3.001906	0.028488
8	-3.282146	-0.807971	0.746915
1	-2.687385	-1.543542	0.474741
6	-4.139950	-0.499710	-0.346109
1	-4.792911	0.318087	-0.034976
1	-4.760189	-1.363103	-0.610009
1	-3.570753	-0.177209	-1.227050
8	-1.676582	0.601508	2.405252
1	-2.358640	0.328791	1.755321
6	-0.935186	-0.570028	2.728892
1	-0.156474	-0.285920	3.440510
1	-0.459989	-1.005334	1.839026
1	-1.578966	-1.324693	3.192919
8	2.692894	-1.574151	-1.052112
1	2.782345	-0.599151	-0.993122
6	2.184976	-1.882042	-2.347975
1	1.950118	-2.948001	-2.366617
1	2.930601	-1.668944	-3.120326
1	1.272770	-1.311704	-2.562422
8	0.033942	0.956294	-1.788335
1	0.981033	1.190395	-1.804525
6	-0.206245	0.256326	-0.577113
1	-1.284662	0.089141	-0.490475
1	0.124635	0.835081	0.294520
1	0.299053	-0.716323	-0.566207
8	-1.636299	-2.748064	-0.181946
1	-0.715212	-2.742349	0.157433
6	-1.596692	-2.773272	-1.603828
1	-2.604034	-2.995003	-1.961124
1	-0.915380	-3.551507	-1.962154
1	-1.282317	-1.805361	-2.015570
8	2.488475	1.641657	1.460556
1	1.618345	2.020898	1.738934
6	2.580355	0.304894	1.942165
1	3.558164	-0.087506	1.653619
1	1.801146	-0.330637	1.499334
1	2.493743	0.273020	3.032775

Cartesian coordinates of : MeOH_N10_10r.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	-2.044296	3.401647	2.485083
1	-2.968623	3.045870	2.943709
1	-2.240824	4.361291	1.992972
1	-1.294603	3.548932	3.268698
8	-1.615848	2.417827	1.551265
1	-0.785179	2.742678	1.127944
6	0.167559	4.522153	-0.532046
1	0.135294	4.029685	-1.509819
1	0.879022	5.353823	-0.573482
1	-0.824345	4.921022	-0.306503
8	0.512988	3.607786	0.498736
1	1.385865	3.205227	0.276297
6	3.938484	3.613215	0.394692
1	4.846380	3.677917	-0.214323
1	4.192506	3.192265	1.373216
1	3.539842	4.619988	0.537192
8	2.940756	2.840867	-0.259310
1	3.283022	1.922587	-0.369838
6	4.838581	0.506243	-1.869119

1	4.146466	0.197493	-2.659656
1	5.702908	-0.166376	-1.866851
1	5.184876	1.520219	-2.080636
8	4.201813	0.521397	-0.598565
1	3.863226	-0.386335	-0.414952
6	4.661749	-2.727242	0.334255
1	4.681461	-3.788100	0.063047
1	4.587345	-2.637029	1.423124
1	5.595300	-2.264974	0.006070
8	3.592092	-2.054778	-0.316527
1	2.744706	-2.448581	-0.000652
6	1.187369	-4.493497	-0.308719
1	0.561480	-5.245933	0.183715
1	2.127816	-4.962048	-0.606303
1	0.673915	-4.132902	-1.206985
8	1.492809	-3.427052	0.579134
1	0.640352	-3.056103	0.912870
6	-1.319176	-3.755680	2.397422
1	-2.143092	-3.413948	3.032042
1	-0.471426	-4.020110	3.032869
1	-1.638959	-4.647958	1.846947
8	-0.896317	-2.725513	1.513001
1	-1.617314	-2.576313	0.853144
6	-2.563201	-3.478629	-1.335103
1	-3.456995	-3.736131	-1.913028
1	-2.125132	-4.398520	-0.940303
1	-1.834848	-2.997091	-1.996935
8	-2.891966	-2.645695	-0.231495
1	-3.249175	-1.790946	-0.579491
6	-5.320070	-0.560491	-1.461067
1	-5.541463	-1.526415	-1.919496
1	-5.715569	0.232224	-2.104594
1	-5.815241	-0.510565	-0.485329
8	-3.908048	-0.453023	-1.331981
1	-3.703315	0.408509	-0.890795
6	-3.422688	2.966845	-1.142525
1	-4.232170	2.868851	-1.868558
1	-2.464812	2.902565	-1.670895
1	-3.500752	3.947182	-0.659893
8	-3.560612	1.920615	-0.190078
1	-2.835139	2.021224	0.474792

Cartesian coordinates of : MeOH_N10_114.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	2.835250	2.070898	0.846476
1	1.871341	2.071817	1.067011
6	3.563471	2.290912	2.050421
1	4.626416	2.219486	1.813727
1	3.315956	1.537626	2.806540
1	3.356327	3.286652	2.453803
8	-2.799085	-1.459688	0.816059
1	-1.914229	-1.840874	0.992195
6	-3.250418	-0.779679	1.978794
1	-4.336292	-0.686193	1.913758
1	-2.818462	0.227363	2.047972
1	-2.998453	-1.334607	2.888852
8	0.500821	0.819424	-2.839878
1	0.005732	-0.007599	-2.705728
6	0.581562	1.428403	-1.562951
1	1.094284	2.386941	-1.675032
1	1.152679	0.809911	-0.856550

