

Supplementary Material

Theoretical investigation of Fused N-methyl-dithieno-pyrrole derivatives in the context of Acceptor-Donor-Acceptor approach

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Table S1: Coordinates of the studied compounds (in Angstroms) optimized in gas phase at B3LYP/6-31G (d) level of theory.

A. Compound PBDB-C1

C	-10.803371	-0.637271	0.004930
C	-9.994209	-1.788073	0.002849
C	-10.516716	-3.073085	0.007442
C	-11.905666	-3.215437	0.014603
C	-12.726792	-2.081126	0.016920
C	-12.194771	-0.787500	0.012109
H	-9.846115	-3.926266	0.005518
H	-12.353097	-4.204554	0.018445
H	-13.805578	-2.203111	0.022601
H	-12.864256	0.060834	0.014179
C	-9.927078	0.564330	-0.001338
C	-8.569965	-1.390842	-0.004177
C	-8.540409	0.088720	-0.005222
C	-7.404450	0.870095	-0.007426
C	-6.014476	0.595587	-0.011131
C	-3.644320	-0.183962	-0.010662
C	-3.778362	1.228676	-0.016614
S	-5.182083	-0.989241	-0.012157
C	-5.099620	1.664929	-0.013038
C	-2.267214	-0.451795	-0.006598
C	-1.603923	0.797461	-0.010455
N	-2.523845	1.820863	-0.032759
S	-1.150964	-1.806928	-0.007105
S	1.150915	1.806537	0.008055
C	0.198420	-0.673774	0.002343
C	-0.198424	0.673343	-0.001459
C	1.603937	-0.797878	0.011227
C	2.267166	0.451409	0.007247
C	3.644283	0.183683	0.011045
C	3.778409	-1.228925	0.017023
C	5.099690	-1.665132	0.013298
C	6.014493	-0.595734	0.011347

S	5.181990	0.989050	0.012426
N	2.523952	-1.821220	0.033317
C	7.404528	-0.870172	0.007388
C	8.540398	-0.088684	0.004956
C	8.569748	1.390882	0.004077
C	9.927133	-0.564098	0.000737
C	9.993929	1.788309	-0.002930
C	10.803248	0.637624	-0.005349
C	10.516258	3.073402	-0.007267
C	12.194630	0.788043	-0.012643
C	11.905183	3.215943	-0.014528
C	12.726468	2.081741	-0.017202
C	10.384797	-1.870801	0.002801
C	9.534100	-3.018676	0.010206
C	11.769344	-2.222147	-0.001672
N	8.863977	-3.972415	0.016260
N	12.886900	-2.551315	-0.005220
C	-10.384568	1.871088	-0.003704
C	-11.769079	2.222615	0.000569
C	-9.533722	3.018856	-0.011178
N	-12.886594	2.551923	0.003937
N	-8.863471	3.972505	-0.017293
O	-7.613055	-2.157586	-0.007884
O	7.612727	2.157478	0.008003
C	2.241322	-3.243103	-0.055319
H	1.319634	-3.467804	0.486037
H	2.137482	-3.570602	-1.095396
H	3.054737	-3.799289	0.414699
C	-2.240714	3.242673	0.055455
H	-2.132659	3.569632	1.095272
H	-1.321217	3.467670	-0.489549
H	-3.056035	3.799114	-0.410893
H	5.428741	-2.697761	0.009432
H	12.864228	-0.060198	-0.014970
H	13.805236	2.203884	-0.022963
H	12.352484	4.205120	-0.018168
H	9.845536	3.926489	-0.005095
H	7.572785	-1.940241	0.006048
H	-7.572622	1.940178	-0.006089
H	-5.428646	2.697565	-0.009238

B. Compound PBDB-C2

C	-10.818269	-0.112225	0.001121
C	-10.066322	-1.299667	-0.000396
C	-10.642631	-2.562653	0.001032
C	-12.027882	-2.626611	0.004127
C	-12.795938	-1.452279	0.005753
C	-12.216546	-0.189419	0.004312
H	-10.036854	-3.461638	-0.000242
H	-12.870581	0.670931	0.005693
C	-9.885633	1.044780	-0.001194
C	-8.624195	-0.973048	-0.003565
C	-8.524258	0.502047	-0.004017

C	-7.351483	1.228369	-0.006824
C	-5.977254	0.887159	-0.010161
C	-3.647909	-0.006175	-0.007918
C	-3.713273	1.411761	-0.017689
S	-5.222244	-0.736224	-0.007410
C	-5.011370	1.911473	-0.014873
C	-2.285971	-0.340784	-0.003865
C	-1.562727	0.875114	-0.011593
N	-2.431476	1.942001	-0.035885
S	-1.237684	-1.748828	-0.001461
S	1.237589	1.748639	0.002045
C	0.165049	-0.682726	0.003899
C	-0.165101	0.682492	-0.003317
C	1.562693	-0.875327	0.012147
C	2.285877	0.340600	0.004294
C	3.647845	0.006086	0.008173
C	3.713288	-1.411820	0.017977
C	5.011403	-1.911483	0.015028
C	5.977245	-0.887121	0.010245
S	5.222133	0.736223	0.007484
N	2.431534	-1.942166	0.036431
C	7.351481	-1.228307	0.006788
C	8.524265	-0.501981	0.003873
C	8.624188	0.973116	0.003319
C	9.885660	-1.044698	0.000996
C	10.066309	1.299759	0.000084
C	10.818278	0.112329	-0.001405
C	10.642603	2.562750	-0.001383
C	12.216556	0.189546	-0.004585
C	12.027852	2.626730	-0.004505
C	12.795926	1.452418	-0.006085
C	10.282697	-2.370689	0.000575
C	9.379455	-3.477452	0.003175
C	11.650969	-2.779683	-0.002464
N	8.663965	-4.397505	0.005316
N	12.757022	-3.145456	-0.004942
C	-10.282669	2.370759	-0.000669
C	-11.650951	2.779717	0.002229
C	-9.379452	3.477543	-0.003016
N	-12.757025	3.145423	0.004588
N	-8.663966	4.397600	-0.004966
O	-7.709741	-1.789200	-0.005396
O	7.709730	1.789264	0.005155
C	2.079809	-3.349376	-0.043230
H	1.147820	-3.524919	0.498558
H	1.961187	-3.678163	-1.081238
H	2.864521	-3.941335	0.431796
C	-2.079298	3.349136	0.042980
H	-1.957097	3.677598	1.080675
H	-1.149148	3.524814	-0.501969
H	-2.865616	3.941295	-0.429089
H	5.290070	-2.958860	0.013523
H	12.870607	-0.670790	-0.005927
H	10.036812	3.461726	-0.000129

H	7.468748	-2.305140	0.007123
H	-7.468750	2.305204	-0.007140
H	-5.290019	2.958856	-0.013337
F	14.129040	1.571611	-0.009105
F	12.661842	3.804938	-0.006066
F	-14.129055	-1.571442	0.008776
F	-12.661892	-3.804808	0.005626

C. Compound PBDB-C3

C	10.818518	-0.262770	-0.001307
C	10.050826	-1.441691	0.000374
C	10.606466	-2.710953	-0.001874
C	11.995831	-2.778025	-0.006062
C	12.797862	-1.635231	-0.007942
C	12.216419	-0.366545	-0.005565
H	9.989008	-3.601756	-0.000450
H	12.857818	0.503148	-0.007097
C	9.902091	0.905105	0.002114
C	8.610930	-1.093987	0.004641
C	8.531685	0.381425	0.005250
C	7.369053	1.123357	0.007852
C	5.989899	0.801309	0.011264
C	3.647915	-0.058834	0.009417
C	3.733627	1.357838	0.017983
S	5.211856	-0.811172	0.009635
C	5.038870	1.839045	0.015014
C	2.281026	-0.373735	0.005291
C	1.575460	0.852286	0.011753
N	2.459612	1.906561	0.035483
S	1.212226	-1.766383	0.003761
S	-1.212121	1.766364	-0.003823
C	-0.175012	-0.680080	-0.003159
C	0.175092	0.680041	0.003067
C	-1.575387	-0.852319	-0.011846
C	-2.280925	0.373727	-0.005359
C	-3.647825	0.058872	-0.009471
C	-3.733574	-1.357792	-0.018058
C	-5.038827	-1.838981	-0.015079
C	-5.989833	-0.801221	-0.011303
S	-5.211757	0.811227	-0.009641
N	-2.459583	-1.906563	-0.035612
C	-7.368987	-1.123250	-0.007893
C	-8.531724	-0.381453	-0.005271
C	-8.611183	1.094032	-0.004623
C	-9.901987	-0.905327	-0.002130
C	-10.051097	1.441408	-0.000286
C	-10.818665	0.262486	0.001377
C	-10.606413	2.710901	0.002037
C	-12.216519	0.366657	0.005701
C	-11.995795	2.778228	0.006288
C	-12.797878	1.635362	0.008157

C	-10.312817	-2.227745	-0.002553
C	-9.422157	-3.344640	-0.006631
C	-11.684772	-2.624410	0.000846
N	-8.718050	-4.273567	-0.009971
N	-12.792974	-2.983891	0.003601
C	10.312745	2.227504	0.002471
C	11.684731	2.624225	-0.000920
C	9.422185	3.344480	0.006456
N	12.792779	2.984184	-0.003667
N	8.718150	4.273465	0.009722
O	7.685325	-1.897445	0.007042
O	-7.685672	1.897607	-0.007026
C	-2.128149	-3.318435	0.046638
H	-1.199214	-3.508612	-0.495500
H	-2.013372	-3.646845	1.085225
H	-2.921794	-3.899996	-0.426394
C	2.127963	3.318396	-0.046559
H	2.011231	3.646489	-1.085027
H	1.200047	3.508735	0.497288
H	2.922505	3.900094	0.424771
H	-5.332512	-2.882247	-0.012892
H	-12.858160	-0.502898	0.007227
H	-9.988189	3.601108	0.000621
H	-7.500590	-2.198384	-0.007735
H	7.500683	2.198490	0.007674
H	5.332544	2.882316	0.012806
F	12.593172	-3.981214	-0.008401
H	13.875446	-1.754690	-0.011249
F	-12.592963	3.981362	0.008701
H	-13.875388	1.754950	0.011516

D. Compound PBDB-C4

C	10.819969	-0.354388	-0.003594
C	10.038596	-1.527868	-0.001849
C	10.642504	-2.776428	-0.004967
C	12.031516	-2.884483	-0.009961
C	12.799793	-1.718924	-0.011735
C	12.214169	-0.447281	-0.008597
H	12.847981	0.427011	-0.010147
C	9.906088	0.821298	0.000637
C	8.602450	-1.174216	0.003241
C	8.537909	0.305699	0.004156
C	7.378376	1.053555	0.007224
C	5.997034	0.742529	0.010939
C	3.647059	-0.094307	0.009570
C	3.746271	1.321743	0.017866
C	5.203650	-0.862114	0.009662
C	5.055801	1.789975	0.014689
C	2.277244	-0.395742	0.005516
C	1.583370	0.837084	0.011719
N	2.477553	1.882849	0.035232
S	1.195158	-1.778127	0.004095
S	-1.195103	1.777992	-0.004263

C	-0.181537	-0.678515	-0.003105
C	0.181559	0.678354	0.002922
C	-1.583356	-0.837236	-0.011898
C	-2.277198	0.395618	-0.005667
C	-3.647026	0.094237	-0.009678
C	-3.746283	-1.321803	-0.017994
C	-5.055820	-1.790008	-0.014786
C	-5.997028	-0.742538	-0.010993
S	-5.203594	0.862085	-0.009715
N	-2.477593	-1.882966	-0.035450
C	-7.378378	-1.053529	-0.007242
C	-8.537899	-0.305652	-0.004136
C	-8.602417	1.174263	-0.003197
C	-9.906090	-0.821227	-0.000582
C	-10.038555	1.527942	0.001957
C	-10.819949	0.354477	0.003706
C	-10.642440	2.776513	0.005124
C	-12.214147	0.447396	0.008761
C	-12.031449	2.884595	0.010173
C	-12.799747	1.719050	0.011950
C	-10.326858	-2.140980	-0.001225
C	-9.441766	-3.262477	-0.006042
C	-11.698847	-2.537516	0.002572
N	-8.743337	-4.195699	-0.009974
N	-12.804272	-2.905539	0.005603
C	10.326824	2.141060	0.001260
C	11.698803	2.537632	-0.002504
C	9.441698	3.262530	0.006010
N	12.804223	2.905669	-0.005509
N	8.743209	4.195708	0.009898
O	7.658323	-1.953615	0.005986
O	-7.658278	1.953649	-0.005954
C	-2.159850	-3.297905	0.047381
H	-1.232457	-3.497263	-0.494098
H	-2.048855	-3.627150	1.086129
H	-2.958809	-3.871924	-0.425945
C	2.159530	3.297748	-0.047257
H	2.046063	3.626677	-1.085835
H	1.233422	3.497262	0.496390
H	2.959620	3.871908	0.423954
H	-5.359650	-2.830370	-0.012403
H	-12.847976	-0.426883	0.010317
H	-7.517050	-2.127682	-0.007120
H	7.517028	2.127712	0.007095
H	5.359620	2.830340	0.012297
H	-12.486212	3.868783	0.012627
H	-13.881922	1.800614	0.015906
H	12.486298	-3.868662	-0.012378
H	13.881969	-1.800468	-0.015649
F	9.897723	-3.888411	-0.003249
F	-9.897637	3.888482	0.003402

E. Compound PBDB-C5

C	-10.851940	0.337897	-0.062290
C	-10.147967	-0.875190	-0.043300
C	-10.768659	-2.116031	-0.053936
C	-12.165306	-2.155728	-0.087896
C	-12.901008	-0.935083	-0.097138
C	-12.252738	0.297421	-0.086589
H	-10.155790	-3.009065	-0.047853
H	-12.875317	1.180599	-0.106108
C	-9.883162	1.456757	-0.044938
C	-8.696552	-0.606683	-0.024862
C	-8.538422	0.865061	-0.035713
C	-7.342583	1.546929	-0.045164
C	-5.978731	1.155223	-0.043273
C	-3.682958	0.175101	-0.026501
C	-3.696138	1.592646	-0.057920
S	-5.284831	-0.494618	-0.014842
C	-4.976461	2.140829	-0.062475
C	-2.333371	-0.209500	-0.017838
C	-1.565933	0.977832	-0.045291
N	-2.395785	2.075174	-0.086444
S	-1.335753	-1.654301	0.006433
S	1.265113	1.749132	-0.047655
C	0.105583	-0.640224	-0.005782
C	-0.175803	0.734796	-0.034952
C	1.495706	-0.883039	0.004818
C	2.262542	0.304435	-0.023197
C	3.612497	-0.079247	-0.014577
C	3.626550	-1.496619	0.018529
C	4.907400	-2.043349	0.022951
C	5.908629	-1.056227	-0.000499
S	5.213493	0.592424	-0.028363
N	2.326271	-1.980043	0.047442
C	7.272850	-1.447303	0.002549
C	8.467894	-0.763704	-0.011809
C	8.623592	0.711398	-0.046084
C	9.810878	-1.352813	-0.000771
C	10.072606	0.981632	-0.060887
C	10.777167	-0.231506	-0.034383
C	10.716577	2.209633	-0.077646
C	12.175528	-0.208500	-0.048369
C	12.110010	2.247328	-0.078108
C	12.840466	1.021922	-0.086158
C	10.160349	-2.694680	0.041086
C	9.221716	-3.769883	0.079879
C	11.514382	-3.147548	0.053587
N	8.479044	-4.667993	0.112285
N	12.611836	-3.540155	0.064683
C	-10.227639	2.798265	-0.030585
C	-11.578993	3.260495	-0.024227
C	-9.283582	3.869953	-0.010334
N	-12.667344	3.676191	-0.014063
N	-8.535832	4.764183	0.006216
O	-7.812130	-1.457090	-0.007375
O	7.732208	1.553516	-0.060588

C	1.923277	-3.373563	-0.011688
H	0.990727	-3.509183	0.540918
H	1.782098	-3.711287	-1.044265
H	2.690971	-3.988117	0.462644
C	-1.991823	3.468733	-0.032672
H	-1.849768	3.810018	0.998601
H	-1.059534	3.601927	-0.586317
H	-2.759373	4.082282	-0.508553
H	5.147597	-3.100075	0.039088
H	12.749204	-1.120638	-0.050432
H	10.155518	3.137290	-0.085441
H	7.350892	-2.527660	0.020741
H	-7.419797	2.627311	-0.061812
H	-5.215243	3.197923	-0.075790
O	-12.906832	-3.288968	-0.128543
O	-14.263212	-0.941717	-0.189450
O	14.191301	1.137049	-0.151865
O	12.696355	3.471502	-0.140986
C	13.797131	3.772710	0.730688
H	14.740156	3.398203	0.329380
H	13.824145	4.861790	0.799985
H	13.634365	3.349654	1.728314
C	14.980165	-0.052977	-0.155151
H	14.824430	-0.640301	0.757233
H	14.756779	-0.677416	-1.027859
H	16.016508	0.281787	-0.202436
C	-14.977240	-1.437594	0.952145
H	-16.035798	-1.318376	0.716458
H	-14.757871	-2.492897	1.136702
H	-14.735255	-0.846965	1.844384
C	-12.224900	-4.540443	-0.153671
H	-13.003784	-5.301800	-0.198717
H	-11.580406	-4.624209	-1.036771
H	-11.622169	-4.686182	0.750991

F. Compound PBDB-C6

C	10.861641	-0.157045	0.002154
C	10.142297	1.048803	0.001125
C	10.735567	2.301160	0.001641
C	12.136719	2.350393	0.003251
C	12.881476	1.151943	0.004469
C	12.265667	-0.092529	0.003962
H	10.106902	3.183030	0.000678
H	12.880829	-0.981261	0.004845
C	9.908618	-1.287665	0.000691
C	8.691030	0.757020	-0.000895
C	8.554721	-0.714984	-0.001836
C	7.368078	-1.413514	-0.005769
C	5.999351	-1.041286	-0.009336
C	3.689894	-0.094536	-0.006193
C	3.723596	-1.512099	-0.019025
S	5.281581	0.598655	-0.003670
C	5.011426	-2.041772	-0.016505

C	2.334726	0.270484	-0.002303
C	1.584791	-0.928163	-0.013339
N	2.430443	-2.013900	-0.039641
S	1.316761	1.701006	0.002170
S	-1.234745	-1.740121	-0.003660
C	-0.109770	0.666291	0.004192
C	0.191226	-0.705088	-0.005774
C	-1.503375	0.889151	0.011828
C	-2.252837	-0.309861	0.000829
C	-3.608089	0.054191	0.004910
C	-3.642694	1.472024	0.017827
C	-4.930634	2.000364	0.015551
C	-5.917982	0.998426	0.008504
S	-5.198604	-0.640924	0.002457
N	-2.349589	1.974533	0.038379
C	-7.286347	1.369630	0.005534
C	-8.473213	0.669768	0.001932
C	-8.604807	-0.803230	0.000530
C	-9.826223	1.242151	0.000325
C	-10.056087	-1.099503	-0.000611
C	-10.778673	0.111360	-0.000668
C	-10.656493	-2.340424	-0.001089
C	-12.176044	0.047175	-0.001236
C	-12.060956	-2.393513	-0.001544
C	-12.806125	-1.199489	-0.001642
C	-10.186734	2.580972	-0.000556
C	-9.257269	3.664903	0.000210
C	-11.543964	3.024026	-0.002550
N	-8.521008	4.568950	0.000923
N	-12.640632	3.418057	-0.004199
C	10.268714	-2.625712	0.001869
C	11.625558	-3.071105	0.004766
C	9.338283	-3.709262	0.000524
N	12.720210	-3.470284	0.007149
N	8.601853	-4.613045	-0.000649
O	7.796293	1.595965	-0.001672
O	-7.705148	-1.635941	0.000545
C	-1.967713	3.373437	-0.038476
H	-1.031491	3.527591	0.502671
H	-1.842689	3.702666	-1.075753
H	-2.739107	3.981334	0.438442
C	2.047739	-3.412719	0.036603
H	1.921372	-3.741885	1.073706
H	1.112076	-3.566364	-0.505623
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H	-5.186236	3.053605	0.015949
H	-12.789995	0.936846	-0.001241
H	-10.068389	-3.251223	-0.000947
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H	7.460390	-2.492789	-0.007413
H	5.265787	-3.095308	-0.016726
O	12.869674	3.488639	0.003687
O	-12.601009	-3.635616	-0.001741
C	-14.019345	-3.770300	-0.001574

H	-14.465479	-3.319533	-0.896552
H	-14.215483	-4.842729	-0.001513
H	-14.465253	-3.319468	0.893489
C	12.181656	4.737016	0.001658
H	12.956381	5.503984	0.001953
H	11.558262	4.848323	-0.893815
H	11.555950	4.849986	0.895306
H	-13.888514	-1.229997	-0.001995
H	13.963173	1.231544	0.005720

G. Compound PBDB-C7

C	10.824680	-0.016128	0.002395
C	10.089343	1.185271	0.001242
C	10.724119	2.436038	0.002587
C	12.129512	2.460271	0.005254
C	12.848137	1.263628	0.006441
C	12.221426	0.015182	0.005048
H	12.820631	-0.882714	0.005930
C	9.874456	-1.162021	0.000031
C	8.644123	0.878349	-0.001662
C	8.525778	-0.601407	-0.002719
C	7.342270	-1.307001	-0.006260
C	5.970510	-0.947662	-0.009876
C	3.649876	-0.030580	-0.007224
C	3.700626	-1.447928	-0.018813
S	5.233144	0.682924	-0.005503
C	4.994472	-1.961108	-0.016081
C	2.290333	0.317336	-0.003018
C	1.554676	-0.890280	-0.012629
N	2.413455	-1.965754	-0.038622
S	1.255286	1.735608	0.000645
S	-1.255265	-1.735596	-0.000713
C	-0.158689	0.683934	0.004416
C	0.158701	-0.683914	-0.004510
C	-1.554667	0.890297	0.012590
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C	-3.649862	0.030573	0.007234
C	-3.700625	1.447917	0.018818
C	-4.994472	1.961089	0.016048
C	-5.970509	0.947635	0.009855
S	-5.233123	-0.682944	0.005419
N	-2.413462	1.965761	0.038604
C	-7.342264	1.306989	0.006287
C	-8.525792	0.601422	0.002707
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N	12.693854	-3.361182	0.006671
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O	7.716096	1.678078	-0.003036
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H	2.825595	-3.968429	-0.436302
H	-5.262065	3.011372	0.015528
H	-12.820644	0.882712	-0.006036
H	-7.442105	2.385435	0.007354
H	7.442133	-2.385446	-0.007319
H	5.262066	-3.011391	-0.015559
O	9.934867	3.530732	0.001220
O	-9.934844	-3.530720	-0.001396
C	-10.546856	-4.815828	-0.001554
H	-11.160711	-4.969575	-0.897868
H	-9.725256	-5.532209	0.000506
H	-11.164076	-4.968182	0.892683
C	10.546967	4.815795	0.001954
H	11.164164	4.968506	-0.892243
H	9.725419	5.532236	0.000194
H	11.160871	4.969098	0.898312
H	-13.933056	-1.307051	-0.008524
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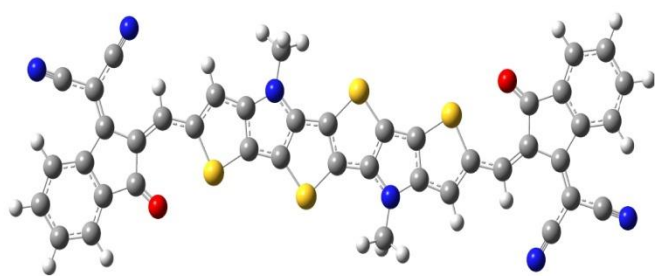
Table S2: Calculated values of HOMO and LUMO energies, $\Delta_{\text{H-L}}$ and Λ_{max} values of the reference compound obtained using various functionals.

Functionals	E _{HOMO} (eV)	E _{LUMO} (eV)	$\Delta_{\text{H-L}}$ (eV)	Λ_{max} (nm)
Reported	-5.87	-3.94	1.93	569
B3LYP	-5.89	-3.55	2.34	-
B3LYP-D3	-5.88	-3.61	2.27	-
B3PW91	-6.01	-3.66	2.35	-
PBEPBE	-5.39	-4.09	1.30	-
HSEH1PBE	-5.78	-3.83	1.95	-
CAM-B3LYP	-6.24	-2.67	3.57	548
M06-2X-D3	-	-	-	578
ω B97XD	-	-	-	439

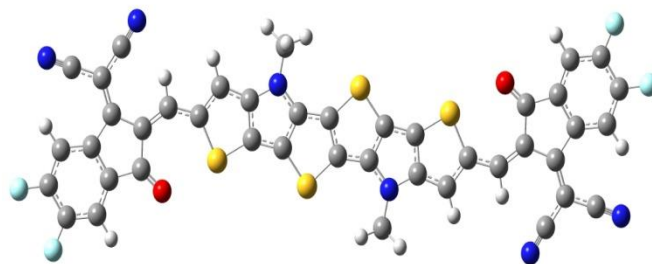
Table S3: Spectral data obtained from PDOS spectra.

Compounds	Groups	Contribution to HOMO (%)	Contribution to LUMO (%)
1	Acceptor Donor	32 68	63 37
2	Acceptor Donor	32 68	62 38
3	Acceptor Donor	32 68	61 39
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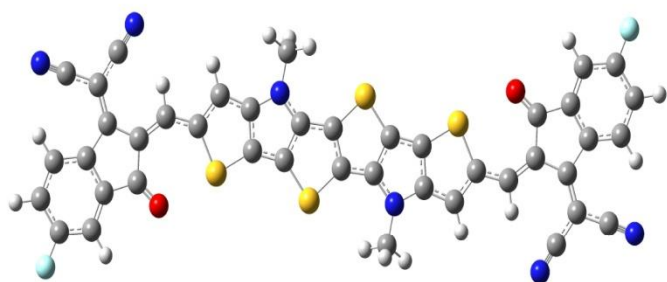
Fig.1: Optimized structures of the studied compounds:



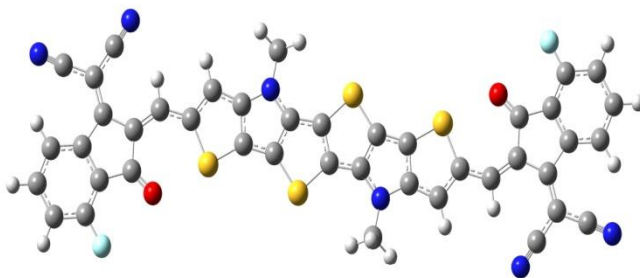
PBDB-C1



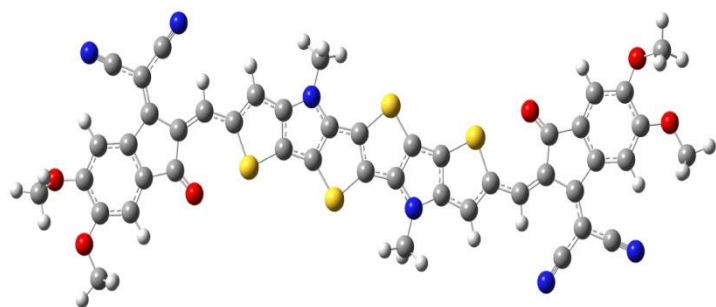
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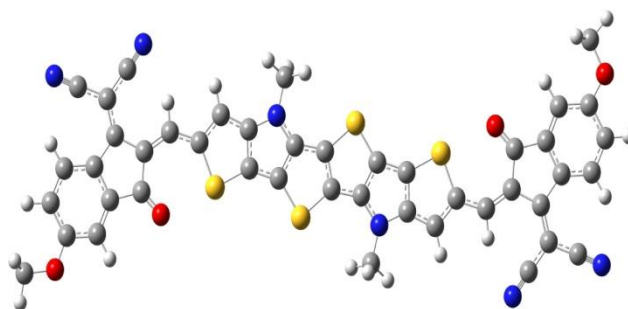
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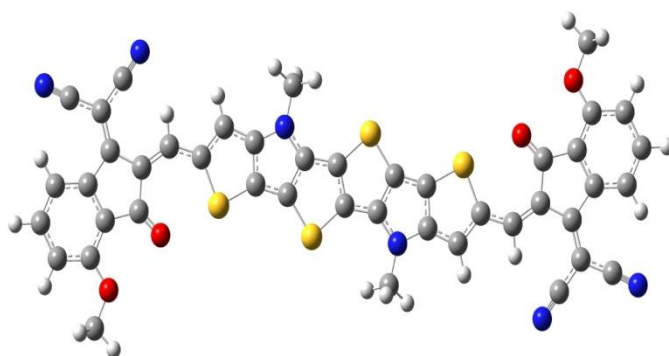
PBDB-C4



PBDB-C5

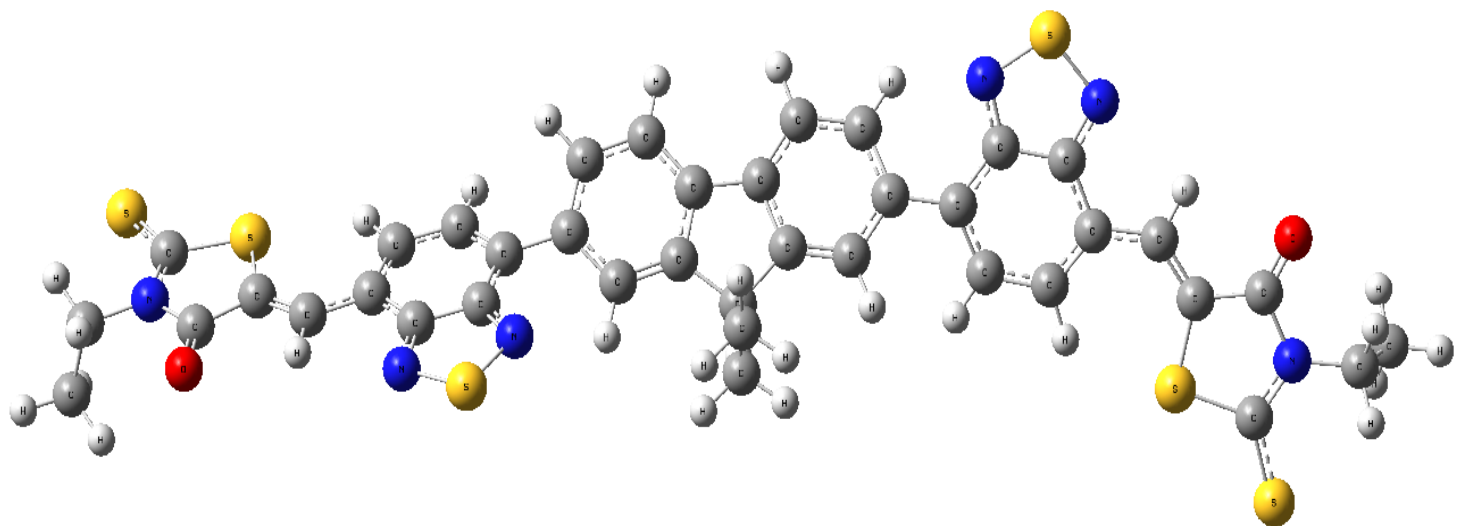


PBDB-C6

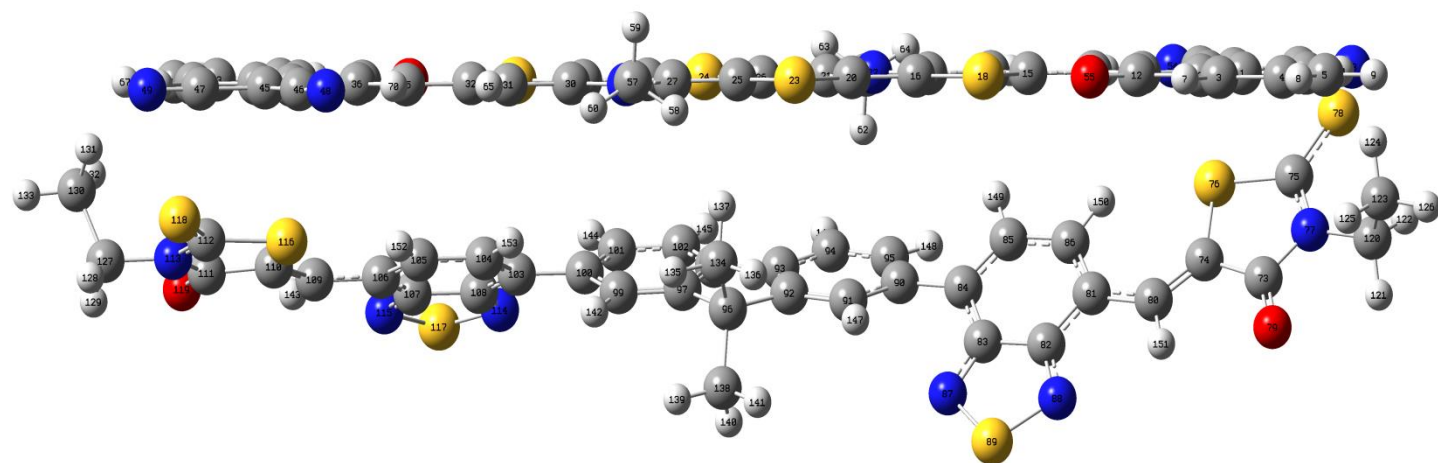


PBDB-C7

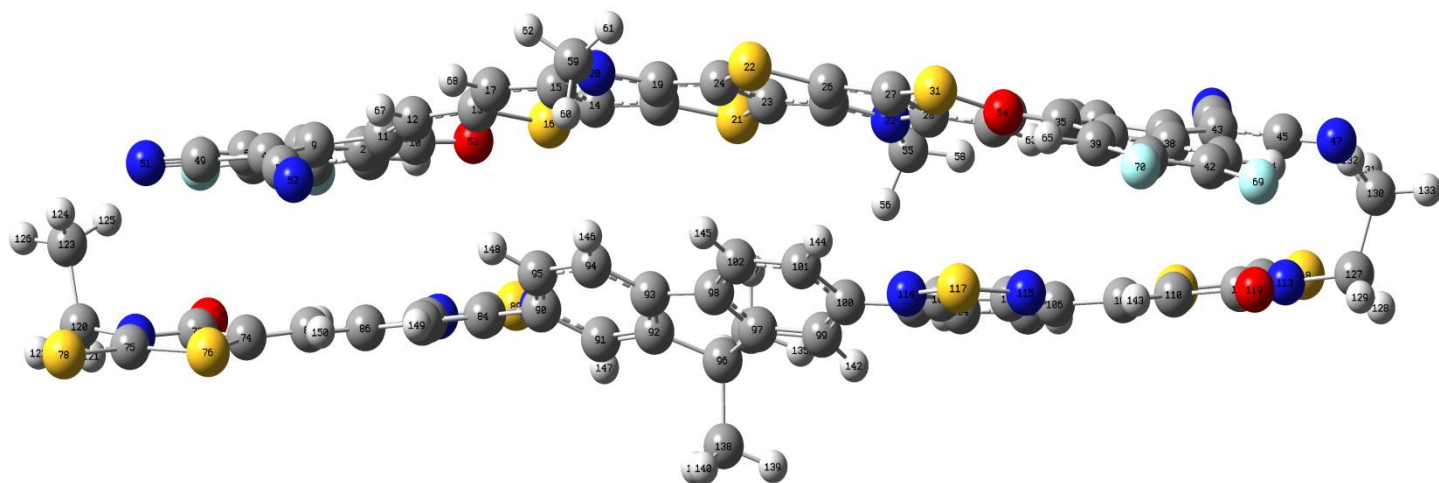
Fig. 2. Optimized structures of the D/A blends:



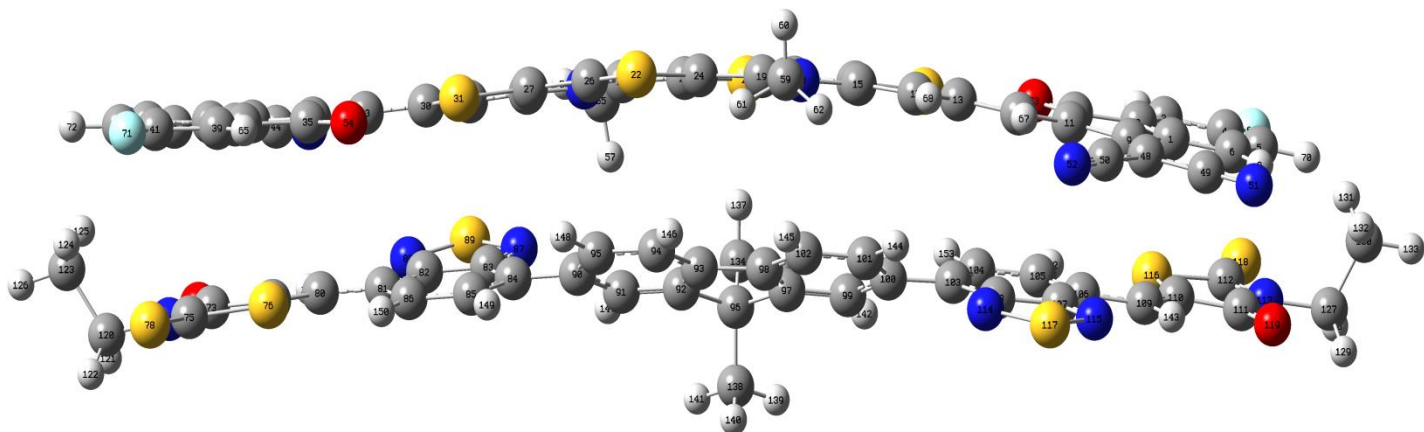
FREA (a76)



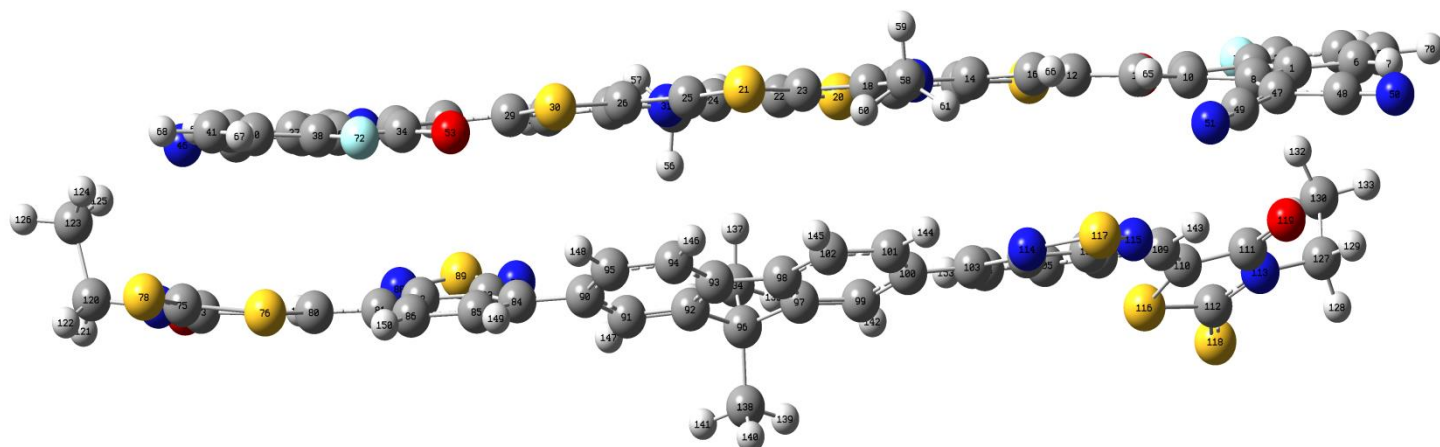
FREA/PBDB-C1



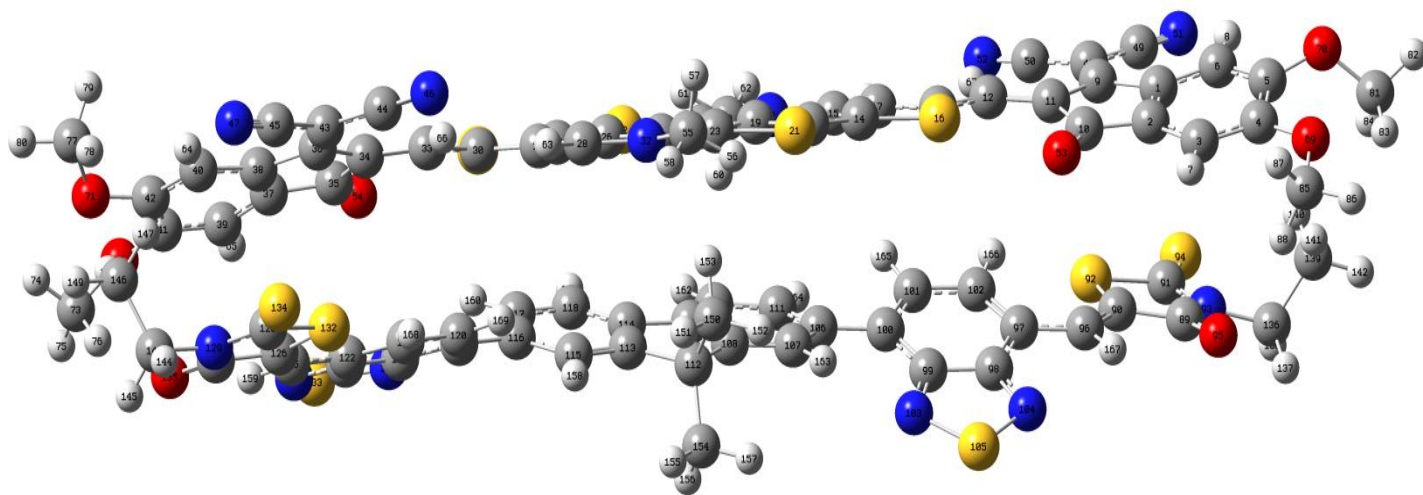
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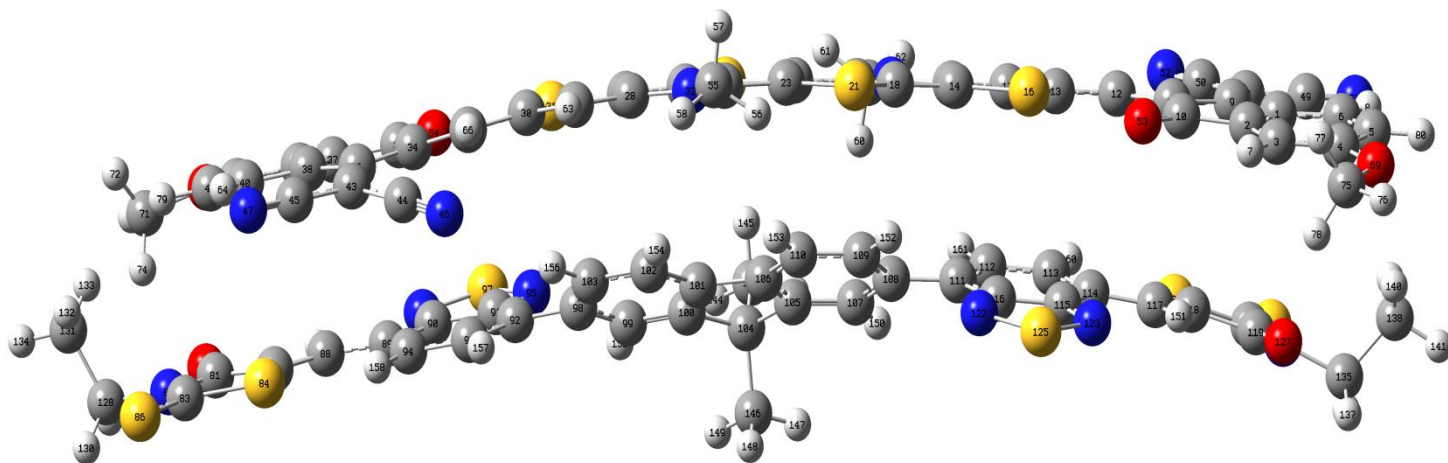
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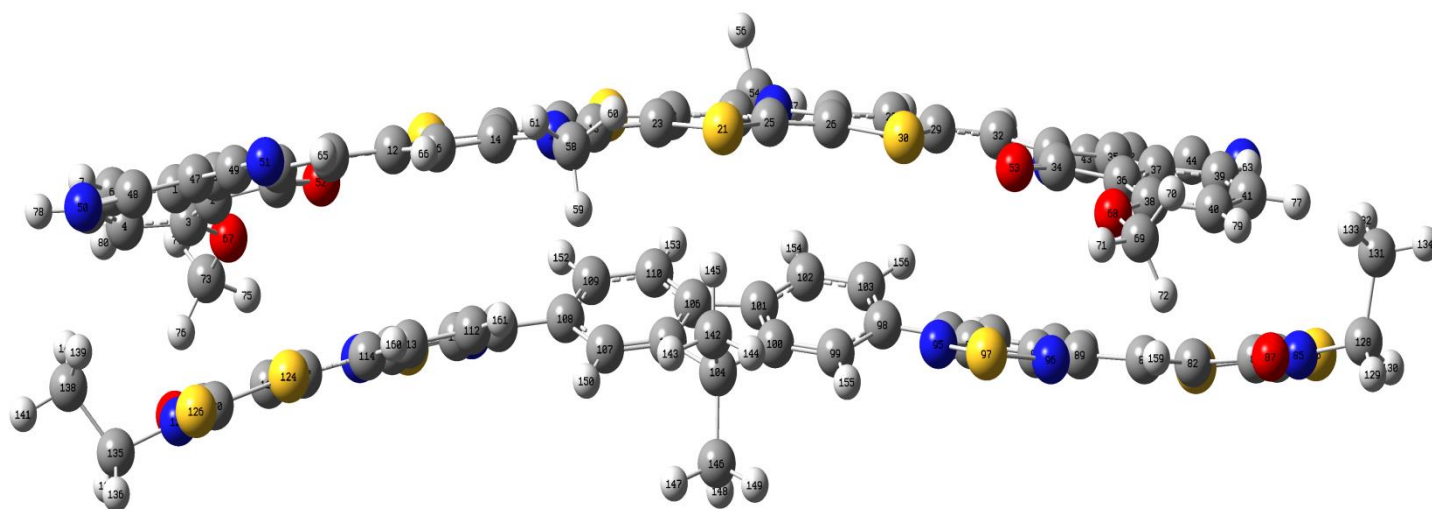
FREA/PBDB-C4



FREA/PBDB-C5



FREA/PBDB-C6



FREA/PBDB-C7

Fig. 3: Frontier molecular orbital diagram of the studied compounds in gas phase:

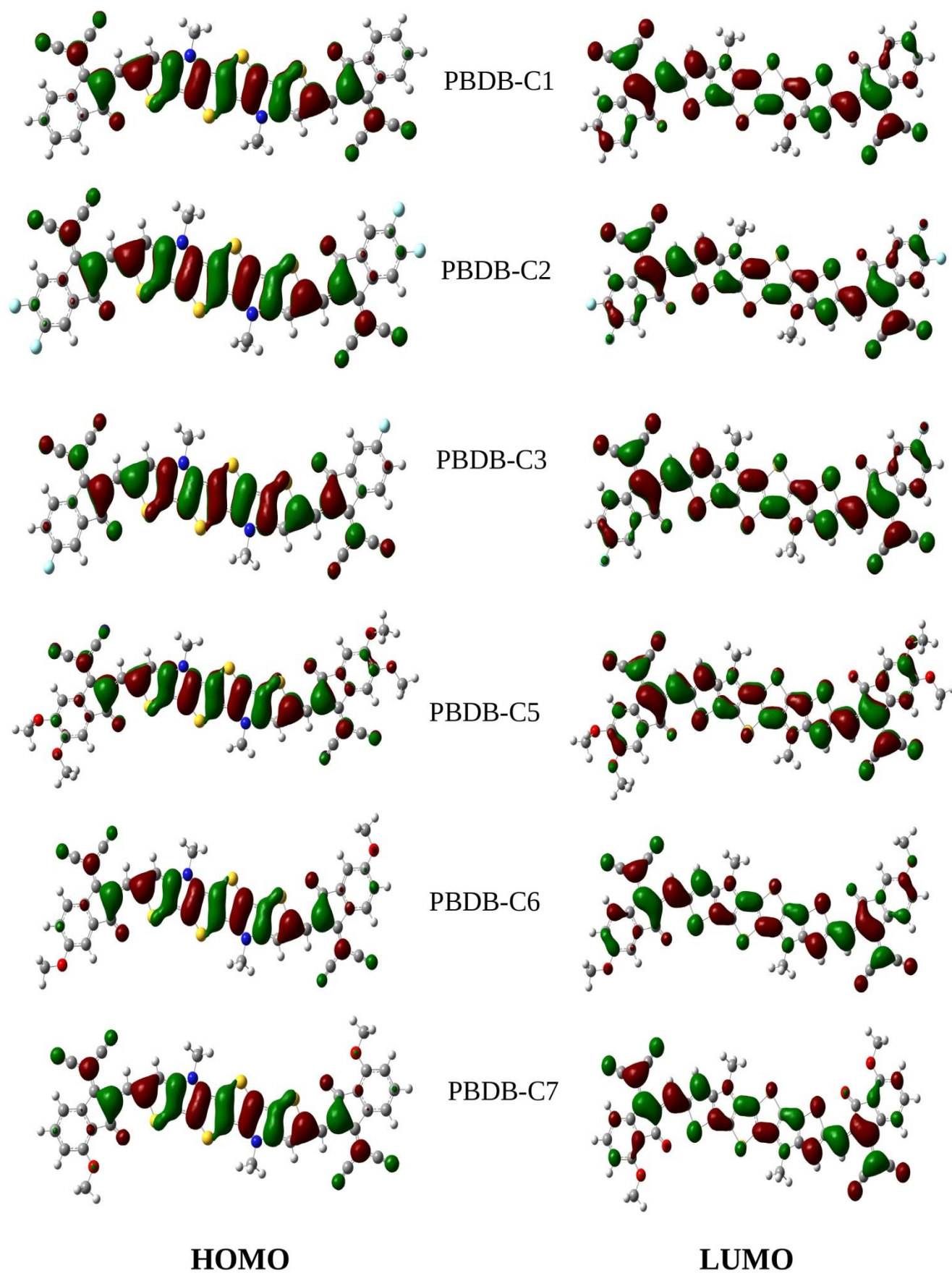


Fig.4: Frontier molecular orbital diagram of the studied compounds in solvent phase:

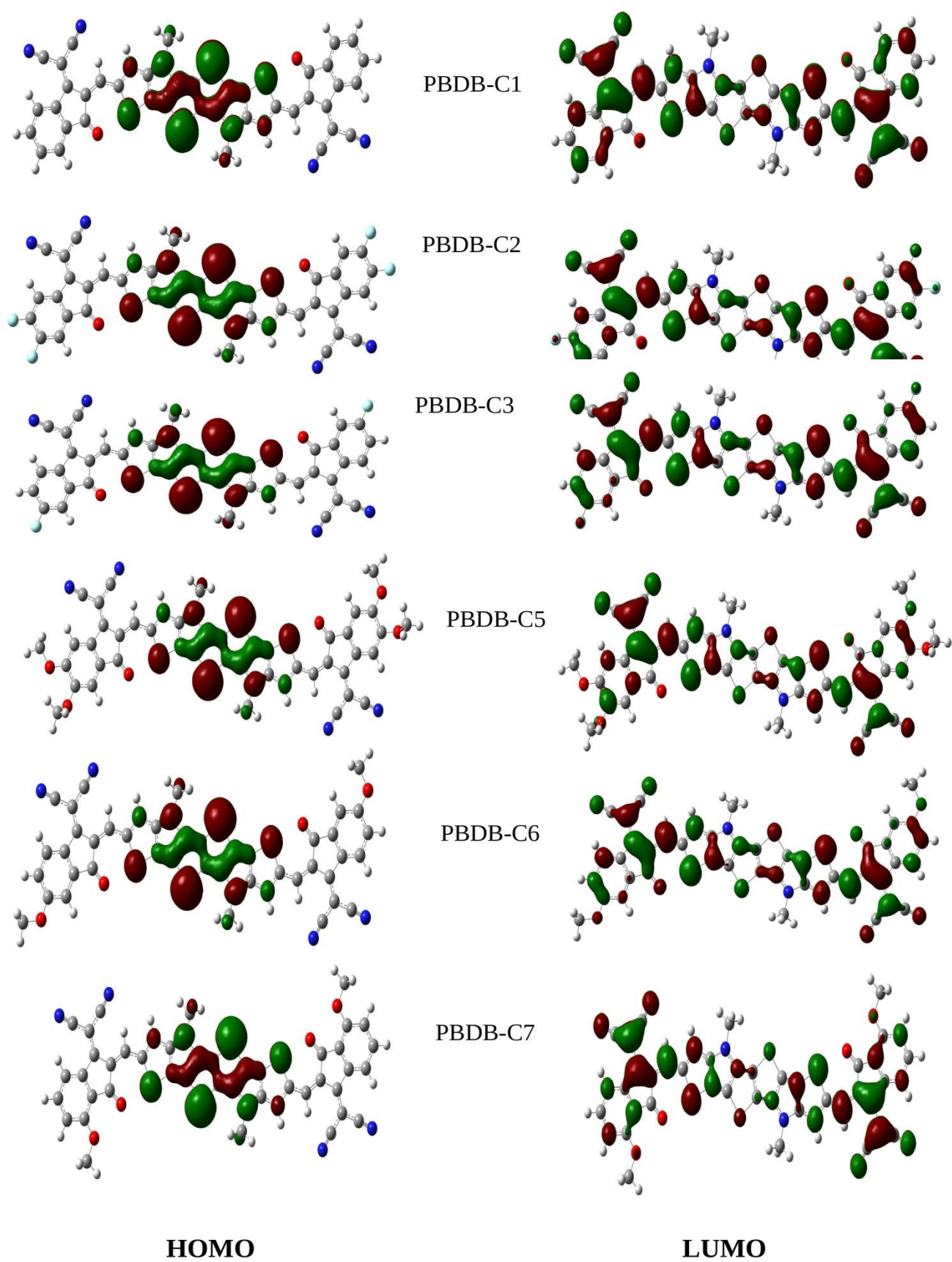


Fig.5: Plot of Density of states of the studied compounds:

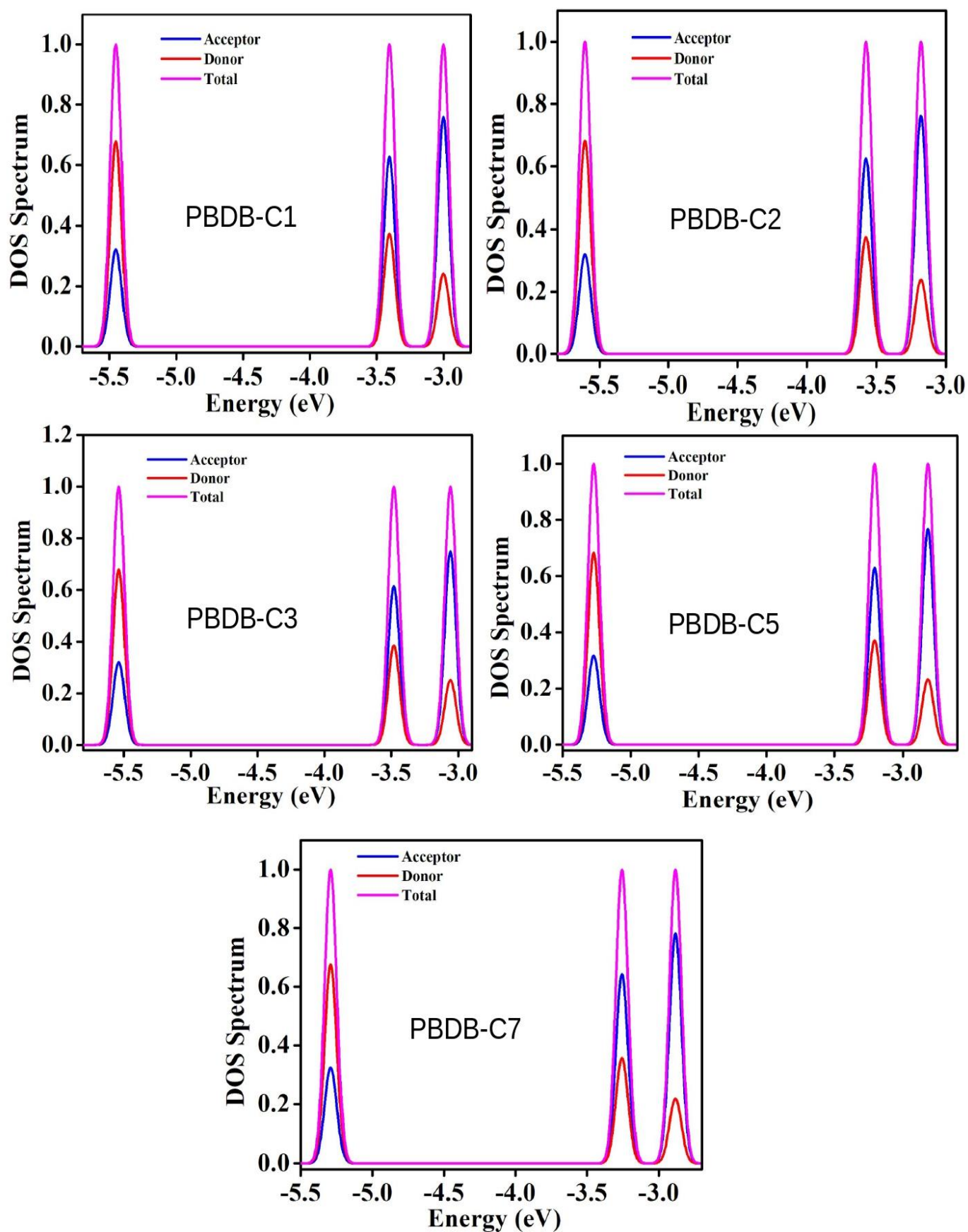


Table S4: Convergence table:

Compounds	Change in energy during convergence (a.u)	Convergence
PBDB-C1	-1.517239×10^{-8}	1×10^{-5}
PBDB-C2	-8.833829×10^{-9}	1×10^{-5}
PBDB-C3	-1.578832×10^{-7}	1×10^{-5}
PBDB-C4	-5.96575×10^{-8}	1×10^{-5}
PBDB-C5	-4.688897×10^{-9}	1×10^{-5}
PBDB-C6	-5.146890×10^{-9}	1×10^{-5}
PBDB-C7	-8.483309×10^{-9}	1×10^{-5}

2. Output file of PBDB-C1:

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Output=/sharehome/chem/Shahnaz/sixth/PBDB.log
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scrdir="/sharehome/chem/Shahnaz/sixth/"
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Gaussian 09, Revision D.01,

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O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,
and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

Gaussian 09: ES64L-G09RevD.01 24-Apr-2013

3-Jan-2019

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C	7.47376	-8.43368	10.73502
C	6.02697	-10.16179	10.00943
C	7.13736	-9.90503	10.68065
C	5.55433	-11.634	9.88043
C	8.00064	-10.99104	11.33997
C	6.31478	-12.62817	10.46652
C	7.61464	-12.27927	11.23878
C	8.65245	-8.25878	11.47188
C	9.66289	-7.22003	12.00995
C	9.50675	-9.38812	12.14205
N	10.48209	-6.53955	12.46329

N	10.14053	-10.22593	12.63922
C	-9.34522	3.21408	-0.06039
C	-10.60056	3.88029	-0.70643
C	-9.77101	1.77218	-0.38314
N	-11.53953	4.34822	-1.20832
N	-10.15968	0.73121	-0.67431
O	-5.35628	5.4996	2.12813
O	4.34833	-8.73755	8.78821
C	3.45173	-0.97642	8.33299
H	3.22154	-0.0001	7.96835
H	2.73197	-1.26409	9.06833
H	4.43052	-0.97049	8.77651
C	-1.5946	-1.32744	1.85635
H	-1.06638	-0.39789	1.72474
H	-0.90674	-2.14006	1.75374
H	-2.35615	-1.40998	1.10778
H	5.57552	-3.36941	9.22353
H	8.8948	-10.72933	11.87113
H	8.20713	-13.05123	11.69132
H	6.01356	-13.65347	10.39343
H	4.66197	-11.88311	9.35217
H	6.8534	-5.57213	10.02981
H	-6.81919	1.4782	1.36192
H	-5.09657	-0.23071	2.48554

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Initialization pass.

 ! Initial Parameters !
 ! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.
! R1	R(1,2)	1.3646	estimate D2E/DX2
! R2	R(1,6)	1.419	estimate D2E/DX2
! R3	R(1,11)	1.5364	estimate D2E/DX2
! R4	R(2,3)	1.4314	estimate D2E/DX2
! R5	R(2,12)	1.5988	estimate D2E/DX2
! R6	R(3,4)	1.4352	estimate D2E/DX2
! R7	R(3,7)	1.0658	estimate D2E/DX2
! R8	R(4,5)	1.4095	estimate D2E/DX2
! R9	R(4,8)	1.076	estimate D2E/DX2
! R10	R(5,6)	1.4033	estimate D2E/DX2
! R11	R(5,9)	1.0772	estimate D2E/DX2

!	R12	R(6,10)	1.0737	estimate	D2E/DX2
!					
!	R13	R(11,13)	1.6515	estimate	D2E/DX2
!					
!	R14	R(11,50)	1.3909	estimate	D2E/DX2
!					
!	R15	R(12,13)	1.5948	estimate	D2E/DX2
!					
!	R16	R(12,55)	1.2579	estimate	D2E/DX2
!					
!	R17	R(13,14)	1.5075	estimate	D2E/DX2
!					
!	R18	R(14,15)	1.7175	estimate	D2E/DX2
!					
!	R19	R(14,71)	1.0752	estimate	D2E/DX2
!					
!	R20	R(15,18)	1.8581	estimate	D2E/DX2
!					
!	R21	R(15,19)	1.3867	estimate	D2E/DX2
!					
!	R22	R(16,17)	1.3076	estimate	D2E/DX2
!					
!	R23	R(16,18)	1.9137	estimate	D2E/DX2
!					
!	R24	R(16,20)	1.6439	estimate	D2E/DX2
!					
!	R25	R(17,19)	1.5578	estimate	D2E/DX2
!					
!	R26	R(17,22)	1.5128	estimate	D2E/DX2
!					
!	R27	R(19,72)	1.0468	estimate	D2E/DX2
!					
!	R28	R(20,21)	1.3601	estimate	D2E/DX2
!					
!	R29	R(20,23)	1.8398	estimate	D2E/DX2
!					
!	R30	R(21,22)	1.5337	estimate	D2E/DX2
!					
!	R31	R(21,26)	1.6329	estimate	D2E/DX2
!					
!	R32	R(22,61)	1.4943	estimate	D2E/DX2
!					
!	R33	R(23,25)	1.853	estimate	D2E/DX2
!					
!	R34	R(24,26)	1.8257	estimate	D2E/DX2
!					
!	R35	R(24,28)	1.8204	estimate	D2E/DX2
!					
!	R36	R(25,26)	1.3786	estimate	D2E/DX2
!					
!	R37	R(25,27)	1.6665	estimate	D2E/DX2
!					
!	R38	R(27,28)	1.3657	estimate	D2E/DX2
!					
!	R39	R(27,34)	1.5564	estimate	D2E/DX2
!					
!	R40	R(28,29)	1.6179	estimate	D2E/DX2
!					
!	R41	R(29,30)	1.3195	estimate	D2E/DX2
!					

!	R42	R(29,33)	1.8407	estimate	D2E/DX2
!					
!	R43	R(30,31)	1.6059	estimate	D2E/DX2
!					
!	R44	R(30,34)	1.541	estimate	D2E/DX2
!					
!	R45	R(31,32)	1.4201	estimate	D2E/DX2
!					
!	R46	R(31,65)	1.0698	estimate	D2E/DX2
!					
!	R47	R(32,33)	1.8514	estimate	D2E/DX2
!					
!	R48	R(32,35)	1.6888	estimate	D2E/DX2
!					
!	R49	R(34,57)	1.4705	estimate	D2E/DX2
!					
!	R50	R(35,36)	1.462	estimate	D2E/DX2
!					
!	R51	R(35,70)	1.0701	estimate	D2E/DX2
!					
!	R52	R(36,37)	1.564	estimate	D2E/DX2
!					
!	R53	R(36,38)	1.6425	estimate	D2E/DX2
!					
!	R54	R(37,39)	1.5737	estimate	D2E/DX2
!					
!	R55	R(37,56)	1.2548	estimate	D2E/DX2
!					
!	R56	R(38,40)	1.5103	estimate	D2E/DX2
!					
!	R57	R(38,45)	1.401	estimate	D2E/DX2
!					
!	R58	R(39,40)	1.3227	estimate	D2E/DX2
!					
!	R59	R(39,41)	1.5516	estimate	D2E/DX2
!					
!	R60	R(40,42)	1.536	estimate	D2E/DX2
!					
!	R61	R(41,43)	1.3821	estimate	D2E/DX2
!					
!	R62	R(41,69)	1.0665	estimate	D2E/DX2
!					
!	R63	R(42,44)	1.3486	estimate	D2E/DX2
!					
!	R64	R(42,66)	1.0724	estimate	D2E/DX2
!					
!	R65	R(43,44)	1.5517	estimate	D2E/DX2
!					
!	R66	R(43,68)	1.0711	estimate	D2E/DX2
!					
!	R67	R(44,67)	1.0732	estimate	D2E/DX2
!					
!	R68	R(45,46)	1.5458	estimate	D2E/DX2
!					
!	R69	R(45,47)	1.5666	estimate	D2E/DX2
!					
!	R70	R(46,48)	1.1574	estimate	D2E/DX2
!					
!	R71	R(47,49)	1.1622	estimate	D2E/DX2
!					

!	R72	R(50,51)	1.5611	estimate	D2E/DX2
!					
!	R73	R(50,52)	1.5377	estimate	D2E/DX2
!					
!	R74	R(51,53)	1.163	estimate	D2E/DX2
!					
!	R75	R(52,54)	1.1487	estimate	D2E/DX2
!					
!	R76	R(57,58)	1.0673	estimate	D2E/DX2
!					
!	R77	R(57,59)	1.0684	estimate	D2E/DX2
!					
!	R78	R(57,60)	1.0746	estimate	D2E/DX2
!					
!	R79	R(61,62)	1.0772	estimate	D2E/DX2
!					
!	R80	R(61,63)	1.0696	estimate	D2E/DX2
!					
!	R81	R(61,64)	1.071	estimate	D2E/DX2
!					
!	A1	A(2,1,6)	123.0221	estimate	D2E/DX2
!					
!	A2	A(2,1,11)	111.7891	estimate	D2E/DX2
!					
!	A3	A(6,1,11)	125.1887	estimate	D2E/DX2
!					
!	A4	A(1,2,3)	118.6466	estimate	D2E/DX2
!					
!	A5	A(1,2,12)	109.4176	estimate	D2E/DX2
!					
!	A6	A(3,2,12)	131.9358	estimate	D2E/DX2
!					
!	A7	A(2,3,4)	119.2366	estimate	D2E/DX2
!					
!	A8	A(2,3,7)	121.3287	estimate	D2E/DX2
!					
!	A9	A(4,3,7)	119.4343	estimate	D2E/DX2
!					
!	A10	A(3,4,5)	120.4803	estimate	D2E/DX2
!					
!	A11	A(3,4,8)	120.6003	estimate	D2E/DX2
!					
!	A12	A(5,4,8)	118.9191	estimate	D2E/DX2
!					
!	A13	A(4,5,6)	119.3323	estimate	D2E/DX2
!					
!	A14	A(4,5,9)	120.4323	estimate	D2E/DX2
!					
!	A15	A(6,5,9)	120.2351	estimate	D2E/DX2
!					
!	A16	A(1,6,5)	119.2556	estimate	D2E/DX2
!					
!	A17	A(1,6,10)	120.9297	estimate	D2E/DX2
!					
!	A18	A(5,6,10)	119.8139	estimate	D2E/DX2
!					
!	A19	A(1,11,13)	109.7152	estimate	D2E/DX2
!					
!	A20	A(1,11,50)	110.3683	estimate	D2E/DX2
!					

!	A21	A(13,11,50)	139.916	estimate	D2E/DX2
!					
!	A22	A(2,12,13)	110.0411	estimate	D2E/DX2
!					
!	A23	A(2,12,55)	123.922	estimate	D2E/DX2
!					
!	A24	A(13,12,55)	126.0362	estimate	D2E/DX2
!					
!	A25	A(11,13,12)	98.9492	estimate	D2E/DX2
!					
!	A26	A(11,13,14)	129.5451	estimate	D2E/DX2
!					
!	A27	A(12,13,14)	131.5046	estimate	D2E/DX2
!					
!	A28	A(13,14,15)	137.005	estimate	D2E/DX2
!					
!	A29	A(13,14,71)	111.3772	estimate	D2E/DX2
!					
!	A30	A(15,14,71)	111.6103	estimate	D2E/DX2
!					
!	A31	A(14,15,18)	140.7924	estimate	D2E/DX2
!					
!	A32	A(14,15,19)	127.396	estimate	D2E/DX2
!					
!	A33	A(18,15,19)	91.7651	estimate	D2E/DX2
!					
!	A34	A(17,16,18)	108.1784	estimate	D2E/DX2
!					
!	A35	A(17,16,20)	105.2224	estimate	D2E/DX2
!					
!	A36	A(18,16,20)	146.5992	estimate	D2E/DX2
!					
!	A37	A(16,17,19)	105.526	estimate	D2E/DX2
!					
!	A38	A(16,17,22)	113.1507	estimate	D2E/DX2
!					
!	A39	A(19,17,22)	141.2869	estimate	D2E/DX2
!					
!	A40	A(15,18,16)	99.7867	estimate	D2E/DX2
!					
!	A41	A(15,19,17)	133.1484	estimate	D2E/DX2
!					
!	A42	A(15,19,72)	113.5926	estimate	D2E/DX2
!					
!	A43	A(17,19,72)	113.2578	estimate	D2E/DX2
!					
!	A44	A(16,20,21)	107.2937	estimate	D2E/DX2
!					
!	A45	A(16,20,23)	143.5016	estimate	D2E/DX2
!					
!	A46	A(21,20,23)	109.2042	estimate	D2E/DX2
!					
!	A47	A(20,21,22)	108.7043	estimate	D2E/DX2
!					
!	A48	A(20,21,26)	113.417	estimate	D2E/DX2
!					
!	A49	A(22,21,26)	137.873	estimate	D2E/DX2
!					
!	A50	A(17,22,21)	103.4616	estimate	D2E/DX2
!					

!	A51	A(17,22,61)	105.204	estimate	D2E/DX2
!					
!	A52	A(21,22,61)	108.9449	estimate	D2E/DX2
!					
!	A53	A(20,23,25)	95.0419	estimate	D2E/DX2
!					
!	A54	A(26,24,28)	94.8889	estimate	D2E/DX2
!					
!	A55	A(23,25,26)	108.4265	estimate	D2E/DX2
!					
!	A56	A(23,25,27)	140.0796	estimate	D2E/DX2
!					
!	A57	A(26,25,27)	111.4206	estimate	D2E/DX2
!					
!	A58	A(21,26,24)	136.195	estimate	D2E/DX2
!					
!	A59	A(21,26,25)	113.2622	estimate	D2E/DX2
!					
!	A60	A(24,26,25)	110.465	estimate	D2E/DX2
!					
!	A61	A(25,27,28)	111.9172	estimate	D2E/DX2
!					
!	A62	A(25,27,34)	140.1982	estimate	D2E/DX2
!					
!	A63	A(28,27,34)	107.8828	estimate	D2E/DX2
!					
!	A64	A(24,28,27)	110.5497	estimate	D2E/DX2
!					
!	A65	A(24,28,29)	140.9663	estimate	D2E/DX2
!					
!	A66	A(27,28,29)	108.4569	estimate	D2E/DX2
!					
!	A67	A(28,29,30)	106.6806	estimate	D2E/DX2
!					
!	A68	A(28,29,33)	143.7763	estimate	D2E/DX2
!					
!	A69	A(30,29,33)	109.536	estimate	D2E/DX2
!					
!	A70	A(29,30,31)	114.1459	estimate	D2E/DX2
!					
!	A71	A(29,30,34)	111.9873	estimate	D2E/DX2
!					
!	A72	A(31,30,34)	133.8532	estimate	D2E/DX2
!					
!	A73	A(30,31,32)	114.9599	estimate	D2E/DX2
!					
!	A74	A(30,31,65)	122.813	estimate	D2E/DX2
!					
!	A75	A(32,31,65)	122.2168	estimate	D2E/DX2
!					
!	A76	A(31,32,33)	104.8427	estimate	D2E/DX2
!					
!	A77	A(31,32,35)	121.1152	estimate	D2E/DX2
!					
!	A78	A(33,32,35)	134.0418	estimate	D2E/DX2
!					
!	A79	A(29,33,32)	96.2012	estimate	D2E/DX2
!					
!	A80	A(27,34,30)	103.5108	estimate	D2E/DX2
!					

!	A81	A(27,34,57)	116.9906	estimate	D2E/DX2
!					
!	A82	A(30,34,57)	111.1663	estimate	D2E/DX2
!					
!	A83	A(32,35,36)	132.0473	estimate	D2E/DX2
!					
!	A84	A(32,35,70)	114.2436	estimate	D2E/DX2
!					
!	A85	A(36,35,70)	113.7083	estimate	D2E/DX2
!					
!	A86	A(35,36,37)	127.1699	estimate	D2E/DX2
!					
!	A87	A(35,36,38)	132.5497	estimate	D2E/DX2
!					
!	A88	A(37,36,38)	100.2798	estimate	D2E/DX2
!					
!	A89	A(36,37,39)	108.8039	estimate	D2E/DX2
!					
!	A90	A(36,37,56)	125.8102	estimate	D2E/DX2
!					
!	A91	A(39,37,56)	125.3858	estimate	D2E/DX2
!					
!	A92	A(36,38,40)	107.5452	estimate	D2E/DX2
!					
!	A93	A(36,38,45)	143.3103	estimate	D2E/DX2
!					
!	A94	A(40,38,45)	109.1444	estimate	D2E/DX2
!					
!	A95	A(37,39,40)	110.1423	estimate	D2E/DX2
!					
!	A96	A(37,39,41)	131.0342	estimate	D2E/DX2
!					
!	A97	A(40,39,41)	118.8235	estimate	D2E/DX2
!					
!	A98	A(38,40,39)	113.2274	estimate	D2E/DX2
!					
!	A99	A(38,40,42)	123.2404	estimate	D2E/DX2
!					
!	A100	A(39,40,42)	123.5322	estimate	D2E/DX2
!					
!	A101	A(39,41,43)	118.6635	estimate	D2E/DX2
!					
!	A102	A(39,41,69)	121.1774	estimate	D2E/DX2
!					
!	A103	A(43,41,69)	120.1591	estimate	D2E/DX2
!					
!	A104	A(40,42,44)	118.8354	estimate	D2E/DX2
!					
!	A105	A(40,42,66)	120.5733	estimate	D2E/DX2
!					
!	A106	A(44,42,66)	120.5912	estimate	D2E/DX2
!					
!	A107	A(41,43,44)	120.6793	estimate	D2E/DX2
!					
!	A108	A(41,43,68)	120.3237	estimate	D2E/DX2
!					
!	A109	A(44,43,68)	118.9969	estimate	D2E/DX2
!					
!	A110	A(42,44,43)	119.4649	estimate	D2E/DX2
!					

!	A111	A(42,44,67)	119.8308	estimate	D2E/DX2
!	A112	A(43,44,67)	120.7042	estimate	D2E/DX2
!	A113	A(38,45,46)	144.7756	estimate	D2E/DX2
!	A114	A(38,45,47)	126.4243	estimate	D2E/DX2
!	A115	A(46,45,47)	88.8	estimate	D2E/DX2
!	A116	A(11,50,51)	124.5614	estimate	D2E/DX2
!	A117	A(11,50,52)	140.2356	estimate	D2E/DX2
!	A118	A(51,50,52)	95.2	estimate	D2E/DX2
!	A119	A(34,57,58)	109.6869	estimate	D2E/DX2
!	A120	A(34,57,59)	109.8077	estimate	D2E/DX2
!	A121	A(34,57,60)	108.9423	estimate	D2E/DX2
!	A122	A(58,57,59)	109.6422	estimate	D2E/DX2
!	A123	A(58,57,60)	109.4146	estimate	D2E/DX2
!	A124	A(59,57,60)	109.3304	estimate	D2E/DX2
!	A125	A(22,61,62)	108.9438	estimate	D2E/DX2
!	A126	A(22,61,63)	110.4838	estimate	D2E/DX2
!	A127	A(22,61,64)	109.5888	estimate	D2E/DX2
!	A128	A(62,61,63)	109.1791	estimate	D2E/DX2
!	A129	A(62,61,64)	109.2545	estimate	D2E/DX2
!	A130	A(63,61,64)	109.3703	estimate	D2E/DX2
!	A131	L(45,46,48,2,-1)	186.243	estimate	D2E/DX2
!	A132	L(45,47,49,41,-1)	180.0009	estimate	D2E/DX2
!	A133	L(50,51,53,3,-1)	181.5506	estimate	D2E/DX2
!	A134	L(50,52,54,16,-1)	184.6602	estimate	D2E/DX2
!	A135	L(45,46,48,2,-2)	179.6612	estimate	D2E/DX2
!	A136	L(45,47,49,41,-2)	180.0	estimate	D2E/DX2
!	A137	L(50,51,53,3,-2)	179.1728	estimate	D2E/DX2
!	A138	L(50,52,54,16,-2)	180.4428	estimate	D2E/DX2
!	D1	D(6,1,2,3)	-1.0184	estimate	D2E/DX2
!	D2	D(6,1,2,12)	178.9889	estimate	D2E/DX2
!					

!	D3	D(11,1,2,3)	179.0977	estimate D2E/DX2
!				
!	D4	D(11,1,2,12)	-0.8951	estimate D2E/DX2
!				
!	D5	D(2,1,6,5)	-0.4676	estimate D2E/DX2
!				
!	D6	D(2,1,6,10)	179.8316	estimate D2E/DX2
!				
!	D7	D(11,1,6,5)	179.4006	estimate D2E/DX2
!				
!	D8	D(11,1,6,10)	-0.3003	estimate D2E/DX2
!				
!	D9	D(2,1,11,13)	2.5658	estimate D2E/DX2
!				
!	D10	D(2,1,11,50)	-177.2168	estimate D2E/DX2
!				
!	D11	D(6,1,11,13)	-177.3151	estimate D2E/DX2
!				
!	D12	D(6,1,11,50)	2.9023	estimate D2E/DX2
!				
!	D13	D(1,2,3,4)	1.7644	estimate D2E/DX2
!				
!	D14	D(1,2,3,7)	-178.4591	estimate D2E/DX2
!				
!	D15	D(12,2,3,4)	-178.2448	estimate D2E/DX2
!				
!	D16	D(12,2,3,7)	1.5316	estimate D2E/DX2
!				
!	D17	D(1,2,12,13)	-1.1557	estimate D2E/DX2
!				
!	D18	D(1,2,12,55)	178.5441	estimate D2E/DX2
!				
!	D19	D(3,2,12,13)	178.8529	estimate D2E/DX2
!				
!	D20	D(3,2,12,55)	-1.4473	estimate D2E/DX2
!				
!	D21	D(2,3,4,5)	-1.077	estimate D2E/DX2
!				
!	D22	D(2,3,4,8)	178.7462	estimate D2E/DX2
!				
!	D23	D(7,3,4,5)	179.1422	estimate D2E/DX2
!				
!	D24	D(7,3,4,8)	-1.0346	estimate D2E/DX2
!				
!	D25	D(3,4,5,6)	-0.401	estimate D2E/DX2
!				
!	D26	D(3,4,5,9)	179.3816	estimate D2E/DX2
!				
!	D27	D(8,4,5,6)	179.7729	estimate D2E/DX2
!				
!	D28	D(8,4,5,9)	-0.4445	estimate D2E/DX2
!				
!	D29	D(4,5,6,1)	1.1741	estimate D2E/DX2
!				
!	D30	D(4,5,6,10)	-179.1217	estimate D2E/DX2
!				
!	D31	D(9,5,6,1)	-178.6089	estimate D2E/DX2
!				
!	D32	D(9,5,6,10)	1.0953	estimate D2E/DX2
!				

!	D33	D(1,11,13,12)	-2.9232	estimate D2E/DX2
!				
!	D34	D(1,11,13,14)	177.4242	estimate D2E/DX2
!				
!	D35	D(50,11,13,12)	176.7603	estimate D2E/DX2
!				
!	D36	D(50,11,13,14)	-2.8923	estimate D2E/DX2
!				
!	D37	D(1,11,50,51)	-2.6456	estimate D2E/DX2
!				
!	D38	D(1,11,50,52)	178.1648	estimate D2E/DX2
!				
!	D39	D(13,11,50,51)	177.6723	estimate D2E/DX2
!				
!	D40	D(13,11,50,52)	-1.5173	estimate D2E/DX2
!				
!	D41	D(2,12,13,11)	2.4118	estimate D2E/DX2
!				
!	D42	D(2,12,13,14)	-177.946	estimate D2E/DX2
!				
!	D43	D(55,12,13,11)	-177.2801	estimate D2E/DX2
!				
!	D44	D(55,12,13,14)	2.3621	estimate D2E/DX2
!				
!	D45	D(11,13,14,15)	-175.7068	estimate D2E/DX2
!				
!	D46	D(11,13,14,71)	5.4119	estimate D2E/DX2
!				
!	D47	D(12,13,14,15)	4.7515	estimate D2E/DX2
!				
!	D48	D(12,13,14,71)	-174.1298	estimate D2E/DX2
!				
!	D49	D(13,14,15,18)	3.9633	estimate D2E/DX2
!				
!	D50	D(13,14,15,19)	-172.7799	estimate D2E/DX2
!				
!	D51	D(71,14,15,18)	-177.1572	estimate D2E/DX2
!				
!	D52	D(71,14,15,19)	6.0996	estimate D2E/DX2
!				
!	D53	D(14,15,18,16)	-172.1565	estimate D2E/DX2
!				
!	D54	D(19,15,18,16)	5.2554	estimate D2E/DX2
!				
!	D55	D(14,15,19,17)	164.4177	estimate D2E/DX2
!				
!	D56	D(14,15,19,72)	-15.1653	estimate D2E/DX2
!				
!	D57	D(18,15,19,17)	-13.5233	estimate D2E/DX2
!				
!	D58	D(18,15,19,72)	166.8938	estimate D2E/DX2
!				
!	D59	D(18,16,17,19)	-7.2627	estimate D2E/DX2
!				
!	D60	D(18,16,17,22)	171.0239	estimate D2E/DX2
!				
!	D61	D(20,16,17,19)	172.724	estimate D2E/DX2
!				
!	D62	D(20,16,17,22)	-8.9895	estimate D2E/DX2
!				

!	D63	D(17,16,18,15)	1.7087	estimate D2E/DX2
!				
!	D64	D(20,16,18,15)	-178.2679	estimate D2E/DX2
!				
!	D65	D(17,16,20,21)	-0.5471	estimate D2E/DX2
!				
!	D66	D(17,16,20,23)	179.7672	estimate D2E/DX2
!				
!	D67	D(18,16,20,21)	179.4299	estimate D2E/DX2
!				
!	D68	D(18,16,20,23)	-0.2558	estimate D2E/DX2
!				
!	D69	D(16,17,19,15)	16.4088	estimate D2E/DX2
!				
!	D70	D(16,17,19,72)	-164.0072	estimate D2E/DX2
!				
!	D71	D(22,17,19,15)	-161.0717	estimate D2E/DX2
!				
!	D72	D(22,17,19,72)	18.5123	estimate D2E/DX2
!				
!	D73	D(16,17,22,21)	14.5347	estimate D2E/DX2
!				
!	D74	D(16,17,22,61)	-99.7325	estimate D2E/DX2
!				
!	D75	D(19,17,22,21)	-168.1055	estimate D2E/DX2
!				
!	D76	D(19,17,22,61)	77.6273	estimate D2E/DX2
!				
!	D77	D(16,20,21,22)	9.4417	estimate D2E/DX2
!				
!	D78	D(16,20,21,26)	-171.2664	estimate D2E/DX2
!				
!	D79	D(23,20,21,22)	-170.7563	estimate D2E/DX2
!				
!	D80	D(23,20,21,26)	8.5357	estimate D2E/DX2
!				
!	D81	D(16,20,23,25)	173.5145	estimate D2E/DX2
!				
!	D82	D(21,20,23,25)	-6.1678	estimate D2E/DX2
!				
!	D83	D(20,21,22,17)	-14.1998	estimate D2E/DX2
!				
!	D84	D(20,21,22,61)	97.3478	estimate D2E/DX2
!				
!	D85	D(26,21,22,17)	166.7689	estimate D2E/DX2
!				
!	D86	D(26,21,22,61)	-81.6835	estimate D2E/DX2
!				
!	D87	D(20,21,26,24)	175.7181	estimate D2E/DX2
!				
!	D88	D(20,21,26,25)	-7.9045	estimate D2E/DX2
!				
!	D89	D(22,21,26,24)	-5.2818	estimate D2E/DX2
!				
!	D90	D(22,21,26,25)	171.0956	estimate D2E/DX2
!				
!	D91	D(17,22,61,62)	54.6446	estimate D2E/DX2
!				
!	D92	D(17,22,61,63)	174.5782	estimate D2E/DX2
!				

!	D93	D(17,22,61,64)	-64.8414	estimate	D2E/DX2
!					
!	D94	D(21,22,61,62)	-55.7412	estimate	D2E/DX2
!					
!	D95	D(21,22,61,63)	64.1924	estimate	D2E/DX2
!					
!	D96	D(21,22,61,64)	-175.2272	estimate	D2E/DX2
!					
!	D97	D(20,23,25,26)	1.5375	estimate	D2E/DX2
!					
!	D98	D(20,23,25,27)	177.9544	estimate	D2E/DX2
!					
!	D99	D(28,24,26,21)	178.4939	estimate	D2E/DX2
!					
!	D100	D(28,24,26,25)	2.0461	estimate	D2E/DX2
!					
!	D101	D(26,24,28,27)	-7.03	estimate	D2E/DX2
!					
!	D102	D(26,24,28,29)	170.7364	estimate	D2E/DX2
!					
!	D103	D(23,25,26,21)	2.82	estimate	D2E/DX2
!					
!	D104	D(23,25,26,24)	-179.8557	estimate	D2E/DX2
!					
!	D105	D(27,25,26,21)	-174.7109	estimate	D2E/DX2
!					
!	D106	D(27,25,26,24)	2.6134	estimate	D2E/DX2
!					
!	D107	D(23,25,27,28)	175.566	estimate	D2E/DX2
!					
!	D108	D(23,25,27,34)	-5.0139	estimate	D2E/DX2
!					
!	D109	D(26,25,27,28)	-8.0857	estimate	D2E/DX2
!					
!	D110	D(26,25,27,34)	171.3344	estimate	D2E/DX2
!					
!	D111	D(25,27,28,24)	9.2723	estimate	D2E/DX2
!					
!	D112	D(25,27,28,29)	-169.2449	estimate	D2E/DX2
!					
!	D113	D(34,27,28,24)	-170.3376	estimate	D2E/DX2
!					
!	D114	D(34,27,28,29)	11.1451	estimate	D2E/DX2
!					
!	D115	D(25,27,34,30)	168.2839	estimate	D2E/DX2
!					
!	D116	D(25,27,34,57)	45.6598	estimate	D2E/DX2
!					
!	D117	D(28,27,34,30)	-12.2814	estimate	D2E/DX2
!					
!	D118	D(28,27,34,57)	-134.9055	estimate	D2E/DX2
!					
!	D119	D(24,28,29,30)	176.4513	estimate	D2E/DX2
!					
!	D120	D(24,28,29,33)	-4.7124	estimate	D2E/DX2
!					
!	D121	D(27,28,29,30)	-5.7536	estimate	D2E/DX2
!					
!	D122	D(27,28,29,33)	173.0828	estimate	D2E/DX2
!					

!	D123	D(28,29,30,31)	178.6097	estimate	D2E/DX2
!					
!	D124	D(28,29,30,34)	-2.5437	estimate	D2E/DX2
!					
!	D125	D(33,29,30,31)	-0.6607	estimate	D2E/DX2
!					
!	D126	D(33,29,30,34)	178.1859	estimate	D2E/DX2
!					
!	D127	D(28,29,33,32)	178.8155	estimate	D2E/DX2
!					
!	D128	D(30,29,33,32)	-2.3673	estimate	D2E/DX2
!					
!	D129	D(29,30,31,32)	4.6906	estimate	D2E/DX2
!					
!	D130	D(29,30,31,65)	-176.4539	estimate	D2E/DX2
!					
!	D131	D(34,30,31,32)	-173.8261	estimate	D2E/DX2
!					
!	D132	D(34,30,31,65)	5.0293	estimate	D2E/DX2
!					
!	D133	D(29,30,34,27)	8.8696	estimate	D2E/DX2
!					
!	D134	D(29,30,34,57)	135.2801	estimate	D2E/DX2
!					
!	D135	D(31,30,34,27)	-172.59	estimate	D2E/DX2
!					
!	D136	D(31,30,34,57)	-46.1795	estimate	D2E/DX2
!					
!	D137	D(30,31,32,33)	-5.8527	estimate	D2E/DX2
!					
!	D138	D(30,31,32,35)	173.9735	estimate	D2E/DX2
!					
!	D139	D(65,31,32,33)	175.2842	estimate	D2E/DX2
!					
!	D140	D(65,31,32,35)	-4.8896	estimate	D2E/DX2
!					
!	D141	D(31,32,33,29)	4.7661	estimate	D2E/DX2
!					
!	D142	D(35,32,33,29)	-175.0269	estimate	D2E/DX2
!					
!	D143	D(31,32,35,36)	176.3632	estimate	D2E/DX2
!					
!	D144	D(31,32,35,70)	-3.2979	estimate	D2E/DX2
!					
!	D145	D(33,32,35,36)	-3.8705	estimate	D2E/DX2
!					
!	D146	D(33,32,35,70)	176.4684	estimate	D2E/DX2
!					
!	D147	D(27,34,57,58)	-61.1579	estimate	D2E/DX2
!					
!	D148	D(27,34,57,59)	59.3949	estimate	D2E/DX2
!					
!	D149	D(27,34,57,60)	179.1034	estimate	D2E/DX2
!					
!	D150	D(30,34,57,58)	-179.7364	estimate	D2E/DX2
!					
!	D151	D(30,34,57,59)	-59.1836	estimate	D2E/DX2
!					
!	D152	D(30,34,57,60)	60.5249	estimate	D2E/DX2
!					

!	D153	D(32,35,36,37)	-0.2241	estimate	D2E/DX2
!					
!	D154	D(32,35,36,38)	-179.8806	estimate	D2E/DX2
!					
!	D155	D(70,35,36,37)	179.4384	estimate	D2E/DX2
!					
!	D156	D(70,35,36,38)	-0.2182	estimate	D2E/DX2
!					
!	D157	D(35,36,37,39)	-179.8638	estimate	D2E/DX2
!					
!	D158	D(35,36,37,56)	0.0319	estimate	D2E/DX2
!					
!	D159	D(38,36,37,39)	-0.1209	estimate	D2E/DX2
!					
!	D160	D(38,36,37,56)	179.7747	estimate	D2E/DX2
!					
!	D161	D(35,36,38,40)	-179.9824	estimate	D2E/DX2
!					
!	D162	D(35,36,38,45)	0.1681	estimate	D2E/DX2
!					
!	D163	D(37,36,38,40)	0.2957	estimate	D2E/DX2
!					
!	D164	D(37,36,38,45)	-179.5537	estimate	D2E/DX2
!					
!	D165	D(36,37,39,40)	-0.1169	estimate	D2E/DX2
!					
!	D166	D(36,37,39,41)	179.8162	estimate	D2E/DX2
!					
!	D167	D(56,37,39,40)	179.9869	estimate	D2E/DX2
!					
!	D168	D(56,37,39,41)	-0.08	estimate	D2E/DX2
!					
!	D169	D(36,38,40,39)	-0.4123	estimate	D2E/DX2
!					
!	D170	D(36,38,40,42)	179.5884	estimate	D2E/DX2
!					
!	D171	D(45,38,40,39)	179.4925	estimate	D2E/DX2
!					
!	D172	D(45,38,40,42)	-0.5068	estimate	D2E/DX2
!					
!	D173	D(36,38,45,46)	0.0585	estimate	D2E/DX2
!					
!	D174	D(36,38,45,47)	179.9126	estimate	D2E/DX2
!					
!	D175	D(40,38,45,46)	-179.7895	estimate	D2E/DX2
!					
!	D176	D(40,38,45,47)	0.0645	estimate	D2E/DX2
!					
!	D177	D(37,39,40,38)	0.3328	estimate	D2E/DX2
!					
!	D178	D(37,39,40,42)	-179.6679	estimate	D2E/DX2
!					
!	D179	D(41,39,40,38)	-179.6097	estimate	D2E/DX2
!					
!	D180	D(41,39,40,42)	0.3896	estimate	D2E/DX2
!					
!	D181	D(37,39,41,43)	179.749	estimate	D2E/DX2
!					
!	D182	D(37,39,41,69)	-0.2589	estimate	D2E/DX2
!					

!	D183	D(40,39,41,43)	-0.3227	estimate	D2E/DX2
!					
!	D184	D(40,39,41,69)	179.6694	estimate	D2E/DX2
!					
!	D185	D(38,40,42,44)	179.838	estimate	D2E/DX2
!					
!	D186	D(38,40,42,66)	-0.1824	estimate	D2E/DX2
!					
!	D187	D(39,40,42,44)	-0.1612	estimate	D2E/DX2
!					
!	D188	D(39,40,42,66)	179.8184	estimate	D2E/DX2
!					
!	D189	D(39,41,43,44)	0.0361	estimate	D2E/DX2
!					
!	D190	D(39,41,43,68)	-179.9654	estimate	D2E/DX2
!					
!	D191	D(69,41,43,44)	-179.9561	estimate	D2E/DX2
!					
!	D192	D(69,41,43,68)	0.0424	estimate	D2E/DX2
!					
!	D193	D(40,42,44,43)	-0.14	estimate	D2E/DX2
!					
!	D194	D(40,42,44,67)	179.851	estimate	D2E/DX2
!					
!	D195	D(66,42,44,43)	179.8804	estimate	D2E/DX2
!					
!	D196	D(66,42,44,67)	-0.1286	estimate	D2E/DX2
!					
!	D197	D(41,43,44,42)	0.1906	estimate	D2E/DX2
!					
!	D198	D(41,43,44,67)	-179.8003	estimate	D2E/DX2
!					
!	D199	D(68,43,44,42)	-179.8079	estimate	D2E/DX2
!					
!	D200	D(68,43,44,67)	0.2012	estimate	D2E/DX2
!					

 Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06
 Number of steps in this run= 429 maximum allowed number of steps= 432.
 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4
 Framework group C1[X(C42H18N6O2S4)]
 Deg. of freedom 210
 Full point group C1 NOp 1
 Largest Abelian subgroup C1 NOp 1
 Largest concise Abelian subgroup C1 NOp 1
 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-12.305458	-0.170767	-0.318804
2	6	0	-11.791538	-1.432760	-0.245774
3	6	0	-12.693306	-2.543890	-0.278690
4	6	0	-14.100191	-2.300795	-0.425321
5	6	0	-14.592716	-0.983086	-0.513106
6	6	0	-13.693913	0.092561	-0.447224
7	1	0	-12.340405	-3.546538	-0.200091

8	1	0	-14.795671	-3.120506	-0.472885
9	1	0	-15.647723	-0.801804	-0.633110
10	1	0	-14.062095	1.099800	-0.499083
11	6	0	-11.204336	0.898424	-0.247842
12	6	0	-10.198678	-1.352346	-0.133542
13	6	0	-9.724146	0.169695	-0.173241
14	6	0	-8.349925	0.788764	-0.143869
15	6	0	-6.723284	0.237622	-0.157349
16	6	0	-3.987830	-0.647285	0.083136
17	6	0	-4.094885	0.631664	0.333641
18	16	0	-5.735413	-1.330283	-0.293120
19	6	0	-5.575464	0.996526	0.014835
20	6	0	-2.385187	-0.982922	0.228564
21	6	0	-1.755073	0.181119	0.541366
22	7	0	-2.814355	1.244597	0.856171
23	16	0	-1.141342	-2.334200	0.120119
24	16	0	1.278875	1.215903	0.705874
25	6	0	0.326053	-1.221773	0.326794
26	6	0	-0.126533	0.068827	0.500423
27	6	0	1.987080	-1.303761	0.433434
28	6	0	2.555998	-0.063554	0.491720
29	6	0	4.155126	-0.224341	0.305948
30	6	0	4.405427	-1.519726	0.283111
31	6	0	5.954219	-1.885834	0.068423
32	6	0	6.834910	-0.772120	0.039994
33	16	0	5.727033	0.710115	0.095729
34	7	0	3.130405	-2.357632	0.499828
35	6	0	8.508944	-0.984777	-0.025791
36	6	0	9.613439	-0.032898	-0.132604
37	6	0	9.512640	1.525198	-0.223247
38	6	0	11.243173	-0.225600	-0.200008
39	6	0	10.964914	2.122252	-0.327299
40	6	0	11.860114	1.148795	-0.306820
41	6	0	11.457334	3.589015	-0.443701
42	6	0	13.375482	1.387832	-0.383731
43	6	0	12.816672	3.828254	-0.515258
44	6	0	13.830166	2.653775	-0.480759
45	6	0	12.261791	-1.187509	-0.197078
46	6	0	12.569172	-2.701030	-0.131604
47	6	0	13.801424	-0.912231	-0.287173
48	7	0	12.921330	-3.802807	-0.090034
49	7	0	14.943623	-0.708030	-0.354010
50	6	0	-11.764200	2.171582	-0.261529
51	6	0	-13.291243	2.466108	-0.397460
52	6	0	-11.343204	3.648791	-0.189685
53	7	0	-14.423726	2.716566	-0.482793
54	7	0	-11.119852	4.774072	-0.132008
55	8	0	-9.450950	-2.358040	-0.024427
56	8	0	8.450893	2.193828	-0.216650
57	6	0	3.062481	-3.476813	-0.451520
58	1	0	2.169968	-4.037572	-0.283855
59	1	0	3.068692	-3.102308	-1.452146
60	1	0	3.916516	-4.112190	-0.304206
61	6	0	-2.994776	1.326080	2.337263
62	1	0	-3.243902	0.347948	2.713547
63	1	0	-2.094710	1.664115	2.805935
64	1	0	-3.790766	2.005472	2.565200
65	1	0	6.304137	-2.892239	-0.027383
66	1	0	14.059800	0.562420	-0.360335
67	1	0	14.885912	2.839292	-0.533089

68	1	0	13.185897	4.830529	-0.595584
69	1	0	10.768066	4.402469	-0.468826
70	1	0	8.823924	-2.006755	0.013054
71	1	0	-8.404268	1.860932	-0.084259
72	1	0	-5.735380	2.026318	-0.083736

Rotational constants (GHZ): 0.1681493 0.0078165 0.0075097

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6042.0582661359 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T
Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6041.9819955852 Hartrees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.73D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1

AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-yADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlgl= 2001

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 IlCent= 200000004 NGrid=

0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0=

0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Integral accuracy reduced to 1.0D-05 until final iterations.

Initial convergence to 1.0D-05 achieved. Increase integral accuracy.

SCF Done: E(RB3LYP) = -3682.23033302 A.U. after 16 cycles

NFock= 16 Conv=0.86D-08 -V/T= 2.0084

Population analysis using the SCF density.

Orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

[illegible]

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
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 (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

The electronic state is 1-A.

Alpha occ. eigenvalues --	-88.94057	-88.93638	-88.93626	-88.93170	-19.17563
Alpha occ. eigenvalues --	-19.17465	-14.40549	-14.39954	-14.36488	-14.36324
Alpha occ. eigenvalues --	-14.36294	-14.36083	-10.32797	-10.32453	-10.32226
Alpha occ. eigenvalues --	-10.32029	-10.31803	-10.30973	-10.30757	-10.30613
Alpha occ. eigenvalues --	-10.30410	-10.29908	-10.29709	-10.29320	-10.28609
Alpha occ. eigenvalues --	-10.28503	-10.28269	-10.28264	-10.28132	-10.27970
Alpha occ. eigenvalues --	-10.27836	-10.27715	-10.27287	-10.26769	-10.26663
Alpha occ. eigenvalues --	-10.26629	-10.26442	-10.26250	-10.25899	-10.24950
Alpha occ. eigenvalues --	-10.24743	-10.24387	-10.24261	-10.23962	-10.23384
Alpha occ. eigenvalues --	-10.23188	-10.23150	-10.23038	-10.22969	-10.22800
Alpha occ. eigenvalues --	-10.22495	-10.22341	-10.20559	-10.20043	-7.99769
Alpha occ. eigenvalues --	-7.99407	-7.99294	-7.98909	-5.96292	-5.95927
Alpha occ. eigenvalues --	-5.95918	-5.95817	-5.95545	-5.95426	-5.95419
Alpha occ. eigenvalues --	-5.95292	-5.95066	-5.94936	-5.94829	-5.94387
Alpha occ. eigenvalues --	-1.04779	-1.04355	-0.97103	-0.96542	-0.95812
Alpha occ. eigenvalues --	-0.95709	-0.93309	-0.93124	-0.90174	-0.90074
Alpha occ. eigenvalues --	-0.88876	-0.87872	-0.86995	-0.84945	-0.84066
Alpha occ. eigenvalues --	-0.83906	-0.81397	-0.80857	-0.79735	-0.79083
Alpha occ. eigenvalues --	-0.77726	-0.77026	-0.76697	-0.76339	-0.74601
Alpha occ. eigenvalues --	-0.73498	-0.72832	-0.72394	-0.71320	-0.70254
Alpha occ. eigenvalues --	-0.70083	-0.68407	-0.68188	-0.67953	-0.67153
Alpha occ. eigenvalues --	-0.63506	-0.62710	-0.61259	-0.60901	-0.60652
Alpha occ. eigenvalues --	-0.59199	-0.58036	-0.56609	-0.56156	-0.56028
Alpha occ. eigenvalues --	-0.55058	-0.54267	-0.54005	-0.53706	-0.53504

Alpha occ. eigenvalues -- 0.50034	-0.53330	-0.52913	-0.51111	-0.50698	-
Alpha occ. eigenvalues -- 0.47817	-0.49560	-0.49485	-0.48838	-0.48055	-
Alpha occ. eigenvalues -- 0.45649	-0.46970	-0.46819	-0.46579	-0.45905	-
Alpha occ. eigenvalues -- 0.44300	-0.45581	-0.45270	-0.44816	-0.44532	-
Alpha occ. eigenvalues -- 0.42692	-0.44165	-0.44038	-0.43249	-0.43061	-
Alpha occ. eigenvalues -- 0.41397	-0.41925	-0.41840	-0.41765	-0.41670	-
Alpha occ. eigenvalues -- 0.39806	-0.40663	-0.40286	-0.40103	-0.40013	-
Alpha occ. eigenvalues -- 0.38948	-0.39648	-0.39504	-0.39435	-0.39419	-
Alpha occ. eigenvalues -- 0.37603	-0.38898	-0.38757	-0.38208	-0.37745	-
Alpha occ. eigenvalues -- 0.36098	-0.37500	-0.37400	-0.36770	-0.36725	-
Alpha occ. eigenvalues -- 0.34393	-0.35882	-0.35725	-0.34755	-0.34615	-
Alpha occ. eigenvalues -- 0.30984	-0.34196	-0.32687	-0.31988	-0.31553	-
Alpha occ. eigenvalues -- 0.27829	-0.30373	-0.29776	-0.29708	-0.28032	-
Alpha occ. eigenvalues -- 0.26768	-0.27760	-0.27733	-0.27657	-0.26926	-
Alpha occ. eigenvalues -- 0.24162	-0.26618	-0.26211	-0.25321	-0.24635	-
Alpha occ. eigenvalues --	-0.23177				
Alpha virt. eigenvalues -- 0.07489	-0.13894	-0.13247	-0.10931	-0.10367	-
Alpha virt. eigenvalues -- 0.03493	-0.06317	-0.04912	-0.04111	-0.03945	-
Alpha virt. eigenvalues -- 0.01345	-0.03038	-0.02675	-0.01958	-0.01574	-
Alpha virt. eigenvalues -- 0.00490	-0.00990	-0.00554	-0.00517	0.00233	
Alpha virt. eigenvalues -- 0.02236	0.00824	0.00943	0.01522	0.02002	
Alpha virt. eigenvalues -- 0.03956	0.02645	0.03268	0.03474	0.03693	
Alpha virt. eigenvalues -- 0.07220	0.04355	0.04630	0.04839	0.05782	
Alpha virt. eigenvalues -- 0.09004	0.07702	0.07736	0.08054	0.08817	
Alpha virt. eigenvalues -- 0.10660	0.09255	0.10034	0.10315	0.10316	
Alpha virt. eigenvalues -- 0.13023	0.10931	0.11266	0.12098	0.12329	
Alpha virt. eigenvalues -- 0.14495	0.13515	0.13799	0.13890	0.13988	
Alpha virt. eigenvalues -- 0.15709	0.14621	0.14925	0.15252	0.15506	
Alpha virt. eigenvalues -- 0.16997	0.15790	0.16158	0.16482	0.16727	
Alpha virt. eigenvalues -- 0.20037	0.17371	0.18278	0.19609	0.19786	

Alpha virt. eigenvalues --	0.20201	0.20477	0.20847	0.21399
0.22056				
Alpha virt. eigenvalues --	0.23269	0.23657	0.24367	0.25183
0.25695				
Alpha virt. eigenvalues --	0.25809	0.26233	0.26607	0.27405
0.28114				
Alpha virt. eigenvalues --	0.28589	0.28797	0.29099	0.30440
0.31148				
Alpha virt. eigenvalues --	0.31286	0.31789	0.32262	0.32713
0.33432				
Alpha virt. eigenvalues --	0.33693	0.33876	0.34127	0.34763
0.35083				
Alpha virt. eigenvalues --	0.35435	0.35645	0.35694	0.36517
0.36864				
Alpha virt. eigenvalues --	0.37061	0.37479	0.38384	0.38886
0.39601				
Alpha virt. eigenvalues --	0.40546	0.40777	0.41757	0.42217
0.42726				
Alpha virt. eigenvalues --	0.43737	0.43872	0.44217	0.45155
0.45487				
Alpha virt. eigenvalues --	0.45861	0.46061	0.46453	0.47105
0.47907				
Alpha virt. eigenvalues --	0.48181	0.48864	0.49426	0.49453
0.49881				
Alpha virt. eigenvalues --	0.49956	0.50139	0.50287	0.50466
0.50795				
Alpha virt. eigenvalues --	0.51186	0.51455	0.51825	0.52056
0.52355				
Alpha virt. eigenvalues --	0.52513	0.52634	0.52810	0.52844
0.52991				
Alpha virt. eigenvalues --	0.53253	0.53916	0.54184	0.54474
0.54657				
Alpha virt. eigenvalues --	0.54932	0.55017	0.55086	0.55236
0.55807				
Alpha virt. eigenvalues --	0.56207	0.56213	0.56382	0.56507
0.56820				
Alpha virt. eigenvalues --	0.57170	0.57401	0.57440	0.57897
0.58160				
Alpha virt. eigenvalues --	0.58347	0.58560	0.58744	0.58832
0.58916				
Alpha virt. eigenvalues --	0.59248	0.59425	0.59881	0.59948
0.60184				
Alpha virt. eigenvalues --	0.60488	0.61250	0.61668	0.62104
0.62429				
Alpha virt. eigenvalues --	0.62639	0.62899	0.63153	0.63396
0.63595				
Alpha virt. eigenvalues --	0.63665	0.64305	0.64740	0.65648
0.66476				
Alpha virt. eigenvalues --	0.66659	0.67368	0.67757	0.67855
0.68309				
Alpha virt. eigenvalues --	0.69383	0.69669	0.69917	0.70074
0.70315				
Alpha virt. eigenvalues --	0.70564	0.70924	0.71219	0.71256
0.71915				
Alpha virt. eigenvalues --	0.72290	0.72589	0.73332	0.73515
0.73810				
Alpha virt. eigenvalues --	0.74691	0.75183	0.76108	0.76261
0.77128				
Alpha virt. eigenvalues --	0.77418	0.77833	0.78319	0.78565
0.78697				

Alpha virt. eigenvalues -- 0.80089	0.78971	0.79040	0.79285	0.80056
Alpha virt. eigenvalues -- 0.81170	0.80252	0.80429	0.80515	0.80824
Alpha virt. eigenvalues -- 0.82413	0.81215	0.81419	0.81844	0.82137
Alpha virt. eigenvalues -- 0.83804	0.82710	0.82832	0.83212	0.83408
Alpha virt. eigenvalues -- 0.85398	0.83879	0.84343	0.84671	0.84896
Alpha virt. eigenvalues -- 0.86346	0.85501	0.85653	0.85945	0.86153
Alpha virt. eigenvalues -- 0.88299	0.86741	0.87037	0.87483	0.87787
Alpha virt. eigenvalues -- 0.90113	0.88459	0.89247	0.89406	0.89652
Alpha virt. eigenvalues -- 0.91678	0.90191	0.90652	0.90898	0.91521
Alpha virt. eigenvalues -- 0.93858	0.92040	0.92299	0.93444	0.93539
Alpha virt. eigenvalues -- 0.95288	0.94351	0.94666	0.94744	0.95074
Alpha virt. eigenvalues -- 0.97728	0.95606	0.96604	0.96890	0.97205
Alpha virt. eigenvalues -- 0.99835	0.98142	0.98732	0.99294	0.99673
Alpha virt. eigenvalues -- 1.01677	1.00037	1.00257	1.00359	1.00480
Alpha virt. eigenvalues -- 1.04540	1.02428	1.02679	1.03774	1.04152
Alpha virt. eigenvalues -- 1.06357	1.05071	1.05344	1.05820	1.06245
Alpha virt. eigenvalues -- 1.10838	1.07532	1.07926	1.08487	1.09899
Alpha virt. eigenvalues -- 1.14204	1.11227	1.11772	1.12111	1.13013
Alpha virt. eigenvalues -- 1.17886	1.14745	1.15088	1.16009	1.16634
Alpha virt. eigenvalues -- 1.21005	1.18151	1.19806	1.20386	1.20566
Alpha virt. eigenvalues -- 1.23225	1.21498	1.21840	1.22260	1.22720
Alpha virt. eigenvalues -- 1.25606	1.24019	1.24357	1.24710	1.24862
Alpha virt. eigenvalues -- 1.27518	1.25991	1.26066	1.26577	1.26675
Alpha virt. eigenvalues -- 1.30533	1.28261	1.28430	1.30149	1.30338
Alpha virt. eigenvalues -- 1.33587	1.31633	1.31977	1.32379	1.32817
Alpha virt. eigenvalues -- 1.35781	1.34263	1.34897	1.35283	1.35411
Alpha virt. eigenvalues -- 1.37482	1.35802	1.35979	1.36249	1.36328
Alpha virt. eigenvalues -- 1.38798	1.37861	1.38179	1.38331	1.38372
Alpha virt. eigenvalues -- 1.39809	1.38823	1.39223	1.39595	1.39698
Alpha virt. eigenvalues -- 1.44397	1.41213	1.42175	1.42440	1.43110

Alpha virt. eigenvalues -- 1.47400	1.44680	1.45228	1.46245	1.46388
Alpha virt. eigenvalues -- 1.49349	1.47798	1.48731	1.48938	1.49193
Alpha virt. eigenvalues -- 1.51810	1.50367	1.50530	1.50970	1.51529
Alpha virt. eigenvalues -- 1.54890	1.52581	1.53085	1.53466	1.53844
Alpha virt. eigenvalues -- 1.58556	1.55085	1.56147	1.56997	1.57465
Alpha virt. eigenvalues -- 1.61680	1.58815	1.59396	1.59629	1.60285
Alpha virt. eigenvalues -- 1.64008	1.62060	1.62517	1.63010	1.63330
Alpha virt. eigenvalues -- 1.67151	1.64527	1.64705	1.65354	1.66473
Alpha virt. eigenvalues -- 1.69637	1.67389	1.67874	1.69120	1.69331
Alpha virt. eigenvalues -- 1.72322	1.69992	1.70085	1.70716	1.71801
Alpha virt. eigenvalues -- 1.76645	1.73602	1.73660	1.74513	1.76549
Alpha virt. eigenvalues -- 1.78150	1.76736	1.76895	1.77429	1.77705
Alpha virt. eigenvalues -- 1.80171	1.78701	1.78933	1.79233	1.79716
Alpha virt. eigenvalues -- 1.82753	1.81372	1.81785	1.82020	1.82492
Alpha virt. eigenvalues -- 1.85591	1.83157	1.83577	1.84228	1.84708
Alpha virt. eigenvalues -- 1.87976	1.86004	1.86354	1.86501	1.87639
Alpha virt. eigenvalues -- 1.90664	1.88385	1.89059	1.89926	1.90367
Alpha virt. eigenvalues -- 1.92134	1.91112	1.91209	1.91465	1.91975
Alpha virt. eigenvalues -- 1.95089	1.92814	1.93241	1.93810	1.94924
Alpha virt. eigenvalues -- 1.96303	1.95121	1.95343	1.95762	1.95794
Alpha virt. eigenvalues -- 1.97819	1.96764	1.97075	1.97198	1.97641
Alpha virt. eigenvalues -- 2.00933	1.98693	1.99009	1.99459	2.00312
Alpha virt. eigenvalues -- 2.02833	2.01988	2.02158	2.02181	2.02608
Alpha virt. eigenvalues -- 2.04895	2.03281	2.03803	2.03976	2.04698
Alpha virt. eigenvalues -- 2.08364	2.05886	2.06971	2.07204	2.07675
Alpha virt. eigenvalues -- 2.10931	2.08992	2.09037	2.09504	2.10765
Alpha virt. eigenvalues -- 2.13608	2.11470	2.11573	2.12668	2.13402
Alpha virt. eigenvalues -- 2.17225	2.15354	2.15556	2.15764	2.15928
Alpha virt. eigenvalues -- 2.19540	2.17685	2.18021	2.18683	2.19102
Alpha virt. eigenvalues -- 2.22196	2.19640	2.20681	2.21247	2.21919

Alpha virt. eigenvalues --	2.22819	2.23353	2.23468	2.24980
2.25738				
Alpha virt. eigenvalues --	2.26585	2.29067	2.29191	2.29873
2.30303				
Alpha virt. eigenvalues --	2.30534	2.30715	2.30872	2.31420
2.32166				
Alpha virt. eigenvalues --	2.34606	2.34655	2.34993	2.35533
2.36235				
Alpha virt. eigenvalues --	2.37245	2.37629	2.38562	2.38944
2.39401				
Alpha virt. eigenvalues --	2.40493	2.41272	2.41662	2.41731
2.43324				
Alpha virt. eigenvalues --	2.43610	2.44524	2.45017	2.45269
2.45695				
Alpha virt. eigenvalues --	2.46159	2.46575	2.47078	2.47089
2.48352				
Alpha virt. eigenvalues --	2.48514	2.50302	2.51151	2.51785
2.51912				
Alpha virt. eigenvalues --	2.52108	2.52336	2.52907	2.53510
2.54052				
Alpha virt. eigenvalues --	2.55251	2.55871	2.57232	2.57358
2.57861				
Alpha virt. eigenvalues --	2.58391	2.59434	2.59605	2.61086
2.61614				
Alpha virt. eigenvalues --	2.61631	2.62172	2.62894	2.63141
2.63626				
Alpha virt. eigenvalues --	2.64089	2.64416	2.64468	2.64837
2.65869				
Alpha virt. eigenvalues --	2.66032	2.66392	2.67154	2.67835
2.68876				
Alpha virt. eigenvalues --	2.69596	2.70550	2.70798	2.71151
2.71637				
Alpha virt. eigenvalues --	2.72151	2.72656	2.73092	2.73315
2.73647				
Alpha virt. eigenvalues --	2.73771	2.74708	2.75430	2.76311
2.77223				
Alpha virt. eigenvalues --	2.77567	2.79003	2.79445	2.80680
2.81397				
Alpha virt. eigenvalues --	2.81649	2.83172	2.83317	2.84506
2.87000				
Alpha virt. eigenvalues --	2.87296	2.87716	2.88422	2.89280
2.89987				
Alpha virt. eigenvalues --	2.90485	2.90937	2.93679	2.94657
2.95610				
Alpha virt. eigenvalues --	2.96873	3.00190	3.01469	3.02958
3.05154				
Alpha virt. eigenvalues --	3.06734	3.07412	3.08726	3.09162
3.12168				
Alpha virt. eigenvalues --	3.13231	3.13556	3.14593	3.18945
3.24331				
Alpha virt. eigenvalues --	3.24647	3.25233	3.26700	3.27529
3.28257				
Alpha virt. eigenvalues --	3.33456	3.34341	3.35211	3.35421
3.41227				
Alpha virt. eigenvalues --	3.42827	3.42980	3.43838	3.45331
3.46451				
Alpha virt. eigenvalues --	3.46705	3.47392	3.52247	3.53596
3.76086				
Alpha virt. eigenvalues --	3.80632	3.85400	3.85586	3.86454
3.87796				

Alpha virt. eigenvalues --	3.88657	3.89682	3.89772	3.90476
3.98932				
Alpha virt. eigenvalues --	4.00700	4.01053	4.01165	4.02302
4.03204				
Alpha virt. eigenvalues --	4.04864	4.05898	4.08601	4.09789
4.11056				
Alpha virt. eigenvalues --	4.11601	4.13765	4.14537	4.15272
4.15931				
Alpha virt. eigenvalues --	4.16527	4.17284	4.20424	4.22822
4.24269				
Alpha virt. eigenvalues --	4.25145	4.26450	4.29281	4.30164
4.33466				
Alpha virt. eigenvalues --	4.36869	4.37569	4.39530	4.39978
4.43339				
Alpha virt. eigenvalues --	4.44348	4.44693	4.45231	4.45602
4.46449				
Alpha virt. eigenvalues --	4.47638	4.49591	4.51701	4.56535
4.58774				
Alpha virt. eigenvalues --	4.59474	4.74336	4.75193	4.80594
4.81101				

Condensed to atoms (all electrons):

Mulliken charges:

1		
1	C	0.000356
2	C	0.049463
3	C	-0.130238
4	C	-0.076202
5	C	-0.109504
6	C	-0.074792
7	H	0.120447
8	H	0.108331
9	H	0.113977
10	H	0.150805
11	C	0.114597
12	C	0.357693
13	C	0.033127
14	C	-0.098925
15	C	-0.119614
16	C	-0.156331
17	C	0.270914
18	S	0.270167
19	C	-0.158603
20	C	-0.186554
21	C	0.209120
22	N	-0.521640
23	S	0.275702
24	S	0.285047
25	C	-0.170688
26	C	-0.158271
27	C	0.233553
28	C	-0.195694
29	C	-0.196892
30	C	0.243981
31	C	-0.084995
32	C	-0.165490
33	S	0.321253
34	N	-0.529995
35	C	-0.099791
36	C	0.040840
37	C	0.353443

38	C	0.124587
39	C	0.011410
40	C	-0.006210
41	C	-0.098848
42	C	-0.035232
43	C	-0.083618
44	C	-0.140265
45	C	-0.074026
46	C	0.335718
47	C	0.366389
48	N	-0.456074
49	N	-0.487456
50	C	-0.068106
51	C	0.366204
52	C	0.332801
53	N	-0.491225
54	N	-0.455605
55	O	-0.455632
56	O	-0.460464
57	C	-0.178612
58	H	0.132496
59	H	0.130528
60	H	0.126066
61	C	-0.179237
62	H	0.123221
63	H	0.134785
64	H	0.133012
65	H	0.116825
66	H	0.156317
67	H	0.113418
68	H	0.109810
69	H	0.121747
70	H	0.149090
71	H	0.160138
72	H	0.107448

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

1		
1	C	0.000356
2	C	0.049463
3	C	-0.009792
4	C	0.032129
5	C	0.004472
6	C	0.076012
11	C	0.114597
12	C	0.357693
13	C	0.033127
14	C	0.061213
15	C	-0.119614
16	C	-0.156331
17	C	0.270914
18	S	0.270167
19	C	-0.051154
20	C	-0.186554
21	C	0.209120
22	N	-0.521640
23	S	0.275702
24	S	0.285047
25	C	-0.170688
26	C	-0.158271

27	C	0.233553
28	C	-0.195694
29	C	-0.196892
30	C	0.243981
31	C	0.031829
32	C	-0.165490
33	S	0.321253
34	N	-0.529995
35	C	0.049299
36	C	0.040840
37	C	0.353443
38	C	0.124587
39	C	0.011410
40	C	-0.006210
41	C	0.022900
42	C	0.121086
43	C	0.026192
44	C	-0.026847
45	C	-0.074026
46	C	0.335718
47	C	0.366389
48	N	-0.456074
49	N	-0.487456
50	C	-0.068106
51	C	0.366204
52	C	0.332801
53	N	-0.491225
54	N	-0.455605
55	O	-0.455632
56	O	-0.460464
57	C	0.210478
61	C	0.211781

Electronic spatial extent (au): $\langle R^2 \rangle =$ 124793.2074

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X=	-1.1888	Y=	-1.6207	Z=	0.2672

Tot= 2.0277

Quadrupole moment (field-independent basis, Debye-Ang):

XX=	-399.3371	YY=	-352.9854	ZZ=	-336.6488

XY=	91.0439	XZ=	-6.3846	YZ=	5.8070

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX=	-36.3467	YY=	10.0050	ZZ=	26.3416

XY=	91.0439	XZ=	-6.3846	YZ=	5.8070

Octapole moment (field-independent basis, Debye-Ang**2):

XXX=	-1143.5255	YYY=	-68.3101	ZZZ=	13.9432

XYY=	239.0367

XXY=	-22.4782	XXZ=	-33.0192	XZZ=	-18.0182

YZZ=	9.6364

YYZ=	-9.1646	XYZ=	-42.4175

Hexadecapole moment (field-independent basis, Debye-Ang**3):

XXXX=	-190740.4564	YYYY=	-8174.0075	ZZZZ=	-

847.0563 XXXY=	24499.4702

XXXZ=	251.9327	YYYX=	3294.2201	YYYZ=	

28.7463 ZZZX=	-64.4177

ZZZY=	33.4526	XXYY=	-32973.6302	XXZZ=	-

28873.2151 YYZZ=	-1439.8781

XXYZ=	106.7759	YYXZ=	-153.1095	ZZXY=	-

53.2438

N-N= 6.041981995585D+03 E-N=-2.070811635265D+04 KE= 3.651721820077D+03

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOPClX= 0 NMat=1
NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-0.013859438	-0.036119101	-0.005533378
2	6	0.036114411	0.005776021	0.018258038
3	6	-0.023015204	-0.014371681	-0.010586585
4	6	0.019066870	-0.025848925	0.009035041
5	6	0.021451968	-0.012596794	0.010637197
6	6	0.023119467	0.034137648	0.014838523
7	1	0.011152380	0.005452122	0.006344365
8	1	0.003431137	0.006859127	0.001506357
9	1	-0.004500621	0.001692355	-0.002817653
10	1	0.015539149	0.038878706	0.011686331
11	6	-0.001067438	-0.003215320	-0.002147239
12	6	0.033654385	0.021973990	0.019814181
13	6	0.001252490	-0.021207170	0.001370716
14	6	0.013491910	0.069325280	0.016172872
15	6	0.026962044	-0.004193142	0.005409569
16	6	0.047949788	0.046786669	0.043892433
17	6	-0.044948421	-0.007922198	-0.024993721
18	16	0.025530065	0.039970236	0.014590549
19	6	-0.013334306	-0.067237599	-0.042232172
20	6	-0.002263093	0.017822735	0.005193336
21	6	0.000410464	-0.024667886	-0.003657141
22	7	-0.009698410	0.009170145	0.021914740
23	16	-0.003490708	-0.003712658	0.005706216
24	16	-0.003939813	-0.001360181	0.003706511
25	6	0.027320458	-0.009120750	0.005107514
26	6	-0.018743247	0.009293269	-0.024874514
27	6	0.008563405	0.030962571	0.013002524
28	6	0.005402626	-0.019006543	0.011453823
29	6	-0.044771579	-0.025169887	-0.036018822
30	6	0.055689623	0.050870169	0.036052949
31	6	-0.034710897	-0.006652731	-0.038463231
32	6	0.013914121	0.022840523	0.009744313
33	16	0.002052358	-0.006616755	-0.007293618
34	7	-0.033063710	-0.038743331	0.003916317
35	6	-0.046590236	-0.059344117	-0.019722990
36	6	0.005762669	0.016040559	0.002080260
37	6	-0.029025964	-0.008434350	-0.017128172
38	6	0.008207648	0.002950813	0.004288107
39	6	-0.069281132	-0.040251977	-0.038908665
40	6	0.068327965	-0.005828334	0.043355074
41	6	0.035171568	0.048626278	0.016262131
42	6	-0.064696255	0.017127755	-0.043255226
43	6	0.043322104	0.037352246	0.022912593
44	6	-0.065943318	-0.009855333	-0.040058651
45	6	0.062552519	0.010680448	0.039098255
46	6	-0.067718548	-0.016104176	-0.041912605
47	6	-0.016092968	0.059109295	-0.015901416
48	7	0.011120118	0.010968332	0.006011520
49	7	0.043628962	0.025907390	0.025755883
50	6	-0.051549696	-0.036918695	-0.027912562
51	6	0.036524697	-0.046345593	0.015276396
52	6	0.052457698	0.074150457	0.034099364
53	7	-0.019824536	-0.031876382	-0.012068231

54	7	-0.011906473	-0.033615295	-0.008804069
55	8	-0.058007297	-0.026347928	-0.028481670
56	8	0.051389739	-0.000314621	0.032416916
57	6	-0.001522841	-0.010610129	-0.012793331
58	1	-0.002677958	0.016563422	-0.006445965
59	1	-0.012062822	-0.000702338	0.016407022
60	1	0.011810232	0.001156381	0.003749903
61	6	-0.004472429	-0.001329464	0.014837907
62	1	0.008318661	0.010811636	-0.005419140
63	1	0.008732753	-0.013637687	0.000393940
64	1	-0.011394114	-0.002596467	-0.009013308
65	1	0.007108871	0.008327682	0.001862332
66	1	-0.036722285	-0.036139362	-0.020805893
67	1	0.001818750	-0.008968349	0.002160447
68	1	-0.002536371	-0.009525099	-0.000518946
69	1	-0.011154434	0.002345891	-0.007320147
70	1	0.003430024	0.014580341	0.000641561
71	1	0.001238113	-0.012607650	0.002619898
72	1	-0.018405649	-0.029394494	-0.018494861

Cartesian Forces: Max 0.074150457 RMS 0.027049618

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.383723868 RMS 0.049750233

Search for a local minimum.

Step number 1 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Second derivative matrix not updated -- first step.

ITU= 0

Eigenvalues ---	0.00230	0.00230	0.00230	0.00230	0.00244
Eigenvalues ---	0.00297	0.00403	0.00445	0.00448	0.00453
Eigenvalues ---	0.00474	0.00515	0.00527	0.00564	0.00609
Eigenvalues ---	0.00633	0.00635	0.00667	0.00681	0.00685
Eigenvalues ---	0.00689	0.00717	0.00739	0.00742	0.00745
Eigenvalues ---	0.00747	0.00760	0.00862	0.00878	0.00879
Eigenvalues ---	0.01012	0.01072	0.01089	0.01114	0.01168
Eigenvalues ---	0.01193	0.01232	0.01269	0.01277	0.01344
Eigenvalues ---	0.01356	0.01368	0.01372	0.01386	0.01454
Eigenvalues ---	0.01547	0.01647	0.01655	0.01751	0.01792
Eigenvalues ---	0.01800	0.01931	0.01950	0.02006	0.02016
Eigenvalues ---	0.02075	0.02075	0.02209	0.02210	0.03303
Eigenvalues ---	0.04827	0.04827	0.04837	0.04837	0.04900
Eigenvalues ---	0.04900	0.05016	0.05016	0.05494	0.07234
Eigenvalues ---	0.07400	0.07477	0.07585	0.12984	0.14353
Eigenvalues ---	0.15996	0.15999	0.16000	0.16000	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.17191	0.18383
Eigenvalues ---	0.18556	0.19232	0.20057	0.20912	0.21423
Eigenvalues ---	0.21438	0.21814	0.21998	0.22000	0.22000
Eigenvalues ---	0.22001	0.22044	0.22209	0.22531	0.22588
Eigenvalues ---	0.22603	0.22625	0.22994	0.23016	0.23233
Eigenvalues ---	0.23354	0.23361	0.23980	0.23983	0.24226
Eigenvalues ---	0.24240	0.24527	0.24536	0.24571	0.24688
Eigenvalues ---	0.24769	0.24847	0.24852	0.24869	0.24936
Eigenvalues ---	0.24948	0.24965	0.24971	0.24990	0.24993
Eigenvalues ---	0.24999	0.24999	0.25000	0.25000	0.25000

Eigenvalues	---	0.25000	0.25000	0.25000	0.25000	0.25000
Eigenvalues	---	0.25000	0.25000	0.25000	0.25659	0.26283
Eigenvalues	---	0.26350	0.26712	0.26727	0.26741	0.27120
Eigenvalues	---	0.27326	0.27925	0.28011	0.28358	0.28499
Eigenvalues	---	0.28536	0.28723	0.30080	0.30797	0.31602
Eigenvalues	---	0.32987	0.35686	0.36333	0.36338	0.36476
Eigenvalues	---	0.36581	0.36654	0.36717	0.36769	0.36829
Eigenvalues	---	0.36922	0.37087	0.37099	0.37215	0.37255
Eigenvalues	---	0.37281	0.37429	0.37573	0.37676	0.37761
Eigenvalues	---	0.38025	0.39238	0.40325	0.40945	0.41633
Eigenvalues	---	0.42779	0.43027	0.44433	0.45452	0.45712
Eigenvalues	---	0.46176	0.47055	0.47165	0.48220	0.48357
Eigenvalues	---	0.52991	0.56055	0.56065	0.58665	0.80369
Eigenvalues	---	0.81503	1.25861	1.26344	1.29487	1.35496

RFO step: Lambda=-8.97836376D-01 EMin= 2.30000000D-03

Linear search not attempted -- first point.

Maximum step size (0.300) exceeded in Quadratic search.

