5-Exo-dig radical cyclization of enediynes: the first synthesis of tin-substituted benzofulvenes

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SUPPORTING INFORMATION. COMPUTATIONAL RESULTS.

Optimized Geometries Computed at the UB3LYP/3-21G* Level

Total energy = -842.59138

6	1.074951	0.000851	-3.839078
6	1.177212	0.010072	-2.432168
6	2.466124	0.041192	-1.831053
6	3.594906	0.061080	-2.666496
6	3.477692	0.051520	-4.053553
6	2.210126	0.021350	-4.642630
1	0.087966	-0.022928	-4.284084
1	4.578604	0.084714	-2.209421
1	4.367289	0.067535	-4.672032
1	2.108670	0.013732	-5.721309
6	2.675007	0.054213	-0.371378
6	1.758033	0.043511	0.567283
6	-0.013177	-0.012330	-1.656700
6	-1.081316	-0.033241	-1.076509
1	3.730616	0.075820	-0.075616
6	1.263273	0.044078	1.863983
6	0.979143	-1.181416	2.544058
6	0.425587	-1.169290	3.815703
6	0.124077	0.043014	4.454285
6	0.385292	1.255692	3.798880
6	0.938616	1.268626	2.527333
1	1.204837	-2.116076	2.045894
1	0.222391	-2.107816	4.318961
1	-0.309108	0.042698	5.447242
1	0.150453	2.193749	4.288991
1	1.132834	2.203224	2.016088
6	-2.303471	-0.058211	-0.347588
6	-3.543670	-0.049227	-1.019230
6	-4.733372	-0.073408	-0.295781
6	-4.707855	-0.106650	1.101852
6	-3.482478	-0.115850	1.774813
6	-2.286086	-0.092039	1.062812
1	-3.557351	-0.023104	-2.101833
1	-5.681591	-0.066215	-0.820780
1	-5.636019	-0.125296	1.661192
1	-3.456389	-0.141513	2.857911
1	-1.334893	-0.099743	1.575759

Total energy = -842.59261

6	2.421824	-3.128415	0.407883
6	1.730504	-1.966687	0.031339
6	2.489754	-0.776911	-0.338082
6	3.925268	-0.853054	-0.275458
6	4.559942	-2.017067	0.103583
6	3.813876	-3.164395	0.444867
1	1.845556	-4.005322	0.676600
1	4.493192	0.029794	-0.540992
1	5.642699	-2.051485	0.138077
1	4.323136	-4.073485	0.740141
6	1.861312	0.371216	-0.722949
6	1.260007	1.422258	-1.216377
1	1.105324	1.487962	-2.298697
6	0.319588	-1.923704	0.018891
6	-0.892529	-1.830290	0.006710
6	0.730766	2.574327	-0.445687
6	0.149870	3.653900	-1.130669
6	-0.358791	4.749206	-0.431640
6	-0.295802	4.780514	0.962692
6	0.278495	3.707933	1.654431
6	0.786721	2.614651	0.958811
1	0.100985	3.631445	-2.214540
1	-0.802781	5.575811	-0.974461
1	-0.690771	5.630192	1.507232
1	0.326448	3.726042	2.737219
1	1.228190	1.779624	1.490920
6	-2.303980	-1.669499	-0.011845
6	-3.164968	-2.773438	0.160694
6	-4.545939	-2.596307	0.137056
6	-5.091124	-1.323545	-0.057334
6	-4.245386	-0.222816	-0.227439
6	-2.863212	-0.387460	-0.205888
1	-2.737585	-3.757246	0.309643
1	-5.199275	-3.450854	0.269840
1	-6.166460	-1.190328	-0.074927
1	-4.665205	0.765372	-0.375325
1	-2.200625	0.459977	-0.332263

Total energy = -842.63573

6	-2.583463	0.254864	-0.721994
6	-2.771826	0.235678	0.731929
6	-1.499763	0.089195	1.342582
6	-0.479468	0.017532	0.247840
6	0.821269	-0.093936	0.399799
6	-1.261426	0.131228	-1.036172
6	-3.918157	0.326400	1.519046
6	-3.782624	0.274464	2.912998
6	-2.524473	0.133131	3.508567
6	-1.366474	0.038444	2.721439