1	-0.414426	1.600494	-1.131474
8	-1.972701	2.731894	0.732748
1	-2.390154	1.998340	0.217789
6	-1.967408	3.904317	-0.072653
1	-1.498660	4.703481	0.503834
1	-2.988177	4.205831	-0.328690
1	-1.395754	3.753473	-0.996093
8	-0.420842	-2.672888	1.436536
1	0.400039	-2.448562	0.954289
6	-0.120108	-3.059173	2.770818
1	-1.059436	-3.336780	3.251878
1	0.336058	-2.236285	3.332651
1	0.552351	-3.922552	2.788344
8	3.472372	-0.238467	-0.269862
1	3.235396	0.622990	0.164593
6	3.836327	0.024266	-1.624607
1	4.307036	-0.876399	-2.023839
1	4.553303	0.848759	-1.676225
1	2.956462	0.269335	-2.231483
8	0.333252	1.759715	1.651750
1	-0.479680	2.224616	1.337028
6	0.074488	0.362404	1.634791
1	1.035729	-0.161479	1.582811
1	-0.526807	0.076459	0.761337
1	-0.443899	0.043700	2.546517
8	1.547049	-1.992386	-0.306913
1	2.260703	-1.295348	-0.231067
6	2.028768	-3.054593	-1.129253
1	1.337959	-3.894666	-1.029998
1	3.024241	-3.372748	-0.806643
1	2.067397	-2.744964	-2.179445
8	-3.048017	0.768642	-0.716560
1	-2.753081	-0.126169	-0.442592
6	-3.038784	0.902632	-2.131418
1	-3.379749	1.913496	-2.365235
1	-3.725882	0.186907	-2.595135
1	-2.034805	0.757491	-2.540219
8	-0.816932	-1.210097	-1.484058
1	0.017598	-1.427458	-1.019314
6	-1.455202	-2.425999	-1.855685
1	-2.445243	-2.173411	-2.241708
1	-1.575657	-3.086940	-0.990366
1	-0.893673	-2.949446	-2.638030

 Cartesian coordinates of : MeOH_N10_146.log

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-3.935998	-0.972406	0.301658
1	-3.152689	-1.480869	-0.012361
6	-5.073567	-1.406359	-0.433221
1	-5.918282	-0.780744	-0.138545
1	-5.313336	-2.450865	-0.208709
1	-4.916729	-1.299955	-1.512980
8	2.462046	0.037536	-2.132781
1	2.484673	0.916568	-1.670924
6	3.540503	-0.050571	-3.061713
1	3.513480	-1.046985	-3.504841
1	4.501949	0.090335	-2.557824
1	3.431674	0.696020	-3.853031
8	-0.224422	0.994681	2.395958
1	0.421126	0.251340	2.390796
6	-1.540188	0.456951	2.341116

1	-2.222061	1.258215	2.047011
1	-1.843896	0.064300	3.317323
1	-1.613849	-0.345702	1.598017
8	0.471390	3.019918	0.746345
1	0.216334	2.304713	1.373058
6	-0.708817	3.650042	0.256472
1	-0.443452	4.197788	-0.650856
1	-1.101014	4.361160	0.992042
1	-1.486777	2.915431	0.019122
8	-1.811984	-2.355715	-0.587865
1	-1.250190	-1.848711	-1.211066
6	-0.980594	-2.840635	0.461427
1	-1.592287	-2.949769	1.360619
1	-0.165727	-2.138649	0.674493
1	-0.555171	-3.815372	0.202050
8	-0.226026	-0.594661	-1.862547
1	0.656306	-0.627837	-2.270472
6	-0.188293	0.451500	-0.897760
1	-1.169429	0.506707	-0.418606
1	0.018998	1.416291	-1.373357
1	0.571891	0.256619	-0.128893
8	-3.413264	1.620196	-0.380169
1	-3.643468	0.743574	-0.009308
6	-3.332919	1.475004	-1.786879
1	-2.790343	2.336829	-2.185905
1	-4.327236	1.444264	-2.249951
1	-2.786162	0.565623	-2.071077
8	2.536935	-1.744192	-0.079329
1	2.571831	-1.077961	-0.800273
6	2.316585	-3.025976	-0.656633
1	2.156031	-3.733732	0.158941
1	3.186838	-3.345574	-1.238505
1	1.430414	-3.023146	-1.301753
8	2.646087	2.163197	-0.573775
1	1.806939	2.574940	-0.262529
6	3.244114	1.565854	0.572987
1	4.086380	0.956528	0.236261
1	2.528304	0.919155	1.097868
1	3.611111	2.328810	1.266279
8	1.473666	-1.095179	2.293103
1	1.820155	-1.341188	1.403868
6	2.551879	-1.114948	3.221215
1	2.161672	-0.799532	4.190209
1	3.350656	-0.427117	2.920710
1	2.965670	-2.123669	3.316245

Cartesian coordinates of : MeOH_N10_170.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	4.436197	0.228636	-0.621123
1	3.933340	0.192377	0.227583
6	4.553289	-1.091073	-1.140506
1	5.378057	-1.100797	-1.854993
1	3.635367	-1.398085	-1.657342
1	4.767420	-1.810287	-0.343184
8	-3.187011	1.746255	-0.047577
1	-3.226526	0.758322	-0.053302
6	-4.436411	2.237756	0.424281
1	-4.377353	3.327572	0.449068
1	-4.653253	1.870861	1.433036
1	-5.249021	1.943556	-0.247651
8	0.344982	-2.571112	-0.832317