-- Step size scaled by 0.340

Iteration 1 RMS(Cart)= 0.15178093 RMS(Int)= 0.00447775

Iteration 2 RMS(Cart)= 0.01825829 RMS(Int)= 0.00005757

Iteration 3 RMS(Cart)= 0.00014608 RMS(Int)= 0.00002030

Iteration 4 RMS(Cart)= 0.00000003 RMS(Int)= 0.00002030

Variable (Linear)	Old X (Quad)	-DE/DX (Total)	Delta X	Delta X	Delta X	New X
R1	2.57868	0.06500	0.00000	0.01615	0.01611	2.59479
R2	2.68157	-0.00565	0.00000	-0.00121	-0.00118	2.68039
R3	2.90347	0.07618	0.00000	0.02202	0.02203	2.92549
R4	2.70494	-0.03256	0.00000	-0.00839	-0.00841	2.69653
R5	3.02136	-0.08476	0.00000	-0.02532	-0.02536	2.99600
R6	2.71222	-0.05702	0.00000	-0.01516	-0.01518	2.69703
R7	2.01415	0.01366	0.00000	0.00364	0.00364	2.01779
R8	2.66354	-0.02206	0.00000	-0.00592	-0.00593	2.65761
R9	2.03344	0.00656	0.00000	0.00177	0.00177	2.03520
R10	2.65182	-0.00763	0.00000	-0.00200	-0.00199	2.64983
R11	2.03556	0.00548	0.00000	0.00148	0.00148	2.03704
R12	2.02895	-0.03753	0.00000	-0.01009	-0.01009	2.01887
R13	3.12095	-0.06288	0.00000	-0.01958	-0.01953	3.10142
R14	2.62839	0.03287	0.00000	0.00816	0.00816	2.63656
R15	3.01372	-0.07861	0.00000	-0.02376	-0.02373	2.98999
R16	2.37717	-0.06950	0.00000	-0.01389	-0.01389	2.36328
R17	2.84878	-0.12752	0.00000	-0.03573	-0.03573	2.81306
R18	3.24566	-0.11356	0.00000	-0.03610	-0.03610	3.20955
R19	2.03183	0.00818	0.00000	0.00220	0.00220	2.03403
R20	3.51136	0.00254	0.00000	0.00027	0.00028	3.51164
R21	2.62058	-0.02519	0.00000	-0.00645	-0.00642	2.61415
R22	2.47108	0.07661	0.00000	0.01772	0.01769	2.48877
R23	3.61630	-0.04519	0.00000	-0.01393	-0.01395	3.60235
R24	3.10644	-0.07995	0.00000	-0.02427	-0.02427	3.08217
R25	2.94390	-0.08218	0.00000	-0.02385	-0.02384	2.92006
R26	2.85873	-0.04879	0.00000	-0.01355	-0.01356	2.84517
R27	1.97814	0.03792	0.00000	0.00991	0.00991	1.98805
R28	2.57022	0.00567	0.00000	0.00099	0.00101	2.57123
R29	3.47672	-0.03164	0.00000	-0.00950	-0.00950	3.46722
R30	2.89823	-0.04303	0.00000	-0.01287	-0.01287	2.88536
R31	3.08577	-0.09651	0.00000	-0.02946	-0.02946	3.05632
R32	2.82375	-0.00029	0.00000	-0.00008	-0.00008	2.82367
R33	3.50158	-0.03137	0.00000	-0.00954	-0.00954	3.49205
R34	3.45007	-0.02559	0.00000	-0.00770	-0.00770	3.44237
R35	3.44009	-0.02714	0.00000	-0.00810	-0.00810	3.43199
R36	2.60524	-0.00391	0.00000	-0.00098	-0.00098	2.60426

R37	3.14916	-0.09993	0.00000	-0.03098	-0.03098	3.11818
R38	2.58083	0.00156	0.00000	0.00022	0.00023	2.58106
R39	2.94109	-0.06435	0.00000	-0.01906	-0.01906	2.92203
R40	3.05737	-0.08499	0.00000	-0.02552	-0.02552	3.03186
R41	2.49358	0.04494	0.00000	0.01064	0.01062	2.50419
R42	3.47848	-0.03746	0.00000	-0.01108	-0.01108	3.46739
R43	3.03469	-0.09513	0.00000	-0.02848	-0.02849	3.00620
R44	2.91210	-0.06293	0.00000	-0.01806	-0.01807	2.89403
R45	2.68367	-0.04394	0.00000	-0.01156	-0.01156	2.67211
R46	2.02163	0.01029	0.00000	0.00276	0.00276	2.02438
R47	3.49855	-0.02251	0.00000	-0.00716	-0.00714	3.49141
R48	3.19131	-0.10379	0.00000	-0.03258	-0.03258	3.15873
R49	2.77876	0.00484	0.00000	0.00131	0.00131	2.78007
R50	2.76275	-0.10355	0.00000	-0.02784	-0.02784	2.73491
R51	2.02224	0.01135	0.00000	0.00304	0.00304	2.02528
R52	2.95550	-0.07872	0.00000	-0.02369	-0.02368	2.93182
R53	3.10382	-0.05394	0.00000	-0.01696	-0.01690	3.08692
R54	2.97378	-0.08821	0.00000	-0.02592	-0.02597	2.94781
R55	2.37115	-0.06063	0.00000	-0.01204	-0.01204	2.35911
R56	2.85404	0.12295	0.00000	0.03497	0.03499	2.88903
R57	2.64755	0.04635	0.00000	0.01165	0.01165	2.65920
R58	2.49946	0.09710	0.00000	0.02284	0.02281	2.52226
R59	2.93207	-0.07009	0.00000	-0.02014	-0.02018	2.91190
R60	2.90268	-0.04682	0.00000	-0.01301	-0.01296	2.88972
R61	2.61176	-0.05017	0.00000	-0.01266	-0.01271	2.59905
R62	2.01540	0.01241	0.00000	0.00331	0.00331	2.01871
R63	2.54851	0.01394	0.00000	0.00313	0.00317	2.55168
R64	2.02663	-0.04974	0.00000	-0.01335	-0.01335	2.01328
R65	2.93228	-0.08736	0.00000	-0.02590	-0.02591	2.90637
R66	2.02416	0.00987	0.00000	0.00264	0.00264	2.02680
R67	2.02805	0.00837	0.00000	0.00225	0.00225	2.03030
R68	2.92115	-0.05294	0.00000	-0.01529	-0.01529	2.90586
R69	2.96052	-0.04206	0.00000	-0.01232	-0.01232	2.94820
R70	2.18724	0.01667	0.00000	0.00259	0.00259	2.18982
R71	2.19630	0.01613	0.00000	0.00254	0.00254	2.19884
R72	2.95008	-0.04814	0.00000	-0.01405	-0.01405	2.93603
R73	2.90585	-0.05455	0.00000	-0.01565	-0.01565	2.89019
R74	2.19772	0.00839	0.00000	0.00132	0.00132	2.19904
R75	2.17069	0.03672	0.00000	0.00554	0.00554	2.17624
R76	2.01692	0.01793	0.00000	0.00479	0.00479	2.02170
R77	2.01904	0.01961	0.00000	0.00524	0.00524	2.02428
R78	2.03071	0.01231	0.00000	0.00331	0.00331	2.03403
R79	2.03564	0.01407	0.00000	0.00379	0.00379	2.03944
R80	2.02125	0.01594	0.00000	0.00427	0.00427	2.02551
R81	2.02397	0.01460	0.00000	0.00391	0.00391	2.02789
A1	2.14714	-0.08024	0.00000	-0.02339	-0.02334	2.12380
A2	1.95109	-0.02704	0.00000	-0.00774	-0.00779	1.94329
A3	2.18496	0.10728	0.00000	0.03112	0.03113	2.21609
A4	2.07077	0.04494	0.00000	0.01361	0.01363	2.08441
A5	1.90970	0.02170	0.00000	0.00666	0.00658	1.91628
A6	2.30271	-0.06663	0.00000	-0.02026	-0.02022	2.28250
A7	2.08107	0.00255	0.00000	0.00065	0.00060	2.08167
A8	2.11758	-0.00399	0.00000	-0.00119	-0.00117	2.11642
A9	2.08452	0.00143	0.00000	0.00055	0.00057	2.08510
A10	2.10278	-0.00951	0.00000	-0.00352	-0.00357	2.09921
A11	2.10487	0.00044	0.00000	0.00037	0.00040	2.10527
A12	2.07553	0.00906	0.00000	0.00314	0.00317	2.07870
A13	2.08274	0.01941	0.00000	0.00547	0.00546	2.08820
A14	2.10194	-0.00885	0.00000	-0.00246	-0.00245	2.09949
A15	2.09850	-0.01056	0.00000	-0.00301	-0.00301	2.09549

A16	2.08140	0.02287	0.00000	0.00720	0.00722	2.08863
A17	2.11062	0.01068	0.00000	0.00351	0.00350	2.11412
A18	2.09115	-0.03355	0.00000	-0.01071	-0.01072	2.08043
A19	1.91489	-0.05679	0.00000	-0.01673	-0.01667	1.89822
A20	1.92629	0.29893	0.00000	0.08852	0.08849	2.01478
A21	2.44199	-0.24215	0.00000	-0.07179	-0.07182	2.37017
A22	1.92058	-0.01563	0.00000	-0.00479	-0.00480	1.91578
A23	2.16285	0.01530	0.00000	0.00461	0.00461	2.16746
A24	2.19975	0.00033	0.00000	0.00018	0.00018	2.19993
A25	1.72699	0.07768	0.00000	0.02257	0.02265	1.74964
A26	2.26099	-0.04065	0.00000	-0.01182	-0.01186	2.24913
A27	2.29519	-0.03705	0.00000	-0.01075	-0.01079	2.28440
A28	2.39119	-0.03475	0.00000	-0.01057	-0.01057	2.38062
A29	1.94390	0.02741	0.00000	0.00851	0.00851	1.95241
A30	1.94797	0.00734	0.00000	0.00206	0.00206	1.95003
A31	2.45729	-0.05759	0.00000	-0.01677	-0.01679	2.44050
A32	2.22348	-0.04304	0.00000	-0.01245	-0.01247	2.21101
A33	1.60160	0.10071	0.00000	0.02924	0.02928	1.63089
A34	1.88807	0.02696	0.00000	0.00868	0.00866	1.89673
A35	1.83648	-0.00626	0.00000	-0.00122	-0.00122	1.83526
A36	2.55864	-0.02070	0.00000	-0.00746	-0.00744	2.55120
A37	1.84178	0.02156	0.00000	0.00704	0.00705	1.84883
A38	1.97485	0.00395	0.00000	0.00171	0.00170	1.97655
A39	2.46592	-0.02548	0.00000	-0.00875	-0.00874	2.45718
A40	1.74161	-0.06753	0.00000	-0.01997	-0.01998	1.72163
A41	2.32388	-0.08137	0.00000	-0.02480	-0.02479	2.29909
A42	1.98257	0.04517	0.00000	0.01384	0.01383	1.99640
A43	1.97672	0.03625	0.00000	0.01097	0.01097	1.98769
A44	1.87263	-0.01365	0.00000	-0.00397	-0.00396	1.86867
A45	2.50458	-0.01743	0.00000	-0.00522	-0.00522	2.49935
A46	1.90597	0.03108	0.00000	0.00919	0.00918	1.91515
A47	1.89725	0.03619	0.00000	0.01012	0.01013	1.90738
A48	1.97950	-0.01099	0.00000	-0.00296	-0.00296	1.97654
A49	2.40634	-0.02520	0.00000	-0.00716	-0.00717	2.39917
A50	1.80575	-0.01991	0.00000	-0.00643	-0.00643	1.79932
A51	1.83616	0.01577	0.00000	0.00492	0.00492	1.84108
A52	1.90145	0.00533	0.00000	0.00171	0.00171	1.90316
A53	1.65879	-0.04245	0.00000	-0.01267	-0.01266	1.64613
A54	1.65612	-0.04172	0.00000	-0.01258	-0.01257	1.64355
A55	1.89240	0.03302	0.00000	0.00967	0.00968	1.90208
A56	2.44485	-0.02515	0.00000	-0.00740	-0.00741	2.43745
A57	1.94466	-0.00774	0.00000	-0.00223	-0.00223	1.94243
A58	2.37705	-0.01895	0.00000	-0.00552	-0.00552	2.37153
A59	1.97680	-0.01019	0.00000	-0.00306	-0.00306	1.97374
A60	1.92798	0.02922	0.00000	0.00861	0.00861	1.93659
A61	1.95332	-0.00664	0.00000	-0.00170	-0.00170	1.95162
A62	2.44692	-0.02383	0.00000	-0.00695	-0.00696	2.43996
A63	1.88291	0.03045	0.00000	0.00865	0.00866	1.89157
A64	1.92946	0.02767	0.00000	0.00818	0.00817	1.93763
A65	2.46033	-0.01343	0.00000	-0.00405	-0.00406	2.45627
A66	1.89293	-0.01418	0.00000	-0.00411	-0.00410	1.88883
A67	1.86193	-0.00916	0.00000	-0.00234	-0.00234	1.85959
A68	2.50937	-0.01102	0.00000	-0.00406	-0.00404	2.50533
A69	1.91176	0.02017	0.00000	0.00640	0.00638	1.91814
A70	1.99222	-0.00518	0.00000	-0.00115	-0.00117	1.99106
A71	1.95455	0.00992	0.00000	0.00321	0.00320	1.95774
A72	2.33618	-0.00474	0.00000	-0.00206	-0.00203	2.33414
A73	2.00643	-0.01969	0.00000	-0.00607	-0.00608	2.00035
A74	2.14349	0.00664	0.00000	0.00201	0.00201	2.14550
A75	2.13309	0.01309	0.00000	0.00408	0.00408	2.13716

A76	1.82985	0.05335	0.00000	0.01528	0.01530	1.84515
A77	2.11386	-0.01658	0.00000	-0.00465	-0.00466	2.10920
A78	2.33947	-0.03677	0.00000	-0.01063	-0.01064	2.32883
A79	1.67903	-0.04828	0.00000	-0.01431	-0.01430	1.66473
A80	1.80661	-0.01601	0.00000	-0.00505	-0.00506	1.80154
A81	2.04187	0.00322	0.00000	0.00095	0.00097	2.04284
A82	1.94022	0.01570	0.00000	0.00509	0.00509	1.94531
A83	2.30466	-0.02182	0.00000	-0.00664	-0.00664	2.29802
A84	1.99393	0.00101	0.00000	0.00014	0.00014	1.99406
A85	1.98458	0.02081	0.00000	0.00650	0.00650	1.99109
A86	2.21953	-0.03541	0.00000	-0.00998	-0.01002	2.20951
A87	2.31343	-0.05065	0.00000	-0.01450	-0.01454	2.29889
A88	1.75021	0.08607	0.00000	0.02448	0.02456	1.77478
A89	1.89899	-0.00791	0.00000	-0.00281	-0.00284	1.89614
A90	2.19580	-0.00070	0.00000	0.00003	0.00004	2.19585
A91	2.18839	0.00861	0.00000	0.00279	0.00280	2.19120
A92	1.87702	-0.06132	0.00000	-0.01792	-0.01784	1.85918
A93	2.50124	-0.32240	0.00000	-0.09565	-0.09569	2.40555
A94	1.90493	0.38372	0.00000	0.11356	0.11352	2.01845
A95	1.92235	0.02540	0.00000	0.00802	0.00794	1.93029
A96	2.28698	-0.08284	0.00000	-0.02551	-0.02545	2.26153
A97	2.07386	0.05744	0.00000	0.01749	0.01751	2.09137
A98	1.97619	-0.04224	0.00000	-0.01177	-0.01183	1.96436
A99	2.15095	0.15285	0.00000	0.04405	0.04404	2.19499
A100	2.15604	-0.11061	0.00000	-0.03228	-0.03221	2.12384
A101	2.07107	0.00921	0.00000	0.00265	0.00255	2.07361
A102	2.11494	-0.01008	0.00000	-0.00308	-0.00303	2.11191
A103	2.09717	0.00087	0.00000	0.00043	0.00049	2.09766
A104	2.07407	0.03660	0.00000	0.01148	0.01156	2.08563
A105	2.10440	0.00675	0.00000	0.00231	0.00227	2.10668
A106	2.10471	-0.04335	0.00000	-0.01379	-0.01383	2.09088
A107	2.10625	-0.01487	0.00000	-0.00545	-0.00553	2.10072
A108	2.10005	0.00774	0.00000	0.00282	0.00286	2.10291
A109	2.07689	0.00714	0.00000	0.00263	0.00267	2.07956
A110	2.08506	0.02224	0.00000	0.00611	0.00613	2.09118
A111	2.09144	-0.00677	0.00000	-0.00166	-0.00166	2.08978
A112	2.10669	-0.01547	0.00000	-0.00445	-0.00446	2.10223
A113	2.52681	-0.20113	0.00000	-0.05959	-0.05959	2.46722
A114	2.20652	0.27810	0.00000	0.08240	0.08240	2.28892
A115	1.54985	-0.07698	0.00000	-0.02281	-0.02281	1.52705
A116	2.17401	0.21265	0.00000	0.06300	0.06300	2.23701
A117	2.44757	-0.15199	0.00000	-0.04503	-0.04503	2.40254
A118	1.66155	-0.06066	0.00000	-0.01797	-0.01797	1.64358
A119	1.91440	-0.00198	0.00000	-0.00066	-0.00066	1.91374
A120	1.91651	0.00912	0.00000	0.00297	0.00297	1.91947
A121	1.90140	-0.00202	0.00000	-0.00066	-0.00067	1.90074
A122	1.91362	-0.00235	0.00000	-0.00073	-0.00073	1.91289
A123	1.90965	-0.00105	0.00000	-0.00041	-0.00041	1.90924
A124	1.90818	-0.00174	0.00000	-0.00052	-0.00052	1.90765
A125	1.90143	0.00798	0.00000	0.00260	0.00260	1.90403
A126	1.92831	-0.00489	0.00000	-0.00159	-0.00159	1.92671
A127	1.91269	-0.00302	0.00000	-0.00099	-0.00099	1.91170
A128	1.90553	-0.00044	0.00000	-0.00011	-0.00011	1.90542
A129	1.90685	-0.00055	0.00000	-0.00013	-0.00013	1.90672
A130	1.90887	0.00099	0.00000	0.00025	0.00025	1.90912
A131	3.25055	-0.00316	0.00000	-0.00114	-0.00114	3.24942
A132	3.14161	0.11984	0.00000	0.04307	0.04307	3.18468
A133	3.16866	0.08466	0.00000	0.03043	0.03043	3.19908
A134	3.22293	-0.00169	0.00000	-0.00060	-0.00060	3.22232
A135	3.13568	0.00009	0.00000	0.00003	0.00003	3.13571

A136	3.14159	0.00161	0.00000	0.00058	0.00058	3.14217
A137	3.12716	-0.00164	0.00000	-0.00059	-0.00059	3.12657
A138	3.14932	-0.00038	0.00000	-0.00014	-0.00014	3.14919
D1	-0.01777	-0.00093	0.00000	-0.00036	-0.00035	-0.01812
D2	3.12395	-0.00177	0.00000	-0.00064	-0.00063	3.12332
D3	3.12584	-0.00033	0.00000	-0.00014	-0.00014	3.12571
D4	-0.01562	-0.00117	0.00000	-0.00042	-0.00042	-0.01604
D5	-0.00816	0.00137	0.00000	0.00049	0.00048	-0.00768
D6	3.13865	0.00174	0.00000	0.00064	0.00063	3.13929
D7	3.13113	0.00049	0.00000	0.00018	0.00017	3.13130
D8	-0.00524	0.00086	0.00000	0.00033	0.00032	-0.00492
D9	0.04478	-0.00014	0.00000	0.00007	0.00007	0.04485
D10	-3.09302	0.00219	0.00000	0.00085	0.00087	-3.09214
D11	-3.09473	0.00074	0.00000	0.00038	0.00038	-3.09436
D12	0.05065	0.00307	0.00000	0.00115	0.00118	0.05184
D13	0.03080	0.00031	0.00000	0.00011	0.00010	0.03090
D14	-3.11470	-0.00008	0.00000	-0.00003	-0.00003	-3.11473
D15	-3.11096	0.00140	0.00000	0.00047	0.00045	-3.11050
D16	0.02673	0.00100	0.00000	0.00032	0.00032	0.02705
D17	-0.02017	0.00094	0.00000	0.00028	0.00029	-0.01988
D18	3.11618	0.00162	0.00000	0.00051	0.00052	3.11670
D19	3.12157	-0.00007	0.00000	-0.00005	-0.00004	3.12154
D20	-0.02526	0.00061	0.00000	0.00018	0.00019	-0.02507
D21	-0.01880	0.00103	0.00000	0.00036	0.00036	-0.01844
D22	3.11971	0.00036	0.00000	0.00012	0.00013	3.11984
D23	3.12662	0.00143	0.00000	0.00050	0.00050	3.12712
D24	-0.01806	0.00076	0.00000	0.00027	0.00026	-0.01779
D25	-0.00700	-0.00035	0.00000	-0.00013	-0.00013	-0.00713
D26	3.13080	-0.00042	0.00000	-0.00015	-0.00015	3.13065
D27	3.13763	0.00032	0.00000	0.00010	0.00011	3.13773
D28	-0.00776	0.00025	0.00000	0.00008	0.00008	-0.00768
D29	0.02049	-0.00055	0.00000	-0.00019	-0.00020	0.02030
D30	-3.12626	-0.00079	0.00000	-0.00029	-0.00030	-3.12656
D31	-3.11731	-0.00048	0.00000	-0.00017	-0.00017	-3.11749
D32	0.01912	-0.00072	0.00000	-0.00027	-0.00028	0.01884
D33	-0.05102	-0.00143	0.00000	-0.00050	-0.00052	-0.05154
D34	3.09664	0.00009	0.00000	0.00001	0.00001	3.09664
D35	3.08505	-0.00263	0.00000	-0.00097	-0.00095	3.08410
D36	-0.05048	-0.00110	0.00000	-0.00046	-0.00043	-0.05091
D37	-0.04617	-0.00131	0.00000	-0.00047	-0.00048	-0.04665
D38	3.10956	-0.00092	0.00000	-0.00033	-0.00033	3.10923
D39	3.10097	0.00062	0.00000	0.00022	0.00022	3.10119
D40	-0.02648	0.00101	0.00000	0.00036	0.00037	-0.02612
D41	0.04209	0.00210	0.00000	0.00066	0.00067	0.04276
D42	-3.10574	0.00052	0.00000	0.00013	0.00013	-3.10561
D43	-3.09412	0.00135	0.00000	0.00041	0.00042	-3.09370
D44	0.04123	-0.00022	0.00000	-0.00012	-0.00012	0.04111
D45	-3.06666	-0.00346	0.00000	-0.00128	-0.00127	-3.06794
D46	0.09446	-0.00336	0.00000	-0.00125	-0.00124	0.09321
D47	0.08293	-0.00181	0.00000	-0.00070	-0.00070	0.08223
D48	-3.03914	-0.00171	0.00000	-0.00067	-0.00067	-3.03981
D49	0.06917	0.00196	0.00000	0.00049	0.00048	0.06966
D50	-3.01558	-0.00389	0.00000	-0.00122	-0.00121	-3.01679
D51	-3.09198	0.00202	0.00000	0.00051	0.00050	-3.09147
D52	0.10646	-0.00383	0.00000	-0.00120	-0.00119	0.10527
D53	-3.00470	0.00160	0.00000	0.00035	0.00031	-3.00438
D54	0.09172	0.00461	0.00000	0.00124	0.00119	0.09291
D55	2.86963	0.00787	0.00000	0.00299	0.00296	2.87259
D56	-0.26468	-0.00018	0.00000	0.00030	0.00030	-0.26439
D57	-0.23603	0.00683	0.00000	0.00269	0.00265	-0.23337

D58	2.91285	-0.00123	0.00000	-0.00001	-0.00001	2.91283
D59	-0.12676	-0.00392	0.00000	-0.00100	-0.00098	-0.12773
D60	2.98493	-0.00401	0.00000	-0.00102	-0.00100	2.98393
D61	3.01460	-0.00302	0.00000	-0.00075	-0.00072	3.01388
D62	-0.15690	-0.00310	0.00000	-0.00076	-0.00074	-0.15764
D63	0.02982	-0.00347	0.00000	-0.00107	-0.00102	0.02880
D64	-3.11136	-0.00507	0.00000	-0.00152	-0.00147	-3.11283
D65	-0.00955	0.00416	0.00000	0.00129	0.00127	-0.00828
D66	3.13753	0.00296	0.00000	0.00107	0.00106	3.13859
D67	3.13164	0.00574	0.00000	0.00174	0.00172	3.13336
D68	-0.00447	0.00454	0.00000	0.00151	0.00150	-0.00296
D69	0.28639	-0.01666	0.00000	-0.00554	-0.00552	0.28087
D70	-2.86247	-0.00860	0.00000	-0.00284	-0.00285	-2.86532
D71	-2.81123	-0.01801	0.00000	-0.00603	-0.00599	-2.81722
D72	0.32310	-0.00995	0.00000	-0.00333	-0.00332	0.31978
D73	0.25368	-0.00254	0.00000	-0.00107	-0.00109	0.25259
D74	-1.74066	-0.00642	0.00000	-0.00225	-0.00224	-1.74290
D75	-2.93399	-0.00093	0.00000	-0.00050	-0.00054	-2.93454
D76	1.35485	-0.00480	0.00000	-0.00168	-0.00169	1.35316
D77	0.16479	-0.00159	0.00000	-0.00073	-0.00073	0.16406
D78	-2.98916	-0.00173	0.00000	-0.00067	-0.00066	-2.98983
D79	-2.98026	-0.00095	0.00000	-0.00062	-0.00063	-2.98089
D80	0.14898	-0.00109	0.00000	-0.00056	-0.00056	0.14841
D81	3.02840	0.00404	0.00000	0.00129	0.00127	3.02967
D82	-0.10765	0.00291	0.00000	0.00108	0.00108	-0.10656
D83	-0.24783	-0.00008	0.00000	0.00054	0.00054	-0.24729
D84	1.69904	0.01057	0.00000	0.00378	0.00377	1.70281
D85	2.91067	-0.00027	0.00000	0.00034	0.00034	2.91101
D86	-1.42565	0.01038	0.00000	0.00358	0.00358	-1.42207
D87	3.06686	0.00193	0.00000	0.00065	0.00065	3.06751
D88	-0.13796	0.00474	0.00000	0.00159	0.00158	-0.13638
D89	-0.09218	0.00242	0.00000	0.00094	0.00094	-0.09125
D90	2.98618	0.00523	0.00000	0.00187	0.00187	2.98805
D91	0.95373	-0.00616	0.00000	-0.00202	-0.00202	0.95171
D92	3.04696	-0.00467	0.00000	-0.00150	-0.00150	3.04547
D93	-1.13170	-0.00850	0.00000	-0.00284	-0.00284	-1.13453
D94	-0.97287	0.00688	0.00000	0.00228	0.00228	-0.97059
D95	1.12037	0.00837	0.00000	0.00280	0.00280	1.12317
D96	-3.05829	0.00455	0.00000	0.00146	0.00146	-3.05683
D97	0.02683	-0.00107	0.00000	-0.00041	-0.00042	0.02642
D98	3.10589	0.00239	0.00000	0.00079	0.00079	3.10668
D99	3.11531	0.00029	0.00000	0.00012	0.00012	3.11543
D100	0.03571	-0.00152	0.00000	-0.00052	-0.00051	0.03520
D101	-0.12270	0.00446	0.00000	0.00157	0.00157	-0.12113
D102	2.97991	0.00690	0.00000	0.00232	0.00231	2.98223
D103	0.04922	0.00016	0.00000	0.00001	0.00001	0.04923
D104	-3.13907	0.00080	0.00000	0.00028	0.00029	-3.13879
D105	-3.04928	-0.00106	0.00000	-0.00048	-0.00048	-3.04976
D106	0.04561	-0.00042	0.00000	-0.00021	-0.00021	0.04541
D107	3.06420	0.00139	0.00000	0.00048	0.00048	3.06468
D108	-0.08751	-0.00051	0.00000	-0.00013	-0.00013	-0.08764
D109	-0.14112	0.00581	0.00000	0.00197	0.00196	-0.13916
D110	2.99035	0.00391	0.00000	0.00136	0.00135	2.99170
D111	0.16183	-0.00250	0.00000	-0.00102	-0.00102	0.16081
D112	-2.95388	-0.00381	0.00000	-0.00142	-0.00143	-2.95531
D113	-2.97295	-0.00096	0.00000	-0.00053	-0.00053	-2.97348
D114	0.19452	-0.00227	0.00000	-0.00093	-0.00094	0.19358
D115	2.93711	0.00505	0.00000	0.00181	0.00181	2.93892
D116	0.79691	-0.00483	0.00000	-0.00144	-0.00144	0.79547
D117	-0.21435	0.00307	0.00000	0.00118	0.00118	-0.21317

D118	-2.35454	-0.00681	0.00000	-0.00207	-0.00208	-2.35662
D119	3.07966	0.00236	0.00000	0.00087	0.00087	3.08053
D120	-0.08225	0.00218	0.00000	0.00078	0.00078	-0.08147
D121	-0.10042	0.00534	0.00000	0.00178	0.00178	-0.09864
D122	3.02086	0.00516	0.00000	0.00169	0.00168	3.02255
D123	3.11733	0.00001	0.00000	-0.00002	-0.00003	3.11730
D124	-0.04440	-0.00029	0.00000	-0.00018	-0.00018	-0.04458
D125	-0.01153	0.00041	0.00000	0.00013	0.00013	-0.01140
D126	3.10993	0.00011	0.00000	-0.00002	-0.00003	3.10990
D127	3.12092	0.00267	0.00000	0.00092	0.00092	3.12184
D128	-0.04132	0.00228	0.00000	0.00076	0.00076	-0.04055
D129	0.08187	-0.00431	0.00000	-0.00149	-0.00148	0.08038
D130	-3.07970	-0.00237	0.00000	-0.00079	-0.00078	-3.08048
D131	-3.03384	-0.00415	0.00000	-0.00137	-0.00137	-3.03520
D132	0.08778	-0.00221	0.00000	-0.00067	-0.00066	0.08711
D133	0.15480	-0.00279	0.00000	-0.00086	-0.00087	0.15394
D134	2.36108	-0.00023	0.00000	-0.00005	-0.00006	2.36103
D135	-3.01226	-0.00311	0.00000	-0.00103	-0.00103	-3.01329
D136	-0.80598	-0.00055	0.00000	-0.00021	-0.00022	-0.80620
D137	-0.10215	0.00185	0.00000	0.00085	0.00085	-0.10130
D138	3.03641	0.00207	0.00000	0.00086	0.00086	3.03727
D139	3.05929	0.00001	0.00000	0.00017	0.00018	3.05946
D140	-0.08534	0.00022	0.00000	0.00018	0.00019	-0.08515
D141	0.08319	-0.00229	0.00000	-0.00093	-0.00092	0.08226
D142	-3.05479	-0.00264	0.00000	-0.00096	-0.00096	-3.05575
D143	3.07812	0.00019	0.00000	0.00013	0.00013	3.07825
D144	-0.05756	-0.00020	0.00000	-0.00002	-0.00002	-0.05757
D145	-0.06755	0.00069	0.00000	0.00020	0.00020	-0.06735
D146	3.07995	0.00029	0.00000	0.00005	0.00005	3.08001
D147	-1.06741	-0.00500	0.00000	-0.00160	-0.00160	-1.06901
D148	1.03664	-0.00341	0.00000	-0.00105	-0.00105	1.03559
D149	3.12594	-0.00130	0.00000	-0.00031	-0.00031	3.12564
D150	-3.13699	0.00161	0.00000	0.00042	0.00042	-3.13657
D151	-1.03295	0.00320	0.00000	0.00097	0.00097	-1.03197
D152	1.05636	0.00531	0.00000	0.00171	0.00171	1.05807
D153	-0.00391	-0.00039	0.00000	-0.00015	-0.00015	-0.00406
D154	-3.13951	-0.00023	0.00000	-0.00008	-0.00008	-3.13959
D155	3.13179	-0.00005	0.00000	-0.00002	-0.00002	3.13177
D156	-0.00381	0.00011	0.00000	0.00005	0.00005	-0.00376
D157	-3.13921	-0.00021	0.00000	-0.00007	-0.00008	-3.13929
D158	0.00056	0.00010	0.00000	0.00003	0.00003	0.00059
D159	-0.00211	-0.00060	0.00000	-0.00021	-0.00021	-0.00232
D160	3.13766	-0.00030	0.00000	-0.00010	-0.00011	3.13756
D161	-3.14129	0.00039	0.00000	0.00014	0.00014	-3.14114
D162	0.00293	0.00008	0.00000	0.00005	0.00005	0.00298
D163	0.00516	0.00073	0.00000	0.00026	0.00027	0.00543
D164	-3.13380	0.00041	0.00000	0.00017	0.00017	-3.13364
D165	-0.00204	-0.00001	0.00000	0.00000	-0.00001	-0.00205
D166	3.13839	0.00030	0.00000	0.00011	0.00011	3.13849
D167	3.14136	-0.00030	0.00000	-0.00011	-0.00011	3.14125
D168	-0.00140	0.00001	0.00000	0.00001	0.00001	-0.00139
D169	-0.00720	-0.00039	0.00000	-0.00017	-0.00017	-0.00737
D170	3.13441	-0.00081	0.00000	-0.00034	-0.00034	3.13407
D171	3.13273	-0.00113	0.00000	-0.00039	-0.00039	3.13234
D172	-0.00885	-0.00156	0.00000	-0.00056	-0.00056	-0.00941
D173	0.00102	-0.00019	0.00000	-0.00007	-0.00007	0.00095
D174	3.14007	-0.00184	0.00000	-0.00068	-0.00068	3.13938
D175	-3.13792	-0.00011	0.00000	-0.00004	-0.00004	-3.13796
D176	0.00113	-0.00175	0.00000	-0.00065	-0.00065	0.00048
D177	0.00581	0.00038	0.00000	0.00015	0.00015	0.00596

D178	-3.13580	0.00081	0.00000	0.00031	0.00031	-3.13548
D179	-3.13478	0.00021	0.00000	0.00008	0.00008	-3.13470
D180	0.00680	0.00065	0.00000	0.00025	0.00024	0.00704
D181	3.13721	-0.00074	0.00000	-0.00026	-0.00026	3.13695
D182	-0.00452	-0.00047	0.00000	-0.00017	-0.00017	-0.00469
D183	-0.00563	-0.00043	0.00000	-0.00015	-0.00015	-0.00578
D184	3.13582	-0.00016	0.00000	-0.00005	-0.00005	3.13577
D185	3.13876	-0.00013	0.00000	-0.00005	-0.00004	3.13872
D186	-0.00318	-0.00049	0.00000	-0.00019	-0.00018	-0.00337
D187	-0.00281	-0.00060	0.00000	-0.00023	-0.00022	-0.00304
D188	3.13842	-0.00097	0.00000	-0.00037	-0.00037	3.13805
D189	0.00063	-0.00036	0.00000	-0.00013	-0.00013	0.00050
D190	-3.14099	0.00010	0.00000	0.00003	0.00003	-3.14096
D191	-3.14083	-0.00062	0.00000	-0.00022	-0.00022	-3.14104
D192	0.00074	-0.00017	0.00000	-0.00006	-0.00006	0.00068
D193	-0.00244	0.00028	0.00000	0.00009	0.00009	-0.00235
D194	3.13899	0.00013	0.00000	0.00004	0.00004	3.13903
D195	3.13951	0.00064	0.00000	0.00023	0.00023	3.13974
D196	-0.00224	0.00049	0.00000	0.00018	0.00018	-0.00207
D197	0.00333	0.00034	0.00000	0.00012	0.00012	0.00344
D198	-3.13811	0.00049	0.00000	0.00017	0.00017	-3.13793
D199	-3.13824	-0.00011	0.00000	-0.00004	-0.00004	-3.13828
D200	0.00351	0.00004	0.00000	0.00001	0.00001	0.00353

Item	Value	Threshold	Converged?

Maximum Force	0.383724	0.000450	NO

RMS Force	0.049750	0.000300	NO

Maximum Displacement	1.180006	0.001800	NO

RMS Displacement	0.167891	0.001200	NO

Predicted change in Energy=-2.939400D-01

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-12.179266	-0.236316	-0.314042
2	6	0	-11.624156	-1.489740	-0.235305
3	6	0	-12.474056	-2.635706	-0.259690
4	6	0	-13.882654	-2.456866	-0.403885
5	6	0	-14.427207	-1.163666	-0.498234
6	6	0	-13.579372	-0.048235	-0.441286
7	1	0	-12.075767	-3.622857	-0.175853
8	1	0	-14.542256	-3.307232	-0.445038
9	1	0	-15.490020	-1.028595	-0.617276
10	1	0	-14.002019	0.931204	-0.499719
11	6	0	-11.093933	0.865681	-0.248591
12	6	0	-10.046780	-1.372538	-0.127224
13	6	0	-9.618858	0.149998	-0.174455
14	6	0	-8.272692	0.784980	-0.150333
15	6	0	-6.660470	0.250945	-0.163986
16	6	0	-3.954377	-0.627761	0.073974
17	6	0	-4.063245	0.661802	0.318251
18	16	0	-5.688452	-1.327249	-0.296979

19	6	0	-5.530158	1.030894	0.002552
20	6	0	-2.363476	-0.956442	0.219621
21	6	0	-1.740403	0.213649	0.526207
22	7	0	-2.790440	1.278362	0.834630
23	16	0	-1.127008	-2.308053	0.116264
24	16	0	1.265148	1.264653	0.687651
25	6	0	0.325386	-1.183693	0.319098
26	6	0	-0.127059	0.107181	0.486829
27	6	0	1.970258	-1.260625	0.424970
28	6	0	2.534134	-0.017816	0.479605
29	6	0	4.120091	-0.178026	0.297571
30	6	0	4.368170	-1.479616	0.278194
31	6	0	5.902154	-1.844918	0.068113
32	6	0	6.773729	-0.731873	0.037470
33	16	0	5.683657	0.759010	0.087914
34	7	0	3.101366	-2.312660	0.494070
35	6	0	8.430738	-0.942286	-0.026223
36	6	0	9.517722	0.007132	-0.133952
37	6	0	9.391792	1.550674	-0.226823
38	6	0	11.137121	-0.197244	-0.198727
39	6	0	10.822980	2.162307	-0.331400
40	6	0	11.747616	1.199983	-0.309655
41	6	0	11.254185	3.636966	-0.449056
42	6	0	13.240994	1.518986	-0.389802
43	6	0	12.595634	3.931381	-0.522845
44	6	0	13.641863	2.804601	-0.488736
45	6	0	12.055224	-1.263541	-0.182077
46	6	0	12.112580	-2.797969	-0.099520
47	6	0	13.613468	-1.277720	-0.257257
48	7	0	12.280189	-3.943254	-0.044244
49	7	0	14.774232	-1.338343	-0.310728
50	6	0	-11.570008	2.177105	-0.259483
51	6	0	-13.040054	2.663938	-0.385519
52	6	0	-10.990918	3.590590	-0.182988
53	7	0	-14.119442	3.091703	-0.463598
54	7	0	-10.642588	4.686495	-0.120722
55	8	0	-9.275454	-2.350634	-0.015997
56	8	0	8.324461	2.198163	-0.221096
57	6	0	3.028441	-3.436446	-0.452540
58	1	0	2.132263	-3.994668	-0.279885
59	1	0	3.034432	-3.068527	-1.458563
60	1	0	3.881782	-4.074998	-0.302175
61	6	0	-2.966172	1.375275	2.315313
62	1	0	-3.215554	0.400551	2.705757
63	1	0	-2.061867	1.718625	2.777067
64	1	0	-3.762005	2.059801	2.538119
65	1	0	6.253358	-2.852717	-0.024577
66	1	0	13.965899	0.738554	-0.367905
67	1	0	14.690243	3.033238	-0.542907
68	1	0	12.925797	4.948545	-0.604721
69	1	0	10.529870	4.421785	-0.473498
70	1	0	8.746464	-1.965601	0.015612
71	1	0	-8.336564	1.858055	-0.095678
72	1	0	-5.696683	2.064561	-0.100258

Rotational constants (GHZ): 0.1616229 0.0080786 0.0077356

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions
 196 alpha electrons 196 beta electrons
 nuclear repulsion energy 6071.2297109000 Hartrees.
 NAToms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T
 Big=T
 Integral buffers will be 131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 Nuclear repulsion after empirical dispersion term = 6071.1522397002 Hartrees.
 One-electron integrals computed using PRISM.
 NBasis= 916 RedAO= T EigKep= 3.84D-04 NBF= 916
 NBSUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916
 Initial guess from the checkpoint file: "PBDB.chk"
 B after Tr= 0.000000 0.000000 0.000000
 Rot= 0.999997 0.002356 0.000009 0.000887 Ang= 0.29 deg.
 ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1
 AccDes= 0.00D+00
 Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.
 HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-yADJ=14
 ICTDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
 FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2001
 NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
 wScrn= 0.000000 ICntrl= 500 IOpCl= 0 IlCent= 200000004 NGrid= 0
 NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 Integral accuracy reduced to 1.0D-05 until final iterations.
 Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
 SCF Done: E(RB3LYP) = -3682.41770888 A.U. after 14 cycles
 NFock= 14 Conv=0.65D-08 -V/T= 2.0085
 Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1
 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-0.013149810	-0.037315193	-0.005772310
2	6	0.031434645	0.000529446	0.015717834
3	6	-0.020233510	-0.012753875	-0.009358439
4	6	0.016117846	-0.023424924	0.007666996
5	6	0.015487239	-0.012990723	0.007679301
6	6	0.012285555	0.011287357	0.007581444
7	1	0.010472184	0.003756342	0.006035846
8	1	0.003014552	0.005795069	0.001303227
9	1	-0.003862310	0.001530874	-0.002540490
10	1	-0.002743159	0.004091059	-0.000585389
11	6	0.001149179	-0.003648656	-0.000895026
12	6	0.026399358	0.015671112	0.016270334
13	6	-0.000907876	-0.020170052	-0.000062862
14	6	0.017491233	0.063183786	0.018640934

15	6	0.021943766	-0.000374996	0.003793340
16	6	0.043922805	0.040533600	0.039028749
17	6	-0.041897863	-0.000588985	-0.020898738
18	16	0.023168634	0.031054739	0.011366500
19	6	-0.009988340	-0.066016185	-0.039301286
20	6	-0.004970645	0.020016366	0.003514786
21	6	0.002776715	-0.026697742	-0.002778747
22	7	-0.008691168	0.010739286	0.023226736
23	16	-0.004551144	-0.006054875	0.004450093
24	16	-0.002820514	0.000837773	0.004681767
25	6	0.029876650	-0.009476674	0.006978422
26	6	-0.020783866	0.009758410	-0.026446958
27	6	0.006756593	0.033583225	0.011026276
28	6	0.006931449	-0.021147742	0.012110653
29	6	-0.042232105	-0.021949724	-0.034619361
30	6	0.053240662	0.046352838	0.034537159
31	6	-0.034888125	-0.002797235	-0.038610124
32	6	0.016006932	0.016630537	0.011948748
33	16	0.003007260	-0.002913774	-0.006915580
34	7	-0.034313991	-0.039151805	0.004348863
35	6	-0.046799912	-0.051110652	-0.020891262
36	6	0.008212776	0.013830904	0.003838448
37	6	-0.021547299	-0.005504731	-0.012760666
38	6	0.006688098	0.004807425	0.003159639
39	6	-0.059893127	-0.036080168	-0.033604251
40	6	0.063676288	-0.003766534	0.040379999
41	6	0.032321405	0.049543539	0.014583893
42	6	-0.034477451	0.041397107	-0.025990659
43	6	0.045028733	0.030507909	0.024782688
44	6	-0.059302567	-0.009129084	-0.036125947
45	6	0.056148565	0.015820670	0.034598163
46	6	-0.062731897	-0.020961269	-0.038325441
47	6	-0.051488081	0.005745192	-0.033607194
48	7	0.007619182	0.011722289	0.003716556
49	7	0.004785353	0.002800646	0.002802114
50	6	-0.046298456	-0.036262839	-0.025260386
51	6	0.048949559	-0.002192957	0.024891008
52	6	0.044080875	0.068841747	0.028990804
53	7	-0.002248893	-0.006390276	-0.000950906
54	7	-0.006504092	-0.028713110	-0.005391285
55	8	-0.049326207	-0.020688837	-0.024220090
56	8	0.042656322	-0.002178108	0.027180504
57	6	-0.001412325	-0.009426632	-0.011921070
58	1	-0.002300449	0.014793581	-0.005809673
59	1	-0.010751455	-0.000490422	0.014695139
60	1	0.010568099	0.001266456	0.003262984
61	6	-0.004030359	-0.001776359	0.013241125
62	1	0.007483684	0.009597984	-0.005019458
63	1	0.007648618	-0.012325952	0.000496729
64	1	-0.010213869	-0.002524751	-0.007966423
65	1	0.006588333	0.007184280	0.001504719
66	1	0.003857766	-0.000175175	0.002259662
67	1	0.001227079	-0.007752967	0.001656474
68	1	-0.001924975	-0.008392294	-0.000294186
69	1	-0.010021758	0.003382690	-0.006727603
70	1	0.002925119	0.013675035	0.000472572
71	1	0.001157319	-0.011943071	0.002670877
72	1	-0.015798831	-0.025009926	-0.017440295

Cartesian Forces: Max 0.068841747 RMS 0.023824621

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 GSVD: received Info= 1 from GESDD.
 Internal Forces: Max 0.118167432 RMS 0.025749469
 Search for a local minimum.
 Step number 2 out of a maximum of 429
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- RFO/linear search
 Update second derivatives using D2CorX and points 1 2
 DE= -1.87D-01 DEPred=-2.94D-01 R= 6.37D-01
 TightC=F SS= 1.41D+00 RLast= 3.00D-01 DXNew= 5.0454D-01 9.0134D-01
 Trust test= 6.37D-01 RLast= 3.00D-01 DXMaxT set to 5.05D-01
 ITU= 1 0
 Use linear search instead of GDIIS.
 Linear search step of 0.600 exceeds DXMaxT= 0.505 but not scaled.
 Quartic linear search produced a step of 2.00000.
 Iteration 1 RMS(Cart)= 0.23868493 RMS(Int)= 0.01356182
 Iteration 2 RMS(Cart)= 0.10809723 RMS(Int)= 0.00221783
 Iteration 3 RMS(Cart)= 0.00408876 RMS(Int)= 0.00012067
 Iteration 4 RMS(Cart)= 0.00001326 RMS(Int)= 0.00012061
 Iteration 5 RMS(Cart)= 0.00000000 RMS(Int)= 0.00012061

Variable (Linear)	Old X (Quad)	-DE/DX (Total)	Delta X	Delta X	Delta X	New X
R1	2.59479	0.02916	0.03223	0.00000	0.03201	2.62680
R2	2.68039	-0.01273	-0.00237	0.00000	-0.00222	2.67817
R3	2.92549	-0.01128	0.04405	0.00000	0.04406	2.96955
R4	2.69653	-0.03033	-0.01682	0.00000	-0.01690	2.67963
R5	2.99600	-0.05720	-0.05072	0.00000	-0.05092	2.94507
R6	2.69703	-0.03385	-0.03037	0.00000	-0.03051	2.66652
R7	2.01779	0.01224	0.00728	0.00000	0.00728	2.02508
R8	2.65761	-0.00319	-0.01186	0.00000	-0.01193	2.64568
R9	2.03520	0.00568	0.00353	0.00000	0.00353	2.03873
R10	2.64983	-0.00806	-0.00397	0.00000	-0.00389	2.64594
R11	2.03704	0.00475	0.00295	0.00000	0.00295	2.04000
R12	2.01887	0.00025	-0.02017	0.00000	-0.02017	1.99869
R13	3.10142	-0.07145	-0.03906	0.00000	-0.03877	3.06266
R14	2.63656	-0.03389	0.01633	0.00000	0.01633	2.65288
R15	2.98999	-0.05083	-0.04747	0.00000	-0.04733	2.94266
R16	2.36328	-0.05848	-0.02778	0.00000	-0.02778	2.33550
R17	2.81306	-0.11817	-0.07146	0.00000	-0.07146	2.74160
R18	3.20955	-0.11125	-0.07220	0.00000	-0.07220	3.13735
R19	2.03403	0.00761	0.00440	0.00000	0.00440	2.03843
R20	3.51164	-0.00084	0.00056	0.00000	0.00061	3.51225
R21	2.61415	-0.02163	-0.01285	0.00000	-0.01271	2.60144
R22	2.48877	0.06549	0.03539	0.00000	0.03523	2.52400
R23	3.60235	-0.04613	-0.02790	0.00000	-0.02801	3.57434
R24	3.08217	-0.07776	-0.04853	0.00000	-0.04851	3.03366
R25	2.92006	-0.07843	-0.04768	0.00000	-0.04764	2.87241
R26	2.84517	-0.04567	-0.02712	0.00000	-0.02716	2.81801
R27	1.98805	0.03285	0.01982	0.00000	0.01982	2.00788
R28	2.57123	0.00566	0.00201	0.00000	0.00208	2.57331
R29	3.46722	-0.03070	-0.01901	0.00000	-0.01901	3.44821
R30	2.88536	-0.04201	-0.02575	0.00000	-0.02574	2.85961
R31	3.05632	-0.09292	-0.05891	0.00000	-0.05892	2.99740
R32	2.82367	-0.00033	-0.00016	0.00000	-0.00016	2.82351
R33	3.49205	-0.03034	-0.01907	0.00000	-0.01907	3.47298
R34	3.44237	-0.02462	-0.01539	0.00000	-0.01538	3.42699

R35	3.43199	-0.02610	-0.01619	0.00000	-0.01619	3.41581
R36	2.60426	-0.00263	-0.00197	0.00000	-0.00197	2.60228
R37	3.11818	-0.09675	-0.06197	0.00000	-0.06198	3.05620
R38	2.58106	0.00236	0.00047	0.00000	0.00054	2.58160
R39	2.92203	-0.06241	-0.03811	0.00000	-0.03811	2.88392
R40	3.03186	-0.08177	-0.05103	0.00000	-0.05100	2.98086
R41	2.50419	0.04011	0.02124	0.00000	0.02110	2.52530
R42	3.46739	-0.03634	-0.02217	0.00000	-0.02219	3.44521
R43	3.00620	-0.09105	-0.05698	0.00000	-0.05703	2.94917
R44	2.89403	-0.05976	-0.03613	0.00000	-0.03620	2.85783
R45	2.67211	-0.03854	-0.02311	0.00000	-0.02306	2.64905
R46	2.02438	0.00912	0.00551	0.00000	0.00551	2.02989
R47	3.49141	-0.02197	-0.01429	0.00000	-0.01421	3.47720
R48	3.15873	-0.10021	-0.06516	0.00000	-0.06516	3.09357
R49	2.78007	0.00417	0.00262	0.00000	0.00262	2.78269
R50	2.73491	-0.09270	-0.05568	0.00000	-0.05568	2.67923
R51	2.02528	0.01040	0.00608	0.00000	0.00608	2.03136
R52	2.93182	-0.03670	-0.04735	0.00000	-0.04726	2.88456
R53	3.08692	-0.06742	-0.03379	0.00000	-0.03343	3.05349
R54	2.94781	-0.04858	-0.05195	0.00000	-0.05225	2.89556
R55	2.35911	-0.05058	-0.02408	0.00000	-0.02408	2.33503
R56	2.88903	-0.00970	0.06997	0.00000	0.07006	2.95908
R57	2.65920	-0.05015	0.02331	0.00000	0.02331	2.68251
R58	2.52226	0.04024	0.04561	0.00000	0.04541	2.56767
R59	2.91190	-0.06982	-0.04036	0.00000	-0.04056	2.87134
R60	2.88972	-0.05544	-0.02593	0.00000	-0.02562	2.86409
R61	2.59905	-0.01704	-0.02542	0.00000	-0.02572	2.57333
R62	2.01871	0.01117	0.00662	0.00000	0.00662	2.02533
R63	2.55168	0.01300	0.00634	0.00000	0.00654	2.55823
R64	2.01328	0.00436	-0.02670	0.00000	-0.02670	1.98658
R65	2.90637	-0.05778	-0.05183	0.00000	-0.05192	2.85445
R66	2.02680	0.00857	0.00529	0.00000	0.00529	2.03209
R67	2.03030	0.00711	0.00449	0.00000	0.00449	2.03479
R68	2.90586	-0.04748	-0.03057	0.00000	-0.03057	2.87529
R69	2.94820	-0.05046	-0.02464	0.00000	-0.02464	2.92356
R70	2.18982	0.01430	0.00517	0.00000	0.00517	2.19499
R71	2.19884	0.00310	0.00508	0.00000	0.00508	2.20392
R72	2.93603	-0.05259	-0.02810	0.00000	-0.02810	2.90793
R73	2.89019	-0.04952	-0.03131	0.00000	-0.03131	2.85889
R74	2.19904	0.00075	0.00265	0.00000	0.00265	2.20169
R75	2.17624	0.02991	0.01109	0.00000	0.01109	2.18732
R76	2.02170	0.01601	0.00958	0.00000	0.00958	2.03128
R77	2.02428	0.01750	0.01048	0.00000	0.01048	2.03477
R78	2.03403	0.01098	0.00662	0.00000	0.00662	2.04065
R79	2.03944	0.01260	0.00759	0.00000	0.00759	2.04703
R80	2.02551	0.01425	0.00853	0.00000	0.00853	2.03404
R81	2.02789	0.01303	0.00783	0.00000	0.00783	2.03572
A1	2.12380	-0.02078	-0.04668	0.00000	-0.04639	2.07741
A2	1.94329	-0.01114	-0.01559	0.00000	-0.01594	1.92736
A3	2.21609	0.03192	0.06227	0.00000	0.06233	2.27842
A4	2.08441	0.01813	0.02727	0.00000	0.02742	2.11183
A5	1.91628	0.00486	0.01317	0.00000	0.01273	1.92901
A6	2.28250	-0.02299	-0.04043	0.00000	-0.04015	2.24235
A7	2.08167	-0.00439	0.00119	0.00000	0.00089	2.08256
A8	2.11642	-0.00098	-0.00234	0.00000	-0.00219	2.11423
A9	2.08510	0.00537	0.00115	0.00000	0.00130	2.08639
A10	2.09921	0.00117	-0.00713	0.00000	-0.00741	2.09180
A11	2.10527	-0.00411	0.00079	0.00000	0.00093	2.10620
A12	2.07870	0.00293	0.00634	0.00000	0.00647	2.08517
A13	2.08820	0.01018	0.01092	0.00000	0.01088	2.09908

A14	2.09949	-0.00419	-0.00491	0.00000	-0.00489	2.09460
A15	2.09549	-0.00598	-0.00601	0.00000	-0.00599	2.08950
A16	2.08863	-0.00429	0.01445	0.00000	0.01462	2.10325
A17	2.11412	0.00710	0.00699	0.00000	0.00691	2.12103
A18	2.08043	-0.00281	-0.02144	0.00000	-0.02153	2.05890
A19	1.89822	-0.01945	-0.03334	0.00000	-0.03301	1.86521
A20	2.01478	0.09300	0.17698	0.00000	0.17681	2.19159
A21	2.37017	-0.07355	-0.14364	0.00000	-0.14381	2.22637
A22	1.91578	-0.01618	-0.00959	0.00000	-0.00963	1.90615
A23	2.16746	0.01431	0.00923	0.00000	0.00925	2.17671
A24	2.19993	0.00187	0.00036	0.00000	0.00038	2.20031
A25	1.74964	0.04193	0.04530	0.00000	0.04579	1.79543
A26	2.24913	-0.02233	-0.02372	0.00000	-0.02397	2.22516
A27	2.28440	-0.01960	-0.02159	0.00000	-0.02183	2.26256
A28	2.38062	-0.03346	-0.02115	0.00000	-0.02115	2.35947
A29	1.95241	0.02638	0.01702	0.00000	0.01702	1.96944
A30	1.95003	0.00708	0.00412	0.00000	0.00412	1.95415
A31	2.44050	-0.05414	-0.03358	0.00000	-0.03368	2.40682
A32	2.21101	-0.03789	-0.02494	0.00000	-0.02506	2.18595
A33	1.63089	0.09210	0.05856	0.00000	0.05879	1.68967
A34	1.89673	0.02451	0.01731	0.00000	0.01717	1.91390
A35	1.83526	-0.00472	-0.00244	0.00000	-0.00243	1.83283
A36	2.55120	-0.01979	-0.01487	0.00000	-0.01475	2.53645
A37	1.84883	0.02135	0.01410	0.00000	0.01413	1.86296
A38	1.97655	0.00346	0.00339	0.00000	0.00330	1.97985
A39	2.45718	-0.02479	-0.01748	0.00000	-0.01742	2.43976
A40	1.72163	-0.06113	-0.03995	0.00000	-0.04001	1.68162
A41	2.29909	-0.07627	-0.04958	0.00000	-0.04955	2.24954
A42	1.99640	0.04161	0.02767	0.00000	0.02764	2.02404
A43	1.98769	0.03468	0.02194	0.00000	0.02191	2.00960
A44	1.86867	-0.01221	-0.00792	0.00000	-0.00786	1.86081
A45	2.49935	-0.01570	-0.01045	0.00000	-0.01048	2.48887
A46	1.91515	0.02791	0.01837	0.00000	0.01834	1.93350
A47	1.90738	0.03208	0.02026	0.00000	0.02031	1.92769
A48	1.97654	-0.00944	-0.00592	0.00000	-0.00594	1.97060
A49	2.39917	-0.02264	-0.01433	0.00000	-0.01437	2.38481
A50	1.79932	-0.01816	-0.01286	0.00000	-0.01288	1.78644
A51	1.84108	0.01469	0.00984	0.00000	0.00987	1.85095
A52	1.90316	0.00490	0.00342	0.00000	0.00339	1.90654
A53	1.64613	-0.03864	-0.02533	0.00000	-0.02531	1.62082
A54	1.64355	-0.03807	-0.02514	0.00000	-0.02510	1.61845
A55	1.90208	0.02972	0.01935	0.00000	0.01937	1.92145
A56	2.43745	-0.02312	-0.01481	0.00000	-0.01482	2.42263
A57	1.94243	-0.00648	-0.00446	0.00000	-0.00447	1.93796
A58	2.37153	-0.01692	-0.01104	0.00000	-0.01105	2.36049
A59	1.97374	-0.00909	-0.00613	0.00000	-0.00612	1.96761
A60	1.93659	0.02608	0.01721	0.00000	0.01722	1.95381
A61	1.95162	-0.00547	-0.00341	0.00000	-0.00343	1.94819
A62	2.43996	-0.02198	-0.01392	0.00000	-0.01394	2.42602
A63	1.89157	0.02743	0.01732	0.00000	0.01736	1.90893
A64	1.93763	0.02470	0.01635	0.00000	0.01633	1.95396
A65	2.45627	-0.01182	-0.00811	0.00000	-0.00816	2.44811
A66	1.88883	-0.01283	-0.00820	0.00000	-0.00813	1.88069
A67	1.85959	-0.00815	-0.00468	0.00000	-0.00466	1.85493
A68	2.50533	-0.01024	-0.00808	0.00000	-0.00799	2.49733
A69	1.91814	0.01839	0.01275	0.00000	0.01265	1.93079
A70	1.99106	-0.00453	-0.00233	0.00000	-0.00241	1.98864
A71	1.95774	0.00874	0.00639	0.00000	0.00633	1.96408
A72	2.33414	-0.00421	-0.00407	0.00000	-0.00392	2.33022
A73	2.00035	-0.01763	-0.01215	0.00000	-0.01216	1.98819

A74	2.14550	0.00620	0.00402	0.00000	0.00402	2.14953
A75	2.13716	0.01146	0.00815	0.00000	0.00816	2.14532
A76	1.84515	0.04793	0.03060	0.00000	0.03072	1.87587
A77	2.10920	-0.01482	-0.00932	0.00000	-0.00938	2.09982
A78	2.32883	-0.03311	-0.02128	0.00000	-0.02134	2.30749
A79	1.66473	-0.04379	-0.02860	0.00000	-0.02851	1.63621
A80	1.80154	-0.01416	-0.01012	0.00000	-0.01020	1.79134
A81	2.04284	0.00270	0.00193	0.00000	0.00201	2.04485
A82	1.94531	0.01477	0.01018	0.00000	0.01022	1.95553
A83	2.29802	-0.01805	-0.01328	0.00000	-0.01328	2.28475
A84	1.99406	-0.00045	0.00027	0.00000	0.00027	1.99434
A85	1.99109	0.01850	0.01300	0.00000	0.01300	2.00409
A86	2.20951	-0.00752	-0.02005	0.00000	-0.02030	2.18921
A87	2.29889	-0.02553	-0.02908	0.00000	-0.02933	2.26956
A88	1.77478	0.03304	0.04913	0.00000	0.04963	1.82441
A89	1.89614	-0.01004	-0.00569	0.00000	-0.00585	1.89029
A90	2.19585	0.00252	0.00009	0.00000	0.00017	2.19602
A91	2.19120	0.00752	0.00560	0.00000	0.00568	2.19688
A92	1.85918	-0.00921	-0.03567	0.00000	-0.03518	1.82400
A93	2.40555	-0.06836	-0.19138	0.00000	-0.19162	2.21393
A94	2.01845	0.07756	0.22705	0.00000	0.22680	2.24525
A95	1.93029	0.00007	0.01589	0.00000	0.01542	1.94571
A96	2.26153	-0.01466	-0.05090	0.00000	-0.05055	2.21097
A97	2.09137	0.01459	0.03502	0.00000	0.03513	2.12650
A98	1.96436	-0.01387	-0.02366	0.00000	-0.02402	1.94034
A99	2.19499	0.03319	0.08807	0.00000	0.08799	2.28298
A100	2.12384	-0.01932	-0.06441	0.00000	-0.06397	2.05987
A101	2.07361	-0.00208	0.00509	0.00000	0.00449	2.07810
A102	2.11191	-0.00470	-0.00606	0.00000	-0.00576	2.10615
A103	2.09766	0.00678	0.00097	0.00000	0.00127	2.09893
A104	2.08563	-0.00444	0.02311	0.00000	0.02358	2.10920
A105	2.10668	0.00324	0.00455	0.00000	0.00432	2.11099
A106	2.09088	0.00120	-0.02766	0.00000	-0.02789	2.06299
A107	2.10072	0.00216	-0.01106	0.00000	-0.01156	2.08917
A108	2.10291	-0.00015	0.00572	0.00000	0.00597	2.10888
A109	2.07956	-0.00201	0.00534	0.00000	0.00559	2.08514
A110	2.09118	0.00909	0.01225	0.00000	0.01232	2.10350
A111	2.08978	-0.00077	-0.00333	0.00000	-0.00336	2.08642
A112	2.10223	-0.00833	-0.00892	0.00000	-0.00896	2.09327
A113	2.46722	-0.07002	-0.11918	0.00000	-0.11918	2.34804
A114	2.28892	0.00314	0.16479	0.00000	0.16479	2.45371
A115	1.52705	0.06688	-0.04561	0.00000	-0.04561	1.48143
A116	2.23701	0.02782	0.12601	0.00000	0.12601	2.36302
A117	2.40254	-0.06365	-0.09006	0.00000	-0.09006	2.31248
A118	1.64358	0.03583	-0.03595	0.00000	-0.03595	1.60763
A119	1.91374	-0.00182	-0.00131	0.00000	-0.00132	1.91242
A120	1.91947	0.00834	0.00593	0.00000	0.00593	1.92540
A121	1.90074	-0.00177	-0.00133	0.00000	-0.00133	1.89940
A122	1.91289	-0.00212	-0.00145	0.00000	-0.00145	1.91144
A123	1.90924	-0.00110	-0.00081	0.00000	-0.00082	1.90842
A124	1.90765	-0.00156	-0.00104	0.00000	-0.00105	1.90661
A125	1.90403	0.00738	0.00521	0.00000	0.00521	1.90924
A126	1.92671	-0.00459	-0.00319	0.00000	-0.00319	1.92352
A127	1.91170	-0.00282	-0.00198	0.00000	-0.00198	1.90972
A128	1.90542	-0.00033	-0.00023	0.00000	-0.00022	1.90520
A129	1.90672	-0.00045	-0.00027	0.00000	-0.00027	1.90645
A130	1.90912	0.00085	0.00049	0.00000	0.00048	1.90960
A131	3.24942	-0.00482	-0.00227	0.00000	-0.00227	3.24715
A132	3.18468	0.01184	0.08614	0.00000	0.08614	3.27082
A133	3.19908	0.01494	0.06086	0.00000	0.06086	3.25994

A134	3.22232	-0.00247	-0.00121	0.00000	-0.00121	3.22111
A135	3.13571	0.00020	0.00006	0.00000	0.00006	3.13577
A136	3.14217	0.00009	0.00116	0.00000	0.00116	3.14333
A137	3.12657	0.00063	-0.00118	0.00000	-0.00118	3.12539
A138	3.14919	-0.00042	-0.00027	0.00000	-0.00027	3.14891
D1	-0.01812	0.00005	-0.00070	0.00000	-0.00065	-0.01877
D2	3.12332	-0.00042	-0.00126	0.00000	-0.00121	3.12210
D3	3.12571	0.00027	-0.00027	0.00000	-0.00026	3.12544
D4	-0.01604	-0.00020	-0.00083	0.00000	-0.00083	-0.01687
D5	-0.00768	0.00051	0.00096	0.00000	0.00090	-0.00677
D6	3.13929	0.00035	0.00126	0.00000	0.00123	3.14052
D7	3.13130	0.00018	0.00034	0.00000	0.00028	3.13159
D8	-0.00492	0.00002	0.00064	0.00000	0.00061	-0.00431
D9	0.04485	-0.00064	0.00014	0.00000	0.00013	0.04498
D10	-3.09214	0.00009	0.00175	0.00000	0.00191	-3.09024
D11	-3.09436	-0.00031	0.00076	0.00000	0.00075	-3.09360
D12	0.05184	0.00042	0.00236	0.00000	0.00254	0.05437
D13	0.03090	-0.00050	0.00021	0.00000	0.00018	0.03107
D14	-3.11473	-0.00043	-0.00006	0.00000	-0.00007	-3.11480
D15	-3.11050	0.00008	0.00091	0.00000	0.00085	-3.10965
D16	0.02705	0.00014	0.00064	0.00000	0.00061	0.02766
D17	-0.01988	0.00088	0.00058	0.00000	0.00062	-0.01926
D18	3.11670	0.00087	0.00104	0.00000	0.00107	3.11777
D19	3.12154	0.00035	-0.00007	0.00000	0.00000	3.12154
D20	-0.02507	0.00034	0.00039	0.00000	0.00046	-0.02461
D21	-0.01844	0.00062	0.00072	0.00000	0.00073	-0.01771
D22	3.11984	0.00046	0.00025	0.00000	0.00027	3.12011
D23	3.12712	0.00057	0.00099	0.00000	0.00097	3.12809
D24	-0.01779	0.00041	0.00053	0.00000	0.00052	-0.01728
D25	-0.00713	0.00000	-0.00026	0.00000	-0.00024	-0.00737
D26	3.13065	-0.00003	-0.00030	0.00000	-0.00031	3.13034
D27	3.13773	0.00017	0.00021	0.00000	0.00022	3.13796
D28	-0.00768	0.00014	0.00016	0.00000	0.00015	-0.00752
D29	0.02030	-0.00060	-0.00039	0.00000	-0.00041	0.01989
D30	-3.12656	-0.00041	-0.00060	0.00000	-0.00064	-3.12721
D31	-3.11749	-0.00057	-0.00035	0.00000	-0.00034	-3.11783
D32	0.01884	-0.00038	-0.00056	0.00000	-0.00058	0.01826
D33	-0.05154	-0.00023	-0.00103	0.00000	-0.00112	-0.05265
D34	3.09664	0.00019	0.00001	0.00000	-0.00006	3.09658
D35	3.08410	-0.00046	-0.00190	0.00000	-0.00171	3.08239
D36	-0.05091	-0.00004	-0.00085	0.00000	-0.00065	-0.05155
D37	-0.04665	0.00031	-0.00095	0.00000	-0.00098	-0.04763
D38	3.10923	0.00011	-0.00066	0.00000	-0.00069	3.10854
D39	3.10119	0.00088	0.00044	0.00000	0.00047	3.10166
D40	-0.02612	0.00068	0.00073	0.00000	0.00076	-0.02536
D41	0.04276	0.00025	0.00134	0.00000	0.00140	0.04416
D42	-3.10561	-0.00019	0.00027	0.00000	0.00030	-3.10531
D43	-3.09370	0.00021	0.00084	0.00000	0.00090	-3.09280
D44	0.04111	-0.00023	-0.00023	0.00000	-0.00019	0.04092
D45	-3.06794	-0.00286	-0.00255	0.00000	-0.00253	-3.07046
D46	0.09321	-0.00277	-0.00249	0.00000	-0.00246	0.09075
D47	0.08223	-0.00253	-0.00140	0.00000	-0.00142	0.08081
D48	-3.03981	-0.00244	-0.00134	0.00000	-0.00136	-3.04117
D49	0.06966	0.00163	0.00097	0.00000	0.00093	0.07059
D50	-3.01679	-0.00361	-0.00242	0.00000	-0.00239	-3.01918
D51	-3.09147	0.00169	0.00101	0.00000	0.00097	-3.09050
D52	0.10527	-0.00355	-0.00238	0.00000	-0.00234	0.10292
D53	-3.00438	0.00115	0.00063	0.00000	0.00041	-3.00398
D54	0.09291	0.00386	0.00238	0.00000	0.00208	0.09499
D55	2.87259	0.00790	0.00593	0.00000	0.00576	2.87835

D56	-0.26439	0.00009	0.00060	0.00000	0.00060	-0.26378
D57	-0.23337	0.00700	0.00531	0.00000	0.00512	-0.22825
D58	2.91283	-0.00081	-0.00003	0.00000	-0.00004	2.91279
D59	-0.12773	-0.00314	-0.00195	0.00000	-0.00180	-0.12953
D60	2.98393	-0.00328	-0.00200	0.00000	-0.00188	2.98205
D61	3.01388	-0.00235	-0.00144	0.00000	-0.00128	3.01260
D62	-0.15764	-0.00249	-0.00149	0.00000	-0.00137	-0.15901
D63	0.02880	-0.00319	-0.00204	0.00000	-0.00176	0.02705
D64	-3.11283	-0.00457	-0.00294	0.00000	-0.00263	-3.11546
D65	-0.00828	0.00380	0.00255	0.00000	0.00244	-0.00584
D66	3.13859	0.00291	0.00212	0.00000	0.00210	3.14069
D67	3.13336	0.00514	0.00343	0.00000	0.00329	3.13665
D68	-0.00296	0.00426	0.00301	0.00000	0.00295	-0.00001
D69	0.28087	-0.01616	-0.01104	0.00000	-0.01089	0.26997
D70	-2.86532	-0.00837	-0.00571	0.00000	-0.00576	-2.87108
D71	-2.81722	-0.01734	-0.01198	0.00000	-0.01174	-2.82896
D72	0.31978	-0.00955	-0.00664	0.00000	-0.00660	0.31318
D73	0.25259	-0.00281	-0.00218	0.00000	-0.00232	0.25027
D74	-1.74290	-0.00639	-0.00448	0.00000	-0.00446	-1.74736
D75	-2.93454	-0.00136	-0.00109	0.00000	-0.00131	-2.93585
D76	1.35316	-0.00494	-0.00339	0.00000	-0.00345	1.34970
D77	0.16406	-0.00178	-0.00146	0.00000	-0.00145	0.16261
D78	-2.98983	-0.00181	-0.00133	0.00000	-0.00132	-2.99115
D79	-2.98089	-0.00132	-0.00126	0.00000	-0.00130	-2.98219
D80	0.14841	-0.00135	-0.00113	0.00000	-0.00117	0.14724
D81	3.02967	0.00383	0.00255	0.00000	0.00246	3.03213
D82	-0.10656	0.00300	0.00217	0.00000	0.00216	-0.10440
D83	-0.24729	0.00056	0.00108	0.00000	0.00110	-0.24619
D84	1.70281	0.01058	0.00755	0.00000	0.00753	1.71034
D85	2.91101	0.00025	0.00069	0.00000	0.00071	2.91172
D86	-1.42207	0.01028	0.00715	0.00000	0.00714	-1.41494
D87	3.06751	0.00194	0.00130	0.00000	0.00130	3.06881
D88	-0.13638	0.00458	0.00317	0.00000	0.00315	-0.13323
D89	-0.09125	0.00251	0.00188	0.00000	0.00187	-0.08938
D90	2.98805	0.00516	0.00374	0.00000	0.00372	2.99177
D91	0.95171	-0.00552	-0.00404	0.00000	-0.00404	0.94767
D92	3.04547	-0.00411	-0.00300	0.00000	-0.00301	3.04246
D93	-1.13453	-0.00775	-0.00567	0.00000	-0.00567	-1.14021
D94	-0.97059	0.00619	0.00455	0.00000	0.00456	-0.96603
D95	1.12317	0.00761	0.00559	0.00000	0.00559	1.12875
D96	-3.05683	0.00397	0.00292	0.00000	0.00292	-3.05391
D97	0.02642	-0.00105	-0.00083	0.00000	-0.00084	0.02558
D98	3.10668	0.00230	0.00157	0.00000	0.00155	3.10823
D99	3.11543	0.00035	0.00025	0.00000	0.00026	3.11569
D100	0.03520	-0.00140	-0.00102	0.00000	-0.00100	0.03420
D101	-0.12113	0.00442	0.00313	0.00000	0.00309	-0.11804
D102	2.98223	0.00676	0.00463	0.00000	0.00459	2.98681
D103	0.04923	0.00011	0.00003	0.00000	0.00005	0.04928
D104	-3.13879	0.00080	0.00057	0.00000	0.00060	-3.13819
D105	-3.04976	-0.00117	-0.00096	0.00000	-0.00097	-3.05073
D106	0.04541	-0.00047	-0.00041	0.00000	-0.00042	0.04499
D107	3.06468	0.00139	0.00096	0.00000	0.00097	3.06565
D108	-0.08764	-0.00037	-0.00026	0.00000	-0.00025	-0.08789
D109	-0.13916	0.00560	0.00393	0.00000	0.00390	-0.13526
D110	2.99170	0.00384	0.00271	0.00000	0.00269	2.99439
D111	0.16081	-0.00268	-0.00205	0.00000	-0.00208	0.15873
D112	-2.95531	-0.00398	-0.00285	0.00000	-0.00290	-2.95821
D113	-2.97348	-0.00123	-0.00106	0.00000	-0.00107	-2.97456
D114	0.19358	-0.00252	-0.00187	0.00000	-0.00189	0.19170
D115	2.93892	0.00509	0.00362	0.00000	0.00363	2.94255

D116	0.79547	-0.00467	-0.00289	0.00000	-0.00289	0.79258
D117	-0.21317	0.00325	0.00236	0.00000	0.00236	-0.21082
D118	-2.35662	-0.00652	-0.00415	0.00000	-0.00416	-2.36078
D119	3.08053	0.00239	0.00174	0.00000	0.00174	3.08227
D120	-0.08147	0.00218	0.00156	0.00000	0.00155	-0.07991
D121	-0.09864	0.00520	0.00355	0.00000	0.00353	-0.09511
D122	3.02255	0.00499	0.00337	0.00000	0.00334	3.02589
D123	3.11730	0.00002	-0.00005	0.00000	-0.00007	3.11723
D124	-0.04458	-0.00026	-0.00037	0.00000	-0.00038	-0.04496
D125	-0.01140	0.00042	0.00026	0.00000	0.00025	-0.01115
D126	3.10990	0.00014	-0.00005	0.00000	-0.00006	3.10985
D127	3.12184	0.00256	0.00184	0.00000	0.00184	3.12368
D128	-0.04055	0.00216	0.00153	0.00000	0.00152	-0.03903
D129	0.08038	-0.00421	-0.00297	0.00000	-0.00295	0.07743
D130	-3.08048	-0.00225	-0.00156	0.00000	-0.00154	-3.08203
D131	-3.03520	-0.00405	-0.00273	0.00000	-0.00272	-3.03793
D132	0.08711	-0.00209	-0.00133	0.00000	-0.00132	0.08580
D133	0.15394	-0.00268	-0.00173	0.00000	-0.00174	0.15220
D134	2.36103	-0.00016	-0.00011	0.00000	-0.00014	2.36089
D135	-3.01329	-0.00298	-0.00206	0.00000	-0.00206	-3.01535
D136	-0.80620	-0.00045	-0.00044	0.00000	-0.00046	-0.80666
D137	-0.10130	0.00207	0.00170	0.00000	0.00172	-0.09958
D138	3.03727	0.00217	0.00172	0.00000	0.00174	3.03901
D139	3.05946	0.00019	0.00036	0.00000	0.00037	3.05984
D140	-0.08515	0.00029	0.00037	0.00000	0.00039	-0.08477
D141	0.08226	-0.00240	-0.00185	0.00000	-0.00183	0.08043
D142	-3.05575	-0.00260	-0.00192	0.00000	-0.00190	-3.05765
D143	3.07825	0.00032	0.00026	0.00000	0.00026	3.07851
D144	-0.05757	-0.00010	-0.00003	0.00000	-0.00003	-0.05760
D145	-0.06735	0.00064	0.00040	0.00000	0.00040	-0.06696
D146	3.08001	0.00022	0.00011	0.00000	0.00011	3.08011
D147	-1.06901	-0.00420	-0.00320	0.00000	-0.00320	-1.07221
D148	1.03559	-0.00273	-0.00209	0.00000	-0.00210	1.03349
D149	3.12564	-0.00070	-0.00062	0.00000	-0.00062	3.12501
D150	-3.13657	0.00103	0.00084	0.00000	0.00085	-3.13572
D151	-1.03197	0.00251	0.00195	0.00000	0.00196	-1.03002
D152	1.05807	0.00453	0.00343	0.00000	0.00343	1.06150
D153	-0.00406	-0.00026	-0.00030	0.00000	-0.00030	-0.00437
D154	-3.13959	-0.00041	-0.00016	0.00000	-0.00016	-3.13975
D155	3.13177	0.00011	-0.00005	0.00000	-0.00004	3.13173
D156	-0.00376	-0.00004	0.00010	0.00000	0.00010	-0.00366
D157	-3.13929	-0.00001	-0.00015	0.00000	-0.00016	-3.13945
D158	0.00059	0.00004	0.00006	0.00000	0.00005	0.00064
D159	-0.00232	-0.00004	-0.00043	0.00000	-0.00045	-0.00277
D160	3.13756	0.00001	-0.00021	0.00000	-0.00024	3.13732
D161	-3.14114	0.00011	0.00029	0.00000	0.00031	-3.14084
D162	0.00298	0.00007	0.00009	0.00000	0.00005	0.00303
D163	0.00543	0.00005	0.00053	0.00000	0.00056	0.00598
D164	-3.13364	0.00001	0.00033	0.00000	0.00030	-3.13334
D165	-0.00205	0.00001	-0.00001	0.00000	-0.00003	-0.00208
D166	3.13849	0.00008	0.00022	0.00000	0.00019	3.13868
D167	3.14125	-0.00003	-0.00022	0.00000	-0.00024	3.14102
D168	-0.00139	0.00003	0.00001	0.00000	-0.00002	-0.00140
D169	-0.00737	0.00012	-0.00035	0.00000	-0.00035	-0.00772
D170	3.13407	0.00003	-0.00069	0.00000	-0.00071	3.13336
D171	3.13234	-0.00006	-0.00079	0.00000	-0.00079	3.13155
D172	-0.00941	-0.00014	-0.00113	0.00000	-0.00115	-0.01056
D173	0.00095	-0.00010	-0.00015	0.00000	-0.00017	0.00077
D174	3.13938	-0.00022	-0.00137	0.00000	-0.00139	3.13799
D175	-3.13796	-0.00004	-0.00007	0.00000	-0.00005	-3.13801

D176	0.00048	-0.00016	-0.00129	0.00000	-0.00127	-0.00079
D177	0.00596	-0.00007	0.00030	0.00000	0.00032	0.00628
D178	-3.13548	0.00001	0.00063	0.00000	0.00061	-3.13487
D179	-3.13470	-0.00010	0.00016	0.00000	0.00017	-3.13453
D180	0.00704	-0.00003	0.00049	0.00000	0.00046	0.00751
D181	3.13695	-0.00002	-0.00052	0.00000	-0.00050	3.13645
D182	-0.00469	0.00000	-0.00034	0.00000	-0.00033	-0.00502
D183	-0.00578	0.00004	-0.00029	0.00000	-0.00028	-0.00606
D184	3.13577	0.00006	-0.00011	0.00000	-0.00011	3.13566
D185	3.13872	0.00011	-0.00008	0.00000	-0.00005	3.13868
D186	-0.00337	0.00005	-0.00037	0.00000	-0.00035	-0.00372
D187	-0.00304	0.00002	-0.00045	0.00000	-0.00043	-0.00346
D188	3.13805	-0.00004	-0.00074	0.00000	-0.00073	3.13732
D189	0.00050	-0.00005	-0.00025	0.00000	-0.00026	0.00024
D190	-3.14096	0.00000	0.00007	0.00000	0.00006	-3.14089
D191	-3.14104	-0.00006	-0.00044	0.00000	-0.00043	-3.14148
D192	0.00068	-0.00002	-0.00011	0.00000	-0.00011	0.00057
D193	-0.00235	0.00009	0.00019	0.00000	0.00020	-0.00215
D194	3.13903	0.00005	0.00008	0.00000	0.00008	3.13911
D195	3.13974	0.00015	0.00047	0.00000	0.00049	3.14023
D196	-0.00207	0.00011	0.00036	0.00000	0.00037	-0.00170
D197	0.00344	0.00001	0.00023	0.00000	0.00023	0.00367
D198	-3.13793	0.00005	0.00035	0.00000	0.00035	-3.13758
D199	-3.13828	-0.00003	-0.00008	0.00000	-0.00009	-3.13837
D200	0.00353	0.00000	0.00003	0.00000	0.00004	0.00356

Item	Value	Threshold	Converged?

Maximum Force	0.118167	0.000450	NO

RMS Force	0.025749	0.000300	NO

Maximum Displacement	2.691696	0.001800	NO

RMS Displacement	0.342011	0.001200	NO

Predicted change in Energy=-1.499380D-01

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-11.916860	-0.334552	-0.304748
2	6	0	-11.283199	-1.568674	-0.217374
3	6	0	-12.028843	-2.774763	-0.226845
4	6	0	-13.432033	-2.718614	-0.364677
5	6	0	-14.072965	-1.478258	-0.468679
6	6	0	-13.328149	-0.293333	-0.427608
7	1	0	-11.544598	-3.726326	-0.135128
8	1	0	-14.018822	-3.623442	-0.394470
9	1	0	-15.145263	-1.432614	-0.584673
10	1	0	-13.850773	0.623638	-0.496026
11	6	0	-10.862021	0.828849	-0.248438
12	6	0	-9.738920	-1.384132	-0.117585
13	6	0	-9.399401	0.134452	-0.176442
14	6	0	-8.107938	0.795282	-0.161372
15	6	0	-6.526387	0.290513	-0.176151
16	6	0	-3.882207	-0.583747	0.055364

17	6	0	-3.991426	0.726708	0.289307
18	16	0	-5.590844	-1.310229	-0.305737
19	6	0	-5.430021	1.108160	-0.019538
20	6	0	-2.315646	-0.902971	0.200658
21	6	0	-1.703633	0.276894	0.496780
22	7	0	-2.732395	1.346010	0.794343
23	16	0	-1.097407	-2.258076	0.104957
24	16	0	1.247717	1.351589	0.653393
25	6	0	0.327756	-1.114505	0.301770
26	6	0	-0.121006	0.177730	0.460083
27	6	0	1.940100	-1.185977	0.405756
28	6	0	2.497114	0.060450	0.455232
29	6	0	4.056325	-0.102154	0.280248
30	6	0	4.296571	-1.416628	0.265508
31	6	0	5.800025	-1.783403	0.063804
32	6	0	6.656137	-0.673872	0.030656
33	16	0	5.605634	0.836238	0.073261
34	7	0	3.044131	-2.237101	0.478262
35	6	0	8.278572	-0.883680	-0.029460
36	6	0	9.333092	0.057839	-0.137387
37	6	0	9.161610	1.571681	-0.231766
38	6	0	10.931137	-0.173662	-0.197299
39	6	0	10.551616	2.207876	-0.336536
40	6	0	11.532171	1.267542	-0.314199
41	6	0	10.864908	3.690031	-0.453922
42	6	0	12.970750	1.736716	-0.400494
43	6	0	12.165098	4.087239	-0.531915
44	6	0	13.266462	3.053958	-0.500895
45	6	0	11.613268	-1.417822	-0.154737
46	6	0	11.176114	-2.871366	-0.048953
47	6	0	13.047686	-1.996317	-0.190010
48	7	0	10.961489	-4.010334	0.027628
49	7	0	14.064155	-2.567906	-0.205626
50	6	0	-11.158672	2.200988	-0.252503
51	6	0	-12.441714	3.044107	-0.356863
52	6	0	-10.287811	3.435113	-0.167212
53	7	0	-13.331845	3.793293	-0.418541
54	7	0	-9.699121	4.429174	-0.096131
55	8	0	-8.925528	-2.307740	-0.004574
56	8	0	8.085730	2.179362	-0.226317
57	6	0	2.958196	-3.368099	-0.460794
58	1	0	2.053302	-3.919076	-0.279091
59	1	0	2.964509	-3.011733	-1.476845
60	1	0	3.808452	-4.015431	-0.305442
61	6	0	-2.898251	1.471381	2.273943
62	1	0	-3.150539	0.503927	2.690827
63	1	0	-1.984535	1.821797	2.722167
64	1	0	-3.691910	2.167737	2.487647
65	1	0	6.151358	-2.794650	-0.024481
66	1	0	13.765679	1.049019	-0.383332
67	1	0	14.295985	3.364083	-0.558585
68	1	0	12.419091	5.128835	-0.615056
69	1	0	10.076333	4.415541	-0.475225
70	1	0	8.593260	-1.910507	0.016489
71	1	0	-8.188029	1.869979	-0.114584
72	1	0	-5.607260	2.150080	-0.128821

Rotational constants (GHZ): 0.1503988 0.0086896 0.0082596

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.
 916 basis functions, 1734 primitive gaussians, 916 cartesian basis func-
 tions
 196 alpha electrons 196 beta electrons
 nuclear repulsion energy 6160.3295349014 Hartrees.
 NAToms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T
 Big=T
 Integral buffers will be 131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 Nuclear repulsion after empirical dispersion term = 6160.2502566447 Har-
 trees.
 One-electron integrals computed using PRISM.
 NBasis= 916 RedAO= T EigKep= 3.88D-04 NBF= 916
 NBSUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916
 Initial guess from the checkpoint file: "PBDB.chk"
 B after Tr= 0.000000 0.000000 0.000000
 Rot= 0.999990 0.003667 0.000021 0.002425 Ang= 0.50 deg.
 ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1
 AccDes= 0.00D+00
 Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for in-
 itial guess.
 HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-
 yADJ=14
 ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
 FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2001
 NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
 wScrn= 0.000000 ICntrl= 500 IOpCl= 0 IlCent= 200000004 NGrid=
 0
 NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0=
 0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 Integral accuracy reduced to 1.0D-05 until final iterations.
 Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
 SCF Done: E(RB3LYP) = -3682.55938729 A.U. after 16 cycles
 NFock= 16 Conv=0.62D-08 -V/T= 2.0084
 Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1
 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-0.008714864	-0.033340569	-0.004353504
2	6	0.023175776	-0.008576915	0.011075914
3	6	-0.013457495	-0.010989783	-0.006196980
4	6	0.009505727	-0.015988908	0.004491337
5	6	0.008175201	-0.011391937	0.004012644
6	6	0.014343910	-0.001358749	0.007979275
7	1	0.008881500	0.000555128	0.005277319
8	1	0.002397209	0.004236054	0.000999774
9	1	-0.003130284	0.001119723	-0.002211985
10	1	-0.015487116	-0.011995550	-0.008230165
11	6	0.007686629	-0.005627414	0.002793355
12	6	0.010201426	0.005391875	0.008042584
13	6	-0.005362530	-0.014994959	-0.002944224

14	6	0.025594177	0.047317708	0.023782830
15	6	0.011918187	0.008323885	0.000614370
16	6	0.036658819	0.029557927	0.030544177
17	6	-0.035957814	0.011833288	-0.013726219
18	16	0.018512458	0.013889864	0.005069209
19	6	-0.004000187	-0.063827058	-0.033704049
20	6	-0.010243517	0.024205441	0.000201786
21	6	0.007332761	-0.030420795	-0.001151668
22	7	-0.006569973	0.013664746	0.025528019
23	16	-0.006558029	-0.010451823	0.002027758
24	16	-0.000707897	0.004964232	0.006495247
25	6	0.034522577	-0.009860656	0.010525159
26	6	-0.024390461	0.010244101	-0.029214645
27	6	0.003106056	0.038541442	0.006973783
28	6	0.009833252	-0.025167419	0.013202836
29	6	-0.037339134	-0.016172677	-0.031824256
30	6	0.048484627	0.037775567	0.031416022
31	6	-0.034435939	0.005248691	-0.038173163
32	6	0.019907369	0.003861438	0.016106500
33	16	0.004259544	0.004489041	-0.006515570
34	7	-0.036372605	-0.039312004	0.005305901
35	6	-0.046436314	-0.031922354	-0.022854780
36	6	0.011756741	0.007324365	0.006646894
37	6	-0.006019873	-0.002412453	-0.003287930
38	6	0.000031498	0.013087441	-0.001872644
39	6	-0.044679416	-0.027910239	-0.025081076
40	6	0.047380449	-0.006009251	0.030542999
41	6	0.025816988	0.053101750	0.010511969
42	6	-0.028035772	0.052660325	-0.022666168
43	6	0.046889793	0.012735508	0.028021652
44	6	-0.051828667	-0.007242654	-0.031781973
45	6	0.038950517	0.025475633	0.022871330
46	6	-0.051571149	-0.027812983	-0.030725672
47	6	-0.047509305	-0.036658379	-0.027140259
48	7	0.000626299	0.011278232	-0.000657470
49	7	-0.002343958	-0.003927268	-0.001136886
50	6	-0.033365350	-0.034681428	-0.018603957
51	6	0.042375668	0.032209086	0.023681853
52	6	0.029788639	0.055557771	0.019917033
53	7	0.001434496	0.002604172	0.001434328
54	7	0.000905549	-0.017287374	-0.000353706
55	8	-0.029383583	-0.010975095	-0.014067853
56	8	0.023676282	-0.004391748	0.015542654
57	6	-0.001154396	-0.007066799	-0.010252392
58	1	-0.001557632	0.011354481	-0.004539670
59	1	-0.008197964	-0.000115709	0.011333392
60	1	0.008117771	0.001442770	0.002298591
61	6	-0.003182000	-0.002751215	0.010125101
62	1	0.005819968	0.007245482	-0.004165135
63	1	0.005557418	-0.009732784	0.000647956
64	1	-0.007888900	-0.002354752	-0.005918393
65	1	0.005602395	0.004921298	0.000799917
66	1	0.021923025	0.008605996	0.012939499
67	1	0.000957647	-0.005745677	0.001238711
68	1	-0.001502484	-0.006515980	-0.000269284
69	1	-0.007677270	0.005401454	-0.005470316
70	1	0.001692861	0.012237660	-0.000065659
71	1	0.001967333	-0.010757548	0.003323012
72	1	-0.010706666	-0.016714668	-0.015185041

Cartesian Forces: Max 0.063827058 RMS 0.020750041

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.107497403 RMS 0.022095328

Search for a local minimum.

Step number 3 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 2 3

ITU= 0 1 0

Use linear search instead of GDIIS.

Linear search step of 1.187 exceeds DXMaxT= 0.505 scaled by 0.850

Quartic linear search produced a step of 1.68176.

Iteration 1 RMS(Cart)= 0.32403973 RMS(Int)= 0.02756472

Iteration 2 RMS(Cart)= 0.25234790 RMS(Int)= 0.01507112

Iteration 3 RMS(Cart)= 0.03649101 RMS(Int)= 0.00045976

Iteration 4 RMS(Cart)= 0.00099840 RMS(Int)= 0.00035558

Iteration 5 RMS(Cart)= 0.00000144 RMS(Int)= 0.00035555

Iteration 6 RMS(Cart)= 0.00000000 RMS(Int)= 0.00035555

Iteration 1 RMS(Cart)= 0.32403973 RMS(Int)= 0.02756472

Iteration 2 RMS(Cart)= 0.25234790 RMS(Int)= 0.01507112

Iteration 3 RMS(Cart)= 0.03649101 RMS(Int)= 0.00045976

Iteration 4 RMS(Cart)= 0.00099840 RMS(Int)= 0.00035558

Iteration 5 RMS(Cart)= 0.00000144 RMS(Int)= 0.00035555

Iteration 6 RMS(Cart)= 0.00000000 RMS(Int)= 0.00035555

ITry= 2 IFail=0 DXMaxC= 4.68D+00 DCOld= 4.68D+00 DXMaxT= 5.05D-01 DXLimC=

3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.32403973 RMS(Int)= 0.02756472

Iteration 2 RMS(Cart)= 0.25234790 RMS(Int)= 0.01507112

Iteration 3 RMS(Cart)= 0.03649101 RMS(Int)= 0.00045976

Iteration 4 RMS(Cart)= 0.00099840 RMS(Int)= 0.00035558

Iteration 5 RMS(Cart)= 0.00000144 RMS(Int)= 0.00035555

Iteration 6 RMS(Cart)= 0.00000000 RMS(Int)= 0.00035555

ITry= 3 IFail=0 DXMaxC= 4.68D+00 DCOld= 4.68D+00 DXMaxT= 5.05D-01 DXLimC=

3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.32403973 RMS(Int)= 0.02756472

Iteration 2 RMS(Cart)= 0.25234790 RMS(Int)= 0.01507112

Iteration 3 RMS(Cart)= 0.03649101 RMS(Int)= 0.00045976

Iteration 4 RMS(Cart)= 0.00099840 RMS(Int)= 0.00035558

Iteration 5 RMS(Cart)= 0.00000144 RMS(Int)= 0.00035555

Iteration 6 RMS(Cart)= 0.00000000 RMS(Int)= 0.00035555

ITry= 4 IFail=0 DXMaxC= 4.68D+00 DCOld= 4.68D+00 DXMaxT= 5.05D-01 DXLimC=

3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.32403973 RMS(Int)= 0.02756472

Iteration 2 RMS(Cart)= 0.25234790 RMS(Int)= 0.01507112

Iteration 3 RMS(Cart)= 0.03649101 RMS(Int)= 0.00045976

Iteration 4 RMS(Cart)= 0.00099840 RMS(Int)= 0.00035558

Iteration 5 RMS(Cart)= 0.00000144 RMS(Int)= 0.00035555

Iteration 6 RMS(Cart)= 0.00000000 RMS(Int)= 0.00035555

ITry= 5 IFail=0 DXMaxC= 4.68D+00 DCOld= 4.68D+00 DXMaxT= 5.05D-01 DXLimC=

3.00D+00 Rises=F

Iteration 1 RMS(Cart)= 0.32403973 RMS(Int)= 0.02756472

Iteration 2 RMS(Cart)= 0.25234790 RMS(Int)= 0.01507112

Iteration 3 RMS(Cart)= 0.03649101 RMS(Int)= 0.00045976

Iteration 4 RMS(Cart)= 0.00099840 RMS(Int)= 0.00035558

Iteration 5 RMS(Cart)= 0.00000144 RMS(Int)= 0.00035555

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Iteration 6 RMS(Cart)= 0.00000000 RMS(Int)= 0.00035555
ITry= 6 IFail=0 DXMaxC= 4.68D+00 DCOld= 4.68D+00 DXMaxT= 5.05D-01 DXLimC=
3.00D+00 Rises=F
Iteration 1 RMS(Cart)= 0.32403973 RMS(Int)= 0.02756472
Iteration 2 RMS(Cart)= 0.25234790 RMS(Int)= 0.01507112
Iteration 3 RMS(Cart)= 0.03649101 RMS(Int)= 0.00045976
Iteration 4 RMS(Cart)= 0.00099840 RMS(Int)= 0.00035558
Iteration 5 RMS(Cart)= 0.00000144 RMS(Int)= 0.00035555
Iteration 6 RMS(Cart)= 0.00000000 RMS(Int)= 0.00035555
ITry= 7 IFail=0 DXMaxC= 4.68D+00 DCOld= 4.68D+00 DXMaxT= 5.05D-01 DXLimC=
3.00D+00 Rises=F
Iteration 1 RMS(Cart)= 0.32403973 RMS(Int)= 0.02756472
Iteration 2 RMS(Cart)= 0.25234790 RMS(Int)= 0.01507112
Iteration 3 RMS(Cart)= 0.03649101 RMS(Int)= 0.00045976
Iteration 4 RMS(Cart)= 0.00099840 RMS(Int)= 0.00035558
Iteration 5 RMS(Cart)= 0.00000144 RMS(Int)= 0.00035555
Iteration 6 RMS(Cart)= 0.00000000 RMS(Int)= 0.00035555
ITry= 8 IFail=0 DXMaxC= 4.68D+00 DCOld= 4.68D+00 DXMaxT= 5.05D-01 DXLimC=
3.00D+00 Rises=F
Iteration 1 RMS(Cart)= 0.32403973 RMS(Int)= 0.02756472
Iteration 2 RMS(Cart)= 0.25234790 RMS(Int)= 0.01507112
Iteration 3 RMS(Cart)= 0.03649101 RMS(Int)= 0.00045976
Iteration 4 RMS(Cart)= 0.00099840 RMS(Int)= 0.00035558
Iteration 5 RMS(Cart)= 0.00000144 RMS(Int)= 0.00035555
Iteration 6 RMS(Cart)= 0.00000000 RMS(Int)= 0.00035555
ITry= 9 IFail=0 DXMaxC= 4.68D+00 DCOld= 4.68D+00 DXMaxT= 5.05D-01 DXLimC=
3.00D+00 Rises=F
Iteration 1 RMS(Cart)= 0.32403973 RMS(Int)= 0.02756472
Iteration 2 RMS(Cart)= 0.25234790 RMS(Int)= 0.01507112
Iteration 3 RMS(Cart)= 0.03649101 RMS(Int)= 0.00045976
Iteration 4 RMS(Cart)= 0.00099840 RMS(Int)= 0.00035558
Iteration 5 RMS(Cart)= 0.00000144 RMS(Int)= 0.00035555
Iteration 6 RMS(Cart)= 0.00000000 RMS(Int)= 0.00035555
ITry=10 IFail=0 DXMaxC= 4.68D+00 DCOld= 4.68D+00 DXMaxT= 5.05D-01 DXLimC=
3.00D+00 Rises=F
Variable      Old X      -DE/DX      Delta X      Delta X      Delta X      New X
(Linear)      (Quad)      (Total)
R1      2.62680      0.00589      0.05383      0.00000      0.05313      2.67993
R2      2.67817     -0.01971     -0.00373      0.00000     -0.00331      2.67486
R3      2.96955     -0.05418      0.07410      0.00000      0.07407      3.04362
R4      2.67963     -0.02512     -0.02842      0.00000     -0.02864      2.65099
R5      2.94507     -0.03916     -0.08564      0.00000     -0.08622      2.85885
R6      2.66652     -0.01440     -0.05132      0.00000     -0.05174      2.61478
R7      2.02508      0.00945      0.01225      0.00000      0.01225      2.03732
R8      2.64568      0.00660     -0.02006      0.00000     -0.02025      2.62543
R9      2.03873      0.00436      0.00594      0.00000      0.00594      2.04468
R10     2.64594     -0.00633     -0.00654      0.00000     -0.00631      2.63963
R11     2.04000      0.00377      0.00497      0.00000      0.00497      2.04496
R12     1.99869      0.02091     -0.03392      0.00000     -0.03392      1.96477
R13     3.06266     -0.06627     -0.06519      0.00000     -0.06430      2.99836
R14     2.65288     -0.06191      0.02746      0.00000      0.02746      2.68034
R15     2.94266     -0.03546     -0.07960      0.00000     -0.07911      2.86354
R16     2.33550     -0.03417     -0.04672      0.00000     -0.04672      2.28878
R17     2.74160     -0.09438     -0.12017      0.00000     -0.12017      2.62143
R18     3.13735     -0.10497     -0.12143      0.00000     -0.12143      3.01592
R19     2.03843      0.00591      0.00740      0.00000      0.00740      2.04584
R20     3.51225     -0.00714      0.00103      0.00000      0.00124      3.51350
R21     2.60144     -0.01375     -0.02138      0.00000     -0.02098      2.58047
R22     2.52400      0.04538      0.05925      0.00000      0.05873      2.58274
R23     3.57434     -0.04707     -0.04711      0.00000     -0.04743      3.52690

```

R24	3.03366	-0.07254	-0.08159	0.00000	-0.08152	2.95213
R25	2.87241	-0.06942	-0.08013	0.00000	-0.08005	2.79236
R26	2.81801	-0.03872	-0.04567	0.00000	-0.04580	2.77221
R27	2.00788	0.02309	0.03334	0.00000	0.03334	2.04122
R28	2.57331	0.00589	0.00350	0.00000	0.00372	2.57704
R29	3.44821	-0.02850	-0.03197	0.00000	-0.03198	3.41623
R30	2.85961	-0.03927	-0.04329	0.00000	-0.04326	2.81636
R31	2.99740	-0.08430	-0.09908	0.00000	-0.09909	2.89831
R32	2.82351	-0.00042	-0.00027	0.00000	-0.00027	2.82324
R33	3.47298	-0.02801	-0.03207	0.00000	-0.03206	3.44091
R34	3.42699	-0.02235	-0.02587	0.00000	-0.02585	3.40114
R35	3.41581	-0.02360	-0.02722	0.00000	-0.02720	3.38860
R36	2.60228	0.00005	-0.00331	0.00000	-0.00331	2.59898
R37	3.05620	-0.08915	-0.10423	0.00000	-0.10426	2.95194
R38	2.58160	0.00416	0.00090	0.00000	0.00112	2.58272
R39	2.88392	-0.05773	-0.06409	0.00000	-0.06406	2.81986
R40	2.98086	-0.07419	-0.08576	0.00000	-0.08565	2.89521
R41	2.52530	0.03120	0.03549	0.00000	0.03507	2.56037
R42	3.44521	-0.03337	-0.03731	0.00000	-0.03739	3.40782
R43	2.94917	-0.08168	-0.09591	0.00000	-0.09604	2.85313
R44	2.85783	-0.05249	-0.06088	0.00000	-0.06109	2.79674
R45	2.64905	-0.02679	-0.03879	0.00000	-0.03862	2.61042
R46	2.02989	0.00683	0.00927	0.00000	0.00927	2.03916
R47	3.47720	-0.02020	-0.02390	0.00000	-0.02365	3.45355
R48	3.09357	-0.09113	-0.10958	0.00000	-0.10958	2.98399
R49	2.78269	0.00284	0.00441	0.00000	0.00441	2.78710
R50	2.67923	-0.06654	-0.09364	0.00000	-0.09364	2.58559
R51	2.03136	0.00850	0.01023	0.00000	0.01023	2.04158
R52	2.88456	-0.02119	-0.07948	0.00000	-0.07914	2.80542
R53	3.05349	-0.06336	-0.05623	0.00000	-0.05520	2.99829
R54	2.89556	-0.02973	-0.08787	0.00000	-0.08869	2.80687
R55	2.33503	-0.02864	-0.04049	0.00000	-0.04049	2.29454
R56	2.95908	-0.05517	0.11782	0.00000	0.11803	3.07711
R57	2.68251	-0.07858	0.03920	0.00000	0.03920	2.72171
R58	2.56767	0.01105	0.07637	0.00000	0.07570	2.64337
R59	2.87134	-0.06504	-0.06821	0.00000	-0.06881	2.80252
R60	2.86409	-0.05907	-0.04309	0.00000	-0.04219	2.82191
R61	2.57333	0.00522	-0.04326	0.00000	-0.04416	2.52917
R62	2.02533	0.00872	0.01114	0.00000	0.01114	2.03647
R63	2.55823	0.01260	0.01100	0.00000	0.01161	2.56983
R64	1.98658	0.02609	-0.04491	0.00000	-0.04491	1.94168
R65	2.85445	-0.04444	-0.08732	0.00000	-0.08758	2.76686
R66	2.03209	0.00659	0.00890	0.00000	0.00890	2.04099
R67	2.03479	0.00549	0.00756	0.00000	0.00756	2.04235
R68	2.87529	-0.03536	-0.05141	0.00000	-0.05141	2.82388
R69	2.92356	-0.04557	-0.04145	0.00000	-0.04145	2.88211
R70	2.19499	0.01030	0.00870	0.00000	0.00870	2.20369
R71	2.20392	-0.00211	0.00854	0.00000	0.00854	2.21246
R72	2.90793	-0.04877	-0.04726	0.00000	-0.04726	2.86067
R73	2.85889	-0.03874	-0.05265	0.00000	-0.05265	2.80624
R74	2.20169	-0.00213	0.00445	0.00000	0.00445	2.20614
R75	2.18732	0.01718	0.01865	0.00000	0.01865	2.20597
R76	2.03128	0.01227	0.01611	0.00000	0.01611	2.04739
R77	2.03477	0.01339	0.01763	0.00000	0.01763	2.05240
R78	2.04065	0.00837	0.01114	0.00000	0.01114	2.05179
R79	2.04703	0.00970	0.01276	0.00000	0.01276	2.05979
R80	2.03404	0.01095	0.01435	0.00000	0.01435	2.04839
R81	2.03572	0.00996	0.01316	0.00000	0.01316	2.04888
A1	2.07741	0.00886	-0.07802	0.00000	-0.07711	2.00030
A2	1.92736	-0.00398	-0.02680	0.00000	-0.02793	1.89943

A3	2.27842	-0.00488	0.10482	0.00000	0.10503	2.38345
A4	2.11183	0.00395	0.04612	0.00000	0.04658	2.15840
A5	1.92901	-0.00111	0.02141	0.00000	0.02014	1.94915
A6	2.24235	-0.00285	-0.06753	0.00000	-0.06672	2.17562
A7	2.08256	-0.00672	0.00150	0.00000	0.00065	2.08321
A8	2.11423	-0.00085	-0.00368	0.00000	-0.00325	2.11097
A9	2.08639	0.00756	0.00218	0.00000	0.00261	2.08900
A10	2.09180	0.00382	-0.01246	0.00000	-0.01328	2.07852
A11	2.10620	-0.00433	0.00157	0.00000	0.00198	2.10818
A12	2.08517	0.00050	0.01089	0.00000	0.01130	2.09647
A13	2.09908	0.00356	0.01829	0.00000	0.01814	2.11721
A14	2.09460	-0.00059	-0.00822	0.00000	-0.00814	2.08646
A15	2.08950	-0.00297	-0.01007	0.00000	-0.01000	2.07951
A16	2.10325	-0.01345	0.02459	0.00000	0.02506	2.12830
A17	2.12103	0.00298	0.01162	0.00000	0.01138	2.13241
A18	2.05890	0.01047	-0.03621	0.00000	-0.03644	2.02246
A19	1.86521	0.00008	-0.05552	0.00000	-0.05454	1.81067
A20	2.19159	0.00190	0.29735	0.00000	0.29685	2.48844
A21	2.22637	-0.00198	-0.24185	0.00000	-0.24233	1.98404
A22	1.90615	-0.01574	-0.01620	0.00000	-0.01624	1.88991
A23	2.17671	0.01216	0.01555	0.00000	0.01558	2.19229
A24	2.20031	0.00358	0.00064	0.00000	0.00067	2.20098
A25	1.79543	0.02079	0.07701	0.00000	0.07845	1.87388
A26	2.22516	-0.00832	-0.04030	0.00000	-0.04103	2.18413
A27	2.26256	-0.01247	-0.03672	0.00000	-0.03744	2.22513
A28	2.35947	-0.03124	-0.03556	0.00000	-0.03556	2.32390
A29	1.96944	0.02543	0.02863	0.00000	0.02863	1.99807
A30	1.95415	0.00580	0.00693	0.00000	0.00693	1.96107
A31	2.40682	-0.04701	-0.05664	0.00000	-0.05696	2.34987
A32	2.18595	-0.02758	-0.04214	0.00000	-0.04249	2.14346
A33	1.68967	0.07465	0.09887	0.00000	0.09952	1.78920
A34	1.91390	0.01957	0.02888	0.00000	0.02843	1.94233
A35	1.83283	-0.00190	-0.00408	0.00000	-0.00404	1.82879
A36	2.53645	-0.01767	-0.02480	0.00000	-0.02439	2.51206
A37	1.86296	0.02054	0.02377	0.00000	0.02379	1.88675
A38	1.97985	0.00225	0.00555	0.00000	0.00529	1.98514
A39	2.43976	-0.02278	-0.02930	0.00000	-0.02906	2.41070
A40	1.68162	-0.04801	-0.06729	0.00000	-0.06741	1.61421
A41	2.24954	-0.06582	-0.08332	0.00000	-0.08319	2.16635
A42	2.02404	0.03450	0.04649	0.00000	0.04640	2.07044
A43	2.00960	0.03131	0.03685	0.00000	0.03676	2.04637
A44	1.86081	-0.00910	-0.01322	0.00000	-0.01304	1.84777
A45	2.48887	-0.01232	-0.01763	0.00000	-0.01773	2.47114
A46	1.93350	0.02141	0.03085	0.00000	0.03078	1.96427
A47	1.92769	0.02386	0.03416	0.00000	0.03433	1.96202
A48	1.97060	-0.00638	-0.00999	0.00000	-0.01005	1.96054
A49	2.38481	-0.01747	-0.02416	0.00000	-0.02427	2.36054
A50	1.78644	-0.01441	-0.02165	0.00000	-0.02171	1.76473
A51	1.85095	0.01245	0.01660	0.00000	0.01669	1.86764
A52	1.90654	0.00398	0.00569	0.00000	0.00564	1.91218
A53	1.62082	-0.03063	-0.04256	0.00000	-0.04251	1.57831
A54	1.61845	-0.03040	-0.04221	0.00000	-0.04210	1.57636
A55	1.92145	0.02298	0.03258	0.00000	0.03264	1.95409
A56	2.42263	-0.01897	-0.02492	0.00000	-0.02496	2.39767
A57	1.93796	-0.00390	-0.00752	0.00000	-0.00755	1.93041
A58	2.36049	-0.01264	-0.01858	0.00000	-0.01862	2.34187
A59	1.96761	-0.00689	-0.01030	0.00000	-0.01028	1.95733
A60	1.95381	0.01959	0.02896	0.00000	0.02898	1.98279
A61	1.94819	-0.00308	-0.00577	0.00000	-0.00583	1.94236
A62	2.42602	-0.01821	-0.02345	0.00000	-0.02353	2.40249

A63	1.90893	0.02128	0.02920	0.00000	0.02934	1.93827
A64	1.95396	0.01853	0.02746	0.00000	0.02739	1.98135
A65	2.44811	-0.00850	-0.01372	0.00000	-0.01386	2.43425
A66	1.88069	-0.00998	-0.01368	0.00000	-0.01347	1.86722
A67	1.85493	-0.00630	-0.00783	0.00000	-0.00777	1.84716
A68	2.49733	-0.00846	-0.01344	0.00000	-0.01317	2.48417
A69	1.93079	0.01476	0.02127	0.00000	0.02093	1.95172
A70	1.98864	-0.00328	-0.00406	0.00000	-0.00431	1.98433
A71	1.96408	0.00634	0.01065	0.00000	0.01046	1.97454
A72	2.33022	-0.00306	-0.00660	0.00000	-0.00616	2.32406
A73	1.98819	-0.01315	-0.02045	0.00000	-0.02047	1.96772
A74	2.14953	0.00518	0.00677	0.00000	0.00678	2.15630
A75	2.14532	0.00801	0.01372	0.00000	0.01373	2.15905
A76	1.87587	0.03645	0.05166	0.00000	0.05201	1.92787
A77	2.09982	-0.01282	-0.01577	0.00000	-0.01594	2.08388
A78	2.30749	-0.02363	-0.03589	0.00000	-0.03606	2.27143
A79	1.63621	-0.03440	-0.04795	0.00000	-0.04771	1.58851
A80	1.79134	-0.01030	-0.01716	0.00000	-0.01739	1.77395
A81	2.04485	0.00154	0.00338	0.00000	0.00360	2.04845
A82	1.95553	0.01284	0.01719	0.00000	0.01729	1.97283
A83	2.28475	-0.00764	-0.02233	0.00000	-0.02233	2.26242
A84	1.99434	-0.00529	0.00046	0.00000	0.00046	1.99479
A85	2.00409	0.01293	0.02187	0.00000	0.02187	2.02596
A86	2.18921	0.00811	-0.03414	0.00000	-0.03485	2.15436
A87	2.26956	-0.01849	-0.04933	0.00000	-0.05004	2.21952
A88	1.82441	0.01038	0.08346	0.00000	0.08489	1.90930
A89	1.89029	-0.01095	-0.00984	0.00000	-0.01024	1.88006
A90	2.19602	0.00680	0.00028	0.00000	0.00048	2.19650
A91	2.19688	0.00416	0.00956	0.00000	0.00975	2.20663
A92	1.82400	0.01102	-0.05916	0.00000	-0.05772	1.76629
A93	2.21393	-0.00396	-0.32226	0.00000	-0.32299	1.89094
A94	2.24525	-0.00706	0.38142	0.00000	0.38070	2.62595
A95	1.94571	-0.00402	0.02594	0.00000	0.02463	1.97034
A96	2.21097	0.00368	-0.08502	0.00000	-0.08401	2.12696
A97	2.12650	0.00033	0.05909	0.00000	0.05939	2.18589
A98	1.94034	-0.00642	-0.04040	0.00000	-0.04157	1.89876
A99	2.28298	-0.00543	0.14798	0.00000	0.14774	2.43072
A100	2.05987	0.01185	-0.10758	0.00000	-0.10617	1.95370
A101	2.07810	-0.00520	0.00755	0.00000	0.00579	2.08389
A102	2.10615	-0.00396	-0.00969	0.00000	-0.00881	2.09734
A103	2.09893	0.00916	0.00214	0.00000	0.00302	2.10195
A104	2.10920	-0.01376	0.03965	0.00000	0.04099	2.15020
A105	2.11099	0.00047	0.00726	0.00000	0.00659	2.11758
A106	2.06299	0.01329	-0.04691	0.00000	-0.04758	2.01541
A107	2.08917	0.00413	-0.01943	0.00000	-0.02088	2.06828
A108	2.10888	-0.00087	0.01004	0.00000	0.01076	2.11964
A109	2.08514	-0.00326	0.00939	0.00000	0.01012	2.09526
A110	2.10350	0.00264	0.02072	0.00000	0.02088	2.12438
A111	2.08642	0.00103	-0.00565	0.00000	-0.00574	2.08068
A112	2.09327	-0.00367	-0.01506	0.00000	-0.01515	2.07812
A113	2.34804	-0.04948	-0.20044	0.00000	-0.20043	2.14760
A114	2.45371	-0.05802	0.27714	0.00000	0.27714	2.73085
A115	1.48143	0.10750	-0.07671	0.00000	-0.07671	1.40472
A116	2.36302	-0.03991	0.21191	0.00000	0.21192	2.57493
A117	2.31248	-0.03375	-0.15146	0.00000	-0.15146	2.16102
A118	1.60763	0.07366	-0.06045	0.00000	-0.06045	1.54718
A119	1.91242	-0.00149	-0.00221	0.00000	-0.00222	1.91020
A120	1.92540	0.00679	0.00997	0.00000	0.00997	1.93537
A121	1.89940	-0.00127	-0.00224	0.00000	-0.00225	1.89715
A122	1.91144	-0.00168	-0.00244	0.00000	-0.00245	1.90899

A123	1.90842	-0.00119	-0.00137	0.00000	-0.00138	1.90704
A124	1.90661	-0.00120	-0.00176	0.00000	-0.00176	1.90484
A125	1.90924	0.00617	0.00876	0.00000	0.00877	1.91801
A126	1.92352	-0.00398	-0.00537	0.00000	-0.00537	1.91815
A127	1.90972	-0.00241	-0.00333	0.00000	-0.00334	1.90637
A128	1.90520	-0.00010	-0.00038	0.00000	-0.00036	1.90483
A129	1.90645	-0.00024	-0.00045	0.00000	-0.00044	1.90601
A130	1.90960	0.00060	0.00081	0.00000	0.00078	1.91038
A131	3.24715	-0.01026	-0.00382	0.00000	-0.00382	3.24333
A132	3.27082	-0.00929	0.14487	0.00000	0.14487	3.41570
A133	3.25994	-0.00543	0.10235	0.00000	0.10235	3.36230
A134	3.22111	-0.00479	-0.00203	0.00000	-0.00203	3.21908
A135	3.13577	0.00044	0.00011	0.00000	0.00011	3.13588
A136	3.14333	-0.00006	0.00195	0.00000	0.00195	3.14528
A137	3.12539	0.00082	-0.00198	0.00000	-0.00198	3.12341
A138	3.14891	-0.00045	-0.00046	0.00000	-0.00046	3.14846
D1	-0.01877	0.00031	-0.00109	0.00000	-0.00093	-0.01970
D2	3.12210	-0.00001	-0.00204	0.00000	-0.00192	3.12018
D3	3.12544	0.00047	-0.00045	0.00000	-0.00047	3.12498
D4	-0.01687	0.00016	-0.00140	0.00000	-0.00146	-0.01833
D5	-0.00677	0.00025	0.00152	0.00000	0.00134	-0.00543
D6	3.14052	-0.00002	0.00207	0.00000	0.00198	-3.14068
D7	3.13159	0.00005	0.00048	0.00000	0.00033	3.13192
D8	-0.00431	-0.00022	0.00103	0.00000	0.00097	-0.00333
D9	0.04498	-0.00069	0.00021	0.00000	0.00024	0.04522
D10	-3.09024	-0.00054	0.00320	0.00000	0.00360	-3.08664
D11	-3.09360	-0.00053	0.00127	0.00000	0.00130	-3.09230
D12	0.05437	-0.00038	0.00426	0.00000	0.00466	0.05903
D13	0.03107	-0.00079	0.00030	0.00000	0.00020	0.03127
D14	-3.11480	-0.00056	-0.00011	0.00000	-0.00013	-3.11493
D15	-3.10965	-0.00041	0.00143	0.00000	0.00127	-3.10838
D16	0.02766	-0.00018	0.00102	0.00000	0.00094	0.02860
D17	-0.01926	0.00078	0.00104	0.00000	0.00115	-0.01812
D18	3.11777	0.00057	0.00180	0.00000	0.00194	3.11972
D19	3.12154	0.00044	0.00001	0.00000	0.00020	3.12174
D20	-0.02461	0.00022	0.00077	0.00000	0.00100	-0.02361
D21	-0.01771	0.00046	0.00122	0.00000	0.00124	-0.01647
D22	3.12011	0.00047	0.00045	0.00000	0.00049	3.12060
D23	3.12809	0.00025	0.00164	0.00000	0.00158	3.12967
D24	-0.01728	0.00027	0.00087	0.00000	0.00083	-0.01644
D25	-0.00737	0.00012	-0.00040	0.00000	-0.00036	-0.00772
D26	3.13034	0.00008	-0.00052	0.00000	-0.00052	3.12982
D27	3.13796	0.00012	0.00037	0.00000	0.00040	3.13836
D28	-0.00752	0.00008	0.00026	0.00000	0.00024	-0.00729
D29	0.01989	-0.00061	-0.00069	0.00000	-0.00072	0.01917
D30	-3.12721	-0.00037	-0.00108	0.00000	-0.00118	-3.12839
D31	-3.11783	-0.00058	-0.00057	0.00000	-0.00055	-3.11838
D32	0.01826	-0.00033	-0.00097	0.00000	-0.00102	0.01724
D33	-0.05265	0.00025	-0.00188	0.00000	-0.00224	-0.05489
D34	3.09658	0.00021	-0.00010	0.00000	-0.00039	3.09619
D35	3.08239	0.00012	-0.00287	0.00000	-0.00215	3.08024
D36	-0.05155	0.00007	-0.00109	0.00000	-0.00031	-0.05187
D37	-0.04763	0.00073	-0.00165	0.00000	-0.00175	-0.04938
D38	3.10854	0.00040	-0.00117	0.00000	-0.00126	3.10728
D39	3.10166	0.00090	0.00079	0.00000	0.00089	3.10254
D40	-0.02536	0.00057	0.00128	0.00000	0.00137	-0.02398
D41	0.04416	-0.00066	0.00235	0.00000	0.00258	0.04674
D42	-3.10531	-0.00059	0.00051	0.00000	0.00068	-3.10462
D43	-3.09280	-0.00047	0.00152	0.00000	0.00173	-3.09107
D44	0.04092	-0.00039	-0.00032	0.00000	-0.00017	0.04075

D45	-3.07046	-0.00284	-0.00425	0.00000	-0.00419	-3.07465
D46	0.09075	-0.00269	-0.00415	0.00000	-0.00408	0.08667
D47	0.08081	-0.00304	-0.00239	0.00000	-0.00246	0.07835
D48	-3.04117	-0.00289	-0.00229	0.00000	-0.00235	-3.04352
D49	0.07059	0.00091	0.00156	0.00000	0.00146	0.07205
D50	-3.01918	-0.00314	-0.00402	0.00000	-0.00392	-3.02310
D51	-3.09050	0.00092	0.00164	0.00000	0.00154	-3.08895
D52	0.10292	-0.00313	-0.00394	0.00000	-0.00384	0.09908
D53	-3.00398	0.00028	0.00068	0.00000	0.00006	-3.00392
D54	0.09499	0.00241	0.00350	0.00000	0.00270	0.09769
D55	2.87835	0.00797	0.00969	0.00000	0.00921	2.88756
D56	-0.26378	0.00062	0.00101	0.00000	0.00104	-0.26275
D57	-0.22825	0.00737	0.00861	0.00000	0.00807	-0.22018
D58	2.91279	0.00001	-0.00006	0.00000	-0.00010	2.91269
D59	-0.12953	-0.00166	-0.00302	0.00000	-0.00260	-0.13212
D60	2.98205	-0.00185	-0.00316	0.00000	-0.00283	2.97922
D61	3.01260	-0.00108	-0.00216	0.00000	-0.00173	3.01087
D62	-0.15901	-0.00126	-0.00230	0.00000	-0.00197	-0.16097
D63	0.02705	-0.00270	-0.00295	0.00000	-0.00214	0.02490
D64	-3.11546	-0.00368	-0.00442	0.00000	-0.00354	-3.11900
D65	-0.00584	0.00309	0.00410	0.00000	0.00381	-0.00203
D66	3.14069	0.00276	0.00353	0.00000	0.00347	-3.13903
D67	3.13665	0.00403	0.00553	0.00000	0.00514	-3.14140
D68	-0.00001	0.00370	0.00496	0.00000	0.00480	0.00479
D69	0.26997	-0.01507	-0.01832	0.00000	-0.01788	0.25210
D70	-2.87108	-0.00777	-0.00968	0.00000	-0.00981	-2.88089
D71	-2.82896	-0.01600	-0.01974	0.00000	-0.01905	-2.84801
D72	0.31318	-0.00870	-0.01110	0.00000	-0.01098	0.30219
D73	0.25027	-0.00332	-0.00389	0.00000	-0.00426	0.24601
D74	-1.74736	-0.00635	-0.00750	0.00000	-0.00742	-1.75479
D75	-2.93585	-0.00212	-0.00220	0.00000	-0.00282	-2.93866
D76	1.34970	-0.00514	-0.00581	0.00000	-0.00598	1.34373
D77	0.16261	-0.00218	-0.00244	0.00000	-0.00243	0.16018
D78	-2.99115	-0.00199	-0.00222	0.00000	-0.00219	-2.99334
D79	-2.98219	-0.00204	-0.00219	0.00000	-0.00231	-2.98450
D80	0.14724	-0.00185	-0.00197	0.00000	-0.00208	0.14516
D81	3.03213	0.00343	0.00414	0.00000	0.00391	3.03605
D82	-0.10440	0.00315	0.00364	0.00000	0.00363	-0.10077
D83	-0.24619	0.00179	0.00185	0.00000	0.00190	-0.24429
D84	1.71034	0.01059	0.01266	0.00000	0.01260	1.72294
D85	2.91172	0.00128	0.00120	0.00000	0.00126	2.91298
D86	-1.41494	0.01007	0.01200	0.00000	0.01196	-1.40298
D87	3.06881	0.00195	0.00219	0.00000	0.00219	3.07100
D88	-0.13323	0.00423	0.00530	0.00000	0.00524	-0.12798
D89	-0.08938	0.00267	0.00314	0.00000	0.00312	-0.08626
D90	2.99177	0.00495	0.00625	0.00000	0.00618	2.99794
D91	0.94767	-0.00416	-0.00679	0.00000	-0.00680	0.94087
D92	3.04246	-0.00287	-0.00506	0.00000	-0.00509	3.03737
D93	-1.14021	-0.00615	-0.00954	0.00000	-0.00954	-1.14975
D94	-0.96603	0.00471	0.00766	0.00000	0.00768	-0.95835
D95	1.12875	0.00600	0.00940	0.00000	0.00940	1.13815
D96	-3.05391	0.00273	0.00492	0.00000	0.00494	-3.04897
D97	0.02558	-0.00101	-0.00141	0.00000	-0.00143	0.02415
D98	3.10823	0.00211	0.00260	0.00000	0.00253	3.11075
D99	3.11569	0.00045	0.00044	0.00000	0.00048	3.11618
D100	0.03420	-0.00117	-0.00168	0.00000	-0.00161	0.03259
D101	-0.11804	0.00433	0.00520	0.00000	0.00510	-0.11294
D102	2.98681	0.00644	0.00771	0.00000	0.00759	2.99441
D103	0.04928	0.00002	0.00008	0.00000	0.00013	0.04941
D104	-3.13819	0.00080	0.00101	0.00000	0.00110	-3.13709

D105	-3.05073	-0.00135	-0.00164	0.00000	-0.00168	-3.05241
D106	0.04499	-0.00056	-0.00070	0.00000	-0.00071	0.04428
D107	3.06565	0.00137	0.00162	0.00000	0.00165	3.06730
D108	-0.08789	-0.00010	-0.00042	0.00000	-0.00037	-0.08826
D109	-0.13526	0.00511	0.00656	0.00000	0.00648	-0.12878
D110	2.99439	0.00364	0.00452	0.00000	0.00446	2.99884
D111	0.15873	-0.00302	-0.00350	0.00000	-0.00360	0.15512
D112	-2.95821	-0.00426	-0.00487	0.00000	-0.00500	-2.96320
D113	-2.97456	-0.00176	-0.00180	0.00000	-0.00183	-2.97639
D114	0.19170	-0.00300	-0.00317	0.00000	-0.00322	0.18848
D115	2.94255	0.00513	0.00611	0.00000	0.00613	2.94868
D116	0.79258	-0.00437	-0.00485	0.00000	-0.00485	0.78773
D117	-0.21082	0.00358	0.00396	0.00000	0.00395	-0.20686
D118	-2.36078	-0.00592	-0.00700	0.00000	-0.00703	-2.36781
D119	3.08227	0.00245	0.00293	0.00000	0.00292	3.08519
D120	-0.07991	0.00217	0.00261	0.00000	0.00260	-0.07732
D121	-0.09511	0.00488	0.00594	0.00000	0.00587	-0.08924
D122	3.02589	0.00461	0.00562	0.00000	0.00555	3.03144
D123	3.11723	0.00003	-0.00012	0.00000	-0.00018	3.11706
D124	-0.04496	-0.00019	-0.00064	0.00000	-0.00067	-0.04563
D125	-0.01115	0.00043	0.00042	0.00000	0.00038	-0.01077
D126	3.10985	0.00021	-0.00010	0.00000	-0.00012	3.10973
D127	3.12368	0.00235	0.00309	0.00000	0.00310	3.12677
D128	-0.03903	0.00191	0.00256	0.00000	0.00254	-0.03649
D129	0.07743	-0.00399	-0.00496	0.00000	-0.00490	0.07253
D130	-3.08203	-0.00199	-0.00260	0.00000	-0.00254	-3.08457
D131	-3.03793	-0.00386	-0.00458	0.00000	-0.00454	-3.04247
D132	0.08580	-0.00186	-0.00221	0.00000	-0.00218	0.08362
D133	0.15220	-0.00247	-0.00292	0.00000	-0.00295	0.14925
D134	2.36089	-0.00004	-0.00024	0.00000	-0.00033	2.36056
D135	-3.01535	-0.00271	-0.00346	0.00000	-0.00347	-3.01882
D136	-0.80666	-0.00028	-0.00078	0.00000	-0.00085	-0.80751
D137	-0.09958	0.00253	0.00290	0.00000	0.00296	-0.09661
D138	3.03901	0.00237	0.00292	0.00000	0.00298	3.04198
D139	3.05984	0.00057	0.00063	0.00000	0.00068	3.06052
D140	-0.08477	0.00041	0.00065	0.00000	0.00069	-0.08407
D141	0.08043	-0.00265	-0.00308	0.00000	-0.00304	0.07739
D142	-3.05765	-0.00251	-0.00319	0.00000	-0.00313	-3.06078
D143	3.07851	0.00053	0.00044	0.00000	0.00045	3.07897
D144	-0.05760	0.00006	-0.00005	0.00000	-0.00004	-0.05764
D145	-0.06696	0.00045	0.00067	0.00000	0.00066	-0.06630
D146	3.08011	-0.00001	0.00018	0.00000	0.00017	3.08028
D147	-1.07221	-0.00258	-0.00539	0.00000	-0.00540	-1.07762
D148	1.03349	-0.00133	-0.00353	0.00000	-0.00355	1.02994
D149	3.12501	0.00052	-0.00105	0.00000	-0.00107	3.12394
D150	-3.13572	-0.00015	0.00143	0.00000	0.00145	-3.13427
D151	-1.03002	0.00110	0.00329	0.00000	0.00331	-1.02671
D152	1.06150	0.00294	0.00577	0.00000	0.00579	1.06729
D153	-0.00437	-0.00037	-0.00051	0.00000	-0.00050	-0.00486
D154	-3.13975	-0.00051	-0.00027	0.00000	-0.00028	-3.14003
D155	3.13173	0.00005	-0.00007	0.00000	-0.00006	3.13167
D156	-0.00366	-0.00009	0.00017	0.00000	0.00016	-0.00350
D157	-3.13945	0.00005	-0.00027	0.00000	-0.00032	-3.13977
D158	0.00064	0.00001	0.00008	0.00000	0.00002	0.00066
D159	-0.00277	0.00006	-0.00075	0.00000	-0.00083	-0.00361
D160	3.13732	0.00003	-0.00040	0.00000	-0.00049	3.13683
D161	-3.14084	0.00010	0.00051	0.00000	0.00058	-3.14025
D162	0.00303	0.00014	0.00008	0.00000	-0.00011	0.00292
D163	0.00598	-0.00003	0.00094	0.00000	0.00104	0.00702
D164	-3.13334	0.00001	0.00050	0.00000	0.00035	-3.13299

D165	-0.00208	0.00004	-0.00005	0.00000	-0.00012	-0.00220
D166	3.13868	0.00005	0.00032	0.00000	0.00022	3.13890
D167	3.14102	0.00007	-0.00040	0.00000	-0.00046	3.14056
D168	-0.00140	0.00008	-0.00003	0.00000	-0.00011	-0.00152
D169	-0.00772	0.00012	-0.00059	0.00000	-0.00061	-0.00833
D170	3.13336	0.00010	-0.00119	0.00000	-0.00126	3.13209
D171	3.13155	0.00009	-0.00133	0.00000	-0.00133	3.13022
D172	-0.01056	0.00007	-0.00194	0.00000	-0.00198	-0.01254
D173	0.00077	-0.00003	-0.00029	0.00000	-0.00035	0.00042
D174	3.13799	0.00004	-0.00234	0.00000	-0.00240	3.13559
D175	-3.13801	0.00000	-0.00008	0.00000	-0.00002	-3.13803
D176	-0.00079	0.00006	-0.00213	0.00000	-0.00207	-0.00286
D177	0.00628	-0.00013	0.00054	0.00000	0.00061	0.00688
D178	-3.13487	-0.00010	0.00103	0.00000	0.00099	-3.13388
D179	-3.13453	-0.00014	0.00029	0.00000	0.00033	-3.13420
D180	0.00751	-0.00012	0.00078	0.00000	0.00071	0.00822
D181	3.13645	0.00013	-0.00085	0.00000	-0.00079	3.13566
D182	-0.00502	0.00010	-0.00056	0.00000	-0.00053	-0.00555
D183	-0.00606	0.00014	-0.00047	0.00000	-0.00043	-0.00649
D184	3.13566	0.00011	-0.00018	0.00000	-0.00017	3.13549
D185	3.13868	0.00013	-0.00008	0.00000	0.00001	3.13868
D186	-0.00372	0.00010	-0.00059	0.00000	-0.00055	-0.00427
D187	-0.00346	0.00010	-0.00072	0.00000	-0.00064	-0.00411
D188	3.13732	0.00007	-0.00123	0.00000	-0.00120	3.13613
D189	0.00024	0.00002	-0.00044	0.00000	-0.00045	-0.00020
D190	-3.14089	-0.00002	0.00011	0.00000	0.00009	-3.14080
D191	-3.14148	0.00005	-0.00073	0.00000	-0.00071	3.14100
D192	0.00057	0.00001	-0.00019	0.00000	-0.00017	0.00040
D193	-0.00215	0.00003	0.00034	0.00000	0.00037	-0.00177
D194	3.13911	0.00002	0.00013	0.00000	0.00014	3.13925
D195	3.14023	0.00007	0.00082	0.00000	0.00088	3.14111
D196	-0.00170	0.00005	0.00062	0.00000	0.00064	-0.00106
D197	0.00367	-0.00006	0.00039	0.00000	0.00037	0.00404
D198	-3.13758	-0.00004	0.00059	0.00000	0.00061	-3.13698
D199	-3.13837	-0.00001	-0.00015	0.00000	-0.00016	-3.13853
D200	0.00356	0.00000	0.00006	0.00000	0.00007	0.00364

Item	Value	Threshold	Converged?

Maximum Force	0.107497	0.000450	NO

RMS Force	0.022095	0.000300	NO

Maximum Displacement	4.678782	0.001800	NO

RMS Displacement	0.584382	0.001200	NO

Predicted change in Energy=-4.268179D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-11.457406	-0.373031	-0.291853
2	6	0	-10.707816	-1.572971	-0.194736
3	6	0	-11.284769	-2.851633	-0.183846
4	6	0	-12.656979	-2.977810	-0.309124
5	6	0	-13.433136	-1.831157	-0.423039

6	6	0	-12.856076	-0.559235	-0.404178
7	1	0	-10.674254	-3.734556	-0.083692
8	1	0	-13.124488	-3.953493	-0.323060
9	1	0	-14.505934	-1.921638	-0.532412
10	1	0	-13.516471	0.239910	-0.483215
11	6	0	-10.444026	0.878019	-0.246890
12	6	0	-9.222605	-1.298607	-0.107855
13	6	0	-9.011029	0.200150	-0.179714
14	6	0	-7.803826	0.883508	-0.176507
15	6	0	-6.280422	0.408082	-0.193512
16	6	0	-3.753229	-0.489964	0.025856
17	6	0	-3.847606	0.855638	0.245826
18	16	0	-5.427304	-1.239049	-0.320019
19	6	0	-5.233642	1.273256	-0.050749
20	6	0	-2.231244	-0.811535	0.169481
21	6	0	-1.624063	0.376570	0.451334
22	7	0	-2.604493	1.462965	0.733557
23	16	0	-1.059416	-2.185358	0.082671
24	16	0	1.248555	1.455621	0.602211
25	6	0	0.333101	-1.027568	0.272198
26	6	0	-0.094302	0.271434	0.418561
27	6	0	1.889859	-1.108687	0.372641
28	6	0	2.449836	0.137253	0.417025
29	6	0	3.962122	-0.045697	0.253366
30	6	0	4.173606	-1.383937	0.242678
31	6	0	5.621517	-1.767878	0.053804
32	6	0	6.464051	-0.673724	0.019688
33	16	0	5.498332	0.877450	0.053629
34	7	0	2.936366	-2.169757	0.447719
35	6	0	8.025915	-0.899549	-0.035280
36	6	0	9.036886	0.016356	-0.140755
37	6	0	8.808069	1.480282	-0.232912
38	6	0	10.595153	-0.277676	-0.193053
39	6	0	10.135021	2.139622	-0.336252
40	6	0	11.197595	1.230116	-0.315953
41	6	0	10.271013	3.612157	-0.448181
42	6	0	12.520782	1.915817	-0.410310
43	6	0	11.491622	4.154746	-0.531684
44	6	0	12.654605	3.265527	-0.508782
45	6	0	10.790476	-1.702441	-0.113884
46	6	0	9.661266	-2.674905	-0.003291
47	6	0	11.582657	-3.005071	-0.072913
48	7	0	8.862195	-3.519307	0.088162
49	7	0	11.897942	-4.131115	-0.015064
50	6	0	-10.404404	2.295817	-0.238739
51	6	0	-11.177900	3.595514	-0.302670
52	6	0	-9.151317	3.087061	-0.144309
53	7	0	-11.540919	4.704594	-0.335343
54	7	0	-8.217891	3.783322	-0.062796
55	8	0	-8.355927	-2.137201	0.004194
56	8	0	7.726911	2.032890	-0.225832
57	6	0	2.815248	-3.308464	-0.481757
58	1	0	1.889672	-3.836644	-0.286427
59	1	0	2.825658	-2.969056	-1.513391
60	1	0	3.652368	-3.980649	-0.319682
61	6	0	-2.751323	1.632924	2.210569
62	1	0	-3.019234	0.680840	2.668656
63	1	0	-1.817640	1.981971	2.636457
64	1	0	-3.532724	2.357425	2.410677
65	1	0	5.961767	-2.788471	-0.030037

66	1	0	13.399849	1.383909	-0.403216
67	1	0	13.644717	3.694273	-0.571311
68	1	0	11.629040	5.222878	-0.613542
69	1	0	9.393535	4.237610	-0.461595
70	1	0	8.327194	-1.935854	0.014522
71	1	0	-7.898533	1.961333	-0.139517
72	1	0	-5.417118	2.331310	-0.167433

Rotational constants (GHZ): 0.1405601 0.0099854 0.0093756

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6392.4335296913 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T

Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6392.3526762449 Hartrees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.31D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Initial guess from the checkpoint file: "PDBD.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999969 0.004266 0.000091 0.006668 Ang= 0.91 deg.

ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1

AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-yADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlgl= 2001

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid=

0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0=

0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Integral accuracy reduced to 1.0D-05 until final iterations.

Initial convergence to 1.0D-05 achieved. Increase integral accuracy.

SCF Done: E(RB3LYP) = -3682.55486612 A.U. after 18 cycles

NFock= 18 Conv=0.47D-08 -V/T= 2.0077

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1

NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	0.003651623	-0.020335444	0.001410634
2	6	0.008331102	-0.017742362	0.002237733

3	6	-0.000078676	-0.011415691	0.000156075
4	6	-0.000762223	0.001698996	-0.000328959
5	6	-0.000597646	-0.005925506	-0.000229059
6	6	0.017500558	-0.010488233	0.009410498
7	1	0.005551181	-0.004032167	0.003583029
8	1	0.001153189	0.002214303	0.000345302
9	1	-0.002386020	-0.000059942	-0.001893469
10	1	-0.029982028	-0.014830741	-0.016327411
11	6	0.023992086	-0.011957596	0.012464634
12	6	-0.021162115	-0.008370930	-0.008732792
13	6	-0.013034857	0.008593798	-0.007575843
14	6	0.052323623	0.016041332	0.041765854
15	6	-0.004316089	0.026903805	-0.003896586
16	6	0.026451515	0.015397274	0.019731238
17	6	-0.026111737	0.026830937	-0.004154042
18	16	0.012723022	-0.013088940	-0.003890028
19	6	0.003028368	-0.062018452	-0.025428520
20	6	-0.018794213	0.030616020	-0.005336288
21	6	0.014287243	-0.035366933	0.001008014
22	7	-0.002669747	0.017457274	0.028113696
23	16	-0.009517651	-0.016898791	-0.001674197
24	16	0.002379050	0.011046960	0.009037407
25	6	0.040673202	-0.009185309	0.015789988
26	6	-0.028835574	0.009367568	-0.032582663
27	6	-0.003204759	0.045775676	-0.000203811
28	6	0.014301298	-0.030763918	0.014373654
29	6	-0.029650907	-0.008654511	-0.027258199
30	6	0.040475873	0.024479016	0.025615397
31	6	-0.030633910	0.020350335	-0.034564389
32	6	0.024495643	-0.021073151	0.021904243
33	16	0.001932482	0.019786198	-0.009025039
34	7	-0.038306564	-0.037062062	0.007241999
35	6	-0.071780711	-0.001470450	-0.042359097
36	6	0.009951696	-0.017567978	0.007408260
37	6	0.022937637	0.000871331	0.014971065
38	6	-0.021542275	0.034406565	-0.017755303
39	6	-0.022667633	-0.019872724	-0.012182046
40	6	0.012313900	-0.013950606	0.009243159
41	6	0.013968980	0.061632529	0.002882687
42	6	-0.020103532	0.058327558	-0.017719895
43	6	0.043393968	-0.021231604	0.029346971
44	6	-0.038647036	-0.006946093	-0.023733886
45	6	0.011231055	0.026485316	0.005378486
46	6	0.005667112	-0.018566813	0.005007189
47	6	-0.005242631	-0.058657701	0.001463501
48	7	0.017382615	0.016985460	0.010098719
49	7	0.001567216	-0.015631690	0.002689408
50	6	-0.014848011	-0.026735814	-0.009069255
51	6	0.011985888	0.049099752	0.008663806
52	6	-0.001649579	0.016086841	-0.002458254
53	7	-0.000305865	0.008158724	0.000254849
54	7	-0.010288344	-0.004807268	-0.006758106
55	8	0.010110903	0.001839816	0.006853470
56	8	-0.010560453	-0.008533575	-0.005440532
57	6	-0.000624666	-0.003203045	-0.007793596
58	1	-0.000330570	0.005903894	-0.002367365
59	1	-0.004124341	0.000367429	0.005887331
60	1	0.004105976	0.001532266	0.000716623
61	6	-0.001868869	-0.004626764	0.005293810
62	1	0.003067356	0.003528251	-0.002577130

R26	2.77221	-0.02467	0.01930	0.00000	0.01932	2.79153
R27	2.04122	0.00789	-0.01405	0.00000	-0.01405	2.02717
R28	2.57704	0.00713	-0.00157	0.00000	-0.00160	2.57543
R29	3.41623	-0.02354	0.01347	0.00000	0.01348	3.42970
R30	2.81636	-0.03266	0.01822	0.00000	0.01822	2.83458
R31	2.89831	-0.06515	0.04175	0.00000	0.04175	2.94006
R32	2.82324	-0.00073	0.00011	0.00000	0.00011	2.82335
R33	3.44091	-0.02297	0.01351	0.00000	0.01351	3.45442
R34	3.40114	-0.01759	0.01089	0.00000	0.01089	3.41202
R35	3.38860	-0.01826	0.01146	0.00000	0.01146	3.40006
R36	2.59898	0.00505	0.00139	0.00000	0.00139	2.60037
R37	2.95194	-0.07185	0.04393	0.00000	0.04393	2.99587
R38	2.58272	0.00791	-0.00047	0.00000	-0.00050	2.58221
R39	2.81986	-0.04701	0.02699	0.00000	0.02699	2.84685
R40	2.89521	-0.05775	0.03609	0.00000	0.03607	2.93128
R41	2.56037	0.01796	-0.01478	0.00000	-0.01471	2.54566
R42	3.40782	-0.02645	0.01575	0.00000	0.01576	3.42358
R43	2.85313	-0.06134	0.04046	0.00000	0.04048	2.89361
R44	2.79674	-0.03669	0.02574	0.00000	0.02577	2.82251
R45	2.61042	-0.00306	0.01627	0.00000	0.01625	2.62667
R46	2.03916	0.00321	-0.00390	0.00000	-0.00390	2.03526
R47	3.45355	-0.01297	0.00996	0.00000	0.00992	3.46348
R48	2.98399	-0.06587	0.04617	0.00000	0.04617	3.03016
R49	2.78710	0.00046	-0.00186	0.00000	-0.00186	2.78525
R50	2.58559	-0.00963	0.03945	0.00000	0.03945	2.62504
R51	2.04158	-0.03505	-0.00431	0.00000	-0.00431	2.03728
R52	2.80542	-0.00128	0.03334	0.00000	0.03329	2.83871
R53	2.99829	0.05274	0.02326	0.00000	0.02310	3.02139
R54	2.80687	-0.03548	0.03737	0.00000	0.03749	2.84436
R55	2.29454	0.01029	0.01706	0.00000	0.01706	2.31160
R56	3.07711	-0.05312	-0.04973	0.00000	-0.04975	3.02736
R57	2.72171	-0.00844	-0.01652	0.00000	-0.01652	2.70520
R58	2.64337	-0.03419	-0.03189	0.00000	-0.03180	2.61158
R59	2.80252	-0.05145	0.02899	0.00000	0.02908	2.83160
R60	2.82191	-0.04597	0.01777	0.00000	0.01764	2.83954
R61	2.52917	0.03464	0.01860	0.00000	0.01874	2.54791
R62	2.03647	0.00475	-0.00469	0.00000	-0.00469	2.03178
R63	2.56983	0.01196	-0.00489	0.00000	-0.00498	2.56485
R64	1.94168	0.04790	0.01892	0.00000	0.01892	1.96059
R65	2.76686	-0.03066	0.03690	0.00000	0.03694	2.80380
R66	2.04099	0.00357	-0.00375	0.00000	-0.00375	2.03724
R67	2.04235	0.00294	-0.00318	0.00000	-0.00318	2.03917
R68	2.82388	-0.00770	0.02166	0.00000	0.02166	2.84554
R69	2.88211	-0.02918	0.01746	0.00000	0.01746	2.89957
R70	2.20369	0.01441	-0.00366	0.00000	-0.00366	2.20003
R71	2.21246	-0.00750	-0.00360	0.00000	-0.00360	2.20886
R72	2.86067	-0.03572	0.01991	0.00000	0.01991	2.88058
R73	2.80624	-0.01588	0.02218	0.00000	0.02218	2.82842
R74	2.20614	-0.00464	-0.00187	0.00000	-0.00187	2.20426
R75	2.20597	0.00101	-0.00786	0.00000	-0.00786	2.19812
R76	2.04739	0.00626	-0.00679	0.00000	-0.00679	2.04060
R77	2.05240	0.00677	-0.00743	0.00000	-0.00743	2.04497
R78	2.05179	0.00410	-0.00469	0.00000	-0.00469	2.04709
R79	2.05979	0.00498	-0.00538	0.00000	-0.00538	2.05441
R80	2.04839	0.00564	-0.00605	0.00000	-0.00605	2.04235
R81	2.04888	0.00496	-0.00555	0.00000	-0.00555	2.04333
A1	2.00030	0.02006	0.03249	0.00000	0.03235	2.03265
A2	1.89943	0.01811	0.01177	0.00000	0.01194	1.91137
A3	2.38345	-0.03817	-0.04425	0.00000	-0.04429	2.33916
A4	2.15840	-0.00098	-0.01962	0.00000	-0.01969	2.13871

A5	1.94915	-0.00334	-0.00849	0.00000	-0.00829	1.94086
A6	2.17562	0.00432	0.02811	0.00000	0.02799	2.20361
A7	2.08321	-0.00533	-0.00027	0.00000	-0.00014	2.08306
A8	2.11097	-0.00338	0.00137	0.00000	0.00131	2.11228
A9	2.08900	0.00871	-0.00110	0.00000	-0.00116	2.08784
A10	2.07852	-0.00002	0.00560	0.00000	0.00572	2.08424
A11	2.10818	-0.00076	-0.00083	0.00000	-0.00090	2.10729
A12	2.09647	0.00078	-0.00476	0.00000	-0.00482	2.09165
A13	2.11721	-0.00238	-0.00764	0.00000	-0.00762	2.10960
A14	2.08646	0.00326	0.00343	0.00000	0.00342	2.08988
A15	2.07951	-0.00087	0.00421	0.00000	0.00420	2.08371
A16	2.12830	-0.01133	-0.01056	0.00000	-0.01063	2.11768
A17	2.13241	-0.00031	-0.00480	0.00000	-0.00476	2.12765
A18	2.02246	0.01164	0.01535	0.00000	0.01539	2.03784
A19	1.81067	-0.01165	0.02298	0.00000	0.02284	1.83351
A20	2.48844	-0.14869	-0.12507	0.00000	-0.12500	2.36344
A21	1.98404	0.16033	0.10210	0.00000	0.10216	2.08621
A22	1.88991	-0.00105	0.00684	0.00000	0.00684	1.89676
A23	2.19229	0.00031	-0.00656	0.00000	-0.00656	2.18572
A24	2.20098	0.00074	-0.00028	0.00000	-0.00028	2.20070
A25	1.87388	-0.00210	-0.03305	0.00000	-0.03328	1.84060
A26	2.18413	0.07944	0.01729	0.00000	0.01740	2.20153
A27	2.22513	-0.07733	0.01577	0.00000	0.01588	2.24101
A28	2.32390	-0.03086	0.01498	0.00000	0.01498	2.33889
A29	1.99807	0.03760	-0.01206	0.00000	-0.01206	1.98600
A30	1.96107	-0.00675	-0.00292	0.00000	-0.00292	1.95815
A31	2.34987	-0.02999	0.02400	0.00000	0.02405	2.37391
A32	2.14346	-0.01395	0.01790	0.00000	0.01796	2.16142
A33	1.78920	0.04397	-0.04193	0.00000	-0.04204	1.74716
A34	1.94233	0.01113	-0.01198	0.00000	-0.01191	1.93043
A35	1.82879	0.00182	0.00170	0.00000	0.00170	1.83049
A36	2.51206	-0.01295	0.01028	0.00000	0.01021	2.52227
A37	1.88675	0.01836	-0.01002	0.00000	-0.01002	1.87673
A38	1.98514	-0.00025	-0.00223	0.00000	-0.00219	1.98295
A39	2.41070	-0.01810	0.01225	0.00000	0.01220	2.42290
A40	1.61421	-0.02492	0.02840	0.00000	0.02842	1.64262
A41	2.16635	-0.04713	0.03505	0.00000	0.03503	2.20138
A42	2.07044	0.02204	-0.01955	0.00000	-0.01954	2.05090
A43	2.04637	0.02504	-0.01549	0.00000	-0.01548	2.03089
A44	1.84777	-0.00316	0.00550	0.00000	0.00547	1.85324
A45	2.47114	-0.00658	0.00747	0.00000	0.00749	2.47862
A46	1.96427	0.00974	-0.01297	0.00000	-0.01295	1.95132
A47	1.96202	0.01011	-0.01446	0.00000	-0.01449	1.94753
A48	1.96054	-0.00127	0.00424	0.00000	0.00425	1.96479
A49	2.36054	-0.00883	0.01023	0.00000	0.01024	2.37078
A50	1.76473	-0.00747	0.00915	0.00000	0.00916	1.77388
A51	1.86764	0.00847	-0.00703	0.00000	-0.00705	1.86060
A52	1.91218	0.00217	-0.00238	0.00000	-0.00237	1.90981
A53	1.57831	-0.01583	0.01791	0.00000	0.01790	1.59622
A54	1.57636	-0.01629	0.01774	0.00000	0.01772	1.59407
A55	1.95409	0.01091	-0.01375	0.00000	-0.01376	1.94033
A56	2.39767	-0.01129	0.01051	0.00000	0.01052	2.40819
A57	1.93041	0.00047	0.00318	0.00000	0.00319	1.93359
A58	2.34187	-0.00502	0.00784	0.00000	0.00785	2.34972
A59	1.95733	-0.00306	0.00433	0.00000	0.00433	1.96166
A60	1.98279	0.00813	-0.01221	0.00000	-0.01221	1.97057
A61	1.94236	0.00089	0.00246	0.00000	0.00247	1.94482
A62	2.40249	-0.01115	0.00991	0.00000	0.00992	2.41242
A63	1.93827	0.01025	-0.01236	0.00000	-0.01238	1.92589
A64	1.98135	0.00748	-0.01154	0.00000	-0.01153	1.96982

A65	2.43425	-0.00295	0.00584	0.00000	0.00586	2.44011
A66	1.86722	-0.00449	0.00568	0.00000	0.00564	1.87287
A67	1.84716	-0.00354	0.00327	0.00000	0.00326	1.85043
A68	2.48417	-0.00458	0.00555	0.00000	0.00550	2.48967
A69	1.95172	0.00812	-0.00882	0.00000	-0.00877	1.94295
A70	1.98433	-0.00132	0.00182	0.00000	0.00185	1.98619
A71	1.97454	0.00210	-0.00441	0.00000	-0.00438	1.97016
A72	2.32406	-0.00078	0.00260	0.00000	0.00253	2.32659
A73	1.96772	-0.00317	0.00862	0.00000	0.00863	1.97635
A74	2.15630	0.00280	-0.00286	0.00000	-0.00286	2.15345
A75	2.15905	0.00040	-0.00578	0.00000	-0.00578	2.15327
A76	1.92787	0.01273	-0.02191	0.00000	-0.02197	1.90591
A77	2.08388	-0.02071	0.00672	0.00000	0.00675	2.09062
A78	2.27143	0.00798	0.01519	0.00000	0.01522	2.28665
A79	1.58851	-0.01598	0.02010	0.00000	0.02006	1.60857
A80	1.77395	-0.00329	0.00733	0.00000	0.00736	1.78132
A81	2.04845	-0.00073	-0.00152	0.00000	-0.00155	2.04690
A82	1.97283	0.00928	-0.00729	0.00000	-0.00730	1.96552
A83	2.26242	0.01285	0.00941	0.00000	0.00941	2.27183
A84	1.99479	-0.03742	-0.00019	0.00000	-0.00019	1.99460
A85	2.02596	0.02458	-0.00921	0.00000	-0.00921	2.01675
A86	2.15436	-0.08794	0.01468	0.00000	0.01479	2.16915
A87	2.21952	0.10834	0.02108	0.00000	0.02119	2.24071
A88	1.90930	-0.02040	-0.03577	0.00000	-0.03599	1.87331
A89	1.88006	0.01156	0.00431	0.00000	0.00437	1.88442
A90	2.19650	0.00614	-0.00020	0.00000	-0.00023	2.19627
A91	2.20663	-0.01770	-0.00411	0.00000	-0.00414	2.20250
A92	1.76629	-0.01706	0.02432	0.00000	0.02411	1.79040
A93	1.89094	0.26968	0.13608	0.00000	0.13618	2.02712
A94	2.62595	-0.25261	-0.16039	0.00000	-0.16029	2.46566
A95	1.97034	-0.00671	-0.01038	0.00000	-0.01018	1.96016
A96	2.12696	0.00846	0.03540	0.00000	0.03525	2.16220
A97	2.18589	-0.00175	-0.02502	0.00000	-0.02507	2.16082
A98	1.89876	0.03261	0.01752	0.00000	0.01769	1.91646
A99	2.43072	-0.05761	-0.06225	0.00000	-0.06221	2.36851
A100	1.95370	0.02499	0.04473	0.00000	0.04452	1.99822
A101	2.08389	-0.00496	-0.00244	0.00000	-0.00217	2.08172
A102	2.09734	-0.00568	0.00371	0.00000	0.00358	2.10092
A103	2.10195	0.01064	-0.00127	0.00000	-0.00141	2.10055
A104	2.15020	-0.01204	-0.01727	0.00000	-0.01747	2.13272
A105	2.11758	-0.00175	-0.00278	0.00000	-0.00267	2.11491
A106	2.01541	0.01380	0.02005	0.00000	0.02015	2.03556
A107	2.06828	-0.00173	0.00880	0.00000	0.00902	2.07730
A108	2.11964	0.00216	-0.00454	0.00000	-0.00465	2.11500
A109	2.09526	-0.00043	-0.00426	0.00000	-0.00437	2.09089
A110	2.12438	-0.00451	-0.00880	0.00000	-0.00882	2.11556
A111	2.08068	0.00160	0.00242	0.00000	0.00243	2.08311
A112	2.07812	0.00292	0.00638	0.00000	0.00639	2.08452
A113	2.14760	0.15850	0.08445	0.00000	0.08445	2.23205
A114	2.73085	-0.19358	-0.11676	0.00000	-0.11676	2.61409
A115	1.40472	0.03508	0.03232	0.00000	0.03232	1.43704
A116	2.57493	-0.11852	-0.08928	0.00000	-0.08928	2.48565
A117	2.16102	0.08753	0.06381	0.00000	0.06381	2.22483
A118	1.54718	0.03101	0.02547	0.00000	0.02547	1.57265
A119	1.91020	-0.00086	0.00094	0.00000	0.00094	1.91114
A120	1.93537	0.00418	-0.00420	0.00000	-0.00420	1.93117
A121	1.89715	-0.00054	0.00095	0.00000	0.00095	1.89810
A122	1.90899	-0.00097	0.00103	0.00000	0.00103	1.91002
A123	1.90704	-0.00128	0.00058	0.00000	0.00059	1.90762
A124	1.90484	-0.00059	0.00074	0.00000	0.00074	1.90559

A125	1.91801	0.00414	-0.00369	0.00000	-0.00370	1.91431
A126	1.91815	-0.00292	0.00226	0.00000	0.00226	1.92041
A127	1.90637	-0.00179	0.00141	0.00000	0.00141	1.90779
A128	1.90483	0.00026	0.00015	0.00000	0.00015	1.90499
A129	1.90601	0.00012	0.00019	0.00000	0.00019	1.90619
A130	1.91038	0.00021	-0.00033	0.00000	-0.00033	1.91006
A131	3.24333	0.04836	0.00161	0.00000	0.00161	3.24493
A132	3.41570	-0.03111	-0.06104	0.00000	-0.06104	3.35466
A133	3.36230	-0.01482	-0.04312	0.00000	-0.04312	3.31917
A134	3.21908	0.02907	0.00086	0.00000	0.00086	3.21994
A135	3.13588	-0.00313	-0.00004	0.00000	-0.00004	3.13584
A136	3.14528	-0.00002	-0.00082	0.00000	-0.00082	3.14446
A137	3.12341	0.00025	0.00083	0.00000	0.00083	3.12425
A138	3.14846	0.00006	0.00019	0.00000	0.00019	3.14865
D1	-0.01970	0.00022	0.00039	0.00000	0.00037	-0.01933
D2	3.12018	-0.00051	0.00081	0.00000	0.00079	3.12097
D3	3.12498	-0.00001	0.00020	0.00000	0.00020	3.12518
D4	-0.01833	-0.00074	0.00061	0.00000	0.00062	-0.01771
D5	-0.00543	0.00017	-0.00057	0.00000	-0.00054	-0.00597
D6	-3.14068	-0.00025	-0.00084	0.00000	-0.00082	-3.14151
D7	3.13192	0.00068	-0.00014	0.00000	-0.00012	3.13180
D8	-0.00333	0.00026	-0.00041	0.00000	-0.00040	-0.00373
D9	0.04522	0.00049	-0.00010	0.00000	-0.00010	0.04511
D10	-3.08664	-0.00049	-0.00152	0.00000	-0.00158	-3.08822
D11	-3.09230	-0.00001	-0.00055	0.00000	-0.00055	-3.09285
D12	0.05903	-0.00099	-0.00196	0.00000	-0.00203	0.05700
D13	0.03127	-0.00071	-0.00008	0.00000	-0.00007	0.03121
D14	-3.11493	-0.00067	0.00005	0.00000	0.00006	-3.11487
D15	-3.10838	0.00013	-0.00054	0.00000	-0.00051	-3.10889
D16	0.02860	0.00017	-0.00040	0.00000	-0.00039	0.02822
D17	-0.01812	-0.00003	-0.00048	0.00000	-0.00050	-0.01862
D18	3.11972	0.00133	-0.00082	0.00000	-0.00084	3.11888
D19	3.12174	-0.00079	-0.00009	0.00000	-0.00011	3.12163
D20	-0.02361	0.00058	-0.00042	0.00000	-0.00046	-0.02407
D21	-0.01647	0.00043	-0.00052	0.00000	-0.00053	-0.01700
D22	3.12060	0.00040	-0.00021	0.00000	-0.00021	3.12039
D23	3.12967	0.00042	-0.00067	0.00000	-0.00066	3.12901
D24	-0.01644	0.00039	-0.00035	0.00000	-0.00035	-0.01679
D25	-0.00772	0.00007	0.00015	0.00000	0.00014	-0.00758
D26	3.12982	0.00015	0.00022	0.00000	0.00022	3.13004
D27	3.13836	0.00010	-0.00017	0.00000	-0.00018	3.13819
D28	-0.00729	0.00018	-0.00010	0.00000	-0.00010	-0.00738
D29	0.01917	-0.00046	0.00030	0.00000	0.00031	0.01948
D30	-3.12839	-0.00010	0.00050	0.00000	0.00051	-3.12788
D31	-3.11838	-0.00055	0.00023	0.00000	0.00023	-3.11815
D32	0.01724	-0.00019	0.00043	0.00000	0.00044	0.01768
D33	-0.05489	-0.00015	0.00094	0.00000	0.00100	-0.05389
D34	3.09619	-0.00101	0.00017	0.00000	0.00021	3.09640
D35	3.08024	-0.00121	0.00091	0.00000	0.00080	3.08104
D36	-0.05187	-0.00207	0.00013	0.00000	0.00001	-0.05186
D37	-0.04938	0.00087	0.00074	0.00000	0.00076	-0.04862
D38	3.10728	-0.00322	0.00053	0.00000	0.00056	3.10783
D39	3.10254	0.00059	-0.00037	0.00000	-0.00040	3.10214
D40	-0.02398	-0.00350	-0.00058	0.00000	-0.00060	-0.02459
D41	0.04674	0.00005	-0.00109	0.00000	-0.00113	0.04562
D42	-3.10462	0.00206	-0.00029	0.00000	-0.00032	-3.10494
D43	-3.09107	-0.00133	-0.00073	0.00000	-0.00076	-3.09183
D44	0.04075	0.00068	0.00007	0.00000	0.00005	0.04080
D45	-3.07465	-0.00244	0.00177	0.00000	0.00176	-3.07289
D46	0.08667	-0.00191	0.00172	0.00000	0.00171	0.08838

D47	0.07835	-0.00414	0.00104	0.00000	0.00105	0.07940
D48	-3.04352	-0.00361	0.00099	0.00000	0.00100	-3.04252
D49	0.07205	-0.00041	-0.00062	0.00000	-0.00060	0.07145
D50	-3.02310	-0.00262	0.00165	0.00000	0.00164	-3.02146
D51	-3.08895	-0.00054	-0.00065	0.00000	-0.00064	-3.08959
D52	0.09908	-0.00275	0.00162	0.00000	0.00160	0.10069
D53	-3.00392	-0.00118	-0.00002	0.00000	0.00007	-3.00385
D54	0.09769	-0.00003	-0.00114	0.00000	-0.00102	0.09667
D55	2.88756	0.00843	-0.00388	0.00000	-0.00381	2.88375
D56	-0.26275	0.00182	-0.00044	0.00000	-0.00044	-0.26319
D57	-0.22018	0.00816	-0.00340	0.00000	-0.00332	-0.22351
D58	2.91269	0.00155	0.00004	0.00000	0.00005	2.91274
D59	-0.13212	0.00047	0.00109	0.00000	0.00103	-0.13109
D60	2.97922	0.00043	0.00119	0.00000	0.00114	2.98036
D61	3.01087	0.00077	0.00073	0.00000	0.00066	3.01154
D62	-0.16097	0.00073	0.00083	0.00000	0.00078	-0.16019
D63	0.02490	-0.00197	0.00090	0.00000	0.00079	0.02569
D64	-3.11900	-0.00241	0.00149	0.00000	0.00136	-3.11764
D65	-0.00203	0.00203	-0.00161	0.00000	-0.00156	-0.00359
D66	-3.13903	0.00247	-0.00146	0.00000	-0.00145	-3.14048
D67	-3.14140	0.00245	-0.00217	0.00000	-0.00211	3.13968
D68	0.00479	0.00289	-0.00202	0.00000	-0.00200	0.00279
D69	0.25210	-0.01287	0.00753	0.00000	0.00747	0.25957
D70	-2.88089	-0.00633	0.00413	0.00000	0.00415	-2.87674
D71	-2.84801	-0.01365	0.00803	0.00000	0.00793	-2.84008
D72	0.30219	-0.00711	0.00463	0.00000	0.00461	0.30680
D73	0.24601	-0.00398	0.00180	0.00000	0.00185	0.24786
D74	-1.75479	-0.00621	0.00313	0.00000	0.00312	-1.75167
D75	-2.93866	-0.00290	0.00119	0.00000	0.00128	-2.93739
D76	1.34373	-0.00514	0.00252	0.00000	0.00254	1.34627
D77	0.16018	-0.00288	0.00102	0.00000	0.00102	0.16120
D78	-2.99334	-0.00232	0.00092	0.00000	0.00092	-2.99242
D79	-2.98450	-0.00322	0.00097	0.00000	0.00099	-2.98351
D80	0.14516	-0.00265	0.00088	0.00000	0.00089	0.14606
D81	3.03605	0.00283	-0.00165	0.00000	-0.00161	3.03443
D82	-0.10077	0.00332	-0.00153	0.00000	-0.00153	-0.10230
D83	-0.24429	0.00376	-0.00080	0.00000	-0.00081	-0.24510
D84	1.72294	0.01055	-0.00531	0.00000	-0.00530	1.71764
D85	2.91298	0.00288	-0.00053	0.00000	-0.00054	2.91244
D86	-1.40298	0.00968	-0.00504	0.00000	-0.00503	-1.40801
D87	3.07100	0.00193	-0.00092	0.00000	-0.00092	3.07008
D88	-0.12798	0.00354	-0.00221	0.00000	-0.00220	-0.13018
D89	-0.08626	0.00287	-0.00131	0.00000	-0.00131	-0.08757
D90	2.99794	0.00449	-0.00260	0.00000	-0.00259	2.99535
D91	0.94087	-0.00162	0.00287	0.00000	0.00287	0.94374
D92	3.03737	-0.00053	0.00214	0.00000	0.00215	3.03952
D93	-1.14975	-0.00318	0.00402	0.00000	0.00402	-1.14573
D94	-0.95835	0.00194	-0.00324	0.00000	-0.00324	-0.96159
D95	1.13815	0.00303	-0.00396	0.00000	-0.00396	1.13419
D96	-3.04897	0.00038	-0.00208	0.00000	-0.00209	-3.05105
D97	0.02415	-0.00092	0.00060	0.00000	0.00061	0.02475
D98	3.11075	0.00176	-0.00106	0.00000	-0.00105	3.10970
D99	3.11618	0.00054	-0.00020	0.00000	-0.00021	3.11597
D100	0.03259	-0.00081	0.00068	0.00000	0.00067	0.03326
D101	-0.11294	0.00412	-0.00215	0.00000	-0.00213	-0.11507
D102	2.99441	0.00576	-0.00320	0.00000	-0.00318	2.99122
D103	0.04941	-0.00016	-0.00006	0.00000	-0.00006	0.04934
D104	-3.13709	0.00072	-0.00046	0.00000	-0.00047	-3.13756
D105	-3.05241	-0.00160	0.00071	0.00000	0.00071	-3.05170
D106	0.04428	-0.00072	0.00030	0.00000	0.00030	0.04458

D107	3.06730	0.00132	-0.00070	0.00000	-0.00070	3.06660
D108	-0.08826	0.00036	0.00016	0.00000	0.00015	-0.08811
D109	-0.12878	0.00421	-0.00273	0.00000	-0.00272	-0.13150
D110	2.99884	0.00324	-0.00188	0.00000	-0.00187	2.99697
D111	0.15512	-0.00355	0.00152	0.00000	0.00153	0.15666
D112	-2.96320	-0.00461	0.00210	0.00000	0.00212	-2.96108
D113	-2.97639	-0.00269	0.00077	0.00000	0.00077	-2.97561
D114	0.18848	-0.00375	0.00136	0.00000	0.00136	0.18984
D115	2.94868	0.00511	-0.00258	0.00000	-0.00258	2.94609
D116	0.78773	-0.00377	0.00204	0.00000	0.00204	0.78978
D117	-0.20686	0.00410	-0.00167	0.00000	-0.00166	-0.20853
D118	-2.36781	-0.00479	0.00296	0.00000	0.00297	-2.36484
D119	3.08519	0.00251	-0.00123	0.00000	-0.00123	3.08396
D120	-0.07732	0.00205	-0.00109	0.00000	-0.00109	-0.07841
D121	-0.08924	0.00424	-0.00247	0.00000	-0.00246	-0.09170
D122	3.03144	0.00378	-0.00234	0.00000	-0.00232	3.02911
D123	3.11706	0.00006	0.00007	0.00000	0.00008	3.11714
D124	-0.04563	-0.00004	0.00028	0.00000	0.00029	-0.04534
D125	-0.01077	0.00048	-0.00016	0.00000	-0.00015	-0.01092
D126	3.10973	0.00038	0.00005	0.00000	0.00005	3.10978
D127	3.12677	0.00198	-0.00131	0.00000	-0.00131	3.12547
D128	-0.03649	0.00142	-0.00107	0.00000	-0.00107	-0.03756
D129	0.07253	-0.00343	0.00206	0.00000	0.00205	0.07459
D130	-3.08457	-0.00159	0.00107	0.00000	0.00106	-3.08351
D131	-3.04247	-0.00334	0.00191	0.00000	0.00191	-3.04056
D132	0.08362	-0.00151	0.00092	0.00000	0.00091	0.08453
D133	0.14925	-0.00208	0.00124	0.00000	0.00124	0.15050
D134	2.36056	0.00010	0.00014	0.00000	0.00015	2.36071
D135	-3.01882	-0.00220	0.00146	0.00000	0.00146	-3.01736
D136	-0.80751	-0.00002	0.00036	0.00000	0.00037	-0.80714
D137	-0.09661	0.00332	-0.00125	0.00000	-0.00126	-0.09787
D138	3.04198	0.00241	-0.00125	0.00000	-0.00126	3.04072
D139	3.06052	0.00146	-0.00029	0.00000	-0.00029	3.06022
D140	-0.08407	0.00054	-0.00029	0.00000	-0.00030	-0.08437
D141	0.07739	-0.00318	0.00128	0.00000	0.00127	0.07867
D142	-3.06078	-0.00208	0.00132	0.00000	0.00131	-3.05947
D143	3.07897	0.00086	-0.00019	0.00000	-0.00019	3.07877
D144	-0.05764	0.00017	0.00001	0.00000	0.00001	-0.05762
D145	-0.06630	-0.00026	-0.00028	0.00000	-0.00027	-0.06657
D146	3.08028	-0.00096	-0.00007	0.00000	-0.00007	3.08021
D147	-1.07762	0.00025	0.00228	0.00000	0.00228	-1.07534
D148	1.02994	0.00115	0.00150	0.00000	0.00150	1.03144
D149	3.12394	0.00262	0.00045	0.00000	0.00045	3.12440
D150	-3.13427	-0.00226	-0.00061	0.00000	-0.00062	-3.13488
D151	-1.02671	-0.00136	-0.00139	0.00000	-0.00140	-1.02811
D152	1.06729	0.00012	-0.00244	0.00000	-0.00244	1.06485
D153	-0.00486	-0.00082	0.00021	0.00000	0.00021	-0.00466
D154	-3.14003	-0.00099	0.00012	0.00000	0.00012	-3.13991
D155	3.13167	-0.00027	0.00003	0.00000	0.00002	3.13169
D156	-0.00350	-0.00043	-0.00007	0.00000	-0.00006	-0.00357
D157	-3.13977	-0.00074	0.00013	0.00000	0.00014	-3.13963
D158	0.00066	-0.00062	-0.00001	0.00000	0.00000	0.00066
D159	-0.00361	-0.00011	0.00035	0.00000	0.00036	-0.00324
D160	3.13683	0.00000	0.00021	0.00000	0.00022	3.13705
D161	-3.14025	-0.00008	-0.00025	0.00000	-0.00026	-3.14051
D162	0.00292	0.00056	0.00004	0.00000	0.00007	0.00299
D163	0.00702	0.00006	-0.00044	0.00000	-0.00046	0.00657
D164	-3.13299	0.00070	-0.00015	0.00000	-0.00012	-3.13311
D165	-0.00220	0.00014	0.00005	0.00000	0.00006	-0.00214
D166	3.13890	0.00027	-0.00009	0.00000	-0.00008	3.13883

D167	3.14056	0.00000	0.00019	0.00000	0.00020	3.14077
D168	-0.00152	0.00013	0.00005	0.00000	0.00006	-0.00146
D169	-0.00833	-0.00019	0.00026	0.00000	0.00026	-0.00807
D170	3.13209	-0.00001	0.00053	0.00000	0.00054	3.13264
D171	3.13022	0.00022	0.00056	0.00000	0.00056	3.13078
D172	-0.01254	0.00039	0.00083	0.00000	0.00084	-0.01170
D173	0.00042	0.00052	0.00015	0.00000	0.00016	0.00058
D174	3.13559	0.00024	0.00101	0.00000	0.00102	3.13661
D175	-3.13803	0.00039	0.00001	0.00000	0.00000	-3.13803
D176	-0.00286	0.00011	0.00087	0.00000	0.00086	-0.00200
D177	0.00688	0.00018	-0.00026	0.00000	-0.00027	0.00662
D178	-3.13388	0.00012	-0.00042	0.00000	-0.00041	-3.13429
D179	-3.13420	0.00004	-0.00014	0.00000	-0.00015	-3.13435
D180	0.00822	-0.00002	-0.00030	0.00000	-0.00029	0.00793
D181	3.13566	-0.00003	0.00033	0.00000	0.00032	3.13598
D182	-0.00555	-0.00002	0.00022	0.00000	0.00022	-0.00533
D183	-0.00649	0.00012	0.00018	0.00000	0.00017	-0.00631
D184	3.13549	0.00012	0.00007	0.00000	0.00007	3.13556
D185	3.13868	-0.00016	0.00000	0.00000	-0.00002	3.13866
D186	-0.00427	-0.00008	0.00023	0.00000	0.00022	-0.00405
D187	-0.00411	0.00002	0.00027	0.00000	0.00026	-0.00385
D188	3.13613	0.00010	0.00050	0.00000	0.00050	3.13663
D189	-0.00020	-0.00001	0.00019	0.00000	0.00019	-0.00001
D190	-3.14080	-0.00003	-0.00004	0.00000	-0.00004	-3.14084
D191	3.14100	-0.00002	0.00030	0.00000	0.00030	3.14130
D192	0.00040	-0.00005	0.00007	0.00000	0.00007	0.00047
D193	-0.00177	0.00000	-0.00016	0.00000	-0.00016	-0.00193
D194	3.13925	0.00003	-0.00006	0.00000	-0.00006	3.13919
D195	3.14111	-0.00007	-0.00037	0.00000	-0.00038	3.14073
D196	-0.00106	-0.00004	-0.00027	0.00000	-0.00027	-0.00133
D197	0.00404	-0.00005	-0.00016	0.00000	-0.00015	0.00389
D198	-3.13698	-0.00008	-0.00025	0.00000	-0.00026	-3.13723
D199	-3.13853	-0.00002	0.00007	0.00000	0.00007	-3.13846
D200	0.00364	-0.00005	-0.00003	0.00000	-0.00003	0.00360

Item	Value	Threshold	Converged?

Maximum Force	0.269675	0.000450	NO

RMS Force	0.031316	0.000300	NO

Maximum Displacement	1.912537	0.001800	NO

RMS Displacement	0.247911	0.001200	NO

Predicted change in Energy=-9.190797D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-11.652512	-0.377846	-0.296783
2	6	0	-10.948974	-1.592006	-0.203391
3	6	0	-11.595302	-2.844295	-0.200602
4	6	0	-12.983388	-2.897774	-0.331295
5	6	0	-13.706871	-1.711511	-0.441612
6	6	0	-13.060708	-0.471864	-0.413851
7	1	0	-11.034964	-3.757002	-0.103553

8	1	0	-13.500126	-3.846679	-0.351591
9	1	0	-14.781472	-1.747205	-0.553889
10	1	0	-13.667846	0.378145	-0.489050
11	6	0	-10.623724	0.838843	-0.247426
12	6	0	-9.438651	-1.351619	-0.111266
13	6	0	-9.176777	0.157282	-0.178254
14	6	0	-7.935531	0.834498	-0.170433
15	6	0	-6.386567	0.350063	-0.186624
16	6	0	-3.807847	-0.532758	0.037786
17	6	0	-3.911281	0.797962	0.263441
18	16	0	-5.494956	-1.276115	-0.314422
19	6	0	-5.320394	1.197786	-0.038299
20	6	0	-2.266438	-0.850239	0.182160
21	6	0	-1.659678	0.335720	0.469793
22	7	0	-2.662716	1.413053	0.758317
23	16	0	-1.072234	-2.213932	0.091850
24	16	0	1.243876	1.418970	0.622910
25	6	0	0.331663	-1.059099	0.284255
26	6	0	-0.107432	0.236232	0.435392
27	6	0	1.912005	-1.132970	0.386191
28	6	0	2.468159	0.114320	0.432472
29	6	0	4.000588	-0.057175	0.264051
30	6	0	4.226996	-1.385061	0.251903
31	6	0	5.699074	-1.759159	0.057693
32	6	0	6.545139	-0.656866	0.023753
33	16	0	5.540403	0.875534	0.061041
34	7	0	2.984892	-2.187918	0.460381
35	6	0	8.132973	-0.872989	-0.033339
36	6	0	9.160379	0.055818	-0.140055
37	6	0	8.952437	1.540601	-0.233471
38	6	0	10.736189	-0.208896	-0.195549
39	6	0	10.304755	2.193241	-0.337568
40	6	0	11.334818	1.272154	-0.316219
41	6	0	10.511692	3.672871	-0.452195
42	6	0	12.709256	1.872532	-0.407536
43	6	0	11.766781	4.158695	-0.533607
44	6	0	12.908413	3.211399	-0.507182
45	6	0	11.148475	-1.578234	-0.130670
46	6	0	10.277989	-2.801658	-0.017061
47	6	0	12.268955	-2.626463	-0.121464
48	7	0	9.706581	-3.812139	0.071222
49	7	0	12.934847	-3.586733	-0.094182
50	6	0	-10.730736	2.247033	-0.244202
51	6	0	-11.745528	3.381586	-0.325395
52	6	0	-9.618654	3.244565	-0.152451
53	7	0	-12.357091	4.373861	-0.369852
54	7	0	-8.818228	4.084947	-0.074394
55	8	0	-8.591678	-2.224655	0.001493
56	8	0	7.872068	2.114269	-0.227198
57	6	0	2.880949	-3.323907	-0.472931
58	1	0	1.965124	-3.863653	-0.283222
59	1	0	2.889004	-2.977476	-1.498101
60	1	0	3.725054	-3.983898	-0.313609
61	6	0	-2.818031	1.564349	2.236553
62	1	0	-3.077468	0.605123	2.677539
63	1	0	-1.893486	1.916180	2.671849
64	1	0	-3.606162	2.275468	2.442312
65	1	0	6.046024	-2.775164	-0.027826
66	1	0	13.557859	1.275745	-0.396140
67	1	0	13.915846	3.593256	-0.567832

68	1	0	11.951108	5.217657	-0.616282
69	1	0	9.668705	4.340014	-0.469091
70	1	0	8.441998	-1.904696	0.015045
71	1	0	-8.026323	1.910862	-0.129564
72	1	0	-5.503371	2.248650	-0.152134

Rotational constants (GHZ): 0.1430278 0.0093995 0.0088686

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6281.7266579634 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T
Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6281.6468821724 Hartrees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.59D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Lowest energy guess from the checkpoint file: "PBDB.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999991 0.002629 0.000043 0.003472 Ang= 0.50 deg.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999993 -0.001652 -0.000055 -0.003298 Ang= -0.42 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Integral accuracy reduced to 1.0D-05 until final iterations.

Initial convergence to 1.0D-05 achieved. Increase integral accuracy.

SCF Done: E(RB3LYP) = -3682.61029960 A.U. after 13 cycles

NFock= 13 Conv=0.76D-08 -V/T= 2.0081

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1

NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-0.002220460	-0.026387769	-0.001458772
2	6	0.014820173	-0.014955068	0.006160573
3	6	-0.005921787	-0.010670020	-0.002626619
4	6	0.003360007	-0.006500322	0.001565318
5	6	0.002907067	-0.008543875	0.001445948
6	6	0.016414275	-0.006662041	0.008944308
7	1	0.007036861	-0.002234003	0.004356762
8	1	0.001727690	0.002993625	0.000651979
9	1	-0.002640509	0.000490523	-0.001998393
10	1	-0.023590570	-0.014348409	-0.012759772
11	6	0.016148014	-0.009175004	0.007745184
12	6	-0.007272126	-0.003023861	-0.001174561
13	6	-0.009997114	-0.004285856	-0.005825674
14	6	0.036439799	0.027472390	0.030854327
15	6	0.002440068	0.018274956	-0.002155758
16	6	0.030457501	0.020690475	0.023759561