1	-4.896479	0.436843	1.065039
1	-4.664847	0.345157	3.538862
1	-2.443006	0.095667	4.588581
1	-0.390505	-0.072553	3.179980
1	-3.392242	0.327880	-1.434975
6	2.019016	-0.214381	1.085827
6	2.553654	-1.500728	1.414982
6	3.771803	-1.608266	2.067565
6	4.504692	-0.461969	2.409057
6	4.001194	0.807353	2.087326
6	2.786068	0.942377	1.434539
1	1.984028	-2.383784	1.152989
1	4.159493	-2.589252	2.317430
1	5.456495	-0.556557	2.917460
1	4.567233	1.693390	2.351045
1	2.395787	1.920105	1.181605
6	-0.674001	0.122815	-2.383154
6	0.490397	-0.612254	-2.673023
6	1.023705	-0.622765	-3.961451
6	0.406035	0.096219	-4.987192
6	-0.750136	0.832401	-4.712864
6	-1.281937	0.849853	-3.425558
1	0.965792	-1.184380	-1.886553
1	1.919581	-1.197895	-4.165734
1	0.822402	0.087235	-5.987731
1	-1.229459	1.402943	-5.500252
1	-2.158789	1.449264	-3.210266

Total energy = -1664.04333

6	1.710097	0.000550	-4.089933
6	1.811936	0.000526	-2.682873
6	3.095943	0.000386	-2.077335
6	4.228749	0.000216	-2.905181
6	4.114162	0.000191	-4.293016
6	2.849176	0.000374	-4.887810
1	0.723396	0.000701	-4.535766
1	5.210770	0.000099	-2.445370
1	5.005777	0.000048	-4.908147
1	2.752113	0.000387	-5.966468
6	3.297878	0.000439	-0.617345
6	2.380516	0.000288	0.312539
6	0.604011	0.000663	-1.935501
6	-0.512708	0.000533	-1.460235
1	4.350189	0.000611	-0.312781
6	1.748781	0.000175	1.530846
6	1.380415	-1.209270	2.174074
6	0.689397	-1.145110	3.368641
7	0.364583	-0.000091	3.941928
6	0.688850	1.145048	3.368583
6	1.379844	1.209477	2.174009
6	-1.836809	0.000108	-0.981480

6	-2.907035	0.000146	-1.887895
6	-4.202970	-0.000347	-1.391373
7	-4.458241	-0.000845	-0.098411
6	-3.472416	-0.000881	0.776184
6	-2.140275	-0.000430	0.384743
9	0.329208	2.296779	3.993190
9	0.330340	-2.296973	3.993338
9	1.705095	-2.396355	1.600016
9	1.703980	2.396687	1.599905
9	-1.138307	-0.000529	1.305962
9	-3.779717	-0.001435	2.095940
9	-5.247857	-0.000351	-2.255872
9	-2.661841	0.000645	-3.222916

Total energy = -1664.04907

6	1.077566	4.545647	0.138538
6	0.529009	3.278650	-0.103696
6	-0.886801	3.162046	-0.434122
6	-1.659135	4.367604	-0.505539
6	-1.075424	5.595468	-0.266391
6	0.292128	5.693587	0.061325
1	2.130510	4.617003	0.381357
1	-2.711400	4.289684	-0.747138
1	-1.676725	6.494738	-0.327158
1	0.734526	6.663273	0.251493
6	-1.443676	1.927367	-0.609699
6	-1.733063	0.727312	-1.042989
1	-1.500317	0.447567	-2.071384
6	1.311021	2.106256	-0.073113
6	1.891095	1.040691	-0.092063
6	-2.338559	-0.347394	-0.251412
6	-2.410857	-1.629030	-0.799989
6	-2.980333	-2.649268	-0.050746
7	-3.451650	-2.443830	1.163413
6	-3.391282	-1.243134	1.703307
6	-2.839598	-0.155601	1.036606
6	2.492766	-0.227380	-0.147278
6	3.827433	-0.424354	0.230023
6	4.360826	-1.703529	0.150611
7	3.653482	-2.734802	-0.265793
6	2.395112	-2.578266	-0.627302
6	1.765282	-1.342984	-0.588618
9	-1.933604	-1.849437	-2.057055
9	-3.059787	-3.900085	-0.570501
9	-2.786873	1.073853	1.617940
9	-3.888912	-1.074241	2.955191
9	1.704936	-3.666847	-1.049730
9	0.465732	-1.201862	-0.973446
9	4.569813	0.626375	0.662637
9	5.651974	-1.910418	0.511051

Total energy = -1664.08994

6	-2.411840	2.024469	-0.198118
6	-1.584177	3.226302	-0.274978
6	-0.223472	2.833710	-0.261816
6	-0.183713	1.340760	-0.170097
6	0.882149	0.601504	-0.027758
6	-1.630829	0.903890	-0.168821
6	-1.927911	4.574278	-0.346077
6	-0.899442	5.523225	-0.406050
6	0.443165	5.129083	-0.391878