1	0.385379	-1.714453	-1.318952
6	1.478351	-2.651324	0.025190
1	1.187994	-3.186749	0.934153
1	1.834845	-1.650314	0.300617
1	2.292567	-3.199203	-0.459819
8	-3.543538	-0.880369	-0.107179
1	-2.911437	-1.545575	0.263198
6	-3.980312	-1.352857	-1.375383
1	-4.426985	-0.513978	-1.914373
1	-4.731720	-2.141486	-1.261993
1	-3.141205	-1.742104	-1.964213
8	2.536906	1.536650	-1.976983
1	3.310312	1.070776	-1.577116
6	2.143394	2.558095	-1.066919
1	1.416233	3.194753	-1.574697
1	2.999677	3.170416	-0.767163
1	1.676365	2.133067	-0.167160
8	0.437286	-0.146495	-1.950016
1	1.255209	0.400253	-2.016384
6	-0.680458	0.715054	-1.777342
1	-1.568967	0.090592	-1.652521
1	-0.821603	1.359708	-2.651819
1	-0.570840	1.340656	-0.882555
8	-1.867317	-2.803920	0.608658
1	-1.048155	-2.718430	0.058095
6	-2.458514	-4.074390	0.362307
1	-3.414524	-4.104974	0.888700
1	-1.821722	-4.880789	0.739867
1	-2.638593	-4.230291	-0.707232
8	-1.090421	2.815212	1.159938
1	-1.893311	2.393223	0.761669
6	-0.783902	3.983697	0.413553
1	0.214187	4.320249	0.702260
1	-1.501060	4.783491	0.626973
1	-0.791614	3.780165	-0.663898
8	0.445879	0.763005	1.921031
1	0.021717	1.606629	1.640787
6	-0.461012	-0.294870	1.635534
1	-0.099214	-1.197737	2.132557
1	-0.521710	-0.487626	0.557907
1	-1.463364	-0.066157	2.015982
8	3.025783	0.164674	1.635442
1	2.079243	0.440874	1.680340
6	3.296618	-0.751537	2.686474
1	4.361601	-0.988834	2.655280
1	2.725798	-1.680068	2.565825
1	3.060658	-0.311197	3.660345

Cartesian coordinates of : MeOH_N10_187.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.248108	-1.434623	1.079837
1	-0.138209	-1.798261	0.259212
6	-0.273343	-0.118391	1.237945
1	0.036153	0.244528	2.221851
1	-1.369956	-0.116293	1.196894
1	0.125402	0.555281	0.470209
8	-1.798762	2.402214	-0.298324
1	-1.130342	2.151114	-0.983327
6	-1.102761	3.025402	0.778916
1	-1.471243	2.618134	1.726689
1	-1.277817	4.105942	0.768159

1	-0.026381	2.831964	0.704328
8	-3.339186	-1.974859	0.278331
1	-3.452051	-0.992094	0.313325
6	-3.192341	-2.458292	1.610083
1	-3.221558	-3.548490	1.573772
1	-4.010737	-2.103141	2.243608
1	-2.235800	-2.144192	2.044747
8	-1.163798	-2.189077	-1.192772
1	-2.006210	-2.278958	-0.675690
6	-1.297754	-1.026464	-2.008721
1	-0.349644	-0.864570	-2.526601
1	-1.519658	-0.141284	-1.399693
1	-2.090142	-1.160299	-2.751307
8	2.862670	-0.623274	1.394012
1	2.033669	-1.017610	1.058476
6	2.942332	-0.909653	2.781937
1	3.853218	-0.445616	3.164815
1	2.993837	-1.989119	2.963813
1	2.083957	-0.499954	3.328989
8	1.901429	-0.080503	-1.237782
1	1.721532	-1.036950	-1.377576
6	3.225371	0.200138	-1.683075
1	3.385733	1.274705	-1.571812
1	3.357953	-0.077149	-2.734065
1	3.957628	-0.329666	-1.065167
8	0.178272	1.874077	-1.971256
1	0.773550	1.141011	-1.691536
6	0.949943	3.064665	-2.117991
1	0.251897	3.895463	-2.245376
1	1.587963	3.004492	-3.006333
1	1.565565	3.235731	-1.229662
8	-3.627652	0.659583	0.496313
1	-2.919721	1.273551	0.175002
6	-4.892520	1.168809	0.091836
1	-5.658964	0.477810	0.447905
1	-4.961690	1.243325	-0.998583
1	-5.074194	2.154422	0.532002
8	2.314448	2.084092	0.721262
1	2.451134	1.118425	0.722815
6	2.328545	2.510527	2.070429
1	2.234168	3.599156	2.077851
1	3.263718	2.237656	2.574563
1	1.488870	2.088441	2.640079
8	1.501332	-2.741288	-1.616421
1	0.546722	-2.917040	-1.546157
6	2.207394	-3.528296	-0.658896
1	3.253516	-3.220818	-0.698194
1	2.138238	-4.592198	-0.902310
1	1.825808	-3.358862	0.353912

Cartesian coordinates of : MeOH_N10_188.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.215436	-0.808725	-2.102230
1	1.104401	-1.170456	-1.956916
6	0.040223	0.246590	-1.173633
1	-0.728195	0.920511	-1.561984
1	0.963248	0.821243	-1.029896
1	-0.291773	-0.122530	-0.191176
8	-0.250777	2.644674	0.769252
1	-1.134635	2.339459	0.449821
6	-0.278398	2.816582	2.180563