```

Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.109674585 RMS 0.020059471
Search for a local minimum.
Step number 5 out of a maximum of 429
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 4 3 5
ITU= 0 0 0 1 0
Use linear search instead of GDIIS.
Eigenvalues --- 0.00230 0.00230 0.00230 0.00230 0.00243
Eigenvalues --- 0.00285 0.00392 0.00445 0.00451 0.00472
Eigenvalues --- 0.00494 0.00539 0.00543 0.00584 0.00614
Eigenvalues --- 0.00631 0.00667 0.00670 0.00687 0.00709
Eigenvalues --- 0.00729 0.00739 0.00754 0.00755 0.00760
Eigenvalues --- 0.00763 0.00779 0.00869 0.00887 0.00928
Eigenvalues --- 0.01037 0.01084 0.01124 0.01145 0.01175
Eigenvalues --- 0.01201 0.01257 0.01269 0.01327 0.01349
Eigenvalues --- 0.01372 0.01379 0.01410 0.01430 0.01451
Eigenvalues --- 0.01569 0.01648 0.01662 0.01757 0.01793
Eigenvalues --- 0.01818 0.01926 0.01954 0.02006 0.02034
Eigenvalues --- 0.02075 0.02075 0.02209 0.02210 0.03281
Eigenvalues --- 0.04825 0.04827 0.04837 0.04893 0.04900
Eigenvalues --- 0.04904 0.05014 0.05016 0.05552 0.07281
Eigenvalues --- 0.07354 0.07399 0.07600 0.12655 0.14135
Eigenvalues --- 0.14867 0.15997 0.15999 0.16000 0.16000
Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16000
Eigenvalues --- 0.16000 0.16000 0.16011 0.16649 0.17648
Eigenvalues --- 0.18584 0.18665 0.19354 0.20164 0.21048
Eigenvalues --- 0.21550 0.21759 0.21882 0.21998 0.22000
Eigenvalues --- 0.22012 0.22040 0.22217 0.22488 0.22562
Eigenvalues --- 0.22597 0.22645 0.22726 0.23004 0.23245
Eigenvalues --- 0.23256 0.23361 0.23429 0.23983 0.24009
Eigenvalues --- 0.24235 0.24254 0.24507 0.24549 0.24587
Eigenvalues --- 0.24710 0.24768 0.24848 0.24869 0.24878
Eigenvalues --- 0.24940 0.24952 0.24974 0.24975 0.24988
Eigenvalues --- 0.24992 0.24999 0.24999 0.25000 0.25000
Eigenvalues --- 0.25000 0.25000 0.25000 0.25000 0.25000
Eigenvalues --- 0.25000 0.25000 0.25633 0.26275 0.26316
Eigenvalues --- 0.26680 0.26724 0.26749 0.27084 0.27271
Eigenvalues --- 0.27896 0.27929 0.28342 0.28439 0.28534
Eigenvalues --- 0.28668 0.30056 0.30330 0.30903 0.32986
Eigenvalues --- 0.33800 0.35687 0.36332 0.36338 0.36476
Eigenvalues --- 0.36582 0.36653 0.36763 0.36828 0.36902
Eigenvalues --- 0.37086 0.37097 0.37157 0.37254 0.37278
Eigenvalues --- 0.37424 0.37568 0.37673 0.37757 0.37956
Eigenvalues --- 0.39047 0.39753 0.40419 0.41414 0.41803
Eigenvalues --- 0.42659 0.42678 0.44449 0.45398 0.45816
Eigenvalues --- 0.46198 0.47007 0.47928 0.48178 0.49050
Eigenvalues --- 0.52799 0.55666 0.55941 0.58373 0.80640
Eigenvalues --- 0.81818 1.25853 1.26316 1.29449 1.35399
RFO step: Lambda=-3.04420505D-01 EMin= 2.29993595D-03
Quartic linear search produced a step of 0.00747.
Maximum step size ( 0.505) exceeded in Quadratic search.
-- Step size scaled by 0.683
Iteration 1 RMS(Cart)= 0.23712429 RMS(Int)= 0.00560111
Iteration 2 RMS(Cart)= 0.01297518 RMS(Int)= 0.00009343

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Iteration 3 RMS(Cart)= 0.00002557 RMS(Int)= 0.00009301
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00009301
Variable      Old X      -DE/DX      Delta X      Delta X      Delta X      New X
(Linear)      (Quad)      (Total)
R1            2.65765    -0.00743    0.00023    -0.00811    -0.00789    2.64976
R2            2.67619    -0.01820   -0.00001   -0.01723   -0.01721    2.65897
R3            3.01242    -0.06063    0.00032   -0.07121   -0.07088    2.94155
R4            2.66309    -0.01916   -0.00012   -0.01818   -0.01830    2.64479
R5            2.89526    -0.03086   -0.00037   -0.03777   -0.03819    2.85708
R6            2.63664    -0.00045   -0.00022    0.00085    0.00060    2.63724
R7            2.03216     0.00679    0.00005    0.00659    0.00664    2.03881
R8            2.63399     0.01004   -0.00009    0.01010    0.00999    2.64398
R9            2.04217     0.00320    0.00003    0.00316    0.00319    2.04536
R10           2.64226    -0.00397   -0.00003   -0.00317   -0.00320    2.63905
R11           2.04287     0.00286    0.00002    0.00285    0.00287    2.04574
R12           1.97906     0.02997   -0.00015    0.03106    0.03091    2.00998
R13           3.02531    -0.04248   -0.00028   -0.05483   -0.05506    2.97025
R14           2.66877    -0.05674    0.00012   -0.05010   -0.04998    2.61879
R15           2.89680    -0.02697   -0.00034   -0.03191   -0.03224    2.86456
R16           2.30846    -0.00811   -0.00020   -0.00389   -0.00409    2.30437
R17           2.67206    -0.06326   -0.00052   -0.06740   -0.06792    2.60414
R18           3.06708    -0.09612   -0.00053   -0.13646   -0.13699    2.93009
R19           2.04272    -0.00145    0.00003   -0.00177   -0.00174    2.04098
R20           3.51294    -0.01224    0.00001   -0.01774   -0.01783    3.49511
R21           2.58924    -0.00511   -0.00009   -0.00450   -0.00442    2.58482
R22           2.55807     0.02837    0.00025    0.02117    0.02144    2.57951
R23           3.54694    -0.04667   -0.00020   -0.06365   -0.06402    3.48291
R24           2.98647    -0.06621   -0.00035   -0.08573   -0.08606    2.90041
R25           2.82608    -0.05871   -0.00035   -0.06832   -0.06851    2.75757
R26           2.79153    -0.03099   -0.00020   -0.03348   -0.03367    2.75785
R27           2.02717     0.01413    0.00014    0.01301    0.01316    2.04032
R28           2.57543     0.00646    0.00002    0.00476    0.00481    2.58025
R29           3.42970    -0.02585   -0.00014   -0.03258   -0.03273    3.39698
R30           2.83458    -0.03575   -0.00019   -0.04228   -0.04250    2.79207
R31           2.94006    -0.07397   -0.00043   -0.09542   -0.09584    2.84422
R32           2.82335    -0.00056    0.00000   -0.00060   -0.00060    2.82275
R33           3.45442    -0.02529   -0.00014   -0.03270   -0.03285    3.42157
R34           3.41202    -0.01974   -0.00011   -0.02492   -0.02503    3.38699
R35           3.40006    -0.02069   -0.00012   -0.02569   -0.02581    3.37426
R36           2.60037     0.00285   -0.00001    0.00255    0.00254    2.60291
R37           2.99587    -0.07992   -0.00045   -0.10688   -0.10733    2.88854
R38           2.58221     0.00623    0.00000    0.00514    0.00520    2.58741
R39           2.84685    -0.05201   -0.00028   -0.06240   -0.06268    2.78417
R40           2.93128    -0.06529   -0.00037   -0.08162   -0.08196    2.84931
R41           2.54566     0.02333    0.00015    0.01824    0.01834    2.56400
R42           3.42358    -0.02963   -0.00016   -0.03657   -0.03674    3.38684
R43           2.89361    -0.07075   -0.00042   -0.08804   -0.08846    2.80516
R44           2.82251    -0.04400   -0.00026   -0.05053   -0.05084    2.77167
R45           2.62667    -0.01387   -0.00017   -0.01302   -0.01317    2.61350
R46           2.03526     0.00472    0.00004    0.00460    0.00464    2.03990
R47           3.46348    -0.01708   -0.00010   -0.02304   -0.02313    3.44035
R48           3.03016    -0.07870   -0.00047   -0.10829   -0.10877    2.92140
R49           2.78525     0.00152    0.00002    0.00148    0.00150    2.78674
R50           2.62504    -0.03218   -0.00040   -0.03070   -0.03111    2.59393
R51           2.03728    -0.00045    0.00004   -0.00082   -0.00077    2.03650
R52           2.83871    -0.01116   -0.00034   -0.01133   -0.01172    2.82699
R53           3.02139    -0.03588   -0.00024   -0.04542   -0.04562    2.97578
R54           2.84436    -0.02088   -0.00038   -0.02421   -0.02465    2.81971
R55           2.31160    -0.00613   -0.00018   -0.00278   -0.00295    2.30865
R56           3.02736    -0.06290    0.00051   -0.07161   -0.07103    2.95632

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R57	2.70520	-0.07153	0.00017	-0.06461	-0.06444	2.64075
R58	2.61158	-0.00799	0.00033	-0.00836	-0.00794	2.60364
R59	2.83160	-0.05819	-0.00030	-0.06800	-0.06825	2.76336
R60	2.83954	-0.05306	-0.00018	-0.06094	-0.06107	2.77847
R61	2.54791	0.02286	-0.00019	0.02112	0.02087	2.56878
R62	2.03178	0.00640	0.00005	0.00623	0.00628	2.03806
R63	2.56485	0.01252	0.00005	0.00999	0.01000	2.57485
R64	1.96059	0.03827	-0.00019	0.03962	0.03942	2.00002
R65	2.80380	-0.03555	-0.00038	-0.03989	-0.04037	2.76344
R66	2.03724	0.00481	0.00004	0.00471	0.00475	2.04199
R67	2.03917	0.00399	0.00003	0.00392	0.00395	2.04312
R68	2.84554	-0.02080	-0.00022	-0.02332	-0.02354	2.82200
R69	2.89957	-0.03682	-0.00018	-0.04362	-0.04380	2.85578
R70	2.20003	0.00788	0.00004	0.00320	0.00324	2.20326
R71	2.20886	-0.00562	0.00004	-0.00262	-0.00258	2.20628
R72	2.88058	-0.04170	-0.00020	-0.04910	-0.04930	2.83128
R73	2.82842	-0.02636	-0.00023	-0.02949	-0.02972	2.79870
R74	2.20426	-0.00393	0.00002	-0.00181	-0.00179	2.20248
R75	2.19812	0.00615	0.00008	0.00211	0.00219	2.20031
R76	2.04060	0.00874	0.00007	0.00850	0.00857	2.04917
R77	2.04497	0.00951	0.00008	0.00926	0.00933	2.05430
R78	2.04709	0.00587	0.00005	0.00578	0.00583	2.05293
R79	2.05441	0.00694	0.00006	0.00688	0.00693	2.06135
R80	2.04235	0.00784	0.00006	0.00765	0.00771	2.05006
R81	2.04333	0.00703	0.00006	0.00688	0.00694	2.05027
A1	2.03265	0.01754	-0.00033	0.02214	0.02186	2.05451
A2	1.91137	0.00132	-0.00012	0.00112	0.00096	1.91233
A3	2.33916	-0.01886	0.00045	-0.02326	-0.02283	2.31634
A4	2.13871	-0.00062	0.00020	-0.00200	-0.00175	2.13696
A5	1.94086	-0.00136	0.00009	-0.00238	-0.00236	1.93850
A6	2.20361	0.00198	-0.00029	0.00438	0.00411	2.20772
A7	2.08306	-0.00610	0.00000	-0.00799	-0.00802	2.07504
A8	2.11228	-0.00221	-0.00001	-0.00376	-0.00375	2.10852
A9	2.08784	0.00831	0.00001	0.01175	0.01178	2.09962
A10	2.08424	0.00247	-0.00006	0.00446	0.00435	2.08859
A11	2.10729	-0.00270	0.00001	-0.00431	-0.00427	2.10302
A12	2.09165	0.00022	0.00005	-0.00016	-0.00008	2.09157
A13	2.10960	0.00030	0.00008	0.00132	0.00136	2.11096
A14	2.08988	0.00151	-0.00004	0.00180	0.00178	2.09166
A15	2.08371	-0.00181	-0.00004	-0.00312	-0.00314	2.08056
A16	2.11768	-0.01357	0.00011	-0.01789	-0.01776	2.09992
A17	2.12765	0.00163	0.00005	0.00113	0.00117	2.12882
A18	2.03784	0.01195	-0.00016	0.01676	0.01659	2.05444
A19	1.83351	0.00261	-0.00024	0.00361	0.00344	1.83695
A20	2.36344	-0.04751	0.00128	-0.06283	-0.06158	2.30187
A21	2.08621	0.04490	-0.00105	0.05922	0.05813	2.14434
A22	1.89676	-0.01131	-0.00007	-0.01311	-0.01320	1.88355
A23	2.18572	0.00763	0.00007	0.00883	0.00891	2.19463
A24	2.20070	0.00369	0.00000	0.00428	0.00430	2.20499
A25	1.84060	0.00878	0.00034	0.01084	0.01124	1.85184
A26	2.20153	0.01720	-0.00018	0.02187	0.02166	2.22319
A27	2.24101	-0.02598	-0.00016	-0.03270	-0.03289	2.20812
A28	2.33889	-0.02901	-0.00015	-0.03738	-0.03753	2.30136
A29	1.98600	0.02772	0.00012	0.03817	0.03829	2.02430
A30	1.95815	0.00129	0.00003	-0.00080	-0.00077	1.95738
A31	2.37391	-0.03819	-0.00025	-0.04593	-0.04623	2.32769
A32	2.16142	-0.01897	-0.00018	-0.02239	-0.02264	2.13878
A33	1.74716	0.05720	0.00043	0.06835	0.06890	1.81606
A34	1.93043	0.01472	0.00012	0.01987	0.01996	1.95039
A35	1.83049	0.00042	-0.00002	0.00296	0.00297	1.83345

A36	2.52227	-0.01513	-0.00011	-0.02283	-0.02293	2.49934
A37	1.87673	0.01936	0.00010	0.02605	0.02642	1.90315
A38	1.98295	0.00087	0.00002	0.00243	0.00233	1.98529
A39	2.42290	-0.02022	-0.00013	-0.02844	-0.02872	2.39418
A40	1.64262	-0.03483	-0.00029	-0.04097	-0.04167	1.60095
A41	2.20138	-0.05520	-0.00036	-0.07028	-0.07055	2.13083
A42	2.05090	0.02739	0.00020	0.03473	0.03486	2.08577
A43	2.03089	0.02778	0.00016	0.03549	0.03558	2.06647
A44	1.85324	-0.00578	-0.00006	-0.00548	-0.00549	1.84774
A45	2.47862	-0.00902	-0.00008	-0.01196	-0.01207	2.46656
A46	1.95132	0.01480	0.00013	0.01744	0.01755	1.96887
A47	1.94753	0.01589	0.00015	0.01772	0.01789	1.96542
A48	1.96479	-0.00343	-0.00004	-0.00275	-0.00278	1.96201
A49	2.37078	-0.01245	-0.00010	-0.01495	-0.01509	2.35569
A50	1.77388	-0.01049	-0.00009	-0.01489	-0.01497	1.75892
A51	1.86060	0.01018	0.00007	0.01468	0.01475	1.87534
A52	1.90981	0.00298	0.00002	0.00399	0.00395	1.91376
A53	1.59622	-0.02230	-0.00018	-0.02725	-0.02747	1.56875
A54	1.59407	-0.02244	-0.00018	-0.02853	-0.02871	1.56536
A55	1.94033	0.01614	0.00014	0.01876	0.01890	1.95923
A56	2.40819	-0.01467	-0.00011	-0.01802	-0.01814	2.39005
A57	1.93359	-0.00137	-0.00003	-0.00054	-0.00057	1.93302
A58	2.34972	-0.00829	-0.00008	-0.00992	-0.01002	2.33970
A59	1.96166	-0.00470	-0.00004	-0.00509	-0.00512	1.95654
A60	1.97057	0.01305	0.00013	0.01514	0.01526	1.98583
A61	1.94482	-0.00078	-0.00003	0.00099	0.00096	1.94578
A62	2.41242	-0.01428	-0.00010	-0.01749	-0.01762	2.39480
A63	1.92589	0.01505	0.00013	0.01648	0.01665	1.94253
A64	1.96982	0.01225	0.00012	0.01436	0.01445	1.98427
A65	2.44011	-0.00525	-0.00006	-0.00710	-0.00720	2.43292
A66	1.87287	-0.00695	-0.00006	-0.00720	-0.00720	1.86567
A67	1.85043	-0.00466	-0.00003	-0.00376	-0.00380	1.84663
A68	2.48967	-0.00641	-0.00006	-0.01073	-0.01075	2.47892
A69	1.94295	0.01106	0.00009	0.01448	0.01454	1.95749
A70	1.98619	-0.00217	-0.00002	-0.00087	-0.00088	1.98530
A71	1.97016	0.00393	0.00005	0.00495	0.00492	1.97508
A72	2.32659	-0.00177	-0.00003	-0.00410	-0.00406	2.32253
A73	1.97635	-0.00796	-0.00009	-0.01011	-0.01021	1.96614
A74	2.15345	0.00397	0.00003	0.00514	0.00518	2.15862
A75	2.15327	0.00402	0.00006	0.00503	0.00509	2.15835
A76	1.90591	0.02380	0.00022	0.02670	0.02695	1.93285
A77	2.09062	-0.01498	-0.00007	-0.01753	-0.01761	2.07302
A78	2.28665	-0.00883	-0.00016	-0.00918	-0.00935	2.27730
A79	1.60857	-0.02435	-0.00021	-0.02938	-0.02960	1.57897
A80	1.78132	-0.00634	-0.00007	-0.00843	-0.00859	1.77273
A81	2.04690	0.00029	0.00002	0.00086	0.00092	2.04782
A82	1.96552	0.01085	0.00007	0.01693	0.01703	1.98255
A83	2.27183	0.00653	-0.00010	0.00922	0.00912	2.28095
A84	1.99460	-0.01677	0.00000	-0.02457	-0.02456	1.97004
A85	2.01675	0.01024	0.00009	0.01535	0.01544	2.03219
A86	2.16915	0.00116	-0.00015	0.00085	0.00068	2.16984
A87	2.24071	0.00351	-0.00022	0.00490	0.00467	2.24538
A88	1.87331	-0.00468	0.00037	-0.00575	-0.00535	1.86796
A89	1.88442	-0.00620	-0.00004	-0.00659	-0.00670	1.87772
A90	2.19627	0.00952	0.00000	0.01142	0.01146	2.20773
A91	2.20250	-0.00332	0.00004	-0.00483	-0.00476	2.19774
A92	1.79040	0.01362	-0.00025	0.01693	0.01682	1.80722
A93	2.02712	0.05155	-0.00140	0.06856	0.06710	2.09422
A94	2.46566	-0.06517	0.00165	-0.08549	-0.08392	2.38175
A95	1.96016	-0.00302	0.00011	-0.00440	-0.00440	1.95575

A96	2.16220	0.00741	-0.00036	0.01129	0.01086	2.17307
A97	2.16082	-0.00439	0.00026	-0.00688	-0.00646	2.15437
A98	1.91646	0.00027	-0.00018	-0.00018	-0.00036	1.91610
A99	2.36851	-0.02348	0.00064	-0.02909	-0.02858	2.33993
A100	1.99822	0.02320	-0.00046	0.02928	0.02894	2.02716
A101	2.08172	-0.00530	0.00003	-0.00679	-0.00677	2.07495
A102	2.10092	-0.00481	-0.00004	-0.00757	-0.00760	2.09332
A103	2.10055	0.01011	0.00001	0.01435	0.01437	2.11491
A104	2.13272	-0.01517	0.00018	-0.02034	-0.02015	2.11257
A105	2.11491	0.00044	0.00003	-0.00057	-0.00054	2.11437
A106	2.03556	0.01474	-0.00021	0.02090	0.02069	2.05625
A107	2.07730	0.00245	-0.00009	0.00478	0.00454	2.08184
A108	2.11500	0.00003	0.00005	-0.00055	-0.00043	2.11457
A109	2.09089	-0.00248	0.00004	-0.00423	-0.00411	2.08678
A110	2.11556	-0.00079	0.00009	-0.00005	-0.00010	2.11546
A111	2.08311	0.00106	-0.00002	0.00089	0.00094	2.08405
A112	2.08452	-0.00027	-0.00007	-0.00085	-0.00084	2.08368
A113	2.23205	-0.01993	-0.00087	-0.02168	-0.02255	2.20950
A114	2.61409	-0.08974	0.00120	-0.11411	-0.11291	2.50117
A115	1.43704	0.10967	-0.00033	0.13579	0.13546	1.57250
A116	2.48565	-0.06466	0.00092	-0.08239	-0.08148	2.40418
A117	2.22483	-0.00567	-0.00066	-0.00462	-0.00527	2.21956
A118	1.57265	0.07033	-0.00026	0.08702	0.08676	1.65941
A119	1.91114	-0.00115	-0.00001	-0.00183	-0.00184	1.90930
A120	1.93117	0.00527	0.00004	0.00790	0.00794	1.93911
A121	1.89810	-0.00082	-0.00001	-0.00127	-0.00129	1.89682
A122	1.91002	-0.00126	-0.00001	-0.00160	-0.00161	1.90841
A123	1.90762	-0.00126	-0.00001	-0.00243	-0.00244	1.90519
A124	1.90559	-0.00085	-0.00001	-0.00087	-0.00088	1.90471
A125	1.91431	0.00500	0.00004	0.00755	0.00760	1.92191
A126	1.92041	-0.00338	-0.00002	-0.00509	-0.00512	1.91530
A127	1.90779	-0.00204	-0.00001	-0.00309	-0.00312	1.90467
A128	1.90499	0.00011	0.00000	0.00043	0.00044	1.90542
A129	1.90619	-0.00003	0.00000	0.00035	0.00035	1.90655
A130	1.91006	0.00036	0.00000	-0.00012	-0.00014	1.90992
A131	3.24493	-0.00915	-0.00002	-0.01760	-0.01762	3.22732
A132	3.35466	-0.02047	0.00063	-0.04072	-0.04010	3.31456
A133	3.31917	-0.01022	0.00044	-0.02040	-0.01996	3.29921
A134	3.21994	-0.00022	-0.00001	-0.00017	-0.00018	3.21976
A135	3.13584	0.00019	0.00000	0.00035	0.00035	3.13618
A136	3.14446	-0.00005	0.00001	-0.00010	-0.00009	3.14437
A137	3.12425	0.00047	-0.00001	0.00090	0.00089	3.12514
A138	3.14865	-0.00038	0.00000	-0.00074	-0.00074	3.14791
D1	-0.01933	0.00030	0.00000	0.00074	0.00074	-0.01859
D2	3.12097	-0.00008	-0.00001	-0.00005	-0.00006	3.12091
D3	3.12518	0.00038	0.00000	0.00080	0.00079	3.12597
D4	-0.01771	0.00001	-0.00001	0.00000	-0.00001	-0.01771
D5	-0.00597	0.00020	0.00001	0.00044	0.00045	-0.00552
D6	-3.14151	-0.00010	0.00001	-0.00019	-0.00018	3.14150
D7	3.13180	0.00016	0.00000	0.00046	0.00046	3.13227
D8	-0.00373	-0.00013	0.00000	-0.00017	-0.00016	-0.00390
D9	0.04511	-0.00040	0.00000	-0.00078	-0.00078	0.04433
D10	-3.08822	-0.00047	0.00002	-0.00073	-0.00073	-3.08895
D11	-3.09285	-0.00039	0.00001	-0.00084	-0.00083	-3.09369
D12	0.05700	-0.00046	0.00002	-0.00079	-0.00078	0.05622
D13	0.03121	-0.00079	0.00000	-0.00165	-0.00164	0.02956
D14	-3.11487	-0.00060	0.00000	-0.00126	-0.00125	-3.11612
D15	-3.10889	-0.00036	0.00001	-0.00073	-0.00071	-3.10961
D16	0.02822	-0.00016	0.00000	-0.00033	-0.00032	0.02789
D17	-0.01862	0.00055	0.00000	0.00106	0.00105	-0.01756

D18	3.11888	0.00068	0.00001	0.00154	0.00154	3.12042
D19	3.12163	0.00015	0.00000	0.00022	0.00021	3.12184
D20	-0.02407	0.00028	0.00000	0.00070	0.00070	-0.02337
D21	-0.01700	0.00041	0.00001	0.00089	0.00090	-0.01610
D22	3.12039	0.00044	0.00000	0.00096	0.00097	3.12135
D23	3.12901	0.00025	0.00001	0.00054	0.00055	3.12957
D24	-0.01679	0.00028	0.00000	0.00061	0.00062	-0.01617
D25	-0.00758	0.00012	0.00000	0.00027	0.00027	-0.00731
D26	3.13004	0.00011	0.00000	0.00029	0.00029	3.13033
D27	3.13819	0.00010	0.00000	0.00021	0.00022	3.13840
D28	-0.00738	0.00009	0.00000	0.00023	0.00024	-0.00715
D29	0.01948	-0.00056	0.00000	-0.00111	-0.00111	0.01837
D30	-3.12788	-0.00031	-0.00001	-0.00055	-0.00055	-3.12843
D31	-3.11815	-0.00056	0.00000	-0.00114	-0.00114	-3.11929
D32	0.01768	-0.00031	0.00000	-0.00058	-0.00058	0.01710
D33	-0.05389	0.00027	-0.00001	0.00085	0.00084	-0.05305
D34	3.09640	-0.00001	0.00000	-0.00005	-0.00007	3.09633
D35	3.08104	-0.00016	-0.00001	0.00016	0.00014	3.08118
D36	-0.05186	-0.00044	0.00000	-0.00074	-0.00077	-0.05263
D37	-0.04862	0.00063	-0.00001	0.00128	0.00127	-0.04735
D38	3.10783	-0.00030	-0.00001	-0.00070	-0.00071	3.10712
D39	3.10214	0.00077	0.00000	0.00163	0.00164	3.10379
D40	-0.02459	-0.00016	0.00001	-0.00035	-0.00034	-0.02493
D41	0.04562	-0.00074	0.00001	-0.00141	-0.00140	0.04422
D42	-3.10494	-0.00014	0.00000	-0.00011	-0.00013	-3.10507
D43	-3.09183	-0.00088	0.00001	-0.00191	-0.00190	-3.09373
D44	0.04080	-0.00029	0.00000	-0.00062	-0.00064	0.04016
D45	-3.07289	-0.00285	-0.00002	-0.00617	-0.00619	-3.07909
D46	0.08838	-0.00254	-0.00002	-0.00559	-0.00560	0.08277
D47	0.07940	-0.00345	-0.00001	-0.00757	-0.00759	0.07181
D48	-3.04252	-0.00314	-0.00001	-0.00700	-0.00700	-3.04951
D49	0.07145	0.00018	0.00001	-0.00137	-0.00148	0.06997
D50	-3.02146	-0.00280	-0.00002	-0.00442	-0.00433	-3.02579
D51	-3.08959	0.00010	0.00001	-0.00161	-0.00170	-3.09129
D52	0.10069	-0.00288	-0.00002	-0.00465	-0.00456	0.09613
D53	-3.00385	-0.00056	0.00000	-0.00332	-0.00376	-3.00762
D54	0.09667	0.00101	0.00001	-0.00187	-0.00252	0.09415
D55	2.88375	0.00818	0.00004	0.01701	0.01673	2.90048
D56	-0.26319	0.00125	0.00000	0.00506	0.00517	-0.25802
D57	-0.22351	0.00779	0.00004	0.01691	0.01674	-0.20677
D58	2.91274	0.00086	0.00000	0.00497	0.00517	2.91791
D59	-0.13109	-0.00037	-0.00001	0.00236	0.00271	-0.12838
D60	2.98036	-0.00050	-0.00001	0.00271	0.00304	2.98340
D61	3.01154	0.00004	-0.00001	0.00262	0.00291	3.01444
D62	-0.16019	-0.00009	-0.00001	0.00297	0.00323	-0.15696
D63	0.02569	-0.00227	-0.00001	-0.00269	-0.00232	0.02337
D64	-3.11764	-0.00292	-0.00002	-0.00306	-0.00257	-3.12021
D65	-0.00359	0.00245	0.00002	0.00337	0.00318	-0.00041
D66	-3.14048	0.00259	0.00002	0.00493	0.00489	-3.13559
D67	3.13968	0.00306	0.00002	0.00372	0.00341	-3.14009
D68	0.00279	0.00321	0.00002	0.00528	0.00513	0.00792
D69	0.25957	-0.01386	-0.00008	-0.02429	-0.02386	0.23571
D70	-2.87674	-0.00700	-0.00004	-0.01247	-0.01242	-2.88915
D71	-2.84008	-0.01466	-0.00008	-0.02619	-0.02565	-2.86573
D72	0.30680	-0.00780	-0.00005	-0.01437	-0.01421	0.29259
D73	0.24786	-0.00373	-0.00002	-0.00986	-0.01007	0.23779
D74	-1.75167	-0.00629	-0.00003	-0.01331	-0.01332	-1.76499
D75	-2.93739	-0.00265	-0.00001	-0.00758	-0.00788	-2.94527
D76	1.34627	-0.00520	-0.00003	-0.01103	-0.01113	1.33514
D77	0.16120	-0.00257	-0.00001	-0.00679	-0.00682	0.15438

D78	-2.99242	-0.00217	-0.00001	-0.00531	-0.00530	-2.99772
D79	-2.98351	-0.00272	-0.00001	-0.00790	-0.00806	-2.99156
D80	0.14606	-0.00232	-0.00001	-0.00642	-0.00654	0.13952
D81	3.03443	0.00307	0.00002	0.00527	0.00511	3.03954
D82	-0.10230	0.00326	0.00002	0.00693	0.00695	-0.09535
D83	-0.24510	0.00294	0.00001	0.00965	0.00973	-0.23536
D84	1.71764	0.01057	0.00005	0.02065	0.02071	1.73835
D85	2.91244	0.00222	0.00001	0.00747	0.00752	2.91996
D86	-1.40801	0.00985	0.00005	0.01847	0.01849	-1.38951
D87	3.07008	0.00194	0.00001	0.00374	0.00372	3.07380
D88	-0.13018	0.00385	0.00002	0.00733	0.00730	-0.12288
D89	-0.08757	0.00279	0.00001	0.00607	0.00607	-0.08151
D90	2.99535	0.00470	0.00003	0.00966	0.00964	3.00500
D91	0.94374	-0.00273	-0.00003	-0.00378	-0.00380	0.93993
D92	3.03952	-0.00156	-0.00002	-0.00168	-0.00171	3.03781
D93	-1.14573	-0.00447	-0.00004	-0.00691	-0.00694	-1.15266
D94	-0.96159	0.00315	0.00003	0.00456	0.00458	-0.95701
D95	1.13419	0.00432	0.00004	0.00666	0.00668	1.14087
D96	-3.05105	0.00141	0.00002	0.00143	0.00145	-3.04961
D97	0.02475	-0.00096	-0.00001	-0.00241	-0.00245	0.02230
D98	3.10970	0.00192	0.00001	0.00318	0.00313	3.11282
D99	3.11597	0.00051	0.00000	0.00108	0.00109	3.11706
D100	0.03326	-0.00096	-0.00001	-0.00202	-0.00202	0.03124
D101	-0.11507	0.00421	0.00002	0.00808	0.00803	-0.10704
D102	2.99122	0.00607	0.00003	0.01087	0.01081	3.00203
D103	0.04934	-0.00008	0.00000	-0.00061	-0.00059	0.04875
D104	-3.13756	0.00077	0.00000	0.00143	0.00147	-3.13609
D105	-3.05170	-0.00150	-0.00001	-0.00381	-0.00386	-3.05556
D106	0.04458	-0.00065	0.00000	-0.00177	-0.00180	0.04278
D107	3.06660	0.00134	0.00001	0.00255	0.00257	3.06917
D108	-0.08811	0.00016	0.00000	0.00070	0.00073	-0.08739
D109	-0.13150	0.00460	0.00003	0.00855	0.00853	-0.12297
D110	2.99697	0.00342	0.00002	0.00671	0.00668	3.00366
D111	0.15666	-0.00332	-0.00002	-0.00770	-0.00781	0.14885
D112	-2.96108	-0.00448	-0.00002	-0.00944	-0.00955	-2.97062
D113	-2.97561	-0.00229	-0.00001	-0.00615	-0.00622	-2.98183
D114	0.18984	-0.00344	-0.00001	-0.00789	-0.00796	0.18188
D115	2.94609	0.00512	0.00003	0.01013	0.01015	2.95625
D116	0.78978	-0.00405	-0.00002	-0.00555	-0.00556	0.78421
D117	-0.20853	0.00388	0.00002	0.00822	0.00824	-0.20029
D118	-2.36484	-0.00530	-0.00003	-0.00745	-0.00748	-2.37232
D119	3.08396	0.00249	0.00001	0.00503	0.00500	3.08896
D120	-0.07841	0.00212	0.00001	0.00424	0.00421	-0.07420
D121	-0.09170	0.00453	0.00003	0.00801	0.00795	-0.08376
D122	3.02911	0.00416	0.00002	0.00722	0.00716	3.03627
D123	3.11714	0.00004	0.00000	-0.00002	-0.00005	3.11709
D124	-0.04534	-0.00011	0.00000	-0.00074	-0.00077	-0.04611
D125	-0.01092	0.00045	0.00000	0.00076	0.00074	-0.01018
D126	3.10978	0.00031	0.00000	0.00004	0.00003	3.10981
D127	3.12547	0.00215	0.00001	0.00443	0.00445	3.12992
D128	-0.03756	0.00165	0.00001	0.00347	0.00348	-0.03408
D129	0.07459	-0.00372	-0.00002	-0.00718	-0.00712	0.06747
D130	-3.08351	-0.00174	-0.00001	-0.00314	-0.00308	-3.08659
D131	-3.04056	-0.00362	-0.00002	-0.00642	-0.00637	-3.04693
D132	0.08453	-0.00165	-0.00001	-0.00238	-0.00233	0.08220
D133	0.15050	-0.00225	-0.00001	-0.00418	-0.00422	0.14628
D134	2.36071	0.00005	0.00000	0.00092	0.00088	2.36160
D135	-3.01736	-0.00242	-0.00001	-0.00499	-0.00502	-3.02238
D136	-0.80714	-0.00012	0.00000	0.00010	0.00008	-0.80707
D137	-0.09787	0.00299	0.00001	0.00742	0.00750	-0.09037

D138	3.04072	0.00248	0.00001	0.00580	0.00584	3.04656
D139	3.06022	0.00101	0.00000	0.00338	0.00346	3.06369
D140	-0.08437	0.00051	0.00000	0.00175	0.00180	-0.08257
D141	0.07867	-0.00294	-0.00001	-0.00672	-0.00673	0.07194
D142	-3.05947	-0.00236	-0.00001	-0.00484	-0.00481	-3.06428
D143	3.07877	0.00069	0.00000	0.00185	0.00185	3.08062
D144	-0.05762	0.00018	0.00000	0.00076	0.00077	-0.05686
D145	-0.06657	0.00011	0.00000	-0.00012	-0.00013	-0.06670
D146	3.08021	-0.00039	0.00000	-0.00121	-0.00121	3.07900
D147	-1.07534	-0.00096	-0.00002	-0.00057	-0.00058	-1.07591
D148	1.03144	0.00008	-0.00002	0.00128	0.00127	1.03271
D149	3.12440	0.00173	0.00000	0.00421	0.00422	3.12862
D150	-3.13488	-0.00135	0.00001	-0.00346	-0.00346	-3.13835
D151	-1.02811	-0.00031	0.00001	-0.00162	-0.00161	-1.02972
D152	1.06485	0.00134	0.00003	0.00132	0.00133	1.06618
D153	-0.00466	-0.00057	0.00000	-0.00126	-0.00126	-0.00592
D154	-3.13991	-0.00064	0.00000	-0.00142	-0.00143	-3.14134
D155	3.13169	-0.00013	0.00000	-0.00025	-0.00025	3.13144
D156	-0.00357	-0.00019	0.00000	-0.00042	-0.00041	-0.00398
D157	-3.13963	-0.00004	0.00000	-0.00018	-0.00018	-3.13981
D158	0.00066	-0.00011	0.00000	-0.00027	-0.00027	0.00039
D159	-0.00324	0.00003	0.00000	-0.00001	-0.00002	-0.00326
D160	3.13705	-0.00003	0.00000	-0.00011	-0.00011	3.13694
D161	-3.14051	0.00008	0.00000	0.00018	0.00018	-3.14032
D162	0.00299	0.00024	0.00000	0.00042	0.00041	0.00341
D163	0.00657	0.00001	0.00000	0.00002	0.00003	0.00660
D164	-3.13311	0.00017	0.00000	0.00026	0.00026	-3.13285
D165	-0.00214	0.00006	0.00000	0.00015	0.00015	-0.00199
D166	3.13883	0.00007	0.00000	0.00016	0.00017	3.13899
D167	3.14077	0.00012	0.00000	0.00023	0.00023	3.14099
D168	-0.00146	0.00012	0.00000	0.00025	0.00024	-0.00121
D169	-0.00807	0.00002	0.00000	0.00005	0.00005	-0.00802
D170	3.13264	0.00006	-0.00001	0.00017	0.00016	3.13280
D171	3.13078	0.00008	-0.00001	0.00010	0.00010	3.13088
D172	-0.01170	0.00012	-0.00001	0.00022	0.00021	-0.01149
D173	0.00058	0.00011	0.00000	0.00023	0.00022	0.00081
D174	3.13661	0.00009	-0.00001	0.00018	0.00017	3.13678
D175	-3.13803	0.00011	0.00000	0.00026	0.00026	-3.13777
D176	-0.00200	0.00009	-0.00001	0.00021	0.00021	-0.00179
D177	0.00662	-0.00007	0.00000	-0.00015	-0.00015	0.00647
D178	-3.13429	-0.00008	0.00000	-0.00022	-0.00021	-3.13451
D179	-3.13435	-0.00008	0.00000	-0.00018	-0.00018	-3.13452
D180	0.00793	-0.00009	0.00000	-0.00024	-0.00024	0.00769
D181	3.13598	0.00015	0.00000	0.00028	0.00028	3.13626
D182	-0.00533	0.00011	0.00000	0.00021	0.00021	-0.00512
D183	-0.00631	0.00016	0.00000	0.00030	0.00030	-0.00602
D184	3.13556	0.00011	0.00000	0.00023	0.00023	3.13579
D185	3.13866	0.00003	0.00000	0.00004	0.00004	3.13870
D186	-0.00405	0.00004	0.00000	0.00007	0.00006	-0.00398
D187	-0.00385	0.00007	0.00000	0.00014	0.00014	-0.00371
D188	3.13663	0.00007	-0.00001	0.00018	0.00017	3.13680
D189	-0.00001	0.00002	0.00000	0.00002	0.00002	0.00000
D190	-3.14084	-0.00003	0.00000	-0.00008	-0.00008	-3.14091
D191	3.14130	0.00006	0.00000	0.00009	0.00009	3.14138
D192	0.00047	0.00000	0.00000	-0.00001	-0.00001	0.00046
D193	-0.00193	0.00001	0.00000	0.00004	0.00005	-0.00189
D194	3.13919	0.00002	0.00000	0.00005	0.00005	3.13924
D195	3.14073	0.00002	0.00000	0.00002	0.00003	3.14076
D196	-0.00133	0.00002	0.00000	0.00003	0.00003	-0.00130
D197	0.00389	-0.00006	0.00000	-0.00013	-0.00013	0.00377

D198	-3.13723	-0.00007	0.00000	-0.00013	-0.00013	-3.13736
D199	-3.13846	-0.00001	0.00000	-0.00003	-0.00003	-3.13849
D200	0.00360	-0.00001	0.00000	-0.00004	-0.00004	0.00357

Item	Value	Threshold	Converged?

Maximum Force	0.109675	0.000450	NO

RMS Force	0.020059	0.000300	NO

Maximum Displacement	1.203345	0.001800	NO

RMS Displacement	0.241195	0.001200	NO

Predicted change in Energy=-1.765174D-01

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-11.278091	-0.519789	-0.272211
2	6	0	-10.488070	-1.673585	-0.168438
3	6	0	-11.037744	-2.960538	-0.148814
4	6	0	-12.420360	-3.105135	-0.271577
5	6	0	-13.227572	-1.968648	-0.391518
6	6	0	-12.670783	-0.687955	-0.381615
7	1	0	-10.406718	-3.829412	-0.044567
8	1	0	-12.871234	-4.089090	-0.278459
9	1	0	-14.299384	-2.077892	-0.497427
10	1	0	-13.333317	0.140051	-0.463898
11	6	0	-10.365761	0.741092	-0.243335
12	6	0	-9.019906	-1.321589	-0.088229
13	6	0	-8.896592	0.186831	-0.173635
14	6	0	-7.726631	0.914975	-0.178224
15	6	0	-6.238025	0.481208	-0.186427
16	6	0	-3.748135	-0.398739	0.035880
17	6	0	-3.844511	0.949002	0.229755
18	16	0	-5.394448	-1.161634	-0.287509
19	6	0	-5.210535	1.374746	-0.056787
20	6	0	-2.253057	-0.715766	0.177088
21	6	0	-1.641368	0.477068	0.436557
22	7	0	-2.606174	1.566020	0.694121
23	16	0	-1.097286	-2.090756	0.106576
24	16	0	1.196390	1.553172	0.572272
25	6	0	0.284372	-0.933398	0.279437
26	6	0	-0.140327	0.370644	0.407264
27	6	0	1.807525	-1.018852	0.375203
28	6	0	2.378554	0.225173	0.407349
29	6	0	3.865738	0.028741	0.255242
30	6	0	4.063019	-1.313652	0.254679
31	6	0	5.482968	-1.709158	0.079074
32	6	0	6.337135	-0.622318	0.035686
33	16	0	5.398050	0.937180	0.058061
34	7	0	2.827975	-2.078387	0.457319
35	6	0	7.861376	-0.875323	-0.015255
36	6	0	8.910965	0.002264	-0.126503
37	6	0	8.761379	1.486821	-0.234553
38	6	0	10.453584	-0.310413	-0.174270

39	6	0	10.130231	2.071418	-0.339083
40	6	0	11.110202	1.103561	-0.304400
41	6	0	10.413313	3.500544	-0.464786
42	6	0	12.497486	1.582691	-0.391995
43	6	0	11.707304	3.909007	-0.545753
44	6	0	12.776008	2.911672	-0.505046
45	6	0	10.900851	-1.632427	-0.103328
46	6	0	10.051133	-2.854441	0.018021
47	6	0	12.143026	-2.493101	-0.104226
48	7	0	9.472263	-3.862056	0.112800
49	7	0	12.974335	-3.312701	-0.088044
50	6	0	-10.658478	2.095531	-0.259806
51	6	0	-11.873793	2.966404	-0.356436
52	6	0	-9.697042	3.219739	-0.187837
53	7	0	-12.701665	3.784574	-0.416578
54	7	0	-9.012863	4.159864	-0.126346
55	8	0	-8.102261	-2.116093	0.028708
56	8	0	7.712374	2.112984	-0.238704
57	6	0	2.687548	-3.226081	-0.457975
58	1	0	1.754400	-3.738683	-0.252217
59	1	0	2.699550	-2.902776	-1.495807
60	1	0	3.514729	-3.909597	-0.288394
61	6	0	-2.738156	1.782451	2.166188
62	1	0	-3.004181	0.847184	2.660545
63	1	0	-1.797888	2.143548	2.569173
64	1	0	-3.515203	2.517169	2.349276
65	1	0	5.814256	-2.733900	0.005564
66	1	0	13.312263	0.907627	-0.368384
67	1	0	13.805947	3.234975	-0.565345
68	1	0	11.958304	4.955895	-0.638825
69	1	0	9.601266	4.209773	-0.491603
70	1	0	8.114677	-1.921074	0.044866
71	1	0	-7.837678	1.989063	-0.156124
72	1	0	-5.403747	2.429379	-0.183891

Rotational constants (GHZ): 0.1515736 0.0097780 0.0092347

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6384.7806520586 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T
Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6384.6985704157 Hartrees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.51D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Initial guess from the checkpoint file: "PBDB.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999952 0.009609 0.000064 -0.001848 Ang= 1.12 deg.

ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1

AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

```

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-
yADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2001
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 IlCent= 200000004 NGrid=
0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0=
0

```

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Integral accuracy reduced to 1.0D-05 until final iterations.

Initial convergence to 1.0D-05 achieved. Increase integral accuracy.

SCF Done: E(RB3LYP) = -3682.78836493 A.U. after 15 cycles

NFock= 15 Conv=0.73D-08 -V/T= 2.0077

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1

NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-0.004999199	-0.025300830	-0.003125988
2	6	0.012160950	-0.010121173	0.004620007
3	6	-0.004506420	-0.003703570	-0.002026430
4	6	0.000419370	-0.004871554	0.000040451
5	6	0.003212797	-0.004357257	0.001728495
6	6	0.006059615	-0.005838765	0.003369196
7	1	0.004349362	-0.002222829	0.002983704
8	1	0.0011110577	0.001870661	0.000357741
9	1	-0.001349705	0.000782047	-0.001309263
10	1	-0.012958348	-0.008510270	-0.007239063
11	6	0.021084382	0.002191995	0.011385452
12	6	-0.012089157	-0.003544428	-0.004348279
13	6	-0.017734167	0.014480661	-0.011071021
14	6	0.037228038	0.003625251	0.031416446
15	6	-0.003428916	0.024487077	-0.002037464
16	6	0.025580748	0.019877731	0.021272147
17	6	-0.026892550	0.017730667	-0.008129822
18	16	0.011027572	-0.014835112	-0.004916663
19	6	0.005228968	-0.053508306	-0.021435085
20	6	-0.017680556	0.030645207	-0.004988580
21	6	0.013537619	-0.034209054	0.000493378
22	7	-0.002044175	0.017111917	0.026256538
23	16	-0.008827379	-0.015940108	-0.001552839
24	16	0.002281577	0.010700615	0.008528569
25	6	0.037738783	-0.006187903	0.015234808
26	6	-0.026211071	0.006539955	-0.030512202
27	6	-0.003547911	0.043506745	-0.002005370
28	6	0.012631626	-0.030638999	0.011938418
29	6	-0.028355949	-0.011540560	-0.026129658
30	6	0.039460920	0.025044024	0.024675932
31	6	-0.026956901	0.017812570	-0.030705696
32	6	0.023485257	-0.017567317	0.021188493
33	16	0.004141130	0.016358604	-0.006148808
34	7	-0.035964538	-0.034439387	0.008741034
35	6	-0.041534354	0.001804663	-0.023745370

36	6	0.015375573	-0.014254795	0.010630903
37	6	0.011343213	0.001347321	0.007523517
38	6	-0.017567156	0.008728898	-0.012869564
39	6	-0.028557060	-0.022657036	-0.016104665
40	6	0.030517948	-0.001949432	0.019902194
41	6	0.011073351	0.042569863	0.003263262
42	6	-0.012446469	0.044847335	-0.011486092
43	6	0.035052547	-0.002906805	0.022655019
44	6	-0.034508035	-0.011254664	-0.021196036
45	6	0.030085393	0.031508038	0.017599247
46	6	-0.023607828	-0.021600001	-0.014030359
47	6	-0.027978786	-0.038256285	-0.015501317
48	7	-0.000882991	-0.000417248	-0.000420042
49	7	-0.004593536	-0.005458188	-0.002568425
50	6	-0.028035415	-0.029823659	-0.016780031
51	6	0.026889016	0.030342458	0.016177573
52	6	0.016987948	0.024730861	0.011156415
53	7	0.001389488	0.004221497	0.001438703
54	7	0.000745319	-0.001677369	0.000517036
55	8	-0.001067474	0.000479077	0.001242240
56	8	0.000016875	-0.004679788	0.000644473
57	6	0.000690139	-0.002026852	-0.007122837
58	1	-0.000256974	0.005222519	-0.002118520
59	1	-0.003765973	0.000021943	0.004961912
60	1	0.003579842	0.001731860	0.000662263
61	6	-0.002184310	-0.005445938	0.004386301
62	1	0.002619126	0.003119076	-0.002142658
63	1	0.001989786	-0.004876594	0.000586385
64	1	-0.003502723	-0.001890103	-0.002390724
65	1	0.004100916	0.000747610	-0.000201833
66	1	0.017217249	0.006463137	0.010562338
67	1	0.000820221	-0.002474378	0.000802338
68	1	-0.000668489	-0.003093834	-0.000169973
69	1	-0.003614874	0.004256191	-0.002795646
70	1	-0.003104214	0.007446519	-0.002396757
71	1	0.002640156	-0.006703221	0.003605984
72	1	-0.002449795	-0.003570975	-0.010825834

Cartesian Forces: Max 0.053508306 RMS 0.016618955

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.072839885 RMS 0.014348228

Search for a local minimum.

Step number 6 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 5 6

DE= -1.78D-01 DEPred=-1.77D-01 R= 1.01D+00

TightC=F SS= 1.41D+00 RLast= 5.10D-01 DXNew= 8.4853D-01 1.5311D+00

Trust test= 1.01D+00 RLast= 5.10D-01 DXMaxT set to 8.49D-01

ITU= 1 0 0 0 1 0

Use linear search instead of GDIIS.

Linear search step of 1.009 exceeds DXMaxT= 0.849 but not scaled.

Quartic linear search produced a step of 2.00000.

Iteration 1 RMS(Cart)= 0.42281981 RMS(Int)= 0.01982903

Iteration 2 RMS(Cart)= 0.08565516 RMS(Int)= 0.00139524

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Iteration 3 RMS(Cart)= 0.00257363 RMS(Int)= 0.00052051
Iteration 4 RMS(Cart)= 0.00000761 RMS(Int)= 0.00052050
Iteration 5 RMS(Cart)= 0.00000000 RMS(Int)= 0.00052050
Variable      Old X      -DE/DX      Delta X      Delta X      Delta X      New X
(Linear)      (Quad)      (Total)
R1            2.64976    -0.00384    -0.01577     0.00000     -0.01584     2.63392
R2            2.65897    -0.01106    -0.03443     0.00000     -0.03427     2.62470
R3            2.94155    -0.04713    -0.14176     0.00000     -0.14166     2.79988
R4            2.64479    -0.01032    -0.03660     0.00000     -0.03659     2.60820
R5            2.85708    -0.01917    -0.07637     0.00000     -0.07662     2.78045
R6            2.63724     0.00029     0.00119     0.00000     0.00104     2.63828
R7            2.03881     0.00430     0.01329     0.00000     0.01329     2.05209
R8            2.64398     0.00537     0.01997     0.00000     0.01981     2.66379
R9            2.04536     0.00205     0.00638     0.00000     0.00638     2.05174
R10           2.63905    -0.00112    -0.00640     0.00000    -0.00642     2.63264
R11           2.04574     0.00185     0.00574     0.00000     0.00574     2.05147
R12           2.00998     0.01657     0.06182     0.00000     0.06182     2.07180
R13           2.97025    -0.03997    -0.11013     0.00000    -0.10984     2.86041
R14           2.61879    -0.03485    -0.09996     0.00000    -0.09996     2.51884
R15           2.86456    -0.01625    -0.06448     0.00000    -0.06441     2.80015
R16           2.30437    -0.00031    -0.00818     0.00000    -0.00818     2.29619
R17           2.60414    -0.02488    -0.13584     0.00000    -0.13584     2.46830
R18           2.93009    -0.07149    -0.27398     0.00000    -0.27398     2.65611
R19           2.04098     0.00214    -0.00348     0.00000    -0.00348     2.03750
R20           3.49511    -0.01360    -0.03566     0.00000    -0.03615     3.45896
R21           2.58482     0.00590    -0.00885     0.00000    -0.00811     2.57671
R22           2.57951     0.02079     0.04288     0.00000     0.04296     2.62247
R23           3.48291    -0.04046    -0.12805     0.00000    -0.12887     3.35404
R24           2.90041    -0.05208    -0.17213     0.00000    -0.17200     2.72841
R25           2.75757    -0.04101    -0.13702     0.00000    -0.13622     2.62135
R26           2.75785    -0.01938    -0.06735     0.00000    -0.06736     2.69050
R27           2.04032     0.00740     0.02631     0.00000     0.02631     2.06664
R28           2.58025     0.00988     0.00963     0.00000     0.00986     2.59011
R29           3.39698    -0.01998    -0.06545     0.00000    -0.06553     3.33145
R30           2.79207    -0.02661    -0.08501     0.00000    -0.08518     2.70689
R31           2.84422    -0.05379    -0.19168     0.00000    -0.19160     2.65261
R32           2.82275    -0.00038    -0.00120     0.00000    -0.00120     2.82155
R33           3.42157    -0.01951    -0.06570     0.00000    -0.06576     3.35581
R34           3.38699    -0.01462    -0.05006     0.00000    -0.05005     3.33695
R35           3.37426    -0.01524    -0.05161     0.00000    -0.05163     3.32262
R36           2.60291     0.00706     0.00508     0.00000     0.00514     2.60805
R37           2.88854    -0.06037    -0.21466     0.00000    -0.21467     2.67388
R38           2.58741     0.00994     0.01040     0.00000     0.01076     2.59817
R39           2.78417    -0.03849    -0.12535     0.00000    -0.12536     2.65882
R40           2.84931    -0.04854    -0.16392     0.00000    -0.16374     2.68557
R41           2.56400     0.02054     0.03669     0.00000     0.03635     2.60035
R42           3.38684    -0.02326    -0.07348     0.00000    -0.07354     3.31331
R43           2.80516    -0.05044    -0.17692     0.00000    -0.17695     2.62820
R44           2.77167    -0.03009    -0.10169     0.00000    -0.10199     2.66968
R45           2.61350    -0.00058    -0.02634     0.00000    -0.02623     2.58727
R46           2.03990     0.00292     0.00928     0.00000     0.00928     2.04918
R47           3.44035    -0.01276    -0.04626     0.00000    -0.04617     3.39418
R48           2.92140    -0.05900    -0.21753     0.00000    -0.21753     2.70386
R49           2.78674     0.00068     0.00299     0.00000     0.00299     2.78974
R50           2.59393    -0.01153    -0.06222     0.00000    -0.06222     2.53172
R51           2.03650     0.00186    -0.00155     0.00000    -0.00155     2.03495
R52           2.82699    -0.00583    -0.02343     0.00000    -0.02366     2.80333
R53           2.97578    -0.03339    -0.09123     0.00000    -0.09098     2.88480
R54           2.81971    -0.01154    -0.04931     0.00000    -0.04970     2.77001
R55           2.30865    -0.00079    -0.00591     0.00000    -0.00591     2.30274

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R56	2.95632	-0.05038	-0.14207	0.00000	-0.14169	2.81463
R57	2.64075	-0.04493	-0.12889	0.00000	-0.12889	2.51187
R58	2.60364	0.00070	-0.01588	0.00000	-0.01528	2.58836
R59	2.76336	-0.04168	-0.13649	0.00000	-0.13618	2.62718
R60	2.77847	-0.04031	-0.12214	0.00000	-0.12181	2.65666
R61	2.56878	0.01747	0.04175	0.00000	0.04142	2.61020
R62	2.03806	0.00415	0.01255	0.00000	0.01255	2.05061
R63	2.57485	0.01345	0.01999	0.00000	0.01969	2.59453
R64	2.00002	0.02057	0.07884	0.00000	0.07884	2.07886
R65	2.76344	-0.02676	-0.08073	0.00000	-0.08136	2.68208
R66	2.04199	0.00312	0.00950	0.00000	0.00950	2.05149
R67	2.04312	0.00267	0.00791	0.00000	0.00791	2.05103
R68	2.82200	-0.02265	-0.04708	0.00000	-0.04708	2.77493
R69	2.85578	-0.03614	-0.08759	0.00000	-0.08759	2.76818
R70	2.20326	-0.00053	0.00647	0.00000	0.00647	2.20973
R71	2.20628	-0.00601	-0.00517	0.00000	-0.00517	2.20111
R72	2.83128	-0.03310	-0.09861	0.00000	-0.09861	2.73267
R73	2.79870	-0.02125	-0.05944	0.00000	-0.05944	2.73926
R74	2.20248	-0.00255	-0.00357	0.00000	-0.00357	2.19890
R75	2.20031	0.00167	0.00439	0.00000	0.00439	2.20469
R76	2.04917	0.00552	0.01713	0.00000	0.01713	2.06630
R77	2.05430	0.00597	0.01867	0.00000	0.01867	2.07297
R78	2.05293	0.00363	0.01166	0.00000	0.01166	2.06459
R79	2.06135	0.00436	0.01387	0.00000	0.01387	2.07521
R80	2.05006	0.00501	0.01543	0.00000	0.01543	2.06549
R81	2.05027	0.00439	0.01388	0.00000	0.01388	2.06415
A1	2.05451	0.01226	0.04373	0.00000	0.04406	2.09857
A2	1.91233	0.00003	0.00192	0.00000	0.00169	1.91402
A3	2.31634	-0.01229	-0.04565	0.00000	-0.04575	2.27059
A4	2.13696	-0.00117	-0.00349	0.00000	-0.00316	2.13380
A5	1.93850	-0.00368	-0.00473	0.00000	-0.00520	1.93330
A6	2.20772	0.00484	0.00822	0.00000	0.00836	2.21608
A7	2.07504	-0.00429	-0.01605	0.00000	-0.01624	2.05880
A8	2.10852	-0.00165	-0.00751	0.00000	-0.00741	2.10111
A9	2.09962	0.00593	0.02356	0.00000	0.02365	2.12327
A10	2.08859	0.00223	0.00869	0.00000	0.00832	2.09691
A11	2.10302	-0.00190	-0.00853	0.00000	-0.00835	2.09467
A12	2.09157	-0.00033	-0.00016	0.00000	0.00003	2.09160
A13	2.11096	0.00056	0.00272	0.00000	0.00251	2.11347
A14	2.09166	0.00036	0.00356	0.00000	0.00367	2.09533
A15	2.08056	-0.00092	-0.00629	0.00000	-0.00618	2.07438
A16	2.09992	-0.00958	-0.03552	0.00000	-0.03541	2.06451
A17	2.12882	0.00049	0.00234	0.00000	0.00228	2.13110
A18	2.05444	0.00908	0.03319	0.00000	0.03313	2.08757
A19	1.83695	0.00696	0.00688	0.00000	0.00731	1.84426
A20	2.30187	-0.03182	-0.12315	0.00000	-0.12336	2.17850
A21	2.14434	0.02486	0.11627	0.00000	0.11605	2.26039
A22	1.88355	-0.00796	-0.02641	0.00000	-0.02653	1.85702
A23	2.19463	0.00339	0.01782	0.00000	0.01788	2.21251
A24	2.20499	0.00457	0.00859	0.00000	0.00865	2.21365
A25	1.85184	0.00469	0.02248	0.00000	0.02288	1.87472
A26	2.22319	0.00246	0.04332	0.00000	0.04312	2.26632
A27	2.20812	-0.00714	-0.06579	0.00000	-0.06599	2.14213
A28	2.30136	-0.01138	-0.07506	0.00000	-0.07506	2.22629
A29	2.02430	0.01348	0.07658	0.00000	0.07658	2.10088
A30	1.95738	-0.00210	-0.00154	0.00000	-0.00154	1.95584
A31	2.32769	-0.02419	-0.09246	0.00000	-0.09267	2.23501
A32	2.13878	-0.01202	-0.04528	0.00000	-0.04558	2.09319
A33	1.81606	0.03624	0.13780	0.00000	0.13829	1.95435
A34	1.95039	0.00865	0.03992	0.00000	0.03970	1.99009

A35	1.83345	0.00135	0.00594	0.00000	0.00605	1.83951
A36	2.49934	-0.01000	-0.04586	0.00000	-0.04576	2.45359
A37	1.90315	0.01495	0.05284	0.00000	0.05417	1.95732
A38	1.98529	-0.00107	0.00466	0.00000	0.00399	1.98928
A39	2.39418	-0.01386	-0.05743	0.00000	-0.05810	2.33608
A40	1.60095	-0.01901	-0.08334	0.00000	-0.08569	1.51527
A41	2.13083	-0.03941	-0.14110	0.00000	-0.14046	1.99037
A42	2.08577	0.01820	0.06973	0.00000	0.06931	2.15507
A43	2.06647	0.02112	0.07115	0.00000	0.07064	2.13710
A44	1.84774	-0.00180	-0.01098	0.00000	-0.01071	1.83703
A45	2.46656	-0.00519	-0.02413	0.00000	-0.02430	2.44226
A46	1.96887	0.00698	0.03510	0.00000	0.03499	2.00386
A47	1.96542	0.00807	0.03578	0.00000	0.03591	2.00133
A48	1.96201	-0.00105	-0.00555	0.00000	-0.00548	1.95654
A49	2.35569	-0.00701	-0.03018	0.00000	-0.03040	2.32529
A50	1.75892	-0.00543	-0.02993	0.00000	-0.02989	1.72903
A51	1.87534	0.00739	0.02949	0.00000	0.02948	1.90483
A52	1.91376	0.00179	0.00790	0.00000	0.00768	1.92145
A53	1.56875	-0.01143	-0.05493	0.00000	-0.05517	1.51358
A54	1.56536	-0.01198	-0.05742	0.00000	-0.05742	1.50794
A55	1.95923	0.00815	0.03779	0.00000	0.03778	1.99701
A56	2.39005	-0.00915	-0.03628	0.00000	-0.03634	2.35371
A57	1.93302	0.00108	-0.00114	0.00000	-0.00112	1.93191
A58	2.33970	-0.00324	-0.02003	0.00000	-0.02013	2.31958
A59	1.95654	-0.00219	-0.01023	0.00000	-0.01012	1.94642
A60	1.98583	0.00548	0.03052	0.00000	0.03048	2.01631
A61	1.94578	0.00095	0.00191	0.00000	0.00184	1.94762
A62	2.39480	-0.00932	-0.03524	0.00000	-0.03542	2.35938
A63	1.94253	0.00837	0.03329	0.00000	0.03353	1.97607
A64	1.98427	0.00508	0.02891	0.00000	0.02873	2.01300
A65	2.43292	-0.00126	-0.01439	0.00000	-0.01461	2.41831
A66	1.86567	-0.00380	-0.01440	0.00000	-0.01402	1.85165
A67	1.84663	-0.00228	-0.00759	0.00000	-0.00759	1.83904
A68	2.47892	-0.00349	-0.02151	0.00000	-0.02132	2.45760
A69	1.95749	0.00577	0.02907	0.00000	0.02888	1.98637
A70	1.98530	-0.00133	-0.00176	0.00000	-0.00173	1.98357
A71	1.97508	-0.00001	0.00985	0.00000	0.00942	1.98451
A72	2.32253	0.00133	-0.00812	0.00000	-0.00773	2.31480
A73	1.96614	-0.00360	-0.02042	0.00000	-0.02048	1.94565
A74	2.15862	0.00295	0.01035	0.00000	0.01036	2.16899
A75	2.15835	0.00067	0.01018	0.00000	0.01018	2.16854
A76	1.93285	0.01159	0.05390	0.00000	0.05400	1.98686
A77	2.07302	-0.00911	-0.03521	0.00000	-0.03527	2.03775
A78	2.27730	-0.00248	-0.01870	0.00000	-0.01876	2.25855
A79	1.57897	-0.01210	-0.05920	0.00000	-0.05930	1.51968
A80	1.77273	-0.00131	-0.01718	0.00000	-0.01765	1.75507
A81	2.04782	-0.00085	0.00185	0.00000	0.00214	2.04996
A82	1.98255	0.00787	0.03405	0.00000	0.03417	2.01672
A83	2.28095	0.01310	0.01825	0.00000	0.01825	2.29920
A84	1.97004	-0.01490	-0.04913	0.00000	-0.04913	1.92091
A85	2.03219	0.00181	0.03089	0.00000	0.03089	2.06308
A86	2.16984	0.00958	0.00137	0.00000	0.00126	2.17110
A87	2.24538	-0.00598	0.00934	0.00000	0.00923	2.25461
A88	1.86796	-0.00359	-0.01070	0.00000	-0.01049	1.85747
A89	1.87772	-0.00469	-0.01341	0.00000	-0.01382	1.86390
A90	2.20773	0.00772	0.02292	0.00000	0.02313	2.23085
A91	2.19774	-0.00303	-0.00951	0.00000	-0.00931	2.18843
A92	1.80722	0.01431	0.03364	0.00000	0.03447	1.84168
A93	2.09422	0.03468	0.13419	0.00000	0.13378	2.22800
A94	2.38175	-0.04899	-0.16783	0.00000	-0.16825	2.21350

A95	1.95575	-0.00557	-0.00881	0.00000	-0.00946	1.94629
A96	2.17307	0.00919	0.02172	0.00000	0.02134	2.19441
A97	2.15437	-0.00361	-0.01291	0.00000	-0.01188	2.14249
A98	1.91610	-0.00046	-0.00072	0.00000	-0.00069	1.91541
A99	2.33993	-0.01664	-0.05717	0.00000	-0.05792	2.28200
A100	2.02716	0.01710	0.05788	0.00000	0.05861	2.08578
A101	2.07495	-0.00403	-0.01353	0.00000	-0.01353	2.06142
A102	2.09332	-0.00274	-0.01520	0.00000	-0.01520	2.07812
A103	2.11491	0.00677	0.02874	0.00000	0.02874	2.14365
A104	2.11257	-0.01148	-0.04031	0.00000	-0.04025	2.07231
A105	2.11437	0.00057	-0.00108	0.00000	-0.00111	2.11326
A106	2.05625	0.01091	0.04139	0.00000	0.04136	2.09761
A107	2.08184	0.00247	0.00908	0.00000	0.00815	2.08999
A108	2.11457	-0.00064	-0.00086	0.00000	-0.00039	2.11417
A109	2.08678	-0.00183	-0.00822	0.00000	-0.00776	2.07902
A110	2.11546	-0.00044	-0.00020	0.00000	-0.00110	2.11436
A111	2.08405	0.00080	0.00188	0.00000	0.00233	2.08638
A112	2.08368	-0.00037	-0.00168	0.00000	-0.00123	2.08245
A113	2.20950	-0.00800	-0.04510	0.00000	-0.04510	2.16440
A114	2.50117	-0.06484	-0.22582	0.00000	-0.22582	2.27535
A115	1.57250	0.07284	0.27092	0.00000	0.27092	1.84342
A116	2.40418	-0.04919	-0.16295	0.00000	-0.16295	2.24122
A117	2.21956	-0.00862	-0.01054	0.00000	-0.01054	2.20901
A118	1.65941	0.05781	0.17351	0.00000	0.17351	1.83292
A119	1.90930	-0.00068	-0.00368	0.00000	-0.00371	1.90559
A120	1.93911	0.00307	0.01587	0.00000	0.01585	1.95496
A121	1.89682	-0.00004	-0.00258	0.00000	-0.00261	1.89421
A122	1.90841	-0.00067	-0.00322	0.00000	-0.00323	1.90518
A123	1.90519	-0.00136	-0.00487	0.00000	-0.00491	1.90028
A124	1.90471	-0.00038	-0.00176	0.00000	-0.00179	1.90292
A125	1.92191	0.00325	0.01519	0.00000	0.01521	1.93712
A126	1.91530	-0.00236	-0.01024	0.00000	-0.01027	1.90503
A127	1.90467	-0.00130	-0.00623	0.00000	-0.00628	1.89839
A128	1.90542	0.00030	0.00088	0.00000	0.00092	1.90634
A129	1.90655	0.00016	0.00070	0.00000	0.00071	1.90725
A130	1.90992	-0.00004	-0.00027	0.00000	-0.00038	1.90954
A131	3.22732	-0.00203	-0.03524	0.00000	-0.03524	3.19208
A132	3.31456	-0.01020	-0.08020	0.00000	-0.08020	3.23437
A133	3.29921	-0.00857	-0.03992	0.00000	-0.03992	3.25929
A134	3.21976	-0.00198	-0.00036	0.00000	-0.00036	3.21939
A135	3.13618	-0.00011	0.00070	0.00000	0.00070	3.13688
A136	3.14437	-0.00004	-0.00018	0.00000	-0.00018	3.14419
A137	3.12514	0.00062	0.00178	0.00000	0.00178	3.12692
A138	3.14791	-0.00034	-0.00148	0.00000	-0.00148	3.14643
D1	-0.01859	0.00036	0.00147	0.00000	0.00145	-0.01715
D2	3.12091	-0.00001	-0.00012	0.00000	-0.00013	3.12078
D3	3.12597	0.00047	0.00158	0.00000	0.00156	3.12753
D4	-0.01771	0.00010	-0.00001	0.00000	-0.00002	-0.01773
D5	-0.00552	0.00018	0.00090	0.00000	0.00094	-0.00458
D6	3.14150	-0.00007	-0.00036	0.00000	-0.00032	3.14118
D7	3.13227	0.00009	0.00093	0.00000	0.00096	3.13322
D8	-0.00390	-0.00016	-0.00033	0.00000	-0.00030	-0.00420
D9	0.04433	-0.00044	-0.00156	0.00000	-0.00157	0.04276
D10	-3.08895	-0.00044	-0.00146	0.00000	-0.00159	-3.09054
D11	-3.09369	-0.00038	-0.00167	0.00000	-0.00167	-3.09536
D12	0.05622	-0.00038	-0.00157	0.00000	-0.00169	0.05453
D13	0.02956	-0.00078	-0.00328	0.00000	-0.00324	0.02632
D14	-3.11612	-0.00058	-0.00251	0.00000	-0.00249	-3.11861
D15	-3.10961	-0.00033	-0.00142	0.00000	-0.00137	-3.11098
D16	0.02789	-0.00014	-0.00065	0.00000	-0.00062	0.02728

D17	-0.01756	0.00064	0.00211	0.00000	0.00206	-0.01550
D18	3.12042	0.00082	0.00308	0.00000	0.00304	3.12346
D19	3.12184	0.00024	0.00042	0.00000	0.00037	3.12221
D20	-0.02337	0.00042	0.00140	0.00000	0.00135	-0.02202
D21	-0.01610	0.00040	0.00180	0.00000	0.00183	-0.01427
D22	3.12135	0.00044	0.00193	0.00000	0.00195	3.12330
D23	3.12957	0.00023	0.00111	0.00000	0.00114	3.13070
D24	-0.01617	0.00026	0.00124	0.00000	0.00126	-0.01491
D25	-0.00731	0.00014	0.00055	0.00000	0.00055	-0.00675
D26	3.13033	0.00013	0.00058	0.00000	0.00060	3.13093
D27	3.13840	0.00011	0.00043	0.00000	0.00045	3.13885
D28	-0.00715	0.00010	0.00047	0.00000	0.00049	-0.00665
D29	0.01837	-0.00051	-0.00222	0.00000	-0.00221	0.01616
D30	-3.12843	-0.00029	-0.00110	0.00000	-0.00107	-3.12950
D31	-3.11929	-0.00050	-0.00228	0.00000	-0.00227	-3.12156
D32	0.01710	-0.00029	-0.00116	0.00000	-0.00113	0.01596
D33	-0.05305	0.00053	0.00169	0.00000	0.00173	-0.05132
D34	3.09633	0.00007	-0.00014	0.00000	-0.00025	3.09608
D35	3.08118	0.00020	0.00029	0.00000	0.00028	3.08145
D36	-0.05263	-0.00026	-0.00154	0.00000	-0.00170	-0.05433
D37	-0.04735	0.00068	0.00253	0.00000	0.00251	-0.04484
D38	3.10712	0.00001	-0.00143	0.00000	-0.00145	3.10567
D39	3.10379	0.00082	0.00328	0.00000	0.00331	3.10710
D40	-0.02493	0.00015	-0.00067	0.00000	-0.00065	-0.02558
D41	0.04422	-0.00094	-0.00280	0.00000	-0.00278	0.04144
D42	-3.10507	-0.00043	-0.00026	0.00000	-0.00038	-3.10545
D43	-3.09373	-0.00112	-0.00380	0.00000	-0.00378	-3.09752
D44	0.04016	-0.00060	-0.00127	0.00000	-0.00138	0.03878
D45	-3.07909	-0.00299	-0.01239	0.00000	-0.01246	-3.09155
D46	0.08277	-0.00290	-0.01121	0.00000	-0.01120	0.07157
D47	0.07181	-0.00361	-0.01517	0.00000	-0.01518	0.05663
D48	-3.04951	-0.00352	-0.01399	0.00000	-0.01392	-3.06344
D49	0.06997	-0.00094	-0.00296	0.00000	-0.00356	0.06641
D50	-3.02579	-0.00278	-0.00866	0.00000	-0.00815	-3.03394
D51	-3.09129	-0.00088	-0.00341	0.00000	-0.00393	-3.09522
D52	0.09613	-0.00272	-0.00911	0.00000	-0.00851	0.08762
D53	-3.00762	-0.00213	-0.00753	0.00000	-0.00983	-3.01745
D54	0.09415	-0.00119	-0.00504	0.00000	-0.00855	0.08560
D55	2.90048	0.00815	0.03346	0.00000	0.03162	2.93211
D56	-0.25802	0.00201	0.01033	0.00000	0.01096	-0.24706
D57	-0.20677	0.00787	0.03348	0.00000	0.03230	-0.17447
D58	2.91791	0.00173	0.01034	0.00000	0.01164	2.92956
D59	-0.12838	0.00095	0.00543	0.00000	0.00739	-0.12099
D60	2.98340	0.00119	0.00607	0.00000	0.00796	2.99136
D61	3.01444	0.00116	0.00581	0.00000	0.00734	3.02179
D62	-0.15696	0.00141	0.00646	0.00000	0.00791	-0.14905
D63	0.02337	-0.00127	-0.00463	0.00000	-0.00264	0.02073
D64	-3.12021	-0.00159	-0.00515	0.00000	-0.00245	-3.12266
D65	-0.00041	0.00155	0.00635	0.00000	0.00525	0.00484
D66	-3.13559	0.00226	0.00979	0.00000	0.00946	-3.12612
D67	-3.14009	0.00185	0.00683	0.00000	0.00504	-3.13505
D68	0.00792	0.00255	0.01026	0.00000	0.00925	0.01717
D69	0.23571	-0.01159	-0.04772	0.00000	-0.04451	0.19120
D70	-2.88915	-0.00550	-0.02483	0.00000	-0.02411	-2.91326
D71	-2.86573	-0.01250	-0.05130	0.00000	-0.04761	-2.91334
D72	0.29259	-0.00641	-0.02842	0.00000	-0.02720	0.26539
D73	0.23779	-0.00429	-0.02014	0.00000	-0.02108	0.21671
D74	-1.76499	-0.00653	-0.02664	0.00000	-0.02649	-1.79148
D75	-2.94527	-0.00311	-0.01576	0.00000	-0.01718	-2.96245
D76	1.33514	-0.00535	-0.02226	0.00000	-0.02259	1.31255

D77	0.15438	-0.00296	-0.01364	0.00000	-0.01383	0.14056
D78	-2.99772	-0.00233	-0.01060	0.00000	-0.01050	-3.00822
D79	-2.99156	-0.00347	-0.01611	0.00000	-0.01701	-3.00858
D80	0.13952	-0.00285	-0.01307	0.00000	-0.01369	0.12583
D81	3.03954	0.00243	0.01022	0.00000	0.00927	3.04881
D82	-0.09535	0.00318	0.01389	0.00000	0.01387	-0.08148
D83	-0.23536	0.00395	0.01946	0.00000	0.01986	-0.21551
D84	1.73835	0.01032	0.04141	0.00000	0.04145	1.77980
D85	2.91996	0.00304	0.01504	0.00000	0.01526	2.93522
D86	-1.38951	0.00942	0.03699	0.00000	0.03686	-1.35266
D87	3.07380	0.00187	0.00745	0.00000	0.00729	3.08109
D88	-0.12288	0.00332	0.01461	0.00000	0.01428	-0.10860
D89	-0.08151	0.00283	0.01213	0.00000	0.01204	-0.06946
D90	3.00500	0.00427	0.01929	0.00000	0.01903	3.02403
D91	0.93993	-0.00082	-0.00760	0.00000	-0.00756	0.93238
D92	3.03781	0.00010	-0.00341	0.00000	-0.00344	3.03437
D93	-1.15266	-0.00218	-0.01387	0.00000	-0.01379	-1.16646
D94	-0.95701	0.00107	0.00917	0.00000	0.00915	-0.94786
D95	1.14087	0.00199	0.01336	0.00000	0.01326	1.15413
D96	-3.04961	-0.00029	0.00290	0.00000	0.00291	-3.04670
D97	0.02230	-0.00089	-0.00490	0.00000	-0.00507	0.01724
D98	3.11282	0.00161	0.00625	0.00000	0.00590	3.11872
D99	3.11706	0.00054	0.00219	0.00000	0.00222	3.11928
D100	0.03124	-0.00074	-0.00403	0.00000	-0.00397	0.02728
D101	-0.10704	0.00382	0.01606	0.00000	0.01563	-0.09141
D102	3.00203	0.00531	0.02161	0.00000	0.02102	3.02305
D103	0.04875	-0.00020	-0.00118	0.00000	-0.00109	0.04767
D104	-3.13609	0.00070	0.00294	0.00000	0.00313	-3.13297
D105	-3.05556	-0.00164	-0.00772	0.00000	-0.00798	-3.06354
D106	0.04278	-0.00075	-0.00360	0.00000	-0.00377	0.03901
D107	3.06917	0.00128	0.00514	0.00000	0.00521	3.07439
D108	-0.08739	0.00048	0.00146	0.00000	0.00162	-0.08576
D109	-0.12297	0.00390	0.01705	0.00000	0.01672	-0.10624
D110	3.00366	0.00310	0.01337	0.00000	0.01313	3.01679
D111	0.14885	-0.00361	-0.01562	0.00000	-0.01615	0.13270
D112	-2.97062	-0.00461	-0.01909	0.00000	-0.01958	-2.99020
D113	-2.98183	-0.00288	-0.01244	0.00000	-0.01283	-2.99466
D114	0.18188	-0.00388	-0.01592	0.00000	-0.01625	0.16563
D115	2.95625	0.00483	0.02031	0.00000	0.02026	2.97651
D116	0.78421	-0.00370	-0.01112	0.00000	-0.01110	0.77311
D117	-0.20029	0.00399	0.01647	0.00000	0.01643	-0.18386
D118	-2.37232	-0.00454	-0.01496	0.00000	-0.01493	-2.38725
D119	3.08896	0.00236	0.01001	0.00000	0.00973	3.09869
D120	-0.07420	0.00197	0.00843	0.00000	0.00818	-0.06601
D121	-0.08376	0.00389	0.01589	0.00000	0.01533	-0.06843
D122	3.03627	0.00350	0.01431	0.00000	0.01378	3.05005
D123	3.11709	0.00009	-0.00010	0.00000	-0.00027	3.11682
D124	-0.04611	0.00007	-0.00153	0.00000	-0.00165	-0.04776
D125	-0.01018	0.00045	0.00149	0.00000	0.00137	-0.00881
D126	3.10981	0.00043	0.00006	0.00000	-0.00001	3.10980
D127	3.12992	0.00183	0.00890	0.00000	0.00890	3.13881
D128	-0.03408	0.00136	0.00696	0.00000	0.00694	-0.02714
D129	0.06747	-0.00327	-0.01424	0.00000	-0.01372	0.05374
D130	-3.08659	-0.00138	-0.00616	0.00000	-0.00573	-3.09232
D131	-3.04693	-0.00320	-0.01275	0.00000	-0.01231	-3.05924
D132	0.08220	-0.00131	-0.00467	0.00000	-0.00432	0.07788
D133	0.14628	-0.00217	-0.00843	0.00000	-0.00859	0.13769
D134	2.36160	0.00046	0.00177	0.00000	0.00158	2.36317
D135	-3.02238	-0.00225	-0.01005	0.00000	-0.01014	-3.03252
D136	-0.80707	0.00038	0.00015	0.00000	0.00004	-0.80703

D137	-0.09037	0.00331	0.01501	0.00000	0.01543	-0.07494
D138	3.04656	0.00254	0.01168	0.00000	0.01185	3.05841
D139	3.06369	0.00140	0.00693	0.00000	0.00744	3.07112
D140	-0.08257	0.00063	0.00360	0.00000	0.00386	-0.07871
D141	0.07194	-0.00297	-0.01346	0.00000	-0.01347	0.05847
D142	-3.06428	-0.00207	-0.00961	0.00000	-0.00931	-3.07359
D143	3.08062	0.00095	0.00370	0.00000	0.00370	3.08433
D144	-0.05686	0.00051	0.00154	0.00000	0.00160	-0.05525
D145	-0.06670	0.00004	-0.00026	0.00000	-0.00032	-0.06703
D146	3.07900	-0.00040	-0.00242	0.00000	-0.00242	3.07658
D147	-1.07591	0.00119	-0.00116	0.00000	-0.00110	-1.07701
D148	1.03271	0.00187	0.00254	0.00000	0.00258	1.03530
D149	3.12862	0.00325	0.00844	0.00000	0.00849	3.13710
D150	-3.13835	-0.00283	-0.00692	0.00000	-0.00697	3.13787
D151	-1.02972	-0.00214	-0.00323	0.00000	-0.00329	-1.03301
D152	1.06618	-0.00076	0.00267	0.00000	0.00262	1.06880
D153	-0.00592	-0.00055	-0.00252	0.00000	-0.00255	-0.00847
D154	-3.14134	-0.00059	-0.00286	0.00000	-0.00288	3.13896
D155	3.13144	-0.00012	-0.00050	0.00000	-0.00047	3.13097
D156	-0.00398	-0.00016	-0.00083	0.00000	-0.00080	-0.00478
D157	-3.13981	0.00002	-0.00036	0.00000	-0.00035	-3.14016
D158	0.00039	-0.00005	-0.00055	0.00000	-0.00055	-0.00016
D159	-0.00326	0.00003	-0.00003	0.00000	-0.00003	-0.00329
D160	3.13694	-0.00004	-0.00022	0.00000	-0.00023	3.13671
D161	-3.14032	0.00008	0.00037	0.00000	0.00037	-3.13995
D162	0.00341	0.00020	0.00083	0.00000	0.00083	0.00424
D163	0.00660	0.00001	0.00006	0.00000	0.00007	0.00667
D164	-3.13285	0.00012	0.00052	0.00000	0.00052	-3.13233
D165	-0.00199	0.00007	0.00030	0.00000	0.00029	-0.00169
D166	3.13899	0.00008	0.00033	0.00000	0.00033	3.13932
D167	3.14099	0.00012	0.00045	0.00000	0.00045	3.14144
D168	-0.00121	0.00014	0.00049	0.00000	0.00048	-0.00073
D169	-0.00802	0.00002	0.00010	0.00000	0.00009	-0.00793
D170	3.13280	0.00006	0.00032	0.00000	0.00031	3.13310
D171	3.13088	0.00007	0.00020	0.00000	0.00021	3.13110
D172	-0.01149	0.00010	0.00042	0.00000	0.00043	-0.01105
D173	0.00081	0.00009	0.00045	0.00000	0.00044	0.00124
D174	3.13678	0.00009	0.00033	0.00000	0.00032	3.13710
D175	-3.13777	0.00008	0.00053	0.00000	0.00054	-3.13722
D176	-0.00179	0.00008	0.00041	0.00000	0.00042	-0.00137
D177	0.00647	-0.00009	-0.00030	0.00000	-0.00030	0.00616
D178	-3.13451	-0.00010	-0.00043	0.00000	-0.00044	-3.13494
D179	-3.13452	-0.00011	-0.00035	0.00000	-0.00035	-3.13487
D180	0.00769	-0.00012	-0.00047	0.00000	-0.00048	0.00721
D181	3.13626	0.00012	0.00055	0.00000	0.00055	3.13680
D182	-0.00512	0.00010	0.00041	0.00000	0.00041	-0.00472
D183	-0.00602	0.00013	0.00060	0.00000	0.00059	-0.00543
D184	3.13579	0.00011	0.00045	0.00000	0.00045	3.13623
D185	3.13870	0.00007	0.00007	0.00000	0.00007	3.13877
D186	-0.00398	0.00006	0.00013	0.00000	0.00013	-0.00385
D187	-0.00371	0.00009	0.00028	0.00000	0.00028	-0.00342
D188	3.13680	0.00008	0.00034	0.00000	0.00034	3.13714
D189	0.00000	0.00003	0.00003	0.00000	0.00002	0.00003
D190	-3.14091	-0.00002	-0.00015	0.00000	-0.00016	-3.14107
D191	3.14138	0.00005	0.00017	0.00000	0.00016	3.14154
D192	0.00046	0.00000	-0.00002	0.00000	-0.00002	0.00044
D193	-0.00189	0.00000	0.00009	0.00000	0.00009	-0.00179
D194	3.13924	0.00001	0.00010	0.00000	0.00010	3.13934
D195	3.14076	0.00002	0.00006	0.00000	0.00006	3.14082
D196	-0.00130	0.00002	0.00007	0.00000	0.00007	-0.00123

D197	0.00377	-0.00007	-0.00025	0.00000	-0.00025	0.00351
D198	-3.13736	-0.00007	-0.00026	0.00000	-0.00026	-3.13762
D199	-3.13849	-0.00001	-0.00006	0.00000	-0.00007	-3.13856
D200	0.00357	-0.00002	-0.00007	0.00000	-0.00008	0.00349

Item	Value	Threshold	Converged?

Maximum Force	0.072840	0.000450	NO
RMS Force	0.014348	0.000300	NO
Maximum Displacement	2.303342	0.001800	NO
RMS Displacement	0.492609	0.001200	NO

Predicted change in Energy=-1.724648D-01

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.496241	-0.720111	-0.222604
2	6	0	-9.554076	-1.740331	-0.103483
3	6	0	-9.912970	-3.072004	-0.050646
4	6	0	-11.268762	-3.389098	-0.152719
5	6	0	-12.227242	-2.364296	-0.287315
6	6	0	-11.848511	-1.023885	-0.313283
7	1	0	-9.154891	-3.841049	0.063850
8	1	0	-11.586836	-4.426998	-0.132299
9	1	0	-13.280191	-2.612997	-0.376540
10	1	0	-12.615375	-0.246049	-0.407472
11	6	0	-9.810394	0.593180	-0.233569
12	6	0	-8.191112	-1.188463	-0.051990
13	6	0	-8.330412	0.281996	-0.170351
14	6	0	-7.303505	1.088613	-0.200402
15	6	0	-5.941358	0.742068	-0.193778
16	6	0	-3.636528	-0.140369	0.027651
17	6	0	-3.715566	1.239038	0.157433
18	16	0	-5.202793	-0.932155	-0.237101
19	6	0	-4.991893	1.716401	-0.102027
20	6	0	-2.234670	-0.458390	0.162740
21	6	0	-1.609854	0.744629	0.365133
22	7	0	-2.495880	1.853088	0.560382
23	16	0	-1.159038	-1.854816	0.132327
24	16	0	1.098939	1.800959	0.464609
25	6	0	0.181095	-0.697235	0.264920
26	6	0	-0.211535	0.623403	0.345460
27	6	0	1.589329	-0.806144	0.349272
28	6	0	2.193002	0.429126	0.352513
29	6	0	3.588115	0.186078	0.233201
30	6	0	3.723188	-1.183105	0.257642
31	6	0	5.037384	-1.616649	0.119028
32	6	0	5.909028	-0.562672	0.056832
33	16	0	5.105966	1.043896	0.047659
34	7	0	2.503890	-1.870772	0.448014
35	6	0	7.303416	-0.881338	0.019584
36	6	0	8.391856	-0.109178	-0.098473
37	6	0	8.360766	1.367550	-0.236153

38	6	0	9.863288	-0.514634	-0.128622
39	6	0	9.753601	1.812802	-0.338156
40	6	0	10.624305	0.757406	-0.274190
41	6	0	10.176586	3.129201	-0.482911
42	6	0	12.007840	0.995757	-0.347803
43	6	0	11.534258	3.372014	-0.558054
44	6	0	12.448417	2.288673	-0.486743
45	6	0	10.369523	-1.740930	-0.046405
46	6	0	9.558045	-2.956994	0.091350
47	6	0	11.761444	-2.196577	-0.073821
48	7	0	8.961865	-3.957066	0.199899
49	7	0	12.830150	-2.659616	-0.086834
50	6	0	-10.427526	1.773714	-0.279876
51	6	0	-11.844762	2.043401	-0.378993
52	6	0	-9.797919	3.079062	-0.250474
53	7	0	-12.952228	2.393612	-0.448698
54	7	0	-9.374547	4.165907	-0.224955
55	8	0	-7.156796	-1.814923	0.067090
56	8	0	7.383534	2.094956	-0.264017
57	6	0	2.287275	-3.037751	-0.429824
58	1	0	1.320758	-3.490950	-0.193052
59	1	0	2.305418	-2.762536	-1.491552
60	1	0	3.076741	-3.768114	-0.237612
61	6	0	-2.576422	2.195922	2.011354
62	1	0	-2.854488	1.317142	2.608321
63	1	0	-1.604215	2.565960	2.346853
64	1	0	-3.328363	2.976530	2.146837
65	1	0	5.334916	-2.658296	0.070755
66	1	0	12.730352	0.167892	-0.294891
67	1	0	13.513871	2.487845	-0.542778
68	1	0	11.918601	4.381024	-0.670798
69	1	0	9.434198	3.919121	-0.531991
70	1	0	7.441374	-1.945981	0.103896
71	1	0	-7.449560	2.156777	-0.214917
72	1	0	-5.201211	2.778925	-0.254429

```

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Rotational constants (GHZ):      0.1711645      0.0107126      0.0101324
Standard basis: 6-31G(d,p) (6D, 7F)
There are 916 symmetry adapted cartesian basis functions of A symmetry.
There are 916 symmetry adapted basis functions of A symmetry.
916 basis functions, 1734 primitive gaussians, 916 cartesian basis func-
tions
196 alpha electrons      196 beta electrons
nuclear repulsion energy      6631.7457974182 Hartrees.
NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T
Big=T
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
Nuclear repulsion after empirical dispersion term = 6631.6596059088 Har-
trees.
One-electron integrals computed using PRISM.
NBasis= 916 RedAO= T EigKep= 3.12D-04 NBF= 916
NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916
Initial guess from the checkpoint file: "PBDB.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999803 0.019629 0.000106 -0.003000 Ang= 2.28 deg.
ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1
AccDes= 0.00D+00

```

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-yADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlgl= 2001
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 IlCent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RB3LYP) = -3682.92176234 A.U. after 16 cycles
NFock= 16 Conv=0.97D-08 -V/T= 2.0065
Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1
NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-0.006977355	-0.009891674	-0.003718676
2	6	0.009398800	0.002703608	0.002651298
3	6	0.001158400	0.009856014	0.001429860
4	6	-0.005249510	0.000358747	-0.002902968
5	6	0.006145654	0.004590134	0.003888989
6	6	-0.011641844	0.002530541	-0.006323251
7	1	-0.000589460	-0.000812743	0.000284795
8	1	-0.000361279	-0.000006117	-0.000473309
9	1	0.001150394	0.000800943	0.000138914
10	1	0.007945281	0.001187409	0.004910118
11	6	0.045971749	0.012976852	0.028840568
12	6	-0.038288330	-0.000255621	-0.021829802
13	6	-0.033091587	0.082344590	-0.019864234
14	6	0.012358659	-0.059611000	0.013183943
15	6	0.005219505	0.025636862	0.011145203
16	6	0.007562670	0.014514659	0.017564857
17	6	-0.010919454	0.002212888	-0.006588609
18	16	0.024075791	-0.051193620	0.001756518
19	6	0.003261185	-0.040606440	-0.010900291
20	6	-0.015454656	0.030527245	-0.006471691
21	6	0.007824830	-0.026404682	-0.005127947
22	7	0.002553636	0.013735995	0.018317712
23	16	-0.008849576	-0.015512865	-0.003253996
24	16	0.003099313	0.011834178	0.008023609
25	6	0.020580864	0.010939228	0.009962104
26	6	-0.011887766	-0.009959475	-0.019707723
27	6	-0.001887940	0.032369188	-0.008301948
28	6	0.006127409	-0.031176393	0.001937857
29	6	-0.013952410	-0.016385825	-0.015341418
30	6	0.023030093	0.016825773	0.010532098
31	6	-0.003107249	0.023879148	-0.007561891
32	6	0.011981989	-0.027727377	0.014631304
33	16	0.002371698	0.019905448	-0.004881239

34	7	-0.026560134	-0.017350624	0.015998647
35	6	-0.013146270	0.020562594	-0.007057456
36	6	0.021995183	-0.040370991	0.016177619
37	6	0.013793061	0.007270715	0.009003172
38	6	-0.047514668	-0.018065574	-0.031862125
39	6	-0.019248264	-0.012690589	-0.011672678
40	6	0.024008931	0.010308502	0.015335226
41	6	-0.004858183	-0.000166953	-0.003296195
42	6	0.014802198	0.020697323	0.008648405
43	6	0.011517534	-0.004111840	0.007906902
44	6	-0.011267176	-0.017326314	-0.006454556
45	6	0.050023603	0.048417114	0.031504226
46	6	-0.004419423	-0.005356478	-0.002755073
47	6	-0.017421799	-0.005823301	-0.011558391
48	7	-0.001865299	-0.011991042	-0.000574359
49	7	-0.001981767	-0.001636578	-0.001332463
50	6	-0.042189491	-0.034047954	-0.027409057
51	6	0.009827119	0.004513764	0.004689605
52	6	0.008533355	-0.000327795	0.005357452
53	7	-0.001114542	0.003033314	0.000124719
54	7	0.002931109	0.004690437	0.002451391
55	8	0.005783746	0.029443356	0.004201529
56	8	-0.009308586	-0.003405955	-0.005832500
57	6	0.003598798	0.004021058	-0.004069431
58	1	0.001589145	-0.000298979	0.000867810
59	1	0.000218201	-0.000469936	-0.001141311
60	1	-0.000707626	0.001659041	-0.000820573
61	6	-0.001824494	-0.009455028	-0.000251383
62	1	-0.000452814	-0.000333375	0.000344449
63	1	-0.000981725	-0.000308338	-0.000333841
64	1	0.000766795	-0.001086365	0.000584863
65	1	0.002679697	-0.002878554	-0.001132866
66	1	-0.008514148	-0.002061594	-0.005432565
67	1	-0.000151372	-0.000296453	0.000011530
68	1	-0.000607255	0.000319528	-0.000463300
69	1	0.000077819	-0.000613363	-0.000040231
70	1	0.004326350	0.002338473	0.003568571
71	1	-0.006272462	-0.003403907	-0.003297554
72	1	0.004375350	0.006417047	-0.005938961

Cartesian Forces: Max 0.082344590 RMS 0.016390360

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.159984808 RMS 0.016697483

Search for a local minimum.

Step number 7 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 6 7

ITU= 0 1 0 0 0 1 0

Use linear search instead of GDIIS.

Eigenvalues --- 0.00230 0.00230 0.00230 0.00230 0.00243

Eigenvalues --- 0.00290 0.00389 0.00445 0.00465 0.00497

Eigenvalues --- 0.00523 0.00557 0.00580 0.00608 0.00619

Eigenvalues --- 0.00649 0.00667 0.00693 0.00710 0.00736

Eigenvalues --- 0.00752 0.00760 0.00766 0.00783 0.00792

Eigenvalues	---	0.00835	0.00849	0.00877	0.00891	0.00902
Eigenvalues	---	0.01048	0.01114	0.01151	0.01173	0.01186
Eigenvalues	---	0.01249	0.01269	0.01290	0.01343	0.01380
Eigenvalues	---	0.01381	0.01400	0.01463	0.01470	0.01509
Eigenvalues	---	0.01611	0.01647	0.01666	0.01758	0.01794
Eigenvalues	---	0.01820	0.01929	0.01952	0.02006	0.02028
Eigenvalues	---	0.02075	0.02075	0.02209	0.02210	0.03106
Eigenvalues	---	0.04824	0.04827	0.04837	0.04886	0.04900
Eigenvalues	---	0.04905	0.05015	0.05016	0.05498	0.07203
Eigenvalues	---	0.07245	0.07442	0.07636	0.11384	0.12230
Eigenvalues	---	0.14108	0.15408	0.15986	0.15999	0.16000
Eigenvalues	---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues	---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues	---	0.16000	0.16001	0.16006	0.16038	0.17218
Eigenvalues	---	0.17781	0.18784	0.19028	0.19608	0.20618
Eigenvalues	---	0.21093	0.21723	0.21829	0.21999	0.22001
Eigenvalues	---	0.22044	0.22248	0.22293	0.22554	0.22599
Eigenvalues	---	0.22635	0.22699	0.22750	0.23024	0.23252
Eigenvalues	---	0.23361	0.23386	0.23750	0.23884	0.24104
Eigenvalues	---	0.24177	0.24260	0.24415	0.24516	0.24587
Eigenvalues	---	0.24670	0.24788	0.24820	0.24878	0.24903
Eigenvalues	---	0.24922	0.24957	0.24967	0.24982	0.24989
Eigenvalues	---	0.24991	0.24994	0.24999	0.24999	0.24999
Eigenvalues	---	0.25000	0.25000	0.25000	0.25000	0.25000
Eigenvalues	---	0.25001	0.25585	0.26086	0.26303	0.26411
Eigenvalues	---	0.26725	0.26761	0.27060	0.27199	0.27716
Eigenvalues	---	0.27921	0.28175	0.28342	0.28460	0.28646
Eigenvalues	---	0.29284	0.30075	0.30541	0.32986	0.33750
Eigenvalues	---	0.35686	0.36323	0.36337	0.36466	0.36487
Eigenvalues	---	0.36594	0.36652	0.36827	0.36842	0.37082
Eigenvalues	---	0.37094	0.37149	0.37252	0.37274	0.37417
Eigenvalues	---	0.37563	0.37670	0.37754	0.37982	0.38914
Eigenvalues	---	0.39573	0.40360	0.41295	0.41712	0.42054
Eigenvalues	---	0.42706	0.44433	0.44606	0.44877	0.45613
Eigenvalues	---	0.46721	0.47742	0.47974	0.48293	0.52654
Eigenvalues	---	0.54775	0.55674	0.57768	0.73898	0.80618
Eigenvalues	---	0.81996	1.25853	1.26308	1.29467	1.35393

RFO step: Lambda=-1.71473229D-01 EMin= 2.29985562D-03

Quartic linear search produced a step of -0.14880.