6	0.794139	3.772519	-0.317216
1	-2.966352	4.883973	-0.354150
1	-1.146051	6.576621	-0.463653
1	1.222359	5.880174	-0.440045
1	1.834421	3.469917	-0.306242
1	-3.488769	2.028042	-0.171900
6	2.025195	-0.128863	0.119988
6	2.625602	-0.323784	1.394466
6	3.771735	-1.089944	1.481877
7	4.333880	-1.651876	0.424925
6	3.801645	-1.494952	-0.775789
6	2.656547	-0.752042	-0.992004
6	-2.107691	-0.474643	-0.108410
6	-3.328710	-0.779914	0.511664
6	-3.763262	-2.096473	0.562035
7	-3.068551	-3.087071	0.039273
6	-1.925863	-2.833091	-0.563315
6	-1.406178	-1.548472	-0.670363
9	4.415650	-2.093105	-1.828364
9	2.127375	-0.597315	-2.229833
9	4.355118	-1.280535	2.693019
9	2.059041	0.247751	2.487722
9	-0.232899	-1.355269	-1.341910
9	-1.240831	-3.869940	-1.107163
9	-4.940592	-2.386486	1.170475
9	-4.093466	0.211403	1.056340

Total energy = -1070.38341

6	2.098042	0.106456	-4.376824
6	2.081178	0.097372	-2.965880
6	3.316167	0.095441	-2.258894
6	4.510933	0.105390	-2.997412
6	4.511070	0.115077	-4.389353
6	3.296714	0.114838	-5.082357
1	1.151652	0.108040	-4.903395
1	5.452837	0.104235	-2.458730
1	5.449508	0.122294	-4.931169
1	3.285626	0.122060	-6.165884
6	3.402114	0.077689	-0.786658
6	2.405142	0.056372	0.067529
6	0.829695	0.092769	-2.293563
6	-0.283533	0.095749	-1.803862
1	4.430302	0.079538	-0.404667
6	1.813452	0.022032	1.321387
6	1.464111	-1.213886	1.942433
6	0.802733	-1.245123	3.161575
6	0.452106	-0.053629	3.812887
6	0.779620	1.178838	3.213163
6	1.435637	1.225795	2.001135
1	1.722018	-2.138060	1.440672
1	0.558247	-2.203184	3.600483
1	0.496203	2.083637	3.735073
1	1.675571	2.177757	1.544247
6	-1.556353	0.104771	-1.172270
6	-2.741029	-0.019404	-1.920144
6	-3.986948	-0.008707	-1.297260
6	-4.075425	0.127856	0.092489
6	-2.898057	0.253762	0.847721
6	-1.658627	0.242183	0.232509
1	-2.677407	-0.124752	-2.996200
1	-4.878596	-0.106672	-1.901393
1	-2.990389	0.361065	1.920288
1	-0.755025	0.340393	0.817586
8	-0.211307	0.024791	5.023707
8	-5.257207	0.150023	0.811568
6	-0.585806	-1.221887	5.686425
1	-1.270772	-1.815427	5.069211

1	0.294922	-1.826461	5.933987
1	-1.089288	-0.912793	6.602428
6	-6.512441	0.024462	0.076905
1	-6.645981	0.845576	-0.637703
1	-6.574004	-0.931923	-0.456393
1	-7.290283	0.070861	0.839270

Total energy = -1070.38416

6	1.083002	0.769943	-4.607135
6	1.060869	0.791285	-3.203795
6	2.325130	0.810400	-2.473936
6	3.541005	0.783002	-3.243261
6	3.511830	0.758664	-4.621628
6	2.283009	0.755622	-5.314252
1	0.137687	0.759481	-5.136012
1	4.481355	0.788378	-2.706266
1	4.441617	0.743558	-5.178563
1	2.271709	0.737179	-6.397172
6	2.352445	0.847234	-1.110383
6	2.359416	1.020462	0.186189
1	2.385903	2.040944	0.584196
6	-0.153821	0.780239	-2.485840
6	-1.166320	0.753288	-1.812430
6	2.320209	-0.040111	1.218468
6	2.364538	0.305244	2.575004
6	2.328884	-0.669189	3.574111
6	2.247230	-2.020015	3.227628
6	2.197742	-2.377797	1.869009
6	2.232710	-1.406973	0.883738
1	2.430010	1.351423	2.855971
1	2.365817	-0.364058	4.611028
1	2.129921	-3.429753	1.624906
1	2.190110	-1.689838	-0.161782
6	-2.311725	0.707341	-0.976961
6	-3.608578	0.888354	-1.491286
6	-4.723365	0.841326	-0.657710
6	-4.566683	0.609621	0.713407
6	-3.276026	0.425841	1.237322
6	-2.166797	0.473366	0.412173
1	-3.735036	1.068250	-2.551708
1	-5.706248	0.986315	-1.084920
1	-3.181418	0.245121	2.299784
1	-1.173657	0.327035	0.818563
8	-5.601490	0.543379	1.628081
8	2.207425	-3.070834	4.128343
6	2.268037	-2.755398	5.551791
1	2.234916	-3.721339	6.056112
1	3.198084	-2.234750	5.810923
1	1.413176	-2.144715	5.867107
6	-6.967275	0.704014	1.137044
1	-7.123166	1.695735	0.695606
1	-7.223109	-0.065022	0.398282
1	-7.597949	0.591112	2.018940