1	0.623396	3.364106	2.465893
1	-0.281397	1.847430	2.692361
1	-1.152814	3.400270	2.487277
8	0.868875	-2.208350	0.751157
1	1.580542	-1.882100	0.146474
6	1.315435	-3.388518	1.419221
1	0.511697	-3.711687	2.083177
1	2.209845	-3.181959	2.014828
1	1.529215	-4.185969	0.701179
8	-3.124980	-0.553087	-0.840574
1	-2.451450	-1.259744	-0.686105
6	-4.325958	-0.959916	-0.194472
1	-5.098704	-0.226943	-0.434330
1	-4.199723	-0.997752	0.894133
1	-4.647312	-1.943308	-0.551663
8	2.012301	3.153473	-0.545299
1	1.149150	3.007108	-0.090485
6	1.765778	3.526904	-1.894315
1	2.729420	3.720148	-2.368098
1	1.159656	4.437233	-1.943272
1	1.255236	2.727919	-2.445000
8	-2.672587	1.941396	-0.073932
1	-2.775175	0.993307	-0.343009
6	-3.065599	2.763986	-1.165827
1	-2.978507	3.804494	-0.847863
1	-4.104151	2.566251	-1.449641
1	-2.420607	2.606354	-2.038676
8	-1.596182	-2.680267	-0.332616
1	-0.685901	-2.469590	-0.034199
6	-1.517476	-3.517077	-1.482900
1	-2.539387	-3.738998	-1.796866
1	-1.011559	-4.458375	-1.243797
1	-0.989272	-3.008260	-2.294415
8	3.315637	0.950241	0.248803
1	2.974479	1.775032	-0.170999
6	2.609187	0.791633	1.479239
1	2.857101	-0.194151	1.881474
1	1.525043	0.853354	1.324184
1	2.912956	1.555673	2.202185
8	-0.256585	-0.593328	2.735564
1	0.252213	-1.040425	2.035676
6	-1.611616	-0.544454	2.321141
1	-2.224797	-0.326159	3.198740
1	-1.938842	-1.500403	1.892662
1	-1.780973	0.247701	1.577607
8	2.727343	-1.295511	-0.937760
1	3.020940	-0.409061	-0.586001
6	3.858376	-2.143339	-1.126223
1	3.493714	-3.111093	-1.473890
1	4.402627	-2.281748	-0.186539
1	4.532717	-1.725353	-1.878535

 Cartesian coordinates of : MeOH_N10_244.log

 Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	0.600171	3.833413	-0.313739
1	0.289428	3.049691	-0.811671
6	1.796894	4.282167	-0.924217
1	2.141330	5.163128	-0.378321
1	1.639413	4.561625	-1.972703
1	2.586947	3.519894	-0.881555
8	2.093022	-2.680624	-1.032596

1	2.585326	-1.944866	-0.585366
6	2.542426	-2.800972	-2.375599
1	2.024417	-3.649542	-2.826332
1	3.620447	-2.987514	-2.411108
1	2.316811	-1.899893	-2.958081
8	-0.414851	0.451635	2.284757
1	-0.828668	-0.424589	2.135197
6	-1.140900	1.411463	1.523231
1	-0.460459	2.216985	1.232465
1	-1.961332	1.833847	2.113698
1	-1.550748	0.957890	0.611411
8	3.491050	-0.756934	0.128613
1	2.984041	-0.256304	0.817482
6	4.657385	-1.296705	0.740090
1	5.212089	-1.844530	-0.024008
1	4.399663	-1.984280	1.552790
1	5.294394	-0.498197	1.133639
8	-2.528469	0.954228	-1.839550
1	-2.943636	0.298901	-1.232161
6	-3.092364	2.231629	-1.561910
1	-2.600877	2.960021	-2.209684
1	-2.926972	2.524373	-0.517314
1	-4.166698	2.240886	-1.770928
8	0.095577	1.529017	-1.683289
1	-0.824621	1.187944	-1.754646
6	0.943199	0.569564	-1.070227
1	1.827876	1.092812	-0.696754
1	1.270670	-0.191012	-1.788735
1	0.455230	0.069516	-0.221861
8	2.264242	0.597927	2.041493
1	1.292094	0.476499	2.142513
6	2.547383	1.993855	2.014508
1	3.597907	2.113084	1.739217
1	2.389278	2.440799	3.001605
1	1.923265	2.516556	1.279740
8	-0.509254	-2.771711	-0.645661
1	0.474629	-2.714931	-0.772299
6	-1.173672	-2.258428	-1.794351
1	-2.248727	-2.373622	-1.637408
1	-0.885492	-2.813666	-2.692184
1	-0.955091	-1.194613	-1.945321
8	-1.680473	-1.785886	1.427143
1	-1.142575	-2.178979	0.675843
6	-2.149720	-2.838086	2.270540
1	-2.760958	-2.388659	3.054503
1	-1.311638	-3.369706	2.729467
1	-2.760509	-3.544759	1.700328
8	-3.689330	-0.664474	-0.021296
1	-2.995067	-1.073158	0.542182
6	-4.621980	0.016038	0.812020
1	-5.380000	0.460525	0.165080
1	-4.136780	0.811954	1.388304
1	-5.109779	-0.679989	1.501465

Cartesian coordinates of : MeOH_N10_280.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	2.709608	2.023017	0.389768
1	2.123869	1.691705	1.103971
6	2.047605	3.091326	-0.274853
1	2.639953	3.355471	-1.152822
1	1.967148	3.967338	0.376808