Iteration	1	RMS (Cart)=	0.17465727	RMS (Int)=	0.02310384
Iteration	2	RMS (Cart)=	0.16566898	RMS (Int)=	0.01645206
Iteration	3	RMS (Cart)=	0.20941561	RMS (Int)=	0.00974043
Iteration	4	RMS (Cart)=	0.11643018	RMS (Int)=	0.00182093
Iteration	5	RMS (Cart)=	0.00546215	RMS (Int)=	0.00011705
Iteration	6	RMS (Cart)=	0.00000367	RMS (Int)=	0.00011705
Iteration	7	RMS (Cart)=	0.00000000	RMS (Int)=	0.00011705
Iteration	1	RMS (Cart)=	0.17396060	RMS (Int)=	0.02011431
Iteration	2	RMS (Cart)=	0.17322178	RMS (Int)=	0.01351631
Iteration	3	RMS (Cart)=	0.22368946	RMS (Int)=	0.00758941
Iteration	4	RMS (Cart)=	0.03919654	RMS (Int)=	0.00019133
Iteration	5	RMS (Cart)=	0.00062451	RMS (Int)=	0.00009563
Iteration	6	RMS (Cart)=	0.00000009	RMS (Int)=	0.00009563

ITry= 2 IFail=0 DXMaxC= 3.17D+00 DCOld= 3.48D+00 DXMaxT= 8.49D-01 DXLimC= 3.00D+00 Rises=F

Iteration	1	RMS (Cart)=	0.17267430	RMS (Int)=	0.01719999
Iteration	2	RMS (Cart)=	0.18348553	RMS (Int)=	0.01067726
Iteration	3	RMS (Cart)=	0.18978520	RMS (Int)=	0.00470541
Iteration	4	RMS (Cart)=	0.01371830	RMS (Int)=	0.00007882
Iteration	5	RMS (Cart)=	0.00001634	RMS (Int)=	0.00007878
Iteration	6	RMS (Cart)=	0.00000000	RMS (Int)=	0.00007878

ITry= 3 IFail=0 DXMaxC= 2.87D+00 DCold= 3.17D+00 DXMaxT= 8.49D-01 DXLimC= 3.00D+00 Rises=F

Variable (Linear)	Old X (Quad)	-DE/DX (Total)	Delta X	Delta X	Delta X	New X
R1	2.63392	-0.00611	0.00236	-0.01531	-0.00993	2.62400
R2	2.62470	0.00780	0.00510	-0.00465	0.00138	2.62608
R3	2.79988	-0.00513	0.02108	-0.07574	-0.03935	2.76053
R4	2.60820	0.00958	0.00544	-0.00126	0.00442	2.61262
R5	2.78045	0.00321	0.01140	-0.02135	-0.00585	2.77460
R6	2.63828	0.00067	-0.00015	0.00295	0.00221	2.64049
R7	2.05209	-0.00051	-0.00198	0.00432	0.00148	2.05357
R8	2.66379	-0.00630	-0.00295	0.00158	-0.00167	2.66212
R9	2.05174	-0.00019	-0.00095	0.00212	0.00074	2.05249
R10	2.63264	0.00538	0.00095	0.00409	0.00424	2.63688
R11	2.05147	-0.00013	-0.00085	0.00197	0.00072	2.05220
R12	2.07180	-0.00940	-0.00920	0.01291	0.00113	2.07293
R13	2.86041	-0.01595	0.01634	-0.08727	-0.05335	2.80706
R14	2.51884	0.03362	0.01487	-0.00892	0.00774	2.52658
R15	2.80015	0.01916	0.00958	0.01064	0.01800	2.81816
R16	2.29619	0.00482	0.00122	0.00316	0.00374	2.29993
R17	2.46830	0.12223	0.02021	0.12963	0.12392	2.59222
R18	2.65611	0.05244	0.04077	-0.00731	0.03492	2.69104
R19	2.03750	0.00730	0.00052	0.01096	0.00929	2.04679
R20	3.45896	0.00228	0.00538	-0.01288	-0.00483	3.45413
R21	2.57671	0.04305	0.00121	0.04774	0.03935	2.61605
R22	2.62247	0.00305	-0.00639	0.01732	0.00738	2.62985
R23	3.35404	-0.01528	0.01918	-0.08802	-0.05116	3.30287
R24	2.72841	-0.00862	0.02559	-0.08705	-0.04406	2.68435
R25	2.62135	0.00593	0.02027	-0.04443	-0.01537	2.60597
R26	2.69050	0.01186	0.01002	-0.00967	0.00230	2.69279
R27	2.06664	-0.00528	-0.00392	0.00256	-0.00187	2.06477
R28	2.59011	0.01824	-0.00147	0.02515	0.01862	2.60873
R29	3.33145	-0.00397	0.00975	-0.03432	-0.01769	3.31376
R30	2.70689	-0.00191	0.01267	-0.03792	-0.01765	2.68924
R31	2.65261	0.00912	0.02851	-0.06138	-0.02063	2.63198
R32	2.82155	-0.00014	0.00018	-0.00064	-0.00033	2.82122
R33	3.35581	-0.00344	0.00979	-0.03421	-0.01755	3.33826
R34	3.33695	-0.00080	0.00745	-0.02230	-0.01036	3.32658
R35	3.32262	-0.00040	0.00768	-0.02188	-0.00981	3.31281
R36	2.60805	0.01730	-0.00076	0.02217	0.01697	2.62502
R37	2.67388	0.00507	0.03194	-0.07937	-0.03158	2.64230
R38	2.59817	0.01972	-0.00160	0.02687	0.01980	2.61797
R39	2.65882	0.00204	0.01865	-0.04969	-0.02108	2.63774
R40	2.68557	0.00024	0.02437	-0.06452	-0.02733	2.65824
R41	2.60035	0.01787	-0.00541	0.03141	0.01973	2.62009
R42	3.31331	-0.00539	0.01094	-0.04062	-0.02154	3.29176
R43	2.62820	0.01126	0.02633	-0.05166	-0.01502	2.61318
R44	2.66968	0.00805	0.01518	-0.02956	-0.00838	2.66130
R45	2.58727	0.03086	0.00390	0.02995	0.02786	2.61513
R46	2.04918	-0.00074	-0.00138	0.00249	0.00061	2.04979
R47	3.39418	0.00007	0.00687	-0.01978	-0.00893	3.38525
R48	2.70386	0.00771	0.03237	-0.07627	-0.02864	2.67522
R49	2.78974	-0.00062	-0.00045	0.00018	-0.00030	2.78944
R50	2.53172	0.03868	0.00926	0.02915	0.03258	2.56430
R51	2.03495	0.00551	0.00023	0.00895	0.00739	2.04234
R52	2.80333	0.00498	0.00352	0.00130	0.00453	2.80786
R53	2.88480	-0.02138	0.01354	-0.09098	-0.05922	2.82558
R54	2.77001	0.00818	0.00739	-0.00073	0.00677	2.77678
R55	2.30274	0.01103	0.00088	0.00772	0.00705	2.30979
R56	2.81463	-0.00705	0.02108	-0.08255	-0.04491	2.76972

R57	2.51187	0.03686	0.01918	-0.01829	0.00455	2.51641
R58	2.58836	0.01864	0.00227	0.00882	0.00930	2.59766
R59	2.62718	0.00483	0.02026	-0.04697	-0.01732	2.60985
R60	2.65666	-0.00214	0.01813	-0.05434	-0.02536	2.63130
R61	2.61020	0.00911	-0.00616	0.02838	0.01656	2.62677
R62	2.05061	0.00007	-0.00187	0.00483	0.00199	2.05260
R63	2.59453	0.01802	-0.00293	0.02643	0.01823	2.61276
R64	2.07886	-0.01030	-0.01173	0.01834	0.00294	2.08180
R65	2.68208	-0.00539	0.01211	-0.04066	-0.02039	2.66169
R66	2.05149	-0.00011	-0.00141	0.00340	0.00131	2.05280
R67	2.05103	0.00014	-0.00118	0.00317	0.00136	2.05239
R68	2.77493	-0.01762	0.00700	-0.05264	-0.03511	2.73982
R69	2.76818	-0.01989	0.01303	-0.07554	-0.04740	2.72078
R70	2.20973	-0.01212	-0.00096	-0.00497	-0.00494	2.20479
R71	2.20111	-0.00198	0.00077	-0.00442	-0.00277	2.19834
R72	2.73267	-0.00586	0.01467	-0.05209	-0.02700	2.70568
R73	2.73926	-0.00672	0.00884	-0.03651	-0.02036	2.71890
R74	2.19890	0.00180	0.00053	-0.00105	-0.00031	2.19859
R75	2.20469	-0.00551	-0.00065	-0.00240	-0.00257	2.20212
R76	2.06630	-0.00107	-0.00255	0.00503	0.00147	2.06777
R77	2.07297	-0.00083	-0.00278	0.00589	0.00194	2.07491
R78	2.06459	-0.00077	-0.00174	0.00333	0.00093	2.06552
R79	2.07521	-0.00059	-0.00206	0.00441	0.00146	2.07668
R80	2.06549	-0.00038	-0.00230	0.00531	0.00195	2.06744
R81	2.06415	-0.00076	-0.00206	0.00418	0.00128	2.06543
A1	2.09857	-0.00170	-0.00656	0.02036	0.00964	2.10821
A2	1.91402	-0.00765	-0.00025	-0.01243	-0.01005	1.90397
A3	2.27059	0.00935	0.00681	-0.00793	0.00041	2.27099
A4	2.13380	-0.00004	0.00047	-0.00358	-0.00234	2.13146
A5	1.93330	-0.00439	0.00077	-0.01392	-0.01052	1.92278
A6	2.21608	0.00442	-0.00124	0.01749	0.01286	2.22894
A7	2.05880	0.00071	0.00242	-0.00647	-0.00278	2.05602
A8	2.10111	-0.00108	0.00110	-0.00418	-0.00223	2.09888
A9	2.12327	0.00037	-0.00352	0.01065	0.00501	2.12828
A10	2.09691	-0.00001	-0.00124	0.00427	0.00219	2.09910
A11	2.09467	0.00053	0.00124	-0.00264	-0.00088	2.09379
A12	2.09160	-0.00052	0.00000	-0.00162	-0.00131	2.09028
A13	2.11347	0.00098	-0.00037	0.00206	0.00131	2.11477
A14	2.09533	-0.00184	-0.00055	-0.00255	-0.00260	2.09273
A15	2.07438	0.00086	0.00092	0.00049	0.00130	2.07568
A16	2.06451	0.00006	0.00527	-0.01656	-0.00797	2.05654
A17	2.13110	-0.00044	-0.00034	-0.00066	-0.00088	2.13023
A18	2.08757	0.00037	-0.00493	0.01723	0.00884	2.09641
A19	1.84426	0.02520	-0.00109	0.05289	0.04149	1.88575
A20	2.17850	-0.00012	0.01836	-0.06028	-0.03000	2.14850
A21	2.26039	-0.02508	-0.01727	0.00739	-0.01149	2.24890
A22	1.85702	0.01119	0.00395	0.00678	0.00911	1.86613
A23	2.21251	-0.03994	-0.00266	-0.05912	-0.04982	2.16269
A24	2.21365	0.02875	-0.00129	0.05233	0.04071	2.25435
A25	1.87472	-0.02433	-0.00340	-0.03315	-0.02990	1.84482
A26	2.26632	-0.09223	-0.00642	-0.14581	-0.12308	2.14324
A27	2.14213	0.11656	0.00982	0.17896	0.15297	2.29511
A28	2.22629	0.15998	0.01117	0.26029	0.21939	2.44568
A29	2.10088	-0.08273	-0.01140	-0.12319	-0.10996	1.99092
A30	1.95584	-0.07719	0.00023	-0.13692	-0.10932	1.84652
A31	2.23501	0.08754	0.01379	0.10739	0.09974	2.33476
A32	2.09319	-0.05675	0.00678	-0.11174	-0.08261	2.01059
A33	1.95435	-0.03068	-0.02058	0.00480	-0.01683	1.93752
A34	1.99009	-0.00491	-0.00591	0.00447	-0.00235	1.98774
A35	1.83951	0.00125	-0.00090	0.00644	0.00418	1.84369

A36	2.45359	0.00366	0.00681	-0.01092	-0.00183	2.45176
A37	1.95732	0.00099	-0.00806	0.02485	0.01165	1.96898
A38	1.98928	-0.00263	-0.00059	-0.00574	-0.00518	1.98410
A39	2.33608	0.00172	0.00865	-0.01879	-0.00626	2.32982
A40	1.51527	0.02449	0.01275	0.00761	0.01907	1.53434
A41	1.99037	0.01110	0.02090	-0.03514	-0.00745	1.98293
A42	2.15507	-0.00880	-0.01031	0.00944	-0.00270	2.15237
A43	2.13710	-0.00244	-0.01051	0.02487	0.00948	2.14658
A44	1.83703	0.00667	0.00159	0.00978	0.00934	1.84637
A45	2.44226	0.00330	0.00362	-0.00519	-0.00046	2.44180
A46	2.00386	-0.00998	-0.00521	-0.00465	-0.00893	1.99493
A47	2.00133	-0.00910	-0.00534	-0.00282	-0.00765	1.99368
A48	1.95654	0.00253	0.00082	0.00405	0.00400	1.96053
A49	2.32529	0.00658	0.00452	-0.00118	0.00368	2.32896
A50	1.72903	0.00524	0.00445	0.00064	0.00487	1.73390
A51	1.90483	0.00165	-0.00439	0.02052	0.01207	1.91690
A52	1.92145	-0.00072	-0.00114	0.00400	0.00191	1.92336
A53	1.51358	0.01538	0.00821	0.00498	0.01224	1.52582
A54	1.50794	0.01425	0.00854	0.00188	0.01005	1.51799
A55	1.99701	-0.00929	-0.00562	-0.00245	-0.00757	1.98945
A56	2.35371	0.00512	0.00541	-0.00570	0.00089	2.35460
A57	1.93191	0.00422	0.00017	0.00845	0.00686	1.93877
A58	2.31958	0.00854	0.00300	0.00720	0.00880	2.32838
A59	1.94642	0.00170	0.00151	0.00042	0.00177	1.94819
A60	2.01631	-0.01022	-0.00454	-0.00738	-0.01042	2.00589
A61	1.94762	0.00222	-0.00027	0.00732	0.00552	1.95315
A62	2.35938	0.00464	0.00527	-0.00561	0.00086	2.36023
A63	1.97607	-0.00686	-0.00499	-0.00173	-0.00639	1.96967
A64	2.01300	-0.01003	-0.00427	-0.00750	-0.01025	2.00275
A65	2.41831	0.00704	0.00217	0.00608	0.00715	2.42546
A66	1.85165	0.00300	0.00209	0.00151	0.00315	1.85480
A67	1.83904	0.00276	0.00113	0.00412	0.00436	1.84341
A68	2.45760	0.00313	0.00317	-0.00398	0.00003	2.45763
A69	1.98637	-0.00589	-0.00430	-0.00016	-0.00440	1.98196
A70	1.98357	-0.00118	0.00026	-0.00070	-0.00039	1.98318
A71	1.98451	-0.00799	-0.00140	-0.01355	-0.01214	1.97237
A72	2.31480	0.00917	0.00115	0.01424	0.01252	2.32732
A73	1.94565	0.00554	0.00305	0.00302	0.00541	1.95107
A74	2.16899	0.00041	-0.00154	0.00588	0.00318	2.17216
A75	2.16854	-0.00594	-0.00152	-0.00886	-0.00859	2.15995
A76	1.98686	-0.01623	-0.00804	-0.00800	-0.01444	1.97241
A77	2.03775	0.00531	0.00525	-0.00292	0.00291	2.04066
A78	2.25855	0.01090	0.00279	0.01086	0.01148	2.27002
A79	1.51968	0.01800	0.00882	0.00737	0.01476	1.53444
A80	1.75507	0.00990	0.00263	0.01456	0.01425	1.76933
A81	2.04996	-0.00327	-0.00032	-0.00029	-0.00081	2.04915
A82	2.01672	0.00061	-0.00508	0.02212	0.01249	2.02922
A83	2.29920	0.02702	-0.00272	0.05874	0.04428	2.34347
A84	1.92091	-0.01097	0.00731	-0.03702	-0.02231	1.89860
A85	2.06308	-0.01605	-0.00460	-0.02171	-0.02197	2.04111
A86	2.17110	0.02237	-0.00019	0.05019	0.03997	2.21107
A87	2.25461	-0.02270	-0.00137	-0.04164	-0.03468	2.21993
A88	1.85747	0.00033	0.00156	-0.00855	-0.00529	1.85217
A89	1.86390	0.00123	0.00206	-0.00571	-0.00260	1.86130
A90	2.23085	0.00314	-0.00344	0.01518	0.00874	2.23960
A91	2.18843	-0.00437	0.00138	-0.00947	-0.00615	2.18228
A92	1.84168	0.01064	-0.00513	0.03984	0.02680	1.86848
A93	2.22800	0.00075	-0.01991	0.06535	0.03235	2.26035
A94	2.21350	-0.01139	0.02504	-0.10519	-0.05915	2.15435
A95	1.94629	-0.00945	0.00141	-0.02313	-0.01712	1.92917

A96	2.19441	0.01099	-0.00318	0.03368	0.02382	2.21822
A97	2.14249	-0.00153	0.00177	-0.01055	-0.00670	2.13579
A98	1.91541	-0.00275	0.00010	-0.00244	-0.00179	1.91362
A99	2.28200	0.00191	0.00862	-0.03104	-0.01620	2.26580
A100	2.08578	0.00085	-0.00872	0.03348	0.01799	2.10377
A101	2.06142	-0.00126	0.00201	-0.00917	-0.00532	2.05610
A102	2.07812	0.00125	0.00226	-0.00202	0.00065	2.07876
A103	2.14365	0.00001	-0.00428	0.01119	0.00467	2.14832
A104	2.07231	-0.00260	0.00599	-0.02367	-0.01295	2.05936
A105	2.11326	0.00101	0.00016	0.00068	0.00071	2.11397
A106	2.09761	0.00159	-0.00615	0.02299	0.01224	2.10985
A107	2.08999	0.00256	-0.00121	0.00853	0.00566	2.09565
A108	2.11417	-0.00212	0.00006	-0.00480	-0.00381	2.11037
A109	2.07902	-0.00044	0.00115	-0.00373	-0.00186	2.07716
A110	2.11436	0.00199	0.00016	0.00139	0.00132	2.11568
A111	2.08638	-0.00069	-0.00035	0.00119	0.00058	2.08696
A112	2.08245	-0.00130	0.00018	-0.00258	-0.00191	2.08054
A113	2.16440	0.00170	0.00671	-0.00499	0.00272	2.16712
A114	2.27535	-0.02288	0.03360	-0.14756	-0.08445	2.19090
A115	1.84342	0.02118	-0.04031	0.15255	0.08173	1.92515
A116	2.24122	-0.01026	0.02425	-0.09840	-0.05447	2.18676
A117	2.20901	-0.01528	0.00157	-0.02965	-0.02215	2.18686
A118	1.83292	0.02554	-0.02582	0.12806	0.07663	1.90955
A119	1.90559	0.00078	0.00055	0.00002	0.00057	1.90616
A120	1.95496	-0.00138	-0.00236	0.00334	0.00031	1.95527
A121	1.89421	0.00134	0.00039	0.00212	0.00209	1.89630
A122	1.90518	0.00045	0.00048	-0.00013	0.00038	1.90556
A123	1.90028	-0.00180	0.00073	-0.00664	-0.00458	1.89570
A124	1.90292	0.00057	0.00027	0.00098	0.00105	1.90397
A125	1.93712	-0.00009	-0.00226	0.00608	0.00260	1.93972
A126	1.90503	-0.00007	0.00153	-0.00446	-0.00204	1.90299
A127	1.89839	0.00012	0.00093	-0.00229	-0.00090	1.89749
A128	1.90634	0.00049	-0.00014	0.00179	0.00130	1.90764
A129	1.90725	0.00044	-0.00011	0.00162	0.00119	1.90845
A130	1.90954	-0.00090	0.00006	-0.00288	-0.00224	1.90730
A131	3.19208	-0.00174	0.00524	-0.01395	-0.00592	3.18616
A132	3.23437	-0.00465	0.01193	-0.03810	-0.01855	3.21582
A133	3.25929	-0.00578	0.00594	-0.03623	-0.02304	3.23625
A134	3.21939	-0.00550	0.00005	-0.02278	-0.01817	3.20123
A135	3.13688	0.00000	-0.00010	0.00012	-0.00001	3.13687
A136	3.14419	-0.00013	0.00003	-0.00055	-0.00042	3.14377
A137	3.12692	0.00098	-0.00027	0.00449	0.00332	3.13025
A138	3.14643	-0.00019	0.00022	-0.00131	-0.00083	3.14561
D1	-0.01715	0.00035	-0.00022	0.00175	0.00119	-0.01596
D2	3.12078	0.00031	0.00002	0.00036	0.00031	3.12109
D3	3.12753	0.00012	-0.00023	0.00120	0.00075	3.12827
D4	-0.01773	0.00009	0.00000	-0.00020	-0.00014	-0.01787
D5	-0.00458	0.00013	-0.00014	0.00111	0.00075	-0.00383
D6	3.14118	-0.00007	0.00005	-0.00035	-0.00023	3.14096
D7	3.13322	0.00037	-0.00014	0.00180	0.00128	3.13450
D8	-0.00420	0.00017	0.00005	0.00035	0.00031	-0.00389
D9	0.04276	0.00036	0.00023	-0.00059	-0.00029	0.04247
D10	-3.09054	0.00040	0.00024	-0.00027	-0.00002	-3.09056
D11	-3.09536	0.00013	0.00025	-0.00129	-0.00080	-3.09616
D12	0.05453	0.00017	0.00025	-0.00097	-0.00053	0.05400
D13	0.02632	-0.00050	0.00048	-0.00342	-0.00226	0.02406
D14	-3.11861	-0.00035	0.00037	-0.00263	-0.00174	-3.12035
D15	-3.11098	-0.00043	0.00020	-0.00171	-0.00116	-3.11213
D16	0.02728	-0.00029	0.00009	-0.00092	-0.00063	0.02664
D17	-0.01550	0.00033	-0.00031	0.00284	0.00199	-0.01351

D18	3.12346	-0.00033	-0.00045	0.00092	0.00034	3.12379
D19	3.12221	0.00028	-0.00006	0.00130	0.00100	3.12321
D20	-0.02202	-0.00038	-0.00020	-0.00061	-0.00065	-0.02267
D21	-0.01427	0.00028	-0.00027	0.00202	0.00135	-0.01292
D22	3.12330	0.00037	-0.00029	0.00228	0.00154	3.12484
D23	3.13070	0.00014	-0.00017	0.00125	0.00084	3.13154
D24	-0.01491	0.00023	-0.00019	0.00151	0.00102	-0.01389
D25	-0.00675	0.00015	-0.00008	0.00072	0.00050	-0.00625
D26	3.13093	0.00021	-0.00009	0.00093	0.00065	3.13158
D27	3.13885	0.00006	-0.00007	0.00047	0.00032	3.13917
D28	-0.00665	0.00012	-0.00007	0.00068	0.00047	-0.00619
D29	0.01616	-0.00032	0.00033	-0.00235	-0.00156	0.01460
D30	-3.12950	-0.00013	0.00016	-0.00097	-0.00063	-3.13013
D31	-3.12156	-0.00037	0.00034	-0.00255	-0.00170	-3.12327
D32	0.01596	-0.00018	0.00017	-0.00117	-0.00077	0.01519
D33	-0.05132	0.00049	-0.00026	0.00301	0.00215	-0.04917
D34	3.09608	0.00036	0.00004	0.00299	0.00233	3.09841
D35	3.08145	0.00063	-0.00004	0.00224	0.00176	3.08322
D36	-0.05433	0.00050	0.00025	0.00222	0.00195	-0.05239
D37	-0.04484	0.00088	-0.00037	0.00421	0.00301	-0.04184
D38	3.10567	0.00055	0.00022	0.00189	0.00174	3.10741
D39	3.10710	0.00064	-0.00049	0.00452	0.00311	3.11021
D40	-0.02558	0.00031	0.00010	0.00220	0.00184	-0.02373
D41	0.04144	-0.00084	0.00041	-0.00442	-0.00313	0.03831
D42	-3.10545	-0.00153	0.00006	-0.00566	-0.00456	-3.11001
D43	-3.09752	-0.00005	0.00056	-0.00228	-0.00118	-3.09870
D44	0.03878	-0.00073	0.00021	-0.00352	-0.00260	0.03617
D45	-3.09155	0.00001	0.00185	-0.00692	-0.00375	-3.09530
D46	0.07157	-0.00263	0.00167	-0.01638	-0.01143	0.06014
D47	0.05663	0.00041	0.00226	-0.00612	-0.00264	0.05400
D48	-3.06344	-0.00223	0.00207	-0.01557	-0.01032	-3.07376
D49	0.06641	-0.00190	0.00053	-0.00895	-0.00654	0.05987
D50	-3.03394	-0.00433	0.00121	-0.02323	-0.01754	-3.05148
D51	-3.09522	0.00022	0.00058	-0.00048	0.00037	-3.09485
D52	0.08762	-0.00221	0.00127	-0.01476	-0.01064	0.07698
D53	-3.01745	-0.00670	0.00146	-0.03522	-0.02725	-3.04470
D54	0.08560	-0.00521	0.00127	-0.02443	-0.01802	0.06758
D55	2.93211	0.01189	-0.00471	0.05563	0.03928	2.97138
D56	-0.24706	0.00803	-0.00163	0.03174	0.02327	-0.22379
D57	-0.17447	0.00699	-0.00481	0.04062	0.02765	-0.14682
D58	2.92956	0.00313	-0.00173	0.01674	0.01164	2.94120
D59	-0.12099	0.00199	-0.00110	0.01027	0.00700	-0.11399
D60	2.99136	0.00407	-0.00118	0.01912	0.01393	3.00529
D61	3.02179	0.00223	-0.00109	0.01208	0.00850	3.03029
D62	-0.14905	0.00431	-0.00118	0.02093	0.01543	-0.13361
D63	0.02073	0.00049	0.00039	0.00499	0.00447	0.02520
D64	-3.12266	0.00012	0.00037	0.00228	0.00221	-3.12046
D65	0.00484	-0.00026	-0.00078	0.00092	-0.00001	0.00483
D66	-3.12612	0.00144	-0.00141	0.00857	0.00545	-3.12067
D67	-3.13505	0.00009	-0.00075	0.00349	0.00215	-3.13291
D68	0.01717	0.00180	-0.00138	0.01114	0.00761	0.02478
D69	0.19120	-0.00377	0.00662	-0.03564	-0.02229	0.16891
D70	-2.91326	0.00020	0.00359	-0.01168	-0.00605	-2.91931
D71	-2.91334	-0.00630	0.00708	-0.04743	-0.03118	-2.94452
D72	0.26539	-0.00233	0.00405	-0.02347	-0.01494	0.25044
D73	0.21671	-0.00488	0.00314	-0.03139	-0.02194	0.19476
D74	-1.79148	-0.00703	0.00394	-0.04308	-0.03054	-1.82202
D75	-2.96245	-0.00225	0.00256	-0.01896	-0.01273	-2.97517
D76	1.31255	-0.00440	0.00336	-0.03065	-0.02132	1.29123
D77	0.14056	-0.00351	0.00206	-0.02087	-0.01459	0.12596

D78	-3.00822	-0.00237	0.00156	-0.01514	-0.01056	-3.01879
D79	-3.00858	-0.00466	0.00253	-0.02632	-0.01842	-3.02700
D80	0.12583	-0.00352	0.00204	-0.02059	-0.01439	0.11143
D81	3.04881	0.00080	-0.00138	0.00848	0.00548	3.05430
D82	-0.08148	0.00254	-0.00206	0.01655	0.01118	-0.07030
D83	-0.21551	0.00601	-0.00295	0.03232	0.02279	-0.19272
D84	1.77980	0.01009	-0.00617	0.05693	0.03932	1.81911
D85	2.93522	0.00460	-0.00227	0.02501	0.01767	2.95290
D86	-1.35266	0.00869	-0.00548	0.04961	0.03420	-1.31846
D87	3.08109	0.00150	-0.00109	0.00911	0.00619	3.08728
D88	-0.10860	0.00197	-0.00212	0.01513	0.01006	-0.09854
D89	-0.06946	0.00283	-0.00179	0.01626	0.01118	-0.05828
D90	3.02403	0.00330	-0.00283	0.02228	0.01506	3.03909
D91	0.93238	0.00321	0.00112	0.00638	0.00621	0.93858
D92	3.03437	0.00371	0.00051	0.00953	0.00812	3.04250
D93	-1.16646	0.00265	0.00205	0.00209	0.00370	-1.16276
D94	-0.94786	-0.00338	-0.00136	-0.00645	-0.00651	-0.95437
D95	1.15413	-0.00288	-0.00197	-0.00330	-0.00459	1.14955
D96	-3.04670	-0.00394	-0.00043	-0.01074	-0.00901	-3.05571
D97	0.01724	-0.00077	0.00075	-0.00632	-0.00435	0.01288
D98	3.11872	0.00082	-0.00088	0.00491	0.00303	3.12175
D99	3.11928	0.00027	-0.00033	0.00175	0.00104	3.12032
D100	0.02728	-0.00049	0.00059	-0.00464	-0.00321	0.02407
D101	-0.09141	0.00271	-0.00233	0.01735	0.01154	-0.07987
D102	3.02305	0.00334	-0.00313	0.02239	0.01478	3.03783
D103	0.04767	-0.00044	0.00016	-0.00257	-0.00192	0.04575
D104	-3.13297	0.00044	-0.00047	0.00272	0.00169	-3.13127
D105	-3.06354	-0.00175	0.00119	-0.01081	-0.00747	-3.07100
D106	0.03901	-0.00087	0.00056	-0.00552	-0.00385	0.03516
D107	3.07439	0.00115	-0.00078	0.00699	0.00481	3.07920
D108	-0.08576	0.00104	-0.00024	0.00565	0.00425	-0.08151
D109	-0.10624	0.00247	-0.00249	0.01775	0.01180	-0.09444
D110	3.01679	0.00236	-0.00195	0.01641	0.01125	3.02804
D111	0.13270	-0.00401	0.00240	-0.02276	-0.01576	0.11695
D112	-2.99020	-0.00458	0.00291	-0.02635	-0.01811	-3.00830
D113	-2.99466	-0.00404	0.00191	-0.02166	-0.01538	-3.01004
D114	0.16563	-0.00460	0.00242	-0.02526	-0.01773	0.14790
D115	2.97651	0.00406	-0.00301	0.02513	0.01712	2.99363
D116	0.77311	-0.00244	0.00165	-0.01443	-0.00987	0.76324
D117	-0.18386	0.00402	-0.00244	0.02385	0.01665	-0.16721
D118	-2.38725	-0.00248	0.00222	-0.01571	-0.01034	-2.39760
D119	3.09869	0.00194	-0.00145	0.01076	0.00714	3.10583
D120	-0.06601	0.00155	-0.00122	0.00971	0.00655	-0.05946
D121	-0.06843	0.00238	-0.00228	0.01540	0.01006	-0.05837
D122	3.05005	0.00199	-0.00205	0.01435	0.00947	3.05952
D123	3.11682	0.00025	0.00004	0.00149	0.00125	3.11807
D124	-0.04776	0.00044	0.00025	0.00104	0.00108	-0.04668
D125	-0.00881	0.00042	-0.00020	0.00229	0.00162	-0.00719
D126	3.10980	0.00061	0.00000	0.00184	0.00145	3.11125
D127	3.13881	0.00117	-0.00132	0.00855	0.00559	-3.13879
D128	-0.02714	0.00084	-0.00103	0.00747	0.00504	-0.02209
D129	0.05374	-0.00225	0.00204	-0.01541	-0.01036	0.04339
D130	-3.09232	-0.00071	0.00085	-0.00554	-0.00362	-3.09594
D131	-3.05924	-0.00215	0.00183	-0.01431	-0.00965	-3.06890
D132	0.07788	-0.00061	0.00064	-0.00444	-0.00291	0.07496
D133	0.13769	-0.00197	0.00128	-0.01346	-0.00958	0.12811
D134	2.36317	0.00165	-0.00024	0.01035	0.00816	2.37133
D135	-3.03252	-0.00199	0.00151	-0.01440	-0.01014	-3.04265
D136	-0.80703	0.00163	-0.00001	0.00941	0.00760	-0.79943
D137	-0.07494	0.00369	-0.00230	0.02151	0.01482	-0.06011

D138	3.05841	0.00248	-0.00176	0.01492	0.01017	3.06858
D139	3.07112	0.00212	-0.00111	0.01160	0.00811	3.07923
D140	-0.07871	0.00092	-0.00057	0.00500	0.00345	-0.07527
D141	0.05847	-0.00282	0.00200	-0.01716	-0.01167	0.04680
D142	-3.07359	-0.00137	0.00139	-0.00944	-0.00617	-3.07976
D143	3.08433	0.00147	-0.00055	0.00775	0.00566	3.08999
D144	-0.05525	0.00122	-0.00024	0.00585	0.00444	-0.05081
D145	-0.06703	-0.00011	0.00005	-0.00017	-0.00009	-0.06712
D146	3.07658	-0.00037	0.00036	-0.00208	-0.00132	3.07526
D147	-1.07701	0.00545	0.00016	0.01679	0.01360	-1.06341
D148	1.03530	0.00566	-0.00038	0.01881	0.01467	1.04997
D149	3.13710	0.00639	-0.00126	0.02354	0.01758	-3.12850
D150	3.13787	-0.00619	0.00104	-0.02214	-0.01669	3.12119
D151	-1.03301	-0.00599	0.00049	-0.02012	-0.01562	-1.04862
D152	1.06880	-0.00525	-0.00039	-0.01539	-0.01271	1.05609
D153	-0.00847	-0.00046	0.00038	-0.00281	-0.00187	-0.01034
D154	3.13896	-0.00039	0.00043	-0.00269	-0.00171	3.13725
D155	3.13097	-0.00018	0.00007	-0.00079	-0.00057	3.13041
D156	-0.00478	-0.00011	0.00012	-0.00066	-0.00041	-0.00519
D157	-3.14016	0.00016	0.00005	0.00033	0.00032	-3.13985
D158	-0.00016	0.00006	0.00008	-0.00005	0.00004	-0.00012
D159	-0.00329	0.00002	0.00000	0.00007	0.00006	-0.00323
D160	3.13671	-0.00008	0.00003	-0.00030	-0.00021	3.13650
D161	-3.13995	0.00001	-0.00006	-0.00006	-0.00010	-3.14005
D162	0.00424	0.00007	-0.00012	0.00040	0.00021	0.00444
D163	0.00667	-0.00001	-0.00001	-0.00014	-0.00012	0.00655
D164	-3.13233	0.00004	-0.00008	0.00033	0.00019	-3.13214
D165	-0.00169	0.00003	-0.00004	0.00028	0.00018	-0.00151
D166	3.13932	0.00004	-0.00005	0.00039	0.00027	3.13959
D167	3.14144	0.00013	-0.00007	0.00062	0.00043	-3.14132
D168	-0.00073	0.00013	-0.00007	0.00073	0.00051	-0.00022
D169	-0.00793	0.00003	-0.00001	0.00026	0.00020	-0.00773
D170	3.13310	0.00007	-0.00005	0.00048	0.00035	3.13345
D171	3.13110	0.00000	-0.00003	0.00014	0.00008	3.13118
D172	-0.01105	0.00004	-0.00006	0.00036	0.00023	-0.01083
D173	0.00124	0.00004	-0.00007	0.00016	0.00007	0.00131
D174	3.13710	0.00007	-0.00005	0.00035	0.00023	3.13733
D175	-3.13722	0.00007	-0.00008	0.00044	0.00027	-3.13695
D176	-0.00137	0.00010	-0.00006	0.00063	0.00044	-0.00093
D177	0.00616	-0.00010	0.00005	-0.00050	-0.00036	0.00581
D178	-3.13494	-0.00013	0.00007	-0.00067	-0.00047	-3.13542
D179	-3.13487	-0.00011	0.00005	-0.00063	-0.00045	-3.13532
D180	0.00721	-0.00014	0.00007	-0.00080	-0.00057	0.00664
D181	3.13680	0.00009	-0.00008	0.00051	0.00032	3.13713
D182	-0.00472	0.00010	-0.00006	0.00051	0.00034	-0.00437
D183	-0.00543	0.00010	-0.00009	0.00063	0.00042	-0.00501
D184	3.13623	0.00010	-0.00007	0.00063	0.00044	3.13667
D185	3.13877	0.00004	-0.00001	0.00025	0.00019	3.13896
D186	-0.00385	0.00005	-0.00002	0.00030	0.00022	-0.00363
D187	-0.00342	0.00008	-0.00004	0.00047	0.00034	-0.00309
D188	3.13714	0.00009	-0.00005	0.00053	0.00037	3.13751
D189	0.00003	0.00002	0.00000	0.00009	0.00007	0.00010
D190	-3.14107	-0.00001	0.00002	-0.00008	-0.00004	-3.14112
D191	3.14154	0.00001	-0.00002	0.00010	0.00005	-3.14159
D192	0.00044	-0.00001	0.00000	-0.00008	-0.00006	0.00038
D193	-0.00179	0.00002	-0.00001	0.00009	0.00006	-0.00173
D194	3.13934	0.00002	-0.00001	0.00010	0.00007	3.13941
D195	3.14082	0.00001	-0.00001	0.00005	0.00003	3.14085
D196	-0.00123	0.00001	-0.00001	0.00006	0.00004	-0.00120
D197	0.00351	-0.00006	0.00004	-0.00038	-0.00027	0.00325

D198	-3.13762	-0.00006	0.00004	-0.00039	-0.00027	-3.13790
D199	-3.13856	-0.00004	0.00001	-0.00021	-0.00016	-3.13872
D200	0.00349	-0.00004	0.00001	-0.00022	-0.00017	0.00332

Item	Value	Threshold	Converged?

Maximum Force	0.159985	0.000450	NO
RMS Force	0.016697	0.000300	NO
Maximum Displacement	2.865422	0.001800	NO
RMS Displacement	0.535674	0.001200	NO

Predicted change in Energy=-1.104525D-01

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.911898	-0.181510	-0.256080
2	6	0	-10.436195	-1.481331	-0.145318
3	6	0	-11.281837	-2.574999	-0.131627
4	6	0	-12.652946	-2.340318	-0.263493
5	6	0	-13.139254	-1.024157	-0.389044
6	6	0	-12.273218	0.069883	-0.377623
7	1	0	-10.878000	-3.578098	-0.023788
8	1	0	-13.347764	-3.175073	-0.273008
9	1	0	-14.205220	-0.849159	-0.500566
10	1	0	-12.671578	1.088127	-0.465826
11	6	0	-9.782886	0.744881	-0.222880
12	6	0	-8.970524	-1.478266	-0.058275
13	6	0	-8.533713	-0.054824	-0.141914
14	6	0	-7.285617	0.514324	-0.144031
15	6	0	-5.912492	0.137311	-0.127835
16	6	0	-3.547877	-0.593433	0.066002
17	6	0	-3.715693	0.781726	0.198254
18	16	0	-5.041711	-1.469202	-0.171306
19	6	0	-5.014445	1.186152	-0.028420
20	6	0	-2.150302	-0.821170	0.178813
21	6	0	-1.581923	0.421386	0.375601
22	7	0	-2.523897	1.471012	0.565719
23	16	0	-0.997741	-2.141683	0.125440
24	16	0	1.061998	1.608867	0.464152
25	6	0	0.278645	-0.927466	0.256372
26	6	0	-0.190104	0.376873	0.348958
27	6	0	1.674801	-0.966066	0.322261
28	6	0	2.226716	0.304483	0.340689
29	6	0	3.618122	0.131486	0.227498
30	6	0	3.824889	-1.239497	0.225266
31	6	0	5.153126	-1.599460	0.089424
32	6	0	5.982859	-0.492963	0.041468
33	16	0	5.085332	1.057110	0.069947
34	7	0	2.636044	-1.975748	0.392261
35	6	0	7.376339	-0.738268	-0.004849
36	6	0	8.474418	0.052327	-0.107512
37	6	0	8.494218	1.533758	-0.220388
38	6	0	9.903806	-0.385485	-0.137313

39	6	0	9.906380	1.930360	-0.307957
40	6	0	10.721780	0.824934	-0.255616
41	6	0	10.405630	3.212477	-0.427518
42	6	0	12.106035	0.963441	-0.314722
43	6	0	11.785554	3.367815	-0.489559
44	6	0	12.626207	2.239226	-0.430568
45	6	0	10.415118	-1.613541	-0.076711
46	6	0	9.621145	-2.821532	0.034782
47	6	0	11.816991	-1.939139	-0.117847
48	7	0	9.026357	-3.821441	0.122303
49	7	0	12.927202	-2.285450	-0.146132
50	6	0	-9.927625	2.073698	-0.252626
51	6	0	-11.174670	2.767571	-0.368465
52	6	0	-8.853830	3.028728	-0.182175
53	7	0	-12.130622	3.425435	-0.451971
54	7	0	-8.032002	3.852739	-0.122537
55	8	0	-8.295420	-2.483559	0.063718
56	8	0	7.546159	2.304930	-0.241876
57	6	0	2.460852	-3.143310	-0.493740
58	1	0	1.515729	-3.639420	-0.253063
59	1	0	2.459163	-2.858936	-1.554267
60	1	0	3.279160	-3.845062	-0.313117
61	6	0	-2.584572	1.854374	2.007306
62	1	0	-2.795708	0.981664	2.640903
63	1	0	-1.625374	2.290915	2.301078
64	1	0	-3.374965	2.597591	2.139634
65	1	0	5.508280	-2.622369	0.025377
66	1	0	12.768654	0.084506	-0.269751
67	1	0	13.702503	2.377116	-0.476765
68	1	0	12.232578	4.353421	-0.583302
69	1	0	9.712414	4.047685	-0.468611
70	1	0	7.544336	-1.804014	0.058431
71	1	0	-7.293976	1.597389	-0.150398
72	1	0	-5.295841	2.232593	-0.168471

Rotational constants (GHZ): 0.1773022 0.0104094 0.0098791

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6586.8056357042 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T
Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6586.7198960077 Hartrees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.12D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Initial guess from the checkpoint file: "PBDB.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999830 -0.016938 0.000181 0.007292 Ang= -2.11 deg.

ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1

AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-
yADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2001
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 IlCent= 200000004 NGrid=
0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0=
0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Integral accuracy reduced to 1.0D-05 until final iterations.

Initial convergence to 1.0D-05 achieved. Increase integral accuracy.

SCF Done: E(RB3LYP) = -3682.95160773 A.U. after 16 cycles

NFock= 16 Conv=0.97D-08 -V/T= 2.0065

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1

NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-0.005580643	-0.003185154	-0.002047479
2	6	0.001452414	0.006789820	-0.000015460
3	6	-0.000883909	0.007789805	-0.000186453
4	6	-0.002761568	-0.001968383	-0.001555387
5	6	0.003020951	0.003716568	0.001849358
6	6	-0.012494787	0.002947968	-0.006543982
7	1	-0.000822561	-0.001115420	0.000225488
8	1	-0.000214506	-0.000360115	-0.000390785
9	1	0.000858494	0.000770193	-0.000047418
10	1	0.008395415	0.008585295	0.005077210
11	6	0.028463973	0.017203985	0.016803914
12	6	0.002228828	-0.006345772	0.002477401
13	6	-0.008004125	0.004385311	-0.005777344
14	6	0.002024781	0.003428931	0.006496252
15	6	-0.004095625	0.019118550	0.003088348
16	6	0.009328486	0.013389363	0.005892228
17	6	-0.007149272	-0.000014319	-0.006186012
18	16	-0.012849204	-0.011865535	-0.013023847
19	6	-0.002739084	-0.020321973	-0.009081489
20	6	-0.002928757	0.021667291	0.000468119
21	6	0.001116385	-0.018523125	-0.005304859
22	7	0.003404982	0.016929675	0.017447616
23	16	-0.006497482	-0.008652860	-0.000990838
24	16	0.002226374	0.007482476	0.005540722
25	6	0.009375260	0.010819406	0.003027781
26	6	-0.004248576	-0.009021482	-0.012518113
27	6	0.003305859	0.018851249	-0.006440610
28	6	-0.000751492	-0.020701635	-0.002517090
29	6	-0.007791771	-0.013177366	-0.009060109
30	6	0.017264019	0.010089169	0.005668877
31	6	0.002157156	0.013469732	-0.002181522
32	6	0.002857251	-0.014660224	0.007114648
33	16	0.006497524	0.008020752	-0.000430348
34	7	-0.021600958	-0.011500900	0.018305083
35	6	-0.002085629	0.006181841	0.000767703

36	6	0.011529714	-0.020778852	0.008072632
37	6	0.002157503	0.005524570	0.000974947
38	6	-0.038331773	-0.010536785	-0.024857012
39	6	-0.014603973	-0.006650827	-0.008572553
40	6	0.015251871	0.005687823	0.009245233
41	6	-0.005217251	-0.006789718	-0.002861521
42	6	0.015676361	0.005367679	0.009609297
43	6	0.004227890	-0.003376881	0.003038623
44	6	-0.004566848	-0.011524278	-0.002040676
45	6	0.038227078	0.039126187	0.022325408
46	6	-0.000213362	-0.004321638	0.000192692
47	6	-0.004379977	0.005473385	-0.003230908
48	7	-0.001627525	-0.005019126	-0.000689830
49	7	0.002031569	-0.000361536	0.001329100
50	6	-0.024774321	-0.040544832	-0.014833699
51	6	0.001874995	-0.003236953	-0.000665165
52	6	-0.001197979	0.001778419	-0.000819285
53	7	-0.002815494	0.000552654	-0.001099122
54	7	0.000445918	0.000033233	0.000314572
55	8	0.014238187	-0.004949829	0.009020533
56	8	-0.005734954	0.003732081	-0.004232541
57	6	0.004968066	0.004448081	-0.003121770
58	1	0.001578485	-0.001017045	0.001028769
59	1	0.000677087	-0.000534406	-0.001823602
60	1	-0.000976107	0.001330443	-0.000830327
61	6	-0.003921400	-0.009442514	-0.002011221
62	1	-0.000951464	-0.000761769	0.000838528
63	1	-0.001380037	0.000609429	-0.000139569
64	1	0.001170126	-0.000965729	0.000809513
65	1	0.002096881	-0.002915078	-0.001291891
66	1	-0.012305868	-0.007922131	-0.007277373
67	1	-0.000136722	0.000267948	-0.000021384
68	1	-0.000832843	0.000712109	-0.000629258
69	1	0.000767648	-0.001340582	0.000475766
70	1	0.003477665	-0.000991078	0.003171305
71	1	-0.001922738	0.003289218	0.000251249
72	1	0.005015389	0.005825205	-0.005601062

Cartesian Forces: Max 0.040544832 RMS 0.009741114

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.051739903 RMS 0.007727845

Search for a local minimum.

Step number 8 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 7 8

DE= -2.98D-02 DEPred=-1.10D-01 R= 2.70D-01

Trust test= 2.70D-01 RLast= 4.97D-01 DXMaxT set to 8.49D-01

ITU= 0 0 1 0 0 0 1 0

Use linear search instead of GDIIS.

Eigenvalues --- 0.00230 0.00230 0.00230 0.00230 0.00243

Eigenvalues --- 0.00292 0.00391 0.00445 0.00460 0.00494

Eigenvalues --- 0.00520 0.00552 0.00575 0.00601 0.00621

Eigenvalues --- 0.00641 0.00667 0.00688 0.00689 0.00728

Eigenvalues --- 0.00753 0.00754 0.00760 0.00771 0.00781

Eigenvalues	---	0.00813	0.00833	0.00862	0.00878	0.00889
Eigenvalues	---	0.01026	0.01106	0.01146	0.01168	0.01178
Eigenvalues	---	0.01244	0.01269	0.01282	0.01337	0.01373
Eigenvalues	---	0.01383	0.01404	0.01465	0.01469	0.01492
Eigenvalues	---	0.01606	0.01647	0.01660	0.01755	0.01794
Eigenvalues	---	0.01815	0.01930	0.01952	0.02006	0.02027
Eigenvalues	---	0.02075	0.02075	0.02209	0.02209	0.02934
Eigenvalues	---	0.04826	0.04827	0.04837	0.04895	0.04900
Eigenvalues	---	0.04910	0.05016	0.05019	0.05304	0.07185
Eigenvalues	---	0.07230	0.07461	0.07629	0.12346	0.14488
Eigenvalues	---	0.15301	0.15956	0.15989	0.15999	0.16000
Eigenvalues	---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues	---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues	---	0.16000	0.16002	0.16024	0.17070	0.17774
Eigenvalues	---	0.18779	0.19023	0.19317	0.20351	0.20834
Eigenvalues	---	0.21148	0.21411	0.21822	0.21999	0.22003
Eigenvalues	---	0.22053	0.22224	0.22309	0.22576	0.22604
Eigenvalues	---	0.22636	0.22709	0.22805	0.23030	0.23246
Eigenvalues	---	0.23362	0.23475	0.23704	0.23775	0.24012
Eigenvalues	---	0.24183	0.24261	0.24427	0.24470	0.24519
Eigenvalues	---	0.24603	0.24736	0.24837	0.24855	0.24903
Eigenvalues	---	0.24922	0.24957	0.24974	0.24977	0.24990
Eigenvalues	---	0.24992	0.24995	0.24997	0.24999	0.24999
Eigenvalues	---	0.24999	0.25000	0.25000	0.25000	0.25001
Eigenvalues	---	0.25234	0.25599	0.26219	0.26296	0.26638
Eigenvalues	---	0.26712	0.26757	0.27060	0.27189	0.27792
Eigenvalues	---	0.27889	0.28260	0.28346	0.28475	0.28654
Eigenvalues	---	0.29150	0.30091	0.30644	0.32986	0.33644
Eigenvalues	---	0.35686	0.36301	0.36337	0.36354	0.36476
Eigenvalues	---	0.36591	0.36651	0.36827	0.36837	0.37082
Eigenvalues	---	0.37094	0.37147	0.37252	0.37274	0.37417
Eigenvalues	---	0.37563	0.37670	0.37754	0.37984	0.38902
Eigenvalues	---	0.39313	0.40350	0.41276	0.41709	0.42069
Eigenvalues	---	0.42701	0.44440	0.44817	0.44903	0.45623
Eigenvalues	---	0.46634	0.47662	0.47874	0.48475	0.52654
Eigenvalues	---	0.54378	0.55651	0.57682	0.80240	0.81695
Eigenvalues	---	0.99158	1.25851	1.26319	1.29381	1.35392

RFO step: Lambda=-4.71889891D-02 EMin= 2.29985035D-03

Quartic linear search produced a step of -0.39991.

Iteration 1 RMS(Cart)= 0.22101714 RMS(Int)= 0.00669104

Iteration 2 RMS(Cart)= 0.04380772 RMS(Int)= 0.00025093

Iteration 3 RMS(Cart)= 0.00070618 RMS(Int)= 0.00010403

Iteration 4 RMS(Cart)= 0.00000016 RMS(Int)= 0.00010403

Variable	Old X	-DE/DX	Delta X	Delta X	Delta X	New X
(Linear)	(Quad)	(Total)				
R1	2.62400	0.01564	0.00397	0.02120	0.02525	2.64924
R2	2.62608	0.01156	-0.00055	0.02585	0.02538	2.65146
R3	2.76053	0.02394	0.01574	0.06646	0.08224	2.84277
R4	2.61262	0.00582	-0.00177	0.01900	0.01723	2.62985
R5	2.77460	0.00649	0.00234	0.02160	0.02390	2.79850
R6	2.64049	-0.00224	-0.00088	-0.00539	-0.00635	2.63413
R7	2.05357	-0.00111	-0.00059	-0.00342	-0.00401	2.04956
R8	2.66212	-0.00554	0.00067	-0.01682	-0.01624	2.64589
R9	2.05249	-0.00035	-0.00030	-0.00132	-0.00162	2.05087
R10	2.63688	0.00303	-0.00170	0.00785	0.00615	2.64303
R11	2.05220	-0.00030	-0.00029	-0.00115	-0.00144	2.05076
R12	2.07293	-0.01284	-0.00045	-0.03689	-0.03734	2.03559
R13	2.80706	-0.00033	0.02133	0.00727	0.02863	2.83570
R14	2.52658	0.05174	-0.00309	0.10073	0.09763	2.62421
R15	2.81816	-0.00694	-0.00720	0.00023	-0.00698	2.81117

R16	2.29993	0.01430	-0.00150	0.01325	0.01175	2.31169
R17	2.59222	-0.00732	-0.04956	0.09038	0.04082	2.63304
R18	2.69104	-0.00564	-0.01397	0.03585	0.02188	2.71292
R19	2.04679	-0.00172	-0.00371	0.00233	-0.00138	2.04541
R20	3.45413	-0.01475	0.00193	-0.03115	-0.02910	3.42504
R21	2.61605	0.01872	-0.01573	0.05130	0.03551	2.65157
R22	2.62985	0.00951	-0.00295	0.00658	0.00353	2.63338
R23	3.30287	-0.00886	0.02046	-0.02240	-0.00186	3.30101
R24	2.68435	0.00243	0.01762	0.01949	0.03713	2.72147
R25	2.60597	0.01616	0.00615	0.04973	0.05577	2.66174
R26	2.69279	0.00862	-0.00092	0.02824	0.02730	2.72009
R27	2.06477	-0.00526	0.00075	-0.01380	-0.01306	2.05171
R28	2.60873	0.01389	-0.00745	0.02657	0.01913	2.62786
R29	3.31376	-0.00013	0.00707	0.00352	0.01062	3.32439
R30	2.68924	0.00413	0.00706	0.01293	0.01999	2.70923
R31	2.63198	0.01505	0.00825	0.06003	0.06825	2.70023
R32	2.82122	0.00026	0.00013	0.00042	0.00055	2.82177
R33	3.33826	0.00005	0.00702	0.00414	0.01118	3.34944
R34	3.32658	0.00114	0.00414	0.00688	0.01103	3.33761
R35	3.31281	0.00174	0.00392	0.00876	0.01272	3.32553
R36	2.62502	0.01342	-0.00679	0.02593	0.01909	2.64410
R37	2.64230	0.01522	0.01263	0.06162	0.07421	2.71651
R38	2.61797	0.01473	-0.00792	0.02803	0.02016	2.63812
R39	2.63774	0.00881	0.00843	0.02816	0.03660	2.67434
R40	2.65824	0.00790	0.01093	0.03674	0.04769	2.70593
R41	2.62009	0.01448	-0.00789	0.02129	0.01331	2.63340
R42	3.29176	-0.00246	0.00861	-0.00175	0.00688	3.29865
R43	2.61318	0.01513	0.00601	0.05857	0.06451	2.67769
R44	2.66130	0.00895	0.00335	0.03109	0.03440	2.69570
R45	2.61513	0.01866	-0.01114	0.04880	0.03766	2.65279
R46	2.04979	-0.00091	-0.00024	-0.00287	-0.00311	2.04668
R47	3.38525	-0.00118	0.00357	0.00237	0.00602	3.39126
R48	2.67522	0.00831	0.01146	0.04939	0.06085	2.73607
R49	2.78944	-0.00063	0.00012	-0.00184	-0.00172	2.78771
R50	2.56430	0.01274	-0.01303	0.05630	0.04327	2.60757
R51	2.04234	0.00263	-0.00295	0.00658	0.00363	2.04597
R52	2.80786	-0.00233	-0.00181	-0.00492	-0.00676	2.80110
R53	2.82558	-0.01003	0.02368	-0.01752	0.00618	2.83176
R54	2.77678	0.00496	-0.00271	0.01699	0.01425	2.79103
R55	2.30979	0.00698	-0.00282	0.01006	0.00724	2.31703
R56	2.76972	0.02126	0.01796	0.06292	0.08092	2.85064
R57	2.51641	0.05163	-0.00182	0.11138	0.10956	2.62597
R58	2.59766	0.02483	-0.00372	0.04419	0.04060	2.63826
R59	2.60985	0.01012	0.00693	0.03645	0.04338	2.65324
R60	2.63130	0.01131	0.01014	0.03388	0.04414	2.67544
R61	2.62677	0.00228	-0.00662	0.00023	-0.00651	2.62025
R62	2.05260	-0.00057	-0.00080	-0.00219	-0.00299	2.04962
R63	2.61276	0.01277	-0.00729	0.02231	0.01501	2.62778
R64	2.08180	-0.01591	-0.00118	-0.04553	-0.04671	2.03509
R65	2.66169	-0.00196	0.00815	-0.00420	0.00384	2.66553
R66	2.05280	-0.00047	-0.00052	-0.00177	-0.00229	2.05051
R67	2.05239	-0.00028	-0.00054	-0.00113	-0.00167	2.05072
R68	2.73982	-0.00946	0.01404	-0.02484	-0.01080	2.72902
R69	2.72078	-0.00484	0.01896	-0.01435	0.00461	2.72539
R70	2.20479	-0.00519	0.00198	-0.00763	-0.00565	2.19914
R71	2.19834	0.00240	0.00111	0.00141	0.00252	2.20086
R72	2.70568	0.00129	0.01080	0.00911	0.01991	2.72558
R73	2.71890	-0.00195	0.00814	-0.00123	0.00691	2.72581
R74	2.19859	0.00301	0.00012	0.00286	0.00298	2.20157
R75	2.20212	0.00004	0.00103	-0.00173	-0.00070	2.20142

R76	2.06777	-0.00168	-0.00059	-0.00504	-0.00562	2.06215
R77	2.07491	-0.00163	-0.00077	-0.00503	-0.00581	2.06910
R78	2.06552	-0.00115	-0.00037	-0.00356	-0.00393	2.06159
R79	2.07668	-0.00137	-0.00059	-0.00403	-0.00462	2.07206
R80	2.06744	-0.00126	-0.00078	-0.00381	-0.00459	2.06285
R81	2.06543	-0.00131	-0.00051	-0.00401	-0.00452	2.06091
A1	2.10821	-0.01166	-0.00386	-0.03556	-0.03928	2.06894
A2	1.90397	-0.00129	0.00402	-0.00700	-0.00301	1.90097
A3	2.27099	0.01295	-0.00016	0.04256	0.04228	2.31328
A4	2.13146	0.00266	0.00094	0.01059	0.01162	2.14308
A5	1.92278	-0.00106	0.00421	-0.00146	0.00269	1.92547
A6	2.22894	-0.00160	-0.00514	-0.00913	-0.01431	2.21463
A7	2.05602	0.00128	0.00111	0.00621	0.00724	2.06326
A8	2.09888	-0.00129	0.00089	-0.00435	-0.00342	2.09546
A9	2.12828	0.00001	-0.00200	-0.00186	-0.00382	2.12446
A10	2.09910	0.00076	-0.00088	-0.00455	-0.00559	2.09351
A11	2.09379	0.00002	0.00035	0.00455	0.00498	2.09877
A12	2.09028	-0.00078	0.00052	0.00001	0.00061	2.09090
A13	2.11477	0.00347	-0.00052	0.00627	0.00567	2.12044
A14	2.09273	-0.00278	0.00104	-0.00712	-0.00604	2.08669
A15	2.07568	-0.00069	-0.00052	0.00085	0.00037	2.07605
A16	2.05654	0.00349	0.00319	0.01710	0.02037	2.07691
A17	2.13023	0.00057	0.00035	0.00197	0.00227	2.13250
A18	2.09641	-0.00406	-0.00354	-0.01906	-0.02264	2.07377
A19	1.88575	-0.01080	-0.01659	-0.01112	-0.02762	1.85813
A20	2.14850	0.01581	0.01200	0.06470	0.07665	2.22515
A21	2.24890	-0.00501	0.00460	-0.05360	-0.04905	2.19985
A22	1.86613	-0.00178	-0.00364	0.00642	0.00273	1.86886
A23	2.16269	0.01255	0.01992	-0.00202	0.01790	2.18060
A24	2.25435	-0.01077	-0.01628	-0.00436	-0.02064	2.23371
A25	1.84482	0.01495	0.01196	0.01317	0.02516	1.86997
A26	2.14324	0.02123	0.04922	-0.01398	0.03521	2.17845
A27	2.29511	-0.03617	-0.06118	0.00086	-0.06035	2.23476
A28	2.44568	-0.03791	-0.08774	0.01662	-0.07115	2.37453
A29	1.99092	0.01571	0.04397	-0.02083	0.02311	2.01403
A30	1.84652	0.02220	0.04372	0.00409	0.04778	1.89430
A31	2.33476	-0.03208	-0.03989	-0.00176	-0.04178	2.29298
A32	2.01059	0.03387	0.03304	0.03948	0.07228	2.08287
A33	1.93752	-0.00181	0.00673	-0.03842	-0.03181	1.90571
A34	1.98774	-0.00534	0.00094	-0.02114	-0.02024	1.96749
A35	1.84369	0.00312	-0.00167	0.00841	0.00670	1.85038
A36	2.45176	0.00223	0.00073	0.01277	0.01349	2.46525
A37	1.96898	0.00192	-0.00466	0.00132	-0.00350	1.96548
A38	1.98410	-0.00588	0.00207	-0.01902	-0.01691	1.96720
A39	2.32982	0.00399	0.00251	0.01768	0.02031	2.35013
A40	1.53434	0.01284	-0.00763	0.05338	0.04611	1.58045
A41	1.98293	-0.00672	0.00298	0.00953	0.01233	1.99526
A42	2.15237	0.00032	0.00108	-0.01600	-0.01483	2.13754
A43	2.14658	0.00627	-0.00379	0.00636	0.00270	2.14928
A44	1.84637	0.00251	-0.00373	0.01320	0.00947	1.85584
A45	2.44180	0.00431	0.00018	0.01333	0.01350	2.45530
A46	1.99493	-0.00683	0.00357	-0.02661	-0.02305	1.97188
A47	1.99368	-0.00621	0.00306	-0.02703	-0.02394	1.96974
A48	1.96053	0.00048	-0.00160	0.00589	0.00424	1.96477
A49	2.32896	0.00573	-0.00147	0.02115	0.01971	2.34867
A50	1.73390	0.00759	-0.00195	0.02955	0.02758	1.76148
A51	1.91690	0.00029	-0.00483	0.00450	-0.00046	1.91644
A52	1.92336	-0.00086	-0.00076	0.00249	0.00161	1.92496
A53	1.52582	0.01244	-0.00490	0.04277	0.03796	1.56379
A54	1.51799	0.01289	-0.00402	0.04337	0.03946	1.55745

A55	1.98945	-0.00727	0.00303	-0.02688	-0.02383	1.96561
A56	2.35460	0.00480	-0.00035	0.01784	0.01753	2.37213
A57	1.93877	0.00250	-0.00275	0.00917	0.00637	1.94514
A58	2.32838	0.00658	-0.00352	0.02246	0.01898	2.34736
A59	1.94819	0.00151	-0.00071	0.00637	0.00562	1.95381
A60	2.00589	-0.00806	0.00417	-0.02871	-0.02453	1.98136
A61	1.95315	0.00067	-0.00221	0.00519	0.00293	1.95608
A62	2.36023	0.00527	-0.00034	0.01941	0.01907	2.37931
A63	1.96967	-0.00594	0.00256	-0.02459	-0.02199	1.94768
A64	2.00275	-0.00768	0.00410	-0.02764	-0.02353	1.97922
A65	2.42546	0.00581	-0.00286	0.01854	0.01563	2.44109
A66	1.85480	0.00188	-0.00126	0.00915	0.00792	1.86272
A67	1.84341	0.00295	-0.00175	0.01047	0.00873	1.85213
A68	2.45763	0.00260	-0.00001	0.00967	0.00969	2.46732
A69	1.98196	-0.00555	0.00176	-0.02012	-0.01839	1.96357
A70	1.98318	-0.00058	0.00016	0.00024	0.00030	1.98349
A71	1.97237	-0.00671	0.00485	-0.02378	-0.01893	1.95344
A72	2.32732	0.00729	-0.00501	0.02354	0.01863	2.34596
A73	1.95107	0.00125	-0.00217	0.01095	0.00872	1.95979
A74	2.17216	0.00229	-0.00127	0.00544	0.00420	2.17636
A75	2.15995	-0.00354	0.00343	-0.01639	-0.01293	2.14703
A76	1.97241	-0.00824	0.00578	-0.03689	-0.03105	1.94136
A77	2.04066	0.01809	-0.00117	0.04230	0.04111	2.08177
A78	2.27002	-0.00986	-0.00459	-0.00544	-0.01005	2.25997
A79	1.53444	0.01329	-0.00590	0.04643	0.04069	1.57513
A80	1.76933	0.00846	-0.00570	0.03168	0.02595	1.79527
A81	2.04915	-0.00147	0.00032	0.00085	0.00115	2.05030
A82	2.02922	-0.00024	-0.00500	0.00284	-0.00230	2.02692
A83	2.34347	-0.00836	-0.01771	0.00379	-0.01392	2.32955
A84	1.89860	0.00824	0.00892	0.01192	0.02084	1.91944
A85	2.04111	0.00012	0.00878	-0.01571	-0.00692	2.03419
A86	2.21107	-0.00787	-0.01598	-0.00460	-0.02060	2.19047
A87	2.21993	-0.00383	0.01387	-0.01975	-0.00589	2.21404
A88	1.85217	0.01170	0.00212	0.02435	0.02649	1.87866
A89	1.86130	0.00086	0.00104	0.00407	0.00508	1.86639
A90	2.23960	-0.00504	-0.00350	-0.00897	-0.01246	2.22714
A91	2.18228	0.00418	0.00246	0.00490	0.00737	2.18966
A92	1.86848	-0.00340	-0.01072	-0.00995	-0.02058	1.84790
A93	2.26035	-0.01941	-0.01294	-0.07336	-0.08634	2.17401
A94	2.15435	0.02281	0.02365	0.08331	0.10691	2.26127
A95	1.92917	-0.00425	0.00685	-0.00787	-0.00107	1.92810
A96	2.21822	0.00166	-0.00953	-0.00379	-0.01339	2.20483
A97	2.13579	0.00258	0.00268	0.01166	0.01446	2.15025
A98	1.91362	-0.00490	0.00072	-0.01060	-0.00993	1.90369
A99	2.26580	0.01579	0.00648	0.04804	0.05435	2.32015
A100	2.10377	-0.01089	-0.00719	-0.03744	-0.04442	2.05934
A101	2.05610	0.00077	0.00213	0.00350	0.00552	2.06162
A102	2.07876	0.00116	-0.00026	0.00481	0.00461	2.08337
A103	2.14832	-0.00193	-0.00187	-0.00832	-0.01013	2.13819
A104	2.05936	0.00243	0.00518	0.01550	0.02080	2.08017
A105	2.11397	0.00268	-0.00029	0.00952	0.00917	2.12315
A106	2.10985	-0.00511	-0.00490	-0.02502	-0.02998	2.07987
A107	2.09565	0.00130	-0.00226	-0.00244	-0.00494	2.09071
A108	2.11037	-0.00185	0.00152	-0.00316	-0.00153	2.10884
A109	2.07716	0.00056	0.00074	0.00561	0.00647	2.08363
A110	2.11568	0.00382	-0.00053	0.00922	0.00858	2.12426
A111	2.08696	-0.00201	-0.00023	-0.00579	-0.00596	2.08100
A112	2.08054	-0.00181	0.00076	-0.00344	-0.00262	2.07792
A113	2.16712	-0.00732	-0.00109	-0.01500	-0.01609	2.15103
A114	2.19090	0.00887	0.03377	0.05802	0.09179	2.28269

A115	1.92515	-0.00155	-0.03268	-0.04302	-0.07571	1.84944
A116	2.18676	0.00460	0.02178	0.04129	0.06306	2.24982
A117	2.18686	-0.00217	0.00886	-0.01960	-0.01075	2.17612
A118	1.90955	-0.00242	-0.03064	-0.02165	-0.05230	1.85725
A119	1.90616	0.00084	-0.00023	0.00330	0.00307	1.90923
A120	1.95527	-0.00179	-0.00013	-0.00824	-0.00836	1.94691
A121	1.89630	0.00118	-0.00084	0.00466	0.00382	1.90012
A122	1.90556	0.00060	-0.00015	0.00253	0.00238	1.90794
A123	1.89570	-0.00149	0.00183	-0.00483	-0.00300	1.89270
A124	1.90397	0.00065	-0.00042	0.00259	0.00218	1.90615
A125	1.93972	-0.00058	-0.00104	-0.00377	-0.00480	1.93492
A126	1.90299	-0.00025	0.00082	0.00043	0.00125	1.90424
A127	1.89749	0.00050	0.00036	0.00238	0.00274	1.90023
A128	1.90764	0.00062	-0.00052	0.00203	0.00152	1.90915
A129	1.90845	0.00047	-0.00048	0.00187	0.00140	1.90984
A130	1.90730	-0.00078	0.00090	-0.00298	-0.00209	1.90521
A131	3.18616	-0.00256	0.00237	-0.00673	-0.00436	3.18179
A132	3.21582	0.00108	0.00742	0.01324	0.02065	3.23647
A133	3.23625	-0.00093	0.00921	0.00792	0.01713	3.25338
A134	3.20123	-0.00120	0.00727	0.01107	0.01833	3.21956
A135	3.13687	0.00007	0.00000	-0.00027	-0.00027	3.13660
A136	3.14377	-0.00007	0.00017	0.00008	0.00025	3.14402
A137	3.13025	0.00079	-0.00133	0.00214	0.00081	3.13106
A138	3.14561	-0.00007	0.00033	0.00013	0.00046	3.14606
D1	-0.01596	0.00025	-0.00048	0.00128	0.00083	-0.01513
D2	3.12109	-0.00008	-0.00012	0.00037	0.00028	3.12136
D3	3.12827	0.00025	-0.00030	0.00172	0.00145	3.12972
D4	-0.01787	-0.00008	0.00005	0.00081	0.00089	-0.01698
D5	-0.00383	0.00026	-0.00030	0.00080	0.00048	-0.00336
D6	3.14096	0.00010	0.00009	0.00081	0.00090	-3.14133
D7	3.13450	0.00022	-0.00051	0.00013	-0.00044	3.13406
D8	-0.00389	0.00006	-0.00012	0.00014	-0.00002	-0.00391
D9	0.04247	-0.00044	0.00011	-0.00080	-0.00071	0.04176
D10	-3.09056	-0.00006	0.00001	0.00154	0.00156	-3.08900
D11	-3.09616	-0.00039	0.00032	-0.00013	0.00020	-3.09596
D12	0.05400	0.00000	0.00021	0.00220	0.00247	0.05647
D13	0.02406	-0.00050	0.00090	-0.00231	-0.00143	0.02263
D14	-3.12035	-0.00042	0.00070	-0.00183	-0.00115	-3.12150
D15	-3.11213	-0.00012	0.00046	-0.00126	-0.00084	-3.11298
D16	0.02664	-0.00003	0.00025	-0.00079	-0.00056	0.02608
D17	-0.01351	0.00037	-0.00080	-0.00058	-0.00137	-0.01488
D18	3.12379	0.00081	-0.00013	0.00846	0.00838	3.13218
D19	3.12321	0.00003	-0.00040	-0.00148	-0.00187	3.12134
D20	-0.02267	0.00047	0.00026	0.00755	0.00789	-0.01478
D21	-0.01292	0.00039	-0.00054	0.00182	0.00128	-0.01164
D22	3.12484	0.00036	-0.00061	0.00164	0.00103	3.12586
D23	3.13154	0.00031	-0.00033	0.00135	0.00099	3.13253
D24	-0.01389	0.00027	-0.00041	0.00116	0.00074	-0.01315
D25	-0.00625	0.00005	-0.00020	0.00018	-0.00001	-0.00627
D26	3.13158	0.00008	-0.00026	0.00027	0.00001	3.13159
D27	3.13917	0.00009	-0.00013	0.00036	0.00023	3.13940
D28	-0.00619	0.00012	-0.00019	0.00045	0.00025	-0.00594
D29	0.01460	-0.00036	0.00062	-0.00137	-0.00075	0.01385
D30	-3.13013	-0.00020	0.00025	-0.00134	-0.00111	-3.13124
D31	-3.12327	-0.00039	0.00068	-0.00144	-0.00076	-3.12402
D32	0.01519	-0.00023	0.00031	-0.00142	-0.00112	0.01407
D33	-0.04917	0.00025	-0.00086	0.00009	-0.00074	-0.04991
D34	3.09841	0.00026	-0.00093	-0.00685	-0.00804	3.09037
D35	3.08322	-0.00004	-0.00070	-0.00164	-0.00216	3.08106
D36	-0.05239	-0.00003	-0.00078	-0.00858	-0.00946	-0.06185

D37	-0.04184	0.00043	-0.00120	0.00106	-0.00014	-0.04198
D38	3.10741	-0.00037	-0.00069	-0.00653	-0.00723	3.10018
D39	3.11021	0.00090	-0.00124	0.00350	0.00225	3.11246
D40	-0.02373	0.00009	-0.00074	-0.00409	-0.00483	-0.02856
D41	0.03831	-0.00005	0.00125	0.00084	0.00207	0.04038
D42	-3.11001	0.00025	0.00182	0.00856	0.01017	-3.09984
D43	-3.09870	-0.00060	0.00047	-0.00884	-0.00820	-3.10690
D44	0.03617	-0.00030	0.00104	-0.00112	-0.00011	0.03606
D45	-3.09530	-0.00176	0.00150	-0.01634	-0.01486	-3.11015
D46	0.06014	-0.00174	0.00457	-0.00177	0.00272	0.06286
D47	0.05400	-0.00203	0.00105	-0.02529	-0.02415	0.02985
D48	-3.07376	-0.00201	0.00413	-0.01071	-0.00657	-3.08033
D49	0.05987	-0.00120	0.00261	-0.00638	-0.00383	0.05605
D50	-3.05148	-0.00052	0.00702	0.02723	0.03438	-3.01710
D51	-3.09485	-0.00121	-0.00015	-0.02035	-0.02063	-3.11548
D52	0.07698	-0.00052	0.00425	0.01326	0.01758	0.09456
D53	-3.04470	-0.00215	0.01090	0.02620	0.03582	-3.00888
D54	0.06758	-0.00233	0.00720	-0.00541	0.00196	0.06954
D55	2.97138	0.00437	-0.01571	-0.00284	-0.01918	2.95220
D56	-0.22379	0.00191	-0.00931	-0.00497	-0.01487	-0.23866
D57	-0.14682	0.00560	-0.01106	0.02285	0.01180	-0.13502
D58	2.94120	0.00314	-0.00466	0.02073	0.01611	2.95730
D59	-0.11399	0.00333	-0.00280	0.02810	0.02505	-0.08894
D60	3.00529	0.00435	-0.00557	0.02797	0.02213	3.02742
D61	3.03029	0.00266	-0.00340	0.01686	0.01335	3.04363
D62	-0.13361	0.00369	-0.00617	0.01674	0.01042	-0.12319
D63	0.02520	-0.00060	-0.00179	-0.01286	-0.01496	0.01024
D64	-3.12046	0.00039	-0.00088	0.00409	0.00295	-3.11751
D65	0.00483	0.00000	0.00000	-0.00076	-0.00071	0.00412
D66	-3.12067	0.00136	-0.00218	0.00725	0.00520	-3.11547
D67	-3.13291	-0.00093	-0.00086	-0.01681	-0.01785	3.13243
D68	0.02478	0.00042	-0.00304	-0.00879	-0.01194	0.01284
D69	0.16891	-0.00589	0.00891	-0.02985	-0.02114	0.14777
D70	-2.91931	-0.00323	0.00242	-0.02695	-0.02487	-2.94418
D71	-2.94452	-0.00700	0.01247	-0.02898	-0.01658	-2.96110
D72	0.25044	-0.00435	0.00598	-0.02608	-0.02031	0.23013
D73	0.19476	-0.00460	0.00878	-0.02062	-0.01184	0.18293
D74	-1.82202	-0.00738	0.01221	-0.03914	-0.02693	-1.84895
D75	-2.97517	-0.00339	0.00509	-0.02124	-0.01624	-2.99141
D76	1.29123	-0.00616	0.00853	-0.03976	-0.03133	1.25989
D77	0.12596	-0.00349	0.00583	-0.01509	-0.00917	0.11679
D78	-3.01879	-0.00270	0.00422	-0.01147	-0.00721	-3.02599
D79	-3.02700	-0.00435	0.00737	-0.02044	-0.01295	-3.03995
D80	0.11143	-0.00356	0.00576	-0.01681	-0.01098	0.10045
D81	3.05430	0.00107	-0.00219	0.00360	0.00142	3.05572
D82	-0.07030	0.00244	-0.00447	0.01179	0.00737	-0.06293
D83	-0.19272	0.00474	-0.00911	0.02158	0.01244	-0.18028
D84	1.81911	0.00844	-0.01572	0.04184	0.02618	1.84529
D85	2.95290	0.00376	-0.00707	0.01704	0.00996	2.96286
D86	-1.31846	0.00746	-0.01368	0.03730	0.02370	-1.29476
D87	3.08728	0.00155	-0.00247	0.00734	0.00490	3.09218
D88	-0.09854	0.00219	-0.00402	0.01019	0.00624	-0.09230
D89	-0.05828	0.00250	-0.00447	0.01176	0.00733	-0.05095
D90	3.03909	0.00315	-0.00602	0.01461	0.00866	3.04775
D91	0.93858	0.00434	-0.00248	0.01901	0.01649	0.95507
D92	3.04250	0.00458	-0.00325	0.01945	0.01617	3.05866
D93	-1.16276	0.00379	-0.00148	0.01749	0.01597	-1.14679
D94	-0.95437	-0.00433	0.00260	-0.01934	-0.01671	-0.97107
D95	1.14955	-0.00408	0.00184	-0.01890	-0.01703	1.13251
D96	-3.05571	-0.00487	0.00360	-0.02087	-0.01722	-3.07293

D97	0.01288	-0.00092	0.00174	-0.00497	-0.00324	0.00964
D98	3.12175	0.00047	-0.00121	0.00105	-0.00014	3.12161
D99	3.12032	0.00031	-0.00042	0.00121	0.00081	3.12114
D100	0.02407	-0.00055	0.00128	-0.00243	-0.00114	0.02293
D101	-0.07987	0.00215	-0.00462	0.00891	0.00435	-0.07551
D102	3.03783	0.00269	-0.00591	0.01163	0.00580	3.04363
D103	0.04575	-0.00052	0.00077	-0.00246	-0.00167	0.04408
D104	-3.13127	0.00036	-0.00068	0.00105	0.00040	-3.13088
D105	-3.07100	-0.00167	0.00299	-0.00738	-0.00436	-3.07537
D106	0.03516	-0.00079	0.00154	-0.00388	-0.00230	0.03286
D107	3.07920	0.00098	-0.00192	0.00400	0.00207	3.08127
D108	-0.08151	0.00094	-0.00170	0.00444	0.00272	-0.07879
D109	-0.09444	0.00221	-0.00472	0.00940	0.00473	-0.08971
D110	3.02804	0.00217	-0.00450	0.00983	0.00538	3.03342
D111	0.11695	-0.00345	0.00630	-0.01443	-0.00808	0.10886
D112	-3.00830	-0.00392	0.00724	-0.01659	-0.00932	-3.01762
D113	-3.01004	-0.00353	0.00615	-0.01520	-0.00897	-3.01901
D114	0.14790	-0.00400	0.00709	-0.01736	-0.01021	0.13769
D115	2.99363	0.00341	-0.00685	0.01522	0.00843	3.00206
D116	0.76324	-0.00218	0.00395	-0.01477	-0.01092	0.75233
D117	-0.16721	0.00342	-0.00666	0.01590	0.00927	-0.15794
D118	-2.39760	-0.00217	0.00414	-0.01410	-0.01008	-2.40767
D119	3.10583	0.00145	-0.00285	0.00491	0.00209	3.10792
D120	-0.05946	0.00139	-0.00262	0.00587	0.00328	-0.05618
D121	-0.05837	0.00186	-0.00402	0.00713	0.00319	-0.05518
D122	3.05952	0.00180	-0.00379	0.00808	0.00438	3.06390
D123	3.11807	0.00038	-0.00050	0.00252	0.00202	3.12009
D124	-0.04668	0.00042	-0.00043	0.00296	0.00254	-0.04414
D125	-0.00719	0.00033	-0.00065	0.00153	0.00089	-0.00630
D126	3.11125	0.00037	-0.00058	0.00197	0.00141	3.11266
D127	-3.13879	0.00087	-0.00223	0.00205	-0.00019	-3.13898
D128	-0.02209	0.00089	-0.00202	0.00334	0.00131	-0.02079
D129	0.04339	-0.00202	0.00414	-0.00756	-0.00348	0.03991
D130	-3.09594	-0.00075	0.00145	-0.00287	-0.00146	-3.09740
D131	-3.06890	-0.00178	0.00386	-0.00717	-0.00339	-3.07229
D132	0.07496	-0.00052	0.00117	-0.00248	-0.00137	0.07360
D133	0.12811	-0.00195	0.00383	-0.01003	-0.00622	0.12189
D134	2.37133	0.00269	-0.00326	0.01798	0.01472	2.38605
D135	-3.04265	-0.00211	0.00405	-0.01012	-0.00608	-3.04873
D136	-0.79943	0.00253	-0.00304	0.01789	0.01486	-0.78457
D137	-0.06011	0.00302	-0.00593	0.01163	0.00568	-0.05443
D138	3.06858	0.00224	-0.00407	0.01042	0.00634	3.07491
D139	3.07923	0.00178	-0.00324	0.00701	0.00372	3.08295
D140	-0.07527	0.00100	-0.00138	0.00580	0.00438	-0.07088
D141	0.04680	-0.00220	0.00467	-0.00853	-0.00386	0.04294
D142	-3.07976	-0.00156	0.00247	-0.00751	-0.00505	-3.08481
D143	3.08999	0.00148	-0.00226	0.00820	0.00591	3.09590
D144	-0.05081	0.00138	-0.00178	0.00853	0.00673	-0.04408
D145	-0.06712	0.00062	0.00004	0.00658	0.00664	-0.06049
D146	3.07526	0.00052	0.00053	0.00690	0.00746	3.08272
D147	-1.06341	0.00497	-0.00544	0.02328	0.01779	-1.04562
D148	1.04997	0.00514	-0.00587	0.02335	0.01744	1.06740
D149	-3.12850	0.00561	-0.00703	0.02451	0.01742	-3.11108
D150	3.12119	-0.00558	0.00667	-0.02516	-0.01843	3.10276
D151	-1.04862	-0.00542	0.00624	-0.02508	-0.01879	-1.06741
D152	1.05609	-0.00495	0.00508	-0.02393	-0.01880	1.03729
D153	-0.01034	0.00022	0.00075	0.00376	0.00450	-0.00584
D154	3.13725	0.00016	0.00069	0.00308	0.00376	3.14101
D155	3.13041	0.00032	0.00023	0.00342	0.00365	3.13406
D156	-0.00519	0.00027	0.00016	0.00274	0.00291	-0.00228

D157	-3.13985	0.00002	-0.00013	-0.00013	-0.00026	-3.14011
D158	-0.00012	0.00009	-0.00002	0.00086	0.00083	0.00070
D159	-0.00323	0.00004	-0.00003	0.00033	0.00030	-0.00293
D160	3.13650	0.00011	0.00008	0.00131	0.00139	3.13789
D161	-3.14005	-0.00005	0.00004	0.00030	0.00036	-3.13969
D162	0.00444	0.00002	-0.00008	0.00094	0.00081	0.00526
D163	0.00655	-0.00005	0.00005	-0.00021	-0.00016	0.00639
D164	-3.13214	0.00002	-0.00007	0.00043	0.00029	-3.13185
D165	-0.00151	-0.00004	-0.00007	-0.00045	-0.00052	-0.00203
D166	3.13959	0.00002	-0.00011	-0.00007	-0.00018	3.13941
D167	-3.14132	-0.00010	-0.00017	-0.00137	-0.00155	3.14032
D168	-0.00022	-0.00004	-0.00020	-0.00099	-0.00121	-0.00143
D169	-0.00773	0.00008	-0.00008	0.00005	-0.00004	-0.00777
D170	3.13345	0.00009	-0.00014	0.00013	-0.00001	3.13344
D171	3.13118	-0.00007	-0.00003	-0.00085	-0.00094	3.13024
D172	-0.01083	-0.00006	-0.00009	-0.00077	-0.00090	-0.01173
D173	0.00131	-0.00002	-0.00003	0.00021	0.00017	0.00148
D174	3.13733	-0.00008	-0.00009	-0.00094	-0.00104	3.13629
D175	-3.13695	0.00012	-0.00011	0.00113	0.00103	-3.13592
D176	-0.00093	0.00006	-0.00017	-0.00001	-0.00018	-0.00111
D177	0.00581	-0.00004	0.00014	0.00022	0.00036	0.00616
D178	-3.13542	-0.00006	0.00019	0.00012	0.00030	-3.13511
D179	-3.13532	-0.00010	0.00018	-0.00014	0.00004	-3.13528
D180	0.00664	-0.00011	0.00023	-0.00023	-0.00001	0.00663
D181	3.13713	0.00002	-0.00013	0.00005	-0.00006	3.13706
D182	-0.00437	0.00003	-0.00014	0.00001	-0.00012	-0.00450
D183	-0.00501	0.00009	-0.00017	0.00047	0.00031	-0.00470
D184	3.13667	0.00010	-0.00017	0.00042	0.00025	3.13692
D185	3.13896	0.00002	-0.00007	-0.00036	-0.00043	3.13853
D186	-0.00363	0.00002	-0.00009	-0.00029	-0.00038	-0.00401
D187	-0.00309	0.00003	-0.00013	-0.00026	-0.00039	-0.00347
D188	3.13751	0.00003	-0.00015	-0.00019	-0.00034	3.13718
D189	0.00010	-0.00004	-0.00003	-0.00043	-0.00046	-0.00036
D190	-3.14112	-0.00001	0.00002	-0.00013	-0.00011	-3.14123
D191	-3.14159	-0.00004	-0.00002	-0.00038	-0.00039	3.14120
D192	0.00038	-0.00002	0.00002	-0.00008	-0.00005	0.00033
D193	-0.00173	0.00006	-0.00002	0.00042	0.00040	-0.00133
D194	3.13941	0.00004	-0.00003	0.00027	0.00024	3.13965
D195	3.14085	0.00005	-0.00001	0.00034	0.00033	3.14118
D196	-0.00120	0.00003	-0.00001	0.00018	0.00017	-0.00102
D197	0.00325	-0.00003	0.00011	-0.00004	0.00007	0.00332
D198	-3.13790	-0.00002	0.00011	0.00012	0.00023	-3.13767
D199	-3.13872	-0.00006	0.00006	-0.00033	-0.00027	-3.13899
D200	0.00332	-0.00004	0.00007	-0.00018	-0.00011	0.00321

Item	Value	Threshold	Converged?

Maximum Force	0.051740	0.000450	NO

RMS Force	0.007728	0.000300	NO

Maximum Displacement	1.210933	0.001800	NO

RMS Displacement	0.257730	0.001200	NO

Predicted change in Energy=-2.714753D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.972524	-0.471753	-0.194472
2	6	0	-10.263869	-1.677242	-0.094568
3	6	0	-10.891011	-2.918856	-0.052203
4	6	0	-12.281620	-2.958139	-0.139877
5	6	0	-13.008826	-1.766980	-0.252631
6	6	0	-12.372539	-0.521628	-0.272788
7	1	0	-10.299916	-3.823071	0.044302
8	1	0	-12.803736	-3.909447	-0.124927
9	1	0	-14.090606	-1.805450	-0.329875
10	1	0	-12.974836	0.367977	-0.351331
11	6	0	-9.993650	0.670523	-0.198578
12	6	0	-8.806951	-1.415315	-0.051524
13	6	0	-8.624708	0.057618	-0.152683
14	6	0	-7.430450	0.773768	-0.200463
15	6	0	-6.031507	0.451414	-0.206302
16	6	0	-3.638079	-0.336800	0.012147
17	6	0	-3.768023	1.046898	0.114161
18	16	0	-5.169452	-1.142781	-0.225913
19	6	0	-5.087367	1.485133	-0.112221
20	6	0	-2.229964	-0.613695	0.132764
21	6	0	-1.603023	0.615601	0.304694
22	7	0	-2.531151	1.697324	0.459125
23	16	0	-1.101092	-1.962654	0.106203
24	16	0	1.149062	1.672843	0.387398
25	6	0	0.248402	-0.819411	0.222075
26	6	0	-0.178005	0.511570	0.288591
27	6	0	1.680769	-0.916747	0.294878
28	6	0	2.292459	0.338141	0.297442
29	6	0	3.702766	0.109334	0.202233
30	6	0	3.872474	-1.273702	0.220890
31	6	0	5.224468	-1.681982	0.105825
32	6	0	6.106881	-0.591674	0.049065
33	16	0	5.216028	0.966173	0.050988
34	7	0	2.632620	-1.960315	0.382871
35	6	0	7.533490	-0.836434	0.014598
36	6	0	8.635883	-0.012726	-0.086723
37	6	0	8.598998	1.464649	-0.201373
38	6	0	10.073774	-0.434063	-0.107882
39	6	0	9.999900	1.924709	-0.286216
40	6	0	10.874931	0.838373	-0.228748
41	6	0	10.432605	3.254825	-0.408129
42	6	0	12.264866	1.100787	-0.289193
43	6	0	11.796824	3.495380	-0.468477
44	6	0	12.702224	2.415556	-0.406489
45	6	0	10.510514	-1.751074	-0.032107
46	6	0	9.613476	-2.877704	0.075353
47	6	0	11.842312	-2.304333	-0.046238
48	7	0	8.927860	-3.814219	0.159926
49	7	0	12.870777	-2.850818	-0.050217
50	6	0	-10.280156	2.029062	-0.224982
51	6	0	-11.563494	2.682838	-0.301798
52	6	0	-9.290729	3.077620	-0.178286
53	7	0	-12.534858	3.323737	-0.356381
54	7	0	-8.560211	3.984139	-0.137569
55	8	0	-7.942907	-2.276017	0.043667
56	8	0	7.609873	2.188846	-0.224547
57	6	0	2.427626	-3.142584	-0.475275

58	1	0	1.468136	-3.603167	-0.234344
59	1	0	2.445213	-2.876615	-1.537256
60	1	0	3.218382	-3.866515	-0.273318
61	6	0	-2.574227	2.143356	1.883516
62	1	0	-2.812530	1.304589	2.548319
63	1	0	-1.602387	2.558137	2.157564
64	1	0	-3.335910	2.916839	1.988129
65	1	0	5.555706	-2.712178	0.061230
66	1	0	12.992054	0.307647	-0.245743
67	1	0	13.767486	2.617728	-0.451056
68	1	0	12.179574	4.506360	-0.562401
69	1	0	9.697763	4.051384	-0.451505
70	1	0	7.728219	-1.899184	0.084151
71	1	0	-7.535393	1.850958	-0.214734
72	1	0	-5.350427	2.529280	-0.251295

```

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Rotational constants (GHZ):      0.1678664      0.0102656      0.0097120
Standard basis: 6-31G(d,p) (6D, 7F)
There are 916 symmetry adapted cartesian basis functions of A symmetry.
There are 916 symmetry adapted basis functions of A symmetry.
916 basis functions, 1734 primitive gaussians, 916 cartesian basis func-
tions
196 alpha electrons      196 beta electrons
nuclear repulsion energy      6525.6399180510 Hartrees.
NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T
Big=T
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
Nuclear repulsion after empirical dispersion term = 6525.5550222162 Har-
trees.
One-electron integrals computed using PRISM.
NBasis= 916 RedAO= T EigKep= 3.41D-04 NBF= 916
NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916
Initial guess from the checkpoint file: "PBDB.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999971 0.007381 -0.000129 -0.002051 Ang= 0.88 deg.
ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1
AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for in-
itial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-
yADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2001
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 IlCent= 200000004 NGrid=
0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0=
0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RB3LYP) = -3682.96173035 A.U. after 15 cycles
NFock= 15 Conv=0.89D-08 -V/T= 2.0071

```

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1
NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-0.004615358	-0.008597240	-0.002429375
2	6	0.003298252	0.001135614	0.000492893
3	6	-0.000235530	-0.001606935	-0.000024173
4	6	-0.000287104	-0.000264805	-0.000136134
5	6	-0.000187722	-0.001985892	-0.000009564
6	6	0.001748951	-0.002610932	0.000922857
7	1	0.000405196	-0.001198220	0.000838848
8	1	0.000165364	0.000197660	-0.000151397
9	1	-0.000046007	-0.000002678	-0.000539842
10	1	-0.003746063	-0.004351714	-0.002150769
11	6	0.007770629	-0.001466950	0.004127505
12	6	-0.000689838	-0.003499207	0.001612644
13	6	-0.007656942	-0.008479535	-0.004623420
14	6	0.004527952	0.012130368	0.006571706
15	6	0.003694397	0.002856769	0.002437635
16	6	0.007885150	0.007365066	0.007029724
17	6	-0.013754513	0.001760583	-0.008469671
18	16	-0.002701127	-0.001801467	-0.006692469
19	6	0.008034112	-0.012057798	-0.003636128
20	6	-0.004350087	0.008588685	-0.001183430
21	6	0.006069266	-0.014739228	0.001460958
22	7	0.001289962	0.016860460	0.014246807
23	16	-0.003070301	-0.004339367	0.001910130
24	16	-0.000086144	0.003194478	0.003248826
25	6	0.013207931	-0.001691330	0.003511295
26	6	-0.006197724	0.002486429	-0.012750325
27	6	-0.001546767	0.015526543	-0.006268522
28	6	0.004342956	-0.009241731	0.002795273
29	6	-0.007025462	-0.003588897	-0.008601320
30	6	0.018171342	0.007354376	0.008051020
31	6	-0.010427245	0.005043404	-0.011914298
32	6	0.007096520	-0.003634629	0.008341593
33	16	0.002102206	0.003199191	-0.003442690
34	7	-0.021762695	-0.015942165	0.015550993
35	6	-0.014754395	0.000668931	-0.007274779
36	6	0.007185653	-0.000914806	0.003920087
37	6	0.000834994	0.002313117	0.000529761
38	6	-0.006888898	0.002511264	-0.005129656
39	6	-0.008331328	-0.009296231	-0.004583391
40	6	0.012309363	0.002955853	0.007903648
41	6	0.001506280	0.011350177	0.000253814
42	6	-0.003435598	0.013232299	-0.002862675
43	6	0.006639772	-0.000289725	0.004337543
44	6	-0.004971951	-0.003111482	-0.003114515
45	6	0.004700822	0.006220073	0.002987485
46	6	-0.002728389	-0.009268158	-0.001310003
47	6	-0.011029266	-0.013049579	-0.006782548
48	7	0.001574770	0.003677877	0.000886239
49	7	0.000134614	-0.002689730	0.000184796
50	6	-0.004409207	-0.004930467	-0.002133462
51	6	0.008841373	0.009638621	0.004948152
52	6	0.001372753	0.007318915	0.001164949
53	7	-0.000075472	0.003447550	0.000524660

54	7	0.000757642	-0.001480074	0.000397740
55	8	0.003396194	-0.004233392	0.003248879
56	8	0.000593162	0.000395825	0.000350117
57	6	0.003980842	0.002483778	-0.004087172
58	1	0.000436976	0.000675082	-0.000329015
59	1	-0.000387624	-0.000088436	0.000175834
60	1	0.000434477	0.000815820	-0.000262657
61	6	-0.004180123	-0.008598419	0.000846941
62	1	0.000093924	0.000129102	-0.000095594
63	1	-0.000321225	-0.000715100	0.000014749
64	1	-0.000154481	-0.000949532	-0.000142974
65	1	0.002413856	-0.001107355	-0.000873380
66	1	0.004671231	0.003564805	0.002955550
67	1	0.000519904	0.000270991	0.000414281
68	1	-0.000513498	-0.000083660	-0.000364467
69	1	-0.000167465	0.000445057	-0.000250429
70	1	-0.002822289	-0.000725214	-0.001200655
71	1	-0.000568573	0.000686702	0.001282814
72	1	0.001917622	0.002130616	-0.006657845

Cartesian Forces: Max 0.021762695 RMS 0.005865862

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.040581653 RMS 0.006474263

Search for a local minimum.

Step number 9 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 7 8 9

DE= -1.01D-02 DEPred=-2.71D-02 R= 3.73D-01

Trust test= 3.73D-01 RLast= 4.61D-01 DXMaxT set to 8.49D-01

ITU= 0 0 0 1 0 0 0 1 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00230	0.00230	0.00230	0.00230	0.00243
Eigenvalues ---	0.00288	0.00389	0.00445	0.00461	0.00483
Eigenvalues ---	0.00509	0.00542	0.00563	0.00589	0.00615
Eigenvalues ---	0.00632	0.00667	0.00683	0.00686	0.00717
Eigenvalues ---	0.00742	0.00747	0.00760	0.00765	0.00775
Eigenvalues ---	0.00809	0.00818	0.00863	0.00868	0.00896
Eigenvalues ---	0.01013	0.01094	0.01145	0.01150	0.01156
Eigenvalues ---	0.01230	0.01265	0.01269	0.01341	0.01364
Eigenvalues ---	0.01373	0.01397	0.01448	0.01461	0.01480
Eigenvalues ---	0.01584	0.01647	0.01658	0.01756	0.01794
Eigenvalues ---	0.01811	0.01928	0.01953	0.02006	0.02030
Eigenvalues ---	0.02075	0.02075	0.02209	0.02209	0.02776
Eigenvalues ---	0.04825	0.04827	0.04837	0.04894	0.04900
Eigenvalues ---	0.04912	0.05016	0.05017	0.05026	0.07208
Eigenvalues ---	0.07270	0.07446	0.07604	0.12783	0.15003
Eigenvalues ---	0.15299	0.15919	0.15985	0.15997	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues ---	0.16000	0.16003	0.16028	0.17220	0.17771
Eigenvalues ---	0.18793	0.18821	0.19366	0.20516	0.20934
Eigenvalues ---	0.21071	0.21846	0.21930	0.21999	0.22003
Eigenvalues ---	0.22134	0.22285	0.22490	0.22591	0.22615
Eigenvalues ---	0.22659	0.22717	0.22950	0.23134	0.23227

Eigenvalues	---	0.23352	0.23462	0.23761	0.23893	0.24163
Eigenvalues	---	0.24255	0.24270	0.24368	0.24489	0.24515
Eigenvalues	---	0.24604	0.24809	0.24863	0.24880	0.24914
Eigenvalues	---	0.24935	0.24961	0.24974	0.24979	0.24982
Eigenvalues	---	0.24990	0.24992	0.24997	0.24999	0.24999
Eigenvalues	---	0.25000	0.25000	0.25000	0.25000	0.25071
Eigenvalues	---	0.25561	0.25903	0.26205	0.26310	0.26706
Eigenvalues	---	0.26758	0.27023	0.27189	0.27470	0.27811
Eigenvalues	---	0.28003	0.28347	0.28469	0.28639	0.29075
Eigenvalues	---	0.30116	0.30447	0.32673	0.32986	0.35653
Eigenvalues	---	0.35685	0.36328	0.36337	0.36475	0.36574
Eigenvalues	---	0.36651	0.36826	0.36831	0.37081	0.37094
Eigenvalues	---	0.37128	0.37251	0.37274	0.37417	0.37552
Eigenvalues	---	0.37607	0.37673	0.37755	0.37994	0.38877
Eigenvalues	---	0.40300	0.40881	0.41645	0.42261	0.42560
Eigenvalues	---	0.42998	0.44432	0.44870	0.45644	0.46115
Eigenvalues	---	0.47498	0.47899	0.48185	0.52583	0.53468
Eigenvalues	---	0.54644	0.56034	0.57754	0.80401	0.81655
Eigenvalues	---	1.18997	1.25842	1.26334	1.29771	1.35444

RFO step: Lambda=-3.37458414D-02 EMin= 2.29978534D-03

Quartic linear search produced a step of -0.41080.

Iteration 1 RMS(Cart)= 0.15053913 RMS(Int)= 0.00658041

Iteration 2 RMS(Cart)= 0.01518276 RMS(Int)= 0.00037672

Iteration 3 RMS(Cart)= 0.00011393 RMS(Int)= 0.00037496

Iteration 4 RMS(Cart)= 0.00000007 RMS(Int)= 0.00037496

Variable (Linear)	Old X (Quad)	-DE/DX (Total)	Delta X	Delta X	Delta X	New X
R1	2.64924	-0.00005	-0.01037	0.01143	0.00102	2.65026
R2	2.65146	-0.00564	-0.01042	0.00709	-0.00337	2.64809
R3	2.84277	-0.01778	-0.03378	-0.00101	-0.03481	2.80796
R4	2.62985	-0.00357	-0.00708	0.00410	-0.00299	2.62686
R5	2.79850	-0.00081	-0.00982	0.00972	-0.00008	2.79841
R6	2.63413	0.00245	0.00261	-0.00071	0.00193	2.63606
R7	2.04956	0.00030	0.00165	-0.00051	0.00114	2.05070
R8	2.64589	0.00300	0.00667	-0.00394	0.00277	2.64865
R9	2.05087	0.00020	0.00067	0.00000	0.00067	2.05153
R10	2.64303	-0.00127	-0.00253	0.00229	-0.00023	2.64280
R11	2.05076	0.00023	0.00059	0.00007	0.00066	2.05142
R12	2.03559	0.00552	0.01534	-0.00902	0.00632	2.04191
R13	2.83570	-0.01318	-0.01176	-0.04494	-0.05672	2.77898
R14	2.62421	-0.01535	-0.04011	0.03576	-0.00435	2.61986
R15	2.81117	-0.00539	0.00287	-0.01178	-0.00890	2.80227
R16	2.31169	0.00390	-0.00483	0.00981	0.00498	2.31667
R17	2.63304	-0.02438	-0.01677	-0.00163	-0.01840	2.61463
R18	2.71292	-0.01861	-0.00899	-0.01334	-0.02233	2.69059
R19	2.04541	-0.00070	0.00057	0.00095	0.00152	2.04693
R20	3.42504	-0.00939	0.01195	-0.03954	-0.02751	3.39753
R21	2.65157	-0.00119	-0.01459	0.02711	0.01251	2.66408
R22	2.63338	0.00807	-0.00145	0.01540	0.01406	2.64744
R23	3.30101	-0.01075	0.00076	-0.04753	-0.04672	3.25429
R24	2.72147	-0.01285	-0.01525	-0.02079	-0.03575	2.68573
R25	2.66174	-0.01389	-0.02291	0.00180	-0.02124	2.64050
R26	2.72009	-0.00568	-0.01122	0.00343	-0.00796	2.71214
R27	2.05171	-0.00037	0.00536	-0.00609	-0.00072	2.05099
R28	2.62786	0.00381	-0.00786	0.02059	0.01243	2.64029
R29	3.32439	-0.00493	-0.00436	-0.01129	-0.01576	3.30863
R30	2.70923	-0.00651	-0.00821	-0.00917	-0.01767	2.69156
R31	2.70023	-0.01583	-0.02804	-0.00086	-0.02907	2.67116
R32	2.82177	-0.00036	-0.00023	-0.00022	-0.00045	2.82132
R33	3.34944	-0.00542	-0.00459	-0.01363	-0.01788	3.33155

R34	3.33761	-0.00391	-0.00453	-0.00650	-0.01092	3.32669
R35	3.32553	-0.00393	-0.00523	-0.00490	-0.01017	3.31536
R36	2.64410	0.00286	-0.00784	0.01835	0.01082	2.65492
R37	2.71651	-0.01819	-0.03049	-0.00725	-0.03779	2.67872
R38	2.63812	0.00309	-0.00828	0.02141	0.01270	2.65083
R39	2.67434	-0.00974	-0.01504	-0.00804	-0.02283	2.65152
R40	2.70593	-0.01291	-0.01959	-0.00489	-0.02495	2.68098
R41	2.63340	0.00683	-0.00547	0.02188	0.01653	2.64993
R42	3.29865	-0.00669	-0.00283	-0.01920	-0.02201	3.27664
R43	2.67769	-0.01730	-0.02650	-0.00327	-0.02975	2.64795
R44	2.69570	-0.00891	-0.01413	-0.00451	-0.01816	2.67754
R45	2.65279	-0.00267	-0.01547	0.02255	0.00704	2.65983
R46	2.04668	0.00045	0.00128	-0.00032	0.00096	2.04764
R47	3.39126	-0.00320	-0.00247	-0.00945	-0.01198	3.37928
R48	2.73607	-0.01880	-0.02500	-0.02236	-0.04736	2.68871
R49	2.78771	-0.00062	0.00071	-0.00147	-0.00076	2.78695
R50	2.60757	-0.00728	-0.01778	0.01166	-0.00612	2.60145
R51	2.04597	-0.00271	-0.00149	0.00317	0.00168	2.04764
R52	2.80110	0.00004	0.00278	-0.00315	-0.00039	2.80071
R53	2.83176	-0.00709	-0.00254	-0.05658	-0.05910	2.77265
R54	2.79103	-0.00027	-0.00585	0.01163	0.00575	2.79678
R55	2.31703	-0.00069	-0.00297	0.00449	0.00152	2.31855
R56	2.85064	-0.02170	-0.03324	-0.01309	-0.04631	2.80433
R57	2.62597	-0.01553	-0.04501	0.03567	-0.00934	2.61664
R58	2.63826	-0.00039	-0.01668	0.02220	0.00551	2.64376
R59	2.65324	-0.01091	-0.01782	-0.00172	-0.01953	2.63371
R60	2.67544	-0.01328	-0.01813	-0.00670	-0.02487	2.65057
R61	2.62025	0.00546	0.00268	0.00932	0.01203	2.63228
R62	2.04962	0.00019	0.00123	0.00008	0.00131	2.05093
R63	2.62778	0.00171	-0.00617	0.01588	0.00970	2.63748
R64	2.03509	0.00610	0.01919	-0.01137	0.00782	2.04291
R65	2.66553	-0.00241	-0.00158	-0.01057	-0.01213	2.65340
R66	2.05051	0.00025	0.00094	0.00008	0.00102	2.05153
R67	2.05072	0.00025	0.00069	0.00031	0.00100	2.05172
R68	2.72902	-0.00555	0.00444	-0.03219	-0.02775	2.70127
R69	2.72539	-0.00851	-0.00189	-0.03170	-0.03360	2.69179
R70	2.19914	0.00369	0.00232	-0.00172	0.00061	2.19975
R71	2.20086	0.00062	-0.00103	0.00058	-0.00046	2.20041
R72	2.72558	-0.00803	-0.00818	-0.01551	-0.02369	2.70189
R73	2.72581	-0.00548	-0.00284	-0.01666	-0.01950	2.70631
R74	2.20157	-0.00002	-0.00123	0.00109	-0.00013	2.20144
R75	2.20142	0.00152	0.00029	0.00005	0.00034	2.20176
R76	2.06215	0.00061	0.00231	-0.00082	0.00149	2.06364
R77	2.06910	0.00040	0.00239	-0.00085	0.00153	2.07063
R78	2.06159	0.00038	0.00162	-0.00060	0.00101	2.06260
R79	2.07206	0.00018	0.00190	-0.00099	0.00091	2.07296
R80	2.06285	0.00041	0.00189	-0.00042	0.00147	2.06432
R81	2.06091	0.00035	0.00186	-0.00072	0.00113	2.06204
A1	2.06894	0.00639	0.01613	-0.00368	0.01240	2.08134
A2	1.90097	0.00232	0.00124	-0.00168	-0.00046	1.90050
A3	2.31328	-0.00871	-0.01737	0.00537	-0.01193	2.30134
A4	2.14308	-0.00192	-0.00477	0.00160	-0.00321	2.13987
A5	1.92547	-0.00356	-0.00111	-0.01087	-0.01199	1.91349
A6	2.21463	0.00548	0.00588	0.00925	0.01516	2.22979
A7	2.06326	-0.00192	-0.00298	-0.00222	-0.00518	2.05809
A8	2.09546	-0.00045	0.00141	-0.00360	-0.00220	2.09326
A9	2.12446	0.00238	0.00157	0.00582	0.00738	2.13184
A10	2.09351	0.00122	0.00230	0.00254	0.00489	2.09840
A11	2.09877	-0.00065	-0.00205	-0.00059	-0.00266	2.09611
A12	2.09090	-0.00057	-0.00025	-0.00194	-0.00222	2.08867

A13	2.12044	-0.00030	-0.00233	0.00419	0.00188	2.12232
A14	2.08669	0.00036	0.00248	-0.00496	-0.00249	2.08420
A15	2.07605	-0.00006	-0.00015	0.00077	0.00060	2.07666
A16	2.07691	-0.00345	-0.00837	-0.00224	-0.01065	2.06626
A17	2.13250	-0.00099	-0.00093	-0.00180	-0.00271	2.12979
A18	2.07377	0.00444	0.00930	0.00404	0.01336	2.08713
A19	1.85813	0.00183	0.01135	0.00254	0.01384	1.87197
A20	2.22515	-0.02594	-0.03149	-0.02286	-0.05433	2.17083
A21	2.19985	0.02412	0.02015	0.02028	0.04045	2.24030
A22	1.86886	-0.00381	-0.00112	-0.00531	-0.00645	1.86241
A23	2.18060	0.00752	-0.00736	0.01284	0.00548	2.18608
A24	2.23371	-0.00371	0.00848	-0.00750	0.00098	2.23469
A25	1.86997	0.00325	-0.01033	0.01603	0.00567	1.87564
A26	2.17845	0.01759	-0.01446	0.00860	-0.00585	2.17260
A27	2.23476	-0.02085	0.02479	-0.02463	0.00017	2.23493
A28	2.37453	-0.02373	0.02923	-0.01519	0.01391	2.38844
A29	2.01403	0.01163	-0.00949	-0.00407	-0.01369	2.00034
A30	1.89430	0.01210	-0.01963	0.01986	0.00010	1.89440
A31	2.29298	-0.02047	0.01716	-0.04137	-0.02393	2.26905
A32	2.08287	0.00861	-0.02970	0.03259	0.00320	2.08608
A33	1.90571	0.01188	0.01307	0.01006	0.02211	1.92782
A34	1.96749	0.00169	0.00832	-0.00655	0.00157	1.96907
A35	1.85038	0.00046	-0.00275	0.01130	0.00757	1.85795
A36	2.46525	-0.00215	-0.00554	-0.00466	-0.00909	2.45616
A37	1.96548	0.00314	0.00144	0.01356	0.01450	1.97997
A38	1.96720	-0.00102	0.00694	-0.01313	-0.00783	1.95937
A39	2.35013	-0.00209	-0.00834	0.00072	-0.00641	2.34372
A40	1.58045	-0.00604	-0.01894	0.01869	-0.00144	1.57901
A41	1.99526	-0.00994	-0.00506	-0.02187	-0.02859	1.96666
A42	2.13754	0.00288	0.00609	-0.00276	0.00355	2.14108
A43	2.14928	0.00695	-0.00111	0.02210	0.02093	2.17021
A44	1.85584	-0.00034	-0.00389	0.01058	0.00575	1.86159
A45	2.45530	-0.00162	-0.00555	-0.00050	-0.00479	2.45051
A46	1.97188	0.00194	0.00947	-0.01025	-0.00115	1.97074
A47	1.96974	0.00171	0.00984	-0.01153	-0.00317	1.96656
A48	1.96477	-0.00019	-0.00174	0.00449	0.00251	1.96728
A49	2.34867	-0.00151	-0.00810	0.00706	0.00047	2.34914
A50	1.76148	0.00009	-0.01133	0.02831	0.01469	1.77617
A51	1.91644	0.00354	0.00019	0.03231	0.03237	1.94880
A52	1.92496	0.00180	-0.00066	0.02150	0.02029	1.94526
A53	1.56379	-0.00342	-0.01560	0.01844	0.00232	1.56611
A54	1.55745	-0.00309	-0.01621	0.01912	0.00241	1.55986
A55	1.96561	0.00251	0.00979	-0.00958	0.00022	1.96583
A56	2.37213	-0.00290	-0.00720	0.00353	-0.00348	2.36865
A57	1.94514	0.00043	-0.00262	0.00657	0.00356	1.94870
A58	2.34736	-0.00053	-0.00780	0.01135	0.00395	2.35131
A59	1.95381	-0.00057	-0.00231	0.00275	-0.00008	1.95373
A60	1.98136	0.00112	0.01008	-0.01357	-0.00346	1.97789
A61	1.95608	0.00096	-0.00120	0.00778	0.00612	1.96219
A62	2.37931	-0.00280	-0.00784	0.00692	-0.00055	2.37876
A63	1.94768	0.00183	0.00904	-0.01470	-0.00557	1.94211
A64	1.97922	0.00088	0.00966	-0.01398	-0.00442	1.97480
A65	2.44109	0.00015	-0.00642	0.00827	0.00258	2.44367
A66	1.86272	-0.00102	-0.00325	0.00584	0.00194	1.86466
A67	1.85213	-0.00017	-0.00359	0.00959	0.00554	1.85767
A68	2.46732	-0.00116	-0.00398	-0.00074	-0.00435	2.46297
A69	1.96357	0.00134	0.00756	-0.00881	-0.00117	1.96240
A70	1.98349	-0.00008	-0.00013	0.00249	0.00201	1.98549
A71	1.95344	-0.00086	0.00778	-0.02158	-0.01337	1.94007
A72	2.34596	0.00093	-0.00765	0.01902	0.01128	2.35724

A73	1.95979	-0.00073	-0.00358	0.00167	-0.00232	1.95747
A74	2.17636	0.00207	-0.00172	0.01098	0.00931	2.18567
A75	2.14703	-0.00135	0.00531	-0.01274	-0.00736	2.13966
A76	1.94136	0.00417	0.01275	-0.01008	0.00221	1.94357
A77	2.08177	-0.00114	-0.01689	0.02986	0.01310	2.09487
A78	2.25997	-0.00304	0.00413	-0.02002	-0.01575	2.24422
A79	1.57513	-0.00456	-0.01672	0.01794	0.00071	1.57583
A80	1.79527	0.00077	-0.01066	0.03167	0.01957	1.81484
A81	2.05030	0.00110	-0.00047	0.02521	0.02286	2.07316
A82	2.02692	0.00365	0.00094	0.03678	0.03623	2.06316
A83	2.32955	-0.00160	0.00572	-0.00929	-0.00357	2.32598
A84	1.91944	-0.00074	-0.00856	0.01432	0.00576	1.92520
A85	2.03419	0.00235	0.00284	-0.00503	-0.00219	2.03200
A86	2.19047	-0.00645	0.00846	-0.00742	0.00104	2.19152
A87	2.21404	0.00954	0.00242	-0.00317	-0.00075	2.21329
A88	1.87866	-0.00308	-0.01088	0.01060	-0.00029	1.87837
A89	1.86639	-0.00105	-0.00209	-0.00248	-0.00462	1.86177
A90	2.22714	0.00006	0.00512	-0.00652	-0.00138	2.22576
A91	2.18966	0.00099	-0.00303	0.00900	0.00600	2.19565
A92	1.84790	0.00530	0.00845	0.01174	0.02023	1.86813
A93	2.17401	0.03528	0.03547	0.03294	0.06838	2.24239
A94	2.26127	-0.04058	-0.04392	-0.04468	-0.08862	2.17265
A95	1.92810	-0.00429	0.00044	-0.01842	-0.01801	1.91009
A96	2.20483	0.00733	0.00550	0.02123	0.02675	2.23158
A97	2.15025	-0.00304	-0.00594	-0.00281	-0.00873	2.14152
A98	1.90369	0.00313	0.00408	-0.00142	0.00270	1.90639
A99	2.32015	-0.01207	-0.02233	-0.00294	-0.02525	2.29490
A100	2.05934	0.00894	0.01825	0.00437	0.02255	2.08189
A101	2.06162	-0.00169	-0.00227	-0.00378	-0.00600	2.05562
A102	2.08337	0.00034	-0.00189	0.00506	0.00314	2.08651
A103	2.13819	0.00135	0.00416	-0.00127	0.00286	2.14106
A104	2.08017	-0.00423	-0.00855	-0.00637	-0.01497	2.06519
A105	2.12315	-0.00038	-0.00377	0.00328	-0.00046	2.12268
A106	2.07987	0.00461	0.01231	0.00310	0.01544	2.09531
A107	2.09071	0.00139	0.00203	0.00538	0.00746	2.09818
A108	2.10884	-0.00129	0.00063	-0.00738	-0.00678	2.10206
A109	2.08363	-0.00010	-0.00266	0.00200	-0.00068	2.08295
A110	2.12426	-0.00137	-0.00352	0.00323	-0.00029	2.12397
A111	2.08100	0.00000	0.00245	-0.00258	-0.00013	2.08087
A112	2.07792	0.00137	0.00107	-0.00065	0.00042	2.07835
A113	2.15103	0.01871	0.00661	0.01995	0.02656	2.17759
A114	2.28269	-0.03728	-0.03771	-0.07316	-0.11087	2.17182
A115	1.84944	0.01857	0.03110	0.05322	0.08432	1.93376
A116	2.24982	-0.02802	-0.02591	-0.05315	-0.07905	2.17077
A117	2.17612	0.00862	0.00441	0.00230	0.00671	2.18283
A118	1.85725	0.01940	0.02148	0.05085	0.07234	1.92959
A119	1.90923	-0.00017	-0.00126	0.00113	-0.00013	1.90910
A120	1.94691	0.00006	0.00343	-0.00315	0.00028	1.94719
A121	1.90012	0.00035	-0.00157	0.00388	0.00230	1.90242
A122	1.90794	0.00017	-0.00098	0.00221	0.00123	1.90917
A123	1.89270	-0.00067	0.00123	-0.00778	-0.00654	1.88615
A124	1.90615	0.00024	-0.00089	0.00354	0.00264	1.90878
A125	1.93492	0.00032	0.00197	0.00098	0.00295	1.93787
A126	1.90424	-0.00042	-0.00051	-0.00241	-0.00292	1.90131
A127	1.90023	0.00014	-0.00113	0.00105	-0.00008	1.90015
A128	1.90915	0.00028	-0.00062	0.00292	0.00230	1.91145
A129	1.90984	0.00022	-0.00057	0.00303	0.00245	1.91229
A130	1.90521	-0.00056	0.00086	-0.00573	-0.00488	1.90032
A131	3.18179	0.00390	0.00179	0.00626	0.00806	3.18985
A132	3.23647	-0.00578	-0.00849	-0.02802	-0.03650	3.19997

A133	3.25338	-0.00762	-0.00704	-0.05794	-0.06497	3.18841
A134	3.21956	-0.00174	-0.00753	-0.03669	-0.04422	3.17534
A135	3.13660	-0.00015	0.00011	0.00006	0.00017	3.13677
A136	3.14402	-0.00011	-0.00010	-0.00142	-0.00152	3.14250
A137	3.13106	0.00071	-0.00033	0.01025	0.00992	3.14097
A138	3.14606	-0.00005	-0.00019	-0.00090	-0.00109	3.14498
D1	-0.01513	0.00027	-0.00034	0.00465	0.00425	-0.01087
D2	3.12136	0.00000	-0.00011	-0.00005	-0.00019	3.12118
D3	3.12972	0.00029	-0.00059	0.00328	0.00259	3.13231
D4	-0.01698	0.00001	-0.00037	-0.00142	-0.00184	-0.01882
D5	-0.00336	0.00015	-0.00020	0.00313	0.00298	-0.00038
D6	-3.14133	-0.00006	-0.00037	-0.00056	-0.00091	3.14095
D7	3.13406	0.00017	0.00018	0.00486	0.00513	3.13919
D8	-0.00391	-0.00004	0.00001	0.00117	0.00125	-0.00266
D9	0.04176	-0.00040	0.00029	-0.00728	-0.00698	0.03478
D10	-3.08900	-0.00038	-0.00064	-0.00342	-0.00415	-3.09314
D11	-3.09596	-0.00043	-0.00008	-0.00888	-0.00899	-3.10495
D12	0.05647	-0.00041	-0.00102	-0.00502	-0.00616	0.05031
D13	0.02263	-0.00055	0.00059	-0.00917	-0.00853	0.01411
D14	-3.12150	-0.00045	0.00047	-0.00744	-0.00695	-3.12845
D15	-3.11298	-0.00020	0.00035	-0.00359	-0.00314	-3.11612
D16	0.02608	-0.00010	0.00023	-0.00186	-0.00157	0.02451
D17	-0.01488	0.00048	0.00056	0.01017	0.01063	-0.00426
D18	3.13218	0.00059	-0.00344	0.00567	0.00214	3.13431
D19	3.12134	0.00016	0.00077	0.00519	0.00583	3.12717
D20	-0.01478	0.00027	-0.00324	0.00069	-0.00266	-0.01744
D21	-0.01164	0.00030	-0.00053	0.00589	0.00539	-0.00625
D22	3.12586	0.00033	-0.00042	0.00624	0.00582	3.13168
D23	3.13253	0.00020	-0.00041	0.00415	0.00379	3.13632
D24	-0.01315	0.00023	-0.00030	0.00449	0.00422	-0.00893
D25	-0.00627	0.00011	0.00000	0.00164	0.00164	-0.00463
D26	3.13159	0.00013	0.00000	0.00219	0.00219	3.13378
D27	3.13940	0.00008	-0.00009	0.00129	0.00121	3.14060
D28	-0.00594	0.00010	-0.00010	0.00184	0.00176	-0.00417
D29	0.01385	-0.00036	0.00031	-0.00623	-0.00591	0.00794
D30	-3.13124	-0.00017	0.00046	-0.00267	-0.00216	-3.13340
D31	-3.12402	-0.00038	0.00031	-0.00676	-0.00646	-3.13049
D32	0.01407	-0.00020	0.00046	-0.00321	-0.00271	0.01136
D33	-0.04991	0.00057	0.00030	0.01279	0.01315	-0.03675
D34	3.09037	0.00015	0.00330	0.01415	0.01763	3.10800
D35	3.08106	0.00016	0.00089	0.00866	0.00940	3.09045
D36	-0.06185	-0.00026	0.00389	0.01001	0.01387	-0.04798
D37	-0.04198	0.00043	0.00006	0.00857	0.00862	-0.03336
D38	3.10018	-0.00024	0.00297	0.00094	0.00390	3.10408
D39	3.11246	0.00067	-0.00093	0.01333	0.01242	3.12488
D40	-0.02856	0.00000	0.00198	0.00570	0.00769	-0.02087
D41	0.04038	-0.00072	-0.00085	-0.01386	-0.01470	0.02568
D42	-3.09984	-0.00032	-0.00418	-0.01531	-0.01938	-3.11922
D43	-3.10690	-0.00079	0.00337	-0.00910	-0.00588	-3.11278
D44	0.03606	-0.00039	0.00004	-0.01055	-0.01056	0.02551
D45	-3.11015	-0.00171	0.00610	-0.02246	-0.01639	-3.12654
D46	0.06286	-0.00211	-0.00112	-0.05160	-0.05261	0.01025
D47	0.02985	-0.00219	0.00992	-0.02078	-0.01096	0.01889
D48	-3.08033	-0.00259	0.00270	-0.04992	-0.04719	-3.12751
D49	0.05605	-0.00130	0.00157	-0.03982	-0.03878	0.01727
D50	-3.01710	-0.00208	-0.01412	-0.06768	-0.08142	-3.09852
D51	-3.11548	-0.00088	0.00848	-0.01231	-0.00423	-3.11972
D52	0.09456	-0.00166	-0.00722	-0.04018	-0.04687	0.04769
D53	-3.00888	-0.00337	-0.01472	-0.09454	-0.10902	-3.11790
D54	0.06954	-0.00260	-0.00081	-0.06789	-0.06982	-0.00027

D55	2.95220	0.00432	0.00788	0.12371	0.13171	3.08392
D56	-0.23866	0.00189	0.00611	0.06823	0.07560	-0.16306
D57	-0.13502	0.00491	-0.00485	0.10376	0.09845	-0.03658
D58	2.95730	0.00248	-0.00662	0.04829	0.04233	2.99963
D59	-0.08894	0.00207	-0.01029	0.03277	0.02277	-0.06617
D60	3.02742	0.00295	-0.00909	0.07098	0.06246	3.08988
D61	3.04363	0.00172	-0.00548	0.03959	0.03408	3.07772
D62	-0.12319	0.00259	-0.00428	0.07780	0.07377	-0.04942
D63	0.01024	0.00017	0.00615	0.02008	0.02676	0.03700
D64	-3.11751	0.00068	-0.00121	0.00948	0.00943	-3.10807
D65	0.00412	0.00014	0.00029	-0.00094	-0.00119	0.00293
D66	-3.11547	0.00123	-0.00214	0.01111	0.00901	-3.10645
D67	3.13243	-0.00034	0.00733	0.00916	0.01544	-3.13532
D68	0.01284	0.00075	0.00491	0.02120	0.02564	0.03848
D69	0.14777	-0.00571	0.00869	-0.09209	-0.08193	0.06584
D70	-2.94418	-0.00312	0.01022	-0.03538	-0.02413	-2.96831
D71	-2.96110	-0.00690	0.00681	-0.14144	-0.13334	-3.09444
D72	0.23013	-0.00431	0.00834	-0.08474	-0.07554	0.15459
D73	0.18293	-0.00414	0.00486	-0.11478	-0.11035	0.07258
D74	-1.84895	-0.00762	0.01106	-0.16600	-0.15531	-2.00426
D75	-2.99141	-0.00289	0.00667	-0.06503	-0.05907	-3.05048
D76	1.25989	-0.00637	0.01287	-0.11625	-0.10404	1.15586
D77	0.11679	-0.00269	0.00377	-0.07589	-0.07185	0.04494
D78	-3.02599	-0.00199	0.00296	-0.05573	-0.05244	-3.07843
D79	-3.03995	-0.00348	0.00532	-0.08412	-0.07899	-3.11894
D80	0.10045	-0.00278	0.00451	-0.06396	-0.05958	0.04087
D81	3.05572	0.00120	-0.00058	0.03596	0.03469	3.09041
D82	-0.06293	0.00235	-0.00303	0.04834	0.04525	-0.01769
D83	-0.18028	0.00389	-0.00511	0.11415	0.10941	-0.07087
D84	1.84529	0.00867	-0.01075	0.17372	0.16321	2.00850
D85	2.96286	0.00298	-0.00409	0.08802	0.08427	3.04713
D86	-1.29476	0.00776	-0.00974	0.14759	0.13807	-1.15669
D87	3.09218	0.00137	-0.00201	0.03024	0.02806	3.12024
D88	-0.09230	0.00228	-0.00256	0.04701	0.04434	-0.04796
D89	-0.05095	0.00227	-0.00301	0.05630	0.05321	0.00226
D90	3.04775	0.00318	-0.00356	0.07307	0.06949	3.11724
D91	0.95507	0.00146	-0.00677	0.02949	0.02223	0.97731
D92	3.05866	0.00174	-0.00664	0.03217	0.02504	3.08370
D93	-1.14679	0.00090	-0.00656	0.02445	0.01741	-1.12938
D94	-0.97107	-0.00145	0.00686	-0.03238	-0.02503	-0.99610
D95	1.13251	-0.00117	0.00700	-0.02970	-0.02222	1.11029
D96	-3.07293	-0.00201	0.00708	-0.03742	-0.02986	-3.10279
D97	0.00964	-0.00094	0.00133	-0.02051	-0.01940	-0.00976
D98	3.12161	0.00067	0.00006	0.00512	0.00493	3.12653
D99	3.12114	0.00031	-0.00033	0.00402	0.00360	3.12474
D100	0.02293	-0.00059	0.00047	-0.01325	-0.01291	0.01003
D101	-0.07551	0.00225	-0.00179	0.04164	0.03953	-0.03599
D102	3.04363	0.00303	-0.00238	0.05134	0.04847	3.09210
D103	0.04408	-0.00033	0.00068	-0.01037	-0.00969	0.03439
D104	-3.13088	0.00035	-0.00016	0.00324	0.00308	-3.12779
D105	-3.07537	-0.00146	0.00179	-0.02955	-0.02785	-3.10321
D106	0.03286	-0.00078	0.00094	-0.01594	-0.01508	0.01778
D107	3.08127	0.00085	-0.00085	0.02139	0.02056	3.10183
D108	-0.07879	0.00063	-0.00112	0.02147	0.02032	-0.05847
D109	-0.08971	0.00247	-0.00194	0.04662	0.04467	-0.04503
D110	3.03342	0.00225	-0.00221	0.04670	0.04444	3.07785
D111	0.10886	-0.00281	0.00332	-0.05881	-0.05548	0.05338
D112	-3.01762	-0.00335	0.00383	-0.06546	-0.06152	-3.07914
D113	-3.01901	-0.00260	0.00369	-0.05905	-0.05533	-3.07434
D114	0.13769	-0.00314	0.00419	-0.06570	-0.06137	0.07632

D115	3.00206	0.00327	-0.00346	0.06169	0.05851	3.06057
D116	0.75233	-0.00303	0.00448	-0.03234	-0.02766	0.72467
D117	-0.15794	0.00304	-0.00381	0.06194	0.05837	-0.09957
D118	-2.40767	-0.00326	0.00414	-0.03209	-0.02780	-2.43548
D119	3.10792	0.00123	-0.00086	0.02839	0.02762	3.13554
D120	-0.05618	0.00132	-0.00135	0.03021	0.02876	-0.02742
D121	-0.05518	0.00200	-0.00131	0.03752	0.03616	-0.01902
D122	3.06390	0.00209	-0.00180	0.03934	0.03730	3.10120
D123	3.12009	0.00032	-0.00083	0.00407	0.00313	3.12322
D124	-0.04414	0.00019	-0.00104	0.00165	0.00047	-0.04367
D125	-0.00630	0.00029	-0.00037	0.00280	0.00244	-0.00386
D126	3.11266	0.00016	-0.00058	0.00038	-0.00022	3.11244
D127	-3.13898	0.00092	0.00008	0.02398	0.02435	-3.11462
D128	-0.02079	0.00100	-0.00054	0.02602	0.02558	0.00479
D129	0.03991	-0.00195	0.00143	-0.04130	-0.03969	0.00021
D130	-3.09740	-0.00087	0.00060	-0.01549	-0.01475	-3.11215
D131	-3.07229	-0.00174	0.00139	-0.03734	-0.03569	-3.10798
D132	0.07360	-0.00066	0.00056	-0.01154	-0.01075	0.06284
D133	0.12189	-0.00192	0.00256	-0.03690	-0.03474	0.08715
D134	2.38605	0.00273	-0.00605	0.04846	0.04263	2.42868
D135	-3.04873	-0.00212	0.00250	-0.04052	-0.03849	-3.08722
D136	-0.78457	0.00253	-0.00610	0.04484	0.03888	-0.74569
D137	-0.05443	0.00247	-0.00233	0.06013	0.05782	0.00339
D138	3.07491	0.00185	-0.00260	0.04105	0.03821	3.11312
D139	3.08295	0.00141	-0.00153	0.03489	0.03369	3.11664
D140	-0.07088	0.00080	-0.00180	0.01581	0.01407	-0.05681
D141	0.04294	-0.00203	0.00159	-0.04916	-0.04760	-0.00466
D142	-3.08481	-0.00136	0.00207	-0.02805	-0.02616	-3.11096
D143	3.09590	0.00109	-0.00243	0.03147	0.02905	3.12495
D144	-0.04408	0.00095	-0.00276	0.02821	0.02545	-0.01863
D145	-0.06049	0.00041	-0.00273	0.00861	0.00588	-0.05460
D146	3.08272	0.00026	-0.00306	0.00535	0.00228	3.08500
D147	-1.04562	0.00249	-0.00731	0.04885	0.04203	-1.00358
D148	1.06740	0.00262	-0.00716	0.05034	0.04367	1.11108
D149	-3.11108	0.00319	-0.00716	0.05532	0.04867	-3.06241
D150	3.10276	-0.00300	0.00757	-0.05399	-0.04692	3.05583
D151	-1.06741	-0.00286	0.00772	-0.05250	-0.04528	-1.11269
D152	1.03729	-0.00229	0.00772	-0.04752	-0.04029	0.99700
D153	-0.00584	-0.00003	-0.00185	-0.00113	-0.00298	-0.00882
D154	3.14101	-0.00009	-0.00154	-0.00154	-0.00308	3.13793
D155	3.13406	0.00011	-0.00150	0.00231	0.00079	3.13486
D156	-0.00228	0.00006	-0.00119	0.00189	0.00070	-0.00158
D157	-3.14011	-0.00003	0.00011	0.00056	0.00068	-3.13943
D158	0.00070	-0.00001	-0.00034	0.00081	0.00049	0.00119
D159	-0.00293	0.00005	-0.00012	0.00088	0.00075	-0.00218
D160	3.13789	0.00008	-0.00057	0.00113	0.00056	3.13845
D161	-3.13969	-0.00002	-0.00015	-0.00119	-0.00137	-3.14106
D162	0.00526	0.00013	-0.00033	0.00021	-0.00006	0.00519
D163	0.00639	-0.00005	0.00006	-0.00151	-0.00146	0.00493
D164	-3.13185	0.00010	-0.00012	-0.00011	-0.00015	-3.13200
D165	-0.00203	0.00003	0.00021	0.00021	0.00042	-0.00161
D166	3.13941	0.00007	0.00007	0.00110	0.00119	3.14059
D167	3.14032	0.00000	0.00064	-0.00002	0.00061	3.14093
D168	-0.00143	0.00004	0.00050	0.00086	0.00137	-0.00005
D169	-0.00777	0.00005	0.00002	0.00168	0.00171	-0.00606
D170	3.13344	0.00009	0.00000	0.00223	0.00224	3.13568
D171	3.13024	0.00009	0.00038	0.00040	0.00087	3.13111
D172	-0.01173	0.00013	0.00037	0.00095	0.00139	-0.01034
D173	0.00148	0.00008	-0.00007	0.00007	0.00000	0.00148
D174	3.13629	0.00011	0.00043	0.00076	0.00119	3.13748

D175	-3.13592	0.00013	-0.00042	0.00165	0.00122	-3.13470
D176	-0.00111	0.00016	0.00007	0.00234	0.00241	0.00130
D177	0.00616	-0.00005	-0.00015	-0.00128	-0.00141	0.00475
D178	-3.13511	-0.00008	-0.00012	-0.00173	-0.00185	-3.13697
D179	-3.13528	-0.00010	-0.00002	-0.00213	-0.00213	-3.13741
D180	0.00663	-0.00012	0.00001	-0.00259	-0.00257	0.00405
D181	3.13706	0.00006	0.00003	0.00083	0.00082	3.13788
D182	-0.00450	0.00006	0.00005	0.00125	0.00127	-0.00323
D183	-0.00470	0.00011	-0.00013	0.00182	0.00168	-0.00303
D184	3.13692	0.00011	-0.00010	0.00224	0.00213	3.13905
D185	3.13853	0.00004	0.00018	0.00080	0.00097	3.13950
D186	-0.00401	0.00006	0.00016	0.00134	0.00149	-0.00251
D187	-0.00347	0.00008	0.00016	0.00139	0.00154	-0.00194
D188	3.13718	0.00010	0.00014	0.00193	0.00206	3.13924
D189	-0.00036	0.00002	0.00019	0.00017	0.00034	-0.00002
D190	-3.14123	-0.00001	0.00005	-0.00002	0.00003	-3.14120
D191	3.14120	0.00002	0.00016	-0.00026	-0.00012	3.14108
D192	0.00033	-0.00002	0.00002	-0.00045	-0.00044	-0.00011
D193	-0.00133	0.00001	-0.00016	0.00048	0.00033	-0.00100
D194	3.13965	0.00002	-0.00010	0.00056	0.00047	3.14012
D195	3.14118	-0.00001	-0.00014	-0.00004	-0.00018	3.14100
D196	-0.00102	0.00000	-0.00007	0.00004	-0.00004	-0.00106
D197	0.00332	-0.00007	-0.00003	-0.00128	-0.00130	0.00202
D198	-3.13767	-0.00007	-0.00009	-0.00135	-0.00144	-3.13911
D199	-3.13899	-0.00003	0.00011	-0.00109	-0.00099	-3.13998
D200	0.00321	-0.00004	0.00005	-0.00117	-0.00113	0.00208

Item	Value	Threshold	Converged?