Total energy = -1070.42780

6	-3.201546	-0.186871	0.039418
6	-3.156655	-0.190819	1.504448
6	-1.796056	-0.168290	1.907014
6	-0.958189	-0.141536	0.665625
6	0.355814	-0.078164	0.608623
6	-1.938656	-0.156543	-0.479094

6	-4.167459	-0.219533	2.463686
6	-3.810306	-0.221269	3.818988
6	-2.466829	-0.196673	4.208765
6	-1.444059	-0.170553	3.247792
1	-5.211151	-0.238889	2.170268
1	-4.586070	-0.242271	4.576005
1	-2.212944	-0.198790	5.262407
1	-0.401964	-0.152899	3.545920
1	-4.114495	-0.233425	-0.536955
6	1.615992	-0.040810	1.191474
6	2.328777	-1.245885	1.497748
6	3.599432	-1.198756	2.027791
6	4.236884	0.033997	2.274002
6	3.562153	1.226371	1.973154
6	2.282660	1.195610	1.438982
1	1.846665	-2.197644	1.313009
1	4.142014	-2.102921	2.270956
1	4.031542	2.184048	2.153992
1	1.768414	2.119286	1.205111
6	-1.571732	-0.123090	-1.899583
6	-0.372197	-0.696867	-2.371376
6	-0.048843	-0.672857	-3.719071
6	-0.910414	-0.074397	-4.650114
6	-2.101974	0.502956	-4.199923
6	-2.420586	0.478923	-2.843418
1	0.299693	-1.172033	-1.668453
1	0.867047	-1.116300	-4.086975
1	-2.779896	0.984078	-4.891955
1	-3.331850	0.958246	-2.505132
8	-0.491130	-0.102685	-5.970240
8	5.508750	-0.045464	2.804128
6	-1.355175	0.506423	-6.975682
1	-2.335344	0.015834	-7.018061
1	-1.496985	1.578380	-6.791224
1	-0.831881	0.363062	-7.921323
6	6.227796	1.198400	3.072506
1	6.382594	1.778416	2.155148
1	5.700751	1.816352	3.809014
1	7.189897	0.884055	3.476617

Total energy = -1039.98990

6	1.689687	-0.002785	-4.102782
6	1.684427	-0.003899	-2.692213
6	2.923851	-0.005048	-1.994188
6	4.113520	-0.005984	-2.740430
6	4.102575	-0.005052	-4.132441
6	2.883454	-0.003237	-4.816775
1	0.739649	-0.001969	-4.622523
1	5.059626	-0.007056	-2.209441
1	5.036946	-0.005601	-4.681051
1	2.864740	-0.002443	-5.900038
6	3.019523	-0.004511	-0.522872
6	2.031089	0.002212	0.340659
6	0.438471	-0.004575	-2.009270
6	-0.669577	-0.006479	-1.509221
1	4.049154	-0.009718	-0.145901
6	1.454524	0.008286	1.603854
6	1.096325	-1.211623	2.258280
6	0.462430	-1.194967	3.489470
6	0.157958	0.021407	4.100008
6	0.481330	1.231337	3.486355
6	1.115402	1.235072	2.255462
1	1.330406	-2.150868	1.773984
1	0.195577	-2.115618	3.991303
1	0.228103	2.157218	3.985532
1	1.363332	2.169295	1.768518
6	-1.939047	-0.008962	-0.868796

6	-3.130776	0.034840	-1.621794
6	-4.367053	0.032569	-0.986406
6	-4.424908	-0.013139	0.402196
6	-3.264690	-0.057162	1.167209
6	-2.025195	-0.055333	0.539151
1	-3.073241	0.070643	-2.702062
1	-5.287779	0.065964	-1.552930
1	-3.341787	-0.092378	2.245412
1	-1.114525	-0.090324	1.119434
9	-0.472879	0.027746	5.314729
9	-5.643802	-0.014962	1.024940