1	1.043551	2.799184	-0.605596
8	-1.410247	2.199995	1.094552
1	-0.529803	1.937613	1.436712
6	-2.226222	1.030011	1.123499
1	-3.272312	1.343200	1.114730
1	-2.042272	0.442352	2.027364
1	-2.040216	0.392491	0.247787
8	-1.509172	2.691837	-1.547042
1	-1.402797	2.654241	-0.568189
6	-2.903538	2.755880	-1.835061
1	-3.013697	2.939564	-2.904670
1	-3.380368	3.571696	-1.283637
1	-3.404650	1.812462	-1.583923
8	3.859471	-0.102282	-0.817611
1	3.460003	0.707089	-0.423556
6	4.209447	0.137129	-2.174187
1	4.670231	-0.772939	-2.561604
1	4.928319	0.958503	-2.252636
1	3.328436	0.371493	-2.782577
8	0.851031	1.094194	2.148116
1	0.821063	0.099859	2.014282
6	0.924911	1.372915	3.546787
1	1.012728	2.453601	3.667248
1	1.799468	0.889956	3.991334
1	0.019639	1.028028	4.056139
8	-0.640173	0.206939	-2.111614
1	-0.960780	1.135935	-2.032968
6	0.505248	0.075829	-1.280362
1	0.797984	-0.977321	-1.264043
1	0.295379	0.396949	-0.249375
1	1.342408	0.667578	-1.665802
8	-3.703347	-1.640678	0.953950
1	-3.149726	-1.738877	0.154973
6	-4.959421	-1.143584	0.530429
1	-5.553651	-0.929585	1.421577
1	-5.502036	-1.873822	-0.082698
1	-4.854904	-0.215520	-0.047064
8	0.817843	-1.478195	1.807963
1	1.473521	-1.756423	1.115912
6	-0.440193	-2.072661	1.505337
1	-1.129867	-1.841934	2.319120
1	-0.342334	-3.159839	1.419755
1	-0.856370	-1.674399	0.571768
8	2.498767	-2.263523	-0.079007
1	2.999200	-1.475816	-0.409154
6	3.429446	-3.238796	0.378700
1	2.859612	-4.074432	0.788850
1	4.078248	-2.832596	1.161859
1	4.047193	-3.603814	-0.447564
8	-2.360485	-1.758827	-1.454218
1	-1.810521	-0.989507	-1.726817
6	-1.708490	-2.950410	-1.870519
1	-2.313353	-3.795110	-1.535220
1	-0.708898	-3.038854	-1.426754
1	-1.618530	-2.991164	-2.960998

Cartesian coordinates of : MeOH_N10_33.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-2.993462	-1.522453	-0.719499
1	-2.030571	-1.682410	-0.633993
6	-3.387333	-1.919360	-2.025693

1	-4.468507	-1.788404	-2.099719
1	-3.142024	-2.970928	-2.205602
1	-2.901644	-1.304404	-2.792309
8	3.422000	2.036518	-0.681433
1	2.547418	2.168800	-0.263448
6	3.278374	2.061618	-2.099951
1	4.271701	1.919949	-2.529009
1	2.882641	3.024947	-2.436625
1	2.619490	1.254751	-2.439669
8	-1.061142	-0.387501	1.003263
1	-0.160353	-0.752858	1.112875
6	-1.790210	-0.555869	2.203720
1	-2.783665	-0.127977	2.045689
1	-1.319104	-0.032247	3.045823
1	-1.908062	-1.615144	2.467228
8	-1.315206	2.527911	0.885486
1	-1.934865	1.831358	0.568559
6	-1.571023	3.708151	0.134666
1	-0.875567	4.477019	0.476046
1	-2.594882	4.059464	0.297555
1	-1.417777	3.537732	-0.936766
8	-0.432189	-2.564409	-1.031568
1	0.224875	-1.870677	-0.825060
6	-0.440123	-3.549169	-0.010747
1	-1.139087	-4.330145	-0.319279
1	-0.777711	-3.129515	0.945424
1	0.551728	-3.989574	0.133129
8	0.925662	-0.153821	-1.252742
1	1.087974	0.358349	-0.435210
6	-0.153330	0.482935	-1.925778
1	-0.383195	-0.108555	-2.815023
1	0.121068	1.498220	-2.241350
1	-1.041114	0.531679	-1.284410
8	-3.289253	1.103053	-0.290612
1	-3.135806	0.134744	-0.414748
6	-4.623780	1.301497	0.146369
1	-4.789715	2.376432	0.243504
1	-4.805071	0.830448	1.120129
1	-5.340888	0.900810	-0.578754
8	3.682967	-0.544407	0.153620
1	3.652482	0.397535	-0.128923
6	3.936107	-1.350501	-0.995246
1	3.996471	-2.388261	-0.660439
1	4.887486	-1.075513	-1.461770
1	3.123005	-1.252985	-1.721916
8	1.156415	1.703913	0.778050
1	0.200764	1.998932	0.795864
6	1.575056	1.444213	2.112034
1	2.584996	1.026400	2.075094
1	0.914417	0.714159	2.591837
1	1.590560	2.365503	2.703216
8	1.428481	-1.576068	1.174228
1	2.227215	-1.126566	0.808257
6	1.787270	-2.227253	2.382543
1	0.908147	-2.764193	2.747157
1	2.102164	-1.507358	3.147695
1	2.594765	-2.948976	2.217098

Cartesian coordinates of : MeOH_N10_56.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	-3.023117	-0.997801	0.451622