Maximum Force	0.040582	0.000450	NO

RMS Force	0.006474	0.000300	NO

Maximum Displacement	1.028256	0.001800	NO

RMS Displacement	0.154238	0.001200	NO

Predicted change in Energy=-3.091133D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.893714	-0.487476	-0.223200
2	6	0	-10.196548	-1.698393	-0.102671
3	6	0	-10.836318	-2.932345	-0.083483
4	6	0	-12.225707	-2.949699	-0.206628
5	6	0	-12.937625	-1.749412	-0.336962
6	6	0	-12.289758	-0.510031	-0.342460
7	1	0	-10.254769	-3.842227	0.023929
8	1	0	-12.760622	-3.894393	-0.205334
9	1	0	-14.017963	-1.778696	-0.439264
10	1	0	-12.871496	0.395589	-0.437215
11	6	0	-9.918785	0.633583	-0.197308
12	6	0	-8.742716	-1.429386	-0.019336
13	6	0	-8.575904	0.041756	-0.102448
14	6	0	-7.398565	0.768481	-0.092188
15	6	0	-6.004435	0.486594	-0.027870

16	6	0	-3.630211	-0.279463	0.130726
17	6	0	-3.760903	1.115304	0.146367
18	16	0	-5.146775	-1.091528	0.052022
19	6	0	-5.081400	1.551483	0.010482
20	6	0	-2.237018	-0.553899	0.190539
21	6	0	-1.587219	0.681846	0.243536
22	7	0	-2.495247	1.778562	0.280559
23	16	0	-1.127067	-1.907932	0.181317
24	16	0	1.163525	1.697876	0.239537
25	6	0	0.230929	-0.784305	0.218872
26	6	0	-0.179140	0.559429	0.224443
27	6	0	1.643347	-0.900244	0.250275
28	6	0	2.283491	0.347581	0.220694
29	6	0	3.678282	0.092836	0.171620
30	6	0	3.828238	-1.301134	0.199013
31	6	0	5.161569	-1.726940	0.132873
32	6	0	6.060406	-0.646728	0.053187
33	16	0	5.198640	0.920090	0.068431
34	7	0	2.573691	-1.948141	0.321841
35	6	0	7.462009	-0.888196	0.013508
36	6	0	8.559521	-0.062337	-0.078842
37	6	0	8.520092	1.415938	-0.177232
38	6	0	9.968222	-0.471805	-0.104342
39	6	0	9.925184	1.873710	-0.258095
40	6	0	10.779042	0.766455	-0.211582
41	6	0	10.393813	3.181964	-0.364176
42	6	0	12.166109	0.966855	-0.268370
43	6	0	11.772102	3.375186	-0.421398
44	6	0	12.642602	2.274568	-0.372281
45	6	0	10.494731	-1.751231	-0.048203
46	6	0	9.719329	-2.948316	0.047018
47	6	0	11.886629	-2.051783	-0.084303
48	7	0	9.135810	-3.952759	0.122040
49	7	0	13.008280	-2.363375	-0.109797
50	6	0	-10.266882	1.974891	-0.239149
51	6	0	-11.607916	2.457743	-0.352075
52	6	0	-9.343163	3.067174	-0.171162
53	7	0	-12.680882	2.902024	-0.444116
54	7	0	-8.622276	3.980685	-0.113474
55	8	0	-7.870803	-2.283006	0.098988
56	8	0	7.528099	2.137797	-0.191632
57	6	0	2.335638	-3.164870	-0.476849
58	1	0	1.366689	-3.590917	-0.208238
59	1	0	2.353754	-2.951233	-1.551398
60	1	0	3.106213	-3.901076	-0.241170
61	6	0	-2.398127	2.524647	1.570095
62	1	0	-2.579182	1.860208	2.423953
63	1	0	-1.400269	2.961423	1.652683
64	1	0	-3.136352	3.328208	1.569376
65	1	0	5.487603	-2.760128	0.114629
66	1	0	12.860324	0.138893	-0.233164
67	1	0	13.713724	2.446576	-0.415909
68	1	0	12.184199	4.376158	-0.503891
69	1	0	9.685125	4.003226	-0.398475
70	1	0	7.662199	-1.951502	0.071985
71	1	0	-7.530566	1.841996	-0.150822
72	1	0	-5.371163	2.584307	-0.154640

Rotational constants (GHZ): 0.1743779 0.0103198 0.0097725
Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.
 There are 916 symmetry adapted basis functions of A symmetry.
 916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions
 196 alpha electrons 196 beta electrons
 nuclear repulsion energy 6557.3798146590 Hartrees.
 NAToms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T
 Big=T
 Integral buffers will be 131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 Nuclear repulsion after empirical dispersion term = 6557.2943519956 Hartrees.
 One-electron integrals computed using PRISM.
 NBasis= 916 RedAO= T EigKep= 3.29D-04 NBF= 916
 NBSUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916
 Initial guess from the checkpoint file: "PBDB.chk"
 B after Tr= 0.000000 0.000000 0.000000
 Rot= 0.999977 0.006703 -0.000174 -0.000661 Ang= 0.77 deg.
 ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1
 AccDes= 0.00D+00
 Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.
 HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-yADJ=14
 ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
 FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2001
 NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
 wScrn= 0.000000 ICntrl= 500 IOpCl= 0 IlCent= 200000004 NGrid= 0
 NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 Integral accuracy reduced to 1.0D-05 until final iterations.
 Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
 SCF Done: E(RB3LYP) = -3682.99349426 A.U. after 14 cycles
 NFock= 14 Conv=0.86D-08 -V/T= 2.0069
 Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1
 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-0.003326204	-0.001338739	-0.001455070
2	6	0.001881911	0.001545696	0.001273051
3	6	0.000124968	-0.001723213	-0.000030842
4	6	-0.000469166	0.000374015	-0.000226526
5	6	0.000228659	-0.000853811	0.000277751
6	6	0.001113174	0.000637922	0.000330437
7	1	-0.000118017	-0.000495973	0.000383437
8	1	0.000051362	0.000051940	-0.000158771
9	1	0.000051135	-0.000068172	-0.000317177
10	1	-0.000332651	0.000041842	0.000110216
11	6	-0.001379474	-0.001165599	-0.001211960
12	6	0.004181912	0.000657221	0.001953878

13	6	-0.000254528	-0.006478100	-0.001197719
14	6	0.000745273	0.002924375	0.003281394
15	6	0.002281408	0.000128356	-0.000979399
16	6	0.005197678	0.000375062	0.002033809
17	6	-0.006682855	-0.006059968	-0.003003246
18	16	-0.007495785	0.006589157	-0.002549882
19	6	0.003218284	-0.002209544	0.003755359
20	6	-0.001016755	0.001428894	0.000407545
21	6	-0.002642157	-0.008118374	0.000876414
22	7	0.009639972	0.018707852	0.001031437
23	16	-0.000058590	0.000178110	0.001617811
24	16	-0.000111014	0.000553983	0.000466487
25	6	0.002788844	0.000047288	0.000320512
26	6	-0.000190351	0.000115047	-0.005056206
27	6	0.002393025	0.005855292	-0.001648403
28	6	0.003071353	-0.004168328	0.000671781
29	6	-0.003807521	-0.001780824	-0.004588842
30	6	0.008820975	0.008025170	0.001677198
31	6	-0.006588508	0.001738117	-0.002965889
32	6	0.001461943	0.001671231	-0.000049092
33	16	-0.001811701	0.000126497	-0.002123996
34	7	-0.012929694	-0.008621712	0.012532082
35	6	-0.003595377	0.001425920	-0.001584248
36	6	0.001015104	-0.000135714	0.000173289
37	6	-0.000214732	-0.000785263	-0.000049476
38	6	0.000962151	0.001430260	0.000691945
39	6	-0.005169843	-0.003789700	-0.003218786
40	6	0.005825697	-0.000585626	0.003911611
41	6	0.000275329	0.005187758	-0.000039760
42	6	-0.001078071	0.001769580	-0.000787293
43	6	0.001869426	-0.000913222	0.001332353
44	6	-0.001259356	-0.001384071	-0.000822311
45	6	-0.002548115	0.002101291	-0.001797204
46	6	-0.001919277	-0.002626049	-0.001244683
47	6	0.000903932	-0.002155419	0.000632173
48	7	-0.000547509	0.003457978	-0.000489101
49	7	0.001087923	-0.001180992	0.000781540
50	6	-0.000741945	-0.002005151	-0.000174054
51	6	0.001205932	0.002429671	0.000549536
52	6	0.001629450	0.002834656	0.001314739
53	7	-0.000181008	0.000238469	-0.000036034
54	7	0.000011466	-0.001323273	-0.000069856
55	8	0.000631545	-0.004724270	0.001043074
56	8	0.001961332	-0.001132430	0.001240560
57	6	0.004241460	0.001464202	-0.004967390
58	1	0.000141565	-0.000030613	-0.000088335
59	1	0.000012367	-0.000195787	-0.000334012
60	1	0.000055196	0.000104030	-0.000195756
61	6	-0.006100284	-0.007361739	0.003341085
62	1	-0.000466370	-0.000413514	0.000316540
63	1	-0.000318453	-0.000079583	-0.000359086
64	1	0.000179049	-0.000623024	-0.000004199
65	1	0.001358748	-0.000802537	-0.000655955
66	1	-0.000029540	-0.001116482	0.000022897
67	1	0.000275148	0.000428384	0.000241200
68	1	-0.000398201	0.000115005	-0.000301681
69	1	0.000246614	-0.000328906	0.000124639
70	1	0.000558002	-0.000136733	0.001088775
71	1	-0.000022967	0.000318446	0.000086872
72	1	0.002106705	0.001833735	-0.005111188

Cartesian Forces: Max 0.018707852 RMS 0.003132942

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.023958966 RMS 0.002950026

Search for a local minimum.

Step number 10 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 9 10

DE= -3.18D-02 DEPred=-3.09D-02 R= 1.03D+00

TightC=F SS= 1.41D+00 RLast= 6.58D-01 DXNew= 1.4270D+00 1.9738D+00

Trust test= 1.03D+00 RLast= 6.58D-01 DXMaxT set to 1.43D+00

ITU= 1 0 0 0 1 0 0 0 1 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00230	0.00230	0.00230	0.00231	0.00242
Eigenvalues ---	0.00290	0.00388	0.00445	0.00458	0.00482
Eigenvalues ---	0.00510	0.00532	0.00556	0.00594	0.00615
Eigenvalues ---	0.00624	0.00667	0.00683	0.00683	0.00716
Eigenvalues ---	0.00736	0.00747	0.00760	0.00771	0.00774
Eigenvalues ---	0.00815	0.00849	0.00855	0.00866	0.00884
Eigenvalues ---	0.00981	0.01092	0.01134	0.01137	0.01153
Eigenvalues ---	0.01250	0.01269	0.01293	0.01337	0.01363
Eigenvalues ---	0.01374	0.01399	0.01448	0.01462	0.01533
Eigenvalues ---	0.01582	0.01646	0.01655	0.01754	0.01794
Eigenvalues ---	0.01806	0.01929	0.01953	0.02006	0.02027
Eigenvalues ---	0.02075	0.02075	0.02209	0.02210	0.02344
Eigenvalues ---	0.04248	0.04827	0.04837	0.04841	0.04867
Eigenvalues ---	0.04900	0.04934	0.05016	0.05039	0.07182
Eigenvalues ---	0.07252	0.07469	0.07602	0.13295	0.15517
Eigenvalues ---	0.15637	0.15935	0.15994	0.15996	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16002
Eigenvalues ---	0.16005	0.16025	0.16095	0.17263	0.17637
Eigenvalues ---	0.18243	0.19180	0.19656	0.19872	0.20788
Eigenvalues ---	0.21079	0.21997	0.21999	0.22014	0.22178
Eigenvalues ---	0.22245	0.22390	0.22570	0.22595	0.22602
Eigenvalues ---	0.22688	0.22744	0.22821	0.23083	0.23301
Eigenvalues ---	0.23373	0.23416	0.23777	0.23923	0.24173
Eigenvalues ---	0.24215	0.24272	0.24480	0.24488	0.24513
Eigenvalues ---	0.24619	0.24854	0.24947	0.24971	0.24974
Eigenvalues ---	0.24979	0.24987	0.24990	0.24992	0.24992
Eigenvalues ---	0.24994	0.24994	0.24998	0.24999	0.25000
Eigenvalues ---	0.25000	0.25000	0.25000	0.25012	0.25449
Eigenvalues ---	0.25579	0.25930	0.26302	0.26551	0.26764
Eigenvalues ---	0.26831	0.27025	0.27157	0.27343	0.27903
Eigenvalues ---	0.27960	0.28360	0.28494	0.28640	0.28881
Eigenvalues ---	0.30171	0.30554	0.32525	0.32999	0.35571
Eigenvalues ---	0.35832	0.36333	0.36337	0.36475	0.36595
Eigenvalues ---	0.36651	0.36827	0.36830	0.37080	0.37093
Eigenvalues ---	0.37101	0.37251	0.37274	0.37417	0.37562
Eigenvalues ---	0.37670	0.37754	0.37976	0.38438	0.38870
Eigenvalues ---	0.40333	0.40892	0.41638	0.42273	0.42612
Eigenvalues ---	0.43482	0.44435	0.44889	0.45663	0.46113
Eigenvalues ---	0.47487	0.47934	0.48068	0.52080	0.52737
Eigenvalues ---	0.55341	0.56515	0.57744	0.80384	0.81680

Eigenvalues --- 1.04792 1.25843 1.26315 1.29437 1.35399
 RFO step: Lambda=-1.62119751D-02 EMin= 2.30001903D-03
 Quartic linear search produced a step of 0.24238.
 Iteration 1 RMS(Cart)= 0.27786140 RMS(Int)= 0.00782024
 Iteration 2 RMS(Cart)= 0.02450051 RMS(Int)= 0.00052284
 Iteration 3 RMS(Cart)= 0.00029733 RMS(Int)= 0.00051237
 Iteration 4 RMS(Cart)= 0.00000036 RMS(Int)= 0.00051237
 Variable Old X -DE/DX Delta X Delta X Delta X New X
 (Linear) (Quad) (Total)
 R1 2.65026 0.00377 0.00025 0.00647 0.00671 2.65697
 R2 2.64809 -0.00080 -0.00082 -0.00160 -0.00241 2.64568
 R3 2.80796 0.00066 -0.00084 0.00586 -0.00258 2.80539
 R4 2.62686 -0.00209 -0.00072 -0.00511 -0.00584 2.62102
 R5 2.79841 -0.00098 -0.00002 -0.00810 -0.00812 2.79029
 R6 2.63606 0.00045 0.00047 0.00027 0.00073 2.63680
 R7 2.05070 -0.00009 0.00028 0.00014 0.00042 2.05112
 R8 2.64865 0.00003 0.00067 -0.00139 -0.00072 2.64793
 R9 2.05153 0.00004 0.00016 0.00028 0.00044 2.05198
 R10 2.64280 -0.00062 -0.00006 -0.00113 -0.00119 2.64161
 R11 2.05142 0.00003 0.00016 0.00024 0.00040 2.05182
 R12 2.04191 0.00020 0.00153 -0.00006 0.00147 2.04337
 R13 2.77898 -0.00091 -0.01375 0.00345 -0.01029 2.76869
 R14 2.61986 -0.00330 -0.00105 -0.00547 -0.00653 2.61334
 R15 2.80227 -0.00348 -0.00216 -0.00671 -0.00885 2.79342
 R16 2.31667 0.00041 0.00121 -0.00214 -0.00093 2.31574
 R17 2.61463 -0.01238 -0.00446 -0.00277 -0.00723 2.60740
 R18 2.69059 -0.01002 -0.00541 -0.01789 -0.02330 2.66728
 R19 2.04693 -0.00025 0.00037 -0.00004 0.00033 2.04726
 R20 3.39753 -0.00541 -0.00667 -0.01480 -0.02115 3.37638
 R21 2.66408 -0.00309 0.00303 -0.00438 -0.00106 2.66302
 R22 2.64744 0.00409 0.00341 0.00785 0.01073 2.65816
 R23 3.25429 0.00139 -0.01133 0.01197 0.00046 3.25475
 R24 2.68573 -0.00396 -0.00866 -0.01009 -0.01921 2.66652
 R25 2.64050 -0.00536 -0.00515 -0.02100 -0.02625 2.61425
 R26 2.71214 -0.00538 -0.00193 -0.02161 -0.02322 2.68892
 R27 2.05099 -0.00083 -0.00018 -0.00121 -0.00139 2.04960
 R28 2.64029 0.00163 0.00301 0.00385 0.00645 2.64674
 R29 3.30863 -0.00093 -0.00382 -0.00341 -0.00737 3.30126
 R30 2.69156 -0.00491 -0.00428 -0.02351 -0.02740 2.66417
 R31 2.67116 -0.00511 -0.00705 -0.02013 -0.02729 2.64388
 R32 2.82132 -0.00153 -0.00011 -0.00508 -0.00519 2.81612
 R33 3.33155 -0.00138 -0.00433 -0.00528 -0.00932 3.32223
 R34 3.32669 -0.00106 -0.00265 -0.00382 -0.00651 3.32018
 R35 3.31536 -0.00119 -0.00246 -0.00448 -0.00694 3.30842
 R36 2.65492 0.00101 0.00262 0.00169 0.00454 2.65946
 R37 2.67872 -0.00552 -0.00916 -0.02348 -0.03262 2.64610
 R38 2.65083 0.00182 0.00308 0.00429 0.00709 2.65792
 R39 2.65152 -0.00478 -0.00553 -0.02281 -0.02773 2.62378
 R40 2.68098 -0.00629 -0.00605 -0.02123 -0.02812 2.65286
 R41 2.64993 0.00428 0.00401 0.00888 0.01280 2.66273
 R42 3.27664 -0.00111 -0.00533 -0.00267 -0.00804 3.26860
 R43 2.64795 -0.00801 -0.00721 -0.03104 -0.03816 2.60978
 R44 2.67754 -0.00599 -0.00440 -0.02458 -0.02827 2.64928
 R45 2.65983 -0.00104 0.00171 -0.00153 0.00016 2.65999
 R46 2.04764 0.00007 0.00023 0.00036 0.00059 2.04823
 R47 3.37928 0.00117 -0.00290 0.00758 0.00458 3.38385
 R48 2.68871 -0.00118 -0.01148 0.00646 -0.00502 2.68369
 R49 2.78695 -0.00297 -0.00019 -0.00887 -0.00905 2.77790
 R50 2.60145 0.00192 -0.00148 0.01319 0.01171 2.61316
 R51 2.04764 0.00069 0.00041 0.00203 0.00244 2.05008

R52	2.80071	0.00035	-0.00009	0.00056	0.00045	2.80115
R53	2.77265	-0.00104	-0.01432	0.00175	-0.01257	2.76009
R54	2.79678	-0.00068	0.00139	-0.00503	-0.00366	2.79312
R55	2.31855	-0.00233	0.00037	-0.00378	-0.00341	2.31513
R56	2.80433	0.00088	-0.01122	0.01112	-0.00008	2.80425
R57	2.61664	-0.00337	-0.00226	-0.00422	-0.00648	2.61015
R58	2.64376	0.00416	0.00133	0.00922	0.01057	2.65433
R59	2.63371	-0.00399	-0.00473	-0.01459	-0.01932	2.61438
R60	2.65057	-0.00094	-0.00603	-0.00239	-0.00841	2.64216
R61	2.63228	0.00123	0.00292	0.00243	0.00534	2.63762
R62	2.05093	-0.00020	0.00032	-0.00014	0.00018	2.05111
R63	2.63748	0.00068	0.00235	0.00198	0.00433	2.64180
R64	2.04291	-0.00027	0.00190	-0.00097	0.00093	2.04384
R65	2.65340	-0.00114	-0.00294	-0.00765	-0.01060	2.64279
R66	2.05153	0.00001	0.00025	0.00032	0.00056	2.05209
R67	2.05172	-0.00005	0.00024	0.00008	0.00032	2.05204
R68	2.70127	0.00063	-0.00673	0.00425	-0.00248	2.69879
R69	2.69179	0.00361	-0.00814	0.01556	0.00742	2.69921
R70	2.19975	0.00335	0.00015	0.00314	0.00328	2.20303
R71	2.20041	0.00168	-0.00011	0.00163	0.00152	2.20193
R72	2.70189	-0.00033	-0.00574	-0.00024	-0.00599	2.69590
R73	2.70631	-0.00138	-0.00473	-0.00402	-0.00875	2.69756
R74	2.20144	0.00023	-0.00003	0.00027	0.00024	2.20168
R75	2.20176	0.00132	0.00008	0.00156	0.00164	2.20340
R76	2.06364	-0.00003	0.00036	0.00035	0.00071	2.06435
R77	2.07063	-0.00021	0.00037	-0.00005	0.00032	2.07096
R78	2.06260	-0.00001	0.00025	0.00024	0.00049	2.06309
R79	2.07296	-0.00070	0.00022	-0.00162	-0.00140	2.07156
R80	2.06432	-0.00015	0.00036	0.00005	0.00040	2.06472
R81	2.06204	-0.00002	0.00027	0.00032	0.00059	2.06264
A1	2.08134	-0.00086	0.00301	-0.00635	-0.00334	2.07800
A2	1.90050	0.00008	-0.00011	-0.00250	-0.00263	1.89787
A3	2.30134	0.00078	-0.00289	0.00885	0.00597	2.30731
A4	2.13987	0.00032	-0.00078	0.00328	0.00250	2.14237
A5	1.91349	-0.00019	-0.00291	0.00201	-0.00091	1.91257
A6	2.22979	-0.00013	0.00367	-0.00528	-0.00159	2.22820
A7	2.05809	-0.00009	-0.00125	0.00115	-0.00012	2.05796
A8	2.09326	-0.00044	-0.00053	-0.00320	-0.00372	2.08953
A9	2.13184	0.00053	0.00179	0.00205	0.00385	2.13569
A10	2.09840	-0.00008	0.00118	-0.00280	-0.00163	2.09677
A11	2.09611	0.00008	-0.00065	0.00193	0.00129	2.09739
A12	2.08867	0.00000	-0.00054	0.00088	0.00035	2.08902
A13	2.12232	0.00056	0.00046	0.00177	0.00222	2.12455
A14	2.08420	-0.00014	-0.00060	-0.00002	-0.00062	2.08358
A15	2.07666	-0.00042	0.00015	-0.00175	-0.00160	2.07506
A16	2.06626	0.00015	-0.00258	0.00303	0.00044	2.06671
A17	2.12979	0.00007	-0.00066	0.00131	0.00066	2.13045
A18	2.08713	-0.00021	0.00324	-0.00434	-0.00110	2.08603
A19	1.87197	-0.00279	0.00335	-0.00468	-0.00132	1.87065
A20	2.17083	-0.00006	-0.01317	0.01182	-0.00135	2.16948
A21	2.24030	0.00285	0.00980	-0.00714	0.00266	2.24295
A22	1.86241	-0.00126	-0.00156	0.00114	-0.00046	1.86195
A23	2.18608	0.00619	0.00133	0.00513	0.00642	2.19250
A24	2.23469	-0.00493	0.00024	-0.00622	-0.00603	2.22866
A25	1.87564	0.00417	0.00137	0.00415	0.00554	1.88118
A26	2.17260	0.01534	-0.00142	0.02585	0.02442	2.19702
A27	2.23493	-0.01951	0.00004	-0.02999	-0.02996	2.20498
A28	2.38844	-0.02396	0.00337	-0.02817	-0.02483	2.36361
A29	2.00034	0.01177	-0.00332	0.01523	0.01187	2.01221
A30	1.89440	0.01219	0.00002	0.01297	0.01296	1.90736

A31	2.26905	-0.01593	-0.00580	-0.01890	-0.02482	2.24424
A32	2.08608	0.00910	0.00078	0.00446	0.00511	2.09119
A33	1.92782	0.00683	0.00536	0.01482	0.01993	1.94775
A34	1.96907	0.00053	0.00038	0.00051	0.00075	1.96982
A35	1.85795	-0.00092	0.00183	-0.00104	-0.00071	1.85724
A36	2.45616	0.00039	-0.00220	0.00055	-0.00004	2.45613
A37	1.97997	0.00000	0.00351	0.00194	0.00479	1.98477
A38	1.95937	0.00026	-0.00190	-0.00474	-0.00769	1.95168
A39	2.34372	-0.00026	-0.00155	0.00253	0.00208	2.34580
A40	1.57901	-0.00416	-0.00035	-0.01054	-0.01164	1.56738
A41	1.96666	-0.00309	-0.00693	-0.00401	-0.01179	1.95487
A42	2.14108	-0.00012	0.00086	-0.00524	-0.00447	2.13661
A43	2.17021	0.00330	0.00507	0.01449	0.01945	2.18966
A44	1.86159	-0.00096	0.00139	0.00096	0.00085	1.86244
A45	2.45051	-0.00074	-0.00116	-0.00448	-0.00419	2.44633
A46	1.97074	0.00168	-0.00028	0.00368	0.00342	1.97416
A47	1.96656	0.00127	-0.00077	-0.00387	-0.00553	1.96103
A48	1.96728	-0.00061	0.00061	0.00136	0.00145	1.96873
A49	2.34914	-0.00067	0.00011	0.00210	0.00323	2.35237
A50	1.77617	0.00052	0.00356	0.01644	0.01506	1.79123
A51	1.94880	0.00301	0.00785	0.05211	0.05708	2.00588
A52	1.94526	0.00297	0.00492	0.05292	0.05480	2.00006
A53	1.56611	-0.00241	0.00056	-0.00780	-0.00774	1.55837
A54	1.55986	-0.00146	0.00058	-0.00514	-0.00487	1.55499
A55	1.96583	0.00205	0.00005	0.00736	0.00740	1.97323
A56	2.36865	-0.00173	-0.00084	-0.00570	-0.00650	2.36214
A57	1.94870	-0.00032	0.00086	-0.00162	-0.00093	1.94777
A58	2.35131	-0.00044	0.00096	-0.00042	0.00083	2.35214
A59	1.95373	-0.00067	-0.00002	-0.00330	-0.00367	1.95007
A60	1.97789	0.00111	-0.00084	0.00389	0.00302	1.98091
A61	1.96219	0.00011	0.00148	0.00347	0.00439	1.96659
A62	2.37876	-0.00159	-0.00013	-0.00213	-0.00272	2.37604
A63	1.94211	0.00147	-0.00135	-0.00155	-0.00196	1.94015
A64	1.97480	0.00062	-0.00107	0.00051	-0.00044	1.97436
A65	2.44367	0.00017	0.00062	0.00023	0.00114	2.44481
A66	1.86466	-0.00078	0.00047	-0.00076	-0.00071	1.86395
A67	1.85767	-0.00099	0.00134	-0.00226	-0.00129	1.85638
A68	2.46297	-0.00020	-0.00105	-0.00160	-0.00253	2.46044
A69	1.96240	0.00120	-0.00028	0.00384	0.00381	1.96621
A70	1.98549	-0.00103	0.00049	-0.00202	-0.00192	1.98357
A71	1.94007	0.00079	-0.00324	-0.00255	-0.00477	1.93531
A72	2.35724	0.00023	0.00273	0.00430	0.00634	2.36357
A73	1.95747	0.00127	-0.00056	0.00706	0.00652	1.96399
A74	2.18567	0.00044	0.00226	0.00287	0.00499	2.19066
A75	2.13966	-0.00170	-0.00178	-0.00925	-0.01117	2.12849
A76	1.94357	0.00119	0.00054	-0.00061	-0.00017	1.94340
A77	2.09487	-0.00556	0.00318	-0.02866	-0.02548	2.06939
A78	2.24422	0.00437	-0.00382	0.02966	0.02585	2.27007
A79	1.57583	-0.00263	0.00017	-0.00822	-0.00825	1.56758
A80	1.81484	-0.00036	0.00474	0.00727	0.01008	1.82492
A81	2.07316	0.00149	0.00554	0.03175	0.03373	2.10689
A82	2.06316	0.00223	0.00878	0.03566	0.04117	2.10433
A83	2.32598	0.00896	-0.00087	0.06005	0.05917	2.38516
A84	1.92520	-0.00362	0.00140	-0.02642	-0.02503	1.90017
A85	2.03200	-0.00534	-0.00053	-0.03361	-0.03415	1.99785
A86	2.19152	0.00629	0.00025	0.03495	0.03521	2.22672
A87	2.21329	-0.00605	-0.00018	-0.03177	-0.03195	2.18133
A88	1.87837	-0.00024	-0.00007	-0.00319	-0.00326	1.87511
A89	1.86177	0.00040	-0.00112	0.00306	0.00190	1.86367
A90	2.22576	0.00108	-0.00033	0.00809	0.00778	2.23354

A91	2.19565	-0.00148	0.00145	-0.01114	-0.00967	2.18598
A92	1.86813	0.00179	0.00490	0.00565	0.01059	1.87873
A93	2.24239	-0.00491	0.01657	-0.03601	-0.01946	2.22293
A94	2.17265	0.00312	-0.02148	0.03036	0.00886	2.18151
A95	1.91009	0.00044	-0.00437	0.00546	0.00107	1.91116
A96	2.23158	-0.00043	0.00648	-0.00815	-0.00167	2.22991
A97	2.14152	-0.00002	-0.00212	0.00270	0.00060	2.14212
A98	1.90639	-0.00239	0.00065	-0.01097	-0.01029	1.89610
A99	2.29490	0.00305	-0.00612	0.01828	0.01213	2.30704
A100	2.08189	-0.00066	0.00547	-0.00730	-0.00184	2.08005
A101	2.05562	0.00054	-0.00146	0.00351	0.00205	2.05767
A102	2.08651	0.00012	0.00076	0.00006	0.00083	2.08734
A103	2.14106	-0.00066	0.00069	-0.00357	-0.00288	2.13818
A104	2.06519	0.00005	-0.00363	0.00328	-0.00035	2.06485
A105	2.12268	0.00108	-0.00011	0.00705	0.00693	2.12962
A106	2.09531	-0.00113	0.00374	-0.01033	-0.00659	2.08872
A107	2.09818	-0.00001	0.00181	-0.00265	-0.00085	2.09732
A108	2.10206	-0.00052	-0.00164	-0.00141	-0.00305	2.09901
A109	2.08295	0.00053	-0.00017	0.00406	0.00390	2.08685
A110	2.12397	0.00010	-0.00007	0.00048	0.00039	2.12436
A111	2.08087	-0.00062	-0.00003	-0.00376	-0.00378	2.07709
A112	2.07835	0.00052	0.00010	0.00328	0.00339	2.08173
A113	2.17759	-0.00489	0.00644	-0.03232	-0.02589	2.15170
A114	2.17182	-0.00095	-0.02687	0.01296	-0.01391	2.15791
A115	1.93376	0.00584	0.02044	0.01937	0.03981	1.97357
A116	2.17077	-0.00356	-0.01916	0.00089	-0.01827	2.15249
A117	2.18283	-0.00104	0.00163	-0.01379	-0.01217	2.17066
A118	1.92959	0.00461	0.01753	0.01289	0.03043	1.96001
A119	1.90910	-0.00008	-0.00003	-0.00037	-0.00041	1.90869
A120	1.94719	-0.00039	0.00007	-0.00261	-0.00255	1.94464
A121	1.90242	0.00001	0.00056	0.00004	0.00060	1.90302
A122	1.90917	0.00023	0.00030	0.00106	0.00136	1.91053
A123	1.88615	-0.00005	-0.00159	0.00014	-0.00144	1.88471
A124	1.90878	0.00029	0.00064	0.00182	0.00245	1.91124
A125	1.93787	-0.00002	0.00072	0.00011	0.00083	1.93870
A126	1.90131	0.00031	-0.00071	0.00232	0.00161	1.90293
A127	1.90015	0.00038	-0.00002	0.00198	0.00196	1.90210
A128	1.91145	-0.00004	0.00056	-0.00010	0.00045	1.91190
A129	1.91229	0.00000	0.00059	0.00022	0.00081	1.91310
A130	1.90032	-0.00064	-0.00118	-0.00462	-0.00581	1.89452
A131	3.18985	-0.00246	0.00195	-0.05090	-0.04895	3.14090
A132	3.19997	-0.00135	-0.00885	-0.02336	-0.03221	3.16777
A133	3.18841	-0.00042	-0.01575	0.00644	-0.00931	3.17910
A134	3.17534	0.00015	-0.01072	0.00756	-0.00316	3.17218
A135	3.13677	0.00015	0.00004	0.00262	0.00267	3.13944
A136	3.14250	-0.00003	-0.00037	-0.00015	-0.00052	3.14198
A137	3.14097	0.00009	0.00240	-0.00072	0.00168	3.14266
A138	3.14498	-0.00013	-0.00026	-0.00223	-0.00249	3.14249
D1	-0.01087	0.00016	0.00103	0.00376	0.00479	-0.00609
D2	3.12118	0.00010	-0.00005	0.00463	0.00458	3.12576
D3	3.13231	0.00019	0.00063	0.00464	0.00526	3.13757
D4	-0.01882	0.00013	-0.00045	0.00550	0.00505	-0.01377
D5	-0.00038	0.00009	0.00072	0.00144	0.00217	0.00179
D6	3.14095	0.00006	-0.00022	0.00200	0.00179	-3.14044
D7	3.13919	0.00005	0.00124	0.00031	0.00155	3.14074
D8	-0.00266	0.00002	0.00030	0.00087	0.00118	-0.00149
D9	0.03478	-0.00028	-0.00169	-0.00467	-0.00637	0.02841
D10	-3.09314	-0.00022	-0.00100	-0.00460	-0.00564	-3.09879
D11	-3.10495	-0.00024	-0.00218	-0.00362	-0.00580	-3.11075
D12	0.05031	-0.00018	-0.00149	-0.00355	-0.00507	0.04524

D13	0.01411	-0.00030	-0.00207	-0.00648	-0.00854	0.00556
D14	-3.12845	-0.00025	-0.00169	-0.00541	-0.00710	-3.13555
D15	-3.11612	-0.00023	-0.00076	-0.00756	-0.00831	-3.12443
D16	0.02451	-0.00018	-0.00038	-0.00649	-0.00687	0.01764
D17	-0.00426	0.00000	0.00258	-0.00434	-0.00180	-0.00605
D18	3.13431	0.00037	0.00052	0.01325	0.01379	-3.13508
D19	3.12717	-0.00006	0.00141	-0.00336	-0.00199	3.12518
D20	-0.01744	0.00031	-0.00065	0.01423	0.01361	-0.00384
D21	-0.00625	0.00019	0.00131	0.00408	0.00539	-0.00086
D22	3.13168	0.00021	0.00141	0.00484	0.00625	3.13794
D23	3.13632	0.00014	0.00092	0.00299	0.00391	3.14023
D24	-0.00893	0.00016	0.00102	0.00375	0.00477	-0.00415
D25	-0.00463	0.00005	0.00040	0.00097	0.00137	-0.00326
D26	3.13378	0.00007	0.00053	0.00163	0.00216	3.13594
D27	3.14060	0.00003	0.00029	0.00022	0.00051	3.14111
D28	-0.00417	0.00005	0.00043	0.00087	0.00130	-0.00287
D29	0.00794	-0.00019	-0.00143	-0.00376	-0.00519	0.00274
D30	-3.13340	-0.00017	-0.00052	-0.00431	-0.00483	-3.13823
D31	-3.13049	-0.00022	-0.00157	-0.00442	-0.00598	-3.13647
D32	0.01136	-0.00020	-0.00066	-0.00497	-0.00562	0.00574
D33	-0.03675	0.00019	0.00319	0.00177	0.00500	-0.03175
D34	3.10800	0.00005	0.00427	-0.00445	-0.00025	3.10775
D35	3.09045	0.00008	0.00228	0.00189	0.00419	3.09464
D36	-0.04798	-0.00005	0.00336	-0.00433	-0.00106	-0.04904
D37	-0.03336	0.00026	0.00209	0.00628	0.00837	-0.02499
D38	3.10408	0.00008	0.00094	0.00400	0.00495	3.10903
D39	3.12488	0.00039	0.00301	0.00629	0.00930	3.13418
D40	-0.02087	0.00021	0.00187	0.00402	0.00588	-0.01499
D41	0.02568	-0.00008	-0.00356	0.00150	-0.00206	0.02362
D42	-3.11922	0.00014	-0.00470	0.00815	0.00335	-3.11587
D43	-3.11278	-0.00049	-0.00142	-0.01676	-0.01811	-3.13089
D44	0.02551	-0.00026	-0.00256	-0.01011	-0.01270	0.01281
D45	-3.12654	-0.00070	-0.00397	-0.01063	-0.01463	-3.14116
D46	0.01025	-0.00053	-0.01275	-0.00095	-0.01370	-0.00345
D47	0.01889	-0.00093	-0.00266	-0.01826	-0.02092	-0.00204
D48	-3.12751	-0.00076	-0.01144	-0.00858	-0.02000	3.13567
D49	0.01727	-0.00018	-0.00940	0.00365	-0.00603	0.01124
D50	-3.09852	-0.00064	-0.01973	-0.01782	-0.03730	-3.13582
D51	-3.11972	-0.00035	-0.00103	-0.00565	-0.00692	-3.12663
D52	0.04769	-0.00081	-0.01136	-0.02711	-0.03819	0.00949
D53	-3.11790	-0.00039	-0.02642	0.00989	-0.01646	-3.13436
D54	-0.00027	0.00010	-0.01692	0.02975	0.01261	0.01234
D55	3.08392	0.00085	0.03193	0.01037	0.04257	3.12648
D56	-0.16306	0.00188	0.01832	0.06393	0.08268	-0.08038
D57	-0.03658	0.00081	0.02386	-0.00672	0.01687	-0.01970
D58	2.99963	0.00184	0.01026	0.04684	0.05699	3.05662
D59	-0.06617	0.00166	0.00552	0.05167	0.05715	-0.00903
D60	3.08988	0.00205	0.01514	0.06745	0.08243	-3.11087
D61	3.07772	0.00096	0.00826	0.04658	0.05451	3.13223
D62	-0.04942	0.00135	0.01788	0.06236	0.07980	0.03038
D63	0.03700	-0.00106	0.00649	-0.04609	-0.03905	-0.00206
D64	-3.10807	0.00000	0.00229	-0.03839	-0.03506	3.14005
D65	0.00293	-0.00019	-0.00029	-0.00486	-0.00537	-0.00243
D66	-3.10645	0.00067	0.00218	-0.01248	-0.00991	-3.11637
D67	-3.13532	-0.00121	0.00374	-0.01226	-0.00921	3.13866
D68	0.03848	-0.00035	0.00622	-0.01988	-0.01375	0.02473
D69	0.06584	-0.00175	-0.01986	-0.02822	-0.04730	0.01854
D70	-2.96831	-0.00255	-0.00585	-0.08141	-0.08710	-3.05541
D71	-3.09444	-0.00225	-0.03232	-0.04871	-0.08027	3.10847
D72	0.15459	-0.00305	-0.01831	-0.10190	-0.12007	0.03453

D73	0.07258	-0.00187	-0.02675	-0.08982	-0.11700	-0.04442
D74	-2.00426	-0.00701	-0.03764	-0.18495	-0.22294	-2.22720
D75	-3.05048	-0.00137	-0.01432	-0.06957	-0.08459	-3.13507
D76	1.15586	-0.00652	-0.02522	-0.16470	-0.19052	0.96534
D77	0.04494	-0.00104	-0.01742	-0.05468	-0.07155	-0.02661
D78	-3.07843	-0.00063	-0.01271	-0.03567	-0.04797	-3.12641
D79	-3.11894	-0.00167	-0.01915	-0.04957	-0.06853	3.09572
D80	0.04087	-0.00126	-0.01444	-0.03055	-0.04495	-0.00408
D81	3.09041	0.00002	0.00841	0.02769	0.03521	3.12562
D82	-0.01769	0.00094	0.01097	0.01981	0.03052	0.01283
D83	-0.07087	0.00169	0.02652	0.08684	0.11387	0.04301
D84	2.00850	0.00686	0.03956	0.18122	0.22109	2.22959
D85	3.04713	0.00117	0.02043	0.06216	0.08318	3.13030
D86	-1.15669	0.00634	0.03346	0.15654	0.19040	-0.96630
D87	3.12024	0.00072	0.00680	0.01877	0.02537	-3.13757
D88	-0.04796	0.00106	0.01075	0.02739	0.03781	-0.01015
D89	0.00226	0.00122	0.01290	0.04350	0.05623	0.05849
D90	3.11724	0.00157	0.01684	0.05212	0.06867	-3.09727
D91	0.97731	0.00205	0.00539	0.03796	0.04396	1.02127
D92	3.08370	0.00219	0.00607	0.03941	0.04609	3.12980
D93	-1.12938	0.00182	0.00422	0.03633	0.04116	-1.08822
D94	-0.99610	-0.00216	-0.00607	-0.04504	-0.05171	-1.04782
D95	1.11029	-0.00202	-0.00539	-0.04358	-0.04958	1.06071
D96	-3.10279	-0.00238	-0.00724	-0.04667	-0.05452	3.12588
D97	-0.00976	-0.00035	-0.00470	-0.00413	-0.00891	-0.01866
D98	3.12653	0.00036	0.00119	0.00601	0.00707	3.13361
D99	3.12474	0.00023	0.00087	0.00953	0.01029	3.13502
D100	0.01003	-0.00010	-0.00313	0.00091	-0.00224	0.00779
D101	-0.03599	0.00080	0.00958	0.01197	0.02126	-0.01473
D102	3.09210	0.00116	0.01175	0.00957	0.02090	3.11300
D103	0.03439	-0.00027	-0.00235	-0.01207	-0.01436	0.02003
D104	-3.12779	-0.00002	0.00075	-0.00545	-0.00474	-3.13253
D105	-3.10321	-0.00079	-0.00675	-0.01967	-0.02642	-3.12963
D106	0.01778	-0.00054	-0.00365	-0.01305	-0.01680	0.00099
D107	3.10183	0.00046	0.00498	0.01190	0.01696	3.11879
D108	-0.05847	0.00009	0.00493	-0.00387	0.00106	-0.05741
D109	-0.04503	0.00116	0.01083	0.02200	0.03279	-0.01224
D110	3.07785	0.00080	0.01077	0.00622	0.01689	3.09475
D111	0.05338	-0.00121	-0.01345	-0.02150	-0.03496	0.01842
D112	-3.07914	-0.00146	-0.01491	-0.01989	-0.03474	-3.11388
D113	-3.07434	-0.00091	-0.01341	-0.00977	-0.02312	-3.09746
D114	0.07632	-0.00116	-0.01487	-0.00817	-0.02290	0.05342
D115	3.06057	0.00153	0.01418	0.01815	0.03233	3.09290
D116	0.72467	-0.00260	-0.00670	-0.06806	-0.07440	0.65027
D117	-0.09957	0.00116	0.01415	0.00254	0.01665	-0.08293
D118	-2.43548	-0.00298	-0.00674	-0.08367	-0.09009	-2.52556
D119	3.13554	0.00033	0.00670	0.01224	0.01898	-3.12866
D120	-0.02742	0.00053	0.00697	0.01160	0.01850	-0.00892
D121	-0.01902	0.00068	0.00876	0.00994	0.01864	-0.00039
D122	3.10120	0.00088	0.00904	0.00930	0.01816	3.11936
D123	3.12322	0.00025	0.00076	0.00028	0.00088	3.12410
D124	-0.04367	0.00008	0.00011	-0.00843	-0.00849	-0.05216
D125	-0.00386	0.00012	0.00059	0.00076	0.00128	-0.00258
D126	3.11244	-0.00004	-0.00005	-0.00794	-0.00810	3.10434
D127	-3.11462	-0.00014	0.00590	-0.00609	0.00003	-3.11459
D128	0.00479	0.00005	0.00620	-0.00681	-0.00051	0.00428
D129	0.00021	-0.00030	-0.00962	0.00795	-0.00158	-0.00137
D130	-3.11215	-0.00055	-0.00358	-0.01797	-0.02165	-3.13380
D131	-3.10798	-0.00008	-0.00865	0.01962	0.01118	-3.09680
D132	0.06284	-0.00033	-0.00261	-0.00631	-0.00889	0.05396

D133	0.08715	-0.00077	-0.00842	0.00394	-0.00457	0.08258
D134	2.42868	0.00293	0.01033	0.08746	0.09782	2.52650
D135	-3.08722	-0.00101	-0.00933	-0.00750	-0.01704	-3.10426
D136	-0.74569	0.00269	0.00942	0.07601	0.08534	-0.66035
D137	0.00339	0.00033	0.01401	-0.01286	0.00117	0.00456
D138	3.11312	0.00055	0.00926	-0.00065	0.00845	3.12157
D139	3.11664	0.00061	0.00816	0.01251	0.02072	3.13736
D140	-0.05681	0.00083	0.00341	0.02471	0.02800	-0.02882
D141	-0.00466	-0.00022	-0.01154	0.01122	-0.00036	-0.00502
D142	-3.11096	-0.00022	-0.00634	-0.00088	-0.00744	-3.11840
D143	3.12495	0.00036	0.00704	0.00789	0.01491	3.13986
D144	-0.01863	0.00052	0.00617	0.01632	0.02249	0.00387
D145	-0.05460	0.00051	0.00143	0.02153	0.02295	-0.03165
D146	3.08500	0.00067	0.00055	0.02996	0.03054	3.11554
D147	-1.00358	0.00173	0.01019	0.04290	0.05416	-0.94943
D148	1.11108	0.00171	0.01059	0.04228	0.05394	1.16502
D149	-3.06241	0.00183	0.01180	0.04292	0.05578	-3.00663
D150	3.05583	-0.00178	-0.01137	-0.04269	-0.05513	3.00070
D151	-1.11269	-0.00180	-0.01098	-0.04330	-0.05535	-1.16804
D152	0.99700	-0.00168	-0.00977	-0.04267	-0.05350	0.94350
D153	-0.00882	0.00019	-0.00072	0.00608	0.00534	-0.00347
D154	3.13793	0.00021	-0.00075	0.00824	0.00748	-3.13777
D155	3.13486	0.00003	0.00019	-0.00276	-0.00256	3.13230
D156	-0.00158	0.00005	0.00017	-0.00061	-0.00042	-0.00200
D157	-3.13943	0.00007	0.00016	0.00333	0.00353	-3.13590
D158	0.00119	0.00010	0.00012	0.00418	0.00434	0.00553
D159	-0.00218	0.00004	0.00018	0.00142	0.00160	-0.00058
D160	3.13845	0.00006	0.00014	0.00228	0.00241	3.14086
D161	-3.14106	-0.00004	-0.00033	-0.00306	-0.00336	3.13877
D162	0.00519	-0.00004	-0.00002	-0.00327	-0.00324	0.00195
D163	0.00493	-0.00004	-0.00035	-0.00134	-0.00170	0.00324
D164	-3.13200	-0.00004	-0.00004	-0.00155	-0.00158	-3.13358
D165	-0.00161	-0.00001	0.00010	-0.00098	-0.00087	-0.00248
D166	3.14059	0.00001	0.00029	-0.00023	0.00006	3.14065
D167	3.14093	-0.00004	0.00015	-0.00182	-0.00166	3.13927
D168	-0.00005	-0.00001	0.00033	-0.00108	-0.00073	-0.00078
D169	-0.00606	0.00004	0.00041	0.00078	0.00121	-0.00485
D170	3.13568	0.00005	0.00054	0.00129	0.00184	3.13752
D171	3.13111	0.00002	0.00021	0.00076	0.00100	3.13211
D172	-0.01034	0.00003	0.00034	0.00127	0.00163	-0.00871
D173	0.00148	-0.00002	0.00000	-0.00075	-0.00075	0.00074
D174	3.13748	0.00006	0.00029	0.00158	0.00187	3.13935
D175	-3.13470	-0.00002	0.00030	-0.00089	-0.00059	-3.13529
D176	0.00130	0.00007	0.00058	0.00144	0.00202	0.00332
D177	0.00475	-0.00002	-0.00034	0.00011	-0.00023	0.00452
D178	-3.13697	-0.00003	-0.00045	-0.00032	-0.00076	-3.13773
D179	-3.13741	-0.00005	-0.00052	-0.00059	-0.00111	-3.13852
D180	0.00405	-0.00006	-0.00062	-0.00103	-0.00164	0.00241
D181	3.13788	0.00003	0.00020	0.00066	0.00085	3.13874
D182	-0.00323	0.00002	0.00031	0.00042	0.00072	-0.00251
D183	-0.00303	0.00006	0.00041	0.00150	0.00190	-0.00113
D184	3.13905	0.00005	0.00052	0.00125	0.00176	3.14081
D185	3.13950	0.00000	0.00023	-0.00085	-0.00062	3.13887
D186	-0.00251	0.00002	0.00036	-0.00014	0.00022	-0.00230
D187	-0.00194	0.00001	0.00037	-0.00030	0.00006	-0.00187
D188	3.13924	0.00003	0.00050	0.00040	0.00090	3.14014
D189	-0.00002	-0.00001	0.00008	-0.00068	-0.00060	-0.00062
D190	-3.14120	-0.00001	0.00001	-0.00023	-0.00023	-3.14142
D191	3.14108	-0.00001	-0.00003	-0.00042	-0.00046	3.14061
D192	-0.00011	0.00000	-0.00011	0.00003	-0.00008	-0.00019

D193	-0.00100	0.00003	0.00008	0.00112	0.00120	0.00019
D194	3.14012	0.00003	0.00011	0.00096	0.00108	3.14120
D195	3.14100	0.00002	-0.00004	0.00042	0.00037	3.14137
D196	-0.00106	0.00001	-0.00001	0.00027	0.00026	-0.00081
D197	0.00202	-0.00003	-0.00032	-0.00062	-0.00093	0.00109
D198	-3.13911	-0.00003	-0.00035	-0.00046	-0.00081	-3.13992
D199	-3.13998	-0.00003	-0.00024	-0.00106	-0.00130	-3.14129
D200	0.00208	-0.00003	-0.00027	-0.00091	-0.00118	0.00089

Item	Value	Threshold	Converged?

Maximum Force	0.023959	0.000450	NO

RMS Force	0.002950	0.000300	NO

Maximum Displacement	1.250279	0.001800	NO

RMS Displacement	0.288671	0.001200	NO

Predicted change in Energy=-1.383575D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.797859	-0.648776	-0.087988
2	6	0	-10.003336	-1.806583	-0.016789
3	6	0	-10.540514	-3.085178	0.002286
4	6	0	-11.928778	-3.211397	-0.058910
5	6	0	-12.736341	-2.068867	-0.135734
6	6	0	-12.190154	-0.782183	-0.149713
7	1	0	-9.881039	-3.945071	0.063793
8	1	0	-12.388256	-4.195210	-0.049852
9	1	0	-13.814989	-2.181500	-0.188144
10	1	0	-12.846992	0.074870	-0.206714
11	6	0	-9.909269	0.540454	-0.083692
12	6	0	-8.576915	-1.426606	0.017297
13	6	0	-8.529366	0.049489	-0.045948
14	6	0	-7.392208	0.830608	-0.068440
15	6	0	-6.002631	0.584414	-0.042076
16	6	0	-3.639570	-0.156534	0.026111
17	6	0	-3.782759	1.241982	-0.021708
18	16	0	-5.149912	-0.984367	0.021968
19	6	0	-5.098827	1.665165	-0.073511
20	6	0	-2.252722	-0.414305	0.062140
21	6	0	-1.610874	0.830192	0.031708
22	7	0	-2.522592	1.901794	-0.057859
23	16	0	-1.138861	-1.759578	0.099420
24	16	0	1.114742	1.868223	0.024595
25	6	0	0.201267	-0.621695	0.095984
26	6	0	-0.216088	0.721282	0.043150
27	6	0	1.597303	-0.726937	0.122875
28	6	0	2.236509	0.525017	0.074886
29	6	0	3.617948	0.275300	0.070964
30	6	0	3.768356	-1.124935	0.117420
31	6	0	5.084867	-1.541678	0.097648
32	6	0	5.990221	-0.465789	0.033199
33	16	0	5.133460	1.106353	0.005122

34	7	0	2.521799	-1.758404	0.218617
35	6	0	7.381938	-0.748535	0.031406
36	6	0	8.556141	-0.019993	-0.020335
37	6	0	8.703458	1.452676	-0.102653
38	6	0	9.899027	-0.594316	-0.010989
39	6	0	10.153803	1.734972	-0.140726
40	6	0	10.868292	0.527038	-0.083014
41	6	0	10.775082	2.968648	-0.218518
42	6	0	12.265946	0.560233	-0.101424
43	6	0	12.170423	2.997037	-0.238180
44	6	0	12.898528	1.804464	-0.179426
45	6	0	10.238248	-1.931977	0.047282
46	6	0	9.273511	-2.983234	0.108312
47	6	0	11.585183	-2.407348	0.049270
48	7	0	8.485408	-3.840953	0.156149
49	7	0	12.673448	-2.823740	0.052176
50	6	0	-10.357841	1.848553	-0.094777
51	6	0	-11.738864	2.203249	-0.141535
52	6	0	-9.505769	2.993057	-0.052313
53	7	0	-12.855000	2.535006	-0.181338
54	7	0	-8.838735	3.948747	-0.016878
55	8	0	-7.632080	-2.205014	0.072651
56	8	0	7.817500	2.298223	-0.134857
57	6	0	2.281432	-3.046411	-0.447837
58	1	0	1.312052	-3.440852	-0.134675
59	1	0	2.298066	-2.941885	-1.538616
60	1	0	3.050447	-3.756666	-0.137922
61	6	0	-2.338273	2.960866	0.974214
62	1	0	-2.454261	2.551360	1.984441
63	1	0	-1.340362	3.392734	0.867228
64	1	0	-3.076583	3.748027	0.810966
65	1	0	5.419426	-2.572407	0.119046
66	1	0	12.861573	-0.341474	-0.057748
67	1	0	13.983618	1.843535	-0.194097
68	1	0	12.697761	3.944406	-0.298410
69	1	0	10.172630	3.870483	-0.261381
70	1	0	7.521722	-1.823257	0.079811
71	1	0	-7.565365	1.898697	-0.122057
72	1	0	-5.425134	2.692795	-0.191246

Rotational constants (GHZ): 0.1779182 0.0104010 0.0098375

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6577.4102789241 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T
Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6577.3246651282 Hartrees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.22D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Initial guess from the checkpoint file: "PBDB.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999953 0.009620 0.000143 0.001298 Ang= 1.11 deg.
 ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1
 AccDes= 0.00D+00
 Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for in-
 itial guess.
 HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-
 yADJ=14
 ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
 FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2001
 NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
 wScrn= 0.000000 ICntrl= 500 IOPCl= 0 IICent= 200000004 NGrid=
 0
 NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0=
 0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 Integral accuracy reduced to 1.0D-05 until final iterations.
 Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
 SCF Done: E(RB3LYP) = -3683.00325283 A.U. after 14 cycles
 NFock= 14 Conv=0.88D-08 -V/T= 2.0068
 Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IICent= 0 IOPClX= 0 NMat=1
 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-0.000617753	0.000947331	0.000070093
2	6	-0.000265278	0.001029525	-0.000248647
3	6	0.000420393	0.000031383	0.000014675
4	6	-0.000605711	0.000732514	-0.000247788
5	6	0.000312227	0.000617902	0.000423813
6	6	0.000172612	-0.000267394	-0.000269292
7	1	-0.000263501	-0.000026502	0.000090970
8	1	0.000005787	-0.000129032	-0.000086790
9	1	0.000087260	-0.000099659	-0.000135500
10	1	0.000439983	0.000582684	0.000562487
11	6	-0.000040681	0.000602203	-0.000104586
12	6	-0.000078211	-0.000287780	0.001270990
13	6	0.000692933	-0.003047486	-0.000916883
14	6	-0.004142076	0.000698000	-0.001854761
15	6	0.000948625	0.000646873	0.000191500
16	6	0.002629981	-0.000112090	0.001807124
17	6	-0.001428637	-0.009199594	0.004007528
18	16	-0.001732587	0.003276774	-0.001049971
19	6	-0.003501155	0.002090229	-0.000083943
20	6	-0.002056066	0.001771335	0.000651008
21	6	-0.008619870	-0.003796606	0.000229536
22	7	0.014331358	0.012841306	-0.011859776
23	16	0.000703385	0.000803641	0.000512191
24	16	0.000062260	-0.000163442	-0.000057097
25	6	-0.004521623	0.002763786	-0.002576717
26	6	0.004529632	-0.002315862	0.000875137
27	6	0.004829505	0.000937386	-0.000689305
28	6	-0.000607512	-0.002705973	-0.001463961
29	6	-0.002261979	-0.003212442	-0.001385357
30	6	0.000819384	0.004961385	-0.004392502

31	6	0.005022144	-0.001512548	0.005142668
32	6	0.002900455	-0.002163369	0.001097585
33	16	0.004807731	-0.003394899	0.002543161
34	7	-0.008151564	-0.003131222	0.010680685
35	6	-0.001470945	-0.002145941	0.000062787
36	6	-0.003698447	0.003388183	-0.002626574
37	6	-0.003673946	0.000988577	-0.002691455
38	6	0.000698929	-0.000358758	0.000597397
39	6	0.000478637	0.002337791	0.000350613
40	6	0.000801213	0.000779857	0.000529705
41	6	-0.001091231	-0.002300464	-0.000861912
42	6	0.000847000	0.000193048	0.000715955
43	6	-0.000733015	-0.001597527	-0.000588149
44	6	0.001322522	-0.000351955	0.000850686
45	6	0.003143494	0.001527863	0.002213522
46	6	0.002702726	0.001029954	0.001990857
47	6	0.000019653	0.000020708	-0.000000907
48	7	0.002075913	0.000310413	0.001487181
49	7	-0.000285625	0.000432575	-0.000198522
50	6	0.000182307	-0.000514357	0.000221862
51	6	-0.001439335	0.000048461	-0.001115999
52	6	-0.000176176	-0.001891965	-0.000092826
53	7	0.000093888	-0.000276323	0.000003939
54	7	0.000140101	0.000805206	0.000160431
55	8	0.002275492	-0.001682462	0.001111400
56	8	-0.002230857	0.003988476	-0.001491548
57	6	0.003862590	0.000728700	-0.004528979
58	1	0.000180094	-0.000369712	0.000259130
59	1	0.000263030	0.000009417	-0.000349826
60	1	-0.000228248	-0.000092419	-0.000012064
61	6	-0.006241324	-0.002996850	0.006596384
62	1	-0.000463432	-0.000331918	0.000468522
63	1	-0.000546359	0.000279065	-0.000578274
64	1	0.000222727	-0.000232657	0.000284384
65	1	0.000782768	-0.000639265	-0.000109580
66	1	-0.000339916	-0.000508512	-0.000248042
67	1	0.000076717	0.000345478	0.000094849
68	1	-0.000205478	0.000191428	-0.000131488
69	1	0.000190551	-0.000269458	0.000111061
70	1	-0.003233945	-0.002360665	-0.002302268
71	1	-0.000543051	0.000535473	-0.000457452
72	1	0.001419524	0.001212179	-0.002473076

Cartesian Forces: Max 0.014331358 RMS 0.002699866

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.024668876 RMS 0.003250279

Search for a local minimum.

Step number 11 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 10 11

DE= -9.76D-03 DEPred=-1.38D-02 R= 7.05D-01

TightC=F SS= 1.41D+00 RLast= 6.56D-01 DXNew= 2.4000D+00 1.9692D+00

Trust test= 7.05D-01 RLast= 6.56D-01 DXMaxT set to 1.97D+00

ITU= 1 1 0 0 0 1 0 0 0 1 0

Use linear search instead of GDIIS.

Eigenvalues	---	0.00230	0.00230	0.00231	0.00232	0.00241
Eigenvalues	---	0.00290	0.00387	0.00445	0.00459	0.00483
Eigenvalues	---	0.00509	0.00523	0.00563	0.00600	0.00615
Eigenvalues	---	0.00618	0.00667	0.00682	0.00690	0.00710
Eigenvalues	---	0.00736	0.00745	0.00760	0.00770	0.00773
Eigenvalues	---	0.00820	0.00841	0.00856	0.00866	0.00879
Eigenvalues	---	0.00953	0.01085	0.01097	0.01134	0.01155
Eigenvalues	---	0.01246	0.01268	0.01292	0.01336	0.01363
Eigenvalues	---	0.01369	0.01398	0.01439	0.01459	0.01509
Eigenvalues	---	0.01569	0.01646	0.01654	0.01754	0.01772
Eigenvalues	---	0.01794	0.01801	0.01929	0.01953	0.02006
Eigenvalues	---	0.02025	0.02075	0.02075	0.02208	0.02210
Eigenvalues	---	0.02955	0.04827	0.04837	0.04842	0.04900
Eigenvalues	---	0.04922	0.04999	0.05016	0.05063	0.07158
Eigenvalues	---	0.07266	0.07457	0.07606	0.14311	0.15529
Eigenvalues	---	0.15608	0.15973	0.15998	0.16000	0.16000
Eigenvalues	---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues	---	0.16000	0.16000	0.16000	0.16002	0.16003
Eigenvalues	---	0.16008	0.16026	0.17410	0.17492	0.17775
Eigenvalues	---	0.19009	0.19508	0.19715	0.20599	0.20983
Eigenvalues	---	0.21167	0.21999	0.22007	0.22100	0.22245
Eigenvalues	---	0.22456	0.22551	0.22597	0.22601	0.22623
Eigenvalues	---	0.22780	0.22788	0.22838	0.23115	0.23311
Eigenvalues	---	0.23399	0.23578	0.23779	0.23925	0.24175
Eigenvalues	---	0.24243	0.24276	0.24490	0.24504	0.24548
Eigenvalues	---	0.24623	0.24771	0.24935	0.24972	0.24980
Eigenvalues	---	0.24983	0.24988	0.24993	0.24994	0.24994
Eigenvalues	---	0.24996	0.24996	0.24997	0.24999	0.24999
Eigenvalues	---	0.25000	0.25000	0.25000	0.25015	0.25559
Eigenvalues	---	0.25834	0.26239	0.26319	0.26723	0.26742
Eigenvalues	---	0.26989	0.27140	0.27325	0.27841	0.27883
Eigenvalues	---	0.28328	0.28473	0.28622	0.28853	0.30119
Eigenvalues	---	0.30382	0.32405	0.32848	0.35066	0.35766
Eigenvalues	---	0.36323	0.36331	0.36343	0.36475	0.36650
Eigenvalues	---	0.36716	0.36827	0.36833	0.37081	0.37095
Eigenvalues	---	0.37134	0.37252	0.37276	0.37418	0.37565
Eigenvalues	---	0.37670	0.37755	0.37994	0.38856	0.40279
Eigenvalues	---	0.40704	0.41468	0.41805	0.42230	0.42727
Eigenvalues	---	0.44429	0.44753	0.45600	0.46048	0.47348
Eigenvalues	---	0.47893	0.48032	0.50413	0.52546	0.54091
Eigenvalues	---	0.55573	0.57716	0.65557	0.80382	0.81988
Eigenvalues	---	0.91535	1.25844	1.26321	1.29359	1.35402

RFO step: Lambda=-1.48204711D-02 EMin= 2.29924599D-03

Quartic linear search produced a step of 0.00589.

Iteration	1	RMS(Cart)=	0.17103994	RMS(Int)=	0.00481024
Iteration	2	RMS(Cart)=	0.01461187	RMS(Int)=	0.00058177
Iteration	3	RMS(Cart)=	0.00007395	RMS(Int)=	0.00058117
Iteration	4	RMS(Cart)=	0.00000019	RMS(Int)=	0.00058117

Variable (Linear)	Old X (Quad)	-DE/DX (Total)	Delta X	Delta X	Delta X	New X
R1	2.65697	0.00151	0.00004	0.00603	0.00607	2.66304
R2	2.64568	0.00026	-0.00001	0.00064	0.00062	2.64630
R3	2.80539	0.00300	-0.00002	0.00983	0.00981	2.81520
R4	2.62102	0.00051	-0.00003	-0.00049	-0.00053	2.62049
R5	2.79029	0.00123	-0.00005	0.00109	0.00105	2.79133
R6	2.63680	0.00034	0.00000	0.00035	0.00035	2.63715
R7	2.05112	-0.00017	0.00000	-0.00050	-0.00050	2.05062
R8	2.64793	-0.00058	0.00000	-0.00268	-0.00269	2.64525
R9	2.05198	-0.00014	0.00000	-0.00025	-0.00024	2.05173

R10	2.64161	0.00059	-0.00001	0.00068	0.00067	2.64229
R11	2.05182	-0.00008	0.00000	-0.00013	-0.00013	2.05170
R12	2.04337	-0.00081	0.00001	-0.00402	-0.00401	2.03936
R13	2.76869	0.00079	-0.00006	-0.00387	-0.00393	2.76476
R14	2.61334	0.00222	-0.00004	0.00258	0.00254	2.61588
R15	2.79342	-0.00023	-0.00005	-0.00117	-0.00122	2.79220
R16	2.31574	0.00243	-0.00001	0.00122	0.00121	2.31696
R17	2.60740	-0.00316	-0.00004	0.00360	0.00355	2.61095
R18	2.66728	0.00256	-0.00014	0.00966	0.00952	2.67680
R19	2.04726	0.00014	0.00000	0.00237	0.00237	2.04963
R20	3.37638	0.00064	-0.00012	-0.00452	-0.00476	3.37162
R21	2.66302	-0.00008	-0.00001	0.00105	0.00112	2.66414
R22	2.65816	0.00201	0.00006	0.00673	0.00644	2.66460
R23	3.25475	0.00333	0.00000	0.01948	0.01935	3.27410
R24	2.66652	0.00057	-0.00011	0.00294	0.00148	2.66799
R25	2.61425	0.00623	-0.00015	0.00567	0.00569	2.61994
R26	2.68892	-0.00242	-0.00014	-0.02013	-0.01921	2.66971
R27	2.04960	-0.00063	-0.00001	-0.00268	-0.00269	2.04691
R28	2.64674	0.00220	0.00004	0.00721	0.00698	2.65372
R29	3.30126	0.00176	-0.00004	0.00413	0.00402	3.30528
R30	2.66417	-0.00096	-0.00016	-0.01913	-0.01822	2.64595
R31	2.64388	0.00774	-0.00016	0.01499	0.01496	2.65884
R32	2.81612	-0.00463	-0.00003	-0.01340	-0.01343	2.80270
R33	3.32223	0.00140	-0.00005	0.00242	0.00224	3.32447
R34	3.32018	0.00159	-0.00004	0.00309	0.00298	3.32317
R35	3.30842	0.00130	-0.00004	0.00221	0.00214	3.31056
R36	2.65946	0.00095	0.00003	0.00365	0.00369	2.66315
R37	2.64610	0.00824	-0.00019	0.01664	0.01652	2.66262
R38	2.65792	0.00259	0.00004	0.00774	0.00765	2.66557
R39	2.62378	0.00333	-0.00016	-0.00482	-0.00447	2.61932
R40	2.65286	0.00287	-0.00017	0.00048	-0.00034	2.65252
R41	2.66273	0.00443	0.00008	0.01211	0.01207	2.67480
R42	3.26860	0.00087	-0.00005	0.00148	0.00141	3.27002
R43	2.60978	0.00956	-0.00022	0.01352	0.01338	2.62316
R44	2.64928	0.00103	-0.00017	-0.01139	-0.01103	2.63825
R45	2.65999	-0.00021	0.00000	0.00123	0.00121	2.66121
R46	2.04823	0.00008	0.00000	0.00020	0.00021	2.04844
R47	3.38385	-0.00218	0.00003	-0.00279	-0.00285	3.38100
R48	2.68369	-0.00695	-0.00003	-0.02255	-0.02258	2.66112
R49	2.77790	-0.00272	-0.00005	-0.01107	-0.01112	2.76677
R50	2.61316	-0.00941	0.00007	-0.00917	-0.00910	2.60406
R51	2.05008	-0.00446	0.00001	-0.00578	-0.00577	2.04431
R52	2.80115	-0.00270	0.00000	-0.00646	-0.00647	2.79468
R53	2.76009	0.01020	-0.00007	0.02499	0.02493	2.78502
R54	2.79312	-0.00035	-0.00002	-0.00080	-0.00084	2.79227
R55	2.31513	0.00220	-0.00002	0.00018	0.00016	2.31529
R56	2.80425	0.00291	0.00000	0.01051	0.01054	2.81479
R57	2.61015	0.00942	-0.00004	0.01533	0.01529	2.62544
R58	2.65433	0.00254	0.00006	0.01070	0.01076	2.66509
R59	2.61438	0.00319	-0.00011	0.00254	0.00242	2.61680
R60	2.64216	0.00150	-0.00005	0.00327	0.00322	2.64538
R61	2.63762	0.00050	0.00003	0.00135	0.00137	2.63899
R62	2.05111	-0.00012	0.00000	-0.00053	-0.00052	2.05058
R63	2.64180	0.00085	0.00003	0.00305	0.00308	2.64488
R64	2.04384	-0.00057	0.00001	-0.00468	-0.00468	2.03916
R65	2.64279	0.00166	-0.00006	0.00071	0.00064	2.64344
R66	2.05209	-0.00016	0.00000	-0.00030	-0.00029	2.05180
R67	2.05204	-0.00013	0.00000	-0.00033	-0.00032	2.05172
R68	2.69879	0.00076	-0.00001	0.00074	0.00073	2.69952
R69	2.69921	-0.00045	0.00004	0.00502	0.00506	2.70427

R70	2.20303	0.00006	0.00002	0.00103	0.00105	2.20408
R71	2.20193	-0.00045	0.00001	0.00059	0.00060	2.20253
R72	2.69590	0.00152	-0.00004	0.00387	0.00383	2.69974
R73	2.69756	0.00107	-0.00005	-0.00110	-0.00115	2.69641
R74	2.20168	-0.00017	0.00000	0.00015	0.00015	2.20183
R75	2.20340	-0.00081	0.00001	0.00000	0.00001	2.20342
R76	2.06435	-0.00048	0.00000	-0.00109	-0.00108	2.06327
R77	2.07096	-0.00044	0.00000	-0.00125	-0.00125	2.06971
R78	2.06309	-0.00023	0.00000	-0.00053	-0.00053	2.06256
R79	2.07156	-0.00074	-0.00001	-0.00275	-0.00276	2.06881
R80	2.06472	-0.00063	0.00000	-0.00149	-0.00149	2.06323
R81	2.06264	-0.00028	0.00000	-0.00064	-0.00064	2.06200
A1	2.07800	-0.00115	-0.00002	-0.00639	-0.00641	2.07159
A2	1.89787	0.00010	-0.00002	-0.00220	-0.00223	1.89564
A3	2.30731	0.00105	0.00004	0.00859	0.00864	2.31595
A4	2.14237	0.00027	0.00001	0.00241	0.00242	2.14479
A5	1.91257	-0.00012	-0.00001	-0.00077	-0.00078	1.91180
A6	2.22820	-0.00015	-0.00001	-0.00164	-0.00164	2.22655
A7	2.05796	0.00024	0.00000	0.00129	0.00128	2.05924
A8	2.08953	-0.00008	-0.00002	-0.00154	-0.00156	2.08797
A9	2.13569	-0.00016	0.00002	0.00026	0.00029	2.13598
A10	2.09677	-0.00032	-0.00001	-0.00234	-0.00236	2.09441
A11	2.09739	0.00017	0.00001	0.00141	0.00142	2.09881
A12	2.08902	0.00015	0.00000	0.00094	0.00094	2.08996
A13	2.12455	0.00031	0.00001	0.00191	0.00193	2.12647
A14	2.08358	-0.00007	0.00000	-0.00052	-0.00052	2.08306
A15	2.07506	-0.00024	-0.00001	-0.00139	-0.00140	2.07365
A16	2.06671	0.00065	0.00000	0.00315	0.00315	2.06986
A17	2.13045	0.00008	0.00000	0.00110	0.00110	2.13155
A18	2.08603	-0.00073	-0.00001	-0.00425	-0.00425	2.08178
A19	1.87065	-0.00129	-0.00001	-0.00108	-0.00111	1.86953
A20	2.16948	0.00322	-0.00001	0.01835	0.01835	2.18783
A21	2.24295	-0.00193	0.00002	-0.01729	-0.01726	2.22569
A22	1.86195	-0.00015	0.00000	0.00096	0.00093	1.86288
A23	2.19250	0.00218	0.00004	0.00525	0.00528	2.19777
A24	2.22866	-0.00203	-0.00004	-0.00609	-0.00613	2.22253
A25	1.88118	0.00146	0.00003	0.00353	0.00353	1.88472
A26	2.19702	0.00529	0.00014	0.01347	0.01362	2.21065
A27	2.20498	-0.00675	-0.00018	-0.01701	-0.01718	2.18780
A28	2.36361	-0.00954	-0.00015	-0.02578	-0.02593	2.33768
A29	2.01221	0.00388	0.00007	0.00695	0.00702	2.01923
A30	1.90736	0.00567	0.00008	0.01883	0.01890	1.92626
A31	2.24424	-0.00341	-0.00015	-0.01017	-0.01038	2.23386
A32	2.09119	0.00369	0.00003	0.00631	0.00628	2.09747
A33	1.94775	-0.00028	0.00012	0.00381	0.00397	1.95172
A34	1.96982	-0.00082	0.00000	-0.00445	-0.00409	1.96573
A35	1.85724	-0.00056	0.00000	-0.00160	-0.00228	1.85496
A36	2.45613	0.00138	0.00000	0.00605	0.00636	2.46249
A37	1.98477	-0.00124	0.00003	-0.00071	-0.00120	1.98357
A38	1.95168	-0.00010	-0.00005	-0.01150	-0.01010	1.94158
A39	2.34580	0.00133	0.00001	0.01171	0.01073	2.35653
A40	1.56738	0.00145	-0.00007	0.00001	-0.00039	1.56698
A41	1.95487	0.00089	-0.00007	0.00154	0.00145	1.95632
A42	2.13661	-0.00143	-0.00003	-0.00954	-0.01011	2.12649
A43	2.18966	0.00061	0.00011	0.01098	0.01056	2.20022
A44	1.86244	-0.00006	0.00001	0.00165	0.00098	1.86343
A45	2.44633	0.00049	-0.00002	-0.00004	0.00015	2.44648
A46	1.97416	-0.00043	0.00002	-0.00150	-0.00104	1.97312
A47	1.96103	-0.00095	-0.00003	-0.01414	-0.01268	1.94835
A48	1.96873	-0.00102	0.00001	0.00000	-0.00056	1.96817

A49	2.35237	0.00197	0.00002	0.01344	0.01243	2.36480
A50	1.79123	0.00169	0.00009	0.02253	0.01890	1.81013
A51	2.00588	0.00132	0.00034	0.06165	0.05622	2.06210
A52	2.00006	0.00266	0.00032	0.06828	0.06312	2.06318
A53	1.55837	0.00182	-0.00005	0.00244	0.00219	1.56056
A54	1.55499	0.00255	-0.00003	0.00624	0.00616	1.56115
A55	1.97323	-0.00038	0.00004	0.00255	0.00252	1.97576
A56	2.36214	0.00027	-0.00004	-0.00087	-0.00100	2.36114
A57	1.94777	0.00011	-0.00001	-0.00175	-0.00160	1.94617
A58	2.35214	0.00089	0.00000	0.00468	0.00454	2.35667
A59	1.95007	0.00002	-0.00002	-0.00347	-0.00325	1.94682
A60	1.98091	-0.00091	0.00002	-0.00115	-0.00123	1.97968
A61	1.96659	-0.00073	0.00003	0.00084	0.00056	1.96715
A62	2.37604	0.00131	-0.00002	0.00567	0.00502	2.38107
A63	1.94015	-0.00059	-0.00001	-0.00681	-0.00594	1.93421
A64	1.97436	-0.00103	0.00000	-0.00394	-0.00377	1.97059
A65	2.44481	0.00120	0.00001	0.00421	0.00421	2.44903
A66	1.86395	-0.00017	0.00000	-0.00023	-0.00041	1.86354
A67	1.85638	0.00054	-0.00001	0.00177	0.00156	1.85794
A68	2.46044	0.00097	-0.00001	0.00093	0.00089	2.46133
A69	1.96621	-0.00150	0.00002	-0.00254	-0.00233	1.96388
A70	1.98357	-0.00024	-0.00001	-0.00024	-0.00051	1.98306
A71	1.93531	-0.00119	-0.00003	-0.00829	-0.00743	1.92788
A72	2.36357	0.00143	0.00004	0.00846	0.00787	2.37144
A73	1.96399	-0.00294	0.00004	-0.00566	-0.00548	1.95851
A74	2.19066	0.00235	0.00003	0.01043	0.01037	2.20103
A75	2.12849	0.00059	-0.00007	-0.00469	-0.00485	2.12364
A76	1.94340	0.00283	0.00000	0.00614	0.00610	1.94951
A77	2.06939	0.01127	-0.00015	0.01811	0.01795	2.08734
A78	2.27007	-0.01409	0.00015	-0.02398	-0.02384	2.24623
A79	1.56758	0.00186	-0.00005	0.00226	0.00212	1.56971
A80	1.82492	0.00146	0.00006	0.01420	0.01282	1.83773
A81	2.10689	0.00089	0.00020	0.03452	0.03159	2.13848
A82	2.10433	-0.00028	0.00024	0.03272	0.02976	2.13409
A83	2.38516	-0.02305	0.00035	-0.03968	-0.03933	2.34582
A84	1.90017	0.01030	-0.00015	0.01934	0.01919	1.91936
A85	1.99785	0.01274	-0.00020	0.02034	0.02014	2.01799
A86	2.22672	-0.02467	0.00021	-0.04381	-0.04361	2.18311
A87	2.18133	0.02103	-0.00019	0.03599	0.03580	2.21714
A88	1.87511	0.00364	-0.00002	0.00784	0.00782	1.88293
A89	1.86367	-0.00024	0.00001	0.00013	0.00011	1.86377
A90	2.23354	-0.00483	0.00005	-0.00969	-0.00962	2.22392
A91	2.18598	0.00507	-0.00006	0.00955	0.00951	2.19549
A92	1.87873	-0.00665	0.00006	-0.01322	-0.01312	1.86561
A93	2.22293	0.01781	-0.00011	0.02844	0.02831	2.25124
A94	2.18151	-0.01116	0.00005	-0.01522	-0.01519	2.16633
A95	1.91116	0.00029	0.00001	0.00248	0.00247	1.91363
A96	2.22991	-0.00052	-0.00001	-0.00374	-0.00374	2.22617
A97	2.14212	0.00023	0.00000	0.00125	0.00127	2.14338
A98	1.89610	0.00296	-0.00006	0.00277	0.00273	1.89883
A99	2.30704	-0.00159	0.00007	0.00401	0.00406	2.31110
A100	2.08005	-0.00137	-0.00001	-0.00678	-0.00679	2.07326
A101	2.05767	0.00009	0.00001	0.00217	0.00218	2.05985
A102	2.08734	0.00029	0.00000	0.00227	0.00228	2.08962
A103	2.13818	-0.00038	-0.00002	-0.00444	-0.00446	2.13372
A104	2.06485	0.00104	0.00000	0.00422	0.00423	2.06907
A105	2.12962	-0.00017	0.00004	0.00337	0.00341	2.13303
A106	2.08872	-0.00086	-0.00004	-0.00759	-0.00764	2.08109
A107	2.09732	-0.00030	-0.00001	-0.00170	-0.00171	2.09561
A108	2.09901	-0.00013	-0.00002	-0.00219	-0.00221	2.09680

A109	2.08685	0.00042	0.00002	0.00389	0.00392	2.09077
A110	2.12436	0.00030	0.00000	0.00084	0.00084	2.12520
A111	2.07709	-0.00050	-0.00002	-0.00351	-0.00354	2.07355
A112	2.08173	0.00020	0.00002	0.00268	0.00270	2.08443
A113	2.15170	0.01406	-0.00015	0.02385	0.02369	2.17540
A114	2.15791	-0.00623	-0.00008	-0.01498	-0.01506	2.14285
A115	1.97357	-0.00783	0.00023	-0.00887	-0.00863	1.96494
A116	2.15249	0.00208	-0.00011	0.00393	0.00382	2.15631
A117	2.17066	-0.00125	-0.00007	-0.01538	-0.01545	2.15521
A118	1.96001	-0.00083	0.00018	0.01146	0.01164	1.97165
A119	1.90869	0.00012	0.00000	0.00037	0.00037	1.90906
A120	1.94464	-0.00011	-0.00001	-0.00198	-0.00199	1.94265
A121	1.90302	-0.00002	0.00000	-0.00007	-0.00006	1.90296
A122	1.91053	0.00003	0.00001	0.00097	0.00097	1.91151
A123	1.88471	0.00000	-0.00001	-0.00020	-0.00021	1.88450
A124	1.91124	0.00000	0.00001	0.00095	0.00097	1.91221
A125	1.93870	0.00001	0.00000	0.00066	0.00066	1.93936
A126	1.90293	0.00059	0.00001	0.00391	0.00391	1.90684
A127	1.90210	-0.00010	0.00001	0.00038	0.00039	1.90249
A128	1.91190	-0.00011	0.00000	0.00023	0.00023	1.91213
A129	1.91310	0.00007	0.00000	0.00060	0.00061	1.91371
A130	1.89452	-0.00047	-0.00003	-0.00593	-0.00597	1.88855
A131	3.14090	0.00566	-0.00029	0.04162	0.04133	3.18223
A132	3.16777	0.00070	-0.00019	0.00038	0.00019	3.16796
A133	3.17910	0.00051	-0.00005	0.00724	0.00719	3.18629
A134	3.17218	-0.00039	-0.00002	-0.00863	-0.00865	3.16354
A135	3.13944	-0.00008	0.00002	0.00064	0.00066	3.14010
A136	3.14198	-0.00001	0.00000	-0.00040	-0.00040	3.14158
A137	3.14266	-0.00005	0.00001	-0.00026	-0.00025	3.14241
A138	3.14249	0.00007	-0.00001	-0.00049	-0.00050	3.14198
D1	-0.00609	0.00002	0.00003	0.00217	0.00219	-0.00390
D2	3.12576	0.00001	0.00003	0.00231	0.00235	3.12811
D3	3.13757	0.00000	0.00003	0.00187	0.00189	3.13946
D4	-0.01377	-0.00001	0.00003	0.00201	0.00205	-0.01172
D5	0.00179	0.00004	0.00001	0.00174	0.00175	0.00354
D6	-3.14044	0.00006	0.00001	0.00213	0.00214	-3.13830
D7	3.14074	0.00006	0.00001	0.00210	0.00212	-3.14033
D8	-0.00149	0.00008	0.00001	0.00249	0.00250	0.00101
D9	0.02841	-0.00016	-0.00004	-0.00949	-0.00951	0.01890
D10	-3.09879	-0.00009	-0.00003	-0.00795	-0.00797	-3.10676
D11	-3.11075	-0.00019	-0.00003	-0.00981	-0.00984	-3.12059
D12	0.04524	-0.00011	-0.00003	-0.00828	-0.00830	0.03694
D13	0.00556	-0.00006	-0.00005	-0.00455	-0.00459	0.00097
D14	-3.13555	-0.00010	-0.00004	-0.00510	-0.00513	-3.14068
D15	-3.12443	-0.00005	-0.00005	-0.00473	-0.00479	-3.12922
D16	0.01764	-0.00009	-0.00004	-0.00528	-0.00533	0.01231
D17	-0.00605	0.00017	-0.00001	0.00619	0.00615	0.00010
D18	-3.13508	-0.00009	0.00008	-0.00376	-0.00375	-3.13883
D19	3.12518	0.00016	-0.00001	0.00637	0.00635	3.13153
D20	-0.00384	-0.00010	0.00008	-0.00358	-0.00356	-0.00739
D21	-0.00086	0.00005	0.00003	0.00304	0.00307	0.00220
D22	3.13794	0.00006	0.00004	0.00371	0.00374	-3.14151
D23	3.14023	0.00009	0.00002	0.00361	0.00363	-3.13933
D24	-0.00415	0.00010	0.00003	0.00428	0.00430	0.00015
D25	-0.00326	0.00001	0.00001	0.00077	0.00078	-0.00249
D26	3.13594	0.00005	0.00001	0.00188	0.00190	3.13784
D27	3.14111	0.00000	0.00000	0.00011	0.00010	3.14122
D28	-0.00287	0.00004	0.00001	0.00122	0.00122	-0.00165
D29	0.00274	-0.00005	-0.00003	-0.00319	-0.00322	-0.00048
D30	-3.13823	-0.00007	-0.00003	-0.00357	-0.00360	3.14136

D31	-3.13647	-0.00009	-0.00004	-0.00430	-0.00434	-3.14081
D32	0.00574	-0.00011	-0.00003	-0.00468	-0.00471	0.00103
D33	-0.03175	0.00024	0.00003	0.01310	0.01313	-0.01862
D34	3.10775	0.00009	0.00000	0.00768	0.00760	3.11535
D35	3.09464	0.00022	0.00002	0.01188	0.01194	3.10659
D36	-0.04904	0.00007	-0.00001	0.00646	0.00641	-0.04262
D37	-0.02499	0.00011	0.00005	0.00582	0.00588	-0.01911
D38	3.10903	0.00015	0.00003	0.00736	0.00740	3.11643
D39	3.13418	0.00018	0.00005	0.00746	0.00751	-3.14150
D40	-0.01499	0.00022	0.00003	0.00900	0.00903	-0.00596
D41	0.02362	-0.00023	-0.00001	-0.01185	-0.01188	0.01173
D42	-3.11587	-0.00010	0.00002	-0.00645	-0.00649	-3.12237
D43	-3.13089	0.00007	-0.00011	-0.00153	-0.00169	-3.13257
D44	0.01281	0.00020	-0.00007	0.00387	0.00371	0.01651
D45	-3.14116	-0.00014	-0.00009	-0.00672	-0.00680	3.13522
D46	-0.00345	-0.00005	-0.00008	-0.00583	-0.00591	-0.00936
D47	-0.00204	-0.00031	-0.00012	-0.01309	-0.01322	-0.01526
D48	3.13567	-0.00022	-0.00012	-0.01220	-0.01232	3.12335
D49	0.01124	-0.00019	-0.00004	-0.00830	-0.00831	0.00293
D50	-3.13582	-0.00009	-0.00022	-0.02181	-0.02206	3.12531
D51	-3.12663	-0.00027	-0.00004	-0.00914	-0.00916	-3.13579
D52	0.00949	-0.00018	-0.00022	-0.02265	-0.02290	-0.01341
D53	-3.13436	0.00008	-0.00010	-0.00107	-0.00119	-3.13555
D54	0.01234	-0.00002	0.00007	0.01153	0.01160	0.02394
D55	3.12648	0.00006	0.00025	0.01515	0.01555	-3.14115
D56	-0.08038	0.00116	0.00049	0.06313	0.06339	-0.01699
D57	-0.01970	0.00013	0.00010	0.00375	0.00384	-0.01587
D58	3.05662	0.00123	0.00034	0.05173	0.05167	3.10829
D59	-0.00903	0.00018	0.00034	0.03147	0.03170	0.02267
D60	-3.11087	0.00014	0.00049	0.04168	0.04192	-3.06895
D61	3.13223	-0.00018	0.00032	0.02901	0.02922	-3.12174
D62	0.03038	-0.00022	0.00047	0.03923	0.03945	0.06982
D63	-0.00206	-0.00007	-0.00023	-0.02386	-0.02404	-0.02610
D64	3.14005	0.00048	-0.00021	-0.02014	-0.02025	3.11980
D65	-0.00243	0.00003	-0.00003	-0.00251	-0.00251	-0.00494
D66	-3.11637	0.00031	-0.00006	-0.00828	-0.00823	-3.12460
D67	3.13866	-0.00050	-0.00005	-0.00608	-0.00615	3.13251
D68	0.02473	-0.00022	-0.00008	-0.01186	-0.01188	0.01285
D69	0.01854	-0.00019	-0.00028	-0.02215	-0.02246	-0.00392
D70	-3.05541	-0.00124	-0.00051	-0.07094	-0.07178	-3.12720
D71	3.10847	-0.00020	-0.00047	-0.03626	-0.03671	3.07176
D72	0.03453	-0.00126	-0.00071	-0.08505	-0.08603	-0.05151
D73	-0.04442	0.00028	-0.00069	-0.05864	-0.05968	-0.10410
D74	-2.22720	-0.00507	-0.00131	-0.19768	-0.19880	-2.42599
D75	-3.13507	0.00032	-0.00050	-0.04495	-0.04585	3.10226
D76	0.96534	-0.00503	-0.00112	-0.18398	-0.18497	0.78037
D77	-0.02661	0.00021	-0.00042	-0.03543	-0.03561	-0.06222
D78	-3.12641	0.00016	-0.00028	-0.02204	-0.02221	3.13457
D79	3.09572	0.00003	-0.00040	-0.03140	-0.03161	3.06411
D80	-0.00408	-0.00002	-0.00026	-0.01800	-0.01821	-0.02229
D81	3.12562	-0.00029	0.00021	0.01692	0.01701	-3.14055
D82	0.01283	-0.00001	0.00018	0.01087	0.01104	0.02387
D83	0.04301	-0.00028	0.00067	0.05717	0.05811	0.10112
D84	2.22959	0.00417	0.00130	0.19141	0.19279	2.42239
D85	3.13030	-0.00035	0.00049	0.03903	0.03977	-3.11311
D86	-0.96630	0.00410	0.00112	0.17327	0.17446	-0.79183
D87	-3.13757	0.00008	0.00015	0.01005	0.01016	-3.12742
D88	-0.01015	0.00005	0.00022	0.01677	0.01693	0.00678
D89	0.05849	0.00015	0.00033	0.02856	0.02891	0.08740
D90	-3.09727	0.00012	0.00040	0.03528	0.03568	-3.06160

D91	1.02127	0.00262	0.00026	0.06450	0.06659	1.08786
D92	3.12980	0.00288	0.00027	0.06776	0.06987	-3.08351
D93	-1.08822	0.00259	0.00024	0.06309	0.06516	-1.02306
D94	-1.04782	-0.00274	-0.00030	-0.06670	-0.06884	-1.11665
D95	1.06071	-0.00248	-0.00029	-0.06343	-0.06556	0.99516
D96	3.12588	-0.00277	-0.00032	-0.06811	-0.07027	3.05561
D97	-0.01866	0.00003	-0.00005	-0.00138	-0.00141	-0.02008
D98	3.13361	0.00014	0.00004	0.00659	0.00663	3.14024
D99	3.13502	0.00002	0.00006	0.00721	0.00729	-3.14087
D100	0.00779	0.00005	-0.00001	0.00042	0.00043	0.00822
D101	-0.01473	0.00008	0.00013	0.00858	0.00868	-0.00605
D102	3.11300	0.00035	0.00012	0.01328	0.01332	3.12631
D103	0.02003	-0.00006	-0.00008	-0.00847	-0.00853	0.01150
D104	-3.13253	-0.00007	-0.00003	-0.00322	-0.00325	-3.13579
D105	-3.12963	-0.00015	-0.00016	-0.01450	-0.01461	3.13894
D106	0.00099	-0.00016	-0.00010	-0.00924	-0.00934	-0.00835
D107	3.11879	0.00011	0.00010	0.00784	0.00797	3.12676
D108	-0.05741	-0.00001	0.00001	-0.00471	-0.00473	-0.06214
D109	-0.01224	0.00022	0.00019	0.01571	0.01590	0.00366
D110	3.09475	0.00010	0.00010	0.00316	0.00320	3.09795
D111	0.01842	-0.00021	-0.00021	-0.01571	-0.01586	0.00256
D112	-3.11388	-0.00041	-0.00020	-0.01890	-0.01900	-3.13288
D113	-3.09746	-0.00016	-0.00014	-0.00660	-0.00669	-3.10415
D114	0.05342	-0.00036	-0.00013	-0.00979	-0.00983	0.04359
D115	3.09290	0.00053	0.00019	0.02054	0.02074	3.11364
D116	0.65027	-0.00180	-0.00044	-0.08792	-0.08825	0.56202
D117	-0.08293	0.00040	0.00010	0.00822	0.00828	-0.07464
D118	-2.52556	-0.00192	-0.00053	-0.10024	-0.10070	-2.62627
D119	-3.12866	-0.00023	0.00011	0.00171	0.00189	-3.12677
D120	-0.00892	0.00023	0.00011	0.01305	0.01316	0.00425
D121	-0.00039	0.00003	0.00011	0.00620	0.00633	0.00594
D122	3.11936	0.00049	0.00011	0.01754	0.01760	3.13696
D123	3.12410	0.00022	0.00001	0.00065	0.00056	3.12466
D124	-0.05216	0.00027	-0.00005	-0.00085	-0.00100	-0.05317
D125	-0.00258	-0.00012	0.00001	-0.00711	-0.00715	-0.00973
D126	3.10434	-0.00007	-0.00005	-0.00862	-0.00871	3.09563
D127	-3.11459	-0.00023	0.00000	-0.00368	-0.00357	-3.11817
D128	0.00428	0.00027	0.00000	0.00815	0.00816	0.01245
D129	-0.00137	-0.00014	-0.00001	0.00127	0.00132	-0.00005
D130	-3.13380	-0.00015	-0.00013	-0.00809	-0.00821	3.14118
D131	-3.09680	-0.00013	0.00007	0.00381	0.00393	-3.09287
D132	0.05396	-0.00013	-0.00005	-0.00555	-0.00560	0.04835
D133	0.08258	-0.00044	-0.00003	-0.00429	-0.00428	0.07831
D134	2.52650	0.00247	0.00058	0.10488	0.10530	2.63179
D135	-3.10426	-0.00044	-0.00010	-0.00664	-0.00671	-3.11097
D136	-0.66035	0.00247	0.00050	0.10253	0.10286	-0.55749
D137	0.00456	0.00035	0.00001	0.00490	0.00487	0.00943
D138	3.12157	0.00026	0.00005	0.01423	0.01441	3.13598
D139	3.13736	0.00036	0.00012	0.01397	0.01401	-3.13181
D140	-0.02882	0.00027	0.00016	0.02330	0.02355	-0.00526
D141	-0.00502	-0.00036	0.00000	-0.00745	-0.00748	-0.01250
D142	-3.11840	-0.00077	-0.00004	-0.01901	-0.01893	-3.13733
D143	3.13986	0.00023	0.00009	0.01392	0.01404	-3.12929
D144	0.00387	0.00014	0.00013	0.01401	0.01418	0.01804
D145	-0.03165	0.00052	0.00014	0.02595	0.02605	-0.00560
D146	3.11554	0.00043	0.00018	0.02604	0.02619	-3.14146
D147	-0.94943	0.00170	0.00032	0.05796	0.05903	-0.89039
D148	1.16502	0.00174	0.00032	0.05814	0.05921	1.22423
D149	-3.00663	0.00165	0.00033	0.05803	0.05911	-2.94752
D150	3.00070	-0.00178	-0.00032	-0.06082	-0.06189	2.93881

D151	-1.16804	-0.00174	-0.00033	-0.06064	-0.06171	-1.22975
D152	0.94350	-0.00183	-0.00031	-0.06075	-0.06182	0.88168
D153	-0.00347	0.00017	0.00003	0.00672	0.00675	0.00327
D154	-3.13777	0.00005	0.00004	0.00339	0.00344	-3.13433
D155	3.13230	0.00025	-0.00002	0.00661	0.00659	3.13889
D156	-0.00200	0.00013	0.00000	0.00328	0.00328	0.00128
D157	-3.13590	-0.00020	0.00002	-0.00271	-0.00261	-3.13851
D158	0.00553	-0.00012	0.00003	-0.00086	-0.00079	0.00474
D159	-0.00058	-0.00001	0.00001	0.00029	0.00031	-0.00027
D160	3.14086	0.00006	0.00001	0.00215	0.00213	-3.14020
D161	3.13877	-0.00003	-0.00002	0.00153	0.00159	3.14036
D162	0.00195	-0.00001	-0.00002	0.00003	0.00006	0.00202
D163	0.00324	-0.00001	-0.00001	-0.00103	-0.00104	0.00219
D164	-3.13358	0.00001	-0.00001	-0.00252	-0.00257	-3.13615
D165	-0.00248	0.00002	-0.00001	0.00058	0.00058	-0.00190
D166	3.14065	0.00005	0.00000	0.00104	0.00103	-3.14150
D167	3.13927	-0.00005	-0.00001	-0.00121	-0.00120	3.13807
D168	-0.00078	-0.00003	0.00000	-0.00075	-0.00075	-0.00153
D169	-0.00485	0.00002	0.00001	0.00143	0.00144	-0.00341
D170	3.13752	0.00002	0.00001	0.00116	0.00117	3.13870
D171	3.13211	0.00010	0.00001	0.00303	0.00302	3.13513
D172	-0.00871	0.00010	0.00001	0.00276	0.00276	-0.00595
D173	0.00074	0.00002	0.00000	0.00059	0.00060	0.00134
D174	3.13935	0.00005	0.00001	0.00271	0.00274	-3.14110
D175	-3.13529	0.00001	0.00000	-0.00119	-0.00120	-3.13650
D176	0.00332	0.00004	0.00001	0.00094	0.00094	0.00426
D177	0.00452	-0.00001	0.00000	-0.00120	-0.00122	0.00330
D178	-3.13773	-0.00001	0.00000	-0.00097	-0.00099	-3.13872
D179	-3.13852	-0.00003	-0.00001	-0.00164	-0.00165	-3.14017
D180	0.00241	-0.00003	-0.00001	-0.00141	-0.00142	0.00099
D181	3.13874	-0.00001	0.00001	0.00045	0.00047	3.13921
D182	-0.00251	-0.00001	0.00000	0.00044	0.00045	-0.00206
D183	-0.00113	0.00002	0.00001	0.00097	0.00098	-0.00015
D184	3.14081	0.00002	0.00001	0.00095	0.00096	-3.14141
D185	3.13887	0.00003	0.00000	0.00107	0.00108	3.13996
D186	-0.00230	0.00002	0.00000	0.00106	0.00106	-0.00123
D187	-0.00187	0.00002	0.00000	0.00079	0.00079	-0.00108
D188	3.14014	0.00001	0.00001	0.00077	0.00077	3.14091
D189	-0.00062	0.00000	0.00000	0.00005	0.00005	-0.00057
D190	-3.14142	-0.00001	0.00000	-0.00028	-0.00029	3.14148
D191	3.14061	0.00000	0.00000	0.00007	0.00007	3.14069
D192	-0.00019	-0.00001	0.00000	-0.00026	-0.00026	-0.00045
D193	0.00019	0.00000	0.00001	0.00020	0.00021	0.00040
D194	3.14120	0.00001	0.00001	0.00053	0.00053	-3.14146
D195	3.14137	0.00001	0.00000	0.00022	0.00022	-3.14159
D196	-0.00081	0.00002	0.00000	0.00055	0.00055	-0.00026
D197	0.00109	-0.00001	-0.00001	-0.00063	-0.00064	0.00045
D198	-3.13992	-0.00002	0.00000	-0.00095	-0.00096	-3.14088
D199	-3.14129	0.00000	-0.00001	-0.00030	-0.00031	3.14159
D200	0.00089	-0.00001	-0.00001	-0.00063	-0.00063	0.00026

Item	Value	Threshold	Converged?

Maximum Force	0.024669	0.000450	NO

RMS Force	0.003250	0.000300	NO

Maximum Displacement	0.800116	0.001800	NO

RMS Displacement	0.180142	0.001200	NO

Predicted change in Energy=-9.890688D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.773485	-0.660002	-0.017904
2	6	0	-9.940018	-1.795986	0.009776
3	6	0	-10.433536	-3.091832	0.022942
4	6	0	-11.818117	-3.265446	0.006699
5	6	0	-12.663081	-2.149872	-0.024650
6	6	0	-12.161464	-0.844775	-0.037613
7	1	0	-9.743103	-3.928696	0.045169
8	1	0	-12.244359	-4.263962	0.016297
9	1	0	-13.738628	-2.297220	-0.040603
10	1	0	-12.850674	-0.014696	-0.062120
11	6	0	-9.916455	0.558524	-0.022260
12	6	0	-8.525388	-1.370928	0.008080
13	6	0	-8.525043	0.106329	-0.022340
14	6	0	-7.398068	0.904981	-0.054834
15	6	0	-6.006286	0.641505	-0.053667
16	6	0	-3.651766	-0.144174	-0.030957
17	6	0	-3.771114	1.258944	-0.103425
18	16	0	-5.188687	-0.943713	-0.009836
19	6	0	-5.083539	1.705684	-0.113685
20	6	0	-2.267969	-0.422811	-0.003296
21	6	0	-1.604509	0.813261	-0.066288
22	7	0	-2.504790	1.875359	-0.214382
23	16	0	-1.173080	-1.785451	0.057572
24	16	0	1.151685	1.801352	-0.065642
25	6	0	0.187275	-0.670104	0.039185
26	6	0	-0.203982	0.681597	-0.037535
27	6	0	1.589928	-0.801231	0.064458
28	6	0	2.254119	0.442064	0.012045
29	6	0	3.630451	0.167216	0.032332
30	6	0	3.757150	-1.241421	0.088660
31	6	0	5.073583	-1.681710	0.093497
32	6	0	5.991848	-0.615330	0.040654
33	16	0	5.163145	0.969798	-0.000241
34	7	0	2.499439	-1.841515	0.173199
35	6	0	7.373672	-0.886584	0.044795
36	6	0	8.509473	-0.106834	0.015606
37	6	0	8.524840	1.371307	-0.028530
38	6	0	9.907202	-0.574111	0.017519
39	6	0	9.943791	1.782789	-0.052583
40	6	0	10.769431	0.639810	-0.022896
41	6	0	10.448122	3.071737	-0.095051
42	6	0	12.158716	0.811206	-0.035606
43	6	0	11.835162	3.233403	-0.108483
44	6	0	12.671748	2.112686	-0.078676
45	6	0	10.393861	-1.875094	0.046190
46	6	0	9.577492	-3.046907	0.079046
47	6	0	11.792177	-2.179374	0.044686
48	7	0	8.950393	-4.029979	0.105177
49	7	0	12.924125	-2.457126	0.044377
50	6	0	-10.378999	1.863138	-0.007568
51	6	0	-11.765031	2.209445	-0.008704

52	6	0	-9.520444	3.002539	0.017500
53	7	0	-12.881692	2.542105	-0.010766
54	7	0	-8.839467	3.948780	0.038689
55	8	0	-7.550789	-2.114650	0.025612
56	8	0	7.559632	2.125845	-0.041349
57	6	0	2.233683	-3.178598	-0.360851
58	1	0	1.260667	-3.523823	-0.005658
59	1	0	2.244753	-3.179121	-1.456038
60	1	0	2.992669	-3.868343	0.012607
61	6	0	-2.259846	3.115444	0.561404
62	1	0	-2.333441	2.928464	1.637570
63	1	0	-1.265169	3.498019	0.324101
64	1	0	-2.993442	3.868352	0.268823
65	1	0	5.401778	-2.714071	0.132788
66	1	0	12.841572	-0.024040	-0.013725
67	1	0	13.748648	2.250437	-0.088809
68	1	0	12.267690	4.228744	-0.141649
69	1	0	9.766503	3.915794	-0.116356
70	1	0	7.540381	-1.955089	0.073126
71	1	0	-7.579922	1.973595	-0.092082
72	1	0	-5.405227	2.738034	-0.177275

Rotational constants (GHZ): 0.1752778 0.0104540 0.0098707

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis func-
tions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6580.7237270647 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T
Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6580.6383111623 Har-
trees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.24D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Initial guess from the checkpoint file: "PBDB.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999997 0.000689 -0.000121 -0.002181 Ang= 0.26 deg.

ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1

AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for in-
itial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-
yADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPflag= 0 FMflag= 100000 FMflg1= 2001

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 IlCent= 200000004 NGrid=

0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0=

0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Integral accuracy reduced to 1.0D-05 until final iterations.

Initial convergence to 1.0D-05 achieved. Increase integral accuracy.

SCF Done: E(RB3LYP) = -3683.01112333 A.U. after 14 cycles

NFock= 14 Conv=0.77D-08 -V/T= 2.0068

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1

NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	0.000740243	0.000383010	0.000943404
2	6	-0.001324757	-0.000377634	-0.000438297
3	6	0.000342227	-0.000154138	0.000015513
4	6	-0.000129365	0.000472987	-0.000013887
5	6	-0.000285813	0.000670547	-0.000077599
6	6	0.001044643	-0.001774852	0.000207385
7	1	-0.000025765	0.000091699	0.000068074
8	1	0.000016587	-0.000103577	-0.000002230
9	1	-0.000053001	-0.000108378	-0.000093091
10	1	-0.001270186	-0.000956885	-0.000976984
11	6	-0.000049398	0.000889299	-0.000396349
12	6	-0.001021109	-0.000605505	-0.001263038
13	6	0.001909178	-0.002663927	0.001089220
14	6	-0.000784689	-0.000092940	-0.000491031
15	6	-0.002398678	0.000754329	-0.000709662
16	6	0.001710595	0.000463593	0.001790453
17	6	-0.003205008	-0.006341976	0.004992765
18	16	0.003750971	-0.002086177	0.001396934
19	6	-0.002275738	0.003242044	-0.001357486
20	6	-0.003302952	0.001811530	-0.000444723
21	6	-0.004977691	-0.004378713	0.003497802
22	7	0.013172997	0.006170625	-0.015702575
23	16	0.000970984	0.000481705	0.000168156
24	16	-0.000144028	-0.000498021	-0.000487441
25	6	-0.002155448	-0.001478949	-0.000519653
26	6	0.002871662	0.001214185	0.001331736
27	6	0.001141517	0.001636460	-0.003063302
28	6	0.000010246	0.000975223	-0.000228679
29	6	0.000182205	-0.000403517	0.000758128
30	6	0.002320952	0.001148576	-0.002912620
31	6	0.000579489	-0.000888521	0.001445486
32	6	-0.003499031	0.001793078	-0.003377757
33	16	-0.000152447	-0.000336932	-0.000395461
34	7	-0.006554927	-0.001106377	0.007487794
35	6	0.005119577	-0.001673055	0.004384560
36	6	0.003156624	-0.001522376	0.002454371
37	6	0.002971951	0.000032345	0.002036292
38	6	-0.000580000	0.001175072	-0.000321268
39	6	0.001849004	0.001779957	0.001343722
40	6	-0.001829866	-0.000004141	-0.001381133
41	6	-0.000201488	-0.001530329	-0.000258458
42	6	-0.001028208	-0.000511621	-0.000705531
43	6	-0.000499774	-0.000647662	-0.000404927
44	6	0.000342113	0.000463250	0.000276600
45	6	-0.002476085	-0.003038881	-0.002163794
46	6	-0.000427920	0.001070077	-0.000239836
47	6	-0.000141027	0.001004792	0.000001529
48	7	-0.001019390	-0.001607326	-0.000890794

49	7	-0.000850105	0.001228907	-0.000534026
50	6	-0.000116079	0.002644395	0.000376744
51	6	-0.000061878	-0.000533988	-0.000090166
52	6	-0.001900468	-0.002003643	-0.001540555
53	7	0.000476207	0.000631376	0.000396751
54	7	-0.000486248	0.000885078	-0.000328232
55	8	0.000331798	0.001858761	0.000475745
56	8	-0.001587152	-0.000806431	-0.001025462
57	6	0.002647068	-0.000121323	-0.004078273
58	1	-0.000038046	0.000050898	0.000200968
59	1	0.000135564	0.000360395	0.000192455
60	1	-0.000034360	-0.000055312	0.000223415
61	6	-0.004520076	0.000997549	0.007527826
62	1	0.000018230	-0.000166603	-0.000160924
63	1	-0.000232032	0.000158426	-0.000055629
64	1	-0.000106443	0.000141037	0.000101552
65	1	-0.000305430	0.000088657	-0.000123930
66	1	0.000479779	0.000024480	0.000337156
67	1	0.000044222	0.000107036	0.000042631
68	1	0.000049474	0.000064039	0.000043641
69	1	-0.000067753	0.000028157	-0.000050844
70	1	0.002150425	0.000917963	0.001469250
71	1	0.001474860	0.000790186	0.001005353
72	1	0.000108468	-0.000122014	-0.000777762

Cartesian Forces: Max 0.015702575 RMS 0.002295029

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.010938003 RMS 0.001806774

Search for a local minimum.

Step number 12 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 11 12

DE= -7.87D-03 DEPred=-9.89D-03 R= 7.96D-01

TightC=F SS= 1.41D+00 RLast= 5.60D-01 DXNew= 3.3118D+00 1.6814D+00

Trust test= 7.96D-01 RLast= 5.60D-01 DXMaxT set to 1.97D+00

ITU= 1 1 1 0 0 0 1 0 0 0 1 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00230	0.00230	0.00230	0.00232	0.00241
Eigenvalues ---	0.00289	0.00387	0.00445	0.00458	0.00481
Eigenvalues ---	0.00505	0.00517	0.00573	0.00602	0.00614
Eigenvalues ---	0.00623	0.00668	0.00682	0.00705	0.00710
Eigenvalues ---	0.00737	0.00743	0.00760	0.00771	0.00773
Eigenvalues ---	0.00817	0.00832	0.00849	0.00864	0.00882
Eigenvalues ---	0.00992	0.01013	0.01086	0.01134	0.01152
Eigenvalues ---	0.01240	0.01254	0.01269	0.01336	0.01360
Eigenvalues ---	0.01364	0.01394	0.01406	0.01452	0.01457
Eigenvalues ---	0.01570	0.01575	0.01646	0.01654	0.01754
Eigenvalues ---	0.01794	0.01800	0.01929	0.01953	0.02006
Eigenvalues ---	0.02024	0.02075	0.02075	0.02166	0.02210
Eigenvalues ---	0.02219	0.04827	0.04837	0.04858	0.04900
Eigenvalues ---	0.04927	0.04999	0.05016	0.05099	0.07134
Eigenvalues ---	0.07279	0.07441	0.07608	0.15482	0.15721
Eigenvalues ---	0.15847	0.15997	0.15998	0.15999	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16000

Eigenvalues	---	0.16000	0.16000	0.16000	0.16001	0.16005
Eigenvalues	---	0.16017	0.16028	0.17451	0.17809	0.18960
Eigenvalues	---	0.19055	0.19505	0.19832	0.20619	0.21176
Eigenvalues	---	0.21408	0.22000	0.22005	0.22139	0.22336
Eigenvalues	---	0.22552	0.22569	0.22610	0.22637	0.22668
Eigenvalues	---	0.22826	0.22901	0.22981	0.23132	0.23368
Eigenvalues	---	0.23447	0.23754	0.23800	0.23942	0.24168
Eigenvalues	---	0.24253	0.24277	0.24412	0.24501	0.24564
Eigenvalues	---	0.24612	0.24729	0.24904	0.24959	0.24962
Eigenvalues	---	0.24977	0.24982	0.24987	0.24994	0.24996
Eigenvalues	---	0.24997	0.24998	0.24998	0.24999	0.25000
Eigenvalues	---	0.25000	0.25000	0.25012	0.25407	0.25562
Eigenvalues	---	0.25839	0.26256	0.26465	0.26732	0.26801
Eigenvalues	---	0.26996	0.27168	0.27351	0.27839	0.27996
Eigenvalues	---	0.28314	0.28452	0.28628	0.28916	0.30047
Eigenvalues	---	0.30518	0.32311	0.32773	0.35141	0.35644
Eigenvalues	---	0.36329	0.36337	0.36474	0.36585	0.36650
Eigenvalues	---	0.36698	0.36827	0.36868	0.37081	0.37095
Eigenvalues	---	0.37242	0.37252	0.37274	0.37419	0.37565
Eigenvalues	---	0.37670	0.37755	0.38020	0.38855	0.40305
Eigenvalues	---	0.40694	0.41529	0.42004	0.42270	0.42789
Eigenvalues	---	0.44422	0.44764	0.45610	0.46104	0.47371
Eigenvalues	---	0.47875	0.48047	0.51151	0.52615	0.54383
Eigenvalues	---	0.55864	0.57704	0.73814	0.80372	0.81777
Eigenvalues	---	0.97340	1.25843	1.26318	1.29398	1.35397

RFO step: Lambda=-7.50681917D-03 EMin= 2.29994933D-03

Quartic linear search produced a step of 0.05093.

Iteration 1 RMS(Cart)= 0.07140260 RMS(Int)= 0.00190523

Iteration 2 RMS(Cart)= 0.00378732 RMS(Int)= 0.00079696

Iteration 3 RMS(Cart)= 0.00000627 RMS(Int)= 0.00079696

Iteration 4 RMS(Cart)= 0.00000003 RMS(Int)= 0.00079696

Variable	Old X	-DE/DX	Delta X	Delta X	Delta X	New X
(Linear)	(Quad)	(Total)				
R1	2.66304	-0.00283	0.00031	-0.00388	-0.00357	2.65947
R2	2.64630	-0.00138	0.00003	-0.00408	-0.00405	2.64226
R3	2.81520	-0.00317	0.00050	-0.01115	-0.01065	2.80455
R4	2.62049	0.00043	-0.00003	0.00011	0.00008	2.62057
R5	2.79133	0.00048	0.00005	0.00245	0.00250	2.79384
R6	2.63715	0.00091	0.00002	0.00263	0.00265	2.63979
R7	2.05062	0.00004	-0.00003	0.00008	0.00006	2.05068
R8	2.64525	0.00047	-0.00014	0.00123	0.00110	2.64634
R9	2.05173	-0.00010	-0.00001	-0.00029	-0.00030	2.05143
R10	2.64229	0.00036	0.00003	0.00084	0.00088	2.64316
R11	2.05170	-0.00001	-0.00001	-0.00002	-0.00002	2.05167
R12	2.03936	0.00178	-0.00020	0.00452	0.00431	2.04368
R13	2.76476	0.00414	-0.00020	0.01293	0.01273	2.77749
R14	2.61588	0.00106	0.00013	-0.00048	-0.00035	2.61553
R15	2.79220	0.00198	-0.00006	0.00540	0.00535	2.79755
R16	2.31696	0.00057	0.00006	0.00136	0.00143	2.31838
R17	2.61095	0.00004	0.00018	-0.01051	-0.01032	2.60063
R18	2.67680	0.00142	0.00048	0.00036	0.00084	2.67764
R19	2.04963	-0.00183	0.00012	-0.00383	-0.00371	2.04592
R20	3.37162	0.00318	-0.00024	0.01149	0.01099	3.38261
R21	2.66414	-0.00080	0.00006	-0.00282	-0.00278	2.66136
R22	2.66460	0.00057	0.00033	0.00415	0.00414	2.66874
R23	3.27410	-0.00038	0.00099	0.00397	0.00487	3.27898
R24	2.66799	-0.00177	0.00008	-0.00052	-0.00231	2.66568
R25	2.61994	0.00327	0.00029	0.01170	0.01223	2.63217
R26	2.66971	-0.00230	-0.00098	-0.01902	-0.01852	2.65119
R27	2.04691	0.00037	-0.00014	0.00043	0.00030	2.04721

R28	2.65372	0.00110	0.00036	0.00499	0.00503	2.65875
R29	3.30528	0.00089	0.00020	0.00531	0.00546	3.31073
R30	2.64595	-0.00113	-0.00093	-0.01480	-0.01425	2.63170
R31	2.65884	0.00238	0.00076	0.01224	0.01322	2.67206
R32	2.80270	-0.00621	-0.00068	-0.02245	-0.02313	2.77957
R33	3.32447	0.00057	0.00011	0.00318	0.00304	3.32751
R34	3.32317	0.00072	0.00015	0.00360	0.00369	3.32685
R35	3.31056	0.00062	0.00011	0.00317	0.00323	3.31379
R36	2.66315	-0.00140	0.00019	-0.00217	-0.00201	2.66114
R37	2.66262	0.00110	0.00084	0.00819	0.00911	2.67172
R38	2.66557	0.00024	0.00039	0.00313	0.00336	2.66893
R39	2.61932	0.00085	-0.00023	-0.00112	-0.00078	2.61854
R40	2.65252	0.00203	-0.00002	0.01021	0.00947	2.66199
R41	2.67480	-0.00012	0.00061	0.00420	0.00470	2.67950
R42	3.27002	0.00159	0.00007	0.00592	0.00597	3.27599
R43	2.62316	0.00203	0.00068	0.01141	0.01218	2.63535
R44	2.63825	0.00146	-0.00056	-0.00182	-0.00181	2.63644
R45	2.66121	0.00088	0.00006	0.00068	0.00072	2.66192
R46	2.04844	-0.00021	0.00001	-0.00028	-0.00027	2.04817
R47	3.38100	0.00105	-0.00015	0.00162	0.00137	3.38237
R48	2.66112	0.00780	-0.00115	0.02086	0.01971	2.68083
R49	2.76677	-0.00169	-0.00057	-0.00794	-0.00851	2.75826
R50	2.60406	0.00180	-0.00046	-0.00493	-0.00539	2.59867
R51	2.04431	0.00250	-0.00029	0.00337	0.00307	2.04738
R52	2.79468	0.00007	-0.00033	-0.00243	-0.00276	2.79192
R53	2.78502	-0.00770	0.00127	-0.02441	-0.02313	2.76189
R54	2.79227	0.00047	-0.00004	0.00059	0.00055	2.79282
R55	2.31529	0.00190	0.00001	0.00231	0.00232	2.31761
R56	2.81479	-0.00031	0.00054	-0.00266	-0.00213	2.81266
R57	2.62544	-0.00596	0.00078	-0.01046	-0.00968	2.61576
R58	2.66509	-0.00183	0.00055	-0.00096	-0.00041	2.66468
R59	2.61680	0.00172	0.00012	0.00531	0.00543	2.62223
R60	2.64538	-0.00015	0.00016	-0.00197	-0.00180	2.64358
R61	2.63899	-0.00005	0.00007	0.00077	0.00084	2.63983
R62	2.05058	0.00008	-0.00003	0.00014	0.00011	2.05069
R63	2.64488	-0.00013	0.00016	0.00051	0.00067	2.64555
R64	2.03916	0.00057	-0.00024	0.00156	0.00132	2.04048
R65	2.64344	0.00051	0.00003	0.00268	0.00271	2.64615
R66	2.05180	-0.00008	-0.00001	-0.00022	-0.00024	2.05156
R67	2.05172	-0.00003	-0.00002	-0.00012	-0.00013	2.05158
R68	2.69952	-0.00060	0.00004	-0.00273	-0.00270	2.69682
R69	2.70427	-0.00194	0.00026	-0.00761	-0.00735	2.69692
R70	2.20408	-0.00170	0.00005	-0.00089	-0.00084	2.20324
R71	2.20253	-0.00140	0.00003	-0.00106	-0.00103	2.20150
R72	2.69974	-0.00044	0.00020	-0.00175	-0.00155	2.69819
R73	2.69641	0.00110	-0.00006	0.00235	0.00229	2.69870
R74	2.20183	-0.00036	0.00001	-0.00034	-0.00033	2.20150
R75	2.20342	-0.00087	0.00000	-0.00069	-0.00069	2.20273
R76	2.06327	-0.00005	-0.00006	-0.00032	-0.00037	2.06290
R77	2.06971	0.00004	-0.00006	-0.00011	-0.00018	2.06953
R78	2.06256	0.00003	-0.00003	0.00003	0.00001	2.06256
R79	2.06881	0.00009	-0.00014	-0.00052	-0.00066	2.06815
R80	2.06323	-0.00023	-0.00008	-0.00097	-0.00105	2.06218
R81	2.06200	0.00003	-0.00003	0.00002	-0.00001	2.06199
A1	2.07159	0.00189	-0.00033	0.00623	0.00591	2.07750
A2	1.89564	0.00169	-0.00011	0.00600	0.00588	1.90153
A3	2.31595	-0.00358	0.00044	-0.01223	-0.01179	2.30416
A4	2.14479	-0.00069	0.00012	-0.00301	-0.00288	2.14191
A5	1.91180	-0.00017	-0.00004	-0.00170	-0.00175	1.91005
A6	2.22655	0.00086	-0.00008	0.00474	0.00466	2.23121

A7	2.05924	-0.00011	0.00007	-0.00049	-0.00043	2.05881
A8	2.08797	0.00015	-0.00008	0.00045	0.00037	2.08834
A9	2.13598	-0.00004	0.00001	0.00004	0.00006	2.13603
A10	2.09441	-0.00005	-0.00012	0.00081	0.00068	2.09509
A11	2.09881	-0.00001	0.00007	-0.00075	-0.00068	2.09813
A12	2.08996	0.00006	0.00005	-0.00005	0.00000	2.08996
A13	2.12647	-0.00067	0.00010	-0.00139	-0.00129	2.12518
A14	2.08306	0.00049	-0.00003	0.00182	0.00180	2.08485
A15	2.07365	0.00018	-0.00007	-0.00043	-0.00050	2.07315
A16	2.06986	-0.00037	0.00016	-0.00214	-0.00198	2.06788
A17	2.13155	-0.00038	0.00006	-0.00214	-0.00209	2.12946
A18	2.08178	0.00074	-0.00022	0.00428	0.00406	2.08584
A19	1.86953	0.00059	-0.00006	0.00060	0.00054	1.87008
A20	2.18783	-0.00984	0.00093	-0.03446	-0.03353	2.15430
A21	2.22569	0.00925	-0.00088	0.03394	0.03306	2.25875
A22	1.86288	0.00071	0.00005	0.00137	0.00143	1.86431
A23	2.19777	-0.00251	0.00027	-0.00317	-0.00290	2.19487
A24	2.22253	0.00180	-0.00031	0.00179	0.00147	2.22400
A25	1.88472	-0.00282	0.00018	-0.00620	-0.00603	1.87869
A26	2.21065	0.00018	0.00069	0.01197	0.01264	2.22328
A27	2.18780	0.00265	-0.00087	-0.00584	-0.00673	2.18107
A28	2.33768	0.00661	-0.00132	0.00065	-0.00068	2.33701
A29	2.01923	-0.00262	0.00036	0.00118	0.00153	2.02076
A30	1.92626	-0.00399	0.00096	-0.00181	-0.00086	1.92541
A31	2.23386	0.00736	-0.00053	0.01439	0.01372	2.24758
A32	2.09747	-0.00528	0.00032	-0.01135	-0.01116	2.08631
A33	1.95172	-0.00208	0.00020	-0.00259	-0.00247	1.94925
A34	1.96573	-0.00033	-0.00021	-0.00340	-0.00300	1.96274
A35	1.85496	-0.00002	-0.00012	0.00198	0.00127	1.85623
A36	2.46249	0.00035	0.00032	0.00141	0.00172	2.46421
A37	1.98357	-0.00066	-0.00006	0.00149	0.00069	1.98426
A38	1.94158	-0.00027	-0.00051	-0.01261	-0.01073	1.93085
A39	2.35653	0.00095	0.00055	0.01221	0.01090	2.36743
A40	1.56698	0.00148	-0.00002	0.00346	0.00321	1.57019
A41	1.95632	0.00160	0.00007	0.00129	0.00171	1.95804
A42	2.12649	-0.00089	-0.00052	-0.00393	-0.00486	2.12163
A43	2.20022	-0.00070	0.00054	0.00310	0.00322	2.20344
A44	1.86343	0.00027	0.00005	0.00343	0.00291	1.86634
A45	2.44648	0.00022	0.00001	-0.00045	-0.00048	2.44600
A46	1.97312	-0.00049	-0.00005	-0.00284	-0.00232	1.97080
A47	1.94835	-0.00105	-0.00065	-0.01549	-0.01368	1.93468
A48	1.96817	-0.00043	-0.00003	0.00086	0.00010	1.96826
A49	2.36480	0.00150	0.00063	0.01520	0.01406	2.37886
A50	1.81013	0.00123	0.00096	0.02585	0.02267	1.83280
A51	2.06210	0.00069	0.00286	0.05797	0.05199	2.11410
A52	2.06318	0.00167	0.00321	0.06613	0.06112	2.12430
A53	1.56056	0.00043	0.00011	0.00196	0.00187	1.56243
A54	1.56115	0.00038	0.00031	0.00242	0.00271	1.56386
A55	1.97576	0.00017	0.00013	0.00221	0.00223	1.97799
A56	2.36114	-0.00052	-0.00005	-0.00154	-0.00171	2.35944
A57	1.94617	0.00034	-0.00008	-0.00066	-0.00051	1.94565
A58	2.35667	-0.00016	0.00023	0.00196	0.00192	2.35860
A59	1.94682	0.00033	-0.00017	-0.00194	-0.00170	1.94511
A60	1.97968	-0.00018	-0.00006	-0.00002	-0.00022	1.97945
A61	1.96715	0.00013	0.00003	0.00144	0.00117	1.96832
A62	2.38107	0.00056	0.00026	0.00626	0.00582	2.38689
A63	1.93421	-0.00068	-0.00030	-0.00772	-0.00703	1.92718
A64	1.97059	-0.00068	-0.00019	-0.00322	-0.00323	1.96736
A65	2.44903	0.00002	0.00021	0.00111	0.00130	2.45032
A66	1.86354	0.00065	-0.00002	0.00216	0.00196	1.86550

A67	1.85794	-0.00044	0.00008	-0.00027	-0.00041	1.85752
A68	2.46133	0.00072	0.00005	0.00287	0.00286	2.46418
A69	1.96388	-0.00028	-0.00012	-0.00249	-0.00242	1.96147
A70	1.98306	-0.00043	-0.00003	-0.00024	-0.00058	1.98249
A71	1.92788	0.00001	-0.00038	-0.00610	-0.00551	1.92236
A72	2.37144	0.00042	0.00040	0.00683	0.00650	2.37793
A73	1.95851	0.00112	-0.00028	-0.00057	-0.00069	1.95782
A74	2.20103	-0.00083	0.00053	0.00106	0.00149	2.20253
A75	2.12364	-0.00029	-0.00025	-0.00049	-0.00083	2.12281
A76	1.94951	-0.00133	0.00031	0.00053	0.00078	1.95028
A77	2.08734	-0.00127	0.00091	0.00584	0.00672	2.09406
A78	2.24623	0.00260	-0.00121	-0.00613	-0.00738	2.23884
A79	1.56971	0.00092	0.00011	0.00257	0.00259	1.57229
A80	1.83773	0.00048	0.00065	0.01215	0.01119	1.84892
A81	2.13848	0.00065	0.00161	0.03123	0.02914	2.16762
A82	2.13409	0.00003	0.00152	0.02760	0.02526	2.15936
A83	2.34582	0.00351	-0.00200	-0.01252	-0.01454	2.33129
A84	1.91936	-0.00055	0.00098	0.01190	0.01287	1.93223
A85	2.01799	-0.00296	0.00103	0.00066	0.00167	2.01966
A86	2.18311	0.00735	-0.00222	0.00228	0.00006	2.18317
A87	2.21714	-0.00710	0.00182	-0.00583	-0.00401	2.21313
A88	1.88293	-0.00025	0.00040	0.00356	0.00396	1.88688
A89	1.86377	-0.00040	0.00001	-0.00251	-0.00251	1.86126
A90	2.22392	0.00107	-0.00049	-0.00119	-0.00169	2.22223
A91	2.19549	-0.00067	0.00048	0.00371	0.00419	2.19969
A92	1.86561	0.00246	-0.00067	0.00433	0.00366	1.86927
A93	2.25124	-0.01094	0.00144	-0.01830	-0.01686	2.23439
A94	2.16633	0.00848	-0.00077	0.01398	0.01320	2.17953
A95	1.91363	-0.00048	0.00013	-0.00289	-0.00277	1.91086
A96	2.22617	0.00017	-0.00019	0.00227	0.00208	2.22826
A97	2.14338	0.00031	0.00006	0.00062	0.00069	2.14407
A98	1.89883	-0.00133	0.00014	-0.00247	-0.00233	1.89650
A99	2.31110	0.00139	0.00021	0.00266	0.00287	2.31397
A100	2.07326	-0.00006	-0.00035	-0.00019	-0.00054	2.07272
A101	2.05985	-0.00016	0.00011	-0.00064	-0.00053	2.05932
A102	2.08962	0.00003	0.00012	0.00093	0.00105	2.09067
A103	2.13372	0.00013	-0.00023	-0.00030	-0.00052	2.13320
A104	2.06907	0.00028	0.00022	0.00088	0.00109	2.07016
A105	2.13303	-0.00002	0.00017	0.00054	0.00071	2.13373
A106	2.08109	-0.00026	-0.00039	-0.00141	-0.00180	2.07929
A107	2.09561	-0.00053	-0.00009	-0.00163	-0.00172	2.09389
A108	2.09680	0.00032	-0.00011	0.00017	0.00006	2.09687
A109	2.09077	0.00022	0.00020	0.00146	0.00165	2.09243
A110	2.12520	0.00016	0.00004	0.00096	0.00100	2.12620
A111	2.07355	-0.00020	-0.00018	-0.00204	-0.00222	2.07133
A112	2.08443	0.00004	0.00014	0.00109	0.00122	2.08566
A113	2.17540	-0.00705	0.00121	-0.01004	-0.00883	2.16656
A114	2.14285	0.00648	-0.00077	0.00896	0.00819	2.15104
A115	1.96494	0.00057	-0.00044	0.00108	0.00064	1.96558
A116	2.15631	-0.00487	0.00019	-0.02217	-0.02198	2.13433
A117	2.15521	0.00719	-0.00079	0.02350	0.02271	2.17793
A118	1.97165	-0.00232	0.00059	-0.00133	-0.00074	1.97091
A119	1.90906	0.00019	0.00002	0.00134	0.00136	1.91042
A120	1.94265	0.00053	-0.00010	0.00285	0.00275	1.94540
A121	1.90296	-0.00003	0.00000	-0.00052	-0.00052	1.90244
A122	1.91151	-0.00033	0.00005	-0.00136	-0.00132	1.91019
A123	1.88450	-0.00003	-0.00001	-0.00009	-0.00010	1.88440
A124	1.91221	-0.00035	0.00005	-0.00230	-0.00225	1.90995
A125	1.93936	0.00042	0.00003	0.00333	0.00336	1.94272
A126	1.90684	-0.00003	0.00020	0.00097	0.00116	1.90800

A127	1.90249	-0.00040	0.00002	-0.00279	-0.00277	1.89972
A128	1.91213	-0.00004	0.00001	0.00065	0.00066	1.91279
A129	1.91371	-0.00001	0.00003	0.00017	0.00020	1.91392
A130	1.88855	0.00004	-0.00030	-0.00250	-0.00281	1.88574
A131	3.18223	-0.00271	0.00210	-0.01820	-0.01609	3.16614
A132	3.16796	0.00164	0.00001	0.03160	0.03161	3.19957
A133	3.18629	-0.00178	0.00037	-0.02969	-0.02932	3.15696
A134	3.16354	0.00132	-0.00044	0.01726	0.01682	3.18036
A135	3.14010	0.00003	0.00003	0.00042	0.00046	3.14055
A136	3.14158	0.00001	-0.00002	-0.00004	-0.00006	3.14152
A137	3.14241	-0.00004	-0.00001	-0.00049	-0.00050	3.14190
A138	3.14198	0.00012	-0.00003	0.00217	0.00214	3.14413
D1	-0.00390	0.00001	0.00011	0.00168	0.00182	-0.00208
D2	3.12811	0.00009	0.00012	0.00542	0.00558	3.13368
D3	3.13946	-0.00001	0.00010	0.00011	0.00021	3.13966
D4	-0.01172	0.00006	0.00010	0.00385	0.00396	-0.00776
D5	0.00354	-0.00003	0.00009	-0.00153	-0.00146	0.00208
D6	-3.13830	-0.00001	0.00011	-0.00019	-0.00010	-3.13840
D7	-3.14033	0.00001	0.00011	0.00053	0.00062	-3.13971
D8	0.00101	0.00003	0.00013	0.00186	0.00198	0.00300
D9	0.01890	0.00000	-0.00048	-0.00429	-0.00478	0.01412
D10	-3.10676	-0.00021	-0.00041	-0.01010	-0.01039	-3.11715
D11	-3.12059	-0.00004	-0.00050	-0.00619	-0.00670	-3.12729
D12	0.03694	-0.00025	-0.00042	-0.01200	-0.01232	0.02462
D13	0.00097	0.00001	-0.00023	-0.00044	-0.00069	0.00029
D14	-3.14068	-0.00001	-0.00026	-0.00136	-0.00162	3.14089
D15	-3.12922	-0.00006	-0.00024	-0.00484	-0.00513	-3.13435
D16	0.01231	-0.00009	-0.00027	-0.00576	-0.00606	0.00625
D17	0.00010	-0.00011	0.00031	-0.00198	-0.00167	-0.00157
D18	-3.13883	0.00000	-0.00019	-0.00091	-0.00112	-3.13996
D19	3.13153	-0.00004	0.00032	0.00192	0.00228	3.13381
D20	-0.00739	0.00006	-0.00018	0.00299	0.00282	-0.00457
D21	0.00220	-0.00003	0.00016	-0.00091	-0.00076	0.00145
D22	-3.14151	-0.00001	0.00019	0.00040	0.00059	-3.14092
D23	-3.13933	0.00000	0.00018	0.00003	0.00020	-3.13913
D24	0.00015	0.00002	0.00022	0.00134	0.00155	0.00170
D25	-0.00249	0.00001	0.00004	0.00102	0.00107	-0.00142
D26	3.13784	0.00003	0.00010	0.00190	0.00200	3.13983
D27	3.14122	-0.00001	0.00001	-0.00028	-0.00027	3.14094
D28	-0.00165	0.00001	0.00006	0.00060	0.00066	-0.00099
D29	-0.00048	0.00002	-0.00016	0.00025	0.00008	-0.00039
D30	3.14136	0.00000	-0.00018	-0.00105	-0.00125	3.14011
D31	-3.14081	0.00000	-0.00022	-0.00063	-0.00084	3.14154
D32	0.00103	-0.00002	-0.00024	-0.00192	-0.00217	-0.00114
D33	-0.01862	-0.00002	0.00067	0.00312	0.00377	-0.01485
D34	3.11535	-0.00007	0.00039	-0.00686	-0.00656	3.10879
D35	3.10659	-0.00003	0.00061	0.00827	0.00901	3.11560
D36	-0.04262	-0.00009	0.00033	-0.00171	-0.00133	-0.04395
D37	-0.01911	0.00011	0.00030	0.00636	0.00666	-0.01245
D38	3.11643	0.00007	0.00038	0.00602	0.00641	3.12284
D39	-3.14150	-0.00001	0.00038	-0.00015	0.00023	-3.14127
D40	-0.00596	-0.00005	0.00046	-0.00048	-0.00003	-0.00599
D41	0.01173	0.00006	-0.00061	-0.00085	-0.00144	0.01030
D42	-3.12237	0.00013	-0.00033	0.00887	0.00848	-3.11389
D43	-3.13257	-0.00005	-0.00009	-0.00195	-0.00200	-3.13457
D44	0.01651	0.00001	0.00019	0.00777	0.00791	0.02443
D45	3.13522	0.00002	-0.00035	-0.00294	-0.00326	3.13196
D46	-0.00936	0.00007	-0.00030	0.00627	0.00600	-0.00337
D47	-0.01526	-0.00007	-0.00067	-0.01455	-0.01525	-0.03051
D48	3.12335	-0.00001	-0.00063	-0.00535	-0.00600	3.11735

D49	0.00293	-0.00021	-0.00042	-0.01386	-0.01434	-0.01141
D50	3.12531	0.00018	-0.00112	0.01803	0.01696	-3.14092
D51	-3.13579	-0.00026	-0.00047	-0.02271	-0.02323	3.12417
D52	-0.01341	0.00013	-0.00117	0.00918	0.00807	-0.00534
D53	-3.13555	0.00004	-0.00006	0.01963	0.01979	-3.11576
D54	0.02394	-0.00028	0.00059	-0.00997	-0.00941	0.01452
D55	-3.14115	-0.00034	0.00079	-0.01549	-0.01442	3.12761
D56	-0.01699	0.00021	0.00323	0.01185	0.01517	-0.00182
D57	-0.01587	0.00010	0.00020	0.01179	0.01202	-0.00384
D58	3.10829	0.00065	0.00263	0.03913	0.04162	-3.13327
D59	0.02267	-0.00044	0.00161	-0.00028	0.00138	0.02405
D60	-3.06895	-0.00076	0.00214	-0.01869	-0.01626	-3.08521
D61	-3.12174	-0.00059	0.00149	-0.00173	-0.00005	-3.12179
D62	0.06982	-0.00091	0.00201	-0.02014	-0.01768	0.05214
D63	-0.02610	0.00039	-0.00122	0.00585	0.00459	-0.02151
D64	3.11980	0.00062	-0.00103	0.00806	0.00678	3.12658
D65	-0.00494	0.00014	-0.00013	0.00380	0.00364	-0.00130
D66	-3.12460	0.00017	-0.00042	-0.00579	-0.00638	-3.13098
D67	3.13251	-0.00008	-0.00031	0.00167	0.00153	3.13404
D68	0.01285	-0.00005	-0.00060	-0.00792	-0.00850	0.00435
D69	-0.00392	0.00023	-0.00114	-0.00749	-0.00872	-0.01264
D70	-3.12720	-0.00035	-0.00366	-0.03613	-0.03989	3.11610
D71	3.07176	0.00058	-0.00187	0.01568	0.01389	3.08566
D72	-0.05151	0.00000	-0.00438	-0.01297	-0.01728	-0.06879
D73	-0.10410	0.00123	-0.00304	0.02614	0.02294	-0.08116
D74	-2.42599	-0.00289	-0.01012	-0.14005	-0.14951	-2.57551
D75	3.10226	0.00089	-0.00234	0.00301	0.00053	3.10279
D76	0.78037	-0.00322	-0.00942	-0.16318	-0.17192	0.60845
D77	-0.06222	0.00073	-0.00181	0.01401	0.01181	-0.05041
D78	3.13457	0.00044	-0.00113	0.00498	0.00374	3.13831
D79	3.06411	0.00071	-0.00161	0.02069	0.01879	3.08290
D80	-0.02229	0.00042	-0.00093	0.01167	0.01072	-0.01157
D81	-3.14055	-0.00033	0.00087	0.00130	0.00229	-3.13826
D82	0.02387	-0.00030	0.00056	-0.00873	-0.00816	0.01570
D83	0.10112	-0.00118	0.00296	-0.02384	-0.02073	0.08038
D84	2.42239	0.00238	0.00982	0.13778	0.14761	2.57000
D85	-3.11311	-0.00092	0.00203	-0.01305	-0.01101	-3.12412
D86	-0.79183	0.00264	0.00888	0.14857	0.15733	-0.63450
D87	-3.12742	-0.00012	0.00052	-0.00728	-0.00676	-3.13418
D88	0.00678	-0.00032	0.00086	-0.00856	-0.00769	-0.00091
D89	0.08740	-0.00036	0.00147	-0.01768	-0.01622	0.07118
D90	-3.06160	-0.00056	0.00182	-0.01896	-0.01715	-3.07874
D91	1.08786	0.00220	0.00339	0.09019	0.09589	1.18375
D92	-3.08351	0.00240	0.00356	0.09378	0.09964	-2.98387
D93	-1.02306	0.00220	0.00332	0.08970	0.09533	-0.92773
D94	-1.11665	-0.00222	-0.00351	-0.08127	-0.08709	-1.20374
D95	0.99516	-0.00202	-0.00334	-0.07769	-0.08333	0.91182
D96	3.05561	-0.00222	-0.00358	-0.08176	-0.08765	2.96797
D97	-0.02008	0.00011	-0.00007	0.00377	0.00372	-0.01636
D98	3.14024	0.00001	0.00034	0.00245	0.00278	-3.14016
D99	-3.14087	-0.00010	0.00037	0.00256	0.00294	-3.13793
D100	0.00822	0.00010	0.00002	0.00386	0.00389	0.01211
D101	-0.00605	-0.00018	0.00044	-0.00872	-0.00829	-0.01434
D102	3.12631	0.00006	0.00068	-0.00033	0.00029	3.12660
D103	0.01150	0.00009	-0.00043	0.00194	0.00149	0.01299
D104	-3.13579	-0.00007	-0.00017	0.00097	0.00078	-3.13500
D105	3.13894	0.00016	-0.00074	0.00292	0.00217	3.14111
D106	-0.00835	0.00000	-0.00048	0.00195	0.00147	-0.00688
D107	3.12676	-0.00004	0.00041	-0.00728	-0.00686	3.11990
D108	-0.06214	0.00002	-0.00024	-0.00804	-0.00829	-0.07043

D109	0.00366	-0.00014	0.00081	-0.00860	-0.00781	-0.00414
D110	3.09795	-0.00007	0.00016	-0.00936	-0.00924	3.08871
D111	0.00256	0.00022	-0.00081	0.01166	0.01086	0.01342
D112	-3.13288	0.00006	-0.00097	0.00606	0.00514	-3.12774
D113	-3.10415	0.00014	-0.00034	0.01189	0.01160	-3.09256
D114	0.04359	-0.00001	-0.00050	0.00629	0.00588	0.04947
D115	3.11364	0.00015	0.00106	-0.00078	0.00023	3.11387
D116	0.56202	-0.00159	-0.00449	-0.11634	-0.12076	0.44126
D117	-0.07464	0.00023	0.00042	-0.00136	-0.00103	-0.07567
D118	-2.62627	-0.00151	-0.00513	-0.11693	-0.12202	-2.74828
D119	-3.12677	-0.00043	0.00010	-0.01709	-0.01695	3.13947
D120	0.00425	-0.00004	0.00067	-0.00160	-0.00093	0.00332
D121	0.00594	-0.00021	0.00032	-0.00903	-0.00870	-0.00275
D122	3.13696	0.00018	0.00090	0.00646	0.00732	-3.13890
D123	3.12466	0.00020	0.00003	-0.00198	-0.00204	3.12262
D124	-0.05317	0.00036	-0.00005	0.00895	0.00873	-0.04443
D125	-0.00973	-0.00008	-0.00036	-0.01256	-0.01293	-0.02266
D126	3.09563	0.00009	-0.00044	-0.00163	-0.00216	3.09347
D127	-3.11817	-0.00030	-0.00018	-0.00333	-0.00345	-3.12161
D128	0.01245	0.00010	0.00042	0.01275	0.01318	0.02563
D129	-0.00005	0.00000	0.00007	0.00451	0.00462	0.00457
D130	3.14118	0.00018	-0.00042	0.01398	0.01361	-3.12840
D131	-3.09287	-0.00020	0.00020	-0.00975	-0.00958	-3.10245
D132	0.04835	-0.00003	-0.00029	-0.00028	-0.00058	0.04777
D133	0.07831	-0.00032	-0.00022	-0.00444	-0.00455	0.07376
D134	2.63179	0.00168	0.00536	0.11231	0.11739	2.74918
D135	-3.11097	-0.00013	-0.00034	0.00960	0.00939	-3.10158
D136	-0.55749	0.00187	0.00524	0.12636	0.13133	-0.42616
D137	0.00943	0.00006	0.00025	0.00520	0.00542	0.01485
D138	3.13598	0.00028	0.00073	0.02030	0.02109	-3.12611
D139	-3.13181	-0.00010	0.00071	-0.00379	-0.00310	-3.13492
D140	-0.00526	0.00012	0.00120	0.01131	0.01257	0.00731
D141	-0.01250	-0.00009	-0.00038	-0.01030	-0.01069	-0.02319
D142	-3.13733	-0.00028	-0.00096	-0.02727	-0.02815	3.11771
D143	-3.12929	-0.00019	0.00071	-0.01551	-0.01477	3.13912
D144	0.01804	-0.00030	0.00072	-0.02409	-0.02337	-0.00533
D145	-0.00560	0.00002	0.00133	0.00256	0.00388	-0.00172
D146	-3.14146	-0.00008	0.00133	-0.00603	-0.00471	3.13702
D147	-0.89039	0.00108	0.00301	0.06259	0.06632	-0.82407
D148	1.22423	0.00115	0.00302	0.06363	0.06737	1.29160
D149	-2.94752	0.00103	0.00301	0.06223	0.06597	-2.88156
D150	2.93881	-0.00115	-0.00315	-0.06759	-0.07147	2.86734
D151	-1.22975	-0.00108	-0.00314	-0.06656	-0.07043	-1.30018
D152	0.88168	-0.00120	-0.00315	-0.06795	-0.07183	0.80985
D153	0.00327	-0.00015	0.00034	-0.00519	-0.00485	-0.00157
D154	-3.13433	-0.00018	0.00018	-0.00957	-0.00938	3.13947
D155	3.13889	-0.00003	0.00034	0.00378	0.00410	-3.14020
D156	0.00128	-0.00006	0.00017	-0.00059	-0.00043	0.00085
D157	-3.13851	-0.00002	-0.00013	-0.00449	-0.00463	3.14005
D158	0.00474	-0.00008	-0.00004	-0.01003	-0.01007	-0.00533
D159	-0.00027	-0.00001	0.00002	-0.00084	-0.00082	-0.00109
D160	-3.14020	-0.00007	0.00011	-0.00638	-0.00626	3.13672
D161	3.14036	0.00004	0.00008	0.00343	0.00351	-3.13932
D162	0.00202	0.00000	0.00000	0.00177	0.00179	0.00380
D163	0.00219	-0.00001	-0.00005	-0.00033	-0.00039	0.00180
D164	-3.13615	-0.00005	-0.00013	-0.00199	-0.00211	-3.13826
D165	-0.00190	0.00002	0.00003	0.00178	0.00181	-0.00009
D166	-3.14150	-0.00001	0.00005	-0.00005	0.00001	-3.14149
D167	3.13807	0.00009	-0.00006	0.00721	0.00715	-3.13797
D168	-0.00153	0.00005	-0.00004	0.00538	0.00535	0.00382

D169	-0.00341	0.00002	0.00007	0.00145	0.00153	-0.00188
D170	3.13870	0.00002	0.00006	0.00116	0.00122	3.13991
D171	3.13513	0.00001	0.00015	0.00294	0.00311	3.13824
D172	-0.00595	0.00001	0.00014	0.00265	0.00280	-0.00315
D173	0.00134	-0.00001	0.00003	0.00028	0.00031	0.00164
D174	-3.14110	-0.00002	0.00014	0.00048	0.00061	-3.14048
D175	-3.13650	-0.00003	-0.00006	-0.00161	-0.00167	-3.13816
D176	0.00426	-0.00004	0.00005	-0.00141	-0.00136	0.00289
D177	0.00330	-0.00003	-0.00006	-0.00203	-0.00208	0.00122
D178	-3.13872	-0.00004	-0.00005	-0.00178	-0.00182	-3.14054
D179	-3.14017	0.00000	-0.00008	-0.00030	-0.00038	-3.14055
D180	0.00099	0.00000	-0.00007	-0.00005	-0.00012	0.00087
D181	3.13921	0.00004	0.00002	0.00180	0.00183	3.14104
D182	-0.00206	0.00003	0.00002	0.00174	0.00176	-0.00029
D183	-0.00015	-0.00001	0.00005	-0.00024	-0.00019	-0.00034
D184	-3.14141	-0.00001	0.00005	-0.00030	-0.00026	3.14151
D185	3.13996	0.00000	0.00006	0.00065	0.00071	3.14066
D186	-0.00123	-0.00001	0.00005	0.00012	0.00018	-0.00105
D187	-0.00108	0.00001	0.00004	0.00034	0.00038	-0.00071
D188	3.14091	0.00000	0.00004	-0.00019	-0.00016	3.14076
D189	-0.00057	0.00001	0.00000	0.00025	0.00025	-0.00032
D190	3.14148	0.00000	-0.00001	-0.00011	-0.00013	3.14135
D191	3.14069	0.00001	0.00000	0.00031	0.00032	3.14100
D192	-0.00045	0.00000	-0.00001	-0.00005	-0.00006	-0.00052
D193	0.00040	-0.00001	0.00001	-0.00034	-0.00032	0.00007
D194	-3.14146	0.00000	0.00003	-0.00009	-0.00007	-3.14152
D195	-3.14159	0.00000	0.00001	0.00018	0.00019	-3.14140
D196	-0.00026	0.00001	0.00003	0.00042	0.00045	0.00019
D197	0.00045	0.00000	-0.00003	0.00004	0.00001	0.00046
D198	-3.14088	0.00000	-0.00005	-0.00020	-0.00025	-3.14113
D199	3.14159	0.00000	-0.00002	0.00040	0.00038	-3.14121
D200	0.00026	0.00000	-0.00003	0.00016	0.00012	0.00039

Item	Value	Threshold	Converged?