Total energy = -1039.99133

6	0.772736	0.721909	-4.227900
6	0.770824	0.724845	-2.824520
6	2.044190	0.726107	-2.112684
6	3.249884	0.709463	-2.897973
6	3.201246	0.703856	-4.275874
6	1.963019	0.711778	-4.951425
1	-0.179702	0.724791	-4.743688
1	4.197623	0.705343	-2.374340
1	4.123056	0.694203	-4.845772
1	1.936818	0.707728	-6.034105
6	2.093414	0.730777	-0.749323
6	2.133149	0.870603	0.550238
1	2.162773	1.879020	0.976775
6	-0.436349	0.719669	-2.093060
6	-1.448632	0.698921	-1.420132
6	2.135184	-0.222781	1.550866
6	2.197973	0.088798	2.918730
6	2.203873	-0.917550	3.881769
6	2.145951	-2.245502	3.480611
6	2.080563	-2.581503	2.131381
6	2.074587	-1.576082	1.172797
1	2.245598	1.127193	3.228111
1	2.253634	-0.684212	4.936790
1	2.033462	-3.624864	1.849602
1	2.020599	-1.826928	0.120007
6	-2.602433	0.665427	-0.594190
6	-3.897810	0.775106	-1.142032
6	-5.017313	0.740913	-0.319346
6	-4.856535	0.596383	1.054380
6	-3.590995	0.484044	1.620355
6	-2.467448	0.518467	0.804012
1	-4.011376	0.887765	-2.212475
1	-6.015065	0.824747	-0.728402
1	-3.500033	0.368950	2.691981
1	-1.476331	0.427768	1.229769
9	-5.960791	0.563805	1.861776
9	2.151289	-3.238625	4.423299

Total energy = -1040.03421

6	-2.963322	-0.027355	-0.194474
6	-2.950951	-0.029848	1.271862
6	-1.600050	-0.037088	1.704817
6	-0.734510	-0.032507	0.481618
6	0.579876	0.001156	0.451900
6	-1.689931	-0.028581	-0.684212
6	-3.984111	-0.034078	2.206595
6	-3.657930	-0.041408	3.569697
6	-2.323547	-0.045859	3.989825

6	-1.278297	-0.044195	3.053087
1	-5.020747	-0.030389	1.889169
1	-4.450741	-0.043576	4.308843
1	-2.093989	-0.051396	5.048868
1	-0.243713	-0.048943	3.376565
1	-3.864213	-0.052605	-0.790849
6	1.848310	0.020291	1.015616
6	2.544892	-1.193836	1.310329
6	3.827781	-1.163026	1.828584
6	4.455693	0.060343	2.060588
6	3.810640	1.263981	1.777094
6	2.528140	1.255175	1.257647
1	2.048417	-2.138508	1.129269
1	4.357130	-2.077353	2.061266
1	4.327660	2.194653	1.969027
1	2.020029	2.183304	1.030771
6	-1.290147	-0.013850	-2.097072
6	-0.105031	-0.634586	-2.534184
6	0.251676	-0.628667	-3.879479
6	-0.572481	-0.003146	-4.806057
6	-1.747563	0.621707	-4.404916
6	-2.100438	0.619349	-3.059901
1	0.529956	-1.133609	-1.814230
1	1.159382	-1.109310	-4.218801
1	-2.364766	1.113007	-5.145062
1	-2.998985	1.133280	-2.741156
9	5.723481	0.079889	2.571958
9	-0.221203	0.003530	-6.130036

Total energy = -843.30179

6	-2.514209	-0.116889	-0.662451
6	-2.539105	-0.118482	0.803213
6	-1.195578	-0.067041	1.277263
6	-0.305898	-0.014377	0.080351
6	1.030635	0.155802	-0.035861
6	-1.227599	-0.048101	-1.102578
6	-3.610286	-0.129497	1.692063
6	-3.347877	-0.069436	3.066442
6	-2.033934	0.013897	3.535399
6	-0.949990	0.019123	2.645066
1	-4.630661	-0.170054	1.327623
1	-4.171122	-0.076888	3.771623
1	-1.846621	0.075974	4.601121
1	0.060805	0.088646	3.022166
1	-3.391154	-0.189344	-1.289660
6	2.058570	0.115843	1.017380
6	2.080642	-0.897890	1.993383
6	3.093097	-0.937210	2.951622
6	4.104231	0.027548	2.948396
6	4.106715	1.025192	1.969516
6	3.101170	1.061819	1.005163
1	1.310771	-1.659786	1.979582
1	3.100442	-1.727475	3.693531
1	4.889991	-0.005312	3.693999
1	4.893951	1.770024	1.955827
1	3.106625	1.833179	0.242844
6	-0.792798	-0.027433	-2.511663
6	0.199520	-0.906462	-2.985351
6	0.584886	-0.885039	-4.326150
6	-0.014337	0.008175	-5.217627
6	-1.004931	0.881213	-4.760185
6	-1.389120	0.866084	-3.419821
1	0.645346	-1.619620	-2.302646
1	1.345611	-1.572940	-4.677330
1	0.286988	0.023312	-6.258581
1	-1.471267	1.579389	-5.445942
1	-2.140340	1.558099	-3.057556