1	-2.461655	-0.487428	1.085482
6	-4.147397	-1.515466	1.153671
1	-4.760403	-2.066852	0.438555
1	-4.745679	-0.704253	1.580714
1	-3.837389	-2.195352	1.954373
8	3.031738	0.241947	-2.048514
1	2.952359	-0.619643	-1.581818
6	3.741330	1.113861	-1.172587
1	3.748354	2.107779	-1.623861
1	4.773942	0.777533	-1.036068
1	3.250384	1.176206	-0.193430
8	-1.762434	-2.722258	-1.109999
1	-2.244810	-2.103099	-0.507273
6	-2.006250	-2.330153	-2.452727
1	-1.355136	-2.920171	-3.100310
1	-1.786073	-1.266676	-2.606678
1	-3.048176	-2.518788	-2.732508
8	2.775047	-1.852041	-0.382683
1	1.935653	-2.342214	-0.212996
6	3.834597	-2.451048	0.347183
1	4.742638	-1.878948	0.146613
1	3.995672	-3.489099	0.038288
1	3.635669	-2.425133	1.425230
8	-1.702353	0.573975	2.125866
1	-0.732843	0.539713	2.284613
6	-2.002037	1.882820	1.645274
1	-3.087495	1.959537	1.549199
1	-1.547750	2.065612	0.663329
1	-1.652377	2.644374	2.350493
8	0.931337	1.029747	2.418616
1	1.044583	1.713920	1.719651
6	2.094053	0.214328	2.487315
1	1.952678	-0.495068	3.305027
1	2.983660	0.818475	2.695049
1	2.252718	-0.347437	1.556635
8	0.512721	-3.134479	0.250590
1	-0.228562	-3.055252	-0.392813
6	0.041797	-2.626301	1.493049
1	0.822963	-2.787097	2.238795
1	-0.866782	-3.148312	1.811491
1	-0.171407	-1.550615	1.432582
8	1.125734	2.810355	0.400650
1	0.911375	2.375257	-0.448180
6	0.535104	4.105873	0.452891
1	0.585284	4.446831	1.488475
1	-0.510553	4.074666	0.131095
1	1.087824	4.808058	-0.179262
8	0.530285	1.104648	-1.693303
1	1.424158	0.877231	-2.046101
6	0.141742	0.015857	-0.857389
1	-0.900654	0.168860	-0.559219
1	0.765896	-0.028054	0.043499
1	0.219080	-0.935660	-1.392193
8	-1.756745	2.705645	-1.744631
1	-0.953653	2.200990	-1.954277
6	-2.882710	1.856863	-1.908510
1	-3.776334	2.465668	-1.756199
1	-2.893327	1.039567	-1.174324
1	-2.922918	1.427168	-2.916398

Cartesian coordinates of : MeOH_N10_8r_2_2.log

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

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6 -2.071036 3.425947 1.007964  
8 -2.440229 2.850616 -0.239882  
8 -0.243969 1.654573 -1.111636  
6 -0.493124 0.296377 -0.762514  
8 1.823780 2.233046 0.378885  
6 1.936324 3.606016 0.745660  
8 2.134448 0.252947 2.159241  
6 3.507347 -0.031303 1.888399  
8 1.011703 -1.950583 1.291307  
6 1.497274 -3.012069 2.112325  
8 -4.096046 0.895081 0.401235  
6 -5.453526 1.116901 0.038052  
8 -3.525114 -1.492301 -0.625744  
6 -4.533921 -2.439213 -0.290824  
8 -1.248430 -2.714207 0.027168  
6 -0.624791 -3.312066 -1.105274  
8 2.454001 -1.792058 -1.109075  
6 3.444988 -2.804403 -1.054431  
1 -1.438961 2.743000 1.590198  
1 -2.956407 3.680417 1.598645  
1 -1.510334 4.339945 0.803353  
1 -3.075248 2.110899 -0.057248  
1 -1.279229 -0.133330 -1.393422  
1 -0.789087 0.204072 0.291350  
1 0.432899 -0.264339 -0.923207  
1 -1.061269 2.171396 -0.891893  
1 1.063534 3.932580 1.318642  
1 2.045050 4.235798 -0.143061  
1 2.827870 3.710709 1.366165  
1 1.030807 2.101124 -0.213450  
1 -0.156771 -2.559706 -1.749194  
1 -1.398910 -3.835594 -1.669147  
1 -0.548844 -2.313745 0.584183  
1 4.113864 0.875481 1.974300  
1 3.628743 -0.453035 0.882978  
1 3.850296 -0.756025 2.629102  
1 1.886584 1.015860 1.588121  
1 1.192052 -2.870699 3.152817  
1 2.589192 -3.078742 2.059332  
1 1.067784 -3.944060 1.739375  
1 1.317237 -1.080218 1.668013  
1 -6.118756 0.437554 0.581231  
1 -5.604040 0.984051 -1.038781  
1 -5.707536 2.144463 0.305261  
1 -3.821417 0.010765 0.052747  
1 -4.632211 -2.549879 0.794720  
1 -4.312683 -3.415967 -0.732318  
1 -5.479905 -2.076739 -0.697586  
1 -2.652666 -1.866467 -0.356363  
1 4.032348 -2.744230 -1.972566  
1 4.121805 -2.665297 -0.201292  
1 2.999634 -3.805149 -0.990781  
1 1.906724 -1.866889 -0.306081  
1 0.136334 -4.035748 -0.793654  
6 3.100618 1.716756 -2.547210  
1 3.743802 1.617311 -3.423922  
1 2.530011 2.649847 -2.636396  
1 2.397179 0.875445 -2.530056  
8 3.933528 1.722309 -1.398834  
1 3.340234 1.822100 -0.634323  
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Cartesian coordinates of : MeOH_N10_8r_2_3.log