Maximum Force	0.010938	0.000450	NO

RMS Force	0.001807	0.000300	NO

Maximum Displacement	0.386296	0.001800	NO

RMS Displacement	0.072804	0.001200	NO

Predicted change in Energy=-4.986939D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.773167	-0.639284	-0.042300
2	6	0	-9.945472	-1.777466	-0.048177
3	6	0	-10.448135	-3.069823	-0.062628
4	6	0	-11.835467	-3.232927	-0.071945
5	6	0	-12.673294	-2.110826	-0.068363
6	6	0	-12.160951	-0.809419	-0.053874
7	1	0	-9.763837	-3.912032	-0.067254
8	1	0	-12.268436	-4.228361	-0.082701
9	1	0	-13.750177	-2.248611	-0.077341

10	1	0	-12.841541	0.031037	-0.052953
11	6	0	-9.921412	0.575928	-0.023959
12	6	0	-8.528558	-1.355436	-0.044826
13	6	0	-8.522606	0.124938	-0.038677
14	6	0	-7.392061	0.909196	-0.065389
15	6	0	-6.002827	0.630416	-0.072351
16	6	0	-3.638587	-0.156757	-0.029336
17	6	0	-3.761771	1.248912	-0.087078
18	16	0	-5.177876	-0.957612	-0.030953
19	6	0	-5.081234	1.694919	-0.102150
20	6	0	-2.255758	-0.433193	0.005403
21	6	0	-1.589182	0.805209	-0.033875
22	7	0	-2.497700	1.853393	-0.157735
23	16	0	-1.158011	-1.797238	0.066347
24	16	0	1.178910	1.787433	-0.011348
25	6	0	0.204499	-0.681829	0.065992
26	6	0	-0.182004	0.670685	-0.000232
27	6	0	1.611438	-0.817127	0.099032
28	6	0	2.281443	0.425305	0.052582
29	6	0	3.662114	0.146631	0.073255
30	6	0	3.785494	-1.264543	0.135684
31	6	0	5.107143	-1.709562	0.138997
32	6	0	6.027017	-0.644133	0.084900
33	16	0	5.201476	0.943681	0.053813
34	7	0	2.523413	-1.854258	0.211930
35	6	0	7.420141	-0.910891	0.061053
36	6	0	8.537588	-0.111165	0.008152
37	6	0	8.523603	1.365315	-0.042612
38	6	0	9.930609	-0.553110	-0.007375
39	6	0	9.935209	1.800683	-0.087357
40	6	0	10.777120	0.669724	-0.065832
41	6	0	10.420716	3.099437	-0.142373
42	6	0	12.162448	0.861187	-0.100283
43	6	0	11.805393	3.280819	-0.177104
44	6	0	12.657213	2.169636	-0.155675
45	6	0	10.414101	-1.849764	0.023144
46	6	0	9.587226	-3.011737	0.075151
47	6	0	11.805521	-2.166590	0.005047
48	7	0	8.935224	-3.977366	0.117440
49	7	0	12.924484	-2.490560	-0.007122
50	6	0	-10.429542	1.862801	0.013888
51	6	0	-11.832302	2.128950	0.023645
52	6	0	-9.637692	3.050561	0.054347
53	7	0	-12.973366	2.363676	0.031540
54	7	0	-9.029461	4.044248	0.090976
55	8	0	-7.557287	-2.104923	-0.050037
56	8	0	7.541479	2.099813	-0.051045
57	6	0	2.248863	-3.234028	-0.177066
58	1	0	1.282287	-3.540409	0.227325
59	1	0	2.241600	-3.349462	-1.266091
60	1	0	3.014330	-3.883195	0.251803
61	6	0	-2.248624	3.168605	0.451917
62	1	0	-2.300353	3.117027	1.543892
63	1	0	-1.263259	3.526328	0.148705
64	1	0	-2.993285	3.875245	0.082102
65	1	0	5.434710	-2.742254	0.170101
66	1	0	12.858757	0.036052	-0.085471
67	1	0	13.732139	2.319472	-0.182518
68	1	0	12.223132	4.281925	-0.220636
69	1	0	9.727267	3.934024	-0.156826

70	1	0	7.606603	-1.977610	0.095111
71	1	0	-7.560979	1.978493	-0.079983
72	1	0	-5.408153	2.727565	-0.121678

Rotational constants (GHZ): 0.1752800 0.0104151 0.0098354

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6574.1851124976 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T

Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6574.0999808113 Hartrees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.23D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Initial guess from the checkpoint file: "PBDB.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000410 -0.000007 -0.000459 Ang= 0.07 deg.

ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1

AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-yADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 IlCent= 200000004 NGrid=

0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0=

0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Integral accuracy reduced to 1.0D-05 until final iterations.

Initial convergence to 1.0D-05 achieved. Increase integral accuracy.

SCF Done: E(RB3LYP) = -3683.01456379 A.U. after 13 cycles

NFock= 13 Conv=0.91D-08 -V/T= 2.0068

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1

NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	0.001331970	0.000943467	0.001224888
2	6	-0.000251683	-0.000501975	0.000076342
3	6	-0.000022624	0.000287223	-0.000013792
4	6	0.000125019	-0.000218356	0.000024113
5	6	0.000307583	0.000220810	0.000271924
6	6	-0.000844248	0.001866982	-0.000465728

7	1	-0.000023031	0.000198331	-0.000018545
8	1	0.000056270	0.000006666	0.000072225
9	1	0.000013281	0.000012222	0.000030895
10	1	0.001430000	0.001977962	0.001378764
11	6	0.000952011	-0.000716366	0.000652906
12	6	-0.000507200	0.000833724	-0.000747202
13	6	-0.001780570	0.002702800	-0.000506424
14	6	-0.000480694	-0.001129802	-0.001389379
15	6	0.000601090	-0.000995719	-0.000235245
16	6	0.000810723	0.000278402	0.001548831
17	6	-0.003189741	-0.003845510	0.001430916
18	16	0.001139294	-0.001740629	0.000811996
19	6	0.001784548	0.001500213	0.000535386
20	6	-0.002205344	0.001920621	-0.000626588
21	6	-0.002159516	-0.004336799	0.002609960
22	7	0.008295769	0.002935524	-0.009665857
23	16	0.000594697	0.000194603	0.000410631
24	16	-0.000561185	-0.000301835	-0.000198814
25	6	-0.000308935	-0.002454012	0.000160821
26	6	0.000636535	0.002598402	-0.000421604
27	6	0.001735139	0.001266390	-0.002416691
28	6	0.002313541	0.000503188	0.001541217
29	6	-0.000141456	0.002202997	-0.001300980
30	6	0.002085766	0.000139205	-0.001615763
31	6	-0.001839279	-0.000790412	-0.000618048
32	6	0.000488263	0.000173405	0.000180920
33	16	-0.002615993	0.001485503	-0.000335362
34	7	-0.005550018	-0.001612050	0.005792694
35	6	-0.001615473	0.004283269	-0.001565042
36	6	-0.000852477	-0.001267148	-0.001017930
37	6	0.001081213	-0.000624588	0.001376507
38	6	0.000955420	-0.001047893	0.000692779
39	6	0.000819477	-0.000387657	0.000538599
40	6	-0.001792273	-0.000614686	-0.001481452
41	6	0.000572712	0.000213106	0.000445512
42	6	-0.000330692	-0.000604120	-0.000287272
43	6	-0.000033519	0.000630786	0.000035823
44	6	-0.000048781	0.000387728	0.000021475
45	6	-0.000616805	-0.002399210	-0.000665553
46	6	0.000419920	0.001541124	0.000406429
47	6	0.001178465	0.001399788	0.001009954
48	7	0.000058667	-0.000674214	0.000018074
49	7	-0.000135833	-0.001038106	-0.000170542
50	6	0.001422008	-0.000491118	0.001150368
51	6	-0.001405148	-0.002029157	-0.001462686
52	6	0.000624118	-0.000180220	0.000472783
53	7	-0.000326309	-0.001946552	-0.000543116
54	7	0.001011359	0.000176073	0.000942181
55	8	-0.000961504	0.000969702	-0.000541303
56	8	0.001072670	-0.002701906	0.000101130
57	6	0.001536234	-0.000741876	-0.002944665
58	1	-0.000130450	0.000126231	-0.000049352
59	1	0.000036743	0.000332140	0.000256275
60	1	0.000079069	-0.000038506	0.000242828
61	6	-0.003141337	0.001591000	0.006286668
62	1	0.000186110	-0.000179972	-0.000456403
63	1	0.000178831	-0.000231094	0.000002116
64	1	-0.000110325	-0.000027136	-0.000350420
65	1	-0.000240704	0.000262178	-0.000154875
66	1	0.000658695	0.000715093	0.000569110

67	1	-0.000054592	-0.000094614	-0.000047683
68	1	0.000163792	0.000007873	0.000106937
69	1	-0.000034785	0.000180501	-0.000002839
70	1	-0.000745921	0.000587168	-0.000315509
71	1	-0.001629092	-0.001007412	-0.001277301
72	1	-0.000069463	-0.000681746	0.000478986

Cartesian Forces: Max 0.009665857 RMS 0.001628559

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.019232338 RMS 0.002346050

Search for a local minimum.

Step number 13 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 12 13

DE= -3.44D-03 DEPred=-4.99D-03 R= 6.90D-01

TightC=F SS= 1.41D+00 RLast= 5.24D-01 DXNew= 3.3118D+00 1.5706D+00

Trust test= 6.90D-01 RLast= 5.24D-01 DXMaxT set to 1.97D+00

ITU= 1 1 1 1 0 0 0 1 0 0 0 1 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00230	0.00230	0.00231	0.00233	0.00241
Eigenvalues ---	0.00289	0.00388	0.00444	0.00458	0.00471
Eigenvalues ---	0.00480	0.00511	0.00550	0.00593	0.00613
Eigenvalues ---	0.00619	0.00667	0.00681	0.00685	0.00697
Eigenvalues ---	0.00726	0.00743	0.00745	0.00760	0.00770
Eigenvalues ---	0.00780	0.00817	0.00836	0.00854	0.00868
Eigenvalues ---	0.00881	0.01000	0.01049	0.01084	0.01132
Eigenvalues ---	0.01149	0.01208	0.01251	0.01271	0.01334
Eigenvalues ---	0.01363	0.01363	0.01393	0.01424	0.01457
Eigenvalues ---	0.01510	0.01568	0.01646	0.01653	0.01754
Eigenvalues ---	0.01794	0.01800	0.01894	0.01929	0.01954
Eigenvalues ---	0.02007	0.02024	0.02075	0.02075	0.02209
Eigenvalues ---	0.02210	0.04828	0.04837	0.04900	0.04915
Eigenvalues ---	0.04980	0.05005	0.05018	0.05215	0.07106
Eigenvalues ---	0.07258	0.07454	0.07600	0.15571	0.15683
Eigenvalues ---	0.15980	0.15999	0.15999	0.16000	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues ---	0.16000	0.16001	0.16002	0.16003	0.16027
Eigenvalues ---	0.16048	0.17508	0.17766	0.18145	0.19023
Eigenvalues ---	0.19375	0.19798	0.20575	0.20791	0.21247
Eigenvalues ---	0.21360	0.22001	0.22002	0.22149	0.22318
Eigenvalues ---	0.22538	0.22600	0.22628	0.22650	0.22672
Eigenvalues ---	0.22870	0.22982	0.23188	0.23366	0.23444
Eigenvalues ---	0.23591	0.23783	0.23915	0.24077	0.24196
Eigenvalues ---	0.24264	0.24342	0.24500	0.24526	0.24570
Eigenvalues ---	0.24605	0.24809	0.24891	0.24952	0.24969
Eigenvalues ---	0.24979	0.24983	0.24987	0.24993	0.24995
Eigenvalues ---	0.24998	0.24998	0.24999	0.25000	0.25000
Eigenvalues ---	0.25000	0.25000	0.25011	0.25561	0.25777
Eigenvalues ---	0.26214	0.26325	0.26713	0.26734	0.26852
Eigenvalues ---	0.27080	0.27243	0.27837	0.27860	0.28220
Eigenvalues ---	0.28455	0.28623	0.28754	0.29982	0.30340
Eigenvalues ---	0.32049	0.32293	0.34844	0.35586	0.36156
Eigenvalues ---	0.36331	0.36338	0.36475	0.36650	0.36662
Eigenvalues ---	0.36768	0.36827	0.37080	0.37093	0.37102
Eigenvalues ---	0.37251	0.37273	0.37418	0.37564	0.37670

Eigenvalues --- 0.37755 0.37938 0.38852 0.40263 0.40692
 Eigenvalues --- 0.40951 0.41641 0.42240 0.42708 0.44421
 Eigenvalues --- 0.44774 0.45592 0.45873 0.47327 0.47817
 Eigenvalues --- 0.47900 0.49257 0.52547 0.54108 0.55646
 Eigenvalues --- 0.57618 0.62699 0.75346 0.80372 0.81862
 Eigenvalues --- 0.95923 1.25841 1.26327 1.29341 1.35383

RFO step: Lambda=-6.39742182D-03 EMin= 2.30028725D-03

Quartic linear search produced a step of -0.06762.

Iteration 1 RMS(Cart)= 0.09208884 RMS(Int)= 0.00197861

Iteration 2 RMS(Cart)= 0.00481323 RMS(Int)= 0.00063168

Iteration 3 RMS(Cart)= 0.00000827 RMS(Int)= 0.00063167

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00063167

Variable	Old X	-DE/DX	Delta X	Delta X	Delta X	New X
(Linear)	(Quad)	(Total)				
R1	2.65947	0.00142	0.00024	-0.00059	-0.00035	2.65912
R2	2.64226	0.00277	0.00027	0.00077	0.00104	2.64330
R3	2.80455	0.00605	0.00072	0.00534	0.00606	2.81060
R4	2.62057	0.00032	-0.00001	-0.00049	-0.00050	2.62008
R5	2.79384	-0.00077	-0.00017	-0.00266	-0.00283	2.79101
R6	2.63979	-0.00129	-0.00018	-0.00054	-0.00072	2.63908
R7	2.05068	0.00002	0.00000	0.00039	0.00039	2.05107
R8	2.64634	-0.00097	-0.00007	-0.00022	-0.00030	2.64605
R9	2.05143	0.00003	0.00002	-0.00002	0.00000	2.05144
R10	2.64316	0.00033	-0.00006	0.00081	0.00075	2.64391
R11	2.05167	-0.00001	0.00000	0.00010	0.00010	2.05177
R12	2.04368	-0.00240	-0.00029	0.00038	0.00009	2.04376
R13	2.77749	-0.00544	-0.00086	-0.00729	-0.00815	2.76934
R14	2.61553	0.00117	0.00002	-0.00031	-0.00028	2.61525
R15	2.79755	-0.00074	-0.00036	-0.00253	-0.00289	2.79466
R16	2.31838	-0.00108	-0.00010	0.00003	-0.00007	2.31832
R17	2.60063	0.00327	0.00070	-0.01319	-0.01249	2.58814
R18	2.67764	0.00190	-0.00006	-0.00590	-0.00596	2.67168
R19	2.04592	0.00218	0.00025	0.00005	0.00030	2.04622
R20	3.38261	0.00041	-0.00074	0.00790	0.00696	3.38957
R21	2.66136	-0.00010	0.00019	-0.00419	-0.00404	2.65732
R22	2.66874	0.00036	-0.00028	0.00438	0.00385	2.67259
R23	3.27898	-0.00083	-0.00033	-0.00462	-0.00499	3.27399
R24	2.66568	-0.00259	0.00016	-0.01016	-0.01140	2.65428
R25	2.63217	-0.00179	-0.00083	0.00062	-0.00004	2.63213
R26	2.65119	-0.00207	0.00125	-0.02034	-0.01799	2.63320
R27	2.04721	0.00019	-0.00002	0.00149	0.00147	2.04868
R28	2.65875	0.00095	-0.00034	0.00464	0.00407	2.66281
R29	3.31073	0.00008	-0.00037	0.00313	0.00271	3.31345
R30	2.63170	-0.00246	0.00096	-0.01804	-0.01596	2.61574
R31	2.67206	-0.00257	-0.00089	-0.00480	-0.00553	2.66653
R32	2.77957	-0.00429	0.00156	-0.02532	-0.02375	2.75581
R33	3.32751	-0.00006	-0.00021	0.00076	0.00037	3.32788
R34	3.32685	-0.00027	-0.00025	0.00069	0.00040	3.32725
R35	3.31379	-0.00008	-0.00022	0.00120	0.00095	3.31475
R36	2.66114	-0.00177	0.00014	-0.00515	-0.00503	2.65610
R37	2.67172	-0.00245	-0.00062	-0.00838	-0.00894	2.66278
R38	2.66893	-0.00087	-0.00023	0.00044	0.00012	2.66905
R39	2.61854	-0.00249	0.00005	-0.00956	-0.00910	2.60944
R40	2.66199	-0.00272	-0.00064	-0.00318	-0.00432	2.65767
R41	2.67950	-0.00189	-0.00032	0.00034	-0.00007	2.67943
R42	3.27599	0.00035	-0.00040	0.00384	0.00343	3.27942
R43	2.63535	-0.00330	-0.00082	-0.00613	-0.00689	2.62845
R44	2.63644	-0.00152	0.00012	-0.00687	-0.00636	2.63008
R45	2.66192	-0.00070	-0.00005	-0.00270	-0.00277	2.65915
R46	2.04817	-0.00008	0.00002	-0.00015	-0.00013	2.04804

R47	3.38237	0.00114	-0.00009	0.00346	0.00329	3.38566
R48	2.68083	0.00106	-0.00133	0.01174	0.01041	2.69124
R49	2.75826	-0.00140	0.00058	-0.00765	-0.00708	2.75119
R50	2.59867	0.00714	0.00036	0.00704	0.00740	2.60607
R51	2.04738	-0.00016	-0.00021	0.00040	0.00019	2.04757
R52	2.79192	0.00280	0.00019	0.00493	0.00512	2.79704
R53	2.76189	0.00337	0.00156	-0.00048	0.00108	2.76297
R54	2.79282	0.00026	-0.00004	-0.00124	-0.00128	2.79154
R55	2.31761	-0.00091	-0.00016	0.00067	0.00051	2.31813
R56	2.81266	-0.00169	0.00014	-0.00749	-0.00735	2.80531
R57	2.61576	0.00027	0.00065	-0.00920	-0.00855	2.60721
R58	2.66468	-0.00306	0.00003	-0.00568	-0.00566	2.65902
R59	2.62223	-0.00065	-0.00037	-0.00129	-0.00165	2.62058
R60	2.64358	-0.00019	0.00012	-0.00543	-0.00530	2.63827
R61	2.63983	-0.00017	-0.00006	0.00090	0.00084	2.64067
R62	2.05069	-0.00001	-0.00001	0.00034	0.00033	2.05102
R63	2.64555	-0.00084	-0.00005	-0.00090	-0.00094	2.64461
R64	2.04048	0.00101	-0.00009	0.00540	0.00531	2.04579
R65	2.64615	-0.00044	-0.00018	-0.00019	-0.00037	2.64577
R66	2.05156	-0.00005	0.00002	-0.00008	-0.00006	2.05150
R67	2.05158	0.00002	0.00001	0.00012	0.00012	2.05171
R68	2.69682	0.00088	0.00018	0.00105	0.00123	2.69806
R69	2.69692	0.00108	0.00050	-0.00421	-0.00371	2.69321
R70	2.20324	-0.00067	0.00006	-0.00066	-0.00061	2.20264
R71	2.20150	0.00017	0.00007	-0.00064	-0.00057	2.20092
R72	2.69819	0.00058	0.00011	-0.00167	-0.00157	2.69662
R73	2.69870	-0.00012	-0.00015	0.00141	0.00125	2.69995
R74	2.20150	-0.00030	0.00002	-0.00042	-0.00040	2.20110
R75	2.20273	-0.00032	0.00005	-0.00031	-0.00026	2.20247
R76	2.06290	0.00016	0.00003	0.00049	0.00052	2.06341
R77	2.06953	0.00019	0.00001	0.00073	0.00074	2.07028
R78	2.06256	0.00013	0.00000	0.00055	0.00055	2.06311
R79	2.06815	0.00044	0.00004	0.00101	0.00106	2.06920
R80	2.06218	0.00024	0.00007	0.00012	0.00020	2.06238
R81	2.06199	0.00021	0.00000	0.00073	0.00073	2.06272
A1	2.07750	-0.00306	-0.00040	-0.00321	-0.00361	2.07389
A2	1.90153	-0.00296	-0.00040	-0.00257	-0.00297	1.89856
A3	2.30416	0.00602	0.00080	0.00578	0.00658	2.31073
A4	2.14191	0.00138	0.00020	0.00227	0.00246	2.14437
A5	1.91005	0.00093	0.00012	0.00171	0.00182	1.91187
A6	2.23121	-0.00231	-0.00032	-0.00396	-0.00427	2.22694
A7	2.05881	0.00050	0.00003	0.00052	0.00055	2.05936
A8	2.08834	-0.00005	-0.00003	0.00023	0.00021	2.08855
A9	2.13603	-0.00045	0.00000	-0.00076	-0.00076	2.13527
A10	2.09509	-0.00036	-0.00005	-0.00141	-0.00146	2.09363
A11	2.09813	0.00009	0.00005	0.00004	0.00009	2.09822
A12	2.08996	0.00027	0.00000	0.00137	0.00137	2.09133
A13	2.12518	0.00059	0.00009	0.00025	0.00033	2.12551
A14	2.08485	-0.00033	-0.00012	0.00095	0.00083	2.08568
A15	2.07315	-0.00027	0.00003	-0.00120	-0.00116	2.07199
A16	2.06788	0.00095	0.00013	0.00158	0.00172	2.06960
A17	2.12946	0.00100	0.00014	0.00299	0.00313	2.13259
A18	2.08584	-0.00195	-0.00027	-0.00458	-0.00485	2.08099
A19	1.87008	0.00051	-0.00004	-0.00110	-0.00115	1.86893
A20	2.15430	0.01872	0.00227	0.02362	0.02588	2.18018
A21	2.25875	-0.01923	-0.00224	-0.02248	-0.02471	2.23404
A22	1.86431	-0.00016	-0.00010	-0.00153	-0.00163	1.86268
A23	2.19487	-0.00108	0.00020	-0.00092	-0.00072	2.19415
A24	2.22400	0.00123	-0.00010	0.00245	0.00235	2.22635
A25	1.87869	0.00167	0.00041	0.00357	0.00397	1.88266

A26	2.22328	-0.01071	-0.00085	-0.00859	-0.00945	2.21383
A27	2.18107	0.00903	0.00046	0.00497	0.00543	2.18650
A28	2.33701	0.00687	0.00005	0.00230	0.00234	2.33935
A29	2.02076	-0.00418	-0.00010	-0.00119	-0.00129	2.01947
A30	1.92541	-0.00269	0.00006	-0.00111	-0.00105	1.92436
A31	2.24758	0.00355	-0.00093	0.00972	0.00877	2.25635
A32	2.08631	-0.00258	0.00075	-0.00940	-0.00866	2.07765
A33	1.94925	-0.00097	0.00017	-0.00051	-0.00042	1.94883
A34	1.96274	0.00036	0.00020	-0.00071	-0.00005	1.96268
A35	1.85623	-0.00039	-0.00009	0.00156	0.00102	1.85725
A36	2.46421	0.00003	-0.00012	-0.00085	-0.00097	2.46324
A37	1.98426	-0.00071	-0.00005	0.00111	0.00050	1.98476
A38	1.93085	0.00044	0.00073	-0.00991	-0.00737	1.92348
A39	2.36743	0.00028	-0.00074	0.00933	0.00727	2.37470
A40	1.57019	0.00002	-0.00022	0.00039	0.00000	1.57019
A41	1.95804	0.00131	-0.00012	-0.00004	0.00016	1.95820
A42	2.12163	0.00002	0.00033	0.00115	0.00134	2.12297
A43	2.20344	-0.00133	-0.00022	-0.00117	-0.00153	2.20191
A44	1.86634	-0.00015	-0.00020	0.00226	0.00165	1.86799
A45	2.44600	0.00036	0.00003	-0.00026	-0.00025	2.44574
A46	1.97080	-0.00021	0.00016	-0.00196	-0.00137	1.96944
A47	1.93468	0.00014	0.00092	-0.01133	-0.00857	1.92611
A48	1.96826	-0.00005	-0.00001	0.00132	0.00076	1.96902
A49	2.37886	-0.00009	-0.00095	0.01063	0.00833	2.38719
A50	1.83280	0.00000	-0.00153	0.02028	0.01549	1.84829
A51	2.11410	0.00082	-0.00352	0.05156	0.04073	2.15483
A52	2.12430	0.00070	-0.00413	0.05658	0.04540	2.16970
A53	1.56243	-0.00081	-0.00013	-0.00239	-0.00266	1.55977
A54	1.56386	-0.00094	-0.00018	-0.00281	-0.00300	1.56086
A55	1.97799	0.00062	-0.00015	0.00360	0.00337	1.98135
A56	2.35944	-0.00080	0.00012	-0.00363	-0.00360	2.35583
A57	1.94565	0.00017	0.00003	0.00007	0.00027	1.94592
A58	2.35860	-0.00093	-0.00013	-0.00162	-0.00195	2.35665
A59	1.94511	0.00044	0.00012	-0.00049	-0.00007	1.94504
A60	1.97945	0.00048	0.00002	0.00210	0.00202	1.98147
A61	1.96832	0.00023	-0.00008	0.00188	0.00158	1.96990
A62	2.38689	-0.00025	-0.00039	0.00314	0.00224	2.38913
A63	1.92718	0.00003	0.00048	-0.00455	-0.00342	1.92375
A64	1.96736	0.00005	0.00022	-0.00131	-0.00096	1.96641
A65	2.45032	-0.00035	-0.00009	-0.00123	-0.00133	2.44899
A66	1.86550	0.00030	-0.00013	0.00254	0.00226	1.86776
A67	1.85752	-0.00049	0.00003	-0.00163	-0.00176	1.85577
A68	2.46418	0.00014	-0.00019	0.00221	0.00203	2.46621
A69	1.96147	0.00036	0.00016	-0.00060	-0.00028	1.96118
A70	1.98249	-0.00012	0.00004	-0.00021	-0.00038	1.98210
A71	1.92236	0.00071	0.00037	-0.00255	-0.00154	1.92082
A72	2.37793	-0.00059	-0.00044	0.00305	0.00214	2.38007
A73	1.95782	0.00177	0.00005	0.00401	0.00414	1.96196
A74	2.20253	-0.00127	-0.00010	-0.00356	-0.00371	2.19881
A75	2.12281	-0.00050	0.00006	-0.00040	-0.00040	2.12241
A76	1.95028	-0.00143	-0.00005	-0.00167	-0.00177	1.94852
A77	2.09406	-0.00703	-0.00045	-0.01591	-0.01635	2.07770
A78	2.23884	0.00846	0.00050	0.01757	0.01808	2.25692
A79	1.57229	-0.00056	-0.00017	-0.00118	-0.00145	1.57084
A80	1.84892	-0.00051	-0.00076	0.00789	0.00592	1.85484
A81	2.16762	0.00059	-0.00197	0.02657	0.02185	2.18947
A82	2.15936	0.00056	-0.00171	0.02406	0.01951	2.17886
A83	2.33129	0.01180	0.00098	0.02380	0.02479	2.35607
A84	1.93223	-0.00689	-0.00087	-0.01570	-0.01657	1.91566
A85	2.01966	-0.00490	-0.00011	-0.00810	-0.00822	2.01144

A86	2.18317	0.00846	0.00000	0.01652	0.01651	2.19968
A87	2.21313	-0.00475	0.00027	-0.00905	-0.00879	2.20434
A88	1.88688	-0.00371	-0.00027	-0.00747	-0.00773	1.87916
A89	1.86126	0.00115	0.00017	0.00218	0.00233	1.86359
A90	2.22223	0.00259	0.00011	0.00621	0.00627	2.22850
A91	2.19969	-0.00374	-0.00028	-0.00833	-0.00866	2.19103
A92	1.86927	0.00163	-0.00025	0.00532	0.00507	1.87435
A93	2.23439	0.00215	0.00114	0.00209	0.00323	2.23761
A94	2.17953	-0.00378	-0.00089	-0.00741	-0.00830	2.17123
A95	1.91086	0.00029	0.00019	-0.00080	-0.00061	1.91025
A96	2.22826	0.00021	-0.00014	0.00170	0.00156	2.22982
A97	2.14407	-0.00050	-0.00005	-0.00090	-0.00095	2.14312
A98	1.89650	0.00064	0.00016	0.00078	0.00093	1.89743
A99	2.31397	-0.00180	-0.00019	-0.00415	-0.00435	2.30962
A100	2.07272	0.00116	0.00004	0.00337	0.00341	2.07613
A101	2.05932	0.00012	0.00004	-0.00043	-0.00040	2.05892
A102	2.09067	-0.00025	-0.00007	-0.00133	-0.00140	2.08927
A103	2.13320	0.00013	0.00004	0.00176	0.00180	2.13499
A104	2.07016	-0.00033	-0.00007	-0.00064	-0.00072	2.06945
A105	2.13373	-0.00034	-0.00005	-0.00200	-0.00205	2.13169
A106	2.07929	0.00068	0.00012	0.00264	0.00276	2.08205
A107	2.09389	0.00012	0.00012	-0.00062	-0.00051	2.09338
A108	2.09687	0.00013	0.00000	0.00106	0.00105	2.09792
A109	2.09243	-0.00025	-0.00011	-0.00043	-0.00054	2.09188
A110	2.12620	-0.00056	-0.00007	-0.00077	-0.00084	2.12536
A111	2.07133	0.00040	0.00015	-0.00043	-0.00028	2.07105
A112	2.08566	0.00016	-0.00008	0.00120	0.00112	2.08677
A113	2.16656	0.00123	0.00060	0.00001	0.00061	2.16717
A114	2.15104	-0.00059	-0.00055	0.00276	0.00221	2.15325
A115	1.96558	-0.00064	-0.00004	-0.00277	-0.00282	1.96276
A116	2.13433	0.01444	0.00149	0.02423	0.02571	2.16004
A117	2.17793	-0.01162	-0.00154	-0.01202	-0.01356	2.16436
A118	1.97091	-0.00282	0.00005	-0.01219	-0.01214	1.95877
A119	1.91042	-0.00006	-0.00009	0.00067	0.00057	1.91100
A120	1.94540	0.00051	-0.00019	0.00469	0.00450	1.94990
A121	1.90244	0.00001	0.00004	-0.00037	-0.00034	1.90211
A122	1.91019	-0.00022	0.00009	-0.00216	-0.00207	1.90812
A123	1.88440	0.00006	0.00001	0.00043	0.00043	1.88483
A124	1.90995	-0.00030	0.00015	-0.00337	-0.00322	1.90673
A125	1.94272	0.00030	-0.00023	0.00355	0.00332	1.94604
A126	1.90800	0.00007	-0.00008	0.00069	0.00061	1.90862
A127	1.89972	0.00020	0.00019	-0.00120	-0.00102	1.89871
A128	1.91279	-0.00024	-0.00004	-0.00079	-0.00084	1.91195
A129	1.91392	-0.00032	-0.00001	-0.00159	-0.00160	1.91232
A130	1.88574	-0.00001	0.00019	-0.00078	-0.00059	1.88515
A131	3.16614	0.00019	0.00109	0.00199	0.00308	3.16922
A132	3.19957	-0.00231	-0.00214	-0.01488	-0.01702	3.18255
A133	3.15696	0.00446	0.00198	0.03568	0.03766	3.19462
A134	3.18036	-0.00298	-0.00114	-0.02179	-0.02292	3.15743
A135	3.14055	-0.00004	-0.00003	-0.00101	-0.00104	3.13951
A136	3.14152	0.00001	0.00000	0.00017	0.00018	3.14170
A137	3.14190	-0.00005	0.00003	-0.00126	-0.00123	3.14067
A138	3.14413	-0.00019	-0.00015	-0.00060	-0.00074	3.14339
D1	-0.00208	0.00001	-0.00012	0.00010	-0.00003	-0.00212
D2	3.13368	0.00005	-0.00038	0.00349	0.00310	3.13679
D3	3.13966	0.00002	-0.00001	0.00015	0.00013	3.13979
D4	-0.00776	0.00006	-0.00027	0.00354	0.00327	-0.00449
D5	0.00208	-0.00003	0.00010	-0.00112	-0.00101	0.00106
D6	-3.13840	0.00001	0.00001	0.00054	0.00056	-3.13784
D7	-3.13971	-0.00004	-0.00004	-0.00119	-0.00123	-3.14094

D8	0.00300	0.00000	-0.00013	0.00047	0.00034	0.00334
D9	0.01412	-0.00004	0.00032	-0.00464	-0.00431	0.00981
D10	-3.11715	0.00012	0.00070	-0.00759	-0.00694	-3.12409
D11	-3.12729	-0.00003	0.00045	-0.00457	-0.00411	-3.13140
D12	0.02462	0.00013	0.00083	-0.00752	-0.00674	0.01788
D13	0.00029	0.00001	0.00005	0.00114	0.00120	0.00148
D14	3.14089	0.00002	0.00011	0.00042	0.00053	3.14142
D15	-3.13435	-0.00005	0.00035	-0.00293	-0.00256	-3.13691
D16	0.00625	-0.00004	0.00041	-0.00365	-0.00323	0.00302
D17	-0.00157	-0.00003	0.00011	-0.00106	-0.00095	-0.00252
D18	-3.13996	0.00003	0.00008	-0.00039	-0.00031	-3.14027
D19	3.13381	0.00002	-0.00015	0.00258	0.00241	3.13622
D20	-0.00457	0.00009	-0.00019	0.00325	0.00304	-0.00153
D21	0.00145	-0.00001	0.00005	-0.00134	-0.00128	0.00016
D22	-3.14092	-0.00002	-0.00004	-0.00095	-0.00099	3.14128
D23	-3.13913	-0.00003	-0.00001	-0.00059	-0.00060	-3.13973
D24	0.00170	-0.00003	-0.00010	-0.00021	-0.00031	0.00139
D25	-0.00142	0.00000	-0.00007	0.00033	0.00026	-0.00116
D26	3.13983	-0.00001	-0.00013	0.00064	0.00050	3.14034
D27	3.14094	0.00000	0.00002	-0.00006	-0.00004	3.14091
D28	-0.00099	-0.00001	-0.00004	0.00025	0.00021	-0.00078
D29	-0.00039	0.00002	-0.00001	0.00092	0.00091	0.00052
D30	3.14011	-0.00002	0.00008	-0.00070	-0.00060	3.13951
D31	3.14154	0.00003	0.00006	0.00061	0.00067	-3.14098
D32	-0.00114	-0.00001	0.00015	-0.00100	-0.00085	-0.00199
D33	-0.01485	-0.00001	-0.00026	0.00386	0.00362	-0.01123
D34	3.10879	0.00018	0.00044	0.00075	0.00122	3.11001
D35	3.11560	0.00013	-0.00061	0.00743	0.00676	3.12236
D36	-0.04395	0.00032	0.00009	0.00431	0.00436	-0.03959
D37	-0.01245	0.00003	-0.00045	0.00368	0.00322	-0.00922
D38	3.12284	0.00020	-0.00043	0.00590	0.00547	3.12831
D39	-3.14127	0.00002	-0.00002	-0.00020	-0.00021	-3.14149
D40	-0.00599	0.00019	0.00000	0.00202	0.00203	-0.00396
D41	0.01030	0.00004	0.00010	-0.00179	-0.00170	0.00860
D42	-3.11389	0.00011	-0.00057	0.00141	0.00084	-3.11305
D43	-3.13457	-0.00003	0.00014	-0.00248	-0.00236	-3.13693
D44	0.02443	0.00003	-0.00054	0.00072	0.00018	0.02461
D45	3.13196	0.00007	0.00022	-0.00219	-0.00198	3.12998
D46	-0.00337	-0.00009	-0.00041	-0.00277	-0.00318	-0.00655
D47	-0.03051	0.00017	0.00103	-0.00587	-0.00483	-0.03534
D48	3.11735	0.00002	0.00041	-0.00644	-0.00603	3.11132
D49	-0.01141	-0.00003	0.00097	-0.01575	-0.01480	-0.02621
D50	-3.14092	-0.00023	-0.00115	0.00580	0.00468	-3.13624
D51	3.12417	0.00012	0.00157	-0.01520	-0.01365	3.11052
D52	-0.00534	-0.00008	-0.00055	0.00636	0.00583	0.00049
D53	-3.11576	-0.00008	-0.00134	0.01241	0.01118	-3.10458
D54	0.01452	0.00010	0.00064	-0.00783	-0.00719	0.00733
D55	3.12761	-0.00002	0.00098	-0.01315	-0.01206	3.11555
D56	-0.00182	-0.00002	-0.00103	-0.00830	-0.00927	-0.01109
D57	-0.00384	-0.00023	-0.00081	0.00486	0.00409	0.00024
D58	-3.13327	-0.00023	-0.00281	0.00971	0.00687	-3.12640
D59	0.02405	-0.00019	-0.00009	-0.00802	-0.00802	0.01603
D60	-3.08521	-0.00018	0.00110	-0.02176	-0.02044	-3.10564
D61	-3.12179	-0.00027	0.00000	-0.00902	-0.00880	-3.13059
D62	0.05214	-0.00026	0.00120	-0.02276	-0.02122	0.03093
D63	-0.02151	0.00004	-0.00031	0.00891	0.00853	-0.01298
D64	3.12658	0.00016	-0.00046	0.01043	0.00971	3.13628
D65	-0.00130	0.00005	-0.00025	0.00427	0.00401	0.00272
D66	-3.13098	0.00016	0.00043	-0.00100	-0.00074	-3.13172
D67	3.13404	-0.00007	-0.00010	0.00280	0.00288	3.13691

D68	0.00435	0.00004	0.00057	-0.00247	-0.00187	0.00248
D69	-0.01264	0.00027	0.00059	0.00190	0.00240	-0.01024
D70	3.11610	0.00029	0.00270	-0.00320	-0.00051	3.11559
D71	3.08566	0.00026	-0.00094	0.01973	0.01875	3.10441
D72	-0.06879	0.00027	0.00117	0.01463	0.01584	-0.05295
D73	-0.08116	0.00035	-0.00155	0.03077	0.02905	-0.05210
D74	-2.57551	-0.00186	0.01011	-0.15742	-0.14671	-2.72222
D75	3.10279	0.00038	-0.00004	0.01314	0.01298	3.11577
D76	0.60845	-0.00182	0.01163	-0.17504	-0.16278	0.44566
D77	-0.05041	0.00018	-0.00080	0.01581	0.01466	-0.03575
D78	3.13831	0.00012	-0.00025	0.00495	0.00455	-3.14033
D79	3.08290	0.00011	-0.00127	0.01948	0.01797	3.10087
D80	-0.01157	0.00005	-0.00072	0.00862	0.00785	-0.00372
D81	-3.13826	-0.00014	-0.00015	-0.00004	0.00000	-3.13826
D82	0.01570	-0.00002	0.00055	-0.00553	-0.00494	0.01076
D83	0.08038	-0.00034	0.00140	-0.02806	-0.02651	0.05388
D84	2.57000	0.00194	-0.00998	0.15906	0.14886	2.71886
D85	-3.12412	-0.00025	0.00074	-0.01423	-0.01342	-3.13753
D86	-0.63450	0.00202	-0.01064	0.17290	0.16195	-0.47255
D87	-3.13418	-0.00006	0.00046	-0.00622	-0.00575	-3.13993
D88	-0.00091	-0.00007	0.00052	-0.00765	-0.00709	-0.00800
D89	0.07118	-0.00015	0.00110	-0.01994	-0.01884	0.05233
D90	-3.07874	-0.00016	0.00116	-0.02136	-0.02017	-3.09892
D91	1.18375	0.00120	-0.00648	0.10810	0.10316	1.28690
D92	-2.98387	0.00114	-0.00674	0.10987	0.10467	-2.87920
D93	-0.92773	0.00128	-0.00645	0.10863	0.10372	-0.82401
D94	-1.20374	-0.00114	0.00589	-0.09802	-0.09367	-1.29741
D95	0.91182	-0.00120	0.00564	-0.09625	-0.09216	0.81967
D96	2.96797	-0.00106	0.00593	-0.09749	-0.09310	2.87487
D97	-0.01636	-0.00003	-0.00025	0.00108	0.00084	-0.01552
D98	-3.14016	0.00001	-0.00019	-0.00179	-0.00199	3.14103
D99	-3.13793	-0.00008	-0.00020	-0.00151	-0.00169	-3.13962
D100	0.01211	-0.00006	-0.00026	-0.00006	-0.00033	0.01178
D101	-0.01434	0.00010	0.00056	-0.00442	-0.00386	-0.01820
D102	3.12660	0.00018	-0.00002	0.00648	0.00638	3.13299
D103	0.01299	0.00007	-0.00010	0.00350	0.00338	0.01637
D104	-3.13500	0.00005	-0.00005	0.00239	0.00233	-3.13267
D105	3.14111	0.00003	-0.00015	0.00563	0.00548	-3.13659
D106	-0.00688	0.00001	-0.00010	0.00452	0.00443	-0.00245
D107	3.11990	0.00003	0.00046	-0.00506	-0.00460	3.11530
D108	-0.07043	0.00024	0.00056	0.00900	0.00956	-0.06087
D109	-0.00414	0.00006	0.00053	-0.00792	-0.00741	-0.01156
D110	3.08871	0.00027	0.00062	0.00614	0.00674	3.09545
D111	0.01342	-0.00010	-0.00073	0.00797	0.00726	0.02067
D112	-3.12774	-0.00015	-0.00035	0.00071	0.00042	-3.12733
D113	-3.09256	-0.00025	-0.00078	-0.00248	-0.00318	-3.09574
D114	0.04947	-0.00030	-0.00040	-0.00974	-0.01002	0.03945
D115	3.11387	0.00029	-0.00002	0.00439	0.00434	3.11820
D116	0.44126	-0.00112	0.00817	-0.12000	-0.11172	0.32954
D117	-0.07567	0.00050	0.00007	0.01834	0.01833	-0.05735
D118	-2.74828	-0.00090	0.00825	-0.10605	-0.09773	-2.84601
D119	3.13947	-0.00005	0.00115	-0.01364	-0.01243	3.12704
D120	0.00332	-0.00017	0.00006	-0.00963	-0.00959	-0.00627
D121	-0.00275	0.00003	0.00059	-0.00313	-0.00254	-0.00530
D122	-3.13890	-0.00009	-0.00050	0.00088	0.00030	-3.13861
D123	3.12262	0.00023	0.00014	0.00599	0.00604	3.12866
D124	-0.04443	0.00026	-0.00059	0.01491	0.01420	-0.03024
D125	-0.02266	0.00031	0.00087	0.00328	0.00413	-0.01853
D126	3.09347	0.00034	0.00015	0.01221	0.01229	3.10576
D127	-3.12161	-0.00034	0.00023	-0.01347	-0.01312	-3.13473

D128	0.02563	-0.00046	-0.00089	-0.00931	-0.01017	0.01546
D129	0.00457	0.00007	-0.00031	0.00698	0.00671	0.01128
D130	-3.12840	-0.00014	-0.00092	0.00086	-0.00007	-3.12847
D131	-3.10245	0.00000	0.00065	-0.00499	-0.00430	-3.10675
D132	0.04777	-0.00021	0.00004	-0.01112	-0.01109	0.03668
D133	0.07376	-0.00044	0.00031	-0.02022	-0.01985	0.05391
D134	2.74918	0.00096	-0.00794	0.10432	0.09613	2.84531
D135	-3.10158	-0.00039	-0.00064	-0.00850	-0.00910	-3.11068
D136	-0.42616	0.00102	-0.00888	0.11603	0.10689	-0.31927
D137	0.01485	-0.00042	-0.00037	-0.01386	-0.01425	0.00060
D138	-3.12611	-0.00035	-0.00143	-0.00449	-0.00604	-3.13215
D139	-3.13492	-0.00023	0.00021	-0.00807	-0.00782	3.14045
D140	0.00731	-0.00015	-0.00085	0.00130	0.00039	0.00769
D141	-0.02319	0.00053	0.00072	0.01325	0.01394	-0.00925
D142	3.11771	0.00044	0.00190	0.00289	0.00465	3.12236
D143	3.13912	0.00023	0.00100	0.01765	0.01863	-3.12543
D144	-0.00533	0.00034	0.00158	0.01644	0.01800	0.01267
D145	-0.00172	0.00032	-0.00026	0.02875	0.02850	0.02678
D146	3.13702	0.00043	0.00032	0.02754	0.02787	-3.11830
D147	-0.82407	0.00067	-0.00448	0.06792	0.06392	-0.76015
D148	1.29160	0.00067	-0.00456	0.06871	0.06464	1.35624
D149	-2.88156	0.00063	-0.00446	0.06724	0.06326	-2.81829
D150	2.86734	-0.00071	0.00483	-0.07408	-0.06973	2.79761
D151	-1.30018	-0.00070	0.00476	-0.07329	-0.06901	-1.36919
D152	0.80985	-0.00075	0.00486	-0.07476	-0.07039	0.73947
D153	-0.00157	0.00032	0.00033	0.01007	0.01042	0.00884
D154	3.13947	0.00030	0.00063	0.00558	0.00620	-3.13751
D155	-3.14020	0.00021	-0.00028	0.01134	0.01108	-3.12912
D156	0.00085	0.00020	0.00003	0.00684	0.00686	0.00771
D157	3.14005	-0.00001	0.00031	-0.00445	-0.00418	3.13587
D158	-0.00533	0.00019	0.00068	0.01076	0.01149	0.00616
D159	-0.00109	0.00001	0.00006	-0.00066	-0.00061	-0.00170
D160	3.13672	0.00021	0.00042	0.01455	0.01506	-3.13140
D161	-3.13932	-0.00001	-0.00024	0.00338	0.00313	-3.13619
D162	0.00380	0.00001	-0.00012	0.00326	0.00312	0.00693
D163	0.00180	-0.00002	0.00003	-0.00048	-0.00044	0.00136
D164	-3.13826	0.00000	0.00014	-0.00060	-0.00045	-3.13871
D165	-0.00009	0.00001	-0.00012	0.00164	0.00151	0.00142
D166	-3.14149	0.00003	0.00000	0.00123	0.00122	-3.14027
D167	-3.13797	-0.00020	-0.00048	-0.01336	-0.01376	3.13145
D168	0.00382	-0.00018	-0.00036	-0.01376	-0.01406	-0.01024
D169	-0.00188	0.00003	-0.00010	0.00150	0.00139	-0.00049
D170	3.13991	0.00002	-0.00008	0.00117	0.00109	3.14100
D171	3.13824	0.00001	-0.00021	0.00163	0.00141	3.13965
D172	-0.00315	0.00000	-0.00019	0.00130	0.00111	-0.00204
D173	0.00164	0.00001	-0.00002	0.00075	0.00073	0.00238
D174	-3.14048	-0.00004	-0.00004	-0.00104	-0.00108	-3.14156
D175	-3.13816	0.00003	0.00011	0.00060	0.00071	-3.13745
D176	0.00289	-0.00001	0.00009	-0.00119	-0.00110	0.00179
D177	0.00122	-0.00002	0.00014	-0.00196	-0.00180	-0.00059
D178	-3.14054	-0.00002	0.00012	-0.00167	-0.00155	3.14109
D179	-3.14055	-0.00004	0.00003	-0.00157	-0.00153	3.14110
D180	0.00087	-0.00004	0.00001	-0.00129	-0.00128	-0.00041
D181	3.14104	0.00001	-0.00012	0.00122	0.00109	-3.14106
D182	-0.00029	0.00000	-0.00012	0.00091	0.00079	0.00050
D183	-0.00034	0.00003	0.00001	0.00076	0.00077	0.00042
D184	3.14151	0.00002	0.00002	0.00045	0.00047	-3.14121
D185	3.14066	0.00002	-0.00005	0.00123	0.00117	-3.14135
D186	-0.00105	0.00002	-0.00001	0.00115	0.00113	0.00008
D187	-0.00071	0.00002	-0.00003	0.00087	0.00085	0.00014

D188	3.14076	0.00002	0.00001	0.00079	0.00081	3.14156
D189	-0.00032	0.00000	-0.00002	0.00016	0.00014	-0.00018
D190	3.14135	0.00000	0.00001	-0.00004	-0.00003	3.14131
D191	3.14100	0.00001	-0.00002	0.00048	0.00045	3.14146
D192	-0.00052	0.00001	0.00000	0.00027	0.00028	-0.00024
D193	0.00007	0.00001	0.00002	0.00001	0.00003	0.00010
D194	-3.14152	0.00000	0.00000	-0.00009	-0.00008	3.14158
D195	-3.14140	0.00001	-0.00001	0.00008	0.00006	-3.14133
D196	0.00019	0.00000	-0.00003	-0.00001	-0.00004	0.00015
D197	0.00046	-0.00002	0.00000	-0.00054	-0.00054	-0.00008
D198	-3.14113	0.00000	0.00002	-0.00044	-0.00043	-3.14156
D199	-3.14121	-0.00002	-0.00003	-0.00034	-0.00036	-3.14157
D200	0.00039	0.00000	-0.00001	-0.00024	-0.00025	0.00014

Item	Value	Threshold	Converged?

Maximum Force	0.019232	0.000450	NO

RMS Force	0.002346	0.000300	NO

Maximum Displacement	0.521859	0.001800	NO

RMS Displacement	0.094594	0.001200	NO

Predicted change in Energy=-4.262113D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.791467	-0.659893	-0.013367
2	6	0	-9.969476	-1.801858	-0.030743
3	6	0	-10.475189	-3.092785	-0.040844
4	6	0	-11.862451	-3.253375	-0.035120
5	6	0	-12.696443	-2.128716	-0.019799
6	6	0	-12.180037	-0.828456	-0.008484
7	1	0	-9.793003	-3.936874	-0.054349
8	1	0	-12.297382	-4.247983	-0.042957
9	1	0	-13.773961	-2.262130	-0.016624
10	1	0	-12.862232	0.010700	0.001239
11	6	0	-9.928290	0.551271	-0.003943
12	6	0	-8.551258	-1.389643	-0.039621
13	6	0	-8.537839	0.089135	-0.030212
14	6	0	-7.413374	0.870184	-0.066242
15	6	0	-6.026523	0.596001	-0.083028
16	6	0	-3.653509	-0.166563	-0.033433
17	6	0	-3.794197	1.239348	-0.095004
18	16	0	-5.180685	-0.984670	-0.025286
19	6	0	-5.118819	1.669500	-0.115432
20	6	0	-2.273461	-0.426466	-0.005528
21	6	0	-1.617877	0.820153	-0.046938
22	7	0	-2.541127	1.846687	-0.146045
23	16	0	-1.159803	-1.779451	0.054552
24	16	0	1.135345	1.833112	-0.052787
25	6	0	0.187691	-0.645712	0.042082
26	6	0	-0.212085	0.700068	-0.025928
27	6	0	1.591313	-0.766560	0.069665
28	6	0	2.250911	0.480825	0.007748

29	6	0	3.632261	0.217171	0.023985
30	6	0	3.768206	-1.191978	0.102976
31	6	0	5.090475	-1.623456	0.112033
32	6	0	6.003989	-0.554661	0.054811
33	16	0	5.166341	1.027721	-0.010714
34	7	0	2.513156	-1.789274	0.174631
35	6	0	7.399658	-0.837837	0.044605
36	6	0	8.548875	-0.076213	0.011886
37	6	0	8.613094	1.402288	-0.014447
38	6	0	9.921326	-0.580226	0.002552
39	6	0	10.044520	1.766548	-0.037123
40	6	0	10.825947	0.596422	-0.027686
41	6	0	10.596801	3.038297	-0.064010
42	6	0	12.217093	0.712564	-0.046547
43	6	0	11.989779	3.147571	-0.082808
44	6	0	12.781505	1.992873	-0.074030
45	6	0	10.348760	-1.891948	0.016426
46	6	0	9.474085	-3.020145	0.040629
47	6	0	11.723181	-2.268769	0.005255
48	7	0	8.785749	-3.960597	0.058849
49	7	0	12.832830	-2.622443	-0.003094
50	6	0	-10.392463	1.854504	0.033289
51	6	0	-11.775995	2.203192	0.056798
52	6	0	-9.544766	3.004354	0.057430
53	7	0	-12.888596	2.547253	0.077589
54	7	0	-8.868205	3.953122	0.079491
55	8	0	-7.585656	-2.146198	-0.056171
56	8	0	7.676003	2.193855	-0.005894
57	6	0	2.245894	-3.196766	-0.084374
58	1	0	1.291498	-3.475464	0.366987
59	1	0	2.216112	-3.412933	-1.157966
60	1	0	3.028181	-3.798529	0.382350
61	6	0	-2.294393	3.218533	0.282717
62	1	0	-2.311555	3.307162	1.373965
63	1	0	-1.324512	3.546682	-0.095068
64	1	0	-3.060911	3.864929	-0.148668
65	1	0	5.423783	-2.653789	0.155500
66	1	0	12.867363	-0.152943	-0.040422
67	1	0	13.863212	2.084930	-0.088710
68	1	0	12.460613	4.125526	-0.104309
69	1	0	9.946350	3.907134	-0.069820
70	1	0	7.556181	-1.909640	0.072436
71	1	0	-7.584402	1.939284	-0.082362
72	1	0	-5.456662	2.699380	-0.138045

Rotational constants (GHZ): 0.1755165 0.0104048 0.0098253

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis func-

tions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6571.7203583788 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T

Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6571.6352757133 Har-

trees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.22D-04 NBF= 916
NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916
Initial guess from the checkpoint file: "PBDB.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999999 0.000938 0.000019 0.001219 Ang= 0.18 deg.
ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1
AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-yADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2001
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOPCl= 0 IICent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RB3LYP) = -3683.01776294 A.U. after 13 cycles
NFock= 13 Conv=0.88D-08 -V/T= 2.0068
Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IICent= 0 IOPClX= 0 NMat=1
NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	0.000076938	0.000000626	0.000069432
2	6	-0.000171063	0.000013275	-0.000067101
3	6	-0.000104514	0.000720350	0.000136282
4	6	0.000105804	-0.000348698	-0.000037100
5	6	-0.000192887	0.000022451	-0.000186348
6	6	-0.000835877	0.000016086	-0.000599012
7	1	-0.000091058	0.000003275	-0.000105770
8	1	-0.000047147	0.000003945	-0.000027401
9	1	0.000081688	0.000050957	0.000088709
10	1	0.000243489	-0.000352235	0.000039012
11	6	0.000051564	0.000263463	0.000190936
12	6	0.000528715	0.000436078	-0.000008904
13	6	-0.001854012	0.007094120	-0.000100822
14	6	0.000685656	-0.005248746	-0.000274210
15	6	0.002888111	-0.001238307	0.000582801
16	6	-0.000247789	0.000599047	0.000739478
17	6	-0.002181088	-0.001563545	-0.000168956
18	16	-0.001753646	0.000076280	-0.000216104
19	6	0.002018439	-0.000612253	0.000483566
20	6	0.000223115	0.001851637	0.000421128
21	6	-0.002101222	-0.002327680	0.000981831
22	7	0.004436955	0.001383012	-0.004153465
23	16	0.000184714	-0.000098027	0.000150360
24	16	-0.000387501	-0.000066629	0.000067438
25	6	-0.001140892	0.000186325	-0.000374523

26	6	0.000734648	0.000559631	-0.000914122
27	6	0.002776440	-0.000165400	-0.000003756
28	6	0.001478161	-0.001536401	0.000569140
29	6	-0.000994037	0.001070631	-0.001423527
30	6	-0.000208959	0.000083429	-0.001558491
31	6	0.000674714	-0.000243029	0.000602085
32	6	0.002843734	-0.002131729	0.002489958
33	16	0.002154788	-0.000513465	0.001028540
34	7	-0.003168223	-0.001313375	0.004139987
35	6	-0.002752762	0.001401939	-0.002400859
36	6	-0.002835892	0.001304557	-0.001382161
37	6	-0.001915442	0.000057547	-0.002899132
38	6	-0.000427665	-0.001385804	-0.000467901
39	6	0.000313706	-0.000224084	0.000558431
40	6	-0.001853480	-0.000108414	-0.001447791
41	6	0.000231274	-0.000658310	0.000107032
42	6	0.002581627	-0.001707919	0.001810387
43	6	-0.000378461	0.000809070	-0.000218290
44	6	0.000227002	0.000136139	0.000205939
45	6	0.001002840	0.002255916	0.001059367
46	6	0.000545769	0.000895423	0.000612077
47	6	0.001609995	0.000387277	0.001257346
48	7	0.000050810	0.000139760	-0.000015630
49	7	0.000644473	-0.000248662	0.000470209
50	6	0.000312534	0.000137041	0.000360472
51	6	-0.000364451	-0.000028564	-0.000380840
52	6	0.000491793	-0.000042290	0.000255755
53	7	-0.000365783	0.000992404	-0.000110098
54	7	-0.000363453	-0.000185203	-0.000270758
55	8	-0.000635929	0.000377778	-0.000480189
56	8	-0.000401335	0.001694091	0.000721145
57	6	0.001263202	-0.000165470	-0.001807837
58	1	-0.000033660	0.000009024	-0.000010767
59	1	-0.000037622	-0.000088904	-0.000080483
60	1	-0.000009897	0.000063617	0.000155668
61	6	-0.002347307	-0.000071116	0.003595164
62	1	0.000003913	-0.000317726	-0.000305982
63	1	0.000156711	-0.000486468	-0.000229227
64	1	0.000063010	-0.000371001	-0.000591248
65	1	-0.000094711	0.000178060	-0.000019484
66	1	-0.001091646	-0.000629146	-0.000919210
67	1	-0.000133314	-0.000166231	-0.000119548
68	1	0.000055898	0.000016957	0.000042662
69	1	0.000085467	0.000031337	0.000080300
70	1	-0.000498801	-0.000089635	-0.000498489
71	1	0.000012929	-0.000386990	0.000202920
72	1	0.000180902	-0.000201100	0.000599980

Cartesian Forces: Max 0.007094120 RMS 0.001275252

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.009773698 RMS 0.001227421

Search for a local minimum.

Step number 14 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 13 14
 DE= -3.20D-03 DEPred=-4.26D-03 R= 7.51D-01
 TightC=F SS= 1.41D+00 RLast= 5.02D-01 DXNew= 3.3118D+00 1.5066D+00
 Trust test= 7.51D-01 RLast= 5.02D-01 DXMaxT set to 1.97D+00
 ITU= 1 1 1 1 1 0 0 0 1 0 0 0 1 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00230	0.00230	0.00231	0.00235	0.00241
Eigenvalues ---	0.00290	0.00387	0.00443	0.00454	0.00461
Eigenvalues ---	0.00483	0.00505	0.00516	0.00582	0.00615
Eigenvalues ---	0.00616	0.00662	0.00681	0.00686	0.00694
Eigenvalues ---	0.00715	0.00738	0.00744	0.00760	0.00770
Eigenvalues ---	0.00775	0.00794	0.00828	0.00840	0.00865
Eigenvalues ---	0.00873	0.00880	0.01007	0.01084	0.01132
Eigenvalues ---	0.01150	0.01196	0.01249	0.01274	0.01337
Eigenvalues ---	0.01361	0.01364	0.01394	0.01413	0.01458
Eigenvalues ---	0.01491	0.01573	0.01646	0.01653	0.01754
Eigenvalues ---	0.01794	0.01800	0.01860	0.01929	0.01954
Eigenvalues ---	0.02006	0.02023	0.02075	0.02075	0.02209
Eigenvalues ---	0.02210	0.04828	0.04837	0.04900	0.04933
Eigenvalues ---	0.04976	0.05002	0.05017	0.05286	0.07081
Eigenvalues ---	0.07228	0.07454	0.07593	0.15476	0.15705
Eigenvalues ---	0.15974	0.15998	0.15999	0.16000	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues ---	0.16000	0.16001	0.16003	0.16011	0.16028
Eigenvalues ---	0.16051	0.17515	0.17972	0.19180	0.19277
Eigenvalues ---	0.19811	0.20541	0.20674	0.21299	0.21406
Eigenvalues ---	0.22002	0.22009	0.22157	0.22370	0.22399
Eigenvalues ---	0.22535	0.22599	0.22635	0.22648	0.22680
Eigenvalues ---	0.22900	0.22977	0.23236	0.23370	0.23473
Eigenvalues ---	0.23783	0.23874	0.24052	0.24179	0.24270
Eigenvalues ---	0.24284	0.24469	0.24496	0.24557	0.24607
Eigenvalues ---	0.24709	0.24807	0.24932	0.24973	0.24979
Eigenvalues ---	0.24987	0.24990	0.24992	0.24996	0.24997
Eigenvalues ---	0.24997	0.24998	0.24999	0.25000	0.25000
Eigenvalues ---	0.25000	0.25010	0.25058	0.25567	0.25847
Eigenvalues ---	0.26221	0.26443	0.26705	0.26768	0.27021
Eigenvalues ---	0.27183	0.27358	0.27838	0.27896	0.28243
Eigenvalues ---	0.28429	0.28630	0.29013	0.29961	0.30509
Eigenvalues ---	0.31986	0.32176	0.35044	0.35596	0.36327
Eigenvalues ---	0.36337	0.36405	0.36475	0.36650	0.36702
Eigenvalues ---	0.36773	0.36827	0.37081	0.37094	0.37154
Eigenvalues ---	0.37251	0.37273	0.37419	0.37565	0.37670
Eigenvalues ---	0.37755	0.37944	0.38850	0.40298	0.40684
Eigenvalues ---	0.41357	0.41685	0.42182	0.42718	0.44423
Eigenvalues ---	0.44791	0.45585	0.46133	0.47378	0.47851
Eigenvalues ---	0.47965	0.50595	0.52621	0.54327	0.55819
Eigenvalues ---	0.57614	0.71759	0.78466	0.80306	0.82443
Eigenvalues ---	0.91367	1.25862	1.26318	1.29342	1.35383

RFO step: Lambda=-2.98897486D-03 EMin= 2.30135958D-03

Quartic linear search produced a step of 0.01717.

Iteration 1	RMS(Cart)=	0.06655511	RMS(Int)=	0.00118155
Iteration 2	RMS(Cart)=	0.00258331	RMS(Int)=	0.00041750
Iteration 3	RMS(Cart)=	0.00000335	RMS(Int)=	0.00041750
Iteration 4	RMS(Cart)=	0.00000000	RMS(Int)=	0.00041750

Variable	Old X	-DE/DX	Delta X	Delta X	Delta X	New X
(Linear)	(Quad)	(Total)				
R1	2.65912	-0.00069	-0.00001	-0.00045	-0.00046	2.65866
R2	2.64330	0.00013	0.00002	0.00057	0.00059	2.64388
R3	2.81060	-0.00117	0.00010	-0.00058	-0.00048	2.81012
R4	2.62008	0.00054	-0.00001	0.00011	0.00010	2.62017

R5	2.79101	0.00103	-0.00005	0.00095	0.00091	2.79191
R6	2.63908	0.00012	-0.00001	-0.00052	-0.00053	2.63855
R7	2.05107	-0.00013	0.00001	0.00000	0.00000	2.05107
R8	2.64605	0.00016	-0.00001	0.00014	0.00014	2.64618
R9	2.05144	-0.00001	0.00000	0.00009	0.00009	2.05153
R10	2.64391	-0.00017	0.00001	-0.00029	-0.00028	2.64364
R11	2.05177	-0.00005	0.00000	0.00000	0.00000	2.05177
R12	2.04376	-0.00012	0.00000	-0.00034	-0.00034	2.04342
R13	2.76934	0.00124	-0.00014	0.00069	0.00055	2.76989
R14	2.61525	-0.00022	0.00000	-0.00149	-0.00149	2.61375
R15	2.79466	0.00142	-0.00005	0.00177	0.00173	2.79639
R16	2.31832	-0.00079	0.00000	-0.00155	-0.00156	2.31676
R17	2.58814	0.00977	-0.00021	0.01804	0.01783	2.60596
R18	2.67168	0.00400	-0.00010	0.00943	0.00933	2.68101
R19	2.04622	0.00016	0.00001	0.00058	0.00059	2.04681
R20	3.38957	-0.00113	0.00012	-0.00366	-0.00366	3.38591
R21	2.65732	0.00160	-0.00007	0.00042	0.00032	2.65764
R22	2.67259	0.00096	0.00007	0.00407	0.00399	2.67658
R23	3.27399	0.00103	-0.00009	0.00192	0.00181	3.27581
R24	2.65428	0.00054	-0.00020	-0.00356	-0.00462	2.64966
R25	2.63213	-0.00114	0.00000	-0.00859	-0.00850	2.62364
R26	2.63320	0.00052	-0.00031	-0.00921	-0.00883	2.62437
R27	2.04868	-0.00032	0.00003	0.00025	0.00027	2.04895
R28	2.66281	0.00178	0.00007	0.00523	0.00516	2.66797
R29	3.31345	0.00032	0.00005	0.00152	0.00154	3.31499
R30	2.61574	-0.00066	-0.00027	-0.01209	-0.01168	2.60407
R31	2.66653	0.00015	-0.00009	-0.00830	-0.00830	2.65823
R32	2.75581	-0.00013	-0.00041	-0.01057	-0.01098	2.74483
R33	3.32788	0.00032	0.00001	0.00017	0.00006	3.32794
R34	3.32725	0.00024	0.00001	-0.00005	-0.00008	3.32717
R35	3.31475	0.00032	0.00002	0.00069	0.00068	3.31543
R36	2.65610	-0.00009	-0.00009	-0.00273	-0.00283	2.65327
R37	2.66278	0.00154	-0.00015	-0.00415	-0.00426	2.65853
R38	2.66905	0.00021	0.00000	0.00045	0.00038	2.66943
R39	2.60944	-0.00071	-0.00016	-0.01043	-0.01032	2.59911
R40	2.65767	-0.00182	-0.00007	-0.01301	-0.01342	2.64426
R41	2.67943	-0.00001	0.00000	0.00036	0.00030	2.67973
R42	3.27942	-0.00053	0.00006	-0.00147	-0.00142	3.27800
R43	2.62845	0.00077	-0.00012	-0.00770	-0.00778	2.62067
R44	2.63008	-0.00114	-0.00011	-0.01011	-0.00995	2.62013
R45	2.65915	-0.00072	-0.00005	-0.00360	-0.00366	2.65549
R46	2.04804	0.00003	0.00000	0.00012	0.00012	2.04816
R47	3.38566	-0.00180	0.00006	-0.00484	-0.00483	3.38083
R48	2.69124	-0.00712	0.00018	-0.02981	-0.02964	2.66161
R49	2.75119	-0.00077	-0.00012	-0.00532	-0.00545	2.74574
R50	2.60607	-0.00304	0.00013	-0.00278	-0.00266	2.60341
R51	2.04757	-0.00056	0.00000	-0.00036	-0.00036	2.04721
R52	2.79704	-0.00075	0.00009	-0.00048	-0.00032	2.79672
R53	2.76297	0.00319	0.00002	0.01115	0.01113	2.77410
R54	2.79154	0.00067	-0.00002	0.00064	0.00070	2.79224
R55	2.31813	-0.00023	0.00001	-0.00085	-0.00085	2.31728
R56	2.80531	0.00282	-0.00013	0.00576	0.00553	2.81084
R57	2.60721	0.00617	-0.00015	0.00675	0.00660	2.61381
R58	2.65902	0.00111	-0.00010	0.00032	0.00021	2.65923
R59	2.62058	0.00008	-0.00003	-0.00348	-0.00350	2.61708
R60	2.63827	0.00283	-0.00009	0.00573	0.00564	2.64391
R61	2.64067	-0.00068	0.00001	-0.00130	-0.00129	2.63939
R62	2.05102	-0.00012	0.00001	-0.00005	-0.00005	2.05098
R63	2.64461	-0.00028	-0.00002	-0.00086	-0.00088	2.64372
R64	2.04579	-0.00155	0.00009	-0.00156	-0.00147	2.04432

R65	2.64577	-0.00014	-0.00001	-0.00262	-0.00263	2.64314
R66	2.05150	-0.00003	0.00000	0.00002	0.00002	2.05152
R67	2.05171	-0.00002	0.00000	0.00009	0.00009	2.05180
R68	2.69806	0.00103	0.00002	0.00393	0.00395	2.70200
R69	2.69321	0.00259	-0.00006	0.00878	0.00872	2.70193
R70	2.20264	0.00014	-0.00001	0.00011	0.00010	2.20273
R71	2.20092	0.00084	-0.00001	0.00057	0.00056	2.20148
R72	2.69662	0.00118	-0.00003	0.00250	0.00247	2.69909
R73	2.69995	0.00023	0.00002	0.00026	0.00028	2.70023
R74	2.20110	0.00067	-0.00001	0.00037	0.00037	2.20147
R75	2.20247	0.00019	0.00000	0.00031	0.00030	2.20277
R76	2.06341	0.00002	0.00001	0.00056	0.00057	2.06398
R77	2.07028	-0.00005	0.00001	0.00044	0.00045	2.07073
R78	2.06311	0.00003	0.00001	0.00049	0.00050	2.06361
R79	2.06920	0.00024	0.00002	0.00124	0.00126	2.07046
R80	2.06238	0.00031	0.00000	0.00111	0.00112	2.06349
R81	2.06272	0.00012	0.00001	0.00084	0.00086	2.06358
A1	2.07389	0.00096	-0.00006	0.00107	0.00101	2.07490
A2	1.89856	0.00033	-0.00005	-0.00060	-0.00066	1.89790
A3	2.31073	-0.00129	0.00011	-0.00047	-0.00035	2.31038
A4	2.14437	-0.00066	0.00004	-0.00083	-0.00078	2.14359
A5	1.91187	-0.00021	0.00003	0.00048	0.00050	1.91237
A6	2.22694	0.00087	-0.00007	0.00035	0.00029	2.22722
A7	2.05936	-0.00006	0.00001	-0.00007	-0.00007	2.05930
A8	2.08855	0.00007	0.00000	0.00021	0.00021	2.08877
A9	2.13527	0.00000	-0.00001	-0.00013	-0.00015	2.13512
A10	2.09363	0.00037	-0.00003	0.00092	0.00089	2.09453
A11	2.09822	-0.00013	0.00000	-0.00050	-0.00050	2.09773
A12	2.09133	-0.00024	0.00002	-0.00042	-0.00040	2.09093
A13	2.12551	-0.00027	0.00001	-0.00059	-0.00058	2.12493
A14	2.08568	0.00001	0.00001	0.00015	0.00017	2.08584
A15	2.07199	0.00026	-0.00002	0.00044	0.00042	2.07241
A16	2.06960	-0.00034	0.00003	-0.00050	-0.00047	2.06913
A17	2.13259	-0.00024	0.00005	0.00000	0.00006	2.13265
A18	2.08099	0.00058	-0.00008	0.00050	0.00041	2.08141
A19	1.86893	0.00105	-0.00002	0.00159	0.00155	1.87048
A20	2.18018	-0.00373	0.00044	0.00136	0.00181	2.18199
A21	2.23404	0.00268	-0.00042	-0.00294	-0.00335	2.23069
A22	1.86268	0.00039	-0.00003	0.00002	-0.00005	1.86263
A23	2.19415	-0.00065	-0.00001	-0.00053	-0.00058	2.19357
A24	2.22635	0.00026	0.00004	0.00046	0.00046	2.22681
A25	1.88266	-0.00156	0.00007	-0.00163	-0.00159	1.88107
A26	2.21383	-0.00105	-0.00016	-0.00372	-0.00390	2.20993
A27	2.18650	0.00262	0.00009	0.00558	0.00565	2.19215
A28	2.33935	0.00297	0.00004	0.00379	0.00378	2.34313
A29	2.01947	-0.00112	-0.00002	0.00085	0.00079	2.02026
A30	1.92436	-0.00186	-0.00002	-0.00457	-0.00463	1.91972
A31	2.25635	0.00001	0.00015	-0.00208	-0.00204	2.25431
A32	2.07765	0.00060	-0.00015	0.00112	0.00086	2.07851
A33	1.94883	-0.00059	-0.00001	0.00172	0.00154	1.95037
A34	1.96268	0.00005	0.00000	0.00049	0.00072	1.96340
A35	1.85725	-0.00053	0.00002	-0.00135	-0.00158	1.85567
A36	2.46324	0.00047	-0.00002	0.00092	0.00087	2.46411
A37	1.98476	-0.00080	0.00001	-0.00154	-0.00191	1.98285
A38	1.92348	0.00062	-0.00013	-0.00310	-0.00204	1.92144
A39	2.37470	0.00018	0.00012	0.00455	0.00386	2.37856
A40	1.57019	0.00026	0.00000	-0.00235	-0.00247	1.56772
A41	1.95820	0.00107	0.00000	0.00161	0.00176	1.95995
A42	2.12297	-0.00009	0.00002	0.00247	0.00240	2.12537
A43	2.20191	-0.00097	-0.00003	-0.00394	-0.00406	2.19785

A44	1.86799	-0.00020	0.00003	-0.00042	-0.00062	1.86737
A45	2.44574	0.00071	0.00000	0.00183	0.00179	2.44753
A46	1.96944	-0.00051	-0.00002	-0.00138	-0.00115	1.96829
A47	1.92611	0.00038	-0.00015	-0.00341	-0.00238	1.92373
A48	1.96902	-0.00014	0.00001	0.00084	0.00049	1.96952
A49	2.38719	-0.00024	0.00014	0.00289	0.00218	2.38937
A50	1.84829	-0.00028	0.00027	0.00732	0.00555	1.85385
A51	2.15483	0.00072	0.00070	0.03059	0.02647	2.18130
A52	2.16970	0.00010	0.00078	0.02948	0.02543	2.19513
A53	1.55977	0.00035	-0.00005	-0.00229	-0.00242	1.55736
A54	1.56086	0.00033	-0.00005	-0.00208	-0.00215	1.55872
A55	1.98135	-0.00004	0.00006	0.00243	0.00242	1.98378
A56	2.35583	-0.00001	-0.00006	-0.00225	-0.00238	2.35346
A57	1.94592	0.00005	0.00000	-0.00010	0.00001	1.94593
A58	2.35665	-0.00025	-0.00003	-0.00227	-0.00243	2.35422
A59	1.94504	0.00034	0.00000	0.00047	0.00065	1.94568
A60	1.98147	-0.00008	0.00003	0.00183	0.00181	1.98327
A61	1.96990	-0.00022	0.00003	0.00034	0.00022	1.97012
A62	2.38913	0.00007	0.00004	0.00053	0.00022	2.38935
A63	1.92375	0.00015	-0.00006	-0.00048	-0.00014	1.92361
A64	1.96641	-0.00008	-0.00002	0.00016	0.00024	1.96665
A65	2.44899	0.00043	-0.00002	0.00012	0.00010	2.44909
A66	1.86776	-0.00035	0.00004	-0.00025	-0.00032	1.86745
A67	1.85577	0.00042	-0.00003	0.00039	0.00024	1.85601
A68	2.46621	-0.00005	0.00003	0.00002	0.00004	2.46625
A69	1.96118	-0.00036	0.00000	-0.00035	-0.00026	1.96092
A70	1.98210	0.00044	-0.00001	0.00158	0.00143	1.98354
A71	1.92082	-0.00013	-0.00003	-0.00120	-0.00078	1.92004
A72	2.38007	-0.00031	0.00004	-0.00035	-0.00062	2.37945
A73	1.96196	-0.00134	0.00007	-0.00253	-0.00239	1.95957
A74	2.19881	0.00047	-0.00006	-0.00082	-0.00092	2.19789
A75	2.12241	0.00087	-0.00001	0.00334	0.00330	2.12571
A76	1.94852	0.00129	-0.00003	0.00435	0.00430	1.95282
A77	2.07770	0.00424	-0.00028	0.00207	0.00179	2.07949
A78	2.25692	-0.00552	0.00031	-0.00636	-0.00605	2.25087
A79	1.57084	-0.00003	-0.00002	-0.00290	-0.00297	1.56787
A80	1.85484	-0.00007	0.00010	0.00250	0.00180	1.85664
A81	2.18947	0.00015	0.00038	0.01472	0.01317	2.20264
A82	2.17886	0.00020	0.00033	0.01450	0.01290	2.19177
A83	2.35607	-0.00850	0.00043	-0.01292	-0.01249	2.34358
A84	1.91566	0.00382	-0.00028	0.00247	0.00219	1.91785
A85	2.01144	0.00469	-0.00014	0.01046	0.01031	2.02176
A86	2.19968	-0.00660	0.00028	-0.00755	-0.00734	2.19234
A87	2.20434	0.00476	-0.00015	0.00574	0.00552	2.20986
A88	1.87916	0.00184	-0.00013	0.00182	0.00183	1.88099
A89	1.86359	-0.00048	0.00004	-0.00060	-0.00083	1.86276
A90	2.22850	-0.00178	0.00011	-0.00134	-0.00188	2.22663
A91	2.19103	0.00226	-0.00015	0.00258	0.00178	2.19281
A92	1.87435	-0.00239	0.00009	-0.00468	-0.00462	1.86973
A93	2.23761	0.00093	0.00006	-0.00425	-0.00418	2.23343
A94	2.17123	0.00146	-0.00014	0.00892	0.00879	2.18002
A95	1.91025	0.00055	-0.00001	0.00273	0.00285	1.91310
A96	2.22982	-0.00054	0.00003	-0.00288	-0.00295	2.22687
A97	2.14312	-0.00002	-0.00002	0.00015	0.00010	2.14322
A98	1.89743	0.00048	0.00002	0.00074	0.00073	1.89816
A99	2.30962	0.00032	-0.00007	0.00098	0.00090	2.31052
A100	2.07613	-0.00079	0.00006	-0.00172	-0.00163	2.07450
A101	2.05892	0.00028	-0.00001	0.00105	0.00106	2.05999
A102	2.08927	-0.00014	-0.00002	-0.00139	-0.00143	2.08784
A103	2.13499	-0.00014	0.00003	0.00035	0.00036	2.13536

A104	2.06945	-0.00006	-0.00001	-0.00014	-0.00015	2.06930
A105	2.13169	0.00025	-0.00004	0.00075	0.00071	2.13240
A106	2.08205	-0.00018	0.00005	-0.00061	-0.00056	2.08149
A107	2.09338	0.00057	-0.00001	0.00130	0.00129	2.09468
A108	2.09792	-0.00022	0.00002	0.00007	0.00009	2.09801
A109	2.09188	-0.00035	-0.00001	-0.00137	-0.00138	2.09050
A110	2.12536	0.00003	-0.00001	-0.00064	-0.00067	2.12469
A111	2.07105	0.00024	0.00000	0.00137	0.00137	2.07242
A112	2.08677	-0.00026	0.00002	-0.00072	-0.00070	2.08607
A113	2.16717	0.00050	0.00001	-0.00525	-0.00524	2.16193
A114	2.15325	0.00135	0.00004	0.01034	0.01038	2.16362
A115	1.96276	-0.00186	-0.00005	-0.00509	-0.00514	1.95763
A116	2.16004	-0.00244	0.00044	0.00429	0.00473	2.16478
A117	2.16436	0.00159	-0.00023	-0.00238	-0.00261	2.16176
A118	1.95877	0.00085	-0.00021	-0.00192	-0.00213	1.95665
A119	1.91100	0.00000	0.00001	0.00011	0.00012	1.91112
A120	1.94990	-0.00023	0.00008	0.00054	0.00062	1.95052
A121	1.90211	0.00024	-0.00001	0.00135	0.00134	1.90345
A122	1.90812	0.00004	-0.00004	-0.00113	-0.00117	1.90695
A123	1.88483	0.00000	0.00001	0.00087	0.00087	1.88571
A124	1.90673	-0.00004	-0.00006	-0.00172	-0.00177	1.90496
A125	1.94604	0.00019	0.00006	0.00201	0.00207	1.94811
A126	1.90862	0.00047	0.00001	0.00303	0.00304	1.91165
A127	1.89871	0.00079	-0.00002	0.00468	0.00466	1.90337
A128	1.91195	-0.00049	-0.00001	-0.00401	-0.00403	1.90792
A129	1.91232	-0.00063	-0.00003	-0.00495	-0.00498	1.90734
A130	1.88515	-0.00035	-0.00001	-0.00079	-0.00082	1.88434
A131	3.16922	0.00007	0.00005	-0.01015	-0.01010	3.15913
A132	3.18255	0.00006	-0.00029	-0.00927	-0.00956	3.17299
A133	3.19462	-0.00181	0.00065	-0.01305	-0.01241	3.18222
A134	3.15743	0.00099	-0.00039	0.00827	0.00788	3.16531
A135	3.13951	0.00010	-0.00002	0.00162	0.00161	3.14112
A136	3.14170	-0.00001	0.00000	0.00003	0.00003	3.14173
A137	3.14067	0.00008	-0.00002	0.00068	0.00066	3.14133
A138	3.14339	-0.00008	-0.00001	-0.00210	-0.00212	3.14127
D1	-0.00212	0.00003	0.00000	0.00133	0.00133	-0.00079
D2	3.13679	0.00006	0.00005	0.00518	0.00524	-3.14116
D3	3.13979	0.00000	0.00000	0.00052	0.00052	3.14032
D4	-0.00449	0.00003	0.00006	0.00437	0.00443	-0.00005
D5	0.00106	-0.00001	-0.00002	-0.00150	-0.00151	-0.00045
D6	-3.13784	-0.00005	0.00001	-0.00223	-0.00222	-3.14006
D7	-3.14094	0.00002	-0.00002	-0.00046	-0.00048	-3.14142
D8	0.00334	-0.00002	0.00001	-0.00119	-0.00119	0.00215
D9	0.00981	0.00001	-0.00007	0.00477	0.00470	0.01452
D10	-3.12409	0.00002	-0.00012	0.00384	0.00371	-3.12038
D11	-3.13140	-0.00002	-0.00007	0.00381	0.00375	-3.12765
D12	0.01788	-0.00001	-0.00012	0.00288	0.00276	0.02064
D13	0.00148	-0.00002	0.00002	-0.00026	-0.00024	0.00124
D14	3.14142	0.00001	0.00001	0.00165	0.00166	-3.14010
D15	-3.13691	-0.00006	-0.00004	-0.00485	-0.00489	3.14138
D16	0.00302	-0.00003	-0.00006	-0.00293	-0.00299	0.00004
D17	-0.00252	-0.00006	-0.00002	-0.01171	-0.01173	-0.01426
D18	-3.14027	-0.00004	-0.00001	0.00318	0.00315	-3.13712
D19	3.13622	-0.00003	0.00004	-0.00763	-0.00759	3.12863
D20	-0.00153	-0.00001	0.00005	0.00726	0.00730	0.00577
D21	0.00016	0.00001	-0.00002	-0.00059	-0.00062	-0.00045
D22	3.14128	0.00001	-0.00002	-0.00011	-0.00013	3.14115
D23	-3.13973	-0.00003	-0.00001	-0.00256	-0.00257	3.14089
D24	0.00139	-0.00003	-0.00001	-0.00208	-0.00209	-0.00070
D25	-0.00116	0.00000	0.00000	0.00038	0.00039	-0.00077

D26	3.14034	0.00001	0.00001	0.00041	0.00042	3.14075
D27	3.14091	0.00000	0.00000	-0.00010	-0.00010	3.14081
D28	-0.00078	0.00000	0.00000	-0.00007	-0.00007	-0.00085
D29	0.00052	0.00000	0.00002	0.00069	0.00070	0.00122
D30	3.13951	0.00004	-0.00001	0.00140	0.00139	3.14089
D31	-3.14098	0.00000	0.00001	0.00066	0.00067	-3.14030
D32	-0.00199	0.00004	-0.00001	0.00137	0.00135	-0.00064
D33	-0.01123	-0.00004	0.00006	-0.01194	-0.01187	-0.02311
D34	3.11001	0.00008	0.00002	0.00004	0.00002	3.11002
D35	3.12236	-0.00009	0.00012	-0.01094	-0.01081	3.11155
D36	-0.03959	0.00004	0.00007	0.00104	0.00107	-0.03851
D37	-0.00922	-0.00001	0.00006	0.00087	0.00093	-0.00829
D38	3.12831	-0.00005	0.00009	-0.00007	0.00002	3.12833
D39	-3.14149	0.00002	0.00000	-0.00029	-0.00030	3.14140
D40	-0.00396	-0.00003	0.00003	-0.00123	-0.00120	-0.00516
D41	0.00860	0.00006	-0.00003	0.01446	0.01442	0.02301
D42	-3.11305	-0.00001	0.00001	0.00285	0.00282	-3.11023
D43	-3.13693	0.00003	-0.00004	-0.00080	-0.00085	-3.13778
D44	0.02461	-0.00004	0.00000	-0.01241	-0.01244	0.01217
D45	3.12998	0.00018	-0.00003	0.01546	0.01543	-3.13777
D46	-0.00655	0.00000	-0.00005	-0.00438	-0.00445	-0.01099
D47	-0.03534	0.00027	-0.00008	0.02932	0.02925	-0.00609
D48	3.11132	0.00009	-0.00010	0.00948	0.00937	3.12069
D49	-0.02621	0.00029	-0.00025	0.03677	0.03652	0.01031
D50	-3.13624	-0.00021	0.00008	0.00340	0.00350	-3.13275
D51	3.11052	0.00047	-0.00023	0.05583	0.05558	-3.11709
D52	0.00049	-0.00003	0.00010	0.02246	0.02256	0.02304
D53	-3.10458	-0.00021	0.00019	-0.01120	-0.01102	-3.11560
D54	0.00733	0.00028	-0.00012	0.02018	0.02004	0.02737
D55	3.11555	0.00015	-0.00021	0.00298	0.00280	3.11836
D56	-0.01109	0.00003	-0.00016	-0.00729	-0.00748	-0.01857
D57	0.00024	-0.00028	0.00007	-0.02474	-0.02470	-0.02445
D58	-3.12640	-0.00039	0.00012	-0.03502	-0.03498	3.12180
D59	0.01603	0.00010	-0.00014	-0.00136	-0.00146	0.01457
D60	-3.10564	0.00024	-0.00035	0.00214	0.00186	-3.10379
D61	-3.13059	0.00006	-0.00015	0.00642	0.00637	-3.12422
D62	0.03093	0.00021	-0.00036	0.00993	0.00968	0.04061
D63	-0.01298	-0.00022	0.00015	-0.01065	-0.01053	-0.02351
D64	3.13628	-0.00016	0.00017	-0.02254	-0.02250	3.11379
D65	0.00272	-0.00006	0.00007	-0.00059	-0.00051	0.00221
D66	-3.13172	0.00008	-0.00001	-0.00807	-0.00818	-3.13989
D67	3.13691	-0.00011	0.00005	0.01087	0.01103	-3.13525
D68	0.00248	0.00002	-0.00003	0.00338	0.00335	0.00583
D69	-0.01024	0.00012	0.00004	0.01707	0.01706	0.00682
D70	3.11559	0.00025	-0.00001	0.02797	0.02792	-3.13968
D71	3.10441	-0.00008	0.00032	0.01217	0.01243	3.11683
D72	-0.05295	0.00005	0.00027	0.02308	0.02329	-0.02966
D73	-0.05210	-0.00029	0.00050	-0.01557	-0.01528	-0.06739
D74	-2.72222	-0.00135	-0.00252	-0.15598	-0.15820	-2.88042
D75	3.11577	-0.00008	0.00022	-0.01080	-0.01076	3.10501
D76	0.44566	-0.00114	-0.00279	-0.15121	-0.15368	0.29199
D77	-0.03575	-0.00012	0.00025	-0.00905	-0.00895	-0.04470
D78	-3.14033	-0.00012	0.00008	-0.01601	-0.01603	3.12682
D79	3.10087	-0.00021	0.00031	-0.00383	-0.00362	3.09725
D80	-0.00372	-0.00021	0.00013	-0.01079	-0.01069	-0.01441
D81	-3.13826	-0.00003	0.00000	0.01257	0.01269	-3.12557
D82	0.01076	0.00011	-0.00008	0.00480	0.00473	0.01549
D83	0.05388	0.00024	-0.00046	0.01516	0.01493	0.06880
D84	2.71886	0.00152	0.00256	0.15741	0.15960	2.87847
D85	-3.13753	0.00024	-0.00023	0.02440	0.02437	-3.11316

D86	-0.47255	0.00152	0.00278	0.16665	0.16905	-0.30350
D87	-3.13993	0.00010	-0.00010	0.00755	0.00747	-3.13246
D88	-0.00800	0.00021	-0.00012	0.01233	0.01225	0.00425
D89	0.05233	0.00008	-0.00032	-0.00177	-0.00209	0.05025
D90	-3.09892	0.00020	-0.00035	0.00302	0.00269	-3.09623
D91	1.28690	0.00065	0.00177	0.08696	0.08958	1.37648
D92	-2.87920	0.00048	0.00180	0.08528	0.08792	-2.79129
D93	-0.82401	0.00078	0.00178	0.08875	0.09138	-0.73263
D94	-1.29741	-0.00055	-0.00161	-0.07342	-0.07587	-1.37328
D95	0.81967	-0.00072	-0.00158	-0.07510	-0.07753	0.74214
D96	2.87487	-0.00042	-0.00160	-0.07163	-0.07407	2.80080
D97	-0.01552	0.00000	0.00001	0.00225	0.00226	-0.01326
D98	3.14103	0.00004	-0.00003	-0.00503	-0.00509	3.13595
D99	-3.13962	0.00006	-0.00003	0.00087	0.00085	-3.13877
D100	0.01178	-0.00006	-0.00001	-0.00398	-0.00399	0.00779
D101	-0.01820	0.00017	-0.00007	0.00649	0.00642	-0.01178
D102	3.13299	0.00015	0.00011	0.00159	0.00164	3.13463
D103	0.01637	-0.00012	0.00006	-0.00867	-0.00864	0.00772
D104	-3.13267	-0.00004	0.00004	-0.00501	-0.00498	-3.13765
D105	-3.13659	-0.00015	0.00009	-0.00316	-0.00308	-3.13967
D106	-0.00245	-0.00006	0.00008	0.00050	0.00059	-0.00185
D107	3.11530	0.00016	-0.00008	0.01166	0.01158	3.12688
D108	-0.06087	0.00022	0.00016	0.02813	0.02828	-0.03260
D109	-0.01156	0.00020	-0.00013	0.00447	0.00433	-0.00723
D110	3.09545	0.00025	0.00012	0.02094	0.02103	3.11649
D111	0.02067	-0.00025	0.00012	-0.00756	-0.00742	0.01325
D112	-3.12733	-0.00023	0.00001	-0.00428	-0.00423	-3.13156
D113	-3.09574	-0.00029	-0.00005	-0.01956	-0.01959	-3.11533
D114	0.03945	-0.00027	-0.00017	-0.01629	-0.01640	0.02305
D115	3.11820	0.00021	0.00007	0.00039	0.00042	3.11862
D116	0.32954	-0.00062	-0.00192	-0.09164	-0.09344	0.23610
D117	-0.05735	0.00026	0.00031	0.01657	0.01682	-0.04053
D118	-2.84601	-0.00057	-0.00168	-0.07546	-0.07703	-2.92305
D119	3.12704	0.00019	-0.00021	0.01383	0.01365	3.14069
D120	-0.00627	0.00009	-0.00016	0.00207	0.00190	-0.00437
D121	-0.00530	0.00017	-0.00004	0.00910	0.00904	0.00374
D122	-3.13861	0.00007	0.00001	-0.00266	-0.00271	-3.14132
D123	3.12866	0.00000	0.00010	-0.00031	-0.00025	3.12841
D124	-0.03024	-0.00002	0.00024	0.00095	0.00113	-0.02911
D125	-0.01853	0.00007	0.00007	0.00765	0.00769	-0.01084
D126	3.10576	0.00005	0.00021	0.00890	0.00907	3.11483
D127	-3.13473	0.00012	-0.00023	0.00559	0.00545	-3.12928
D128	0.01546	0.00001	-0.00017	-0.00661	-0.00675	0.00871
D129	0.01128	-0.00014	0.00012	-0.00440	-0.00426	0.00702
D130	-3.12847	0.00001	0.00000	-0.00226	-0.00226	-3.13074
D131	-3.10675	-0.00013	-0.00007	-0.00611	-0.00615	-3.11290
D132	0.03668	0.00002	-0.00019	-0.00397	-0.00416	0.03253
D133	0.05391	-0.00016	-0.00034	-0.01070	-0.01099	0.04292
D134	2.84531	0.00066	0.00165	0.08070	0.08220	2.92751
D135	-3.11068	-0.00017	-0.00016	-0.00900	-0.00912	-3.11980
D136	-0.31927	0.00065	0.00183	0.08239	0.08407	-0.23520
D137	0.00060	0.00016	-0.00024	-0.00064	-0.00090	-0.00029
D138	-3.13215	0.00010	-0.00010	-0.00611	-0.00625	-3.13840
D139	3.14045	0.00001	-0.00013	-0.00268	-0.00281	3.13764
D140	0.00769	-0.00004	0.00001	-0.00815	-0.00816	-0.00046
D141	-0.00925	-0.00010	0.00024	0.00415	0.00438	-0.00487
D142	3.12236	0.00003	0.00008	0.01039	0.01045	3.13281
D143	-3.12543	-0.00032	0.00032	-0.05864	-0.05832	3.09943
D144	0.01267	-0.00028	0.00031	-0.05338	-0.05309	-0.04041
D145	0.02678	-0.00043	0.00049	-0.06528	-0.06478	-0.03800

D146	-3.11830	-0.00040	0.00048	-0.06003	-0.05954	3.10534
D147	-0.76015	0.00051	0.00110	0.05010	0.05148	-0.70867
D148	1.35624	0.00040	0.00111	0.04910	0.05050	1.40674
D149	-2.81829	0.00037	0.00109	0.04820	0.04957	-2.76872
D150	2.79761	-0.00042	-0.00120	-0.05619	-0.05768	2.73993
D151	-1.36919	-0.00052	-0.00118	-0.05719	-0.05866	-1.42785
D152	0.73947	-0.00056	-0.00121	-0.05809	-0.05958	0.67988
D153	0.00884	-0.00022	0.00018	-0.00853	-0.00834	0.00051
D154	-3.13751	-0.00018	0.00011	-0.00483	-0.00472	3.14095
D155	-3.12912	-0.00026	0.00019	-0.01399	-0.01379	3.14027
D156	0.00771	-0.00022	0.00012	-0.01028	-0.01018	-0.00247
D157	3.13587	0.00012	-0.00007	0.01316	0.01305	-3.13427
D158	0.00616	-0.00031	0.00020	-0.04510	-0.04485	-0.03869
D159	-0.00170	0.00007	-0.00001	0.01002	0.00999	0.00830
D160	-3.13140	-0.00036	0.00026	-0.04825	-0.04791	3.10388
D161	-3.13619	-0.00005	0.00005	-0.01034	-0.01027	3.13673
D162	0.00693	-0.00003	0.00005	-0.00730	-0.00725	-0.00033
D163	0.00136	-0.00003	-0.00001	-0.00722	-0.00721	-0.00585
D164	-3.13871	-0.00002	-0.00001	-0.00418	-0.00419	3.14028
D165	0.00142	-0.00009	0.00003	-0.00925	-0.00922	-0.00780
D166	-3.14027	-0.00010	0.00002	-0.00904	-0.00903	3.13388
D167	3.13145	0.00030	-0.00024	0.04738	0.04721	-3.10452
D168	-0.01024	0.00029	-0.00024	0.04759	0.04740	0.03716
D169	-0.00049	-0.00002	0.00002	0.00153	0.00154	0.00105
D170	3.14100	0.00002	0.00002	0.00541	0.00543	-3.13675
D171	3.13965	-0.00004	0.00002	-0.00138	-0.00137	3.13828
D172	-0.00204	0.00001	0.00002	0.00250	0.00252	0.00048
D173	0.00238	-0.00004	0.00001	-0.00268	-0.00267	-0.00029
D174	-3.14156	0.00003	-0.00002	-0.00106	-0.00108	3.14055
D175	-3.13745	-0.00002	0.00001	0.00085	0.00086	-3.13659
D176	0.00179	0.00005	-0.00002	0.00247	0.00245	0.00424
D177	-0.00059	0.00007	-0.00003	0.00484	0.00481	0.00422
D178	3.14109	0.00003	-0.00003	0.00156	0.00153	-3.14056
D179	3.14110	0.00008	-0.00003	0.00464	0.00463	-3.13746
D180	-0.00041	0.00004	-0.00002	0.00137	0.00135	0.00094
D181	-3.14106	-0.00003	0.00002	-0.00128	-0.00126	3.14087
D182	0.00050	-0.00001	0.00001	-0.00123	-0.00121	-0.00071
D183	0.00042	-0.00003	0.00001	-0.00105	-0.00104	-0.00062
D184	-3.14121	-0.00002	0.00001	-0.00100	-0.00100	3.14098
D185	-3.14135	-0.00007	0.00002	-0.00506	-0.00505	3.13679
D186	0.00008	-0.00005	0.00002	-0.00460	-0.00459	-0.00451
D187	0.00014	-0.00002	0.00001	-0.00086	-0.00085	-0.00071
D188	3.14156	0.00000	0.00001	-0.00040	-0.00039	3.14118
D189	-0.00018	0.00001	0.00000	0.00026	0.00026	0.00009
D190	3.14131	0.00001	0.00000	0.00026	0.00026	3.14158
D191	3.14146	-0.00001	0.00001	0.00021	0.00022	-3.14151
D192	-0.00024	-0.00001	0.00000	0.00021	0.00021	-0.00003
D193	0.00010	0.00000	0.00000	0.00012	0.00012	0.00021
D194	3.14158	0.00001	0.00000	0.00017	0.00017	-3.14144
D195	-3.14133	-0.00002	0.00000	-0.00033	-0.00033	3.14152
D196	0.00015	-0.00001	0.00000	-0.00028	-0.00028	-0.00013
D197	-0.00008	0.00001	-0.00001	0.00019	0.00018	0.00010
D198	-3.14156	0.00000	-0.00001	0.00014	0.00013	-3.14143
D199	-3.14157	0.00001	-0.00001	0.00019	0.00019	-3.14138
D200	0.00014	0.00000	0.00000	0.00014	0.00013	0.00027

Item	Value	Threshold	Converged?
Maximum Force	0.009774	0.000450	NO
RMS Force	0.001227	0.000300	NO
Maximum Displacement	0.313960	0.001800	NO
RMS Displacement	0.066843	0.001200	NO

Predicted change in Energy=-1.849370D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.790956	-0.636062	0.019587
2	6	0	-9.982588	-1.787361	-0.001009
3	6	0	-10.504481	-3.071833	-0.016482
4	6	0	-11.893388	-3.214886	-0.012721
5	6	0	-12.714186	-2.080535	0.006774
6	6	0	-12.181873	-0.786927	0.023809
7	1	0	-9.833108	-3.924538	-0.030715
8	1	0	-12.340360	-4.204148	-0.024866
9	1	0	-13.793215	-2.201135	0.008769
10	1	0	-12.853226	0.060637	0.037921
11	6	0	-9.912948	0.564032	0.033784
12	6	0	-8.558911	-1.392512	-0.001209
13	6	0	-8.527404	0.086935	0.000480
14	6	0	-7.389864	0.865704	-0.034311
15	6	0	-5.999488	0.586135	-0.072880
16	6	0	-3.633258	-0.186312	-0.095492
17	6	0	-3.767910	1.223651	-0.098993
18	16	0	-5.164496	-0.998815	-0.105819
19	6	0	-5.087141	1.656246	-0.091337
20	6	0	-2.256333	-0.450622	-0.080689
21	6	0	-1.596668	0.797592	-0.072651
22	7	0	-2.515502	1.822366	-0.139729
23	16	0	-1.143706	-1.806793	-0.068938
24	16	0	1.150437	1.808875	-0.001763
25	6	0	0.202072	-0.671710	-0.026004
26	6	0	-0.195787	0.674735	-0.038345
27	6	0	1.603013	-0.794928	0.010822
28	6	0	2.264162	0.453384	0.016920
29	6	0	3.637941	0.188534	0.040847
30	6	0	3.772130	-1.223154	0.043548
31	6	0	5.089400	-1.656710	0.049789
32	6	0	6.001842	-0.588076	0.061173
33	16	0	5.172438	0.997107	0.063522
34	7	0	2.520152	-1.818719	0.059882
35	6	0	7.382771	-0.865177	0.064702
36	6	0	8.519788	-0.087892	0.033301
37	6	0	8.551651	1.390883	-0.016682
38	6	0	9.907738	-0.565875	0.044413
39	6	0	9.975438	1.784834	-0.046850
40	6	0	10.784793	0.634346	-0.007545
41	6	0	10.496237	3.066783	-0.104518
42	6	0	12.175514	0.786070	-0.026177
43	6	0	11.885388	3.210627	-0.123201
44	6	0	12.706577	2.079054	-0.084160
45	6	0	10.357136	-1.873266	0.088309
46	6	0	9.493253	-3.011792	0.131943

47	6	0	11.738157	-2.243495	0.094442
48	7	0	8.805394	-3.952156	0.167622
49	7	0	12.853363	-2.580307	0.100726
50	6	0	-10.358208	1.872754	0.079222
51	6	0	-11.736074	2.247748	0.109122
52	6	0	-9.491143	3.008157	0.107623
53	7	0	-12.846538	2.598993	0.134452
54	7	0	-8.805992	3.950897	0.131348
55	8	0	-7.603740	-2.160800	-0.021185
56	8	0	7.596684	2.157852	-0.075770
57	6	0	2.249905	-3.225397	-0.183808
58	1	0	1.297388	-3.498553	0.275569
59	1	0	2.212685	-3.452177	-1.255221
60	1	0	3.034493	-3.825196	0.282198
61	6	0	-2.250982	3.220400	0.152322
62	1	0	-2.228717	3.410205	1.231169
63	1	0	-1.293290	3.509850	-0.285181
64	1	0	-3.029663	3.833822	-0.305750
65	1	0	5.419190	-2.689133	0.043219
66	1	0	12.847886	-0.060928	0.002452
67	1	0	13.785466	2.200162	-0.098902
68	1	0	12.331582	4.199296	-0.168100
69	1	0	9.823823	3.918231	-0.133467
70	1	0	7.543640	-1.935964	0.098765
71	1	0	-7.552799	1.936422	-0.047578
72	1	0	-5.418129	2.688746	-0.093997

Rotational constants (GHZ): 0.1749265 0.0104492 0.0098634

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6578.1854985333 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T

Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6578.1003930632 Hartrees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.23D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Initial guess from the checkpoint file: "PBDB.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000112 -0.000019 -0.000052 Ang= 0.01 deg.

ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1

AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-yADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 IlCent= 200000004 NGrid=

0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Integral accuracy reduced to 1.0D-05 until final iterations.

Initial convergence to 1.0D-05 achieved. Increase integral accuracy.

SCF Done: E(RB3LYP) = -3683.01887371 A.U. after 13 cycles

NFock= 13 Conv=0.74D-08 -V/T= 2.0068

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1

NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	0.000058173	-0.000013741	-0.000104505
2	6	0.000343887	0.000154251	-0.000928252
3	6	0.000122929	0.000545129	0.000087873
4	6	-0.000074957	-0.000037682	-0.000006396
5	6	-0.000117854	-0.000021366	-0.000116501
6	6	-0.000621187	-0.000238669	-0.000372443
7	1	-0.000098543	-0.000011981	-0.000086737
8	1	-0.000060991	-0.000004503	-0.000029517
9	1	0.000101779	0.000055406	0.000071255
10	1	0.000087884	-0.000475468	-0.000013820
11	6	0.000578384	0.000052413	0.000604873
12	6	-0.001381625	-0.000884359	0.001646668
13	6	0.000989898	-0.000106005	-0.000193605
14	6	0.000406247	0.000125195	0.002120809
15	6	-0.001976280	0.001476737	-0.000496961
16	6	0.000571470	0.000514238	0.000933562
17	6	-0.001694182	-0.000589081	0.002385292
18	16	-0.000111041	0.000151679	-0.002562551
19	6	-0.001424645	-0.000193108	-0.001677719
20	6	0.000404103	0.001679882	0.000350344
21	6	-0.002622191	-0.000267129	0.001566068
22	7	0.003188380	0.001397232	-0.004070555
23	16	-0.000026924	-0.000368334	-0.000426021
24	16	0.000087281	-0.000014387	-0.000079829
25	6	-0.000912871	0.001456473	-0.000268665
26	6	0.001147537	-0.001411860	0.000461925
27	6	0.000281992	0.000200182	-0.000279644
28	6	-0.001331497	-0.000625623	-0.001656104
29	6	0.001320515	-0.001149344	0.000084629
30	6	-0.000038518	0.000038425	-0.001477780
31	6	0.002019065	0.001324187	0.000994127
32	6	-0.003270169	0.000171515	-0.001577173
33	16	-0.000910137	0.000280901	0.000797698
34	7	-0.001348033	0.000455013	0.002956183
35	6	0.003793432	-0.001338035	0.002713780
36	6	0.002754285	-0.001849970	-0.001222942
37	6	-0.002784804	0.000390133	0.004767726
38	6	-0.001613113	-0.000271690	-0.001177542
39	6	0.001407688	0.001144279	-0.000607434
40	6	0.000053610	0.000114446	-0.000120966
41	6	-0.000348821	-0.001719821	-0.000432612
42	6	0.000805229	0.000609035	0.000721273

43	6	-0.000837039	-0.000340707	-0.000529148
44	6	0.000864636	0.000248824	0.000611622
45	6	0.001613441	0.001577105	0.001332207
46	6	0.000026287	-0.000372171	-0.000124702
47	6	-0.001297955	-0.001070455	-0.000994000
48	7	0.000378730	-0.000060410	0.000324125
49	7	0.000088592	0.000040983	0.000051181
50	6	-0.000792983	-0.000862123	-0.000779714
51	6	0.000325136	0.001036928	0.000447090
52	6	-0.000349855	-0.000360005	-0.000315712
53	7	-0.000074219	0.000413829	0.000010709
54	7	-0.000220216	0.000074878	-0.000204999
55	8	0.000772452	-0.000123674	0.000083136
56	8	0.001261335	0.000151987	-0.002326573
57	6	0.000887397	0.000705080	-0.000857837
58	1	0.000102688	-0.000043351	0.000151969
59	1	-0.000003261	-0.000139885	-0.000219647
60	1	-0.000127445	0.000053713	0.000013410
61	6	-0.001014003	-0.001231528	0.000673862
62	1	-0.000150041	-0.000247318	-0.000026611
63	1	0.000022066	-0.000017877	-0.000040247
64	1	0.000162835	-0.000020223	-0.000186842
65	1	0.000142210	-0.000083713	-0.000113164
66	1	-0.000444293	0.000261943	-0.000240698
67	1	-0.000073825	-0.000030063	-0.000072774
68	1	-0.000030927	0.000008510	-0.000022026
69	1	0.000092826	-0.000111903	0.000035849
70	1	-0.000180863	-0.000899813	0.000602335
71	1	0.000594301	0.000400036	-0.000267464
72	1	0.000506610	0.000296809	-0.000293151

Cartesian Forces: Max 0.004767726 RMS 0.001065404

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.007303019 RMS 0.000964264

Search for a local minimum.

Step number 15 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 14 15

DE= -1.11D-03 DEPred=-1.85D-03 R= 6.01D-01

TightC=F SS= 1.41D+00 RLast= 4.88D-01 DXNew= 3.3118D+00 1.4650D+00

Trust test= 6.01D-01 RLast= 4.88D-01 DXMaxT set to 1.97D+00

ITU= 1 1 1 1 1 1 0 0 0 1 0 0 0 1 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00222	0.00231	0.00231	0.00241	0.00249
Eigenvalues ---	0.00287	0.00389	0.00432	0.00445	0.00456
Eigenvalues ---	0.00480	0.00506	0.00553	0.00579	0.00611
Eigenvalues ---	0.00621	0.00639	0.00678	0.00682	0.00685
Eigenvalues ---	0.00712	0.00725	0.00744	0.00755	0.00760
Eigenvalues ---	0.00773	0.00794	0.00820	0.00843	0.00846
Eigenvalues ---	0.00869	0.00898	0.01048	0.01087	0.01134
Eigenvalues ---	0.01152	0.01188	0.01251	0.01292	0.01339
Eigenvalues ---	0.01361	0.01365	0.01395	0.01444	0.01458
Eigenvalues ---	0.01500	0.01624	0.01647	0.01654	0.01754
Eigenvalues ---	0.01794	0.01802	0.01872	0.01929	0.01954

Eigenvalues	---	0.02006	0.02024	0.02075	0.02076	0.02209
Eigenvalues	---	0.02211	0.04828	0.04837	0.04901	0.04924
Eigenvalues	---	0.04980	0.05013	0.05023	0.05296	0.07056
Eigenvalues	---	0.07224	0.07404	0.07581	0.15586	0.15841
Eigenvalues	---	0.15957	0.15987	0.15999	0.16000	0.16000
Eigenvalues	---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues	---	0.16001	0.16001	0.16002	0.16019	0.16030
Eigenvalues	---	0.16050	0.17491	0.18788	0.19186	0.19795
Eigenvalues	---	0.20421	0.20780	0.21367	0.21509	0.22000
Eigenvalues	---	0.22007	0.22133	0.22267	0.22535	0.22582
Eigenvalues	---	0.22609	0.22637	0.22685	0.22696	0.22958
Eigenvalues	---	0.23039	0.23345	0.23436	0.23503	0.23617
Eigenvalues	---	0.23745	0.23945	0.24140	0.24215	0.24285
Eigenvalues	---	0.24355	0.24513	0.24602	0.24636	0.24701
Eigenvalues	---	0.24768	0.24858	0.24912	0.24960	0.24970
Eigenvalues	---	0.24986	0.24991	0.24992	0.24993	0.24996
Eigenvalues	---	0.24997	0.24998	0.24998	0.25000	0.25000
Eigenvalues	---	0.25000	0.25009	0.25170	0.25589	0.25923
Eigenvalues	---	0.26226	0.26481	0.26718	0.26803	0.27049
Eigenvalues	---	0.27225	0.27682	0.27831	0.28210	0.28264
Eigenvalues	---	0.28518	0.28676	0.29920	0.30152	0.31759
Eigenvalues	---	0.32151	0.32690	0.35483	0.36048	0.36243
Eigenvalues	---	0.36338	0.36344	0.36475	0.36652	0.36667
Eigenvalues	---	0.36771	0.36828	0.37085	0.37091	0.37112
Eigenvalues	---	0.37254	0.37272	0.37421	0.37567	0.37673
Eigenvalues	---	0.37757	0.37980	0.38930	0.40302	0.40704
Eigenvalues	---	0.41647	0.42133	0.42631	0.44133	0.44425
Eigenvalues	---	0.44793	0.45596	0.46512	0.47652	0.47874
Eigenvalues	---	0.48380	0.50704	0.52902	0.54446	0.56456
Eigenvalues	---	0.57445	0.67972	0.72392	0.80311	0.81887
Eigenvalues	---	0.91093	1.25842	1.26308	1.29341	1.35383

RFO step: Lambda=-2.67102093D-03 EMin= 2.21789886D-03

Quartic linear search produced a step of -0.20324.

Iteration 1 RMS(Cart)= 0.12848521 RMS(Int)= 0.00334941

Iteration 2 RMS(Cart)= 0.00788772 RMS(Int)= 0.00058415

Iteration 3 RMS(Cart)= 0.00002101 RMS(Int)= 0.00058400

Iteration 4 RMS(Cart)= 0.00000006 RMS(Int)= 0.00058400

Variable	Old X	-DE/DX	Delta X	Delta X	Delta X	New X
(Linear)	(Quad)	(Total)				
R1	2.65866	-0.00049	0.00009	-0.00088	-0.00077	2.65789
R2	2.64388	-0.00020	-0.00012	0.00089	0.00076	2.64465
R3	2.81012	-0.00108	0.00010	-0.00299	-0.00296	2.80717
R4	2.62017	0.00053	-0.00002	0.00164	0.00162	2.62179
R5	2.79191	0.00083	-0.00018	0.00503	0.00493	2.79684
R6	2.63855	0.00032	0.00011	-0.00024	-0.00012	2.63842
R7	2.05107	-0.00013	0.00000	-0.00046	-0.00046	2.05061
R8	2.64618	0.00017	-0.00003	0.00021	0.00019	2.64637
R9	2.05153	-0.00002	-0.00002	0.00000	-0.00002	2.05150
R10	2.64364	-0.00006	0.00006	-0.00048	-0.00043	2.64321
R11	2.05177	-0.00005	0.00000	-0.00020	-0.00020	2.05157
R12	2.04342	0.00006	0.00007	-0.00151	-0.00144	2.04198
R13	2.76989	0.00122	-0.00011	0.00197	0.00180	2.77169
R14	2.61375	0.00098	0.00030	-0.00004	0.00026	2.61401
R15	2.79639	0.00031	-0.00035	0.00396	0.00364	2.80002
R16	2.31676	0.00065	0.00032	-0.00119	-0.00087	2.31589
R17	2.60596	-0.00061	-0.00362	0.02194	0.01832	2.62428
R18	2.68101	-0.00144	-0.00190	0.00663	0.00473	2.68574
R19	2.04681	-0.00046	-0.00012	0.00091	0.00079	2.04760
R20	3.38591	-0.00059	0.00074	-0.00717	-0.00650	3.37941
R21	2.65764	0.00101	-0.00007	0.00285	0.00278	2.66042

R22	2.67658	0.00116	-0.00081	0.00476	0.00386	2.68044
R23	3.27581	0.00084	-0.00037	0.00832	0.00793	3.28373
R24	2.64966	0.00158	0.00094	0.00331	0.00379	2.65345
R25	2.62364	0.00292	0.00173	-0.00135	0.00045	2.62409
R26	2.62437	0.00150	0.00180	-0.00346	-0.00130	2.62307
R27	2.04895	-0.00032	-0.00006	-0.00081	-0.00086	2.04809
R28	2.66797	0.00135	-0.00105	0.00713	0.00603	2.67400
R29	3.31499	0.00055	-0.00031	0.00372	0.00340	3.31839
R30	2.60407	0.00157	0.00237	-0.00662	-0.00387	2.60020
R31	2.65823	0.00369	0.00169	0.00390	0.00565	2.66388
R32	2.74483	0.00125	0.00223	-0.00614	-0.00391	2.74092
R33	3.32794	0.00063	-0.00001	0.00243	0.00234	3.33028
R34	3.32717	0.00078	0.00002	0.00244	0.00244	3.32961
R35	3.31543	0.00069	-0.00014	0.00307	0.00292	3.31835
R36	2.65327	0.00093	0.00058	-0.00110	-0.00054	2.65273
R37	2.65853	0.00349	0.00087	0.00958	0.01046	2.66899
R38	2.66943	0.00135	-0.00008	0.00234	0.00223	2.67165
R39	2.59911	0.00255	0.00210	-0.00293	-0.00071	2.59841
R40	2.64426	0.00339	0.00273	-0.00368	-0.00111	2.64315
R41	2.67973	0.00073	-0.00006	0.00090	0.00081	2.68054
R42	3.27800	0.00070	0.00029	0.00056	0.00082	3.27883
R43	2.62067	0.00400	0.00158	0.00430	0.00591	2.62658
R44	2.62013	0.00242	0.00202	-0.00402	-0.00187	2.61825
R45	2.65549	0.00278	0.00074	0.00131	0.00207	2.65756
R46	2.04816	-0.00003	-0.00002	0.00001	-0.00002	2.04814
R47	3.38083	0.00096	0.00098	-0.00226	-0.00130	3.37952
R48	2.66161	0.00730	0.00602	-0.00605	-0.00003	2.66157
R49	2.74574	0.00023	0.00111	-0.00490	-0.00380	2.74194
R50	2.60341	0.00178	0.00054	-0.00011	0.00043	2.60385
R51	2.04721	-0.00044	0.00007	-0.00004	0.00003	2.04725
R52	2.79672	0.00006	0.00006	-0.00019	0.00071	2.79743
R53	2.77410	-0.00035	-0.00226	0.00738	0.00470	2.77880
R54	2.79224	0.00066	-0.00014	0.00376	0.00453	2.79678
R55	2.31728	0.00031	0.00017	-0.00083	-0.00066	2.31662
R56	2.81084	-0.00101	-0.00112	0.00464	0.00242	2.81326
R57	2.61381	0.00089	-0.00134	0.00999	0.00865	2.62246
R58	2.65923	-0.00063	-0.00004	0.00044	0.00024	2.65947
R59	2.61708	0.00179	0.00071	0.00212	0.00295	2.62003
R60	2.64391	-0.00025	-0.00115	0.00805	0.00689	2.65080
R61	2.63939	0.00009	0.00026	-0.00209	-0.00182	2.63757
R62	2.05098	-0.00006	0.00001	-0.00039	-0.00038	2.05060
R63	2.64372	0.00022	0.00018	-0.00070	-0.00063	2.64310
R64	2.04432	-0.00042	0.00030	-0.00454	-0.00424	2.04008
R65	2.64314	0.00126	0.00054	0.00147	0.00191	2.64505
R66	2.05152	0.00000	0.00000	-0.00008	-0.00008	2.05144
R67	2.05180	-0.00005	-0.00002	-0.00011	-0.00013	2.05167
R68	2.70200	-0.00044	-0.00080	0.00245	0.00165	2.70365
R69	2.70193	-0.00104	-0.00177	0.00859	0.00682	2.70875
R70	2.20273	-0.00005	-0.00002	-0.00015	-0.00017	2.20257
R71	2.20148	0.00008	-0.00011	0.00072	0.00060	2.20209
R72	2.69909	0.00009	-0.00050	0.00419	0.00369	2.70277
R73	2.70023	0.00028	-0.00006	0.00041	0.00035	2.70058
R74	2.20147	0.00019	-0.00007	0.00057	0.00050	2.20197
R75	2.20277	-0.00007	-0.00006	0.00009	0.00003	2.20280
R76	2.06398	-0.00015	-0.00012	0.00010	-0.00001	2.06397
R77	2.07073	-0.00019	-0.00009	-0.00017	-0.00027	2.07046
R78	2.06361	-0.00012	-0.00010	0.00014	0.00004	2.06365
R79	2.07046	-0.00005	-0.00026	0.00100	0.00074	2.07120
R80	2.06349	-0.00001	-0.00023	0.00108	0.00086	2.06435
R81	2.06358	-0.00011	-0.00017	0.00051	0.00033	2.06391

A1	2.07490	0.00086	-0.00021	0.00376	0.00359	2.07849
A2	1.89790	0.00081	0.00013	0.00129	0.00132	1.89922
A3	2.31038	-0.00166	0.00007	-0.00505	-0.00491	2.30547
A4	2.14359	-0.00053	0.00016	-0.00280	-0.00267	2.14092
A5	1.91237	-0.00037	-0.00010	-0.00114	-0.00122	1.91115
A6	2.22722	0.00091	-0.00006	0.00394	0.00389	2.23111
A7	2.05930	-0.00012	0.00001	-0.00046	-0.00044	2.05885
A8	2.08877	0.00008	-0.00004	0.00093	0.00088	2.08965
A9	2.13512	0.00004	0.00003	-0.00047	-0.00044	2.13468
A10	2.09453	0.00022	-0.00018	0.00229	0.00211	2.09664
A11	2.09773	-0.00005	0.00010	-0.00094	-0.00084	2.09688
A12	2.09093	-0.00018	0.00008	-0.00134	-0.00127	2.08966
A13	2.12493	-0.00016	0.00012	-0.00100	-0.00088	2.12405
A14	2.08584	-0.00005	-0.00003	-0.00056	-0.00059	2.08525
A15	2.07241	0.00021	-0.00009	0.00156	0.00148	2.07389
A16	2.06913	-0.00027	0.00010	-0.00179	-0.00171	2.06742
A17	2.13265	-0.00036	-0.00001	-0.00178	-0.00178	2.13086
A18	2.08141	0.00062	-0.00008	0.00357	0.00349	2.08490
A19	1.87048	-0.00009	-0.00032	0.00301	0.00249	1.87297
A20	2.18199	-0.00518	-0.00037	-0.01157	-0.01185	2.17014
A21	2.23069	0.00527	0.00068	0.00850	0.00926	2.23995
A22	1.86263	0.00005	0.00001	0.00058	0.00015	1.86278
A23	2.19357	0.00020	0.00012	0.00100	0.00063	2.19420
A24	2.22681	-0.00024	-0.00009	-0.00064	-0.00122	2.22559
A25	1.88107	-0.00039	0.00032	-0.00279	-0.00256	1.87851
A26	2.20993	0.00187	0.00079	-0.00242	-0.00158	2.20836
A27	2.19215	-0.00148	-0.00115	0.00522	0.00413	2.19628
A28	2.34313	-0.00110	-0.00077	-0.00014	-0.00096	2.34217
A29	2.02026	0.00050	-0.00016	0.00126	0.00105	2.02130
A30	1.91972	0.00060	0.00094	-0.00092	-0.00003	1.91969
A31	2.25431	-0.00129	0.00041	-0.00804	-0.00759	2.24671
A32	2.07851	0.00168	-0.00017	0.00754	0.00740	2.08590
A33	1.95037	-0.00039	-0.00031	0.00049	0.00016	1.95053
A34	1.96340	-0.00102	-0.00015	-0.00190	-0.00192	1.96148
A35	1.85567	0.00034	0.00032	-0.00079	-0.00063	1.85504
A36	2.46411	0.00067	-0.00018	0.00270	0.00255	2.46666
A37	1.98285	0.00005	0.00039	-0.00241	-0.00219	1.98066
A38	1.92144	-0.00043	0.00042	-0.00162	-0.00062	1.92082
A39	2.37856	0.00039	-0.00079	0.00411	0.00290	2.38146
A40	1.56772	0.00148	0.00050	0.00122	0.00158	1.56930
A41	1.95995	-0.00010	-0.00036	0.00318	0.00282	1.96277
A42	2.12537	-0.00003	-0.00049	0.00182	0.00116	2.12653
A43	2.19785	0.00013	0.00082	-0.00487	-0.00421	2.19364
A44	1.86737	0.00001	0.00013	-0.00077	-0.00082	1.86654
A45	2.44753	0.00081	-0.00036	0.00401	0.00360	2.45113
A46	1.96829	-0.00082	0.00023	-0.00324	-0.00284	1.96545
A47	1.92373	-0.00034	0.00048	-0.00166	-0.00066	1.92307
A48	1.96952	-0.00008	-0.00010	0.00025	-0.00008	1.96943
A49	2.38937	0.00042	-0.00044	0.00227	0.00127	2.39064
A50	1.85385	0.00048	-0.00113	0.00686	0.00450	1.85835
A51	2.18130	0.00014	-0.00538	0.02461	0.01636	2.19767
A52	2.19513	-0.00032	-0.00517	0.02172	0.01363	2.20876
A53	1.55736	0.00158	0.00049	0.00196	0.00239	1.55975
A54	1.55872	0.00131	0.00044	0.00173	0.00217	1.56089
A55	1.98378	-0.00076	-0.00049	0.00019	-0.00035	1.98343
A56	2.35346	0.00073	0.00048	0.00010	0.00056	2.35402
A57	1.94593	0.00004	0.00000	-0.00025	-0.00020	1.94574
A58	2.35422	0.00050	0.00049	-0.00106	-0.00064	2.35358
A59	1.94568	0.00008	-0.00013	0.00081	0.00079	1.94647
A60	1.98327	-0.00058	-0.00037	0.00027	-0.00014	1.98314

A61	1.97012	-0.00013	-0.00004	-0.00058	-0.00069	1.96942
A62	2.38935	0.00075	-0.00004	0.00202	0.00182	2.39117
A63	1.92361	-0.00062	0.00003	-0.00134	-0.00108	1.92253
A64	1.96665	-0.00063	-0.00005	-0.00108	-0.00110	1.96555
A65	2.44909	0.00058	-0.00002	0.00185	0.00181	2.45090
A66	1.86745	0.00006	0.00006	-0.00074	-0.00071	1.86673
A67	1.85601	0.00035	-0.00005	0.00140	0.00130	1.85731
A68	2.46625	0.00032	-0.00001	0.00063	0.00059	2.46684
A69	1.96092	-0.00067	0.00005	-0.00207	-0.00206	1.95886
A70	1.98354	0.00001	-0.00029	0.00162	0.00124	1.98477
A71	1.92004	-0.00046	0.00016	-0.00175	-0.00136	1.91868
A72	2.37945	0.00045	0.00013	0.00008	0.00006	2.37951
A73	1.95957	0.00024	0.00049	-0.00215	-0.00169	1.95789
A74	2.19789	-0.00001	0.00019	-0.00077	-0.00066	2.19724
A75	2.12571	-0.00023	-0.00067	0.00299	0.00225	2.12796
A76	1.95282	-0.00162	-0.00087	0.00071	-0.00024	1.95258
A77	2.07949	0.00133	-0.00036	0.00745	0.00703	2.08652
A78	2.25087	0.00030	0.00123	-0.00809	-0.00691	2.24396
A79	1.56787	0.00204	0.00060	0.00214	0.00265	1.57053
A80	1.85664	0.00068	-0.00037	0.00289	0.00214	1.85878
A81	2.20264	-0.00034	-0.00268	0.01098	0.00731	2.20996
A82	2.19177	-0.00021	-0.00262	0.01118	0.00757	2.19934
A83	2.34358	0.00070	0.00254	-0.01369	-0.01117	2.33241
A84	1.91785	0.00043	-0.00044	0.00829	0.00783	1.92568
A85	2.02176	-0.00112	-0.00210	0.00539	0.00328	2.02503
A86	2.19234	-0.00015	0.00149	-0.00498	-0.00417	2.18817
A87	2.20986	0.00061	-0.00112	0.00377	0.00196	2.21182
A88	1.88099	-0.00046	-0.00037	0.00122	0.00219	1.88318
A89	1.86276	0.00020	0.00017	0.00039	-0.00245	1.86032
A90	2.22663	-0.00003	0.00038	0.00037	-0.00621	2.22042
A91	2.19281	-0.00009	-0.00036	0.00704	-0.00044	2.19236
A92	1.86973	0.00036	0.00094	-0.00296	-0.00255	1.86717
A93	2.23343	0.00356	0.00085	0.00024	0.00133	2.23476
A94	2.18002	-0.00392	-0.00179	0.00276	0.00121	2.18123
A95	1.91310	-0.00059	-0.00058	0.00013	0.00095	1.91405
A96	2.22687	0.00086	0.00060	0.00079	0.00044	2.22731
A97	2.14322	-0.00026	-0.00002	-0.00092	-0.00142	2.14180
A98	1.89816	0.00050	-0.00015	0.00164	0.00106	1.89922
A99	2.31052	-0.00128	-0.00018	-0.00184	-0.00196	2.30856
A100	2.07450	0.00079	0.00033	0.00022	0.00089	2.07540
A101	2.05999	-0.00031	-0.00022	0.00018	0.00020	2.06018
A102	2.08784	0.00029	0.00029	0.00040	0.00057	2.08841
A103	2.13536	0.00002	-0.00007	-0.00058	-0.00077	2.13459
A104	2.06930	-0.00020	0.00003	-0.00121	-0.00120	2.06809
A105	2.13240	-0.00029	-0.00015	-0.00017	-0.00030	2.13210
A106	2.08149	0.00049	0.00011	0.00138	0.00151	2.08299
A107	2.09468	0.00003	-0.00026	0.00243	0.00218	2.09686
A108	2.09801	-0.00006	-0.00002	-0.00078	-0.00081	2.09720
A109	2.09050	0.00002	0.00028	-0.00165	-0.00138	2.08912
A110	2.12469	-0.00005	0.00014	-0.00069	-0.00066	2.12403
A111	2.07242	0.00012	-0.00028	0.00235	0.00213	2.07455
A112	2.08607	-0.00007	0.00014	-0.00166	-0.00147	2.08461
A113	2.16193	0.00285	0.00106	0.00082	0.00189	2.16382
A114	2.16362	-0.00341	-0.00211	0.00201	-0.00010	2.16353
A115	1.95763	0.00056	0.00104	-0.00283	-0.00179	1.95584
A116	2.16478	-0.00424	-0.00096	-0.00898	-0.00994	2.15484
A117	2.16176	0.00349	0.00053	0.00559	0.00612	2.16788
A118	1.95665	0.00075	0.00043	0.00339	0.00382	1.96046
A119	1.91112	0.00019	-0.00002	0.00083	0.00080	1.91192
A120	1.95052	-0.00030	-0.00013	-0.00137	-0.00150	1.94903

A121	1.90345	0.00013	-0.00027	0.00212	0.00185	1.90530
A122	1.90695	0.00002	0.00024	-0.00099	-0.00076	1.90619
A123	1.88571	-0.00009	-0.00018	0.00080	0.00063	1.88633
A124	1.90496	0.00006	0.00036	-0.00132	-0.00096	1.90400
A125	1.94811	0.00036	-0.00042	0.00330	0.00288	1.95099
A126	1.91165	-0.00002	-0.00062	0.00337	0.00274	1.91440
A127	1.90337	0.00011	-0.00095	0.00607	0.00511	1.90848
A128	1.90792	-0.00017	0.00082	-0.00525	-0.00443	1.90349
A129	1.90734	-0.00028	0.00101	-0.00677	-0.00576	1.90158
A130	1.88434	-0.00001	0.00017	-0.00086	-0.00070	1.88363
A131	3.15913	0.00110	0.00205	-0.00104	0.00101	3.16014
A132	3.17299	0.00016	0.00194	-0.00128	0.00066	3.17365
A133	3.18222	-0.00083	0.00252	-0.02372	-0.02120	3.16102
A134	3.16531	0.00066	-0.00160	0.01534	0.01374	3.17905
A135	3.14112	-0.00008	-0.00033	0.00122	0.00090	3.14201
A136	3.14173	-0.00003	-0.00001	-0.00041	-0.00042	3.14131
A137	3.14133	0.00002	-0.00013	0.00130	0.00117	3.14250
A138	3.14127	0.00006	0.00043	-0.00177	-0.00134	3.13993
D1	-0.00079	-0.00004	-0.00027	-0.00009	-0.00038	-0.00117
D2	-3.14116	-0.00019	-0.00106	-0.00351	-0.00460	3.13742
D3	3.14032	-0.00007	-0.00011	-0.00217	-0.00229	3.13803
D4	-0.00005	-0.00021	-0.00090	-0.00559	-0.00651	-0.00656
D5	-0.00045	0.00004	0.00031	0.00007	0.00040	-0.00005
D6	-3.14006	0.00000	0.00045	-0.00248	-0.00202	3.14111
D7	-3.14142	0.00007	0.00010	0.00273	0.00283	-3.13859
D8	0.00215	0.00003	0.00024	0.00018	0.00041	0.00257
D9	0.01452	-0.00008	-0.00096	-0.01731	-0.01829	-0.00377
D10	-3.12038	0.00002	-0.00075	-0.00840	-0.00924	-3.12962
D11	-3.12765	-0.00011	-0.00076	-0.01976	-0.02053	3.13500
D12	0.02064	-0.00001	-0.00056	-0.01086	-0.01148	0.00915
D13	0.00124	0.00002	0.00005	0.00006	0.00011	0.00135
D14	-3.14010	-0.00003	-0.00034	-0.00010	-0.00044	-3.14054
D15	3.14138	0.00019	0.00099	0.00412	0.00515	-3.13666
D16	0.00004	0.00014	0.00061	0.00397	0.00460	0.00463
D17	-0.01426	0.00041	0.00238	0.02607	0.02848	0.01423
D18	-3.13712	-0.00014	-0.00064	-0.02480	-0.02544	3.12063
D19	3.12863	0.00026	0.00154	0.02244	0.02399	-3.13056
D20	0.00577	-0.00029	-0.00148	-0.02842	-0.02993	-0.02416
D21	-0.00045	0.00000	0.00013	-0.00001	0.00012	-0.00033
D22	3.14115	-0.00002	0.00003	-0.00071	-0.00069	3.14047
D23	3.14089	0.00006	0.00052	0.00015	0.00068	3.14157
D24	-0.00070	0.00003	0.00042	-0.00055	-0.00012	-0.00082
D25	-0.00077	0.00000	-0.00008	0.00000	-0.00009	-0.00086
D26	3.14075	0.00000	-0.00008	0.00009	0.00000	3.14075
D27	3.14081	0.00002	0.00002	0.00069	0.00071	3.14152
D28	-0.00085	0.00002	0.00001	0.00078	0.00080	-0.00005
D29	0.00122	-0.00002	-0.00014	-0.00003	-0.00018	0.00105
D30	3.14089	0.00002	-0.00028	0.00244	0.00217	-3.14012
D31	-3.14030	-0.00002	-0.00014	-0.00012	-0.00026	-3.14057
D32	-0.00064	0.00002	-0.00028	0.00235	0.00208	0.00145
D33	-0.02311	0.00034	0.00241	0.03318	0.03560	0.01249
D34	3.11002	0.00020	0.00000	0.03486	0.03489	-3.13827
D35	3.11155	0.00019	0.00220	0.02385	0.02596	3.13751
D36	-0.03851	0.00005	-0.00022	0.02553	0.02526	-0.01325
D37	-0.00829	-0.00010	-0.00019	-0.00578	-0.00597	-0.01426
D38	3.12833	-0.00011	0.00000	-0.00569	-0.00570	3.12263
D39	3.14140	0.00005	0.00006	0.00503	0.00510	-3.13669
D40	-0.00516	0.00004	0.00024	0.00512	0.00537	0.00020
D41	0.02301	-0.00046	-0.00293	-0.03639	-0.03928	-0.01627
D42	-3.11023	-0.00035	-0.00057	-0.03800	-0.03854	3.13441

D43	-3.13778	0.00011	0.00017	0.01578	0.01594	-3.12184
D44	0.01217	0.00022	0.00253	0.01417	0.01668	0.02884
D45	-3.13777	-0.00045	-0.00314	-0.02141	-0.02456	3.12085
D46	-0.01099	-0.00008	0.00090	-0.00253	-0.00163	-0.01262
D47	-0.00609	-0.00060	-0.00594	-0.01949	-0.02543	-0.03152
D48	3.12069	-0.00023	-0.00190	-0.00061	-0.00250	3.11819
D49	0.01031	-0.00054	-0.00742	-0.03690	-0.04433	-0.03402
D50	-3.13275	-0.00023	-0.00071	-0.05271	-0.05342	3.09702
D51	-3.11709	-0.00090	-0.01130	-0.05501	-0.06630	3.09979
D52	0.02304	-0.00059	-0.00458	-0.07082	-0.07540	-0.05235
D53	-3.11560	-0.00057	0.00224	-0.03110	-0.02881	3.13878
D54	0.02737	-0.00086	-0.00407	-0.01624	-0.02030	0.00708
D55	3.11836	0.00068	-0.00057	0.02812	0.02762	-3.13721
D56	-0.01857	0.00037	0.00152	-0.00135	0.00017	-0.01840
D57	-0.02445	0.00093	0.00502	0.01492	0.01997	-0.00448
D58	3.12180	0.00062	0.00711	-0.01455	-0.00748	3.11433
D59	0.01457	-0.00021	0.00030	-0.00785	-0.00753	0.00704
D60	-3.10379	-0.00045	-0.00038	-0.01031	-0.01062	-3.11441
D61	-3.12422	-0.00019	-0.00129	-0.00786	-0.00911	-3.13332
D62	0.04061	-0.00043	-0.00197	-0.01032	-0.01219	0.02842
D63	-0.02351	0.00060	0.00214	0.01348	0.01562	-0.00789
D64	3.11379	0.00056	0.00457	0.01348	0.01802	3.13181
D65	0.00221	-0.00002	0.00010	-0.00639	-0.00626	-0.00405
D66	-3.13989	0.00009	0.00166	0.00708	0.00873	-3.13117
D67	-3.13525	0.00002	-0.00224	-0.00639	-0.00858	3.13936
D68	0.00583	0.00013	-0.00068	0.00708	0.00642	0.01225
D69	0.00682	-0.00048	-0.00347	-0.00489	-0.00833	-0.00152
D70	-3.13968	-0.00015	-0.00568	0.02608	0.02039	-3.11928
D71	3.11683	-0.00018	-0.00253	-0.00169	-0.00423	3.11261
D72	-0.02966	0.00015	-0.00473	0.02927	0.02450	-0.00516
D73	-0.06739	0.00070	0.00311	0.02272	0.02581	-0.04158
D74	-2.88042	-0.00013	0.03215	-0.14011	-0.10796	-2.98837
D75	3.10501	0.00039	0.00219	0.01962	0.02182	3.12683
D76	0.29199	-0.00043	0.03123	-0.14321	-0.11194	0.18004
D77	-0.04470	0.00047	0.00182	0.02116	0.02286	-0.02184
D78	3.12682	0.00022	0.00326	-0.00163	0.00154	3.12836
D79	3.09725	0.00039	0.00074	0.01181	0.01252	3.10977
D80	-0.01441	0.00013	0.00217	-0.01098	-0.00881	-0.02322
D81	-3.12557	-0.00026	-0.00258	-0.01093	-0.01344	-3.13901
D82	0.01549	-0.00014	-0.00096	0.00305	0.00210	0.01759
D83	0.06880	-0.00071	-0.00303	-0.02688	-0.02987	0.03894
D84	2.87847	0.00024	-0.03244	0.13830	0.10565	2.98412
D85	-3.11316	-0.00038	-0.00495	0.00378	-0.00111	-3.11428
D86	-0.30350	0.00057	-0.03436	0.16896	0.13440	-0.16910
D87	-3.13246	0.00004	-0.00152	0.00937	0.00786	-3.12460
D88	0.00425	-0.00003	-0.00249	0.01504	0.01257	0.01682
D89	0.05025	-0.00029	0.00042	-0.02182	-0.02142	0.02883
D90	-3.09623	-0.00036	-0.00055	-0.01615	-0.01670	-3.11293
D91	1.37648	0.00060	-0.01821	0.10497	0.08705	1.46353
D92	-2.79129	0.00061	-0.01787	0.10281	0.08522	-2.70607
D93	-0.73263	0.00065	-0.01857	0.10727	0.08899	-0.64364
D94	-1.37328	-0.00055	0.01542	-0.08675	-0.07161	-1.44489
D95	0.74214	-0.00055	0.01576	-0.08891	-0.07344	0.66870
D96	2.80080	-0.00051	0.01505	-0.08444	-0.06967	2.73113
D97	-0.01326	0.00012	-0.00046	0.00556	0.00511	-0.00815
D98	3.13595	0.00007	0.00103	-0.00108	-0.00005	3.13590
D99	-3.13877	0.00000	-0.00017	0.00469	0.00453	-3.13424
D100	0.00779	0.00007	0.00081	-0.00108	-0.00026	0.00753
D101	-0.01178	-0.00003	-0.00130	0.00525	0.00394	-0.00784
D102	3.13463	-0.00010	-0.00033	-0.00406	-0.00440	3.13023

D103	0.00772	-0.00008	0.00176	-0.01279	-0.01104	-0.00332
D104	-3.13765	-0.00013	0.00101	-0.00840	-0.00739	3.13815
D105	-3.13967	-0.00004	0.00063	-0.00773	-0.00711	3.13641
D106	-0.00185	-0.00009	-0.00012	-0.00334	-0.00346	-0.00531
D107	3.12688	0.00012	-0.00235	0.01389	0.01155	3.13842
D108	-0.03260	0.00003	-0.00575	0.02195	0.01621	-0.01638
D109	-0.00723	0.00007	-0.00088	0.00735	0.00647	-0.00076
D110	3.11649	-0.00002	-0.00427	0.01541	0.01113	3.12762
D111	0.01325	-0.00003	0.00151	-0.00829	-0.00677	0.00648
D112	-3.13156	0.00002	0.00086	-0.00207	-0.00120	-3.13276
D113	-3.11533	0.00002	0.00398	-0.01419	-0.01018	-3.12551
D114	0.02305	0.00007	0.00333	-0.00797	-0.00462	0.01843
D115	3.11862	0.00011	-0.00008	0.00213	0.00204	3.12066
D116	0.23610	-0.00037	0.01899	-0.09810	-0.07907	0.15703
D117	-0.04053	0.00003	-0.00342	0.01005	0.00662	-0.03391
D118	-2.92305	-0.00046	0.01566	-0.09018	-0.07449	-2.99754
D119	3.14069	-0.00009	-0.00277	0.01147	0.00872	-3.13378
D120	-0.00437	-0.00015	-0.00039	-0.01063	-0.01102	-0.01539
D121	0.00374	-0.00016	-0.00184	0.00250	0.00066	0.00440
D122	-3.14132	-0.00022	0.00055	-0.01960	-0.01907	3.12280
D123	3.12841	0.00019	0.00005	0.00622	0.00627	3.13468
D124	-0.02911	0.00019	-0.00023	0.00371	0.00346	-0.02565
D125	-0.01084	0.00023	-0.00156	0.02116	0.01958	0.00874
D126	3.11483	0.00023	-0.00184	0.01864	0.01677	3.13160
D127	-3.12928	-0.00015	-0.00111	-0.00050	-0.00161	-3.13090
D128	0.00871	-0.00021	0.00137	-0.02342	-0.02206	-0.01335
D129	0.00702	-0.00008	0.00087	-0.00486	-0.00402	0.00300
D130	-3.13074	-0.00021	0.00046	-0.02351	-0.02306	3.12939
D131	-3.11290	-0.00008	0.00125	-0.00142	-0.00018	-3.11308
D132	0.03253	-0.00021	0.00084	-0.02006	-0.01922	0.01331
D133	0.04292	-0.00013	0.00223	-0.00845	-0.00620	0.03672
D134	2.92751	0.00033	-0.01671	0.09095	0.07423	3.00174
D135	-3.11980	-0.00013	0.00185	-0.01178	-0.00992	-3.12972
D136	-0.23520	0.00032	-0.01709	0.08762	0.07051	-0.16469
D137	-0.00029	-0.00008	0.00018	-0.01297	-0.01278	-0.01307
D138	-3.13840	-0.00031	0.00127	-0.03300	-0.03180	3.11298
D139	3.13764	0.00004	0.00057	0.00478	0.00539	-3.14015
D140	-0.00046	-0.00019	0.00166	-0.01525	-0.01364	-0.01410
D141	-0.00487	0.00017	-0.00089	0.02086	0.01999	0.01512
D142	3.13281	0.00043	-0.00212	0.04340	0.04119	-3.10918
D143	3.09943	0.00106	0.01185	0.10451	0.11635	-3.06741
D144	-0.04041	0.00113	0.01079	0.11648	0.12727	0.08685
D145	-0.03800	0.00079	0.01317	0.08057	0.09374	0.05574
D146	3.10534	0.00086	0.01210	0.09254	0.10466	-3.07318
D147	-0.70867	0.00035	-0.01046	0.05450	0.04411	-0.66456
D148	1.40674	0.00031	-0.01026	0.05291	0.04272	1.44946
D149	-2.76872	0.00027	-0.01008	0.05180	0.04180	-2.72692
D150	2.73993	-0.00034	0.01172	-0.06313	-0.05149	2.68845
D151	-1.42785	-0.00038	0.01192	-0.06472	-0.05287	-1.48072
D152	0.67988	-0.00042	0.01211	-0.06583	-0.05379	0.62609
D153	0.00051	0.00037	0.00169	0.01007	0.01173	0.01224
D154	3.14095	0.00047	0.00096	0.01969	0.02068	-3.12155
D155	3.14027	0.00030	0.00280	-0.00243	0.00034	3.14061
D156	-0.00247	0.00040	0.00207	0.00718	0.00929	0.00682
D157	-3.13427	-0.00047	-0.00265	-0.03744	-0.03988	3.10904
D158	-0.03869	0.00130	0.00911	0.14409	0.15261	0.11392
D159	0.00830	-0.00055	-0.00203	-0.04554	-0.04742	-0.03913
D160	3.10388	0.00122	0.00974	0.13599	0.14506	-3.03425
D161	3.13673	0.00026	0.00209	0.02856	0.03045	-3.11601
D162	-0.00033	0.00012	0.00147	0.01835	0.01973	0.01940

D163	-0.00585	0.00034	0.00147	0.03676	0.03812	0.03227
D164	3.14028	0.00020	0.00085	0.02656	0.02740	-3.11550
D165	-0.00780	0.00056	0.00187	0.03785	0.03959	0.03179
D166	3.13388	0.00049	0.00184	0.03123	0.03301	-3.11629
D167	-3.10452	-0.00116	-0.00959	-0.13895	-0.14873	3.02993
D168	0.03716	-0.00123	-0.00963	-0.14557	-0.15531	-0.11815
D169	0.00105	0.00001	-0.00031	-0.01361	-0.01384	-0.01279
D170	-3.13675	-0.00016	-0.00110	-0.02001	-0.02103	3.12540
D171	3.13828	0.00016	0.00028	-0.00381	-0.00353	3.13475
D172	0.00048	0.00000	-0.00051	-0.01020	-0.01072	-0.01025
D173	-0.00029	0.00007	0.00054	0.00395	0.00444	0.00416
D174	3.14055	0.00005	0.00022	0.00558	0.00576	-3.13688
D175	-3.13659	-0.00011	-0.00018	-0.00793	-0.00807	3.13853
D176	0.00424	-0.00013	-0.00050	-0.00629	-0.00675	-0.00251
D177	0.00422	-0.00036	-0.00098	-0.01524	-0.01617	-0.01195
D178	-3.14056	-0.00022	-0.00031	-0.00985	-0.01010	3.13252
D179	-3.13746	-0.00029	-0.00094	-0.00900	-0.00997	3.13575
D180	0.00094	-0.00016	-0.00027	-0.00361	-0.00390	-0.00296
D181	3.14087	0.00021	0.00026	0.01075	0.01094	-3.13138
D182	-0.00071	0.00011	0.00025	0.00888	0.00906	0.00835
D183	-0.00062	0.00013	0.00021	0.00333	0.00357	0.00295
D184	3.14098	0.00004	0.00020	0.00146	0.00170	-3.14051
D185	3.13679	0.00026	0.00103	0.00871	0.00974	-3.13666
D186	-0.00451	0.00019	0.00093	0.00872	0.00966	0.00515
D187	-0.00071	0.00008	0.00017	0.00179	0.00197	0.00125
D188	3.14118	0.00001	0.00008	0.00180	0.00188	-3.14013
D189	0.00009	-0.00004	-0.00005	-0.00131	-0.00139	-0.00130
D190	3.14158	-0.00005	-0.00005	-0.00079	-0.00086	3.14072
D191	-3.14151	0.00006	-0.00004	0.00061	0.00054	-3.14097
D192	-0.00003	0.00005	-0.00004	0.00113	0.00107	0.00105
D193	0.00021	0.00001	-0.00002	0.00009	0.00008	0.00030
D194	-3.14144	-0.00003	-0.00003	-0.00036	-0.00039	3.14136
D195	3.14152	0.00008	0.00007	0.00008	0.00016	-3.14150
D196	-0.00013	0.00004	0.00006	-0.00037	-0.00031	-0.00044
D197	0.00010	-0.00003	-0.00004	-0.00035	-0.00039	-0.00028
D198	-3.14143	0.00001	-0.00003	0.00011	0.00009	-3.14134
D199	-3.14138	-0.00002	-0.00004	-0.00086	-0.00092	3.14089
D200	0.00027	0.00002	-0.00003	-0.00041	-0.00044	-0.00017

Item	Value	Threshold	Converged?