1 1.407808 0.351764 -1.038011

Total energy = -843.29788

6 -2.400519 0.572691 0.496330
 6 -2.411746 0.330889 1.939648
 6 -1.129289 -0.157262 2.303785
 6 -0.273706 -0.168230 1.078474
 6 1.043690 -0.485068 1.129071
 6 -1.173606 0.279260 -0.030631
 6 -3.414408 0.479128 2.894667
 6 -3.132935 0.135776 4.223434
 6 -1.868778 -0.341432 4.584762
 6 -0.854943 -0.484233 3.625755
 1 -4.393577 0.853837 2.618466
 1 -3.901854 0.241883 4.979956
 1 -1.669059 -0.604150 5.617080
 1 0.121695 -0.849828 3.923959
 1 -3.264362 0.871247 -0.080500
 6 2.119768 -0.370903 0.139003
 6 2.160724 0.633864 -0.846257
 6 3.242519 0.724976 -1.719294
 6 4.304502 -0.179049 -1.628893
 6 4.286795 -1.171835 -0.645078
 6 3.212689 -1.257940 0.236632
 1 1.349124 1.343349 -0.916775
 1 3.258316 1.506344 -2.469922
 1 5.143604 -0.103164 -2.310640
 1 5.111683 -1.869916 -0.561596
 1 3.205165 -2.021671 1.007384
 6 -0.902121 0.273273 -1.483370
 6 -0.329236 -0.847854 -2.108371
 6 -0.137887 -0.867951 -3.488542
 6 -0.512285 0.229242 -4.269664
 6 -1.082220 1.348862 -3.659412
 6 -1.276270 1.371430 -2.277296
 1 -0.040690 -1.699870 -1.505911
 1 0.302249 -1.740993 -3.956484
 1 -0.359977 0.211549 -5.342605
 1 -1.371579 2.205484 -4.257639
 1 -1.705049 2.245050 -1.799471
 1 1.389881 -0.874955 2.086176

Total energy = -1664.75705

6 1.461686 2.459062 0.305627
 6 0.139316 3.074187 0.286861
 6 -0.820332 2.056821 0.038518
 6 -0.087779 0.769795 -0.120509
 6 -0.561070 -0.480733 -0.322720
 6 1.369986 1.129111 0.007473
 6 -0.238004 4.405215 0.429054
 6 -1.593751 4.732650 0.300931
 6 -2.537805 3.742550 0.016682
 6 -2.158657 2.398905 -0.120495
 1 0.500908 5.174472 0.620644
 1 -1.911194 5.762975 0.407494
 1 -3.579789 4.014016 -0.102875
 1 -2.903583 1.659171 -0.373871
 1 2.374523 2.985318 0.531332
 6 -1.927320 -0.980943 -0.210486
 6 -2.319693 -2.009095 -1.078187
 6 -3.581973 -2.568006 -0.946712
 7 -4.427505 -2.166801 -0.016890
 6 -4.078126 -1.219085 0.827479
 6 -2.834072 -0.596825 0.781643

6 2.528665 0.226537 0.004159
 6 3.563936 0.410853 0.934397
 6 4.659435 -0.441975 0.919260
 7 4.774165 -1.428552 0.052983
 6 3.827290 -1.620346 -0.841308
 6 2.696101 -0.816426 -0.910435
 1 0.136700 -1.238385 -0.648378
 9 3.975685 -2.634538 -1.729779
 9 1.756146 -1.063500 -1.873634
 9 -4.969409 -0.845084 1.780361
 9 -3.973486 -3.554008 -1.791413
 9 -1.446531 -2.447963 -2.026858
 9 5.651378 -0.266127 1.827838
 9 3.510046 1.426337 1.843545
 9 -2.513962 0.360038 1.692787