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Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	0.868603	2.847521	0.712335
8	1.616736	2.620155	-0.480135
8	3.507049	0.895006	-0.040975
6	4.792395	1.455531	-0.297041
8	3.040809	-1.633394	-0.819350
6	3.860310	-2.351911	0.099646
8	0.558952	-2.484026	-0.656012
6	0.182091	-3.095786	-1.882425
8	-1.381554	-1.551790	0.756392
6	-1.664628	-2.557182	1.726603
8	-0.259387	1.755019	-2.154542
6	-0.226165	0.384505	-1.773924
8	-2.507583	2.423002	-0.863613
6	-2.705117	3.768703	-0.445625
8	-2.162333	0.975094	1.391687
6	-3.436365	0.684971	1.965052
8	-3.530371	-1.189002	-1.019665
6	-4.316100	-2.311171	-0.654665
1	-0.074774	2.287406	0.700809
1	0.651356	3.913373	0.831310
1	1.464722	2.506107	1.563518
1	0.983477	2.419233	-1.211254
1	4.944264	2.361308	0.297245
1	4.909927	1.693035	-1.358371
1	5.541129	0.714294	-0.012693
1	2.796478	1.558351	-0.272272
1	3.725530	-1.981210	1.122271
1	4.915781	-2.272025	-0.178067
1	3.562147	-3.401274	0.059919
1	3.185480	-0.672187	-0.664383
1	-4.009322	0.008066	1.321013
1	-3.978107	1.627815	2.058591
1	-1.717138	0.119373	1.217732
1	0.711862	-4.042883	-2.024157
1	0.385566	-2.438300	-2.734219
1	-0.891977	-3.292706	-1.839012
1	1.484088	-2.128597	-0.714507
1	-0.847566	-2.640370	2.450810
1	-1.822105	-3.527239	1.244438
1	-2.577427	-2.270429	2.253083
1	-0.591137	-1.843619	0.217628
1	-0.961541	-0.204636	-2.332951
1	-0.425584	0.269752	-0.700259
1	0.774832	-0.002265	-1.982273
1	-1.111741	2.120218	-1.818011
1	-1.886844	4.111820	0.197081
1	-3.652292	3.875620	0.092765
1	-2.736618	4.393103	-1.339756
1	-2.412461	1.858065	-0.062276
1	-5.208868	-2.310985	-1.282878
1	-3.777766	-3.253526	-0.815122
1	-4.632352	-2.262551	0.395745
1	-2.722132	-1.220319	-0.477617
1	-3.324013	0.242679	2.959855
6	1.330287	-0.470157	1.847855
1	0.493601	-0.291259	2.529824
1	1.419203	-1.552980	1.680187
1	1.097968	0.005551	0.885023
8	2.508668	0.068396	2.419762
1	3.074619	0.366353	1.685956

Cartesian coordinates of : MeOH_N10_8r_2_4.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	4.007692	2.392748	0.345973
8	3.066043	1.953062	-0.625699
8	3.189235	-0.637743	-0.651347
6	4.136370	-0.881414	-1.689975
8	1.438505	-2.698469	-0.651822
6	2.296817	-3.661875	-0.049197
8	-1.061669	-2.965265	0.194494
6	-1.610431	-3.840701	-0.784953
8	-2.909476	-1.196746	0.668179
6	-3.592601	-1.747239	1.793161
8	1.119914	3.719583	-0.386265
6	1.165180	4.697593	-1.416958
8	-1.485842	3.556864	0.122327
6	-1.784948	4.488404	1.154828
8	-3.020121	1.501630	0.874381
6	-4.354742	1.657305	0.404807
8	-4.603682	-1.320338	-1.568382
6	-5.831753	-1.635326	-0.935917
1	3.580525	2.369305	1.353854
1	4.351732	3.407582	0.122851
1	4.864135	1.714808	0.311379
1	2.261575	2.526177	-0.563897
1	5.046934	-0.294304	-1.532110
1	3.713738	-0.636402	-2.668897
1	4.392331	-1.943034	-1.668569
1	2.995516	0.340516	-0.636711
1	2.776616	-3.256925	0.848352
1	3.066440	-3.994077	-0.754664
1	1.686459	-4.522822	0.231742
1	1.925118	-1.848246	-0.700227
1	-4.515847	1.098467	-0.523340
1	-4.519850	2.719673	0.212097
1	-2.793849	0.549081	0.828056
1	-1.090241	-4.803648	-0.781379
1	-1.553684	-3.402514	-1.786704
1	-2.660278	-4.006918	-0.532078
1	-0.130778	-2.757166	-0.062664
1	-2.955271	-1.732924	2.682185
1	-3.909362	-2.775789	1.591526
1	-4.477687	-1.135188	1.980447
1	-2.113447	-1.767194	0.482111
1	0.707301	5.635715	-1.086267
1	0.655868	4.348854	-2.321402
1	2.215025	4.884075	-1.652538
1	0.173931	3.531608	-0.176106
1	-1.494782	4.101825	2.137400
1	-2.852375	4.732120	1.165769
1	-1.219712	5.400845	0.953784
1	-1.963229	2.718893	0.321687
1	-6.599553	-1.694945	-1.709738
1	-5.786513	-2.601033	-0.417112
1	-6.128304	-0.862571	-0.214321
1	-3.924208	-1.263030	-0.872192
1	-5.076220	1.323303	1.159018
6	5.507831	-1.976627	1.366912
1	6.063628	-2.307276	2.246457
1	6.137910	-1.279897	0.799997
1	5.301562	-2.853781	0.739154
8	4.314236	-1.359247	1.815906
1	3.835226	-1.047017	1.026790