Maximum Force	0.007303	0.000450	NO

RMS Force	0.000964	0.000300	NO

Maximum Displacement	0.710541	0.001800	NO

RMS Displacement	0.129675	0.001200	NO

Predicted change in Energy=-1.905616D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.800519	-0.624757	0.042376
2	6	0	-9.996952	-1.779081	0.036199
3	6	0	-10.527326	-3.060840	0.061802

4	6	0	-11.916809	-3.193907	0.093240
5	6	0	-12.732044	-2.055274	0.098645
6	6	0	-12.192598	-0.764990	0.074189
7	1	0	-9.862528	-3.918475	0.056659
8	1	0	-12.369670	-4.180354	0.112851
9	1	0	-13.811236	-2.171050	0.122401
10	1	0	-12.855509	0.088321	0.080706
11	6	0	-9.920590	0.571752	0.014707
12	6	0	-8.570213	-1.387654	-0.004666
13	6	0	-8.534119	0.093614	-0.003526
14	6	0	-7.389116	0.879047	-0.027541
15	6	0	-5.995653	0.599463	-0.026255
16	6	0	-3.631355	-0.186736	-0.010850
17	6	0	-3.757557	1.223036	-0.103307
18	16	0	-5.172767	-0.986083	0.057052
19	6	0	-5.075161	1.661324	-0.110801
20	6	0	-2.253910	-0.459183	-0.004301
21	6	0	-1.586917	0.785261	-0.097926
22	7	0	-2.502053	1.808671	-0.189789
23	16	0	-1.142807	-1.817220	0.064799
24	16	0	1.169042	1.783946	-0.146131
25	6	0	0.209440	-0.689105	-0.002458
26	6	0	-0.183245	0.656117	-0.084465
27	6	0	1.615909	-0.817883	0.004169
28	6	0	2.281327	0.427081	-0.073633
29	6	0	3.653694	0.157014	-0.070058
30	6	0	3.784498	-1.253463	0.004326
31	6	0	5.103013	-1.693239	0.008591
32	6	0	6.018281	-0.627646	-0.058707
33	16	0	5.191928	0.955717	-0.150126
34	7	0	2.531815	-1.840709	0.079095
35	6	0	7.400539	-0.896340	-0.028994
36	6	0	8.523863	-0.098844	-0.001803
37	6	0	8.523693	1.381368	0.017401
38	6	0	9.923178	-0.550717	0.004116
39	6	0	9.940436	1.803148	0.090291
40	6	0	10.773715	0.669160	0.073053
41	6	0	10.435984	3.096228	0.158469
42	6	0	12.164055	0.848411	0.123224
43	6	0	11.820406	3.266560	0.208081
44	6	0	12.666777	2.151892	0.190109
45	6	0	10.401580	-1.852737	-0.037262
46	6	0	9.563789	-3.010810	-0.099772
47	6	0	11.793366	-2.195309	-0.021723
48	7	0	8.898911	-3.966744	-0.151042
49	7	0	12.915332	-2.509912	-0.010427
50	6	0	-10.377986	1.877166	0.026392
51	6	0	-11.764649	2.226767	0.049842
52	6	0	-9.528403	3.026283	0.022104
53	7	0	-12.888646	2.533473	0.067764
54	7	0	-8.871015	3.988886	0.016877
55	8	0	-7.616661	-2.157452	0.001518
56	8	0	7.552176	2.121474	0.123427
57	6	0	2.250061	-3.262081	0.003962
58	1	0	1.317049	-3.477896	0.529155
59	1	0	2.167156	-3.603817	-1.033715
60	1	0	3.052646	-3.813294	0.498498
61	6	0	-2.219168	3.229449	-0.118216
62	1	0	-2.143875	3.577469	0.918366
63	1	0	-1.281487	3.444516	-0.635764

64	1	0	-3.015270	3.782690	-0.621199
65	1	0	5.428437	-2.725213	0.070340
66	1	0	12.851544	0.016136	0.111597
67	1	0	13.741939	2.297561	0.229410
68	1	0	12.245671	4.263959	0.261176
69	1	0	9.747737	3.935094	0.169836
70	1	0	7.576604	-1.965226	-0.041179
71	1	0	-7.551999	1.950131	-0.045413
72	1	0	-5.397954	2.692567	-0.194288

Rotational constants (GHZ): 0.1746678 0.0104237 0.0098402

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6572.5720229116 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T
Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6572.4870744224 Hartrees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.25D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Initial guess from the checkpoint file: "PBDB.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000398 0.000002 -0.000434 Ang= 0.07 deg.

ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1

AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-yADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 IlCent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Integral accuracy reduced to 1.0D-05 until final iterations.

Initial convergence to 1.0D-05 achieved. Increase integral accuracy.

SCF Done: E(RB3LYP) = -3683.01773575 A.U. after 14 cycles

NFock= 14 Conv=0.64D-08 -V/T= 2.0068

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1
NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center	Atomic	Forces (Hartrees/Bohr)		
Number	Number	X	Y	Z

1	6	-0.000217266	0.000279212	0.000525785
2	6	-0.001021184	-0.000390761	0.001520561
3	6	0.000037492	-0.000364224	0.000107943
4	6	0.000017277	0.000294389	-0.000063406
5	6	0.000146322	-0.000173759	0.000080739
6	6	0.000288152	0.000523080	0.000158948
7	1	-0.000023606	0.000027271	0.000073764
8	1	0.000031647	0.000037074	-0.000032642
9	1	0.000019271	0.000038178	0.000001618
10	1	0.000171052	0.000442098	0.000236644
11	6	0.001213329	-0.000524402	-0.000200170
12	6	0.002492867	-0.000416340	-0.004702239
13	6	0.000981378	-0.006986298	0.001808480
14	6	0.000532208	0.006253457	0.000323418
15	6	-0.003737822	0.001619851	-0.000948483
16	6	0.002181328	0.000158296	0.000102861
17	6	-0.000319367	0.000709333	0.001913066
18	16	0.000066250	-0.001297401	0.000949836
19	6	-0.002720250	0.000196271	-0.001430439
20	6	-0.000905805	0.000268601	0.000067786
21	6	0.000552385	0.000964126	0.000486501
22	7	0.000867793	0.001785993	-0.001802492
23	16	-0.000235043	-0.000528965	-0.000459877
24	16	0.000158725	0.000034611	0.000134806
25	6	0.001242953	0.000011598	0.000829825
26	6	0.000040594	-0.000796445	0.000526513
27	6	-0.002006377	0.001460416	-0.002246155
28	6	-0.002566114	0.000859711	-0.001273924
29	6	-0.000277038	-0.001705070	0.004163122
30	6	0.001781654	-0.000508163	-0.000729767
31	6	-0.000036358	0.000834466	0.000403533
32	6	-0.002732687	0.001795817	-0.003401793
33	16	0.000602081	0.001706687	-0.004244082
34	7	-0.000845550	0.000273880	0.001016659
35	6	0.002649441	-0.001954585	0.004184993
36	6	-0.001646877	-0.002612500	0.007345914
37	6	0.014036802	0.002636893	-0.011298272
38	6	-0.000108626	0.001348793	-0.000448701
39	6	-0.002821859	-0.000184573	0.004023023
40	6	0.001014669	-0.000667758	0.001671447
41	6	-0.000391828	-0.000348306	-0.000145184
42	6	-0.002066955	0.001755516	-0.001476172
43	6	0.000111120	-0.000652210	-0.000599526
44	6	0.000217441	0.000435928	0.000286897
45	6	0.000841941	-0.000897515	0.000319576
46	6	-0.000530257	-0.001626306	-0.000452478
47	6	-0.002620352	-0.000515957	-0.002345255
48	7	0.000275206	0.000153465	0.000172832
49	7	-0.000581155	0.000259502	-0.000362749
50	6	-0.001171071	-0.001349651	-0.001277495
51	6	0.000649023	0.000318716	0.000652957
52	6	-0.000853667	0.000174516	-0.000091458
53	7	0.000236019	-0.001136799	0.000031273
54	7	0.000508475	0.000048094	0.000302899
55	8	-0.000017981	-0.000175213	0.001654441
56	8	-0.005328448	-0.003026244	0.005318349
57	6	0.000441647	0.001113990	-0.000154063
58	1	0.000099741	0.000043412	0.000112493
59	1	0.000024326	0.000003194	-0.000097928
60	1	-0.000130543	0.000007871	-0.000065700

61	6	-0.000514714	-0.002065080	-0.000510685
62	1	0.000013567	0.000237728	0.000238842
63	1	0.000011161	0.000340289	0.000097738
64	1	0.000137068	0.000387774	0.000193712
65	1	-0.000171978	-0.000228723	0.000382945
66	1	0.000859466	0.000750065	0.000606354
67	1	-0.000005815	0.000064039	0.000072094
68	1	-0.000036197	-0.000050417	-0.000042085
69	1	-0.000076155	-0.000090935	0.000027638
70	1	0.001340374	-0.000227069	-0.001187776
71	1	-0.000582254	0.000546817	0.000029875
72	1	0.000408954	0.000300648	-0.001067701

Cartesian Forces: Max 0.014036802 RMS 0.001976811

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.009967095 RMS 0.001417842

Search for a local minimum.

Step number 16 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 14 16 15

DE= 1.14D-03 DEPred=-1.91D-03 R=-5.97D-01

Trust test=-5.97D-01 RLast= 5.72D-01 DXMaxT set to 9.85D-01

ITU= -1 1 1 1 1 1 0 0 0 1 0 0 0 1 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.64323.

Iteration 1 RMS(Cart)= 0.08333838 RMS(Int)= 0.00138336

Iteration 2 RMS(Cart)= 0.00322945 RMS(Int)= 0.00014368

Iteration 3 RMS(Cart)= 0.00000315 RMS(Int)= 0.00014367

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00014367

Variable	Old X	-DE/DX	Delta X	Delta X	Delta X	New X
(Linear)	(Quad)	(Total)				
R1	2.65789	0.00071	0.00050	0.00000	0.00049	2.65838
R2	2.64465	0.00043	-0.00049	0.00000	-0.00049	2.64416
R3	2.80717	0.00201	0.00190	0.00000	0.00192	2.80908
R4	2.62179	-0.00016	-0.00104	0.00000	-0.00104	2.62075
R5	2.79684	-0.00089	-0.00317	0.00000	-0.00319	2.79365
R6	2.63842	-0.00021	0.00008	0.00000	0.00008	2.63850
R7	2.05061	0.00004	0.00030	0.00000	0.00030	2.05091
R8	2.64637	-0.00025	-0.00012	0.00000	-0.00012	2.64625
R9	2.05150	0.00003	0.00001	0.00000	0.00001	2.05152
R10	2.64321	0.00009	0.00028	0.00000	0.00028	2.64348
R11	2.05157	0.00001	0.00013	0.00000	0.00013	2.05170
R12	2.04198	-0.00039	0.00093	0.00000	0.00093	2.04291
R13	2.77169	-0.00135	-0.00116	0.00000	-0.00114	2.77055
R14	2.61401	0.00167	-0.00017	0.00000	-0.00017	2.61385
R15	2.80002	-0.00162	-0.00234	0.00000	-0.00235	2.79768
R16	2.31589	0.00100	0.00056	0.00000	0.00056	2.31645
R17	2.62428	-0.00097	-0.01178	0.00000	-0.01178	2.61250
R18	2.68574	-0.00422	-0.00304	0.00000	-0.00304	2.68270
R19	2.04760	-0.00009	-0.00051	0.00000	-0.00051	2.04709
R20	3.37941	0.00067	0.00418	0.00000	0.00421	3.38361
R21	2.66042	-0.00083	-0.00179	0.00000	-0.00179	2.65864
R22	2.68044	0.00035	-0.00248	0.00000	-0.00246	2.67798
R23	3.28373	-0.00119	-0.00510	0.00000	-0.00509	3.27864

R24	2.65345	-0.00062	-0.00244	0.00000	-0.00229	2.65116
R25	2.62409	0.00253	-0.00029	0.00000	-0.00031	2.62378
R26	2.62307	0.00003	0.00083	0.00000	0.00072	2.62379
R27	2.04809	0.00008	0.00056	0.00000	0.00056	2.04864
R28	2.67400	-0.00061	-0.00388	0.00000	-0.00386	2.67014
R29	3.31839	-0.00020	-0.00219	0.00000	-0.00218	3.31621
R30	2.60020	0.00111	0.00249	0.00000	0.00237	2.60257
R31	2.66388	0.00114	-0.00363	0.00000	-0.00365	2.66023
R32	2.74092	0.00106	0.00251	0.00000	0.00251	2.74344
R33	3.33028	-0.00015	-0.00151	0.00000	-0.00148	3.32880
R34	3.32961	0.00014	-0.00157	0.00000	-0.00156	3.32804
R35	3.31835	-0.00007	-0.00188	0.00000	-0.00188	3.31647
R36	2.65273	0.00036	0.00035	0.00000	0.00036	2.65308
R37	2.66899	-0.00086	-0.00673	0.00000	-0.00673	2.66225
R38	2.67165	0.00062	-0.00143	0.00000	-0.00142	2.67023
R39	2.59841	0.00168	0.00045	0.00000	0.00041	2.59882
R40	2.64315	0.00357	0.00072	0.00000	0.00077	2.64391
R41	2.68054	0.00010	-0.00052	0.00000	-0.00051	2.68003
R42	3.27883	0.00049	-0.00053	0.00000	-0.00053	3.27830
R43	2.62658	0.00115	-0.00380	0.00000	-0.00381	2.62277
R44	2.61825	0.00242	0.00121	0.00000	0.00116	2.61942
R45	2.65756	0.00196	-0.00133	0.00000	-0.00133	2.65623
R46	2.04814	-0.00005	0.00001	0.00000	0.00001	2.04815
R47	3.37952	0.00176	0.00084	0.00000	0.00084	3.38037
R48	2.66157	0.00905	0.00002	0.00000	0.00002	2.66159
R49	2.74194	0.00107	0.00244	0.00000	0.00244	2.74439
R50	2.60385	0.00370	-0.00028	0.00000	-0.00028	2.60357
R51	2.04725	-0.00008	-0.00002	0.00000	-0.00002	2.04723
R52	2.79743	0.00117	-0.00046	0.00000	-0.00065	2.79678
R53	2.77880	-0.00251	-0.00302	0.00000	-0.00293	2.77587
R54	2.79678	-0.00039	-0.00292	0.00000	-0.00313	2.79365
R55	2.31662	0.00024	0.00042	0.00000	0.00042	2.31705
R56	2.81326	-0.00270	-0.00156	0.00000	-0.00130	2.81196
R57	2.62246	-0.00456	-0.00556	0.00000	-0.00556	2.61690
R58	2.65947	-0.00181	-0.00015	0.00000	-0.00012	2.65935
R59	2.62003	0.00075	-0.00190	0.00000	-0.00192	2.61811
R60	2.65080	-0.00297	-0.00443	0.00000	-0.00443	2.64637
R61	2.63757	0.00039	0.00117	0.00000	0.00116	2.63874
R62	2.05060	0.00006	0.00024	0.00000	0.00024	2.05084
R63	2.64310	0.00000	0.00041	0.00000	0.00043	2.64353
R64	2.04008	0.00119	0.00273	0.00000	0.00273	2.04281
R65	2.64505	0.00068	-0.00123	0.00000	-0.00120	2.64384
R66	2.05144	0.00006	0.00005	0.00000	0.00005	2.05149
R67	2.05167	-0.00002	0.00008	0.00000	0.00008	2.05175
R68	2.70365	-0.00147	-0.00106	0.00000	-0.00106	2.70259
R69	2.70875	-0.00375	-0.00439	0.00000	-0.00439	2.70436
R70	2.20257	0.00016	0.00011	0.00000	0.00011	2.20267
R71	2.20209	-0.00073	-0.00039	0.00000	-0.00039	2.20170
R72	2.70277	-0.00135	-0.00237	0.00000	-0.00237	2.70040
R73	2.70058	-0.00026	-0.00023	0.00000	-0.00023	2.70035
R74	2.20197	-0.00061	-0.00032	0.00000	-0.00032	2.20164
R75	2.20280	-0.00007	-0.00002	0.00000	-0.00002	2.20278
R76	2.06397	-0.00006	0.00001	0.00000	0.00001	2.06398
R77	2.07046	-0.00010	0.00017	0.00000	0.00017	2.07063
R78	2.06365	-0.00014	-0.00003	0.00000	-0.00003	2.06363
R79	2.07120	-0.00024	-0.00048	0.00000	-0.00048	2.07073
R80	2.06435	-0.00018	-0.00055	0.00000	-0.00055	2.06380
R81	2.06391	-0.00018	-0.00021	0.00000	-0.00021	2.06370
A1	2.07849	-0.00111	-0.00231	0.00000	-0.00232	2.07617
A2	1.89922	-0.00049	-0.00085	0.00000	-0.00082	1.89839

A3	2.30547	0.00160	0.00316	0.00000	0.00314	2.30862
A4	2.14092	0.00061	0.00172	0.00000	0.00172	2.14264
A5	1.91115	0.00026	0.00079	0.00000	0.00078	1.91193
A6	2.23111	-0.00087	-0.00250	0.00000	-0.00250	2.22861
A7	2.05885	0.00012	0.00029	0.00000	0.00029	2.05914
A8	2.08965	-0.00003	-0.00057	0.00000	-0.00057	2.08908
A9	2.13468	-0.00008	0.00028	0.00000	0.00028	2.13497
A10	2.09664	-0.00031	-0.00136	0.00000	-0.00136	2.09528
A11	2.09688	0.00016	0.00054	0.00000	0.00054	2.09743
A12	2.08966	0.00015	0.00081	0.00000	0.00082	2.09048
A13	2.12405	0.00031	0.00057	0.00000	0.00057	2.12462
A14	2.08525	-0.00019	0.00038	0.00000	0.00038	2.08563
A15	2.07389	-0.00012	-0.00095	0.00000	-0.00095	2.07294
A16	2.06742	0.00039	0.00110	0.00000	0.00110	2.06852
A17	2.13086	0.00017	0.00115	0.00000	0.00115	2.13201
A18	2.08490	-0.00056	-0.00225	0.00000	-0.00225	2.08265
A19	1.87297	-0.00117	-0.00160	0.00000	-0.00155	1.87142
A20	2.17014	0.00413	0.00762	0.00000	0.00760	2.17775
A21	2.23995	-0.00295	-0.00596	0.00000	-0.00598	2.23397
A22	1.86278	-0.00031	-0.00010	0.00000	0.00001	1.86279
A23	2.19420	0.00028	-0.00041	0.00000	-0.00029	2.19391
A24	2.22559	0.00007	0.00078	0.00000	0.00089	2.22649
A25	1.87851	0.00173	0.00165	0.00000	0.00167	1.88018
A26	2.20836	-0.00040	0.00101	0.00000	0.00100	2.20936
A27	2.19628	-0.00133	-0.00266	0.00000	-0.00267	2.19361
A28	2.34217	-0.00122	0.00062	0.00000	0.00063	2.34280
A29	2.02130	-0.00014	-0.00067	0.00000	-0.00066	2.02064
A30	1.91969	0.00135	0.00002	0.00000	0.00004	1.91973
A31	2.24671	-0.00018	0.00488	0.00000	0.00488	2.25160
A32	2.08590	0.00006	-0.00476	0.00000	-0.00476	2.08114
A33	1.95053	0.00012	-0.00010	0.00000	-0.00009	1.95044
A34	1.96148	-0.00100	0.00123	0.00000	0.00119	1.96268
A35	1.85504	0.00087	0.00040	0.00000	0.00045	1.85549
A36	2.46666	0.00014	-0.00164	0.00000	-0.00164	2.46502
A37	1.98066	0.00101	0.00141	0.00000	0.00147	1.98212
A38	1.92082	-0.00101	0.00040	0.00000	0.00021	1.92103
A39	2.38146	0.00001	-0.00186	0.00000	-0.00173	2.37973
A40	1.56930	0.00101	-0.00101	0.00000	-0.00098	1.56832
A41	1.96277	-0.00113	-0.00181	0.00000	-0.00182	1.96095
A42	2.12653	0.00018	-0.00074	0.00000	-0.00070	2.12583
A43	2.19364	0.00097	0.00271	0.00000	0.00275	2.19639
A44	1.86654	0.00005	0.00053	0.00000	0.00058	1.86712
A45	2.45113	0.00015	-0.00231	0.00000	-0.00230	2.44883
A46	1.96545	-0.00019	0.00183	0.00000	0.00178	1.96723
A47	1.92307	-0.00036	0.00042	0.00000	0.00025	1.92333
A48	1.96943	0.00020	0.00005	0.00000	0.00012	1.96956
A49	2.39064	0.00016	-0.00081	0.00000	-0.00065	2.38999
A50	1.85835	0.00047	-0.00290	0.00000	-0.00253	1.85582
A51	2.19767	0.00002	-0.01052	0.00000	-0.00967	2.18800
A52	2.20876	-0.00043	-0.00877	0.00000	-0.00789	2.20087
A53	1.55975	0.00055	-0.00154	0.00000	-0.00152	1.55823
A54	1.56089	0.00008	-0.00140	0.00000	-0.00140	1.55949
A55	1.98343	-0.00037	0.00022	0.00000	0.00024	1.98366
A56	2.35402	0.00034	-0.00036	0.00000	-0.00035	2.35366
A57	1.94574	0.00004	0.00013	0.00000	0.00011	1.94585
A58	2.35358	0.00029	0.00041	0.00000	0.00044	2.35401
A59	1.94647	-0.00019	-0.00051	0.00000	-0.00054	1.94593
A60	1.98314	-0.00011	0.00009	0.00000	0.00010	1.98324
A61	1.96942	0.00026	0.00045	0.00000	0.00047	1.96989
A62	2.39117	0.00021	-0.00117	0.00000	-0.00112	2.39005

A63	1.92253	-0.00047	0.00070	0.00000	0.00062	1.92316
A64	1.96555	-0.00027	0.00071	0.00000	0.00069	1.96624
A65	2.45090	0.00006	-0.00117	0.00000	-0.00116	2.44974
A66	1.86673	0.00021	0.00046	0.00000	0.00047	1.86720
A67	1.85731	-0.00005	-0.00084	0.00000	-0.00082	1.85649
A68	2.46684	0.00031	-0.00038	0.00000	-0.00037	2.46647
A69	1.95886	-0.00024	0.00133	0.00000	0.00133	1.96019
A70	1.98477	-0.00023	-0.00080	0.00000	-0.00077	1.98401
A71	1.91868	-0.00027	0.00088	0.00000	0.00080	1.91948
A72	2.37951	0.00051	-0.00004	0.00000	0.00001	2.37952
A73	1.95789	0.00139	0.00108	0.00000	0.00109	1.95897
A74	2.19724	-0.00045	0.00042	0.00000	0.00044	2.19768
A75	2.12796	-0.00092	-0.00144	0.00000	-0.00143	2.12653
A76	1.95258	-0.00222	0.00015	0.00000	0.00017	1.95275
A77	2.08652	-0.00345	-0.00452	0.00000	-0.00451	2.08201
A78	2.24396	0.00568	0.00445	0.00000	0.00446	2.24842
A79	1.57053	0.00134	-0.00171	0.00000	-0.00169	1.56884
A80	1.85878	0.00058	-0.00138	0.00000	-0.00126	1.85752
A81	2.20996	-0.00058	-0.00470	0.00000	-0.00439	2.20556
A82	2.19934	0.00004	-0.00487	0.00000	-0.00456	2.19478
A83	2.33241	0.00927	0.00718	0.00000	0.00719	2.33960
A84	1.92568	-0.00405	-0.00504	0.00000	-0.00503	1.92065
A85	2.02503	-0.00522	-0.00211	0.00000	-0.00210	2.02293
A86	2.18817	0.00646	0.00268	0.00000	0.00285	2.19101
A87	2.21182	-0.00421	-0.00126	0.00000	-0.00110	2.21072
A88	1.88318	-0.00225	-0.00141	0.00000	-0.00173	1.88145
A89	1.86032	0.00080	0.00157	0.00000	0.00228	1.86259
A90	2.22042	0.00218	0.00399	0.00000	0.00563	2.22605
A91	2.19236	-0.00220	0.00029	0.00000	0.00193	2.19430
A92	1.86717	0.00226	0.00164	0.00000	0.00177	1.86894
A93	2.23476	0.00161	-0.00086	0.00000	-0.00091	2.23385
A94	2.18123	-0.00387	-0.00078	0.00000	-0.00084	2.18040
A95	1.91405	-0.00075	-0.00061	0.00000	-0.00094	1.91311
A96	2.22731	0.00077	-0.00029	0.00000	-0.00006	2.22725
A97	2.14180	-0.00002	0.00091	0.00000	0.00102	2.14282
A98	1.89922	0.00002	-0.00068	0.00000	-0.00058	1.89863
A99	2.30856	-0.00111	0.00126	0.00000	0.00124	2.30981
A100	2.07540	0.00108	-0.00058	0.00000	-0.00066	2.07474
A101	2.06018	-0.00047	-0.00013	0.00000	-0.00018	2.06000
A102	2.08841	0.00030	-0.00037	0.00000	-0.00034	2.08807
A103	2.13459	0.00017	0.00050	0.00000	0.00052	2.13511
A104	2.06809	0.00000	0.00077	0.00000	0.00078	2.06887
A105	2.13210	-0.00048	0.00020	0.00000	0.00019	2.13229
A106	2.08299	0.00047	-0.00097	0.00000	-0.00097	2.08202
A107	2.09686	-0.00057	-0.00140	0.00000	-0.00141	2.09545
A108	2.09720	0.00024	0.00052	0.00000	0.00052	2.09772
A109	2.08912	0.00033	0.00089	0.00000	0.00089	2.09001
A110	2.12403	-0.00003	0.00043	0.00000	0.00045	2.12448
A111	2.07455	-0.00007	-0.00137	0.00000	-0.00138	2.07317
A112	2.08461	0.00010	0.00094	0.00000	0.00093	2.08554
A113	2.16382	0.00155	-0.00121	0.00000	-0.00121	2.16261
A114	2.16353	-0.00334	0.00006	0.00000	0.00006	2.16359
A115	1.95584	0.00179	0.00115	0.00000	0.00115	1.95699
A116	2.15484	0.00233	0.00639	0.00000	0.00639	2.16123
A117	2.16788	-0.00162	-0.00394	0.00000	-0.00394	2.16394
A118	1.96046	-0.00071	-0.00246	0.00000	-0.00246	1.95801
A119	1.91192	0.00019	-0.00052	0.00000	-0.00052	1.91140
A120	1.94903	-0.00001	0.00096	0.00000	0.00096	1.94999
A121	1.90530	-0.00005	-0.00119	0.00000	-0.00119	1.90411
A122	1.90619	-0.00007	0.00049	0.00000	0.00049	1.90668

A123	1.88633	-0.00009	-0.00040	0.00000	-0.00040	1.88593
A124	1.90400	0.00002	0.00062	0.00000	0.00062	1.90462
A125	1.95099	-0.00014	-0.00185	0.00000	-0.00185	1.94914
A126	1.91440	-0.00030	-0.00176	0.00000	-0.00176	1.91263
A127	1.90848	-0.00051	-0.00329	0.00000	-0.00329	1.90519
A128	1.90349	0.00030	0.00285	0.00000	0.00285	1.90634
A129	1.90158	0.00036	0.00371	0.00000	0.00371	1.90529
A130	1.88363	0.00033	0.00045	0.00000	0.00045	1.88409
A131	3.16014	0.00069	-0.00065	0.00000	-0.00065	3.15949
A132	3.17365	0.00001	-0.00042	0.00000	-0.00042	3.17323
A133	3.16102	0.00217	0.01364	0.00000	0.01364	3.17465
A134	3.17905	-0.00129	-0.00884	0.00000	-0.00884	3.17021
A135	3.14201	0.00013	-0.00058	0.00000	-0.00058	3.14144
A136	3.14131	0.00007	0.00027	0.00000	0.00027	3.14158
A137	3.14250	-0.00003	-0.00075	0.00000	-0.00075	3.14175
A138	3.13993	0.00018	0.00086	0.00000	0.00086	3.14079
D1	-0.00117	0.00007	0.00024	0.00000	0.00025	-0.00092
D2	3.13742	0.00029	0.00296	0.00000	0.00296	3.14039
D3	3.13803	0.00015	0.00147	0.00000	0.00147	3.13950
D4	-0.00656	0.00037	0.00419	0.00000	0.00419	-0.00237
D5	-0.00005	-0.00001	-0.00026	0.00000	-0.00026	-0.00031
D6	3.14111	0.00002	0.00130	0.00000	0.00130	-3.14078
D7	-3.13859	-0.00010	-0.00182	0.00000	-0.00182	-3.14041
D8	0.00257	-0.00007	-0.00027	0.00000	-0.00027	0.00230
D9	-0.00377	0.00020	0.01176	0.00000	0.01177	0.00800
D10	-3.12962	-0.00024	0.00594	0.00000	0.00596	-3.12366
D11	3.13500	0.00029	0.01321	0.00000	0.01321	-3.13498
D12	0.00915	-0.00015	0.00739	0.00000	0.00740	0.01655
D13	0.00135	-0.00009	-0.00007	0.00000	-0.00007	0.00128
D14	-3.14054	0.00002	0.00028	0.00000	0.00028	-3.14026
D15	-3.13666	-0.00035	-0.00331	0.00000	-0.00332	-3.13998
D16	0.00463	-0.00024	-0.00296	0.00000	-0.00296	0.00167
D17	0.01423	-0.00079	-0.01832	0.00000	-0.01833	-0.00410
D18	3.12063	0.00053	0.01636	0.00000	0.01636	3.13699
D19	-3.13056	-0.00055	-0.01543	0.00000	-0.01543	3.13719
D20	-0.02416	0.00076	0.01925	0.00000	0.01926	-0.00490
D21	-0.00033	0.00004	-0.00008	0.00000	-0.00008	-0.00041
D22	3.14047	0.00008	0.00044	0.00000	0.00044	3.14091
D23	3.14157	-0.00007	-0.00044	0.00000	-0.00044	3.14113
D24	-0.00082	-0.00004	0.00008	0.00000	0.00008	-0.00074
D25	-0.00086	0.00002	0.00006	0.00000	0.00006	-0.00080
D26	3.14075	0.00000	0.00000	0.00000	0.00000	3.14075
D27	3.14152	-0.00001	-0.00046	0.00000	-0.00046	3.14106
D28	-0.00005	-0.00003	-0.00051	0.00000	-0.00051	-0.00057
D29	0.00105	-0.00004	0.00011	0.00000	0.00012	0.00116
D30	-3.14012	-0.00007	-0.00139	0.00000	-0.00140	-3.14152
D31	-3.14057	-0.00002	0.00017	0.00000	0.00017	-3.14040
D32	0.00145	-0.00005	-0.00134	0.00000	-0.00134	0.00011
D33	0.01249	-0.00067	-0.02290	0.00000	-0.02290	-0.01041
D34	-3.13827	-0.00046	-0.02244	0.00000	-0.02245	3.12247
D35	3.13751	-0.00012	-0.01670	0.00000	-0.01668	3.12083
D36	-0.01325	0.00009	-0.01625	0.00000	-0.01623	-0.02949
D37	-0.01426	0.00023	0.00384	0.00000	0.00384	-0.01042
D38	3.12263	0.00061	0.00367	0.00000	0.00367	3.12630
D39	-3.13669	-0.00035	-0.00328	0.00000	-0.00328	-3.13997
D40	0.00020	0.00004	-0.00345	0.00000	-0.00345	-0.00325
D41	-0.01627	0.00088	0.02527	0.00000	0.02526	0.00899
D42	3.13441	0.00066	0.02479	0.00000	0.02479	-3.12398
D43	-3.12184	-0.00048	-0.01025	0.00000	-0.01025	-3.13209
D44	0.02884	-0.00069	-0.01073	0.00000	-0.01072	0.01812

D45	3.12085	0.00074	0.01580	0.00000	0.01580	3.13665
D46	-0.01262	0.00062	0.00105	0.00000	0.00105	-0.01157
D47	-0.03152	0.00101	0.01636	0.00000	0.01635	-0.01517
D48	3.11819	0.00088	0.00161	0.00000	0.00160	3.11979
D49	-0.03402	0.00075	0.02851	0.00000	0.02851	-0.00551
D50	3.09702	0.00122	0.03436	0.00000	0.03436	3.13138
D51	3.09979	0.00086	0.04265	0.00000	0.04265	-3.14074
D52	-0.05235	0.00133	0.04850	0.00000	0.04850	-0.00386
D53	3.13878	0.00061	0.01853	0.00000	0.01852	-3.12589
D54	0.00708	0.00017	0.01305	0.00000	0.01305	0.02013
D55	-3.13721	-0.00050	-0.01776	0.00000	-0.01778	3.12820
D56	-0.01840	0.00020	-0.00011	0.00000	-0.00011	-0.01851
D57	-0.00448	-0.00010	-0.01285	0.00000	-0.01285	-0.01733
D58	3.11433	0.00059	0.00481	0.00000	0.00482	3.11915
D59	0.00704	0.00017	0.00484	0.00000	0.00484	0.01188
D60	-3.11441	-0.00015	0.00683	0.00000	0.00681	-3.10759
D61	-3.13332	0.00006	0.00586	0.00000	0.00585	-3.12748
D62	0.02842	-0.00025	0.00784	0.00000	0.00782	0.03624
D63	-0.00789	-0.00018	-0.01005	0.00000	-0.01005	-0.01794
D64	3.13181	-0.00002	-0.01159	0.00000	-0.01158	3.12023
D65	-0.00405	0.00007	0.00403	0.00000	0.00402	-0.00003
D66	-3.13117	-0.00004	-0.00561	0.00000	-0.00561	-3.13678
D67	3.13936	-0.00009	0.00552	0.00000	0.00550	-3.13832
D68	0.01225	-0.00019	-0.00413	0.00000	-0.00413	0.00812
D69	-0.00152	-0.00004	0.00536	0.00000	0.00536	0.00384
D70	-3.11928	-0.00075	-0.01312	0.00000	-0.01312	-3.13240
D71	3.11261	0.00038	0.00272	0.00000	0.00272	3.11533
D72	-0.00516	-0.00033	-0.01576	0.00000	-0.01575	-0.02091
D73	-0.04158	0.00034	-0.01660	0.00000	-0.01659	-0.05817
D74	-2.98837	0.00006	0.06944	0.00000	0.06944	-2.91893
D75	3.12683	-0.00008	-0.01404	0.00000	-0.01404	3.11280
D76	0.18004	-0.00037	0.07200	0.00000	0.07199	0.25204
D77	-0.02184	0.00014	-0.01471	0.00000	-0.01468	-0.03651
D78	3.12836	0.00018	-0.00099	0.00000	-0.00097	3.12740
D79	3.10977	0.00022	-0.00805	0.00000	-0.00804	3.10172
D80	-0.02322	0.00025	0.00567	0.00000	0.00567	-0.01755
D81	-3.13901	-0.00003	0.00864	0.00000	0.00863	-3.13039
D82	0.01759	-0.00014	-0.00135	0.00000	-0.00135	0.01623
D83	0.03894	-0.00028	0.01921	0.00000	0.01920	0.05813
D84	2.98412	0.00008	-0.06796	0.00000	-0.06791	2.91621
D85	-3.11428	-0.00032	0.00072	0.00000	0.00070	-3.11358
D86	-0.16910	0.00003	-0.08645	0.00000	-0.08640	-0.25550
D87	-3.12460	-0.00010	-0.00505	0.00000	-0.00506	-3.12966
D88	0.01682	-0.00024	-0.00809	0.00000	-0.00809	0.00873
D89	0.02883	-0.00005	0.01378	0.00000	0.01378	0.04261
D90	-3.11293	-0.00019	0.01074	0.00000	0.01074	-3.10219
D91	1.46353	0.00023	-0.05599	0.00000	-0.05609	1.40743
D92	-2.70607	0.00030	-0.05481	0.00000	-0.05491	-2.76098
D93	-0.64364	0.00021	-0.05724	0.00000	-0.05734	-0.70098
D94	-1.44489	-0.00022	0.04606	0.00000	0.04616	-1.39872
D95	0.66870	-0.00015	0.04724	0.00000	0.04734	0.71604
D96	2.73113	-0.00024	0.04481	0.00000	0.04491	2.77604
D97	-0.00815	0.00001	-0.00329	0.00000	-0.00329	-0.01143
D98	3.13590	-0.00004	0.00003	0.00000	0.00003	3.13593
D99	-3.13424	-0.00012	-0.00291	0.00000	-0.00292	-3.13715
D100	0.00753	0.00002	0.00017	0.00000	0.00017	0.00769
D101	-0.00784	-0.00010	-0.00254	0.00000	-0.00254	-0.01037
D102	3.13023	0.00026	0.00283	0.00000	0.00284	3.13306
D103	-0.00332	0.00013	0.00710	0.00000	0.00710	0.00379
D104	3.13815	0.00003	0.00475	0.00000	0.00475	-3.14028

D105	3.13641	0.00017	0.00457	0.00000	0.00457	3.14098
D106	-0.00531	0.00007	0.00222	0.00000	0.00222	-0.00309
D107	3.13842	-0.00009	-0.00743	0.00000	-0.00743	3.13099
D108	-0.01638	-0.00007	-0.01043	0.00000	-0.01043	-0.02681
D109	-0.00076	-0.00014	-0.00416	0.00000	-0.00416	-0.00492
D110	3.12762	-0.00012	-0.00716	0.00000	-0.00716	3.12046
D111	0.00648	0.00016	0.00435	0.00000	0.00435	0.01083
D112	-3.13276	-0.00008	0.00077	0.00000	0.00077	-3.13199
D113	-3.12551	0.00014	0.00655	0.00000	0.00654	-3.11897
D114	0.01843	-0.00010	0.00297	0.00000	0.00296	0.02140
D115	3.12066	0.00013	-0.00131	0.00000	-0.00131	3.11935
D116	0.15703	-0.00012	0.05086	0.00000	0.05085	0.20788
D117	-0.03391	0.00015	-0.00426	0.00000	-0.00425	-0.03816
D118	-2.99754	-0.00010	0.04791	0.00000	0.04790	-2.94963
D119	-3.13378	-0.00034	-0.00561	0.00000	-0.00561	-3.13939
D120	-0.01539	0.00052	0.00709	0.00000	0.00709	-0.00830
D121	0.00440	0.00001	-0.00043	0.00000	-0.00043	0.00398
D122	3.12280	0.00087	0.01227	0.00000	0.01227	3.13507
D123	3.13468	-0.00027	-0.00403	0.00000	-0.00403	3.13065
D124	-0.02565	0.00010	-0.00222	0.00000	-0.00222	-0.02787
D125	0.00874	-0.00086	-0.01260	0.00000	-0.01259	-0.00385
D126	3.13160	-0.00049	-0.01079	0.00000	-0.01078	3.12082
D127	-3.13090	0.00030	0.00104	0.00000	0.00104	-3.12986
D128	-0.01335	0.00119	0.01419	0.00000	0.01419	0.00084
D129	0.00300	-0.00013	0.00258	0.00000	0.00259	0.00559
D130	3.12939	0.00092	0.01483	0.00000	0.01483	-3.13896
D131	-3.11308	-0.00062	0.00011	0.00000	0.00011	-3.11296
D132	0.01331	0.00043	0.01236	0.00000	0.01236	0.02567
D133	0.03672	-0.00014	0.00399	0.00000	0.00398	0.04070
D134	3.00174	0.00003	-0.04775	0.00000	-0.04774	2.95400
D135	-3.12972	0.00034	0.00638	0.00000	0.00638	-3.12334
D136	-0.16469	0.00051	-0.04535	0.00000	-0.04535	-0.21004
D137	-0.01307	0.00106	0.00822	0.00000	0.00822	-0.00486
D138	3.11298	0.00162	0.02046	0.00000	0.02047	3.13346
D139	-3.14015	0.00005	-0.00347	0.00000	-0.00348	3.13956
D140	-0.01410	0.00062	0.00877	0.00000	0.00878	-0.00532
D141	0.01512	-0.00130	-0.01286	0.00000	-0.01286	0.00226
D142	-3.10918	-0.00182	-0.02650	0.00000	-0.02648	-3.13566
D143	-3.06741	-0.00199	-0.07484	0.00000	-0.07484	3.14094
D144	0.08685	-0.00251	-0.08186	0.00000	-0.08186	0.00499
D145	0.05574	-0.00142	-0.06030	0.00000	-0.06030	-0.00456
D146	-3.07318	-0.00193	-0.06732	0.00000	-0.06732	-3.14051
D147	-0.66456	0.00013	-0.02837	0.00000	-0.02840	-0.69296
D148	1.44946	0.00017	-0.02748	0.00000	-0.02751	1.42195
D149	-2.72692	0.00016	-0.02689	0.00000	-0.02692	-2.75384
D150	2.68845	-0.00020	0.03312	0.00000	0.03315	2.72159
D151	-1.48072	-0.00017	0.03401	0.00000	0.03404	-1.44668
D152	0.62609	-0.00017	0.03460	0.00000	0.03463	0.66072
D153	0.01224	-0.00083	-0.00754	0.00000	-0.00753	0.00470
D154	-3.12155	-0.00133	-0.01330	0.00000	-0.01331	-3.13487
D155	3.14061	-0.00027	-0.00022	0.00000	-0.00021	3.14040
D156	0.00682	-0.00078	-0.00598	0.00000	-0.00599	0.00083
D157	3.10904	0.00167	0.02565	0.00000	0.02563	3.13467
D158	0.11392	-0.00371	-0.09816	0.00000	-0.09807	0.01584
D159	-0.03913	0.00208	0.03050	0.00000	0.03049	-0.00863
D160	-3.03425	-0.00330	-0.09331	0.00000	-0.09321	-3.12745
D161	-3.11601	-0.00090	-0.01959	0.00000	-0.01956	-3.13557
D162	0.01940	-0.00037	-0.01269	0.00000	-0.01268	0.00673
D163	0.03227	-0.00137	-0.02452	0.00000	-0.02452	0.00775
D164	-3.11550	-0.00084	-0.01762	0.00000	-0.01763	-3.13314

D165	0.03179	-0.00202	-0.02547	0.00000	-0.02546	0.00633
D166	-3.11629	-0.00171	-0.02123	0.00000	-0.02124	-3.13753
D167	3.02993	0.00371	0.09567	0.00000	0.09575	3.12568
D168	-0.11815	0.00403	0.09990	0.00000	0.09997	-0.01818
D169	-0.01279	0.00008	0.00890	0.00000	0.00888	-0.00390
D170	3.12540	0.00053	0.01353	0.00000	0.01352	3.13892
D171	3.13475	-0.00045	0.00227	0.00000	0.00226	3.13701
D172	-0.01025	0.00000	0.00690	0.00000	0.00690	-0.00335
D173	0.00416	-0.00020	-0.00286	0.00000	-0.00285	0.00130
D174	-3.13688	-0.00027	-0.00370	0.00000	-0.00370	-3.14058
D175	3.13853	0.00044	0.00519	0.00000	0.00518	-3.13947
D176	-0.00251	0.00037	0.00434	0.00000	0.00434	0.00183
D177	-0.01195	0.00120	0.01040	0.00000	0.01041	-0.00154
D178	3.13252	0.00083	0.00650	0.00000	0.00649	3.13901
D179	3.13575	0.00090	0.00642	0.00000	0.00644	-3.14099
D180	-0.00296	0.00053	0.00251	0.00000	0.00252	-0.00044
D181	-3.13138	-0.00084	-0.00704	0.00000	-0.00703	-3.13841
D182	0.00835	-0.00046	-0.00583	0.00000	-0.00582	0.00253
D183	0.00295	-0.00048	-0.00230	0.00000	-0.00231	0.00064
D184	-3.14051	-0.00011	-0.00109	0.00000	-0.00110	3.14158
D185	-3.13666	-0.00072	-0.00627	0.00000	-0.00628	3.14025
D186	0.00515	-0.00055	-0.00621	0.00000	-0.00622	-0.00107
D187	0.00125	-0.00024	-0.00126	0.00000	-0.00127	-0.00001
D188	-3.14013	-0.00007	-0.00121	0.00000	-0.00121	-3.14134
D189	-0.00130	0.00016	0.00089	0.00000	0.00090	-0.00040
D190	3.14072	0.00019	0.00055	0.00000	0.00055	3.14127
D191	-3.14097	-0.00023	-0.00035	0.00000	-0.00035	-3.14132
D192	0.00105	-0.00019	-0.00069	0.00000	-0.00069	0.00036
D193	0.00030	-0.00007	-0.00005	0.00000	-0.00006	0.00024
D194	3.14136	0.00008	0.00025	0.00000	0.00025	-3.14158
D195	-3.14150	-0.00024	-0.00011	0.00000	-0.00011	3.14157
D196	-0.00044	-0.00009	0.00020	0.00000	0.00020	-0.00025
D197	-0.00028	0.00012	0.00025	0.00000	0.00025	-0.00003
D198	-3.14134	-0.00003	-0.00006	0.00000	-0.00006	-3.14140
D199	3.14089	0.00008	0.00059	0.00000	0.00059	3.14148
D200	-0.00017	-0.00007	0.00028	0.00000	0.00028	0.00011

Item	Value	Threshold	Converged?

Maximum Force	0.009967	0.000450	NO

RMS Force	0.001418	0.000300	NO

Maximum Displacement	0.456933	0.001800	NO

RMS Displacement	0.083399	0.001200	NO

Predicted change in Energy=-4.964579D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.795600	-0.631076	0.027736
2	6	0	-9.989447	-1.783827	0.012220
3	6	0	-10.514970	-3.067241	0.011257
4	6	0	-11.904202	-3.206247	0.024847
5	6	0	-12.722526	-2.069993	0.039390

6	6	0	-12.187056	-0.777667	0.041759
7	1	0	-9.846303	-3.922006	0.000197
8	1	0	-12.353742	-4.194415	0.023924
9	1	0	-13.801708	-2.188494	0.049098
10	1	0	-12.855047	0.072244	0.053246
11	6	0	-9.916359	0.567516	0.027123
12	6	0	-8.564428	-1.390646	-0.002369
13	6	0	-8.530668	0.089435	-0.000761
14	6	0	-7.390115	0.870092	-0.031595
15	6	0	-5.998635	0.589874	-0.055911
16	6	0	-3.633119	-0.187975	-0.065110
17	6	0	-3.764651	1.222595	-0.100265
18	16	0	-5.168149	-0.996388	-0.047450
19	6	0	-5.083249	1.657412	-0.097955
20	6	0	-2.255907	-0.455124	-0.053350
21	6	0	-1.593336	0.792557	-0.081548
22	7	0	-2.511019	1.816686	-0.157397
23	16	0	-1.143890	-1.812298	-0.021208
24	16	0	1.157181	1.800319	-0.053279
25	6	0	0.204481	-0.678783	-0.017628
26	6	0	-0.191409	0.667682	-0.054772
27	6	0	1.607499	-0.803654	0.008366
28	6	0	2.270329	0.444036	-0.015464
29	6	0	3.643715	0.177558	0.001112
30	6	0	3.776631	-1.234129	0.029354
31	6	0	5.094365	-1.669842	0.034807
32	6	0	6.007960	-0.601752	0.018122
33	16	0	5.179859	0.983536	-0.012954
34	7	0	2.524275	-1.827080	0.066611
35	6	0	7.389336	-0.876301	0.031111
36	6	0	8.522005	-0.091991	0.020700
37	6	0	8.543526	1.387632	-0.004394
38	6	0	9.913943	-0.561223	0.029879
39	6	0	9.965338	1.792449	0.002200
40	6	0	10.782557	0.646937	0.021161
41	6	0	10.478130	3.079437	-0.010474
42	6	0	12.173577	0.808647	0.027030
43	6	0	11.866022	3.232880	-0.004777
44	6	0	12.695570	2.106435	0.013746
45	6	0	10.372973	-1.867664	0.043222
46	6	0	9.517627	-3.013823	0.048888
47	6	0	11.757799	-2.228472	0.052607
48	7	0	8.837329	-3.960295	0.053451
49	7	0	12.875366	-2.557729	0.060610
50	6	0	-10.365401	1.875359	0.060564
51	6	0	-11.746308	2.241911	0.087955
52	6	0	-9.504066	3.015426	0.077506
53	7	0	-12.861669	2.577819	0.110338
54	7	0	-8.828355	3.965160	0.091172
55	8	0	-7.610161	-2.159981	-0.013013
56	8	0	7.582392	2.148954	-0.004408
57	6	0	2.249179	-3.241175	-0.117066
58	1	0	1.303305	-3.494705	0.366638
59	1	0	2.195540	-3.509481	-1.178087
60	1	0	3.040077	-3.823903	0.359823
61	6	0	-2.238883	3.226645	0.056089
62	1	0	-2.197581	3.473922	1.122806
63	1	0	-1.287890	3.490829	-0.411389
64	1	0	-3.023583	3.819096	-0.419143
65	1	0	5.422443	-2.702675	0.052568

66	1	0	12.850912	-0.033727	0.041172
67	1	0	13.773491	2.236438	0.018220
68	1	0	12.305581	4.225465	-0.014610
69	1	0	9.800504	3.927023	-0.024956
70	1	0	7.555024	-1.946759	0.048572
71	1	0	-7.552564	1.941014	-0.046430
72	1	0	-5.411171	2.690244	-0.129399

Rotational constants (GHZ): 0.1748697 0.0104386 0.0098527

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6575.9551145675 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T

Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6575.8700732372 Hartrees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.24D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Lowest energy guess from the checkpoint file: "PBDB.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000106 -0.000004 -0.000129 Ang= 0.02 deg.

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000290 -0.000007 0.000305 Ang= -0.05 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Integral accuracy reduced to 1.0D-05 until final iterations.

Initial convergence to 1.0D-05 achieved. Increase integral accuracy.

SCF Done: E(RB3LYP) = -3683.01939063 A.U. after 11 cycles

NFock= 11 Conv=0.84D-08 -V/T= 2.0068

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1

NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-0.000043295	0.000083026	0.000120027
2	6	-0.000134280	-0.000068720	-0.000048792
3	6	0.000095514	0.000218976	0.000088815
4	6	-0.000043134	0.000081152	-0.000025581
5	6	-0.000026765	-0.000074922	-0.000049996
6	6	-0.000299914	0.000013525	-0.000180250
7	1	-0.000071771	0.000001683	-0.000029281
8	1	-0.000028234	0.000010030	-0.000030656
9	1	0.000072519	0.000049398	0.000046412
10	1	0.000103548	-0.000162786	0.000072544
11	6	0.000819912	-0.000143776	0.000332425
12	6	-0.000023995	-0.000709724	-0.000628275
13	6	0.000985339	-0.002576871	0.000542164
14	6	0.000490011	0.002338307	0.001480430

15	6	-0.002621894	0.001539051	-0.000697340
16	6	0.001218364	0.000375812	0.000675427
17	6	-0.001139393	-0.000166600	0.002261339
18	16	-0.000068515	-0.000348170	-0.001310543
19	6	-0.001892794	-0.000058458	-0.001599335
20	6	-0.000105914	0.001215764	0.000185657
21	6	-0.001567007	0.000219903	0.001134323
22	7	0.002302142	0.001374201	-0.003257176
23	16	-0.000092645	-0.000423261	-0.000430448
24	16	0.000110889	0.000002806	-0.000009103
25	6	-0.000131760	0.000941869	0.000111388
26	6	0.000759330	-0.001204329	0.000494127
27	6	-0.000537971	0.000656636	-0.000957940
28	6	-0.001749962	-0.000114613	-0.001476998
29	6	0.000790078	-0.001336288	0.001516764
30	6	0.000582725	-0.000119074	-0.001229094
31	6	0.001274117	0.001172803	0.000764959
32	6	-0.002965282	0.000718796	-0.002130196
33	16	-0.000392706	0.000579433	-0.001080803
34	7	-0.001131172	0.000490781	0.002272948
35	6	0.003254097	-0.001441395	0.003169772
36	6	0.001266540	-0.002299503	0.001844854
37	6	0.002883653	0.000929062	-0.001291228
38	6	-0.001062126	0.000308922	-0.000957983
39	6	-0.000104771	0.000946899	0.001099602
40	6	0.000410593	-0.000132575	0.000545997
41	6	-0.000354655	-0.001207112	-0.000357633
42	6	-0.000233896	0.001026849	-0.000080951
43	6	-0.000480039	-0.000468256	-0.000537078
44	6	0.000618794	0.000302862	0.000481277
45	6	0.001306388	0.000659363	0.001008216
46	6	-0.000183535	-0.000817046	-0.000212840
47	6	-0.001774601	-0.000883669	-0.001475403
48	7	0.000337145	0.000011029	0.000260235
49	7	-0.000153933	0.000117826	-0.000097211
50	6	-0.000930535	-0.001041465	-0.000962756
51	6	0.000451647	0.000800777	0.000523270
52	6	-0.000531348	-0.000170616	-0.000233369
53	7	0.000053972	-0.000119925	0.000024965
54	7	0.000039909	0.000068892	-0.000014791
55	8	0.000492916	-0.000171806	0.000638266
56	8	-0.000820258	-0.000734832	0.000746342
57	6	0.000705901	0.000797619	-0.000610261
58	1	0.000095856	-0.000008959	0.000140766
59	1	0.000006495	-0.000099598	-0.000171113
60	1	-0.000127264	0.000034409	-0.000017209
61	6	-0.000776226	-0.001414032	0.000248755
62	1	-0.000106482	-0.000062037	0.000080354
63	1	0.000016501	0.000110078	0.000020526
64	1	0.000142919	0.000124735	-0.000037177
65	1	0.000028452	-0.000139699	0.000066098
66	1	0.000028442	0.000436392	0.000043050
67	1	-0.000048123	0.000007359	-0.000022807
68	1	-0.000033829	-0.000009756	-0.000029204
69	1	0.000032658	-0.000104169	0.000033567
70	1	0.000355067	-0.000698738	-0.000051999
71	1	0.000177119	0.000459063	-0.000170588
72	1	0.000480472	0.000306692	-0.000572255

Cartesian Forces: Max 0.003257176 RMS 0.000928062

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 GSVD: received Info= 1 from GESDD.
 Internal Forces: Max 0.007747513 RMS 0.000851644
 Search for a local minimum.
 Step number 17 out of a maximum of 429
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Update second derivatives using D2CorX and points 14 16 15 17
 ITU= 0 -1 1 1 1 1 1 1 0 0 0 1 0 0 0 1 0
 Use linear search instead of GDIIS.

Eigenvalues ---	0.00229	0.00231	0.00231	0.00238	0.00281
Eigenvalues ---	0.00346	0.00388	0.00434	0.00447	0.00465
Eigenvalues ---	0.00488	0.00506	0.00571	0.00587	0.00606
Eigenvalues ---	0.00623	0.00641	0.00672	0.00682	0.00700
Eigenvalues ---	0.00713	0.00721	0.00744	0.00760	0.00770
Eigenvalues ---	0.00781	0.00816	0.00832	0.00844	0.00851
Eigenvalues ---	0.00872	0.01007	0.01086	0.01130	0.01143
Eigenvalues ---	0.01182	0.01207	0.01257	0.01336	0.01360
Eigenvalues ---	0.01365	0.01387	0.01430	0.01456	0.01468
Eigenvalues ---	0.01571	0.01646	0.01652	0.01754	0.01771
Eigenvalues ---	0.01794	0.01838	0.01929	0.01953	0.02006
Eigenvalues ---	0.02022	0.02075	0.02075	0.02208	0.02210
Eigenvalues ---	0.03422	0.04828	0.04837	0.04901	0.04944
Eigenvalues ---	0.04979	0.05011	0.05018	0.05308	0.07045
Eigenvalues ---	0.07227	0.07385	0.07575	0.15522	0.15602
Eigenvalues ---	0.15963	0.15985	0.15999	0.16000	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues ---	0.16001	0.16002	0.16002	0.16018	0.16030
Eigenvalues ---	0.16049	0.17482	0.18393	0.19157	0.19648
Eigenvalues ---	0.19829	0.20582	0.21337	0.21422	0.22001
Eigenvalues ---	0.22012	0.22134	0.22263	0.22535	0.22601
Eigenvalues ---	0.22637	0.22643	0.22682	0.22961	0.23027
Eigenvalues ---	0.23178	0.23348	0.23410	0.23506	0.23767
Eigenvalues ---	0.23796	0.23918	0.24074	0.24220	0.24285
Eigenvalues ---	0.24317	0.24496	0.24572	0.24604	0.24751
Eigenvalues ---	0.24783	0.24879	0.24912	0.24978	0.24988
Eigenvalues ---	0.24991	0.24994	0.24995	0.24996	0.24998
Eigenvalues ---	0.24999	0.25000	0.25000	0.25000	0.25000
Eigenvalues ---	0.25001	0.25009	0.25133	0.25583	0.25902
Eigenvalues ---	0.26227	0.26492	0.26718	0.26804	0.27053
Eigenvalues ---	0.27224	0.27640	0.27829	0.28130	0.28268
Eigenvalues ---	0.28519	0.28652	0.29822	0.30008	0.31387
Eigenvalues ---	0.32137	0.32595	0.35341	0.35741	0.36314
Eigenvalues ---	0.36337	0.36456	0.36475	0.36626	0.36653
Eigenvalues ---	0.36775	0.36827	0.37081	0.37094	0.37141
Eigenvalues ---	0.37252	0.37270	0.37421	0.37565	0.37673
Eigenvalues ---	0.37757	0.37915	0.38829	0.40304	0.40638
Eigenvalues ---	0.41574	0.42051	0.42285	0.42759	0.44422
Eigenvalues ---	0.44788	0.45592	0.46411	0.47460	0.47833
Eigenvalues ---	0.48016	0.51068	0.52798	0.54437	0.56032
Eigenvalues ---	0.57389	0.72224	0.73891	0.80346	0.81959
Eigenvalues ---	0.90761	1.25851	1.26315	1.29341	1.35383

 RFO step: Lambda=-1.92984346D-03 EMin= 2.29221216D-03
 Quartic linear search produced a step of 0.00191.
 Iteration 1 RMS(Cart)= 0.07523679 RMS(Int)= 0.00061842
 Iteration 2 RMS(Cart)= 0.00236022 RMS(Int)= 0.00033210

Iteration	3	RMS(Cart)=	0.00000099	RMS(Int)=	0.00033210	
Variable	Old X	-DE/DX	Delta X	Delta X	Delta X	New X
(Linear)	(Quad)	(Total)				
R1	2.65838	-0.00008	0.00000	-0.00016	-0.00016	2.65822
R2	2.64416	0.00000	0.00000	0.00130	0.00130	2.64545
R3	2.80908	-0.00003	0.00000	-0.00147	-0.00147	2.80762
R4	2.62075	0.00028	0.00000	0.00222	0.00222	2.62297
R5	2.79365	0.00022	0.00000	0.00562	0.00563	2.79928
R6	2.63850	0.00014	0.00000	-0.00009	-0.00009	2.63841
R7	2.05091	-0.00007	0.00000	-0.00065	-0.00065	2.05026
R8	2.64625	0.00003	0.00000	-0.00010	-0.00010	2.64615
R9	2.05152	0.00000	0.00000	-0.00006	-0.00006	2.05146
R10	2.64348	0.00000	0.00000	-0.00032	-0.00032	2.64317
R11	2.05170	-0.00003	0.00000	-0.00028	-0.00028	2.05142
R12	2.04291	-0.00008	0.00000	-0.00246	-0.00246	2.04044
R13	2.77055	0.00027	0.00000	-0.00295	-0.00295	2.76759
R14	2.61385	0.00119	0.00000	0.00217	0.00217	2.61602
R15	2.79768	-0.00041	0.00000	0.00173	0.00173	2.79941
R16	2.31645	0.00078	0.00000	0.00021	0.00021	2.31666
R17	2.61250	-0.00401	0.00001	0.00568	0.00570	2.61819
R18	2.68270	-0.00248	0.00000	-0.00584	-0.00584	2.67686
R19	2.04709	-0.00033	0.00000	0.00120	0.00120	2.04830
R20	3.38361	-0.00012	0.00000	-0.00655	-0.00664	3.37697
R21	2.65864	0.00034	0.00000	0.00344	0.00340	2.66203
R22	2.67798	0.00088	0.00000	0.00437	0.00428	2.68226
R23	3.27864	0.00015	0.00001	0.00890	0.00892	3.28756
R24	2.65116	0.00071	0.00000	0.00668	0.00614	2.65730
R25	2.62378	0.00277	0.00000	0.00892	0.00897	2.63275
R26	2.62379	0.00092	0.00000	0.00097	0.00140	2.62519
R27	2.04864	-0.00018	0.00000	-0.00144	-0.00144	2.04720
R28	2.67014	0.00067	0.00000	0.00635	0.00628	2.67642
R29	3.31621	0.00029	0.00000	0.00407	0.00405	3.32026
R30	2.60257	0.00135	0.00000	-0.00006	0.00039	2.60296
R31	2.66023	0.00279	0.00000	0.01539	0.01547	2.67570
R32	2.74344	0.00108	0.00000	-0.00059	-0.00060	2.74284
R33	3.32880	0.00035	0.00000	0.00334	0.00326	3.33207
R34	3.32804	0.00055	0.00000	0.00393	0.00391	3.33195
R35	3.31647	0.00043	0.00000	0.00397	0.00395	3.32043
R36	2.65308	0.00072	0.00000	0.00119	0.00118	2.65427
R37	2.66225	0.00192	0.00001	0.01700	0.01703	2.67929
R38	2.67023	0.00111	0.00000	0.00413	0.00408	2.67432
R39	2.59882	0.00221	0.00000	0.00617	0.00636	2.60518
R40	2.64391	0.00343	0.00000	0.01107	0.01083	2.65474
R41	2.68003	0.00053	0.00000	0.00180	0.00176	2.68179
R42	3.27830	0.00075	0.00000	0.00314	0.00314	3.28144
R43	2.62277	0.00292	0.00000	0.01514	0.01517	2.63794
R44	2.61942	0.00240	0.00000	0.00480	0.00499	2.62440
R45	2.65623	0.00248	0.00000	0.00684	0.00684	2.66306
R46	2.04815	-0.00003	0.00000	-0.00011	-0.00011	2.04804
R47	3.38037	0.00137	0.00000	0.00386	0.00382	3.38419
R48	2.66159	0.00775	0.00000	0.03126	0.03126	2.69286
R49	2.74439	0.00048	0.00000	-0.00247	-0.00247	2.74191
R50	2.60357	0.00243	0.00000	0.00535	0.00535	2.60892
R51	2.04723	-0.00032	0.00000	-0.00028	-0.00028	2.04695
R52	2.79678	0.00018	0.00000	0.00165	0.00184	2.79862
R53	2.77587	-0.00117	0.00000	-0.00192	-0.00204	2.77384
R54	2.79365	0.00021	0.00000	0.00501	0.00525	2.79889
R55	2.31705	0.00020	0.00000	-0.00037	-0.00037	2.31668
R56	2.81196	-0.00167	0.00000	-0.00345	-0.00371	2.80825
R57	2.61690	-0.00108	0.00001	0.00566	0.00566	2.62256

R58	2.65935	-0.00104	0.00000	-0.00087	-0.00089	2.65846
R59	2.61811	0.00141	0.00000	0.00717	0.00720	2.62531
R60	2.64637	-0.00125	0.00000	0.00271	0.00271	2.64909
R61	2.63874	0.00021	0.00000	-0.00123	-0.00123	2.63751
R62	2.05084	-0.00002	0.00000	-0.00047	-0.00047	2.05037
R63	2.64353	0.00015	0.00000	-0.00010	-0.00013	2.64340
R64	2.04281	0.00016	0.00000	-0.00397	-0.00398	2.03883
R65	2.64384	0.00104	0.00000	0.00549	0.00547	2.64931
R66	2.05149	0.00002	0.00000	-0.00010	-0.00010	2.05139
R67	2.05175	-0.00004	0.00000	-0.00027	-0.00027	2.05148
R68	2.70259	-0.00081	0.00000	-0.00200	-0.00200	2.70059
R69	2.70436	-0.00201	0.00000	-0.00040	-0.00040	2.70397
R70	2.20267	0.00002	0.00000	-0.00029	-0.00029	2.20239
R71	2.20170	-0.00021	0.00000	0.00033	0.00033	2.20203
R72	2.70040	-0.00042	0.00000	0.00216	0.00216	2.70256
R73	2.70035	0.00009	0.00000	-0.00029	-0.00029	2.70006
R74	2.20164	-0.00010	0.00000	0.00032	0.00033	2.20197
R75	2.20278	-0.00007	0.00000	-0.00021	-0.00021	2.20257
R76	2.06398	-0.00012	0.00000	-0.00041	-0.00041	2.06357
R77	2.07063	-0.00016	0.00000	-0.00075	-0.00075	2.06989
R78	2.06363	-0.00013	0.00000	-0.00034	-0.00034	2.06328
R79	2.07073	-0.00012	0.00000	0.00010	0.00010	2.07082
R80	2.06380	-0.00007	0.00000	0.00042	0.00042	2.06422
R81	2.06370	-0.00014	0.00000	-0.00014	-0.00014	2.06356
A1	2.07617	0.00019	0.00000	0.00307	0.00307	2.07924
A2	1.89839	0.00035	0.00000	0.00114	0.00113	1.89952
A3	2.30862	-0.00054	0.00000	-0.00421	-0.00420	2.30442
A4	2.14264	-0.00014	0.00000	-0.00243	-0.00243	2.14021
A5	1.91193	-0.00016	0.00000	-0.00212	-0.00213	1.90980
A6	2.22861	0.00030	0.00000	0.00455	0.00456	2.23317
A7	2.05914	-0.00004	0.00000	-0.00050	-0.00051	2.05863
A8	2.08908	0.00004	0.00000	0.00118	0.00118	2.09026
A9	2.13497	0.00000	0.00000	-0.00067	-0.00067	2.13430
A10	2.09528	0.00004	0.00000	0.00197	0.00198	2.09725
A11	2.09743	0.00002	0.00000	-0.00069	-0.00069	2.09674
A12	2.09048	-0.00006	0.00000	-0.00128	-0.00128	2.08920
A13	2.12462	0.00000	0.00000	-0.00042	-0.00042	2.12420
A14	2.08563	-0.00010	0.00000	-0.00133	-0.00133	2.08430
A15	2.07294	0.00010	0.00000	0.00174	0.00174	2.07468
A16	2.06852	-0.00005	0.00000	-0.00169	-0.00169	2.06684
A17	2.13201	-0.00017	0.00000	-0.00191	-0.00191	2.13010
A18	2.08265	0.00022	0.00000	0.00360	0.00360	2.08625
A19	1.87142	-0.00047	0.00000	0.00182	0.00180	1.87322
A20	2.17775	-0.00194	-0.00001	-0.01039	-0.01039	2.16736
A21	2.23397	0.00241	0.00001	0.00859	0.00860	2.24257
A22	1.86279	-0.00009	0.00000	-0.00047	-0.00049	1.86230
A23	2.19391	0.00025	0.00000	0.00221	0.00223	2.19613
A24	2.22649	-0.00016	0.00000	-0.00174	-0.00173	2.22476
A25	1.88018	0.00037	0.00000	-0.00023	-0.00026	1.87992
A26	2.20936	0.00110	0.00000	-0.00213	-0.00213	2.20723
A27	2.19361	-0.00147	0.00000	0.00242	0.00243	2.19604
A28	2.34280	-0.00118	0.00000	-0.00513	-0.00525	2.33755
A29	2.02064	0.00030	0.00000	-0.00046	-0.00058	2.02006
A30	1.91973	0.00089	0.00000	0.00574	0.00562	1.92534
A31	2.25160	-0.00091	-0.00001	-0.00998	-0.00992	2.24168
A32	2.08114	0.00109	0.00001	0.01032	0.01040	2.09154
A33	1.95044	-0.00018	0.00000	-0.00028	-0.00051	1.94992
A34	1.96268	-0.00100	0.00000	-0.00477	-0.00462	1.95805
A35	1.85549	0.00051	0.00000	0.00125	0.00093	1.85642
A36	2.46502	0.00048	0.00000	0.00354	0.00366	2.46868

A37	1.98212	0.00038	0.00000	-0.00044	-0.00076	1.98137
A38	1.92103	-0.00061	0.00000	-0.00244	-0.00190	1.91914
A39	2.37973	0.00023	0.00000	0.00333	0.00294	2.38266
A40	1.56832	0.00128	0.00000	0.00514	0.00489	1.57321
A41	1.96095	-0.00047	0.00000	0.00115	0.00106	1.96201
A42	2.12583	0.00005	0.00000	0.00030	0.00030	2.12613
A43	2.19639	0.00042	0.00000	-0.00151	-0.00151	2.19489
A44	1.86712	0.00002	0.00000	-0.00046	-0.00082	1.86630
A45	2.44883	0.00057	0.00000	0.00460	0.00462	2.45344
A46	1.96723	-0.00059	0.00000	-0.00420	-0.00399	1.96324
A47	1.92333	-0.00033	0.00000	-0.00187	-0.00143	1.92189
A48	1.96956	0.00001	0.00000	0.00003	-0.00023	1.96932
A49	2.38999	0.00033	0.00000	0.00257	0.00197	2.39196
A50	1.85582	0.00045	0.00000	0.00705	0.00515	1.86098
A51	2.18800	0.00008	0.00001	0.01687	0.01326	2.20126
A52	2.20087	-0.00034	0.00001	0.01345	0.00977	2.21064
A53	1.55823	0.00121	0.00000	0.00593	0.00586	1.56408
A54	1.55949	0.00087	0.00000	0.00481	0.00480	1.56430
A55	1.98366	-0.00061	0.00000	-0.00205	-0.00209	1.98157
A56	2.35366	0.00058	0.00000	0.00238	0.00234	2.35600
A57	1.94585	0.00004	0.00000	-0.00031	-0.00024	1.94561
A58	2.35401	0.00042	0.00000	0.00112	0.00103	2.35505
A59	1.94593	-0.00001	0.00000	0.00032	0.00045	1.94638
A60	1.98324	-0.00041	0.00000	-0.00143	-0.00148	1.98176
A61	1.96989	0.00002	0.00000	-0.00054	-0.00064	1.96925
A62	2.39005	0.00054	0.00000	0.00340	0.00316	2.39321
A63	1.92316	-0.00056	0.00000	-0.00287	-0.00254	1.92062
A64	1.96624	-0.00052	0.00000	-0.00250	-0.00243	1.96381
A65	2.44974	0.00038	0.00000	0.00291	0.00291	2.45264
A66	1.86720	0.00014	0.00000	-0.00041	-0.00048	1.86673
A67	1.85649	0.00016	0.00000	0.00172	0.00164	1.85813
A68	2.46647	0.00028	0.00000	0.00157	0.00157	2.46804
A69	1.96019	-0.00044	0.00000	-0.00326	-0.00319	1.95701
A70	1.98401	-0.00009	0.00000	0.00068	0.00057	1.98458
A71	1.91948	-0.00035	0.00000	-0.00259	-0.00229	1.91720
A72	2.37952	0.00044	0.00000	0.00210	0.00186	2.38138
A73	1.95897	0.00063	0.00000	0.00069	0.00072	1.95969
A74	2.19768	-0.00016	0.00000	-0.00042	-0.00046	2.19722
A75	2.12653	-0.00047	0.00000	-0.00024	-0.00028	2.12625
A76	1.95275	-0.00174	0.00000	-0.00520	-0.00523	1.94752
A77	2.08201	-0.00041	0.00000	0.00520	0.00519	2.08720
A78	2.24842	0.00215	0.00000	-0.00003	-0.00004	2.24838
A79	1.56884	0.00165	0.00000	0.00714	0.00709	1.57594
A80	1.85752	0.00062	0.00000	0.00469	0.00410	1.86163
A81	2.20556	-0.00041	0.00001	0.00653	0.00503	2.21059
A82	2.19478	-0.00013	0.00001	0.00771	0.00622	2.20100
A83	2.33960	0.00352	-0.00001	0.00258	0.00257	2.34217
A84	1.92065	-0.00105	0.00001	0.00532	0.00532	1.92597
A85	2.02293	-0.00247	0.00000	-0.00789	-0.00789	2.01504
A86	2.19101	0.00193	0.00000	0.00431	0.00420	2.19521
A87	2.21072	-0.00095	0.00000	-0.00271	-0.00282	2.20790
A88	1.88145	-0.00097	0.00000	-0.00160	-0.00138	1.88007
A89	1.86259	0.00035	0.00000	0.00068	-0.00018	1.86242
A90	2.22605	0.00055	0.00000	-0.00012	-0.00184	2.22421
A91	2.19430	-0.00089	0.00000	0.00149	-0.00024	2.19405
A92	1.86894	0.00096	0.00000	0.00221	0.00198	1.87092
A93	2.23385	0.00288	0.00000	0.01208	0.01219	2.24604
A94	2.18040	-0.00384	0.00000	-0.01430	-0.01419	2.16620
A95	1.91311	-0.00062	0.00000	-0.00295	-0.00265	1.91046
A96	2.22725	0.00081	0.00000	0.00530	0.00510	2.23234

A97	2.14282	-0.00019	0.00000	-0.00233	-0.00245	2.14037
A98	1.89863	0.00029	0.00000	0.00200	0.00186	1.90050
A99	2.30981	-0.00119	0.00000	-0.00615	-0.00610	2.30371
A100	2.07474	0.00091	0.00000	0.00414	0.00424	2.07898
A101	2.06000	-0.00037	0.00000	-0.00126	-0.00121	2.05879
A102	2.08807	0.00030	0.00000	0.00240	0.00238	2.09045
A103	2.13511	0.00007	0.00000	-0.00114	-0.00117	2.13394
A104	2.06887	-0.00013	0.00000	-0.00218	-0.00219	2.06668
A105	2.13229	-0.00035	0.00000	-0.00196	-0.00195	2.13034
A106	2.08202	0.00048	0.00000	0.00413	0.00414	2.08616
A107	2.09545	-0.00018	0.00000	0.00211	0.00212	2.09758
A108	2.09772	0.00005	0.00000	-0.00129	-0.00129	2.09643
A109	2.09001	0.00013	0.00000	-0.00082	-0.00083	2.08918
A110	2.12448	-0.00004	0.00000	-0.00049	-0.00051	2.12397
A111	2.07317	0.00005	0.00000	0.00201	0.00202	2.07519
A112	2.08554	-0.00001	0.00000	-0.00153	-0.00151	2.08402
A113	2.16261	0.00236	0.00000	0.01163	0.01164	2.17424
A114	2.16359	-0.00336	0.00000	-0.01526	-0.01526	2.14833
A115	1.95699	0.00101	0.00000	0.00363	0.00362	1.96061
A116	2.16123	-0.00198	-0.00001	-0.01356	-0.01357	2.14766
A117	2.16394	0.00170	0.00000	0.00597	0.00597	2.16991
A118	1.95801	0.00029	0.00000	0.00761	0.00761	1.96562
A119	1.91140	0.00020	0.00000	0.00160	0.00160	1.91300
A120	1.94999	-0.00021	0.00000	-0.00243	-0.00243	1.94756
A121	1.90411	0.00006	0.00000	0.00181	0.00181	1.90592
A122	1.90668	-0.00001	0.00000	-0.00056	-0.00056	1.90612
A123	1.88593	-0.00009	0.00000	0.00013	0.00013	1.88606
A124	1.90462	0.00005	0.00000	-0.00047	-0.00047	1.90414
A125	1.94914	0.00016	0.00000	0.00308	0.00308	1.95222
A126	1.91263	-0.00013	0.00000	0.00185	0.00185	1.91448
A127	1.90519	-0.00013	0.00000	0.00366	0.00366	1.90885
A128	1.90634	0.00001	0.00000	-0.00346	-0.00347	1.90287
A129	1.90529	-0.00004	0.00000	-0.00494	-0.00494	1.90034
A130	1.88409	0.00012	0.00000	-0.00032	-0.00033	1.88376
A131	3.15949	0.00094	0.00000	0.01777	0.01777	3.17726
A132	3.17323	0.00011	0.00000	0.00428	0.00429	3.17751
A133	3.17465	0.00020	-0.00001	-0.00674	-0.00675	3.16790
A134	3.17021	-0.00004	0.00001	0.00279	0.00280	3.17301
A135	3.14144	0.00000	0.00000	0.00115	0.00115	3.14259
A136	3.14158	0.00001	0.00000	-0.00024	-0.00024	3.14134
A137	3.14175	0.00000	0.00000	0.00118	0.00118	3.14293
A138	3.14079	0.00010	0.00000	0.00012	0.00012	3.14091
D1	-0.00092	-0.00001	0.00000	-0.00025	-0.00025	-0.00117
D2	3.14039	-0.00002	0.00000	-0.00256	-0.00256	3.13783
D3	3.13950	0.00001	0.00000	-0.00016	-0.00017	3.13933
D4	-0.00237	-0.00001	0.00000	-0.00247	-0.00248	-0.00485
D5	-0.00031	0.00003	0.00000	0.00145	0.00145	0.00114
D6	-3.14078	0.00001	0.00000	-0.00075	-0.00075	-3.14153
D7	-3.14041	0.00001	0.00000	0.00133	0.00134	-3.13907
D8	0.00230	-0.00001	0.00000	-0.00086	-0.00085	0.00145
D9	0.00800	0.00001	-0.00001	-0.00610	-0.00611	0.00188
D10	-3.12366	-0.00010	-0.00001	-0.00778	-0.00778	-3.13143
D11	-3.13498	0.00003	-0.00001	-0.00599	-0.00601	-3.14099
D12	0.01655	-0.00008	-0.00001	-0.00767	-0.00768	0.00888
D13	0.00128	-0.00002	0.00000	-0.00105	-0.00105	0.00023
D14	-3.14026	-0.00001	0.00000	-0.00068	-0.00067	-3.14093
D15	-3.13998	0.00000	0.00000	0.00170	0.00171	-3.13826
D16	0.00167	0.00000	0.00000	0.00208	0.00208	0.00376
D17	-0.00410	-0.00001	0.00002	0.01000	0.01000	0.00590
D18	3.13699	0.00010	-0.00002	0.00914	0.00912	-3.13708

D19	3.13719	-0.00002	0.00002	0.00754	0.00754	-3.13845
D20	-0.00490	0.00008	-0.00002	0.00668	0.00665	0.00175
D21	-0.00041	0.00002	0.00000	0.00112	0.00112	0.00070
D22	3.14091	0.00001	0.00000	0.00046	0.00046	3.14137
D23	3.14113	0.00002	0.00000	0.00073	0.00073	-3.14133
D24	-0.00074	0.00001	0.00000	0.00008	0.00008	-0.00066
D25	-0.00080	0.00000	0.00000	0.00009	0.00009	-0.00072
D26	3.14075	0.00000	0.00000	-0.00015	-0.00015	3.14060
D27	3.14106	0.00001	0.00000	0.00074	0.00074	-3.14138
D28	-0.00057	0.00000	0.00000	0.00050	0.00050	-0.00007
D29	0.00116	-0.00003	0.00000	-0.00139	-0.00139	-0.00023
D30	-3.14152	-0.00001	0.00000	0.00074	0.00075	-3.14077
D31	-3.14040	-0.00002	0.00000	-0.00115	-0.00115	-3.14155
D32	0.00011	0.00000	0.00000	0.00098	0.00098	0.00109
D33	-0.01041	-0.00002	0.00002	0.01217	0.01221	0.00180
D34	3.12247	-0.00002	0.00002	0.01938	0.01940	-3.14132
D35	3.12083	0.00006	0.00002	0.01379	0.01382	3.13465
D36	-0.02949	0.00006	0.00002	0.02099	0.02101	-0.00847
D37	-0.01042	0.00003	0.00000	0.00013	0.00012	-0.01030
D38	3.12630	0.00016	0.00000	0.00673	0.00672	3.13302
D39	-3.13997	-0.00008	0.00000	-0.00184	-0.00183	3.14139
D40	-0.00325	0.00005	0.00000	0.00476	0.00477	0.00152
D41	0.00899	0.00002	-0.00003	-0.01359	-0.01361	-0.00462
D42	-3.12398	0.00000	-0.00003	-0.02069	-0.02071	3.13849
D43	-3.13209	-0.00009	0.00001	-0.01271	-0.01270	3.13839
D44	0.01812	-0.00011	0.00001	-0.01981	-0.01981	-0.00169
D45	3.13665	-0.00002	-0.00002	-0.01410	-0.01410	3.12255
D46	-0.01157	0.00018	0.00000	0.01839	0.01837	0.00680
D47	-0.01517	-0.00001	-0.00002	-0.00567	-0.00567	-0.02084
D48	3.11979	0.00019	0.00000	0.02682	0.02680	-3.13659
D49	-0.00551	-0.00007	-0.00003	0.00340	0.00339	-0.00211
D50	3.13138	0.00031	-0.00004	0.01881	0.01879	-3.13302
D51	-3.14074	-0.00026	-0.00005	-0.02772	-0.02778	3.11466
D52	-0.00386	0.00011	-0.00005	-0.01231	-0.01239	-0.01624
D53	-3.12589	-0.00013	-0.00002	-0.01841	-0.01856	3.13874
D54	0.02013	-0.00049	-0.00001	-0.03292	-0.03296	-0.01284
D55	3.12820	0.00025	0.00002	0.02517	0.02509	-3.12990
D56	-0.01851	0.00030	0.00000	0.01212	0.01206	-0.00645
D57	-0.01733	0.00056	0.00001	0.03803	0.03804	0.02071
D58	3.11915	0.00061	-0.00001	0.02498	0.02500	-3.13903
D59	0.01188	-0.00008	-0.00001	-0.00230	-0.00229	0.00959
D60	-3.10759	-0.00034	-0.00001	-0.01852	-0.01844	-3.12603
D61	-3.12748	-0.00010	-0.00001	-0.01115	-0.01109	-3.13857
D62	0.03624	-0.00036	-0.00001	-0.02737	-0.02724	0.00900
D63	-0.01794	0.00032	0.00001	0.01988	0.01991	0.00197
D64	3.12023	0.00035	0.00001	0.03343	0.03344	-3.12952
D65	-0.00003	0.00001	0.00000	-0.00581	-0.00580	-0.00583
D66	-3.13678	0.00005	0.00001	0.01387	0.01388	-3.12289
D67	-3.13832	-0.00001	-0.00001	-0.01886	-0.01886	3.12601
D68	0.00812	0.00002	0.00000	0.00083	0.00083	0.00894
D69	0.00384	-0.00032	-0.00001	-0.02343	-0.02340	-0.01956
D70	-3.13240	-0.00037	0.00001	-0.00976	-0.00976	3.14103
D71	3.11533	0.00003	0.00000	-0.00148	-0.00146	3.11387
D72	-0.02091	-0.00002	0.00002	0.01219	0.01219	-0.00872
D73	-0.05817	0.00057	0.00002	0.04967	0.04966	-0.00851
D74	-2.91893	-0.00005	-0.00007	-0.08504	-0.08516	-3.00409
D75	3.11280	0.00022	0.00001	0.02823	0.02824	3.14104
D76	0.25204	-0.00040	-0.00008	-0.10648	-0.10657	0.14546
D77	-0.03651	0.00035	0.00002	0.03742	0.03728	0.00076
D78	3.12740	0.00019	0.00000	0.01176	0.01164	3.13903

D79	3.10172	0.00033	0.00001	0.02382	0.02377	3.12550
D80	-0.01755	0.00017	-0.00001	-0.00185	-0.00187	-0.01942
D81	-3.13039	-0.00017	-0.00001	-0.02296	-0.02292	3.12988
D82	0.01623	-0.00014	0.00000	-0.00256	-0.00254	0.01369
D83	0.05813	-0.00055	-0.00002	-0.05340	-0.05339	0.00475
D84	2.91621	0.00016	0.00007	0.08330	0.08309	2.99930
D85	-3.11358	-0.00035	0.00000	-0.01883	-0.01877	-3.13235
D86	-0.25550	0.00036	0.00009	0.11786	0.11770	-0.13780
D87	-3.12966	-0.00001	0.00001	0.00417	0.00419	-3.12547
D88	0.00873	-0.00010	0.00001	0.00676	0.00679	0.01552
D89	0.04261	-0.00021	-0.00001	-0.03101	-0.03106	0.01155
D90	-3.10219	-0.00030	-0.00001	-0.02842	-0.02847	-3.13066
D91	1.40743	0.00045	0.00006	0.08831	0.08864	1.49608
D92	-2.76098	0.00048	0.00006	0.08722	0.08755	-2.67343
D93	-0.70098	0.00048	0.00006	0.09007	0.09040	-0.61058
D94	-1.39872	-0.00043	-0.00005	-0.07179	-0.07211	-1.47084
D95	0.71604	-0.00040	-0.00005	-0.07287	-0.07320	0.64284
D96	2.77604	-0.00040	-0.00005	-0.07003	-0.07035	2.70569
D97	-0.01143	0.00008	0.00000	0.00648	0.00650	-0.00493
D98	3.13593	0.00003	0.00000	0.00214	0.00214	3.13807
D99	-3.13715	-0.00004	0.00000	0.00369	0.00371	-3.13344
D100	0.00769	0.00005	0.00000	0.00106	0.00107	0.00877
D101	-0.01037	-0.00005	0.00000	0.00164	0.00164	-0.00874
D102	3.13306	0.00003	0.00000	-0.00034	-0.00036	3.13270
D103	0.00379	-0.00001	-0.00001	-0.00880	-0.00881	-0.00502
D104	-3.14028	-0.00007	-0.00001	-0.00679	-0.00680	3.13610
D105	3.14098	0.00003	0.00000	-0.00548	-0.00548	3.13550
D106	-0.00309	-0.00003	0.00000	-0.00347	-0.00348	-0.00656
D107	3.13099	0.00004	0.00001	0.00899	0.00901	3.14000
D108	-0.02681	-0.00001	0.00001	0.00775	0.00777	-0.01904
D109	-0.00492	0.00000	0.00000	0.00472	0.00472	-0.00020
D110	3.12046	-0.00006	0.00001	0.00348	0.00348	3.12394
D111	0.01083	0.00004	0.00000	-0.00400	-0.00399	0.00684
D112	-3.13199	-0.00001	0.00000	-0.00267	-0.00266	-3.13465
D113	-3.11897	0.00007	-0.00001	-0.00315	-0.00314	-3.12211
D114	0.02140	0.00002	0.00000	-0.00183	-0.00181	0.01959
D115	3.11935	0.00012	0.00000	0.01028	0.01027	3.12963
D116	0.20788	-0.00028	-0.00005	-0.07524	-0.07524	0.13264
D117	-0.03816	0.00007	0.00000	0.00907	0.00907	-0.02909
D118	-2.94963	-0.00033	-0.00005	-0.07644	-0.07645	-3.02608
D119	-3.13939	-0.00018	0.00001	-0.00422	-0.00421	3.13959
D120	-0.00830	0.00008	-0.00001	0.00046	0.00047	-0.00784
D121	0.00398	-0.00010	0.00000	-0.00613	-0.00613	-0.00215
D122	3.13507	0.00016	-0.00001	-0.00145	-0.00146	3.13361
D123	3.13065	0.00003	0.00000	0.00244	0.00245	3.13310
D124	-0.02787	0.00016	0.00000	0.01208	0.01205	-0.01582
D125	-0.00385	-0.00015	0.00001	-0.00074	-0.00072	-0.00457
D126	3.12082	-0.00002	0.00001	0.00889	0.00888	3.12970
D127	-3.12986	0.00001	0.00000	0.00198	0.00199	-3.12787
D128	0.00084	0.00028	-0.00002	0.00685	0.00685	0.00769
D129	0.00559	-0.00011	0.00000	-0.00810	-0.00812	-0.00253
D130	-3.13896	0.00017	-0.00002	0.00365	0.00361	-3.13535
D131	-3.11296	-0.00028	0.00000	-0.02115	-0.02116	-3.13413
D132	0.02567	0.00001	-0.00001	-0.00940	-0.00943	0.01624
D133	0.04070	-0.00013	0.00000	-0.01302	-0.01302	0.02768
D134	2.95400	0.00022	0.00005	0.07162	0.07169	3.02570
D135	-3.12334	0.00003	-0.00001	-0.00028	-0.00030	-3.12364
D136	-0.21004	0.00038	0.00005	0.08436	0.08441	-0.12563
D137	-0.00486	0.00033	-0.00001	0.01318	0.01314	0.00828
D138	3.13346	0.00033	-0.00002	0.00356	0.00352	3.13698

D139	3.13956	0.00005	0.00000	0.00198	0.00195	3.14151
D140	-0.00532	0.00005	-0.00001	-0.00764	-0.00766	-0.01298
D141	0.00226	-0.00035	0.00001	-0.01141	-0.01139	-0.00913
D142	-3.13566	-0.00034	0.00003	-0.00066	-0.00067	-3.13633
D143	3.14094	-0.00004	0.00008	0.01502	0.01511	-3.12713
D144	0.00499	-0.00019	0.00009	0.01044	0.01052	0.01552
D145	-0.00456	-0.00004	0.00006	0.00356	0.00363	-0.00093
D146	-3.14051	-0.00020	0.00007	-0.00102	-0.00096	-3.14147
D147	-0.69296	0.00027	0.00003	0.04623	0.04634	-0.64662
D148	1.42195	0.00026	0.00003	0.04502	0.04513	1.46708
D149	-2.75384	0.00023	0.00003	0.04409	0.04419	-2.70965
D150	2.72159	-0.00028	-0.00004	-0.05479	-0.05490	2.66669
D151	-1.44668	-0.00029	-0.00004	-0.05600	-0.05611	-1.50279
D152	0.66072	-0.00033	-0.00004	-0.05694	-0.05705	0.60366
D153	0.00470	-0.00012	0.00001	0.00028	0.00030	0.00500
D154	-3.13487	-0.00022	0.00001	-0.00137	-0.00135	-3.13621
D155	3.14040	0.00004	0.00000	0.00510	0.00510	-3.13769
D156	0.00083	-0.00006	0.00001	0.00345	0.00345	0.00428
D157	3.13467	0.00029	-0.00003	0.03451	0.03445	-3.11407
D158	0.01584	-0.00057	0.00010	-0.06162	-0.06143	-0.04558
D159	-0.00863	0.00038	-0.00003	0.03590	0.03583	0.02720
D160	-3.12745	-0.00049	0.00010	-0.06022	-0.06004	3.09569
D161	-3.13557	-0.00017	0.00002	-0.03046	-0.03045	3.11717
D162	0.00673	-0.00007	0.00001	-0.02370	-0.02362	-0.01690
D163	0.00775	-0.00026	0.00003	-0.03188	-0.03185	-0.02410
D164	-3.13314	-0.00016	0.00002	-0.02512	-0.02503	3.12502
D165	0.00633	-0.00035	0.00003	-0.02670	-0.02666	-0.02033
D166	-3.13753	-0.00028	0.00002	-0.01976	-0.01970	3.12595
D167	3.12568	0.00051	-0.00010	0.06715	0.06706	-3.09044
D168	-0.01818	0.00059	-0.00011	0.07410	0.07403	0.05585
D169	-0.00390	0.00004	-0.00001	0.01562	0.01562	0.01172
D170	3.13892	0.00009	-0.00001	0.01492	0.01492	-3.12935
D171	3.13701	-0.00005	0.00000	0.00914	0.00920	-3.13697
D172	-0.00335	-0.00001	-0.00001	0.00844	0.00850	0.00515
D173	0.00130	-0.00003	0.00000	-0.00443	-0.00442	-0.00312
D174	-3.14058	-0.00006	0.00000	-0.00428	-0.00428	3.13833
D175	-3.13947	0.00009	-0.00001	0.00345	0.00344	-3.13603
D176	0.00183	0.00005	0.00000	0.00359	0.00358	0.00542
D177	-0.00154	0.00019	-0.00001	0.00701	0.00700	0.00546
D178	3.13901	0.00015	-0.00001	0.00759	0.00759	-3.13658
D179	-3.14099	0.00012	-0.00001	0.00045	0.00047	-3.14053
D180	-0.00044	0.00008	0.00000	0.00103	0.00106	0.00062
D181	-3.13841	-0.00017	0.00001	-0.00983	-0.00985	3.13493
D182	0.00253	-0.00010	0.00001	-0.00880	-0.00881	-0.00628
D183	0.00064	-0.00008	0.00000	-0.00204	-0.00205	-0.00141
D184	3.14158	-0.00001	0.00000	-0.00101	-0.00101	3.14057
D185	3.14025	-0.00008	0.00001	0.00125	0.00124	3.14149
D186	-0.00107	-0.00006	0.00001	0.00023	0.00023	-0.00084
D187	-0.00001	-0.00003	0.00000	0.00050	0.00048	0.00047
D188	-3.14134	-0.00002	0.00000	-0.00052	-0.00053	3.14132
D189	-0.00040	0.00003	0.00000	0.00152	0.00152	0.00112
D190	3.14127	0.00004	0.00000	0.00077	0.00078	-3.14113
D191	-3.14132	-0.00004	0.00000	0.00046	0.00045	-3.14087
D192	0.00036	-0.00003	0.00000	-0.00028	-0.00029	0.00007
D193	0.00024	-0.00002	0.00000	-0.00098	-0.00098	-0.00074
D194	-3.14158	0.00001	0.00000	-0.00047	-0.00046	3.14115
D195	3.14157	-0.00003	0.00000	0.00001	0.00000	3.14158
D196	-0.00025	-0.00001	0.00000	0.00053	0.00053	0.00028
D197	-0.00003	0.00002	0.00000	-0.00005	-0.00004	-0.00007
D198	-3.14140	-0.00001	0.00000	-0.00057	-0.00056	3.14123

D199	3.14148	0.00001	0.00000	0.00070	0.00070	-3.14101
D200	0.00011	-0.00001	0.00000	0.00018	0.00018	0.00029

Item	Value	Threshold	Converged?

Maximum Force	0.007748	0.000450	NO
RMS Force	0.000852	0.000300	NO
Maximum Displacement	0.298303	0.001800	NO
RMS Displacement	0.074873	0.001200	NO

Predicted change in Energy=-1.133164D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.809544	-0.649749	-0.048929
2	6	0	-9.994273	-1.796069	-0.046629
3	6	0	-10.513194	-3.083429	-0.050740
4	6	0	-11.901725	-3.229283	-0.057700
5	6	0	-12.727949	-2.098735	-0.061204
6	6	0	-12.201009	-0.803093	-0.057060
7	1	0	-9.841027	-3.935077	-0.048099
8	1	0	-12.345642	-4.219949	-0.061292
9	1	0	-13.805996	-2.226109	-0.067552
10	1	0	-12.870726	0.043871	-0.059196
11	6	0	-9.941658	0.556103	-0.040117
12	6	0	-8.570327	-1.387831	-0.043063
13	6	0	-8.552128	0.093418	-0.034919
14	6	0	-7.418876	0.890436	-0.026004
15	6	0	-6.028351	0.621440	-0.000606
16	6	0	-3.658642	-0.164455	0.042185
17	6	0	-3.786103	1.249058	0.021915
18	16	0	-5.203889	-0.963645	0.033944
19	6	0	-5.108281	1.688073	0.012247
20	6	0	-2.279325	-0.437764	0.053745
21	6	0	-1.611234	0.810877	0.032344
22	7	0	-2.528210	1.838457	0.009108
23	16	0	-1.164936	-1.796142	0.057951
24	16	0	1.153938	1.807742	0.050487
25	6	0	0.190741	-0.668670	0.054969
26	6	0	-0.201431	0.680008	0.044598
27	6	0	1.602580	-0.798675	0.059194
28	6	0	2.268971	0.449773	0.051755
29	6	0	3.647338	0.178420	0.047586
30	6	0	3.779095	-1.234572	0.055572
31	6	0	5.103714	-1.674846	0.041791
32	6	0	6.021847	-0.605980	0.019551
33	16	0	5.188169	0.978937	0.029938
34	7	0	2.522493	-1.825142	0.085103
35	6	0	7.420259	-0.879749	0.008956
36	6	0	8.554906	-0.093280	0.002330
37	6	0	8.582102	1.387411	0.011032
38	6	0	9.944597	-0.565557	-0.014936
39	6	0	10.007259	1.787438	-0.039895

40	6	0	10.816885	0.637021	-0.050890
41	6	0	10.532280	3.073350	-0.068332
42	6	0	12.210408	0.783986	-0.091364
43	6	0	11.920464	3.212679	-0.107590
44	6	0	12.742766	2.077261	-0.118781
45	6	0	10.417543	-1.870273	-0.009797
46	6	0	9.587879	-3.033537	0.018099
47	6	0	11.810588	-2.196344	-0.032438
48	7	0	8.945541	-4.005693	0.042508
49	7	0	12.934790	-2.502458	-0.049958
50	6	0	-10.416870	1.856264	-0.028167
51	6	0	-11.810451	2.177461	-0.035345
52	6	0	-9.585221	3.017950	-0.009551
53	7	0	-12.938615	2.468945	-0.042392
54	7	0	-8.936899	3.986448	0.004611
55	8	0	-7.606573	-2.145497	-0.044944
56	8	0	7.623159	2.150587	-0.019070
57	6	0	2.241314	-3.243585	-0.034210
58	1	0	1.307489	-3.476697	0.481618
59	1	0	2.160820	-3.551698	-1.082232
60	1	0	3.042835	-3.810027	0.444150
61	6	0	-2.245723	3.255345	0.148148
62	1	0	-2.178329	3.556594	1.199603
63	1	0	-1.304133	3.493719	-0.351640
64	1	0	-3.037817	3.831618	-0.334482
65	1	0	5.429720	-2.708425	0.039241
66	1	0	12.875786	-0.065253	-0.101126
67	1	0	13.820929	2.200258	-0.149764
68	1	0	12.368234	4.201319	-0.130218
69	1	0	9.864348	3.928352	-0.059242
70	1	0	7.594789	-1.948786	0.004542
71	1	0	-7.595522	1.959810	-0.016004
72	1	0	-5.431986	2.721805	-0.002689

Rotational constants (GHZ): 0.1750913 0.0103592 0.0097825

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6561.4927996339 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T
Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6561.4080435361 Hartrees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.25D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Initial guess from the checkpoint file: "PBDB.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000078 -0.000001 -0.000339 Ang= 0.04 deg.

ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1

AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

```

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-
yADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2001
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 IlCent= 200000004 NGrid=
0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0=
0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RB3LYP) = -3683.01918595 A.U. after 13 cycles
NFock= 13 Conv=0.62D-08 -V/T= 2.0069
Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1
NMatS=1 NMatT=0.
***** Axes restored to original set *****

```

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-0.000094489	0.000461248	0.000148124
2	6	0.000187185	-0.000428692	0.000607394
3	6	0.000012752	-0.000924630	-0.000157148
4	6	0.000039603	0.000317027	0.000115082
5	6	0.000114112	-0.000215332	0.000103352
6	6	0.001062707	0.000682810	0.000751572
7	1	0.000091014	0.000031987	0.000132029
8	1	0.000046262	0.000050308	0.000010701
9	1	-0.000070750	0.000004474	-0.000067136
10	1	-0.000130141	0.000632586	0.000051530
11	6	-0.000175689	-0.000359977	-0.000751475
12	6	-0.000689034	-0.000002586	-0.001071773
13	6	0.001101687	-0.004663386	0.000917661
14	6	-0.000122684	0.004872493	-0.002059431
15	6	0.000656624	-0.000976788	-0.000694711
16	6	0.000865237	-0.000376922	0.000545571
17	6	0.000279196	0.001176403	-0.001228088
18	16	0.001640547	-0.001701388	0.002734482
19	6	-0.000620924	-0.000241615	0.001496009
20	6	-0.001698804	-0.001308606	0.000084621
21	6	0.003424516	0.000308094	-0.000317718
22	7	-0.000469853	0.001481052	0.000624580
23	16	-0.000166130	-0.000235309	0.000047409
24	16	0.000024474	0.000046709	0.000253446
25	6	0.002140874	-0.001825229	0.001443215
26	6	-0.001274756	0.001262298	-0.000691290
27	6	-0.001513802	0.001287871	-0.002098086
28	6	-0.000187095	0.001083827	0.000588886
29	6	0.000260056	0.000606645	0.000311626
30	6	0.001710129	-0.000743947	0.000550030
31	6	-0.002254055	-0.001171460	-0.000697087
32	6	0.003376601	0.000291361	0.001000959
33	16	0.000008792	-0.000453668	0.000259133
34	7	-0.001115751	-0.001779108	-0.000473669
35	6	-0.002990165	-0.000078852	-0.002355016

36	6	0.002063228	0.002237633	-0.001804449
37	6	-0.005133571	-0.001582969	0.007497712
38	6	0.001096051	0.001629646	0.001856509
39	6	0.001516803	-0.000141248	-0.002468384
40	6	0.001106836	-0.000927631	-0.000088768
41	6	0.000227966	0.001671879	0.000263585
42	6	-0.002283322	-0.000513120	-0.001828561
43	6	0.000539488	-0.000015645	0.000795566
44	6	-0.000891848	0.000407356	-0.000639123
45	6	-0.001133912	-0.001839808	-0.000964891
46	6	-0.000031678	-0.001172073	-0.000596991
47	6	-0.000489964	0.001472009	-0.000188660
48	7	-0.000646789	0.000480452	-0.000329455
49	7	-0.000397801	0.000682931	-0.000257772
50	6	-0.000839994	0.000013842	-0.000408977
51	6	0.000207119	-0.001198023	0.000008001
52	6	-0.000500158	0.000659916	-0.000071839
53	7	0.000299761	-0.001013308	0.000025942
54	7	0.000372717	-0.000227311	0.000169456
55	8	-0.000077051	0.000756114	-0.000099028
56	8	0.002057760	0.000231280	-0.002706276
57	6	0.000076303	0.000766668	0.000239146
58	1	-0.000040472	0.000081016	-0.000084233
59	1	0.000014238	0.000196671	0.000090449
60	1	0.000014400	-0.000070853	-0.000029262
61	6	-0.000493879	-0.001512460	-0.000068015
62	1	0.000206636	0.000500054	0.000260417
63	1	0.000028385	0.000257323	0.000155739
64	1	-0.000050290	0.000423394	0.000245986
65	1	-0.000015341	0.000008591	-0.000010763
66	1	0.000507906	-0.000374297	0.000477235
67	1	0.000068921	0.000039578	0.000036281
68	1	0.000020370	-0.000079661	0.000012511
69	1	-0.000031196	0.000065158	-0.000144694
70	1	-0.000059193	0.000728358	0.000396733
71	1	-0.000564105	0.000282580	0.000596487
72	1	-0.000212568	-0.000033739	-0.000452398

Cartesian Forces: Max 0.007497712 RMS 0.001236444

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.007162442 RMS 0.001207389

Search for a local minimum.

Step number 18 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 14 16 15 18 17

DE= 2.05D-04 DEPred=-1.13D-03 R=-1.81D-01

Trust test=-1.81D-01 RLast= 4.20D-01 DXMaxT set to 4.92D-01

ITU= -1 0 -1 1 1 1 1 1 1 0 0 0 1 0 0 0 1 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.54934.