Total energy = -1664.75582

6 -2.720806 -0.689992 1.040007
 6 -2.767898 -0.409231 2.473730
 6 -1.528943 0.173707 2.841778
 6 -0.658783 0.205852 1.629420
 6 0.643141 0.556595 1.682955
 6 -1.516839 -0.304717 0.517182
 6 -3.768827 -0.613803 3.418007
 6 -3.527742 -0.221692 4.742064
 6 -2.306562 0.353742 5.105641
 6 -1.291297 0.548982 4.155795
 1 -4.713006 -1.067254 3.140039
 1 -4.295353 -0.367401 5.492597
 1 -2.140193 0.653969 6.133204
 1 -0.348013 0.992057 4.455036
 1 -3.533124 -1.111769 0.469824
 6 1.692135 0.415304 0.679621
 6 2.698440 1.385206 0.630386
 6 3.745128 1.232178 -0.266603
 7 3.825782 0.188891 -1.069760
 6 2.904863 -0.750956 -1.027647
 6 1.815712 -0.690498 -0.164038
 6 -1.236640 -0.285250 -0.919513
 6 -0.570872 0.778128 -1.533329
 6 -0.372518 0.748663 -2.908710
 7 -0.802846 -0.240569 -3.663225
 6 -1.453216 -1.247476 -3.113428
 6 -1.697592 -1.313269 -1.749106
 1 0.997979 0.988187 2.615120
 9 -1.891757 -2.246502 -3.919901
 9 -2.399435 -2.357916 -1.221948
 9 3.035349 -1.818883 -1.854321
 9 4.719797 2.172522 -0.330891
 9 2.634444 2.453257 1.473521
 9 0.279154 1.778819 -3.506133
 9 -0.135827 1.843698 -0.802457
 9 0.912258 -1.708871 -0.124557

Total energy = -1071.09330

6 -2.987859 -0.162222 -0.423048
 6 -3.021272 -0.131536 1.040462
 6 -1.680909 -0.040046 1.520884
 6 -0.786649 0.007945 0.328359
 6 0.548975 0.203594 0.213327
 6 -1.699492 -0.069318 -0.857985
 6 -4.097285 -0.145293 1.924289
 6 -3.845712 -0.045211 3.297972
 6 -2.537004 0.083417 3.772135

6 -1.448283 0.090772 2.888118
 1 -5.114206 -0.217233 1.554803
 1 -4.673137 -0.054643 3.998392
 1 -2.358185 0.180682 4.836812
 1 -0.442634 0.199951 3.269751
 1 -3.858186 -0.273946 -1.053663
 6 1.582951 0.173429 1.252888
 6 1.590985 -0.785405 2.279406
 6 2.613301 -0.823739 3.226611
 6 3.663551 0.098550 3.165036
 6 3.684370 1.043777 2.126364
 6 2.671756 1.070582 1.182598
 1 0.798603 -1.522692 2.319388
 1 2.589690 -1.583240 3.996180
 1 4.512902 1.738443 2.088855
 1 2.703272 1.801993 0.382617
 6 -1.259057 -0.066181 -2.263967
 6 -0.231965 -0.918282 -2.722615
 6 0.150642 -0.921075 -4.055861
 6 -0.480593 -0.076466 -4.981349
 6 -1.503512 0.769945 -4.543377
 6 -1.882153 0.771974 -3.200650
 1 0.244078 -1.597190 -2.025920
 1 0.930516 -1.577908 -4.418205
 1 -2.003842 1.435790 -5.233478
 1 -2.660968 1.446564 -2.864614
 1 0.917367 0.408055 -0.790710
 8 -0.021233 -0.159020 -6.285656
 8 4.721822 0.155404 4.051956
 6 4.753296 -0.805674 5.151497
 1 3.875423 -0.703260 5.800518
 1 4.813628 -1.837119 4.784100
 1 5.655880 -0.561619 5.711695
 6 -0.654839 0.688780 -7.290198
 1 -1.724574 0.467531 -7.389469
 1 -0.527147 1.753655 -7.060008
 1 -0.142671 0.451206 -8.222825

Total energy = -1071.08956

6 -2.956443 -0.152637 1.269096
 6 -2.904691 -0.085928 2.728628
 6 -1.536230 -0.067051 3.109818
 6 -0.709952 -0.058096 1.865685
 6 0.641652 0.073489 1.911307
 6 -1.693190 -0.149562 0.743019
 6 -3.911430 -0.067570 3.691553
 6 -3.548961 -0.031316 5.043917
 6 -2.201883 -0.008414 5.421217
 6 -1.186393 -0.018744 4.453995
 1 -4.956320 -0.079793 3.402069
 1 -4.319261 -0.019439 5.806516
 1 -1.939155 0.018000 6.472448
 1 -0.147167 0.006361 4.763876
 1 -3.863891 -0.266927 0.693286
 6 1.650829 0.331358 0.886928
 6 1.394918 1.005683 -0.328616
 6 2.416423 1.271415 -1.222983
 6 3.735667 0.875659 -0.947817
 6 4.013517 0.222945 0.258289
 6 2.984701 -0.029267 1.160970
 1 0.389596 1.324458 -0.059103
 1 2.227214 1.791586 -2.152344
 1 5.021299 -0.082392 0.504686
 1 3.214300 -0.525347 2.098380
 6 -1.416008 -0.365389 -0.690862
 6 -0.509345 -1.356672 -1.118050
 6 -0.303175 -1.598201 -2.466400