Cartesian coordinates of : MeOH_N10_8r_2.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
6	4.507719	-0.645201	-1.257011
8	3.366238	-0.412107	-0.433833
8	2.617792	2.167549	-0.770753
6	3.621183	2.748514	0.055702
8	0.324797	3.509430	-0.531076
6	0.498149	4.529786	-1.506416
8	-2.199079	2.732303	-0.423302
6	-2.687971	3.414820	0.725691
8	-3.366239	0.412102	-0.433844
6	-4.507722	0.645206	-1.257016
8	2.199089	-2.732311	-0.423313
6	2.687976	-3.414825	0.725684
8	-0.324795	-3.509433	-0.531069
6	-0.498158	-4.529801	-1.506395
8	-2.617800	-2.167555	-0.770755
6	-3.621194	-2.748509	0.055703
8	-4.204558	0.028862	2.218366
6	-5.603138	-0.091604	2.026927
1	4.211284	-0.815069	-2.296299
1	5.077668	-1.508504	-0.898025
1	5.142872	0.242082	-1.209066
1	2.797500	-1.230830	-0.457492
1	4.598717	2.721051	-0.438637
1	3.687284	2.232497	1.019559
1	3.348311	3.791701	0.229813
1	2.723993	1.193678	-0.733507
1	0.591188	4.108479	-2.512789
1	1.384234	5.134332	-1.286778
1	-0.382822	5.174039	-1.473123
1	1.102465	2.905566	-0.574029
1	-3.687302	-2.232478	1.019553
1	-3.348322	-3.791693	0.229832
1	-2.723996	-1.193683	-0.733517
1	-2.595568	4.498518	0.603051
1	-2.153006	3.106290	1.629849
1	-3.745024	3.162185	0.838999
1	-1.230141	2.915039	-0.505873
1	-4.211293	0.815048	-2.296311
1	-5.077647	1.508530	-0.898042
1	-5.142895	-0.242061	-1.209047
1	-2.797498	1.230821	-0.457501
1	2.595576	-4.498523	0.603045
1	2.153006	-3.106294	1.629839
1	3.745029	-3.162187	0.838996
1	1.230151	-2.915043	-0.505885
1	-0.591211	-4.108505	-2.512772
1	-1.384240	-5.134344	-1.286739
1	0.382814	-5.174052	-1.473106
1	-1.102462	-2.905570	-0.574020
1	-6.060139	-0.259187	3.004138
1	-6.034740	0.819418	1.593833
1	-5.853738	-0.941529	1.378319
1	-3.803419	0.182278	1.343557
1	-4.598726	-2.721053	-0.438641
6	5.603146	0.091624	2.026919
1	6.060146	0.259222	3.004128
1	5.853737	0.941545	1.378303
1	6.034756	-0.819398	1.593835
8	4.204568	-0.028853	2.218362

1 3.803426 -0.182281 1.343555

Cartesian coordinates of : MeOH_N10_91.log

Atomic number (AN) and Cartesian coordinates

AN	X	Y	Z
8	1.087311	1.183351	2.315943
1	0.700842	0.309020	2.542982
6	0.006209	2.100015	2.166444
1	0.417267	3.053668	1.829713
1	-0.510290	2.250839	3.120983
1	-0.712641	1.747983	1.416454
8	0.831659	-1.159588	-1.299031
1	1.789129	-1.078304	-1.524249
6	0.359466	0.173988	-1.075323
1	-0.728244	0.177740	-1.195741
1	0.797409	0.863727	-1.801786
1	0.609487	0.514518	-0.063525
8	-0.578045	3.036626	-0.956763
1	-1.331036	2.533822	-0.589281
6	-0.801009	3.210054	-2.343532
1	0.107671	3.635627	-2.776877
1	-1.634492	3.895494	-2.540545
1	-1.008296	2.256023	-2.845583
8	-2.729050	1.619594	-0.013221
1	-2.947065	0.666332	-0.137786
6	-3.484055	2.151681	1.063288
1	-3.209008	3.203235	1.173264
1	-3.263883	1.635125	2.005138
1	-4.559412	2.087848	0.865426
8	1.364243	-2.531446	1.034178
1	1.082911	-2.097300	0.201766
6	2.749874	-2.250053	1.213573
1	3.055310	-2.687373	2.164956
1	2.936881	-1.169284	1.239546
1	3.343555	-2.695618	0.408899
8	-0.226142	-1.173613	2.731287
1	0.395931	-1.789623	2.285018
6	-1.388407	-1.123002	1.910663
1	-2.041144	-0.334973	2.292065
1	-1.933774	-2.072661	1.932249
1	-1.128835	-0.885615	0.870643
8	-3.407509	-0.949209	-0.388562
1	-2.687399	-1.510275	-0.758761
6	-4.529324	-1.028801	-1.261522
1	-5.323039	-0.410590	-0.838286
1	-4.888675	-2.059635	-1.340536
1	-4.283280	-0.655070	-2.261165
8	3.324674	-0.305263	-1.513438
1	3.278057	0.335643	-0.763038
6	4.635263	-0.843520	-1.604358
1	4.613439	-1.656932	-2.331438
1	4.972652	-1.240459	-0.640447
1	5.346762	-0.083842	-1.944409
8	-1.529512	-2.554877	-1.452637
1	-0.642844	-2.178108	-1.606027
6	-1.399773	-3.767394	-0.713705
1	-2.401907	-4.065649	-0.400038
1	-0.774997	-3.628185	0.175118
1	-0.971141	-4.558265	-1.336293
8	3.082918	1.475026	0.471604
1	2.417085	1.284240	1.168123
6	2.742800	2.729902	-0.119883

1	3.380056	2.862300	-0.997177
1	2.935577	3.550223	0.579924
1	1.690739	2.752328	-0.428028