6	-0.991881	-0.856256	-3.439134
6	-1.892677	0.130700	-3.031428
6	-2.099637	0.367869	-1.670075
1	0.027437	-1.936452	-0.377997
1	0.387346	-2.359297	-2.804785
1	-2.433461	0.722192	-3.757873
1	-2.790278	1.144344	-1.361046
1	1.070979	0.006211	2.911150
8	4.672863	1.187794	-1.913304
8	-0.706409	-1.177230	-4.756927
6	-1.401561	-0.440124	-5.806053
1	-2.487943	-0.580371	-5.747379
1	-1.174727	0.632447	-5.765928
1	-1.027513	-0.858930	-6.740577
6	6.062383	0.805789	-1.675788
1	6.468299	1.297462	-0.783609
1	6.168956	-0.280500	-1.570892
1	6.601777	1.144742	-2.560223

Total energy = -1040.70036

6	-2.793196	-0.023578	-0.485513
6	-2.796854	-0.021775	0.980116
6	-1.445599	-0.008578	1.434859
6	-0.572229	0.015805	0.225148
6	0.767686	0.140932	0.086627
6	-1.511536	0.008589	-0.943843
6	-3.855446	0.000479	1.883358
6	-3.572484	0.056517	3.253845
6	-2.250463	0.104922	3.704274
6	-1.179310	0.076750	2.799065
1	-4.881443	-0.011248	1.533129
1	-4.385638	0.074319	3.970344
1	-2.046591	0.166338	4.766930
1	-0.162651	0.122595	3.163800
1	-3.680740	-0.073262	-1.099937
6	1.813268	0.055314	1.116629
6	1.802893	-0.943225	2.108995
6	2.831196	-1.030529	3.042651
6	3.885440	-0.126055	2.989631
6	3.936011	0.854174	2.005143
6	2.911927	0.935112	1.067560
1	0.993065	-1.661470	2.128727
1	2.832993	-1.799925	3.802983
1	4.774197	1.537260	1.980988
1	2.949694	1.694495	0.295034
6	-1.097568	0.015513	-2.358613
6	-0.145084	-0.896133	-2.851822
6	0.217338	-0.890793	-4.196588
6	-0.371751	0.022120	-5.062472
6	-1.318649	0.930210	-4.604475
6	-1.677003	0.927423	-3.259406
1	0.289972	-1.625484	-2.180279
1	0.942120	-1.594444	-4.583545
1	-1.757032	1.633129	-5.300093
1	-2.397913	1.646082	-2.889367
1	1.133025	0.330455	-0.921118
9	4.894903	-0.211383	3.909376
9	-0.014299	0.027159	-6.384777

Total energy = -1040.69695

6	-2.728651	-0.146764	0.808889
6	-2.730964	-0.146553	2.272366
6	-1.378678	-0.152553	2.704714
6	-0.506157	-0.093886	1.493513

6	0.841968	0.020254	1.584209
6	-1.447886	-0.127174	0.330898
6	-3.773389	-0.163255	3.195556
6	-3.461063	-0.186842	4.561061
6	-2.129378	-0.188139	4.988870
6	-1.077757	-0.163547	4.060813
1	-4.806591	-0.156389	2.867222
1	-4.259176	-0.202670	5.294168
1	-1.906315	-0.208121	6.049201
1	-0.050851	-0.158034	4.409734
1	-3.615352	-0.227231	0.196130
6	1.866072	0.309478	0.576770
6	1.635222	1.123655	-0.549307
6	2.661703	1.412369	-1.440945
6	3.932581	0.893763	-1.221434
6	4.198338	0.102967	-0.109309
6	3.174104	-0.174913	0.788002
1	0.651834	1.538123	-0.714567
1	2.489274	2.040529	-2.304205
1	5.199142	-0.277112	0.044280
1	3.379384	-0.782436	1.662420
6	-1.117542	-0.281014	-1.100392
6	-0.194675	-1.249574	-1.533270
6	0.063375	-1.430975	-2.887982
6	-0.597209	-0.644782	-3.825002
6	-1.513854	0.319320	-3.426313
6	-1.772600	0.499190	-2.068792
1	0.314671	-1.861407	-0.800388
1	0.769320	-2.176641	-3.227937
1	-2.010601	0.920282	-4.176165
1	-2.475798	1.258750	-1.748466
1	1.251904	-0.093028	2.587576
9	4.939822	1.177921	-2.102462
9	-0.338712	-0.821896	-5.158811