Iteration 1 RMS(Cart)= 0.04066114 RMS(Int)= 0.00017779

Iteration 2 RMS(Cart)= 0.00074940 RMS(Int)= 0.00008155

Iteration 3 RMS(Cart)= 0.00000009 RMS(Int)= 0.00008155

Variable	Old X	-DE/DX	Delta X	Delta X	Delta X	New X

(Linear)	(Quad)	(Total)				
R1	2.65822	0.00059	0.00009	0.00000	0.00009	2.65831
R2	2.64545	0.00038	-0.00071	0.00000	-0.00071	2.64474
R3	2.80762	0.00245	0.00081	0.00000	0.00081	2.80842
R4	2.62297	-0.00066	-0.00122	0.00000	-0.00122	2.62175
R5	2.79928	-0.00183	-0.00309	0.00000	-0.00309	2.79619
R6	2.63841	-0.00041	0.00005	0.00000	0.00005	2.63846
R7	2.05026	0.00016	0.00035	0.00000	0.00035	2.05062
R8	2.64615	-0.00033	0.00005	0.00000	0.00005	2.64621
R9	2.05146	0.00006	0.00003	0.00000	0.00003	2.05149
R10	2.64317	0.00002	0.00018	0.00000	0.00017	2.64334
R11	2.05142	0.00007	0.00015	0.00000	0.00015	2.05157
R12	2.04044	-0.00010	0.00135	0.00000	0.00135	2.04180
R13	2.76759	-0.00009	0.00162	0.00000	0.00162	2.76922
R14	2.61602	0.00140	-0.00119	0.00000	-0.00119	2.61482
R15	2.79941	-0.00120	-0.00095	0.00000	-0.00095	2.79846
R16	2.31666	-0.00010	-0.00011	0.00000	-0.00011	2.31654
R17	2.61819	-0.00546	-0.00313	0.00000	-0.00313	2.61507
R18	2.67686	0.00021	0.00321	0.00000	0.00321	2.68007
R19	2.04830	-0.00021	-0.00066	0.00000	-0.00066	2.04763
R20	3.37697	0.00163	0.00365	0.00000	0.00367	3.38064
R21	2.66203	-0.00144	-0.00187	0.00000	-0.00186	2.66018
R22	2.68226	-0.00070	-0.00235	0.00000	-0.00233	2.67993
R23	3.28756	-0.00203	-0.00490	0.00000	-0.00490	3.28266
R24	2.65730	-0.00251	-0.00337	0.00000	-0.00324	2.65406
R25	2.63275	-0.00181	-0.00493	0.00000	-0.00494	2.62781
R26	2.62519	-0.00158	-0.00077	0.00000	-0.00087	2.62432
R27	2.04720	0.00039	0.00079	0.00000	0.00079	2.04799
R28	2.67642	-0.00180	-0.00345	0.00000	-0.00343	2.67299
R29	3.32026	-0.00091	-0.00223	0.00000	-0.00222	3.31804
R30	2.60296	-0.00096	-0.00021	0.00000	-0.00033	2.60263
R31	2.67570	-0.00382	-0.00850	0.00000	-0.00852	2.66718
R32	2.74284	0.00011	0.00033	0.00000	0.00033	2.74317
R33	3.33207	-0.00096	-0.00179	0.00000	-0.00177	3.33029
R34	3.33195	-0.00078	-0.00215	0.00000	-0.00214	3.32981
R35	3.32043	-0.00095	-0.00217	0.00000	-0.00217	3.31826
R36	2.65427	-0.00088	-0.00065	0.00000	-0.00065	2.65362
R37	2.67929	-0.00520	-0.00936	0.00000	-0.00936	2.66992
R38	2.67432	-0.00111	-0.00224	0.00000	-0.00223	2.67208
R39	2.60518	-0.00195	-0.00349	0.00000	-0.00354	2.60164
R40	2.65474	-0.00148	-0.00595	0.00000	-0.00589	2.64885
R41	2.68179	-0.00074	-0.00097	0.00000	-0.00096	2.68084
R42	3.28144	-0.00060	-0.00172	0.00000	-0.00172	3.27972
R43	2.63794	-0.00377	-0.00833	0.00000	-0.00834	2.62960
R44	2.62440	-0.00130	-0.00274	0.00000	-0.00279	2.62162
R45	2.66306	-0.00260	-0.00376	0.00000	-0.00375	2.65931
R46	2.04804	-0.00001	0.00006	0.00000	0.00006	2.04810
R47	3.38419	-0.00080	-0.00210	0.00000	-0.00209	3.38210
R48	2.69286	-0.00644	-0.01717	0.00000	-0.01717	2.67568
R49	2.74191	0.00096	0.00136	0.00000	0.00136	2.74327
R50	2.60892	-0.00283	-0.00294	0.00000	-0.00294	2.60598
R51	2.04695	0.00067	0.00015	0.00000	0.00015	2.04710
R52	2.79862	-0.00084	-0.00101	0.00000	-0.00106	2.79756
R53	2.77384	-0.00263	0.00112	0.00000	0.00115	2.77499
R54	2.79889	-0.00148	-0.00288	0.00000	-0.00294	2.79595
R55	2.31668	-0.00004	0.00020	0.00000	0.00020	2.31688
R56	2.80825	0.00179	0.00204	0.00000	0.00211	2.81035
R57	2.62256	-0.00320	-0.00311	0.00000	-0.00311	2.61945
R58	2.65846	0.00044	0.00049	0.00000	0.00050	2.65896
R59	2.62531	-0.00157	-0.00395	0.00000	-0.00396	2.62135

R60	2.64909	-0.00100	-0.00149	0.00000	-0.00149	2.64760
R61	2.63751	-0.00035	0.00067	0.00000	0.00067	2.63818
R62	2.05037	0.00010	0.00026	0.00000	0.00026	2.05063
R63	2.64340	-0.00050	0.00007	0.00000	0.00008	2.64348
R64	2.03883	0.00058	0.00219	0.00000	0.00219	2.04102
R65	2.64931	-0.00137	-0.00301	0.00000	-0.00300	2.64631
R66	2.05139	0.00007	0.00006	0.00000	0.00006	2.05145
R67	2.05148	0.00003	0.00015	0.00000	0.00015	2.05163
R68	2.70059	-0.00074	0.00110	0.00000	0.00110	2.70169
R69	2.70397	-0.00176	0.00022	0.00000	0.00022	2.70419
R70	2.20239	0.00045	0.00016	0.00000	0.00016	2.20255
R71	2.20203	-0.00069	-0.00018	0.00000	-0.00018	2.20185
R72	2.70256	-0.00129	-0.00119	0.00000	-0.00119	2.70138
R73	2.70006	-0.00045	0.00016	0.00000	0.00016	2.70022
R74	2.20197	-0.00062	-0.00018	0.00000	-0.00018	2.20179
R75	2.20257	0.00022	0.00011	0.00000	0.00011	2.20269
R76	2.06357	0.00012	0.00023	0.00000	0.00023	2.06379
R77	2.06989	0.00010	0.00041	0.00000	0.00041	2.07030
R78	2.06328	0.00001	0.00019	0.00000	0.00019	2.06347
R79	2.07082	-0.00019	-0.00005	0.00000	-0.00005	2.07077
R80	2.06422	-0.00008	-0.00023	0.00000	-0.00023	2.06399
R81	2.06356	-0.00002	0.00008	0.00000	0.00008	2.06363
A1	2.07924	-0.00158	-0.00169	0.00000	-0.00169	2.07756
A2	1.89952	-0.00086	-0.00062	0.00000	-0.00062	1.89891
A3	2.30442	0.00244	0.00231	0.00000	0.00231	2.30672
A4	2.14021	0.00094	0.00134	0.00000	0.00133	2.14154
A5	1.90980	0.00075	0.00117	0.00000	0.00118	1.91098
A6	2.23317	-0.00169	-0.00251	0.00000	-0.00251	2.23066
A7	2.05863	0.00025	0.00028	0.00000	0.00028	2.05891
A8	2.09026	-0.00013	-0.00065	0.00000	-0.00065	2.08961
A9	2.13430	-0.00012	0.00037	0.00000	0.00037	2.13466
A10	2.09725	-0.00053	-0.00109	0.00000	-0.00109	2.09617
A11	2.09674	0.00023	0.00038	0.00000	0.00038	2.09712
A12	2.08920	0.00030	0.00071	0.00000	0.00071	2.08990
A13	2.12420	0.00029	0.00023	0.00000	0.00023	2.12443
A14	2.08430	-0.00008	0.00073	0.00000	0.00073	2.08503
A15	2.07468	-0.00021	-0.00096	0.00000	-0.00096	2.07372
A16	2.06684	0.00063	0.00093	0.00000	0.00093	2.06776
A17	2.13010	0.00034	0.00105	0.00000	0.00105	2.13115
A18	2.08625	-0.00096	-0.00198	0.00000	-0.00198	2.08427
A19	1.87322	-0.00098	-0.00099	0.00000	-0.00099	1.87224
A20	2.16736	0.00587	0.00571	0.00000	0.00571	2.17306
A21	2.24257	-0.00489	-0.00473	0.00000	-0.00473	2.23784
A22	1.86230	0.00016	0.00027	0.00000	0.00028	1.86257
A23	2.19613	-0.00095	-0.00122	0.00000	-0.00123	2.19491
A24	2.22476	0.00079	0.00095	0.00000	0.00095	2.22570
A25	1.87992	0.00093	0.00015	0.00000	0.00015	1.88007
A26	2.20723	-0.00212	0.00117	0.00000	0.00117	2.20840
A27	2.19604	0.00119	-0.00133	0.00000	-0.00134	2.19470
A28	2.33755	0.00324	0.00288	0.00000	0.00291	2.34047
A29	2.02006	-0.00195	0.00032	0.00000	0.00035	2.02041
A30	1.92534	-0.00127	-0.00309	0.00000	-0.00306	1.92229
A31	2.24168	0.00290	0.00545	0.00000	0.00543	2.24711
A32	2.09154	-0.00298	-0.00571	0.00000	-0.00573	2.08581
A33	1.94992	0.00008	0.00028	0.00000	0.00034	1.95026
A34	1.95805	0.00009	0.00254	0.00000	0.00250	1.96056
A35	1.85642	0.00036	-0.00051	0.00000	-0.00043	1.85599
A36	2.46868	-0.00046	-0.00201	0.00000	-0.00204	2.46664
A37	1.98137	0.00093	0.00042	0.00000	0.00049	1.98186
A38	1.91914	-0.00041	0.00104	0.00000	0.00091	1.92004

A39	2.38266	-0.00053	-0.00161	0.00000	-0.00151	2.38115
A40	1.57321	-0.00058	-0.00268	0.00000	-0.00262	1.57059
A41	1.96201	-0.00051	-0.00058	0.00000	-0.00056	1.96145
A42	2.12613	0.00004	-0.00017	0.00000	-0.00017	2.12596
A43	2.19489	0.00048	0.00083	0.00000	0.00083	2.19571
A44	1.86630	0.00002	0.00045	0.00000	0.00054	1.86684
A45	2.45344	-0.00062	-0.00254	0.00000	-0.00254	2.45090
A46	1.96324	0.00061	0.00219	0.00000	0.00214	1.96538
A47	1.92189	0.00015	0.00079	0.00000	0.00068	1.92257
A48	1.96932	0.00037	0.00013	0.00000	0.00019	1.96952
A49	2.39196	-0.00052	-0.00108	0.00000	-0.00094	2.39102
A50	1.86098	-0.00013	-0.00283	0.00000	-0.00236	1.85862
A51	2.20126	0.00022	-0.00728	0.00000	-0.00640	2.19486
A52	2.21064	-0.00010	-0.00537	0.00000	-0.00446	2.20618
A53	1.56408	-0.00135	-0.00322	0.00000	-0.00320	1.56089
A54	1.56430	-0.00157	-0.00264	0.00000	-0.00264	1.56166
A55	1.98157	0.00060	0.00115	0.00000	0.00116	1.98273
A56	2.35600	-0.00060	-0.00129	0.00000	-0.00128	2.35473
A57	1.94561	0.00000	0.00013	0.00000	0.00011	1.94572
A58	2.35505	-0.00039	-0.00057	0.00000	-0.00055	2.35450
A59	1.94638	-0.00023	-0.00025	0.00000	-0.00028	1.94610
A60	1.98176	0.00062	0.00081	0.00000	0.00083	1.98258
A61	1.96925	0.00042	0.00035	0.00000	0.00038	1.96963
A62	2.39321	-0.00088	-0.00174	0.00000	-0.00168	2.39153
A63	1.92062	0.00046	0.00139	0.00000	0.00131	1.92193
A64	1.96381	0.00053	0.00134	0.00000	0.00132	1.96513
A65	2.45264	-0.00043	-0.00160	0.00000	-0.00160	2.45105
A66	1.86673	-0.00010	0.00026	0.00000	0.00028	1.86701
A67	1.85813	-0.00031	-0.00090	0.00000	-0.00088	1.85725
A68	2.46804	-0.00026	-0.00086	0.00000	-0.00086	2.46718
A69	1.95701	0.00057	0.00175	0.00000	0.00173	1.95874
A70	1.98458	0.00007	-0.00031	0.00000	-0.00028	1.98429
A71	1.91720	0.00024	0.00126	0.00000	0.00118	1.91838
A72	2.38138	-0.00030	-0.00102	0.00000	-0.00096	2.38042
A73	1.95969	-0.00021	-0.00039	0.00000	-0.00040	1.95929
A74	2.19722	0.00009	0.00025	0.00000	0.00027	2.19748
A75	2.12625	0.00012	0.00015	0.00000	0.00017	2.12641
A76	1.94752	0.00145	0.00287	0.00000	0.00288	1.95040
A77	2.08720	-0.00118	-0.00285	0.00000	-0.00285	2.08435
A78	2.24838	-0.00026	0.00002	0.00000	0.00002	2.24840
A79	1.57594	-0.00188	-0.00390	0.00000	-0.00389	1.57205
A80	1.86163	-0.00029	-0.00225	0.00000	-0.00211	1.85952
A81	2.21059	-0.00015	-0.00276	0.00000	-0.00239	2.20820
A82	2.20100	0.00046	-0.00342	0.00000	-0.00305	2.19795
A83	2.34217	0.00002	-0.00141	0.00000	-0.00141	2.34076
A84	1.92597	-0.00043	-0.00293	0.00000	-0.00292	1.92305
A85	2.01504	0.00041	0.00433	0.00000	0.00433	2.01937
A86	2.19521	0.00095	-0.00231	0.00000	-0.00228	2.19293
A87	2.20790	-0.00200	0.00155	0.00000	0.00158	2.20947
A88	1.88007	0.00105	0.00076	0.00000	0.00070	1.88078
A89	1.86242	-0.00024	0.00010	0.00000	0.00031	1.86273
A90	2.22421	0.00029	0.00101	0.00000	0.00144	2.22565
A91	2.19405	0.00013	0.00013	0.00000	0.00056	2.19461
A92	1.87092	-0.00017	-0.00109	0.00000	-0.00103	1.86989
A93	2.24604	-0.00699	-0.00669	0.00000	-0.00672	2.23932
A94	2.16620	0.00716	0.00780	0.00000	0.00777	2.17398
A95	1.91046	0.00053	0.00146	0.00000	0.00138	1.91184
A96	2.23234	-0.00131	-0.00280	0.00000	-0.00275	2.22960
A97	2.14037	0.00079	0.00135	0.00000	0.00138	2.14174
A98	1.90050	-0.00113	-0.00102	0.00000	-0.00099	1.89951

A99	2.30371	0.00248	0.00335	0.00000	0.00334	2.30705
A100	2.07898	-0.00134	-0.00233	0.00000	-0.00235	2.07663
A101	2.05879	0.00013	0.00067	0.00000	0.00065	2.05944
A102	2.09045	-0.00015	-0.00131	0.00000	-0.00130	2.08915
A103	2.13394	0.00003	0.00064	0.00000	0.00065	2.13459
A104	2.06668	0.00061	0.00120	0.00000	0.00121	2.06789
A105	2.13034	0.00024	0.00107	0.00000	0.00107	2.13141
A106	2.08616	-0.00085	-0.00227	0.00000	-0.00228	2.08389
A107	2.09758	-0.00054	-0.00117	0.00000	-0.00117	2.09641
A108	2.09643	0.00031	0.00071	0.00000	0.00071	2.09714
A109	2.08918	0.00023	0.00046	0.00000	0.00046	2.08964
A110	2.12397	0.00037	0.00028	0.00000	0.00029	2.12426
A111	2.07519	-0.00027	-0.00111	0.00000	-0.00112	2.07408
A112	2.08402	-0.00010	0.00083	0.00000	0.00083	2.08485
A113	2.17424	-0.00482	-0.00639	0.00000	-0.00639	2.16785
A114	2.14833	0.00506	0.00838	0.00000	0.00838	2.15671
A115	1.96061	-0.00025	-0.00199	0.00000	-0.00199	1.95862
A116	2.14766	0.00487	0.00746	0.00000	0.00746	2.15511
A117	2.16991	-0.00282	-0.00328	0.00000	-0.00328	2.16663
A118	1.96562	-0.00205	-0.00418	0.00000	-0.00418	1.96144
A119	1.91300	-0.00006	-0.00088	0.00000	-0.00088	1.91212
A120	1.94756	0.00032	0.00134	0.00000	0.00134	1.94889
A121	1.90592	-0.00016	-0.00099	0.00000	-0.00099	1.90492
A122	1.90612	-0.00010	0.00031	0.00000	0.00031	1.90643
A123	1.88606	0.00004	-0.00007	0.00000	-0.00007	1.88599
A124	1.90414	-0.00004	0.00026	0.00000	0.00026	1.90441
A125	1.95222	-0.00064	-0.00169	0.00000	-0.00169	1.95053
A126	1.91448	-0.00019	-0.00102	0.00000	-0.00102	1.91347
A127	1.90885	-0.00052	-0.00201	0.00000	-0.00201	1.90684
A128	1.90287	0.00044	0.00191	0.00000	0.00191	1.90478
A129	1.90034	0.00059	0.00272	0.00000	0.00272	1.90306
A130	1.88376	0.00035	0.00018	0.00000	0.00018	1.88394
A131	3.17726	-0.00163	-0.00976	0.00000	-0.00976	3.16750
A132	3.17751	0.00102	-0.00235	0.00000	-0.00235	3.17516
A133	3.16790	0.00188	0.00371	0.00000	0.00371	3.17161
A134	3.17301	-0.00090	-0.00154	0.00000	-0.00154	3.17148
A135	3.14259	-0.00016	-0.00063	0.00000	-0.00063	3.14196
A136	3.14134	-0.00003	0.00013	0.00000	0.00013	3.14147
A137	3.14293	-0.00009	-0.00065	0.00000	-0.00065	3.14228
A138	3.14091	0.00014	-0.00006	0.00000	-0.00006	3.14084
D1	-0.00117	0.00000	0.00014	0.00000	0.00014	-0.00103
D2	3.13783	0.00006	0.00140	0.00000	0.00140	3.13923
D3	3.13933	0.00002	0.00009	0.00000	0.00010	3.13943
D4	-0.00485	0.00008	0.00136	0.00000	0.00136	-0.00349
D5	0.00114	-0.00001	-0.00080	0.00000	-0.00080	0.00034
D6	-3.14153	0.00003	0.00041	0.00000	0.00041	-3.14112
D7	-3.13907	-0.00004	-0.00074	0.00000	-0.00074	-3.13981
D8	0.00145	0.00000	0.00047	0.00000	0.00047	0.00192
D9	0.00188	0.00002	0.00336	0.00000	0.00336	0.00524
D10	-3.13143	-0.00010	0.00427	0.00000	0.00427	-3.12716
D11	-3.14099	0.00005	0.00330	0.00000	0.00330	-3.13768
D12	0.00888	-0.00007	0.00422	0.00000	0.00422	0.01309
D13	0.00023	0.00001	0.00057	0.00000	0.00057	0.00081
D14	-3.14093	0.00000	0.00037	0.00000	0.00037	-3.14056
D15	-3.13826	-0.00006	-0.00094	0.00000	-0.00094	-3.13921
D16	0.00376	-0.00007	-0.00115	0.00000	-0.00115	0.00261
D17	0.00590	-0.00015	-0.00550	0.00000	-0.00549	0.00041
D18	-3.13708	-0.00006	-0.00501	0.00000	-0.00501	3.14110
D19	-3.13845	-0.00008	-0.00414	0.00000	-0.00414	3.14059
D20	0.00175	0.00001	-0.00365	0.00000	-0.00365	-0.00190

D21	0.00070	-0.00001	-0.00061	0.00000	-0.00061	0.00009
D22	3.14137	0.00001	-0.00025	0.00000	-0.00025	3.14112
D23	-3.14133	0.00000	-0.00040	0.00000	-0.00040	3.14146
D24	-0.00066	0.00001	-0.00004	0.00000	-0.00004	-0.00071
D25	-0.00072	0.00000	-0.00005	0.00000	-0.00005	-0.00076
D26	3.14060	0.00000	0.00008	0.00000	0.00008	3.14069
D27	-3.14138	-0.00001	-0.00041	0.00000	-0.00041	3.14139
D28	-0.00007	-0.00001	-0.00027	0.00000	-0.00027	-0.00034
D29	-0.00023	0.00001	0.00076	0.00000	0.00076	0.00053
D30	-3.14077	-0.00003	-0.00041	0.00000	-0.00041	-3.14119
D31	-3.14155	0.00000	0.00063	0.00000	0.00063	-3.14092
D32	0.00109	-0.00003	-0.00054	0.00000	-0.00054	0.00055
D33	0.00180	-0.00012	-0.00671	0.00000	-0.00671	-0.00491
D34	-3.14132	-0.00013	-0.01066	0.00000	-0.01065	3.13121
D35	3.13465	0.00008	-0.00759	0.00000	-0.00760	3.12705
D36	-0.00847	0.00007	-0.01154	0.00000	-0.01154	-0.02002
D37	-0.01030	0.00015	-0.00007	0.00000	-0.00007	-0.01037
D38	3.13302	0.00014	-0.00369	0.00000	-0.00369	3.12933
D39	3.14139	-0.00003	0.00101	0.00000	0.00101	-3.14079
D40	0.00152	-0.00004	-0.00262	0.00000	-0.00262	-0.00110
D41	-0.00462	0.00016	0.00748	0.00000	0.00747	0.00286
D42	3.13849	0.00018	0.01138	0.00000	0.01138	-3.13332
D43	3.13839	0.00007	0.00698	0.00000	0.00698	-3.13781
D44	-0.00169	0.00009	0.01088	0.00000	0.01088	0.00920
D45	3.12255	0.00061	0.00775	0.00000	0.00774	3.13029
D46	0.00680	-0.00009	-0.01009	0.00000	-0.01009	-0.00329
D47	-0.02084	0.00060	0.00311	0.00000	0.00311	-0.01773
D48	-3.13659	-0.00011	-0.01472	0.00000	-0.01472	3.13188
D49	-0.00211	0.00018	-0.00186	0.00000	-0.00187	-0.00398
D50	-3.13302	-0.00020	-0.01032	0.00000	-0.01032	3.13984
D51	3.11466	0.00084	0.01526	0.00000	0.01527	3.12993
D52	-0.01624	0.00047	0.00680	0.00000	0.00681	-0.00943
D53	3.13874	0.00044	0.01020	0.00000	0.01023	-3.13422
D54	-0.01284	0.00077	0.01811	0.00000	0.01812	0.00528
D55	-3.12990	-0.00055	-0.01378	0.00000	-0.01376	3.13953
D56	-0.00645	0.00010	-0.00662	0.00000	-0.00661	-0.01306
D57	0.02071	-0.00088	-0.02090	0.00000	-0.02090	-0.00019
D58	-3.13903	-0.00024	-0.01374	0.00000	-0.01374	3.13041
D59	0.00959	0.00008	0.00126	0.00000	0.00126	0.01085
D60	-3.12603	0.00024	0.01013	0.00000	0.01011	-3.11592
D61	-3.13857	0.00009	0.00609	0.00000	0.00608	-3.13249
D62	0.00900	0.00025	0.01496	0.00000	0.01494	0.02393
D63	0.00197	-0.00048	-0.01094	0.00000	-0.01094	-0.00897
D64	-3.12952	-0.00050	-0.01837	0.00000	-0.01838	3.13529
D65	-0.00583	0.00012	0.00319	0.00000	0.00318	-0.00265
D66	-3.12289	-0.00018	-0.00763	0.00000	-0.00763	-3.13052
D67	3.12601	0.00014	0.01036	0.00000	0.01036	3.13637
D68	0.00894	-0.00015	-0.00045	0.00000	-0.00045	0.00849
D69	-0.01956	0.00052	0.01286	0.00000	0.01285	-0.00672
D70	3.14103	-0.00015	0.00536	0.00000	0.00536	-3.13679
D71	3.11387	0.00030	0.00080	0.00000	0.00079	3.11466
D72	-0.00872	-0.00036	-0.00670	0.00000	-0.00669	-0.01541
D73	-0.00851	-0.00053	-0.02728	0.00000	-0.02728	-0.03579
D74	-3.00409	-0.00048	0.04678	0.00000	0.04680	-2.95728
D75	3.14104	-0.00032	-0.01551	0.00000	-0.01552	3.12552
D76	0.14546	-0.00027	0.05855	0.00000	0.05856	0.20403
D77	0.00076	-0.00046	-0.02048	0.00000	-0.02044	-0.01968
D78	3.13903	-0.00008	-0.00639	0.00000	-0.00637	3.13267
D79	3.12550	-0.00027	-0.01306	0.00000	-0.01305	3.11245
D80	-0.01942	0.00010	0.00103	0.00000	0.00103	-0.01839

D81	3.12988	0.00029	0.01259	0.00000	0.01258	-3.14072
D82	0.01369	-0.00001	0.00140	0.00000	0.00140	0.01508
D83	0.00475	0.00061	0.02933	0.00000	0.02933	0.03407
D84	2.99930	0.00059	-0.04564	0.00000	-0.04559	2.95371
D85	-3.13235	0.00010	0.01031	0.00000	0.01030	-3.12205
D86	-0.13780	0.00008	-0.06466	0.00000	-0.06461	-0.20241
D87	-3.12547	-0.00025	-0.00230	0.00000	-0.00231	-3.12777
D88	0.01552	-0.00020	-0.00373	0.00000	-0.00373	0.01178
D89	0.01155	0.00027	0.01706	0.00000	0.01707	0.02862
D90	-3.13066	0.00032	0.01564	0.00000	0.01565	-3.11501
D91	1.49608	-0.00002	-0.04869	0.00000	-0.04877	1.44731
D92	-2.67343	-0.00001	-0.04810	0.00000	-0.04817	-2.72160
D93	-0.61058	0.00000	-0.04966	0.00000	-0.04973	-0.66031
D94	-1.47084	0.00003	0.03961	0.00000	0.03969	-1.43115
D95	0.64284	0.00004	0.04021	0.00000	0.04028	0.68313
D96	2.70569	0.00005	0.03865	0.00000	0.03872	2.74441
D97	-0.00493	-0.00011	-0.00357	0.00000	-0.00357	-0.00851
D98	3.13807	-0.00005	-0.00118	0.00000	-0.00118	3.13689
D99	-3.13344	-0.00009	-0.00204	0.00000	-0.00204	-3.13548
D100	0.00877	-0.00014	-0.00059	0.00000	-0.00059	0.00818
D101	-0.00874	0.00006	-0.00090	0.00000	-0.00090	-0.00963
D102	3.13270	0.00019	0.00020	0.00000	0.00020	3.13290
D103	-0.00502	0.00019	0.00484	0.00000	0.00484	-0.00018
D104	3.13610	0.00023	0.00373	0.00000	0.00373	3.13984
D105	3.13550	0.00015	0.00301	0.00000	0.00301	3.13851
D106	-0.00656	0.00019	0.00191	0.00000	0.00191	-0.00466
D107	3.14000	-0.00020	-0.00495	0.00000	-0.00495	3.13505
D108	-0.01904	-0.00005	-0.00427	0.00000	-0.00427	-0.02331
D109	-0.00020	-0.00015	-0.00259	0.00000	-0.00259	-0.00279
D110	3.12394	0.00001	-0.00191	0.00000	-0.00191	3.12203
D111	0.00684	0.00005	0.00219	0.00000	0.00219	0.00903
D112	-3.13465	-0.00004	0.00146	0.00000	0.00146	-3.13319
D113	-3.12211	-0.00005	0.00173	0.00000	0.00172	-3.12038
D114	0.01959	-0.00014	0.00099	0.00000	0.00099	0.02058
D115	3.12963	-0.00001	-0.00564	0.00000	-0.00564	3.12398
D116	0.13264	-0.00017	0.04133	0.00000	0.04133	0.17396
D117	-0.02909	0.00014	-0.00498	0.00000	-0.00498	-0.03407
D118	-3.02608	-0.00002	0.04200	0.00000	0.04199	-2.98409
D119	3.13959	-0.00004	0.00231	0.00000	0.00231	-3.14129
D120	-0.00784	-0.00002	-0.00026	0.00000	-0.00026	-0.00809
D121	-0.00215	0.00009	0.00337	0.00000	0.00337	0.00122
D122	3.13361	0.00011	0.00080	0.00000	0.00080	3.13441
D123	3.13310	-0.00006	-0.00134	0.00000	-0.00135	3.13175
D124	-0.01582	0.00000	-0.00662	0.00000	-0.00661	-0.02243
D125	-0.00457	-0.00007	0.00040	0.00000	0.00039	-0.00418
D126	3.12970	-0.00001	-0.00488	0.00000	-0.00487	3.12483
D127	-3.12787	-0.00012	-0.00110	0.00000	-0.00110	-3.12896
D128	0.00769	-0.00010	-0.00376	0.00000	-0.00376	0.00393
D129	-0.00253	0.00025	0.00446	0.00000	0.00447	0.00194
D130	-3.13535	0.00005	-0.00198	0.00000	-0.00198	-3.13733
D131	-3.13413	0.00017	0.01162	0.00000	0.01163	-3.12250
D132	0.01624	-0.00003	0.00518	0.00000	0.00519	0.02142
D133	0.02768	-0.00008	0.00715	0.00000	0.00715	0.03483
D134	3.02570	0.00001	-0.03938	0.00000	-0.03939	2.98630
D135	-3.12364	-0.00001	0.00016	0.00000	0.00017	-3.12347
D136	-0.12563	0.00008	-0.04637	0.00000	-0.04637	-0.17200
D137	0.00828	-0.00031	-0.00722	0.00000	-0.00721	0.00107
D138	3.13698	-0.00004	-0.00193	0.00000	-0.00193	3.13505
D139	3.14151	-0.00012	-0.00107	0.00000	-0.00107	3.14044
D140	-0.01298	0.00015	0.00421	0.00000	0.00421	-0.00876

D141	-0.00913	0.00023	0.00626	0.00000	0.00626	-0.00287
D142	-3.13633	-0.00006	0.00037	0.00000	0.00038	-3.13595
D143	-3.12713	-0.00033	-0.00830	0.00000	-0.00831	-3.13544
D144	0.01552	-0.00024	-0.00578	0.00000	-0.00578	0.00974
D145	-0.00093	0.00001	-0.00199	0.00000	-0.00199	-0.00292
D146	-3.14147	0.00010	0.00053	0.00000	0.00053	-3.14094
D147	-0.64662	0.00001	-0.02546	0.00000	-0.02548	-0.67210
D148	1.46708	0.00005	-0.02479	0.00000	-0.02481	1.44227
D149	-2.70965	0.00010	-0.02428	0.00000	-0.02430	-2.73394
D150	2.66669	-0.00010	0.03016	0.00000	0.03018	2.69687
D151	-1.50279	-0.00006	0.03083	0.00000	0.03085	-1.47195
D152	0.60366	-0.00002	0.03134	0.00000	0.03136	0.63503
D153	0.00500	-0.00035	-0.00016	0.00000	-0.00016	0.00483
D154	-3.13621	-0.00009	0.00074	0.00000	0.00074	-3.13548
D155	-3.13769	-0.00045	-0.00280	0.00000	-0.00280	-3.14049
D156	0.00428	-0.00018	-0.00190	0.00000	-0.00189	0.00239
D157	-3.11407	-0.00102	-0.01892	0.00000	-0.01892	-3.13299
D158	-0.04558	0.00167	0.03374	0.00000	0.03373	-0.01185
D159	0.02720	-0.00124	-0.01969	0.00000	-0.01968	0.00752
D160	3.09569	0.00144	0.03298	0.00000	0.03297	3.12866
D161	3.11717	0.00067	0.01673	0.00000	0.01673	3.13390
D162	-0.01690	0.00015	0.01298	0.00000	0.01296	-0.00394
D163	-0.02410	0.00089	0.01750	0.00000	0.01750	-0.00660
D164	3.12502	0.00037	0.01375	0.00000	0.01374	3.13875
D165	-0.02033	0.00117	0.01465	0.00000	0.01464	-0.00569
D166	3.12595	0.00088	0.01082	0.00000	0.01081	3.13677
D167	-3.09044	-0.00147	-0.03684	0.00000	-0.03685	-3.12729
D168	0.05585	-0.00175	-0.04067	0.00000	-0.04068	0.01517
D169	0.01172	-0.00019	-0.00858	0.00000	-0.00858	0.00313
D170	-3.12935	-0.00033	-0.00820	0.00000	-0.00820	-3.13754
D171	-3.13697	0.00023	-0.00506	0.00000	-0.00507	3.14115
D172	0.00515	0.00009	-0.00467	0.00000	-0.00469	0.00047
D173	-0.00312	0.00010	0.00243	0.00000	0.00243	-0.00069
D174	3.13833	0.00027	0.00235	0.00000	0.00235	3.14068
D175	-3.13603	-0.00046	-0.00189	0.00000	-0.00189	-3.13792
D176	0.00542	-0.00029	-0.00197	0.00000	-0.00197	0.00345
D177	0.00546	-0.00061	-0.00385	0.00000	-0.00385	0.00161
D178	-3.13658	-0.00048	-0.00417	0.00000	-0.00417	-3.14075
D179	-3.14053	-0.00035	-0.00026	0.00000	-0.00026	-3.14079
D180	0.00062	-0.00022	-0.00058	0.00000	-0.00059	0.00003
D181	3.13493	0.00054	0.00541	0.00000	0.00542	3.14035
D182	-0.00628	0.00035	0.00484	0.00000	0.00484	-0.00144
D183	-0.00141	0.00022	0.00113	0.00000	0.00113	-0.00028
D184	3.14057	0.00003	0.00056	0.00000	0.00056	3.14112
D185	3.14149	0.00024	-0.00068	0.00000	-0.00068	3.14081
D186	-0.00084	0.00020	-0.00013	0.00000	-0.00012	-0.00097
D187	0.00047	0.00008	-0.00026	0.00000	-0.00026	0.00021
D188	3.14132	0.00004	0.00029	0.00000	0.00029	-3.14157
D189	0.00112	-0.00008	-0.00084	0.00000	-0.00083	0.00028
D190	-3.14113	-0.00010	-0.00043	0.00000	-0.00043	-3.14156
D191	-3.14087	0.00011	-0.00025	0.00000	-0.00024	-3.14111
D192	0.00007	0.00009	0.00016	0.00000	0.00016	0.00023
D193	-0.00074	0.00005	0.00054	0.00000	0.00054	-0.00020
D194	3.14115	-0.00001	0.00025	0.00000	0.00025	3.14140
D195	3.14158	0.00008	0.00000	0.00000	0.00000	3.14158
D196	0.00028	0.00002	-0.00029	0.00000	-0.00029	-0.00001
D197	-0.00007	-0.00005	0.00002	0.00000	0.00002	-0.00005
D198	3.14123	0.00001	0.00031	0.00000	0.00031	3.14153
D199	-3.14101	-0.00003	-0.00038	0.00000	-0.00039	-3.14139
D200	0.00029	0.00003	-0.00010	0.00000	-0.00010	0.00019

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Full point group	C1	NOp	1
Largest Abelian subgroup	C1	NOp	1
Largest concise Abelian subgroup	C1	NOp	1
Standard orientation:			

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.802608	-0.639940	-0.006938
2	6	0	-9.992159	-1.789707	-0.014620
3	6	0	-10.514554	-3.074967	-0.017190
4	6	0	-11.903495	-3.217227	-0.012864
5	6	0	-12.725563	-2.083634	-0.006264
6	6	0	-12.194098	-0.789740	-0.002899
7	1	0	-9.844174	-3.928251	-0.022210
8	1	0	-12.350382	-4.206580	-0.015135
9	1	0	-13.804258	-2.206264	-0.003803
10	1	0	-12.863001	0.058765	0.002576
11	6	0	-9.928612	0.562044	-0.003113
12	6	0	-8.567622	-1.389573	-0.020981
13	6	0	-8.541018	0.091060	-0.016174
14	6	0	-7.403658	0.879249	-0.028982
15	6	0	-6.012333	0.604318	-0.030922
16	6	0	-3.644609	-0.176900	-0.016720
17	6	0	-3.774436	1.235019	-0.045114
18	16	0	-5.184230	-0.981309	-0.010768
19	6	0	-5.094674	1.671669	-0.048178
20	6	0	-2.266372	-0.446819	-0.005061
21	6	0	-1.601217	0.801261	-0.030154
22	7	0	-2.518767	1.827040	-0.082221
23	16	0	-1.153288	-1.804613	0.014409
24	16	0	1.155951	1.804046	-0.006440
25	6	0	0.198459	-0.673890	0.015071
26	6	0	-0.195732	0.673649	-0.009941
27	6	0	1.605485	-0.801161	0.031245
28	6	0	2.269958	0.446885	0.014826
29	6	0	3.645642	0.178115	0.022029
30	6	0	3.778035	-1.234203	0.041088
31	6	0	5.098872	-1.672062	0.037843
32	6	0	6.014579	-0.603673	0.018681
33	16	0	5.183934	0.981575	0.006357
34	7	0	2.523744	-1.825991	0.074863
35	6	0	7.403662	-0.877976	0.021044
36	6	0	8.537233	-0.092705	0.012331
37	6	0	8.561328	1.387473	0.002530
38	6	0	9.928216	-0.563376	0.009551
39	6	0	9.984927	1.790055	-0.016768
40	6	0	10.798722	0.642222	-0.011397
41	6	0	10.503408	3.076522	-0.036417

42	6	0	12.191096	0.797152	-0.026400
43	6	0	11.891644	3.223455	-0.050981
44	6	0	12.717946	2.092867	-0.045942
45	6	0	10.393444	-1.869090	0.019236
46	6	0	9.549480	-3.022970	0.035046
47	6	0	11.782149	-2.214362	0.014218
48	7	0	8.886039	-3.981165	0.048598
49	7	0	12.902816	-2.533282	0.010741
50	6	0	-10.389702	1.866444	0.020933
51	6	0	-11.776649	2.212459	0.032800
52	6	0	-9.541847	3.016469	0.038939
53	7	0	-12.898127	2.528290	0.041976
54	7	0	-8.878557	3.974852	0.053107
55	8	0	-7.608966	-2.153555	-0.027821
56	8	0	7.601227	2.149838	-0.010997
57	6	0	2.245587	-3.242352	-0.079787
58	1	0	1.305044	-3.486742	0.418571
59	1	0	2.179750	-3.528693	-1.135208
60	1	0	3.041243	-3.817786	0.397858
61	6	0	-2.241803	3.240615	0.097504
62	1	0	-2.188682	3.512527	1.157707
63	1	0	-1.294981	3.493294	-0.384801
64	1	0	-3.029863	3.825683	-0.381225
65	1	0	5.426008	-2.705285	0.046395
66	1	0	12.863069	-0.048406	-0.023152
67	1	0	13.796140	2.219598	-0.057452
68	1	0	12.335060	4.214225	-0.066493
69	1	0	9.830125	3.927533	-0.040174
70	1	0	7.573343	-1.947857	0.028622
71	1	0	-7.572443	1.949579	-0.032416
72	1	0	-5.420680	2.704946	-0.072146

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Rotational constants (GHZ):      0.1750329      0.0104016      0.0098197
Standard basis: 6-31G(d,p) (6D, 7F)
There are 916 symmetry adapted cartesian basis functions of A symmetry.
There are 916 symmetry adapted basis functions of A symmetry.
916 basis functions, 1734 primitive gaussians, 916 cartesian basis func-
tions
196 alpha electrons      196 beta electrons
nuclear repulsion energy      6569.2560474620 Hartrees.
NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T
Big=T
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
Nuclear repulsion after empirical dispersion term = 6569.1711369947 Har-
trees.
One-electron integrals computed using PRISM.
NBasis= 916 RedAO= T EigKep= 3.25D-04 NBF= 916
NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916
Lowest energy guess from the checkpoint file: "PBDB.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 -0.000005 -0.000001 -0.000154 Ang= -0.02 deg.
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 -0.000080 0.000000 0.000186 Ang= -0.02 deg.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
Integral accuracy reduced to 1.0D-05 until final iterations.

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Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
 SCF Done: E(RB3LYP) = -3683.01982429 A.U. after 10 cycles
 NFock= 10 Conv=0.58D-08 -V/T= 2.0068
 Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1
 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-0.000068173	0.000251455	0.000130443
2	6	0.000010784	-0.000231690	0.000249759
3	6	0.000058762	-0.000297456	-0.000020939
4	6	-0.000005097	0.000186529	0.000038544
5	6	0.000031725	-0.000138562	0.000016663
6	6	0.000306888	0.000299750	0.000240979
7	1	0.000000922	0.000015640	0.000044055
8	1	0.000004938	0.000028046	-0.000012005
9	1	0.000008608	0.000028883	-0.000005146
10	1	-0.000012636	0.000182686	0.000052091
11	6	0.000373715	-0.000246884	-0.000165140
12	6	-0.000322691	-0.000393074	-0.000830041
13	6	0.001036567	-0.003527457	0.000729741
14	6	0.000236677	0.003463478	-0.000139446
15	6	-0.001138864	0.000375199	-0.000657312
16	6	0.001115332	0.000018825	0.000650568
17	6	-0.000409847	0.000347256	0.000705637
18	16	0.000660752	-0.000942006	0.000507990
19	6	-0.001323901	-0.000106689	-0.000209437
20	6	-0.000871840	0.000115626	0.000104418
21	6	0.000603630	0.000250633	0.000382375
22	7	0.001042292	0.001393696	-0.001497376
23	16	-0.000116379	-0.000339625	-0.000207442
24	16	0.000071961	0.000026307	0.000105546
25	6	0.000911036	-0.000323473	0.000709774
26	6	-0.000164663	-0.000074464	-0.000035529
27	6	-0.000977865	0.000955835	-0.001448436
28	6	-0.001000629	0.000401968	-0.000530707
29	6	0.000513895	-0.000447171	0.000943739
30	6	0.001098099	-0.000379217	-0.000420557
31	6	-0.000337600	0.000109586	0.000104437
32	6	0.000007341	0.000483357	-0.000676634
33	16	-0.000192767	0.000106838	-0.000468300
34	7	-0.001122417	-0.000502330	0.001033684
35	6	0.000303316	-0.000779637	0.000646082
36	6	0.001615450	-0.000287864	0.000192124
37	6	-0.000761002	-0.000231210	0.002631761
38	6	-0.000083494	0.000905616	0.000302476
39	6	0.000602085	0.000511111	-0.000521354
40	6	0.000728048	-0.000481973	0.000254974
41	6	-0.000092785	0.000097655	-0.000065993
42	6	-0.001161147	0.000363109	-0.000858814
43	6	-0.000008100	-0.000265490	0.000062724
44	6	-0.000071539	0.000352755	-0.000013548
45	6	0.000211101	-0.000482203	0.000119950
46	6	-0.000130341	-0.000976374	-0.000393197
47	6	-0.001219537	0.000155925	-0.000909457
48	7	-0.000119205	0.000213239	-0.000018972
49	7	-0.000271190	0.000351826	-0.000172158
50	6	-0.000894854	-0.000563778	-0.000715865

51	6	0.000361757	-0.000081555	0.000306543
52	6	-0.000521473	0.000206273	-0.000160644
53	7	0.000172214	-0.000505426	0.000036953
54	7	0.000191461	-0.000063324	0.000073752
55	8	0.000243594	0.000235034	0.000300569
56	8	0.000538800	-0.000278173	-0.000755489
57	6	0.000409597	0.000741079	-0.000237249
58	1	0.000030375	0.000030779	0.000037932
59	1	0.000008508	0.000030345	-0.000049722
60	1	-0.000062386	-0.000014919	-0.000024806
61	6	-0.000615532	-0.001379676	0.000123797
62	1	0.000030930	0.000191496	0.000164566
63	1	0.000026648	0.000181260	0.000087155
64	1	0.000053385	0.000262378	0.000095619
65	1	0.000010457	-0.000073489	0.000031293
66	1	0.000263603	0.000085651	0.000241099
67	1	0.000004728	0.000022029	0.000003166
68	1	-0.000008684	-0.000040844	-0.000011001
69	1	0.000002226	-0.000026572	-0.000045607
70	1	0.000175061	-0.000044527	0.000160950
71	1	-0.000155447	0.000387933	0.000171947
72	1	0.000164815	0.000160045	-0.000517551

Cartesian Forces: Max 0.003527457 RMS 0.000624036

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.004691716 RMS 0.000455515

Search for a local minimum.

Step number 19 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 16 15 18 17 19

ITU= 0 -1 0 -1 1 1 1 1 1 1 0 0 0 1 0 0 0 1 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00228	0.00231	0.00235	0.00249	0.00288
Eigenvalues ---	0.00380	0.00393	0.00417	0.00447	0.00472
Eigenvalues ---	0.00484	0.00504	0.00576	0.00596	0.00603
Eigenvalues ---	0.00631	0.00664	0.00665	0.00685	0.00700
Eigenvalues ---	0.00717	0.00721	0.00744	0.00760	0.00769
Eigenvalues ---	0.00779	0.00816	0.00828	0.00842	0.00850
Eigenvalues ---	0.00878	0.01053	0.01087	0.01131	0.01160
Eigenvalues ---	0.01184	0.01221	0.01266	0.01335	0.01360
Eigenvalues ---	0.01365	0.01386	0.01437	0.01457	0.01482
Eigenvalues ---	0.01593	0.01646	0.01651	0.01754	0.01771
Eigenvalues ---	0.01794	0.01835	0.01929	0.01953	0.02006
Eigenvalues ---	0.02022	0.02075	0.02076	0.02208	0.02210
Eigenvalues ---	0.03824	0.04828	0.04837	0.04906	0.04937
Eigenvalues ---	0.04981	0.05017	0.05032	0.05295	0.07032
Eigenvalues ---	0.07233	0.07369	0.07568	0.15577	0.15923
Eigenvalues ---	0.15970	0.15988	0.15999	0.16000	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues ---	0.16001	0.16002	0.16005	0.16015	0.16029
Eigenvalues ---	0.16071	0.17556	0.18996	0.19213	0.19780
Eigenvalues ---	0.20558	0.21268	0.21400	0.21857	0.22002
Eigenvalues ---	0.22008	0.22262	0.22443	0.22580	0.22632
Eigenvalues ---	0.22636	0.22683	0.22762	0.22941	0.23070

Eigenvalues	---	0.23348	0.23467	0.23700	0.23741	0.23826
Eigenvalues	---	0.23996	0.24137	0.24200	0.24268	0.24314
Eigenvalues	---	0.24382	0.24539	0.24605	0.24722	0.24828
Eigenvalues	---	0.24877	0.24911	0.24930	0.24990	0.24992
Eigenvalues	---	0.24994	0.24996	0.24996	0.24997	0.24999
Eigenvalues	---	0.24999	0.25000	0.25000	0.25000	0.25000
Eigenvalues	---	0.25009	0.25060	0.25541	0.25745	0.25908
Eigenvalues	---	0.26249	0.26456	0.26738	0.26811	0.27036
Eigenvalues	---	0.27207	0.27717	0.27838	0.28273	0.28390
Eigenvalues	---	0.28539	0.28802	0.29848	0.30148	0.30589
Eigenvalues	---	0.32140	0.32934	0.35540	0.35919	0.36336
Eigenvalues	---	0.36340	0.36467	0.36481	0.36652	0.36733
Eigenvalues	---	0.36805	0.36842	0.37086	0.37099	0.37124
Eigenvalues	---	0.37257	0.37275	0.37426	0.37568	0.37674
Eigenvalues	---	0.37758	0.38015	0.38974	0.40305	0.40650
Eigenvalues	---	0.41644	0.42157	0.42649	0.44420	0.44786
Eigenvalues	---	0.45583	0.45878	0.46239	0.47772	0.47917
Eigenvalues	---	0.48279	0.51866	0.53263	0.55087	0.57390
Eigenvalues	---	0.58463	0.71817	0.72735	0.80314	0.81951
Eigenvalues	---	0.92291	1.25858	1.26315	1.29342	1.35384

RFO step: Lambda=-8.30834386D-04 EMin= 2.27925887D-03

Quartic linear search produced a step of -0.00012.

Iteration 1 RMS(Cart)= 0.04968832 RMS(Int)= 0.00069108

Iteration 2 RMS(Cart)= 0.00237792 RMS(Int)= 0.00021487

Iteration 3 RMS(Cart)= 0.00000245 RMS(Int)= 0.00021487

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00021487

Variable (Linear)	Old X (Quad)	-DE/DX (Total)	Delta X	Delta X	Delta X	New X
R1	2.65831	0.00021	0.00000	0.00002	0.00002	2.65833
R2	2.64474	0.00016	0.00000	0.00039	0.00039	2.64513
R3	2.80842	0.00104	0.00000	0.00159	0.00158	2.81000
R4	2.62175	-0.00015	0.00000	0.00027	0.00027	2.62202
R5	2.79619	-0.00069	0.00000	-0.00106	-0.00106	2.79513
R6	2.63846	-0.00010	0.00000	-0.00006	-0.00006	2.63840
R7	2.05062	0.00003	0.00000	-0.00008	-0.00008	2.05054
R8	2.64621	-0.00012	0.00000	-0.00013	-0.00013	2.64608
R9	2.05149	0.00003	0.00000	0.00008	0.00008	2.05157
R10	2.64334	0.00001	0.00000	-0.00013	-0.00013	2.64321
R11	2.05157	0.00002	0.00000	-0.00003	-0.00003	2.05155
R12	2.04180	-0.00007	0.00000	-0.00041	-0.00041	2.04138
R13	2.76922	0.00010	0.00000	0.00010	0.00009	2.76931
R14	2.61482	0.00124	0.00000	0.00265	0.00265	2.61747
R15	2.79846	-0.00076	0.00000	-0.00244	-0.00243	2.79602
R16	2.31654	0.00038	0.00000	0.00055	0.00055	2.31710
R17	2.61507	-0.00469	0.00000	-0.01201	-0.01201	2.60306
R18	2.68007	-0.00129	0.00000	-0.00897	-0.00897	2.67109
R19	2.04763	-0.00027	0.00000	-0.00057	-0.00057	2.04707
R20	3.38064	0.00065	0.00000	0.00042	0.00038	3.38102
R21	2.66018	-0.00049	0.00000	0.00017	0.00017	2.66035
R22	2.67993	0.00017	0.00000	0.00256	0.00253	2.68246
R23	3.28266	-0.00083	0.00000	-0.00129	-0.00131	3.28135
R24	2.65406	-0.00084	0.00000	-0.00235	-0.00260	2.65146
R25	2.62781	0.00070	0.00000	0.00563	0.00568	2.63348
R26	2.62432	-0.00029	0.00000	-0.00148	-0.00128	2.62304
R27	2.04799	0.00008	0.00000	-0.00020	-0.00020	2.04779
R28	2.67299	-0.00044	0.00000	0.00184	0.00178	2.67477
R29	3.31804	-0.00025	0.00000	0.00032	0.00032	3.31836
R30	2.60263	0.00023	0.00000	-0.00043	-0.00023	2.60240
R31	2.66718	-0.00021	0.00000	0.00477	0.00479	2.67197
R32	2.74317	0.00055	0.00000	0.00054	0.00054	2.74371

R33	3.33029	-0.00025	0.00000	0.00009	0.00006	3.33035
R34	3.32981	-0.00005	0.00000	0.00117	0.00115	3.33096
R35	3.31826	-0.00020	0.00000	0.00057	0.00057	3.31883
R36	2.65362	-0.00001	0.00000	0.00043	0.00042	2.65403
R37	2.66992	-0.00132	0.00000	-0.00003	-0.00002	2.66990
R38	2.67208	0.00011	0.00000	0.00204	0.00201	2.67410
R39	2.60164	0.00030	0.00000	0.00272	0.00282	2.60446
R40	2.64885	0.00117	0.00000	0.00866	0.00853	2.65738
R41	2.68084	-0.00004	0.00000	0.00107	0.00106	2.68190
R42	3.27972	0.00014	0.00000	0.00137	0.00135	3.28107
R43	2.62960	-0.00013	0.00000	0.00562	0.00566	2.63526
R44	2.62162	0.00070	0.00000	0.00348	0.00358	2.62520
R45	2.65931	0.00017	0.00000	0.00266	0.00266	2.66197
R46	2.04810	-0.00002	0.00000	-0.00001	-0.00001	2.04809
R47	3.38210	0.00038	0.00000	0.00221	0.00218	3.38427
R48	2.67568	0.00118	0.00000	0.01401	0.01401	2.68969
R49	2.74327	0.00066	0.00000	0.00052	0.00052	2.74379
R50	2.60598	0.00003	0.00000	0.00053	0.00053	2.60651
R51	2.04710	0.00014	0.00000	-0.00052	-0.00052	2.04658
R52	2.79756	-0.00029	0.00000	-0.00110	-0.00087	2.79669
R53	2.77499	-0.00188	0.00000	-0.00664	-0.00680	2.76819
R54	2.79595	-0.00054	0.00000	-0.00087	-0.00058	2.79537
R55	2.31688	0.00004	0.00000	0.00001	0.00001	2.31689
R56	2.81035	-0.00020	0.00000	-0.00232	-0.00263	2.80772
R57	2.61945	-0.00212	0.00000	-0.00239	-0.00239	2.61706
R58	2.65896	-0.00039	0.00000	-0.00118	-0.00120	2.65775
R59	2.62135	0.00006	0.00000	0.00226	0.00229	2.62364
R60	2.64760	-0.00116	0.00000	-0.00378	-0.00379	2.64380
R61	2.63818	-0.00003	0.00000	-0.00007	-0.00005	2.63813
R62	2.05063	0.00003	0.00000	-0.00001	-0.00001	2.05062
R63	2.64348	-0.00015	0.00000	-0.00019	-0.00022	2.64326
R64	2.04102	0.00037	0.00000	0.00018	0.00018	2.04119
R65	2.64631	-0.00004	0.00000	0.00167	0.00165	2.64796
R66	2.05145	0.00004	0.00000	0.00013	0.00013	2.05158
R67	2.05163	-0.00001	0.00000	-0.00008	-0.00008	2.05155
R68	2.70169	-0.00078	0.00000	-0.00333	-0.00333	2.69836
R69	2.70419	-0.00189	0.00000	-0.00786	-0.00786	2.69633
R70	2.20255	0.00021	0.00000	0.00016	0.00016	2.20270
R71	2.20185	-0.00043	0.00000	-0.00023	-0.00023	2.20162
R72	2.70138	-0.00081	0.00000	-0.00264	-0.00264	2.69874
R73	2.70022	-0.00016	0.00000	-0.00064	-0.00064	2.69958
R74	2.20179	-0.00033	0.00000	-0.00015	-0.00015	2.20164
R75	2.20269	0.00006	0.00000	0.00002	0.00002	2.20271
R76	2.06379	-0.00001	0.00000	-0.00008	-0.00008	2.06371
R77	2.07030	-0.00004	0.00000	-0.00029	-0.00029	2.07001
R78	2.06347	-0.00007	0.00000	-0.00024	-0.00024	2.06323
R79	2.07077	-0.00015	0.00000	-0.00028	-0.00028	2.07049
R80	2.06399	-0.00008	0.00000	0.00005	0.00005	2.06404
R81	2.06363	-0.00008	0.00000	-0.00018	-0.00018	2.06345
A1	2.07756	-0.00058	0.00000	-0.00048	-0.00048	2.07708
A2	1.89891	-0.00019	0.00000	0.00007	0.00006	1.89896
A3	2.30672	0.00076	0.00000	0.00042	0.00042	2.30714
A4	2.14154	0.00033	0.00000	0.00021	0.00020	2.14175
A5	1.91098	0.00024	0.00000	0.00015	0.00016	1.91113
A6	2.23066	-0.00057	0.00000	-0.00035	-0.00036	2.23031
A7	2.05891	0.00009	0.00000	0.00010	0.00010	2.05901
A8	2.08961	-0.00003	0.00000	0.00021	0.00021	2.08982
A9	2.13466	-0.00005	0.00000	-0.00031	-0.00031	2.13435
A10	2.09617	-0.00021	0.00000	-0.00024	-0.00024	2.09593
A11	2.09712	0.00011	0.00000	0.00031	0.00031	2.09743

A12	2.08990	0.00010	0.00000	-0.00007	-0.00007	2.08983
A13	2.12443	0.00013	0.00000	0.00022	0.00022	2.12464
A14	2.08503	-0.00009	0.00000	-0.00075	-0.00075	2.08429
A15	2.07372	-0.00004	0.00000	0.00053	0.00053	2.07425
A16	2.06776	0.00024	0.00000	0.00020	0.00020	2.06796
A17	2.13115	0.00006	0.00000	-0.00035	-0.00035	2.13080
A18	2.08427	-0.00030	0.00000	0.00015	0.00015	2.08442
A19	1.87224	-0.00068	0.00000	-0.00182	-0.00186	1.87038
A20	2.17306	0.00149	0.00000	-0.00098	-0.00101	2.17206
A21	2.23784	-0.00080	0.00000	0.00292	0.00289	2.24074
A22	1.86257	0.00002	0.00000	-0.00006	-0.00014	1.86244
A23	2.19491	-0.00028	0.00000	-0.00071	-0.00081	2.19409
A24	2.22570	0.00026	0.00000	0.00079	0.00069	2.22639
A25	1.88007	0.00061	0.00000	0.00161	0.00161	1.88168
A26	2.20840	-0.00032	0.00000	-0.00115	-0.00116	2.20724
A27	2.19470	-0.00029	0.00000	-0.00043	-0.00044	2.19426
A28	2.34047	0.00076	0.00000	0.00268	0.00257	2.34303
A29	2.02041	-0.00069	0.00000	-0.00379	-0.00390	2.01651
A30	1.92229	-0.00007	0.00000	0.00128	0.00117	1.92345
A31	2.24711	0.00078	0.00000	0.00017	0.00016	2.24726
A32	2.08581	-0.00074	0.00000	0.00013	0.00011	2.08592
A33	1.95026	-0.00005	0.00000	-0.00031	-0.00029	1.94997
A34	1.96056	-0.00050	0.00000	-0.00354	-0.00346	1.95710
A35	1.85599	0.00043	0.00000	0.00211	0.00205	1.85803
A36	2.46664	0.00007	0.00000	0.00143	0.00140	2.46804
A37	1.98186	0.00062	0.00000	0.00261	0.00251	1.98437
A38	1.92004	-0.00050	0.00000	-0.00314	-0.00284	1.91720
A39	2.38115	-0.00012	0.00000	0.00076	0.00046	2.38161
A40	1.57059	0.00042	0.00000	0.00348	0.00344	1.57403
A41	1.96145	-0.00050	0.00000	-0.00226	-0.00223	1.95922
A42	2.12596	0.00005	0.00000	0.00021	0.00008	2.12604
A43	2.19571	0.00045	0.00000	0.00229	0.00215	2.19786
A44	1.86684	0.00001	0.00000	-0.00018	-0.00026	1.86659
A45	2.45090	0.00004	0.00000	0.00209	0.00208	2.45298
A46	1.96538	-0.00004	0.00000	-0.00181	-0.00176	1.96362
A47	1.92257	-0.00009	0.00000	-0.00174	-0.00140	1.92117
A48	1.96952	0.00016	0.00000	0.00056	0.00045	1.96997
A49	2.39102	-0.00007	0.00000	0.00116	0.00092	2.39195
A50	1.85862	0.00016	0.00000	0.00344	0.00285	1.86146
A51	2.19486	0.00015	0.00000	0.00884	0.00730	2.20216
A52	2.20618	-0.00023	0.00000	0.00627	0.00471	2.21089
A53	1.56089	0.00004	0.00000	0.00251	0.00248	1.56336
A54	1.56166	-0.00024	0.00000	0.00071	0.00071	1.56237
A55	1.98273	-0.00006	0.00000	-0.00078	-0.00081	1.98192
A56	2.35473	0.00004	0.00000	0.00072	0.00071	2.35544
A57	1.94572	0.00002	0.00000	0.00007	0.00010	1.94582
A58	2.35450	0.00005	0.00000	0.00060	0.00057	2.35508
A59	1.94610	-0.00010	0.00000	-0.00026	-0.00022	1.94588
A60	1.98258	0.00006	0.00000	-0.00033	-0.00035	1.98223
A61	1.96963	0.00020	0.00000	0.00073	0.00068	1.97031
A62	2.39153	-0.00011	0.00000	0.00092	0.00079	2.39233
A63	1.92193	-0.00009	0.00000	-0.00161	-0.00144	1.92049
A64	1.96513	-0.00004	0.00000	-0.00118	-0.00114	1.96399
A65	2.45105	0.00001	0.00000	0.00130	0.00128	2.45233
A66	1.86701	0.00003	0.00000	-0.00013	-0.00018	1.86683
A67	1.85725	-0.00006	0.00000	0.00052	0.00046	1.85771
A68	2.46718	0.00004	0.00000	0.00097	0.00091	2.46809
A69	1.95874	0.00002	0.00000	-0.00138	-0.00140	1.95734
A70	1.98429	-0.00002	0.00000	0.00031	0.00022	1.98451
A71	1.91838	-0.00008	0.00000	-0.00170	-0.00156	1.91682

A72	2.38042	0.00010	0.00000	0.00163	0.00144	2.38185
A73	1.95929	0.00025	0.00000	0.00048	0.00046	1.95975
A74	2.19748	-0.00005	0.00000	0.00031	0.00022	2.19770
A75	2.12641	-0.00020	0.00000	-0.00084	-0.00092	2.12549
A76	1.95040	-0.00028	0.00000	-0.00225	-0.00229	1.94811
A77	2.08435	-0.00076	0.00000	0.00086	0.00085	2.08520
A78	2.24840	0.00104	0.00000	0.00147	0.00146	2.24987
A79	1.57205	0.00004	0.00000	0.00274	0.00266	1.57471
A80	1.85952	0.00020	0.00000	0.00358	0.00321	1.86273
A81	2.20820	-0.00029	0.00000	0.00315	0.00228	2.21048
A82	2.19795	0.00013	0.00000	0.00533	0.00447	2.20242
A83	2.34076	0.00191	0.00000	0.00456	0.00455	2.34531
A84	1.92305	-0.00075	0.00000	0.00031	0.00031	1.92335
A85	2.01937	-0.00116	0.00000	-0.00486	-0.00486	2.01451
A86	2.19293	0.00150	0.00000	0.00201	0.00190	2.19483
A87	2.20947	-0.00144	0.00000	-0.00181	-0.00192	2.20756
A88	1.88078	-0.00006	0.00000	-0.00021	0.00001	1.88078
A89	1.86273	0.00005	0.00000	0.00061	-0.00058	1.86215
A90	2.22565	0.00040	0.00000	0.00137	-0.00080	2.22485
A91	2.19461	-0.00044	0.00000	0.00010	-0.00206	2.19255
A92	1.86989	0.00047	0.00000	0.00162	0.00128	1.87117
A93	2.23932	-0.00153	0.00000	0.00351	0.00363	2.24294
A94	2.17398	0.00105	0.00000	-0.00508	-0.00496	2.16902
A95	1.91184	-0.00010	0.00000	-0.00167	-0.00133	1.91051
A96	2.22960	-0.00013	0.00000	0.00157	0.00134	2.23094
A97	2.14174	0.00023	0.00000	0.00010	-0.00004	2.14171
A98	1.89951	-0.00036	0.00000	0.00003	-0.00018	1.89933
A99	2.30705	0.00042	0.00000	-0.00136	-0.00127	2.30577
A100	2.07663	-0.00006	0.00000	0.00133	0.00145	2.07808
A101	2.05944	-0.00015	0.00000	-0.00111	-0.00105	2.05840
A102	2.08915	0.00010	0.00000	0.00112	0.00109	2.09024
A103	2.13459	0.00005	0.00000	-0.00001	-0.00004	2.13455
A104	2.06789	0.00018	0.00000	-0.00027	-0.00029	2.06760
A105	2.13141	-0.00008	0.00000	-0.00113	-0.00112	2.13029
A106	2.08389	-0.00010	0.00000	0.00140	0.00141	2.08529
A107	2.09641	-0.00033	0.00000	-0.00054	-0.00053	2.09588
A108	2.09714	0.00016	0.00000	0.00018	0.00018	2.09731
A109	2.08964	0.00017	0.00000	0.00036	0.00035	2.08999
A110	2.12426	0.00014	0.00000	0.00048	0.00045	2.12471
A111	2.07408	-0.00009	0.00000	0.00021	0.00022	2.07430
A112	2.08485	-0.00005	0.00000	-0.00069	-0.00068	2.08418
A113	2.16785	-0.00090	0.00000	0.00336	0.00335	2.17120
A114	2.15671	0.00035	0.00000	-0.00678	-0.00678	2.14994
A115	1.95862	0.00055	0.00000	0.00342	0.00342	1.96204
A116	2.15511	0.00101	0.00000	-0.00297	-0.00297	2.15214
A117	2.16663	-0.00030	0.00000	0.00230	0.00230	2.16893
A118	1.96144	-0.00071	0.00000	0.00068	0.00068	1.96211
A119	1.91212	0.00008	0.00000	0.00113	0.00113	1.91326
A120	1.94889	0.00003	0.00000	-0.00068	-0.00068	1.94822
A121	1.90492	-0.00004	0.00000	0.00047	0.00047	1.90539
A122	1.90643	-0.00005	0.00000	-0.00053	-0.00053	1.90590
A123	1.88599	-0.00003	0.00000	-0.00014	-0.00014	1.88584
A124	1.90441	0.00001	0.00000	-0.00024	-0.00024	1.90417
A125	1.95053	-0.00019	0.00000	0.00010	0.00010	1.95063
A126	1.91347	-0.00016	0.00000	-0.00002	-0.00002	1.91345
A127	1.90684	-0.00031	0.00000	-0.00050	-0.00051	1.90634
A128	1.90478	0.00021	0.00000	-0.00010	-0.00010	1.90468
A129	1.90306	0.00025	0.00000	-0.00066	-0.00066	1.90239
A130	1.88394	0.00023	0.00000	0.00123	0.00123	1.88517
A131	3.16750	-0.00025	0.00000	0.00738	0.00738	3.17488

A132	3.17516	0.00047	0.00000	0.00955	0.00955	3.18471
A133	3.17161	0.00092	0.00000	0.01259	0.01259	3.18420
A134	3.17148	-0.00044	0.00000	-0.00568	-0.00568	3.16579
A135	3.14196	-0.00007	0.00000	-0.00087	-0.00087	3.14109
A136	3.14147	0.00000	0.00000	-0.00013	-0.00013	3.14134
A137	3.14228	-0.00004	0.00000	-0.00048	-0.00048	3.14181
A138	3.14084	0.00012	0.00000	0.00241	0.00241	3.14325
D1	-0.00103	-0.00001	0.00000	-0.00013	-0.00013	-0.00116
D2	3.13923	0.00001	0.00000	0.00180	0.00181	3.14104
D3	3.13943	0.00002	0.00000	0.00153	0.00153	3.14095
D4	-0.00349	0.00003	0.00000	0.00346	0.00346	-0.00003
D5	0.00034	0.00001	0.00000	0.00098	0.00098	0.00132
D6	-3.14112	0.00002	0.00000	0.00074	0.00073	-3.14039
D7	-3.13981	-0.00001	0.00000	-0.00114	-0.00113	-3.14094
D8	0.00192	0.00000	0.00000	-0.00138	-0.00138	0.00054
D9	0.00524	0.00002	0.00000	0.00580	0.00579	0.01103
D10	-3.12716	-0.00010	0.00000	-0.00798	-0.00796	-3.13512
D11	-3.13768	0.00004	0.00000	0.00775	0.00774	-3.12994
D12	0.01309	-0.00007	0.00000	-0.00603	-0.00601	0.00709
D13	0.00081	0.00000	0.00000	-0.00070	-0.00070	0.00011
D14	-3.14056	-0.00001	0.00000	-0.00011	-0.00011	-3.14067
D15	-3.13921	-0.00003	0.00000	-0.00301	-0.00301	3.14097
D16	0.00261	-0.00003	0.00000	-0.00241	-0.00241	0.00020
D17	0.00041	-0.00007	0.00000	-0.01126	-0.01126	-0.01085
D18	3.14110	0.00003	0.00000	0.01290	0.01289	-3.12919
D19	3.14059	-0.00005	0.00000	-0.00921	-0.00921	3.13139
D20	-0.00190	0.00005	0.00000	0.01496	0.01495	0.01305
D21	0.00009	0.00001	0.00000	0.00066	0.00066	0.00075
D22	3.14112	0.00001	0.00000	0.00085	0.00085	-3.14122
D23	3.14146	0.00001	0.00000	0.00005	0.00005	3.14151
D24	-0.00071	0.00001	0.00000	0.00024	0.00024	-0.00046
D25	-0.00076	0.00000	0.00000	0.00020	0.00020	-0.00056
D26	3.14069	0.00000	0.00000	-0.00001	-0.00001	3.14068
D27	3.14139	0.00000	0.00000	0.00001	0.00001	3.14140
D28	-0.00034	0.00000	0.00000	-0.00020	-0.00020	-0.00054
D29	0.00053	-0.00001	0.00000	-0.00103	-0.00103	-0.00050
D30	-3.14119	-0.00002	0.00000	-0.00079	-0.00079	3.14121
D31	-3.14092	-0.00001	0.00000	-0.00082	-0.00082	3.14145
D32	0.00055	-0.00002	0.00000	-0.00058	-0.00058	-0.00003
D33	-0.00491	-0.00006	0.00000	-0.01267	-0.01267	-0.01758
D34	3.13121	-0.00006	0.00000	-0.00744	-0.00744	3.12377
D35	3.12705	0.00007	0.00000	0.00175	0.00176	3.12881
D36	-0.02002	0.00007	0.00000	0.00698	0.00699	-0.01303
D37	-0.01037	0.00008	0.00000	0.00851	0.00852	-0.00185
D38	3.12933	0.00016	0.00000	0.01410	0.01410	-3.13976
D39	-3.14079	-0.00006	0.00000	-0.00820	-0.00820	3.13419
D40	-0.00110	0.00002	0.00000	-0.00262	-0.00262	-0.00373
D41	0.00286	0.00008	0.00000	0.01465	0.01466	0.01751
D42	-3.13332	0.00008	0.00000	0.00947	0.00948	-3.12384
D43	-3.13781	-0.00002	0.00000	-0.01008	-0.01008	3.13529
D44	0.00920	-0.00002	0.00000	-0.01526	-0.01526	-0.00606
D45	3.13029	0.00026	0.00000	0.04157	0.04156	-3.11133
D46	-0.00329	0.00006	0.00000	0.01028	0.01030	0.00701
D47	-0.01773	0.00026	0.00000	0.04772	0.04770	0.02997
D48	3.13188	0.00006	0.00000	0.01643	0.01644	-3.13487
D49	-0.00398	0.00004	0.00000	0.04390	0.04388	0.03990
D50	3.13984	0.00008	0.00000	0.04959	0.04957	-3.09377
D51	3.12993	0.00023	0.00000	0.07389	0.07391	-3.07935
D52	-0.00943	0.00027	0.00000	0.07959	0.07961	0.07018
D53	-3.13422	0.00011	0.00000	0.00559	0.00559	-3.12863

D54	0.00528	0.00008	0.00000	0.00026	0.00025	0.00553
D55	3.13953	-0.00012	0.00000	-0.00356	-0.00356	3.13597
D56	-0.01306	0.00020	0.00000	0.01935	0.01933	0.00627
D57	-0.00019	-0.00009	0.00000	0.00123	0.00123	0.00103
D58	3.13041	0.00023	0.00000	0.02413	0.02411	-3.12867
D59	0.01085	0.00000	0.00000	0.00270	0.00269	0.01354
D60	-3.11592	-0.00007	0.00000	-0.00981	-0.00980	-3.12572
D61	-3.13249	-0.00001	0.00000	0.00130	0.00131	-3.13118
D62	0.02393	-0.00008	0.00000	-0.01121	-0.01118	0.01276
D63	-0.00897	-0.00004	0.00000	-0.00162	-0.00162	-0.01059
D64	3.13529	-0.00003	0.00000	0.00052	0.00051	3.13580
D65	-0.00265	0.00006	0.00000	0.00455	0.00456	0.00191
D66	-3.13052	-0.00005	0.00000	-0.00604	-0.00606	-3.13659
D67	3.13637	0.00006	0.00000	0.00248	0.00250	3.13887
D68	0.00849	-0.00006	0.00000	-0.00811	-0.00812	0.00037
D69	-0.00672	0.00006	0.00000	-0.00251	-0.00251	-0.00923
D70	-3.13679	-0.00027	0.00000	-0.02650	-0.02651	3.11988
D71	3.11466	0.00016	0.00000	0.01450	0.01451	3.12917
D72	-0.01541	-0.00018	0.00000	-0.00948	-0.00949	-0.02490
D73	-0.03579	0.00007	0.00000	0.01331	0.01329	-0.02250
D74	-2.95728	-0.00024	0.00000	-0.07278	-0.07283	-3.03011
D75	3.12552	-0.00003	0.00000	-0.00333	-0.00332	3.12220
D76	0.20403	-0.00034	0.00001	-0.08942	-0.08944	0.11459
D77	-0.01968	-0.00002	0.00000	0.00361	0.00358	-0.01610
D78	3.13267	0.00007	0.00000	0.00512	0.00509	3.13775
D79	3.11245	0.00005	0.00000	0.01095	0.01092	3.12336
D80	-0.01839	0.00014	0.00000	0.01246	0.01242	-0.00597
D81	-3.14072	0.00004	0.00000	0.00182	0.00187	-3.13885
D82	0.01508	-0.00008	0.00000	-0.00916	-0.00914	0.00594
D83	0.03407	-0.00002	0.00000	-0.01033	-0.01032	0.02375
D84	2.95371	0.00035	0.00000	0.07691	0.07678	3.03049
D85	-3.12205	-0.00014	0.00000	-0.01238	-0.01236	-3.13441
D86	-0.20241	0.00023	-0.00001	0.07485	0.07474	-0.12767
D87	-3.12777	-0.00012	0.00000	-0.01094	-0.01093	-3.13871
D88	0.01178	-0.00015	0.00000	-0.00938	-0.00936	0.00242
D89	0.02862	0.00001	0.00000	-0.00883	-0.00884	0.01978
D90	-3.11501	-0.00002	0.00000	-0.00727	-0.00727	-3.12227
D91	1.44731	0.00022	0.00000	0.05813	0.05823	1.50554
D92	-2.72160	0.00024	0.00000	0.05806	0.05816	-2.66344
D93	-0.66031	0.00024	0.00000	0.05924	0.05934	-0.60098
D94	-1.43115	-0.00021	0.00000	-0.04456	-0.04465	-1.47580
D95	0.68313	-0.00018	0.00000	-0.04462	-0.04472	0.63841
D96	2.74441	-0.00018	0.00000	-0.04345	-0.04355	2.70087
D97	-0.00851	0.00000	0.00000	0.00387	0.00387	-0.00464
D98	3.13689	-0.00001	0.00000	0.00211	0.00210	3.13900
D99	-3.13548	-0.00007	0.00000	-0.00134	-0.00133	-3.13681
D100	0.00818	-0.00004	0.00000	-0.00292	-0.00292	0.00526
D101	-0.00963	0.00000	0.00000	0.00019	0.00019	-0.00945
D102	3.13290	0.00010	0.00000	0.01080	0.01079	-3.13949
D103	-0.00018	0.00009	0.00000	0.00236	0.00235	0.00217
D104	3.13984	0.00006	0.00000	0.00356	0.00356	-3.13979
D105	3.13851	0.00009	0.00000	0.00370	0.00369	-3.14098
D106	-0.00466	0.00007	0.00000	0.00490	0.00491	0.00025
D107	3.13505	-0.00007	0.00000	-0.00300	-0.00300	3.13205
D108	-0.02331	-0.00003	0.00000	0.00031	0.00032	-0.02299
D109	-0.00279	-0.00007	0.00000	-0.00473	-0.00473	-0.00752
D110	3.12203	-0.00003	0.00000	-0.00142	-0.00141	3.12062
D111	0.00903	0.00004	0.00000	0.00256	0.00256	0.01160
D112	-3.13319	-0.00002	0.00000	-0.00451	-0.00449	-3.13768
D113	-3.12038	0.00002	0.00000	0.00014	0.00014	-3.12024

D114	0.02058	-0.00005	0.00000	-0.00693	-0.00691	0.01367
D115	3.12398	0.00006	0.00000	0.01169	0.01169	3.13567
D116	0.17396	-0.00023	0.00000	-0.05408	-0.05403	0.11993
D117	-0.03407	0.00010	0.00000	0.01495	0.01495	-0.01912
D118	-2.98409	-0.00019	0.00000	-0.05082	-0.05076	-3.03485
D119	-3.14129	-0.00012	0.00000	-0.01412	-0.01412	3.12777
D120	-0.00809	0.00004	0.00000	0.00653	0.00654	-0.00155
D121	0.00122	-0.00002	0.00000	-0.00388	-0.00388	-0.00267
D122	3.13441	0.00014	0.00000	0.01677	0.01678	-3.13199
D123	3.13175	-0.00001	0.00000	-0.00177	-0.00176	3.12999
D124	-0.02243	0.00008	0.00000	0.01337	0.01334	-0.00909
D125	-0.00418	-0.00011	0.00000	-0.01571	-0.01568	-0.01986
D126	3.12483	-0.00002	0.00000	-0.00057	-0.00058	3.12424
D127	-3.12896	-0.00005	0.00000	-0.00195	-0.00194	-3.13091
D128	0.00393	0.00011	0.00000	0.01946	0.01946	0.02339
D129	0.00194	0.00005	0.00000	0.00084	0.00082	0.00276
D130	-3.13733	0.00012	0.00000	0.02215	0.02214	-3.11518
D131	-3.12250	-0.00008	0.00000	-0.01975	-0.01977	3.14092
D132	0.02142	-0.00001	0.00000	0.00156	0.00156	0.02298
D133	0.03483	-0.00011	0.00000	-0.01744	-0.01745	0.01739
D134	2.98630	0.00012	0.00000	0.04752	0.04757	3.03387
D135	-3.12347	0.00001	0.00000	0.00262	0.00260	-3.12087
D136	-0.17200	0.00024	0.00000	0.06759	0.06762	-0.10438
D137	0.00107	0.00003	0.00000	0.01390	0.01389	0.01496
D138	3.13505	0.00016	0.00000	0.02525	0.02524	-3.12290
D139	3.14044	-0.00003	0.00000	-0.00642	-0.00642	3.13403
D140	-0.00876	0.00010	0.00000	0.00493	0.00493	-0.00384
D141	-0.00287	-0.00008	0.00000	-0.01911	-0.01911	-0.02198
D142	-3.13595	-0.00022	0.00000	-0.03179	-0.03180	3.11544
D143	-3.13544	-0.00017	0.00000	-0.06970	-0.06971	3.07804
D144	0.00974	-0.00021	0.00000	-0.07797	-0.07798	-0.06825
D145	-0.00292	-0.00002	0.00000	-0.05619	-0.05618	-0.05910
D146	-3.14094	-0.00007	0.00000	-0.06445	-0.06445	3.07780
D147	-0.67210	0.00015	0.00000	0.03563	0.03566	-0.63644
D148	1.44227	0.00016	0.00000	0.03529	0.03532	1.47759
D149	-2.73394	0.00016	0.00000	0.03487	0.03490	-2.69904
D150	2.69687	-0.00019	0.00000	-0.04218	-0.04221	2.65466
D151	-1.47195	-0.00018	0.00000	-0.04252	-0.04255	-1.51450
D152	0.63503	-0.00018	0.00000	-0.04294	-0.04297	0.59206
D153	0.00483	-0.00023	0.00000	-0.02194	-0.02193	-0.01710
D154	-3.13548	-0.00016	0.00000	-0.01796	-0.01797	3.12974
D155	-3.14049	-0.00019	0.00000	-0.01333	-0.01333	3.12937
D156	0.00239	-0.00012	0.00000	-0.00935	-0.00936	-0.00697
D157	-3.13299	-0.00029	0.00000	-0.04332	-0.04331	3.10689
D158	-0.01185	0.00043	0.00000	0.06534	0.06533	0.05347
D159	0.00752	-0.00035	0.00000	-0.04668	-0.04666	-0.03914
D160	3.12866	0.00037	0.00000	0.06199	0.06198	-3.09255
D161	3.13390	0.00019	0.00000	0.03659	0.03661	-3.11268
D162	-0.00394	0.00003	0.00000	0.02163	0.02160	0.01766
D163	-0.00660	0.00026	0.00000	0.03999	0.03999	0.03339
D164	3.13875	0.00009	0.00000	0.02503	0.02498	-3.11946
D165	-0.00569	0.00033	0.00000	0.03632	0.03628	0.03059
D166	3.13677	0.00024	0.00000	0.02739	0.02733	-3.11909
D167	-3.12729	-0.00039	0.00000	-0.06988	-0.06980	3.08609
D168	0.01517	-0.00047	0.00000	-0.07881	-0.07875	-0.06358
D169	0.00313	-0.00005	0.00000	-0.01782	-0.01783	-0.01470
D170	-3.13754	-0.00010	0.00000	-0.02064	-0.02063	3.12501
D171	3.14115	0.00009	0.00000	-0.00354	-0.00359	3.13755
D172	0.00047	0.00004	0.00000	-0.00636	-0.00639	-0.00593
D173	-0.00069	0.00002	0.00000	0.00525	0.00525	0.00456

D174	3.14068	0.00008	0.00000	0.00821	0.00821	-3.13430
D175	-3.13792	-0.00017	0.00000	-0.01213	-0.01212	3.13314
D176	0.00345	-0.00011	0.00000	-0.00917	-0.00916	-0.00572
D177	0.00161	-0.00017	0.00000	-0.01166	-0.01166	-0.01005
D178	-3.14075	-0.00013	0.00000	-0.00928	-0.00929	3.13314
D179	-3.14079	-0.00009	0.00000	-0.00326	-0.00326	3.13913
D180	0.00003	-0.00005	0.00000	-0.00088	-0.00089	-0.00086
D181	3.14035	0.00015	0.00000	0.01181	0.01182	-3.13102
D182	-0.00144	0.00010	0.00000	0.01098	0.01100	0.00956
D183	-0.00028	0.00005	0.00000	0.00180	0.00180	0.00152
D184	3.14112	0.00001	0.00000	0.00098	0.00097	-3.14109
D185	3.14081	0.00007	0.00000	0.00265	0.00265	-3.13972
D186	-0.00097	0.00006	0.00000	0.00326	0.00326	0.00229
D187	0.00021	0.00001	0.00000	-0.00039	-0.00038	-0.00017
D188	-3.14157	0.00001	0.00000	0.00022	0.00023	-3.14135
D189	0.00028	-0.00002	0.00000	-0.00145	-0.00144	-0.00116
D190	-3.14156	-0.00003	0.00000	-0.00048	-0.00048	3.14114
D191	-3.14111	0.00002	0.00000	-0.00060	-0.00060	3.14148
D192	0.00023	0.00002	0.00000	0.00036	0.00036	0.00059
D193	-0.00020	0.00001	0.00000	0.00070	0.00070	0.00050
D194	3.14140	0.00000	0.00000	0.00032	0.00032	-3.14147
D195	3.14158	0.00002	0.00000	0.00011	0.00011	-3.14150
D196	-0.00001	0.00001	0.00000	-0.00027	-0.00027	-0.00028
D197	-0.00005	-0.00001	0.00000	0.00023	0.00023	0.00018
D198	3.14153	0.00000	0.00000	0.00062	0.00061	-3.14104
D199	-3.14139	-0.00001	0.00000	-0.00073	-0.00073	3.14107
D200	0.00019	0.00001	0.00000	-0.00034	-0.00034	-0.00015

Item Value Threshold Converged?

Maximum Force	0.004692	0.000450	NO
RMS Force	0.000456	0.000300	NO
Maximum Displacement	0.237765	0.001800	NO
RMS Displacement	0.049446	0.001200	NO

Predicted change in Energy=-4.740957D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4
Framework group C1[X(C42H18N6O2S4)]
Deg. of freedom 210
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.804222	-0.644226	-0.011295
2	6	0	-9.992337	-1.792238	0.030998
3	6	0	-10.512602	-3.078416	0.047326
4	6	0	-11.900945	-3.223649	0.020160
5	6	0	-12.724424	-2.091970	-0.023071
6	6	0	-12.195282	-0.797298	-0.039642
7	1	0	-9.841230	-3.930211	0.081074
8	1	0	-12.346370	-4.213636	0.032099
9	1	0	-13.802559	-2.217472	-0.044751
10	1	0	-12.865173	0.049487	-0.073554
11	6	0	-9.931725	0.559869	-0.017311
12	6	0	-8.569171	-1.389915	0.054115
13	6	0	-8.544294	0.088750	0.008038
14	6	0	-7.412639	0.873952	-0.008149

15	6	0	-6.025180	0.604229	-0.019798
16	6	0	-3.652922	-0.175923	-0.027576
17	6	0	-3.787095	1.236674	0.011707
18	16	0	-5.192170	-0.978286	-0.072996
19	6	0	-5.110407	1.673467	0.022800
20	6	0	-2.275853	-0.444782	-0.019922
21	6	0	-1.611837	0.804375	0.026164
22	7	0	-2.531887	1.829070	0.026201
23	16	0	-1.158625	-1.799143	-0.052105
24	16	0	1.147323	1.808636	0.100097
25	6	0	0.192414	-0.669087	0.007331
26	6	0	-0.203667	0.677872	0.043561
27	6	0	1.599487	-0.795432	0.025517
28	6	0	2.263786	0.453381	0.065549
29	6	0	3.643901	0.183796	0.074618
30	6	0	3.777409	-1.228763	0.043256
31	6	0	5.101354	-1.666649	0.032972
32	6	0	6.017905	-0.597296	0.059865
33	16	0	5.183056	0.985806	0.123661
34	7	0	2.520674	-1.820566	0.027409
35	6	0	7.414363	-0.870967	0.030513
36	6	0	8.549718	-0.089292	-0.018901
37	6	0	8.579815	1.389172	-0.077849
38	6	0	9.935085	-0.565189	-0.028856
39	6	0	10.004826	1.785910	-0.067553
40	6	0	10.811801	0.634221	-0.046925
41	6	0	10.531080	3.070562	-0.084851
42	6	0	12.203300	0.779281	-0.044598
43	6	0	11.920300	3.208352	-0.083246
44	6	0	12.738926	2.071282	-0.063194
45	6	0	10.398786	-1.870016	-0.011006
46	6	0	9.558791	-3.024392	0.016339
47	6	0	11.785469	-2.206105	-0.014850
48	7	0	8.904840	-3.989030	0.038583
49	7	0	12.904853	-2.529069	-0.016932
50	6	0	-10.396689	1.864246	-0.047797
51	6	0	-11.783980	2.201767	-0.079424
52	6	0	-9.554829	3.018360	-0.055636
53	7	0	-12.902961	2.525079	-0.106155
54	7	0	-8.890909	3.976411	-0.060244
55	8	0	-7.609923	-2.153243	0.079201
56	8	0	7.624531	2.156787	-0.040575
57	6	0	2.241841	-3.236672	-0.130902
58	1	0	1.301192	-3.483033	0.366193
59	1	0	2.175998	-3.519530	-1.187100
60	1	0	3.037155	-3.814047	0.344679
61	6	0	-2.253954	3.244052	0.195362
62	1	0	-2.191493	3.522140	1.253297
63	1	0	-1.311537	3.494332	-0.296778
64	1	0	-3.047306	3.825503	-0.278797
65	1	0	5.429385	-2.698583	-0.013223
66	1	0	12.868393	-0.071687	-0.029355
67	1	0	13.817927	2.191077	-0.061624
68	1	0	12.370588	4.196122	-0.096852
69	1	0	9.863552	3.925961	-0.099970
70	1	0	7.586627	-1.939831	0.058003
71	1	0	-7.586250	1.942841	-0.036297
72	1	0	-5.439156	2.704947	0.070350

Rotational constants (GHZ): 0.1750622 0.0103827 0.0098039

Standard basis: 6-31G(d,p) (6D, 7F)
 There are 916 symmetry adapted cartesian basis functions of A symmetry.
 There are 916 symmetry adapted basis functions of A symmetry.
 916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions
 196 alpha electrons 196 beta electrons
 nuclear repulsion energy 6566.0665124990 Hartrees.
 NAToms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T
 Big=T
 Integral buffers will be 131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 Nuclear repulsion after empirical dispersion term = 6565.9816600236 Hartrees.
 One-electron integrals computed using PRISM.
 NBasis= 916 RedAO= T EigKep= 3.25D-04 NBF= 916
 NBSUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916
 Initial guess from the checkpoint file: "PBDB.chk"
 B after Tr= 0.000000 0.000000 0.000000
 Rot= 1.000000 0.000029 0.000001 -0.000008 Ang= 0.00 deg.
 ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1
 AccDes= 0.00D+00
 Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.
 HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-yADJ=14
 ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
 FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlgl= 2001
 NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
 wScrn= 0.000000 ICntrl= 500 IOpCl= 0 IlCent= 200000004 NGrid= 0
 NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 Integral accuracy reduced to 1.0D-05 until final iterations.
 Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
 SCF Done: E(RB3LYP) = -3683.01905625 A.U. after 13 cycles
 NFock= 13 Conv=0.78D-08 -V/T= 2.0068
 Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1
 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	0.000006219	0.000126700	-0.000348337
2	6	0.000814024	0.000250315	-0.001013050
3	6	0.000067967	-0.000282816	-0.000167658
4	6	0.000001581	0.000123725	0.000157006
5	6	-0.000033681	-0.000063651	0.000014498
6	6	0.000455471	0.000175859	0.000352919
7	1	0.000056353	-0.000024654	0.000035110
8	1	-0.000003974	-0.000011757	0.000021393
9	1	-0.000045409	-0.000023332	-0.000052182
10	1	-0.000133506	0.000177352	-0.000076526
11	6	-0.000567360	-0.000052461	-0.000083620

12	6	-0.002090645	0.000218584	0.002602371
13	6	-0.000192842	0.000797278	-0.000800981
14	6	-0.002506018	-0.000272858	0.000131772
15	6	0.002959770	-0.001632418	0.000181856
16	6	-0.001492806	-0.000279937	0.000540303
17	6	-0.000503506	0.000585088	-0.000889569
18	16	0.001881264	0.000160955	-0.000783204
19	6	0.001036827	-0.000369047	0.001527886
20	6	0.000269930	-0.001267625	-0.000165926
21	6	0.000863527	-0.000296688	0.001126584
22	7	0.000483960	0.000656634	-0.000198053
23	16	-0.000027907	0.000180475	0.000213247
24	16	0.000143065	0.000152760	0.000061208
25	6	0.000313342	-0.000428003	0.000151116
26	6	-0.000979635	0.000704130	-0.000713301
27	6	0.000396553	-0.000490129	0.000378428
28	6	0.001558400	0.000010498	0.000712745
29	6	0.000356373	0.001405806	-0.002008214
30	6	-0.000223783	-0.000200225	0.000907532
31	6	-0.001251306	-0.000839245	-0.000716538
32	6	0.001861491	-0.000120908	0.001677041
33	16	-0.001331471	-0.000625798	0.002390755
34	7	-0.000176642	-0.001255718	-0.000500247
35	6	-0.002162307	0.000821125	-0.002446068
36	6	-0.002623285	0.001479803	0.002038837
37	6	0.006685118	0.000334739	-0.009358939
38	6	0.001358326	0.000444995	0.000061209
39	6	-0.002649210	-0.001073788	0.002868632
40	6	-0.000639114	-0.000187289	0.000425563
41	6	0.000035453	0.000895239	0.000366806
42	6	-0.000141313	-0.001012007	-0.000387354
43	6	0.000625842	0.000149877	0.000019863
44	6	-0.000427799	-0.000072397	-0.000315951
45	6	-0.001217491	-0.000623594	-0.001224879
46	6	-0.000106102	0.000323865	0.000321723
47	6	0.001339678	0.000891580	0.001124665
48	7	-0.000396995	0.000084291	-0.000292449
49	7	-0.000016073	0.000036896	0.000036597
50	6	0.000353038	0.000610409	0.000726046
51	6	-0.000432520	-0.000793353	-0.000547927
52	6	0.000346695	0.000123195	-0.000134027
53	7	0.000057763	0.000052033	0.000039864
54	7	-0.000017527	-0.000064615	0.000073896
55	8	0.000224413	0.000242528	-0.000453337
56	8	-0.002402066	-0.000080506	0.002531241
57	6	0.000025294	0.000242191	0.000130162
58	1	-0.000042491	-0.000001467	-0.000092309
59	1	0.000012039	0.000084816	0.000019321
60	1	0.000038632	-0.000068802	0.000009818
61	6	-0.000158226	-0.000745984	-0.000185598
62	1	0.000079828	0.000202558	0.000163032
63	1	0.000016237	0.000147007	0.000081139
64	1	-0.000022497	0.000208499	0.000115273
65	1	0.000218921	0.000085435	-0.000334893
66	1	0.000128388	-0.000453466	-0.000057395
67	1	0.000017153	0.000009624	0.000052856
68	1	0.000043226	0.000011743	0.000010115
69	1	-0.000097252	0.000054542	0.000085997
70	1	-0.000262850	0.000630979	0.000466434
71	1	0.000563610	-0.000069346	-0.000888835

72 1 -0.000320164 -0.000110240 0.000284508

Cartesian Forces: Max 0.009358939 RMS 0.001150202

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.005229785 RMS 0.000773113

Search for a local minimum.

Step number 20 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 16 18 17 19 20

DE= 7.68D-04 DEPred=-4.74D-04 R=-1.62D+00

Trust test=-1.62D+00 RLast= 3.82D-01 DXMaxT set to 2.46D-01

ITU= -1 0 -1 0 -1 1 1 1 1 1 1 0 0 0 1 0 0 0 1 0

Eigenvalues ---	0.00231	0.00232	0.00239	0.00271	0.00363
Eigenvalues ---	0.00385	0.00393	0.00435	0.00448	0.00481
Eigenvalues ---	0.00503	0.00519	0.00570	0.00599	0.00603
Eigenvalues ---	0.00632	0.00655	0.00678	0.00685	0.00701
Eigenvalues ---	0.00715	0.00744	0.00760	0.00768	0.00771
Eigenvalues ---	0.00789	0.00813	0.00823	0.00842	0.00856
Eigenvalues ---	0.01001	0.01085	0.01128	0.01130	0.01151
Eigenvalues ---	0.01180	0.01248	0.01333	0.01358	0.01362
Eigenvalues ---	0.01378	0.01431	0.01457	0.01460	0.01538
Eigenvalues ---	0.01644	0.01651	0.01715	0.01754	0.01794
Eigenvalues ---	0.01812	0.01929	0.01953	0.02006	0.02018
Eigenvalues ---	0.02064	0.02074	0.02206	0.02208	0.02397
Eigenvalues ---	0.03538	0.04828	0.04837	0.04902	0.04951
Eigenvalues ---	0.04985	0.05020	0.05026	0.05287	0.07034
Eigenvalues ---	0.07234	0.07370	0.07560	0.15520	0.15796
Eigenvalues ---	0.15932	0.15984	0.15994	0.15997	0.15999
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues ---	0.16001	0.16001	0.16003	0.16016	0.16028
Eigenvalues ---	0.16050	0.17504	0.18558	0.19149	0.19800
Eigenvalues ---	0.20322	0.20767	0.21381	0.21512	0.21965
Eigenvalues ---	0.22004	0.22025	0.22268	0.22549	0.22596
Eigenvalues ---	0.22638	0.22658	0.22691	0.22927	0.23054
Eigenvalues ---	0.23347	0.23452	0.23635	0.23774	0.23986
Eigenvalues ---	0.24111	0.24215	0.24287	0.24338	0.24489
Eigenvalues ---	0.24496	0.24603	0.24615	0.24644	0.24784
Eigenvalues ---	0.24808	0.24894	0.24924	0.24936	0.24965
Eigenvalues ---	0.24989	0.24992	0.24996	0.24997	0.24997
Eigenvalues ---	0.24998	0.24999	0.24999	0.24999	0.25000
Eigenvalues ---	0.25000	0.25009	0.25236	0.25596	0.25918
Eigenvalues ---	0.26226	0.26481	0.26717	0.26821	0.27043
Eigenvalues ---	0.27212	0.27720	0.27823	0.28168	0.28292
Eigenvalues ---	0.28550	0.28644	0.29964	0.30079	0.30550
Eigenvalues ---	0.32170	0.32562	0.35512	0.35895	0.36282
Eigenvalues ---	0.36338	0.36440	0.36478	0.36638	0.36660
Eigenvalues ---	0.36799	0.36834	0.37082	0.37089	0.37129
Eigenvalues ---	0.37258	0.37278	0.37430	0.37569	0.37675
Eigenvalues ---	0.37758	0.37977	0.38927	0.40306	0.40666
Eigenvalues ---	0.41621	0.42152	0.42651	0.44412	0.44636
Eigenvalues ---	0.44981	0.45628	0.46511	0.47673	0.47869
Eigenvalues ---	0.48129	0.52097	0.53447	0.55151	0.57259
Eigenvalues ---	0.59720	0.65287	0.72394	0.80287	0.81852


```

Eigenvalues ---      0.91321    1.25829    1.26297    1.29339    1.35383
En-DIIS/RFO-DIIS IScMMF=      0 using points:      20    19
RFO step: Lambda=-5.98297439D-04.
DidBck=T Rises=T RFO-DIIS coefs:      0.26018      0.73982
Iteration 1 RMS(Cart)= 0.05515459 RMS(Int)= 0.00059650
Iteration 2 RMS(Cart)= 0.00191374 RMS(Int)= 0.00016457
Iteration 3 RMS(Cart)= 0.00000121 RMS(Int)= 0.00016457
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00016457
Variable      Old X      -DE/DX      Delta X      Delta X      Delta X      New X
(Linear)      (Quad)      (Total)
R1      2.65833      0.00017      -0.00001      0.00001      0.00001      2.65833
R2      2.64513      0.00004      -0.00029      -0.00020      -0.00049      2.64464
R3      2.81000      0.00060      -0.00117      0.00404      0.00285      2.81284
R4      2.62202      -0.00025      -0.00020      -0.00095      -0.00115      2.62087
R5      2.79513      -0.00029      0.00078      -0.00531      -0.00450      2.79064
R6      2.63840      -0.00009      0.00004      -0.00011      -0.00006      2.63834
R7      2.05054      0.00006      0.00006      0.00029      0.00035      2.05088
R8      2.64608      -0.00001      0.00009      -0.00011      -0.00001      2.64607
R9      2.05157      -0.00001      -0.00006      0.00016      0.00010      2.05167
R10     2.64321      -0.00001      0.00009      -0.00004      0.00005      2.64326
R11     2.05155      0.00003      0.00002      0.00014      0.00016      2.05170
R12     2.04138      0.00010      0.00031      0.00095      0.00125      2.04264
R13     2.76931      0.00009      -0.00007      0.00397      0.00387      2.77318
R14     2.61747      -0.00024      -0.00196      0.00300      0.00104      2.61851
R15     2.79602      0.00025      0.00180      -0.00463      -0.00282      2.79320
R16     2.31710      -0.00009      -0.00041      0.00064      0.00023      2.31733
R17     2.60306      0.00180      0.00888      -0.02159      -0.01270      2.59035
R18     2.67109      0.00301      0.00664      -0.00774      -0.00110      2.66999
R19     2.04707      0.00017      0.00042      -0.00181      -0.00139      2.04568
R20     3.38102      0.00045      -0.00028      0.00543      0.00519      3.38621
R21     2.66035      -0.00031      -0.00013      -0.00212      -0.00225      2.65810
R22     2.68246      -0.00061      -0.00187      0.00130      -0.00056      2.68191
R23     3.28135      -0.00040      0.00097      -0.00738      -0.00640      3.27495
R24     2.65146      -0.00022      0.00193      -0.00699      -0.00487      2.64659
R25     2.63348      -0.00202      -0.00420      0.00287      -0.00137      2.63211
R26     2.62304      -0.00056      0.00095      -0.00302      -0.00224      2.62080
R27     2.04779      0.00008      0.00015      0.00069      0.00083      2.04863
R28     2.67477      -0.00084      -0.00132      -0.00127      -0.00253      2.67223
R29     3.31836      -0.00029      -0.00023      -0.00181      -0.00203      3.31633
R30     2.60240      -0.00069      0.00017      -0.00066      -0.00064      2.60176
R31     2.67197      -0.00231      -0.00355      -0.00285      -0.00641      2.66556
R32     2.74371      0.00011      -0.00040      0.00139      0.00099      2.74469
R33     3.33035      -0.00032      -0.00004      -0.00172      -0.00174      3.32861
R34     3.33096      -0.00045      -0.00085      -0.00055      -0.00139      3.32957
R35     3.31883      -0.00046      -0.00042      -0.00155      -0.00196      3.31686
R36     2.65403      -0.00036      -0.00031      -0.00045      -0.00077      2.65327
R37     2.66990      -0.00146      0.00002      -0.01047      -0.01046      2.65944
R38     2.67410      -0.00084      -0.00149      0.00025      -0.00122      2.67288
R39     2.60446      -0.00163      -0.00209      0.00002      -0.00213      2.60233
R40     2.65738      -0.00261      -0.00631      0.00596      -0.00027      2.65712
R41     2.68190      -0.00059      -0.00079      0.00007      -0.00072      2.68118
R42     3.28107      -0.00057      -0.00100      0.00026      -0.00073      3.28034
R43     2.63526      -0.00254      -0.00418      -0.00120      -0.00541      2.62985
R44     2.62520      -0.00175      -0.00265      0.00206      -0.00067      2.62453
R45     2.66197      -0.00193      -0.00197      -0.00076      -0.00273      2.65924
R46     2.04809      -0.00002      0.00001      0.00002      0.00003      2.04812
R47     3.38427      -0.00091      -0.00161      0.00066      -0.00092      3.38335
R48     2.68969      -0.00523      -0.01037      0.00052      -0.00985      2.67985
R49     2.74379      0.00026      -0.00038      0.00263      0.00224      2.74604
R50     2.60651      -0.00153      -0.00039      -0.00301      -0.00340      2.60311

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R51	2.04658	0.00052	0.00038	-0.00052	-0.00013	2.04645
R52	2.79669	-0.00001	0.00065	-0.00292	-0.00209	2.79460
R53	2.76819	0.00001	0.00503	-0.00813	-0.00322	2.76496
R54	2.79537	-0.00027	0.00043	-0.00491	-0.00425	2.79112
R55	2.31689	0.00023	-0.00001	0.00028	0.00027	2.31716
R56	2.80772	0.00190	0.00195	0.00060	0.00229	2.81001
R57	2.61706	0.00012	0.00177	-0.00692	-0.00515	2.61191
R58	2.65775	0.00087	0.00089	-0.00133	-0.00046	2.65729
R59	2.62364	-0.00091	-0.00170	-0.00086	-0.00253	2.62111
R60	2.64380	0.00096	0.00281	-0.00667	-0.00388	2.63993
R61	2.63813	-0.00015	0.00004	0.00029	0.00034	2.63847
R62	2.05062	0.00001	0.00001	0.00027	0.00028	2.05090
R63	2.64326	-0.00018	0.00016	-0.00052	-0.00038	2.64288
R64	2.04119	-0.00006	-0.00013	0.00256	0.00243	2.04362
R65	2.64796	-0.00080	-0.00122	-0.00096	-0.00219	2.64577
R66	2.05158	-0.00002	-0.00010	0.00026	0.00017	2.05175
R67	2.05155	0.00002	0.00006	0.00004	0.00010	2.05165
R68	2.69836	0.00043	0.00247	-0.00327	-0.00081	2.69755
R69	2.69633	0.00125	0.00581	-0.01103	-0.00521	2.69111
R70	2.20270	0.00006	-0.00012	0.00042	0.00030	2.20301
R71	2.20162	-0.00001	0.00017	-0.00055	-0.00038	2.20123
R72	2.69874	0.00026	0.00195	-0.00498	-0.00303	2.69571
R73	2.69958	-0.00004	0.00048	-0.00039	0.00009	2.69967
R74	2.20164	-0.00005	0.00011	-0.00041	-0.00031	2.20134
R75	2.20271	0.00006	-0.00001	0.00020	0.00018	2.20289
R76	2.06371	0.00007	0.00006	0.00017	0.00023	2.06394
R77	2.07001	0.00002	0.00022	0.00000	0.00021	2.07022
R78	2.06323	0.00004	0.00018	-0.00015	0.00003	2.06326
R79	2.07049	-0.00012	0.00021	-0.00050	-0.00029	2.07020
R80	2.06404	-0.00005	-0.00004	-0.00016	-0.00020	2.06384
R81	2.06345	-0.00001	0.00013	-0.00019	-0.00006	2.06339
A1	2.07708	-0.00044	0.00036	-0.00291	-0.00254	2.07454
A2	1.89896	-0.00031	-0.00004	-0.00038	-0.00046	1.89850
A3	2.30714	0.00075	-0.00031	0.00329	0.00300	2.31015
A4	2.14175	0.00028	-0.00015	0.00193	0.00177	2.14352
A5	1.91113	0.00022	-0.00012	0.00193	0.00182	1.91295
A6	2.23031	-0.00050	0.00027	-0.00386	-0.00359	2.22671
A7	2.05901	0.00007	-0.00008	0.00058	0.00050	2.05951
A8	2.08982	-0.00008	-0.00015	-0.00041	-0.00057	2.08925
A9	2.13435	0.00001	0.00023	-0.00016	0.00007	2.13442
A10	2.09593	-0.00017	0.00018	-0.00172	-0.00154	2.09438
A11	2.09743	0.00007	-0.00023	0.00100	0.00077	2.09819
A12	2.08983	0.00010	0.00005	0.00072	0.00078	2.09061
A13	2.12464	0.00006	-0.00016	0.00052	0.00036	2.12501
A14	2.08429	0.00003	0.00055	-0.00026	0.00029	2.08458
A15	2.07425	-0.00010	-0.00039	-0.00026	-0.00065	2.07360
A16	2.06796	0.00019	-0.00015	0.00161	0.00145	2.06942
A17	2.13080	0.00012	0.00026	0.00061	0.00087	2.13167
A18	2.08442	-0.00031	-0.00011	-0.00222	-0.00232	2.08210
A19	1.87038	0.00011	0.00137	-0.00433	-0.00301	1.86737
A20	2.17206	0.00179	0.00074	0.00509	0.00589	2.17795
A21	2.24074	-0.00191	-0.00214	-0.00081	-0.00289	2.23785
A22	1.86244	0.00013	0.00010	0.00048	0.00048	1.86291
A23	2.19409	-0.00028	0.00060	-0.00260	-0.00211	2.19198
A24	2.22639	0.00017	-0.00051	0.00247	0.00185	2.22824
A25	1.88168	-0.00014	-0.00119	0.00258	0.00134	1.88302
A26	2.20724	-0.00078	0.00085	-0.00009	0.00078	2.20803
A27	2.19426	0.00092	0.00033	-0.00248	-0.00213	2.19213
A28	2.34303	0.00138	-0.00190	0.00739	0.00555	2.34858
A29	2.01651	-0.00066	0.00288	-0.00565	-0.00271	2.01381

A30	1.92345	-0.00072	-0.00086	-0.00231	-0.00311	1.92034
A31	2.24726	0.00094	-0.00012	0.00678	0.00667	2.25394
A32	2.08592	-0.00089	-0.00008	-0.00631	-0.00639	2.07954
A33	1.94997	-0.00005	0.00021	-0.00045	-0.00026	1.94971
A34	1.95710	0.00040	0.00256	-0.00263	-0.00016	1.95694
A35	1.85803	-0.00018	-0.00151	0.00272	0.00124	1.85928
A36	2.46804	-0.00022	-0.00104	-0.00006	-0.00110	2.46694
A37	1.98437	0.00012	-0.00186	0.00455	0.00276	1.98713
A38	1.91720	0.00009	0.00210	-0.00352	-0.00165	1.91556
A39	2.38161	-0.00021	-0.00034	-0.00101	-0.00112	2.38049
A40	1.57403	-0.00068	-0.00255	0.00237	-0.00015	1.57388
A41	1.95922	0.00022	0.00165	-0.00378	-0.00218	1.95704
A42	2.12604	-0.00011	-0.00006	-0.00008	-0.00005	2.12599
A43	2.19786	-0.00011	-0.00159	0.00354	0.00203	2.19989
A44	1.86659	0.00002	0.00019	0.00007	0.00029	1.86687
A45	2.45298	-0.00041	-0.00154	0.00042	-0.00116	2.45182
A46	1.96362	0.00039	0.00130	-0.00043	0.00080	1.96442
A47	1.92117	0.00010	0.00103	-0.00142	-0.00068	1.92050
A48	1.96997	0.00019	-0.00033	0.00105	0.00078	1.97074
A49	2.39195	-0.00030	-0.00068	0.00017	-0.00038	2.39157
A50	1.86146	-0.00003	-0.00211	0.00203	0.00034	1.86180
A51	2.20216	0.00011	-0.00540	0.00458	0.00030	2.20247
A52	2.21089	-0.00006	-0.00348	0.00241	0.00008	2.21097
A53	1.56336	-0.00087	-0.00183	-0.00002	-0.00182	1.56154
A54	1.56237	-0.00056	-0.00052	-0.00209	-0.00261	1.55976
A55	1.98192	0.00036	0.00060	0.00012	0.00073	1.98265
A56	2.35544	-0.00027	-0.00053	-0.00030	-0.00080	2.35464
A57	1.94582	-0.00008	-0.00007	0.00018	0.00007	1.94590
A58	2.35508	-0.00016	-0.00042	0.00009	-0.00031	2.35477
A59	1.94588	-0.00007	0.00016	-0.00063	-0.00051	1.94537
A60	1.98223	0.00023	0.00026	0.00054	0.00082	1.98305
A61	1.97031	0.00007	-0.00051	0.00146	0.00098	1.97129
A62	2.39233	-0.00046	-0.00059	-0.00074	-0.00123	2.39109
A63	1.92049	0.00039	0.00107	-0.00068	0.00028	1.92076
A64	1.96399	0.00034	0.00085	-0.00016	0.00066	1.96465
A65	2.45233	-0.00025	-0.00095	0.00006	-0.00088	2.45145
A66	1.86683	-0.00009	0.00013	-0.00001	0.00015	1.86698
A67	1.85771	-0.00010	-0.00034	-0.00033	-0.00063	1.85708
A68	2.46809	-0.00027	-0.00068	0.00034	-0.00029	2.46780
A69	1.95734	0.00037	0.00104	-0.00016	0.00088	1.95822
A70	1.98451	0.00007	-0.00016	0.00019	0.00007	1.98458
A71	1.91682	0.00030	0.00115	-0.00094	0.00012	1.91694
A72	2.38185	-0.00037	-0.00106	0.00072	-0.00020	2.38166
A73	1.95975	-0.00030	-0.00034	0.00018	-0.00017	1.95957
A74	2.19770	0.00011	-0.00016	0.00047	0.00036	2.19806
A75	2.12549	0.00020	0.00068	-0.00073	0.00001	2.12550
A76	1.94811	0.00116	0.00170	0.00014	0.00182	1.94993
A77	2.08520	-0.00021	-0.00063	-0.00207	-0.00273	2.08248
A78	2.24987	-0.00096	-0.00108	0.00185	0.00074	2.25061
A79	1.57471	-0.00128	-0.00197	-0.00050	-0.00242	1.57229
A80	1.86273	-0.00051	-0.00238	0.00225	0.00012	1.86285
A81	2.21048	0.00019	-0.00169	0.00125	0.00017	2.21065
A82	2.20242	0.00032	-0.00331	0.00394	0.00123	2.20366
A83	2.34531	-0.00131	-0.00337	0.00456	0.00120	2.34651
A84	1.92335	0.00023	-0.00023	-0.00284	-0.00306	1.92029
A85	2.01451	0.00108	0.00360	-0.00175	0.00186	2.01637
A86	2.19483	-0.00027	-0.00141	0.00008	-0.00142	2.19341
A87	2.20756	-0.00048	0.00142	-0.00112	0.00020	2.20776
A88	1.88078	0.00075	0.00000	0.00106	0.00122	1.88201
A89	1.86215	-0.00016	0.00043	0.00099	0.00049	1.86264

A90	2.22485	-0.00005	0.00059	0.00317	0.00205	2.22690
A91	2.19255	0.00047	0.00153	0.00028	0.00010	2.19265
A92	1.87117	-0.00046	-0.00095	0.00055	-0.00064	1.87053
A93	2.24294	-0.00401	-0.00268	-0.00583	-0.00838	2.23456
A94	2.16902	0.00448	0.00367	0.00528	0.00908	2.17810
A95	1.91051	0.00051	0.00099	-0.00026	0.00099	1.91150
A96	2.23094	-0.00084	-0.00099	-0.00185	-0.00302	2.22791
A97	2.14171	0.00033	0.00003	0.00214	0.00206	2.14377
A98	1.89933	-0.00057	0.00013	-0.00137	-0.00141	1.89792
A99	2.30577	0.00161	0.00094	0.00297	0.00399	2.30976
A100	2.07808	-0.00104	-0.00107	-0.00160	-0.00258	2.07550
A101	2.05840	0.00031	0.00078	-0.00074	0.00008	2.05848
A102	2.09024	-0.00023	-0.00081	-0.00001	-0.00084	2.08940
A103	2.13455	-0.00008	0.00003	0.00075	0.00076	2.13531
A104	2.06760	0.00032	0.00021	0.00147	0.00167	2.06927
A105	2.13029	0.00032	0.00083	-0.00039	0.00045	2.13074
A106	2.08529	-0.00063	-0.00104	-0.00108	-0.00212	2.08318
A107	2.09588	-0.00005	0.00039	-0.00242	-0.00202	2.09386
A108	2.09731	0.00006	-0.00013	0.00140	0.00127	2.09858
A109	2.08999	-0.00001	-0.00026	0.00102	0.00075	2.09074
A110	2.12471	0.00014	-0.00033	0.00114	0.00079	2.12550
A111	2.07430	-0.00011	-0.00017	-0.00088	-0.00104	2.07326
A112	2.08418	-0.00003	0.00050	-0.00027	0.00025	2.08442
A113	2.17120	-0.00285	-0.00248	-0.00421	-0.00669	2.16452
A114	2.14994	0.00356	0.00501	0.00344	0.00845	2.15839
A115	1.96204	-0.00071	-0.00253	0.00077	-0.00176	1.96028
A116	2.15214	0.00180	0.00220	0.00542	0.00762	2.15976
A117	2.16893	-0.00124	-0.00170	0.00041	-0.00129	2.16764
A118	1.96211	-0.00056	-0.00050	-0.00583	-0.00633	1.95578
A119	1.91326	-0.00012	-0.00084	0.00077	-0.00006	1.91319
A120	1.94822	0.00016	0.00050	0.00057	0.00107	1.94929
A121	1.90539	-0.00010	-0.00034	-0.00044	-0.00078	1.90461
A122	1.90590	-0.00001	0.00039	-0.00061	-0.00022	1.90568
A123	1.88584	0.00008	0.00011	-0.00010	0.00001	1.88586
A124	1.90417	-0.00001	0.00018	-0.00023	-0.00005	1.90411
A125	1.95063	-0.00025	-0.00007	-0.00187	-0.00195	1.94868
A126	1.91345	-0.00013	0.00002	-0.00131	-0.00130	1.91215
A127	1.90634	-0.00026	0.00037	-0.00328	-0.00291	1.90342
A128	1.90468	0.00020	0.00007	0.00200	0.00207	1.90676
A129	1.90239	0.00027	0.00049	0.00200	0.00249	1.90489
A130	1.88517	0.00018	-0.00091	0.00264	0.00173	1.88690
A131	3.17488	-0.00109	-0.00546	-0.00222	-0.00768	3.16720
A132	3.18471	0.00009	-0.00706	0.01348	0.00642	3.19113
A133	3.18420	-0.00016	-0.00932	0.02236	0.01304	3.19725
A134	3.16579	-0.00007	0.00420	-0.00847	-0.00427	3.16152
A135	3.14109	0.00000	0.00064	-0.00203	-0.00139	3.13970
A136	3.14134	0.00007	0.00010	0.00037	0.00046	3.14180
A137	3.14181	-0.00001	0.00035	-0.00172	-0.00136	3.14044
A138	3.14325	-0.00016	-0.00178	0.00313	0.00134	3.14460
D1	-0.00116	-0.00002	0.00009	-0.00050	-0.00039	-0.00155
D2	3.14104	-0.00020	-0.00134	-0.00033	-0.00165	3.13939
D3	3.14095	-0.00006	-0.00113	0.00099	-0.00012	3.14084
D4	-0.00003	-0.00024	-0.00256	0.00116	-0.00138	-0.00141
D5	0.00132	-0.00001	-0.00072	0.00067	-0.00006	0.00126
D6	-3.14039	-0.00001	-0.00054	0.00119	0.00065	-3.13973
D7	-3.14094	0.00004	0.00084	-0.00123	-0.00041	-3.14135
D8	0.00054	0.00004	0.00102	-0.00071	0.00030	0.00084
D9	0.01103	-0.00018	-0.00428	-0.00904	-0.01331	-0.00227
D10	-3.13512	0.00015	0.00589	-0.02062	-0.01475	3.13332
D11	-3.12994	-0.00023	-0.00573	-0.00728	-0.01298	3.14026

D12	0.00709	0.00010	0.00444	-0.01886	-0.01442	-0.00733
D13	0.00011	0.00005	0.00052	0.00013	0.00064	0.00075
D14	-3.14067	-0.00005	0.00008	-0.00081	-0.00073	-3.14140
D15	3.14097	0.00025	0.00222	-0.00007	0.00214	-3.14007
D16	0.00020	0.00016	0.00179	-0.00101	0.00077	0.00096
D17	-0.01085	0.00056	0.00833	0.00702	0.01536	0.00451
D18	-3.12919	-0.00022	-0.00954	-0.00838	-0.01787	3.13612
D19	3.13139	0.00038	0.00681	0.00721	0.01402	-3.13777
D20	0.01305	-0.00040	-0.01106	-0.00820	-0.01921	-0.00616
D21	0.00075	-0.00004	-0.00049	0.00005	-0.00044	0.00031
D22	-3.14122	-0.00005	-0.00063	0.00029	-0.00034	-3.14156
D23	3.14151	0.00006	-0.00004	0.00101	0.00097	-3.14071
D24	-0.00046	0.00005	-0.00018	0.00125	0.00107	0.00061
D25	-0.00056	0.00000	-0.00015	0.00015	0.00001	-0.00056
D26	3.14068	0.00001	0.00001	0.00010	0.00010	3.14078
D27	3.14140	0.00001	-0.00001	-0.00009	-0.00009	3.14131
D28	-0.00054	0.00003	0.00015	-0.00014	0.00001	-0.00054
D29	-0.00050	0.00002	0.00076	-0.00052	0.00024	-0.00025
D30	3.14121	0.00002	0.00059	-0.00103	-0.00045	3.14076
D31	3.14145	0.00001	0.00061	-0.00046	0.00015	-3.14159
D32	-0.00003	0.00001	0.00043	-0.00097	-0.00054	-0.00058
D33	-0.01758	0.00053	0.00938	0.01324	0.02261	0.00503
D34	3.12377	0.00043	0.00551	0.01372	0.01922	-3.14020
D35	3.12881	0.00017	-0.00130	0.02540	0.02408	-3.13029
D36	-0.01303	0.00007	-0.00517	0.02587	0.02069	0.00767
D37	-0.00185	-0.00007	-0.00630	0.00872	0.00242	0.00057
D38	-3.13976	-0.00042	-0.01043	0.01023	-0.00020	-3.13995
D39	3.13419	0.00034	0.00607	-0.00539	0.00067	3.13486
D40	-0.00373	0.00000	0.00194	-0.00388	-0.00194	-0.00567
D41	0.01751	-0.00066	-0.01084	-0.01248	-0.02336	-0.00584
D42	-3.12384	-0.00057	-0.00701	-0.01296	-0.02001	3.13934
D43	3.13529	0.00012	0.00746	0.00321	0.01072	-3.13718
D44	-0.00606	0.00022	0.01129	0.00273	0.01407	0.00800
D45	-3.11133	-0.00114	-0.03075	0.03034	-0.00040	-3.11173
D46	0.00701	-0.00055	-0.00762	-0.00586	-0.01350	-0.00648
D47	0.02997	-0.00125	-0.03529	0.03090	-0.00437	0.02561
D48	-3.13487	-0.00067	-0.01216	-0.00529	-0.01746	3.13086
D49	0.03990	-0.00092	-0.03246	-0.04389	-0.07634	-0.03644
D50	-3.09377	-0.00124	-0.03668	-0.04794	-0.08461	3.10481
D51	-3.07935	-0.00148	-0.05468	-0.00905	-0.06374	3.14010
D52	0.07018	-0.00180	-0.05890	-0.01310	-0.07201	-0.00184
D53	-3.12863	-0.00072	-0.00413	0.00172	-0.00244	-3.13107
D54	0.00553	-0.00042	-0.00019	0.00548	0.00531	0.01084
D55	3.13597	0.00057	0.00263	-0.00644	-0.00383	3.13214
D56	0.00627	0.00014	-0.01430	0.02190	0.00759	0.01386
D57	0.00103	0.00029	-0.00091	-0.00988	-0.01077	-0.00974
D58	-3.12867	-0.00013	-0.01784	0.01847	0.00065	-3.12802
D59	0.01354	-0.00036	-0.00199	-0.00598	-0.00797	0.00556
D60	-3.12572	-0.00018	0.00725	-0.01330	-0.00606	-3.13178
D61	-3.13118	-0.00020	-0.00097	0.00160	0.00063	-3.13055
D62	0.01276	-0.00002	0.00827	-0.00572	0.00254	0.01529
D63	-0.01059	0.00044	0.00120	0.00023	0.00141	-0.00918
D64	3.13580	0.00019	-0.00038	-0.01143	-0.01180	3.12400
D65	0.00191	0.00003	-0.00337	0.00955	0.00618	0.00809
D66	-3.13659	0.00002	0.00449	-0.01657	-0.01205	3.13454
D67	3.13887	0.00027	-0.00185	0.02080	0.01894	-3.12538
D68	0.00037	0.00026	0.00601	-0.00532	0.00071	0.00108
D69	-0.00923	0.00004	0.00186	0.01023	0.01209	0.00286
D70	3.11988	0.00049	0.01961	-0.01955	0.00007	3.11995
D71	3.12917	-0.00020	-0.01073	0.02022	0.00949	3.13866

D72	-0.02490	0.00024	0.00702	-0.00956	-0.00253	-0.02744
D73	-0.02250	0.00000	-0.00983	-0.00059	-0.01041	-0.03291
D74	-3.03011	-0.00009	0.05388	-0.06999	-0.01606	-3.04617
D75	3.12220	0.00024	0.00246	-0.01032	-0.00788	3.11432
D76	0.11459	0.00015	0.06617	-0.07972	-0.01353	0.10106
D77	-0.01610	-0.00003	-0.00265	-0.01034	-0.01297	-0.02907
D78	3.13775	-0.00007	-0.00376	0.00274	-0.00100	3.13675
D79	3.12336	-0.00003	-0.00808	0.00763	-0.00041	3.12295
D80	-0.00597	-0.00006	-0.00919	0.02071	0.01156	0.00559
D81	-3.13885	0.00006	-0.00138	0.01434	0.01292	-3.12593
D82	0.00594	0.00004	0.00676	-0.01271	-0.00596	-0.00001
D83	0.02375	0.00002	0.00763	0.00678	0.01442	0.03817
D84	3.03049	0.00013	-0.05680	0.07684	0.02012	3.05062
D85	-3.13441	0.00007	0.00915	-0.01090	-0.00175	-3.13616
D86	-0.12767	0.00018	-0.05529	0.05917	0.00396	-0.12371
D87	-3.13871	0.00006	0.00809	-0.01841	-0.01033	3.13415
D88	0.00242	0.00004	0.00693	-0.01907	-0.01216	-0.00974
D89	0.01978	0.00001	0.00654	-0.00037	0.00617	0.02595
D90	-3.12227	-0.00001	0.00538	-0.00103	0.00434	-3.11794
D91	1.50554	0.00008	-0.04308	0.04979	0.00665	1.51219
D92	-2.66344	0.00007	-0.04303	0.05020	0.00710	-2.65634
D93	-0.60098	0.00007	-0.04390	0.05069	0.00672	-0.59426
D94	-1.47580	-0.00003	0.03303	-0.03323	-0.00013	-1.47593
D95	0.63841	-0.00004	0.03309	-0.03283	0.00032	0.63873
D96	2.70087	-0.00005	0.03222	-0.03234	-0.00006	2.70081
D97	-0.00464	-0.00002	-0.00286	0.00188	-0.00098	-0.00562
D98	3.13900	0.00001	-0.00156	0.00137	-0.00018	3.13882
D99	-3.13681	-0.00001	0.00098	-0.00500	-0.00403	-3.14084
D100	0.00526	0.00001	0.00216	-0.00433	-0.00217	0.00309
D101	-0.00945	0.00004	-0.00014	-0.00169	-0.00182	-0.01127
D102	-3.13949	-0.00013	-0.00798	0.01327	0.00529	-3.13420
D103	0.00217	0.00000	-0.00174	0.00936	0.00763	0.00980
D104	-3.13979	-0.00002	-0.00264	0.00885	0.00622	-3.13357
D105	-3.14098	-0.00003	-0.00273	0.00975	0.00702	-3.13396
D106	0.00025	-0.00005	-0.00363	0.00924	0.00561	0.00586
D107	3.13205	0.00004	0.00222	-0.00999	-0.00777	3.12429
D108	-0.02299	0.00001	-0.00024	-0.00459	-0.00483	-0.02782
D109	-0.00752	0.00007	0.00350	-0.01049	-0.00698	-0.01451
D110	3.12062	0.00004	0.00105	-0.00509	-0.00405	3.11657
D111	0.01160	-0.00007	-0.00190	0.00733	0.00543	0.01703
D112	-3.13768	0.00004	0.00332	-0.00262	0.00069	-3.13699
D113	-3.12024	-0.00004	-0.00010	0.00342	0.00332	-3.11693
D114	0.01367	0.00007	0.00511	-0.00653	-0.00143	0.01224
D115	3.13567	-0.00006	-0.00865	0.00798	-0.00067	3.13500
D116	0.11993	-0.00013	0.03997	-0.05405	-0.01410	0.10583
D117	-0.01912	-0.00009	-0.01106	0.01328	0.00222	-0.01690
D118	-3.03485	-0.00016	0.03756	-0.04874	-0.01122	-3.04607
D119	3.12777	0.00015	0.01045	-0.01726	-0.00680	3.12097
D120	-0.00155	-0.00030	-0.00484	0.00228	-0.00257	-0.00412
D121	-0.00267	-0.00001	0.00287	-0.00281	0.00007	-0.00260
D122	-3.13199	-0.00046	-0.01242	0.01672	0.00430	-3.12769
D123	3.12999	0.00020	0.00130	0.00093	0.00223	3.13222
D124	-0.00909	-0.00005	-0.00987	0.01117	0.00131	-0.00778
D125	-0.01986	0.00050	0.01160	-0.01221	-0.00062	-0.02049
D126	3.12424	0.00025	0.00043	-0.00198	-0.00155	3.12270
D127	-3.13091	-0.00036	0.00144	-0.01322	-0.01178	3.14049
D128	0.02339	-0.00082	-0.01440	0.00700	-0.00739	0.01599
D129	0.00276	0.00023	-0.00061	0.01182	0.01122	0.01398
D130	-3.11518	-0.00058	-0.01638	0.01545	-0.00094	-3.11612
D131	3.14092	0.00058	0.01462	-0.00215	0.01248	-3.12979

D132	0.02298	-0.00023	-0.00115	0.00148	0.00032	0.02330
D133	0.01739	0.00009	0.01291	-0.01509	-0.00217	0.01521
D134	3.03387	0.00014	-0.03519	0.04632	0.01109	3.04496
D135	-3.12087	-0.00026	-0.00192	-0.00148	-0.00340	-3.12427
D136	-0.10438	-0.00020	-0.05003	0.05992	0.00986	-0.09452
D137	0.01496	-0.00083	-0.01028	-0.00628	-0.01656	-0.00160
D138	-3.12290	-0.00086	-0.01867	0.01666	-0.00202	-3.12492
D139	3.13403	-0.00006	0.00475	-0.00972	-0.00498	3.12905
D140	-0.00384	-0.00009	-0.00364	0.01321	0.00956	0.00573
D141	-0.02198	0.00094	0.01414	-0.00049	0.01365	-0.00833
D142	3.11544	0.00098	0.02352	-0.02616	-0.00266	3.11277
D143	3.07804	0.00137	0.05157	0.00624	0.05782	3.13586
D144	-0.06825	0.00152	0.05769	-0.00226	0.05544	-0.01280
D145	-0.05910	0.00133	0.04156	0.03364	0.07519	0.01609
D146	3.07780	0.00147	0.04768	0.02514	0.07282	-3.13257
D147	-0.63644	-0.00002	-0.02638	0.03321	0.00681	-0.62963
D148	1.47759	-0.00001	-0.02613	0.03334	0.00719	1.48478
D149	-2.69904	0.00002	-0.02582	0.03313	0.00729	-2.69175
D150	2.65466	-0.00004	0.03123	-0.04030	-0.00906	2.64560
D151	-1.51450	-0.00003	0.03148	-0.04017	-0.00868	-1.52317
D152	0.59206	0.00000	0.03179	-0.04038	-0.00858	0.58348
D153	-0.01710	0.00136	0.01623	-0.00890	0.00731	-0.00978
D154	3.12974	0.00092	0.01329	-0.01342	-0.00013	3.12962
D155	3.12937	0.00121	0.00986	-0.00007	0.00979	3.13916
D156	-0.00697	0.00077	0.00693	-0.00458	0.00235	-0.00462
D157	3.10689	0.00145	0.03204	0.01885	0.05092	-3.12538
D158	0.05347	-0.00175	-0.04833	-0.03482	-0.08322	-0.02975
D159	-0.03914	0.00182	0.03452	0.02266	0.05720	0.01806
D160	-3.09255	-0.00138	-0.04585	-0.03101	-0.07694	3.11369
D161	-3.11268	-0.00096	-0.02708	-0.01535	-0.04243	3.12808
D162	0.01766	-0.00017	-0.01598	-0.01412	-0.03013	-0.01247
D163	0.03339	-0.00134	-0.02958	-0.01920	-0.04878	-0.01539
D164	-3.11946	-0.00055	-0.01848	-0.01797	-0.03647	3.12726
D165	0.03059	-0.00167	-0.02684	-0.01792	-0.04471	-0.01412
D166	-3.11909	-0.00119	-0.02022	-0.01442	-0.03460	3.12950
D167	3.08609	0.00142	0.05164	0.03466	0.08619	-3.11090
D168	-0.06358	0.00190	0.05826	0.03816	0.09630	0.03271
D169	-0.01470	0.00032	0.01319	0.00825	0.02146	0.00676
D170	3.12501	0.00053	0.01527	0.01006	0.02534	-3.13284
D171	3.13755	-0.00036	0.00266	0.00717	0.00979	-3.13584
D172	-0.00593	-0.00015	0.00473	0.00898	0.01367	0.00775
D173	0.00456	-0.00010	-0.00388	-0.00158	-0.00546	-0.00090
D174	-3.13430	-0.00050	-0.00607	-0.00209	-0.00816	3.14073
D175	3.13314	0.00077	0.00897	-0.00019	0.00877	-3.14127
D176	-0.00572	0.00037	0.00678	-0.00071	0.00607	0.00035
D177	-0.01005	0.00085	0.00863	0.00609	0.01470	0.00465
D178	3.13314	0.00067	0.00687	0.00455	0.01142	-3.13862
D179	3.13913	0.00040	0.00241	0.00283	0.00521	-3.13885
D180	-0.00086	0.00022	0.00066	0.00128	0.00192	0.00106
D181	-3.13102	-0.00076	-0.00875	-0.00480	-0.01353	3.13864
D182	0.00956	-0.00052	-0.00814	-0.00385	-0.01199	-0.00243
D183	0.00152	-0.00022	-0.00133	-0.00089	-0.00221	-0.00069
D184	-3.14109	0.00002	-0.00072	0.00005	-0.00066	3.14144
D185	-3.13972	-0.00032	-0.00196	-0.00301	-0.00495	3.13851
D186	0.00229	-0.00025	-0.00241	-0.00245	-0.00485	-0.00256
D187	-0.00017	-0.00009	0.00028	-0.00105	-0.00075	-0.00092
D188	-3.14135	-0.00002	-0.00017	-0.00049	-0.00065	3.14119
D189	-0.00116	0.00009	0.00107	0.00030	0.00136	0.00020
D190	3.14114	0.00012	0.00036	0.00053	0.00088	-3.14117
D191	3.14148	-0.00015	0.00044	-0.00067	-0.00023	3.14125

D192	0.00059	-0.00013	-0.00027	-0.00044	-0.00071	-0.00012
D193	0.00050	-0.00003	-0.00052	0.00050	-0.00002	0.00048
D194	-3.14147	0.00002	-0.00024	0.00050	0.00027	-3.14120
D195	-3.14150	-0.00010	-0.00008	-0.00004	-0.00011	3.14157
D196	-0.00028	-0.00004	0.00020	-0.00004	0.00017	-0.00011
D197	0.00018	0.00003	-0.00017	-0.00012	-0.00029	-0.00011
D198	-3.14104	-0.00002	-0.00045	-0.00012	-0.00058	3.14157
D199	3.14107	0.00000	0.00054	-0.00035	0.00019	3.14126
D200	-0.00015	-0.00005	0.00025	-0.00035	-0.00010	-0.00025

Item	Value	Threshold	Converged?

Maximum Force	0.005230	0.000450	NO

RMS Force	0.000773	0.000300	NO

Maximum Displacement	0.249174	0.001800	NO

RMS Displacement	0.055460	0.001200	NO

Predicted change in Energy=-1.171159D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.800151	-0.634376	-0.006410
2	6	0	-9.993443	-1.786693	-0.022966
3	6	0	-10.517323	-3.070673	-0.044241
4	6	0	-11.906302	-3.211880	-0.050152
5	6	0	-12.725523	-2.076396	-0.035152
6	6	0	-12.191624	-0.783727	-0.013435
7	1	0	-9.847649	-3.924620	-0.056187
8	1	0	-12.354976	-4.200391	-0.066621
9	1	0	-13.804529	-2.196778	-0.040672
10	1	0	-12.861040	0.064895	-0.003191
11	6	0	-9.920377	0.566098	0.015324
12	6	0	-8.569643	-1.394914	-0.014865
13	6	0	-8.534847	0.082488	0.014299
14	6	0	-7.401810	0.853766	0.032323
15	6	0	-6.015874	0.580454	0.004643
16	6	0	-3.642363	-0.193467	-0.026078
17	6	0	-3.782825	1.218765	-0.022625
18	16	0	-5.175278	-1.001867	-0.019357
19	6	0	-5.106118	1.653179	-0.007572
20	6	0	-2.266881	-0.457069	-0.026641
21	6	0	-1.607102	0.793584	-0.012599
22	7	0	-2.530512	1.814401	-0.041048
23	16	0	-1.147536	-1.808663	-0.022015
24	16	0	1.144372	1.809927	0.002518
25	6	0	0.198481	-0.672698	-0.001211
26	6	0	-0.201723	0.673099	-0.005336
27	6	0	1.600483	-0.793637	0.016029
28	6	0	2.261988	0.456531	0.006062
29	6	0	3.642603	0.190423	0.018880
30	6	0	3.778272	-1.221737	0.039884
31	6	0	5.100141	-1.656890	0.042788
32	6	0	6.013987	-0.586785	0.042238

33	16	0	5.179508	0.997230	0.035305
34	7	0	2.522853	-1.815616	0.050300
35	6	0	7.405093	-0.861654	0.024338
36	6	0	8.541930	-0.083839	0.013052
37	6	0	8.575292	1.394604	0.005819
38	6	0	9.924322	-0.563209	0.008661
39	6	0	9.998687	1.787391	-0.028492
40	6	0	10.804406	0.634949	-0.023184
41	6	0	10.522826	3.071204	-0.059394
42	6	0	12.193430	0.781713	-0.048780
43	6	0	11.911853	3.210324	-0.085313
44	6	0	12.728841	2.073343	-0.079893
45	6	0	10.372301	-1.870611	0.028357
46	6	0	9.511889	-3.009245	0.058497
47	6	0	11.749352	-2.233468	0.020853
48	7	0	8.833272	-3.956864	0.081803
49	7	0	12.859659	-2.585676	0.015634
50	6	0	-10.371011	1.876389	0.025948
51	6	0	-11.750354	2.240075	0.017932
52	6	0	-9.514785	3.019815	0.044884
53	7	0	-12.858492	2.599238	0.013572
54	7	0	-8.834850	3.966502	0.064103
55	8	0	-7.616940	-2.166979	-0.019900
56	8	0	7.621072	2.164228	-0.020354
57	6	0	2.244593	-3.238934	-0.041090
58	1	0	1.307919	-3.463259	0.473887
59	1	0	2.171420	-3.571059	-1.082476
60	1	0	3.044391	-3.792379	0.455010
61	6	0	-2.255441	3.236384	0.067812
62	1	0	-2.180436	3.554680	1.113368
63	1	0	-1.320695	3.468423	-0.447133
64	1	0	-3.058557	3.793196	-0.419232
65	1	0	5.430015	-2.689261	0.035149
66	1	0	12.861062	-0.069031	-0.045706
67	1	0	13.807863	2.191709	-0.100224
68	1	0	12.362109	4.198003	-0.109483
69	1	0	9.853563	3.925564	-0.062213
70	1	0	7.571704	-1.931695	0.025926
71	1	0	-7.568635	1.923314	0.042454
72	1	0	-5.438627	2.684733	0.016432

Rotational constants (GHZ): 0.1748680 0.0104164 0.0098324

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis func-

tions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6572.0916910288 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T

Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6572.0067148685 Har-

trees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.23D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Initial guess from the checkpoint file: "PBDB.chk"

B after Tr= 0.000000 0.000000 0.000000
 Rot= 1.000000 0.000098 0.000002 0.000275 Ang= 0.03 deg.
 ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1
 AccDes= 0.00D+00
 Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for in-
 itial guess.
 HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-
 yADJ=14
 ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
 FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2001
 NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
 wScrn= 0.000000 ICntrl= 500 IOPCl= 0 IICent= 200000004 NGrid=
 0
 NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0=
 0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 Integral accuracy reduced to 1.0D-05 until final iterations.
 Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
 SCF Done: E(RB3LYP) = -3683.01964574 A.U. after 13 cycles
 NFock= 13 Conv=0.78D-08 -V/T= 2.0068
 Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IICent= 0 IOPClX= 0 NMat=1
 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-0.000336350	-0.000460744	-0.000200873
2	6	-0.000546607	0.000543891	0.000071316
3	6	-0.000042309	0.000434727	0.000117112
4	6	0.000036863	-0.000058032	-0.000022369
5	6	-0.000138795	0.000089281	-0.000070195
6	6	-0.000268573	-0.000366310	-0.000274710
7	1	-0.000031221	-0.000094331	-0.000032939
8	1	-0.000020950	-0.000064695	-0.000020852
9	1	0.000005034	-0.000039690	-0.000019534
10	1	-0.000057209	-0.000335062	-0.000181783
11	6	0.000011958	0.000298789	0.000246915
12	6	0.001258212	0.000916431	-0.000662877
13	6	-0.002405009	0.005670654	-0.001404332
14	6	-0.001911434	-0.005097735	0.000996042
15	6	0.002387991	-0.001321492	0.001847884
16	6	-0.001551299	0.000125476	-0.001310836
17	6	-0.001048670	-0.000291161	0.000205596
18	16	-0.001103509	0.001656264	-0.000785049
19	6	0.002697048	-0.000389550	-0.000048199
20	6	0.001935643	-0.000501200	-0.000565709
21	6	-0.002056445	-0.000631448	0.001638262
22	7	0.000986813	-0.000344538	-0.000678460
23	16	0.000113274	0.000455874	0.000203688
24	16	0.000142365	0.000236011	0.000000953
25	6	-0.001481747	0.001330349	-0.001133774
26	6	-0.000224851	-0.000381607	-0.000565825
27	6	0.002303663	-0.001830691	0.002332501
28	6	0.002235493	-0.001272961	0.000869436
29	6	-0.000652601	0.001229184	-0.002228079

30	6	-0.001405729	0.000726459	0.000322044
31	6	-0.000109604	0.000113755	-0.000088760
32	6	-0.000248863	-0.000505655	0.001218887
33	16	-0.000256070	-0.000206655	0.000713391
34	7	0.000439630	-0.000251663	0.000226360
35	6	-0.000518940	0.001487181	-0.001444044
36	6	0.000209452	0.000232674	-0.002410511
37	6	-0.004167549	-0.000537357	0.003820996
38	6	-0.000604577	-0.001168840	-0.000219821
39	6	0.000827253	-0.000502888	-0.001514317
40	6	-0.000512696	0.000948532	-0.000603065
41	6	0.000042283	-0.000142357	-0.000097051
42	6	0.001616788	-0.000554406	0.001321122
43	6	-0.000128753	0.000044424	0.000062085
44	6	0.000300655	-0.000541680	0.000130961
45	6	-0.000802415	0.000780212	-0.000501831
46	6	0.000353357	0.001574811	0.000463937
47	6	0.002091548	-0.000497645	0.001611591
48	7	0.000170153	-0.000315686	0.000038948
49	7	0.000377133	-0.000770820	0.000187447
50	6	0.001466713	0.000769397	0.001308306
51	6	-0.000712212	0.000171122	-0.000756114
52	6	0.000857184	-0.000455305	0.000238986
53	7	-0.000250299	0.000962210	0.000036426
54	7	-0.000306107	0.000156253	-0.000002319
55	8	-0.000007606	-0.000613169	0.000432687
56	8	0.001055211	0.000566598	-0.002075467
57	6	-0.000029709	-0.000311359	-0.000093262
58	1	-0.000017809	-0.000093346	-0.000063273
59	1	0.000002544	-0.000071713	-0.000089656
60	1	0.000020108	-0.000045141	0.000030325
61	6	0.000032462	0.000080129	0.000002489
62	1	-0.000066794	-0.000080072	0.000069447
63	1	-0.000036938	-0.000028301	-0.000049446
64	1	0.000057732	-0.000098969	-0.000048473
65	1	0.000179600	0.000026830	-0.000247771
66	1	-0.000226446	-0.000049691	-0.000111319
67	1	0.000017166	-0.000000584	-0.000002620
68	1	0.000003227	0.000097960	0.000043933
69	1	0.000076607	0.000052486	0.000020187
70	1	-0.000380737	0.000077910	0.000008452
71	1	0.000353400	-0.000524480	-0.000712303
72	1	0.000002862	-0.000006847	0.000499106

Cartesian Forces: Max 0.005670654 RMS 0.001051806

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.007689499 RMS 0.000760686

Search for a local minimum.

Step number 21 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 16 18 17 19 20

21

DE= -5.89D-04 DEPred=-1.17D-03 R= 5.03D-01

TightC=F SS= 1.41D+00 RLast= 3.17D-01 DXNew= 4.1397D-01 9.5136D-01

Trust test= 5.03D-01 RLast= 3.17D-01 DXMaxT set to 4.14D-01

ITU= 1 -1 0 -1 0 -1 1 1 1 1 1 1 0 0 0 1 0 0 0 1

ITU= 0

Eigenvalues	---	0.00229	0.00231	0.00242	0.00271	0.00343
Eigenvalues	---	0.00384	0.00394	0.00447	0.00481	0.00488
Eigenvalues	---	0.00505	0.00530	0.00580	0.00599	0.00601
Eigenvalues	---	0.00632	0.00656	0.00678	0.00699	0.00716
Eigenvalues	---	0.00743	0.00745	0.00760	0.00769	0.00773
Eigenvalues	---	0.00790	0.00816	0.00829	0.00842	0.00854
Eigenvalues	---	0.01030	0.01084	0.01127	0.01140	0.01174
Eigenvalues	---	0.01204	0.01252	0.01339	0.01361	0.01363
Eigenvalues	---	0.01380	0.01429	0.01457	0.01462	0.01549
Eigenvalues	---	0.01646	0.01653	0.01744	0.01755	0.01794
Eigenvalues	---	0.01813	0.01929	0.01953	0.02006	0.02021
Eigenvalues	---	0.02066	0.02075	0.02206	0.02208	0.03135
Eigenvalues	---	0.03902	0.04828	0.04838	0.04903	0.04978
Eigenvalues	---	0.05007	0.05020	0.05095	0.05345	0.07056
Eigenvalues	---	0.07228	0.07395	0.07564	0.15538	0.15870
Eigenvalues	---	0.15932	0.15985	0.15996	0.15998	0.15999
Eigenvalues	---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues	---	0.16001	0.16001	0.16003	0.16016	0.16029
Eigenvalues	---	0.16062	0.17917	0.18975	0.19374	0.19822
Eigenvalues	---	0.20618	0.21307	0.21435	0.21854	0.21998
Eigenvalues	---	0.22010	0.22174	0.22459	0.22582	0.22628
Eigenvalues	---	0.22641	0.22691	0.22847	0.23052	0.23200
Eigenvalues	---	0.23351	0.23496	0.23758	0.23852	0.24015
Eigenvalues	---	0.24194	0.24288	0.24316	0.24351	0.24507
Eigenvalues	---	0.24542	0.24603	0.24684	0.24743	0.24862
Eigenvalues	---	0.24919	0.24930	0.24956	0.24969	0.24985
Eigenvalues	---	0.24991	0.24995	0.24995	0.24997	0.24997
Eigenvalues	---	0.24998	0.24999	0.25000	0.25000	0.25000
Eigenvalues	---	0.25009	0.25179	0.25594	0.25797	0.25979
Eigenvalues	---	0.26231	0.26548	0.26793	0.26840	0.27102
Eigenvalues	---	0.27230	0.27722	0.27847	0.28278	0.28456
Eigenvalues	---	0.28546	0.28821	0.29948	0.30226	0.31993
Eigenvalues	---	0.32489	0.34808	0.35500	0.36261	0.36280
Eigenvalues	---	0.36341	0.36474	0.36622	0.36650	0.36796
Eigenvalues	---	0.36831	0.37066	0.37089	0.37110	0.37247
Eigenvalues	---	0.37264	0.37399	0.37565	0.37649	0.37738
Eigenvalues	---	0.37787	0.37970	0.38929	0.40306	0.40847
Eigenvalues	---	0.41617	0.42124	0.42647	0.44425	0.44754
Eigenvalues	---	0.45354	0.45653	0.46667	0.47752	0.47851
Eigenvalues	---	0.48101	0.52141	0.53417	0.55350	0.57290
Eigenvalues	---	0.61341	0.67307	0.73021	0.80314	0.82000
Eigenvalues	---	0.91164	1.25850	1.26324	1.29344	1.35387

En-DIIS/RFO-DIIS IScMMF= 0 using points: 21 20 19

RFO step: Lambda=-4.09428646D-04.

DidBck=T Rises=F RFO-DIIS coefs: 0.34657 0.17587 0.47756

Iteration 1 RMS(Cart)= 0.03181161 RMS(Int)= 0.00022844

Iteration 2 RMS(Cart)= 0.00098923 RMS(Int)= 0.00009712

Iteration 3 RMS(Cart)= 0.00000064 RMS(Int)= 0.00009712

Variable	Old X	-DE/DX	Delta X	Delta X	Delta X	New X
(Linear)	(Quad)	(Total)				
R1	2.65833	-0.00024	-0.00001	-0.00003	-0.00005	2.65828
R2	2.64464	-0.00031	0.00013	-0.00012	0.00001	2.64465
R3	2.81284	-0.00153	-0.00261	0.00057	-0.00213	2.81072
R4	2.62087	0.00025	0.00062	-0.00022	0.00041	2.62128
R5	2.79064	0.00133	0.00344	-0.00078	0.00274	2.79337
R6	2.63834	0.00029	0.00007	-0.00001	0.00006	2.63840

R7	2.05088	-0.00007	-0.00019	0.00007	-0.00012	2.05077
R8	2.64607	0.00031	0.00007	0.00013	0.00020	2.64627
R9	2.05167	-0.00007	-0.00010	0.00003	-0.00007	2.05159
R10	2.64326	-0.00003	0.00003	-0.00009	-0.00007	2.64319
R11	2.05170	-0.00002	-0.00009	0.00004	-0.00005	2.05166
R12	2.04264	0.00024	-0.00062	0.00035	-0.00027	2.04237
R13	2.77318	-0.00047	-0.00258	0.00012	-0.00249	2.77069
R14	2.61851	-0.00200	-0.00194	0.00017	-0.00177	2.61674
R15	2.79320	0.00127	0.00301	-0.00063	0.00244	2.79564
R16	2.31733	0.00024	-0.00041	0.00025	-0.00017	2.31716
R17	2.59035	0.00769	0.01404	-0.00228	0.01176	2.60211
R18	2.66999	0.00352	0.00501	0.00287	0.00787	2.67786
R19	2.04568	0.00054	0.00118	-0.00014	0.00103	2.04671
R20	3.38621	-0.00087	-0.00357	0.00098	-0.00256	3.38364
R21	2.65810	0.00095	0.00139	-0.00027	0.00112	2.65922
R22	2.68191	-0.00021	-0.00085	0.00079	-0.00004	2.68187
R23	3.27495	0.00145	0.00481	-0.00129	0.00353	3.27848
R24	2.64659	0.00181	0.00443	-0.00122	0.00335	2.64993
R25	2.63211	-0.00123	-0.00182	-0.00075	-0.00259	2.62952
R26	2.62080	0.00064	0.00207	-0.00113	0.00082	2.62162
R27	2.04863	-0.00028	-0.00045	0.00011	-0.00034	2.04829
R28	2.67223	0.00050	0.00081	0.00006	0.00090	2.67314
R29	3.31633	0.00041	0.00117	-0.00035	0.00083	3.31715
R30	2.60176	-0.00023	0.00053	-0.00105	-0.00063	2.60113
R31	2.66556	0.00038	0.00190	-0.00182	0.00007	2.66563
R32	2.74469	0.00013	-0.00090	0.00052	-0.00038	2.74431
R33	3.32861	0.00040	0.00111	-0.00041	0.00072	3.32932
R34	3.32957	0.00008	0.00036	-0.00019	0.00018	3.32975
R35	3.31686	0.00023	0.00101	-0.00050	0.00051	3.31737
R36	2.65327	0.00046	0.00030	-0.00004	0.00027	2.65354
R37	2.65944	0.00291	0.00685	-0.00151	0.00532	2.66476
R38	2.67288	-0.00007	-0.00017	0.00012	-0.00003	2.67285
R39	2.60233	-0.00058	0.00005	-0.00133	-0.00136	2.60097
R40	2.65712	-0.00246	-0.00390	-0.00143	-0.00524	2.65188
R41	2.68118	-0.00001	-0.00003	0.00003	0.00001	2.68119
R42	3.28034	-0.00015	-0.00017	-0.00036	-0.00053	3.27981
R43	2.62985	-0.00018	0.00083	-0.00180	-0.00097	2.62887
R44	2.62453	-0.00130	-0.00127	-0.00105	-0.00239	2.62213
R45	2.65924	-0.00009	0.00051	-0.00063	-0.00011	2.65913
R46	2.04812	-0.00002	-0.00002	0.00000	-0.00002	2.04811
R47	3.38335	-0.00030	-0.00044	-0.00046	-0.00089	3.38247
R48	2.67985	-0.00116	-0.00026	-0.00330	-0.00355	2.67629
R49	2.74604	-0.00055	-0.00171	0.00059	-0.00112	2.74491
R50	2.60311	0.00098	0.00197	-0.00082	0.00115	2.60426
R51	2.04645	-0.00014	0.00033	-0.00001	0.00032	2.04678
R52	2.79460	0.00083	0.00178	-0.00011	0.00164	2.79624
R53	2.76496	0.00266	0.00535	-0.00137	0.00401	2.76897
R54	2.79112	0.00106	0.00306	-0.00067	0.00234	2.79346
R55	2.31716	0.00039	-0.00018	0.00015	-0.00003	2.31713
R56	2.81001	-0.00004	-0.00024	0.00039	0.00020	2.81021
R57	2.61191	0.00278	0.00451	-0.00123	0.00328	2.61519
R58	2.65729	0.00050	0.00088	-0.00025	0.00063	2.65792
R59	2.62111	0.00014	0.00056	-0.00045	0.00011	2.62122
R60	2.63993	0.00185	0.00434	-0.00073	0.00362	2.64355
R61	2.63847	0.00039	-0.00020	0.00008	-0.00012	2.63835
R62	2.05090	-0.00008	-0.00018	0.00005	-0.00013	2.05077
R63	2.64288	0.00026	0.00035	-0.00021	0.00015	2.64302
R64	2.04362	-0.00025	-0.00167	0.00061	-0.00106	2.04256
R65	2.64577	0.00031	0.00064	-0.00034	0.00031	2.64607
R66	2.05175	-0.00010	-0.00017	0.00005	-0.00012	2.05162

R67	2.05165	0.00001	-0.00002	0.00003	0.00000	2.05165
R68	2.69755	0.00126	0.00212	-0.00044	0.00168	2.69923
R69	2.69111	0.00331	0.00716	-0.00112	0.00604	2.69716
R70	2.20301	-0.00032	-0.00027	0.00011	-0.00016	2.20284
R71	2.20123	0.00065	0.00036	-0.00007	0.00029	2.20152
R72	2.69571	0.00154	0.00324	-0.00061	0.00264	2.69834
R73	2.69967	0.00031	0.00025	-0.00016	0.00009	2.69976
R74	2.20134	0.00048	0.00027	-0.00006	0.00021	2.20155
R75	2.20289	-0.00017	-0.00013	0.00006	-0.00006	2.20282
R76	2.06394	-0.00002	-0.00011	0.00010	-0.00001	2.06393
R77	2.07022	-0.00009	0.00000	-0.00006	-0.00006	2.07016
R78	2.06326	0.00003	0.00010	-0.00003	0.00007	2.06333
R79	2.07020	-0.00008	0.00032	-0.00024	0.00009	2.07028
R80	2.06384	-0.00002	0.00011	0.00000	0.00011	2.06394
R81	2.06339	-0.00005	0.00013	-0.00008	0.00004	2.06344
A1	2.07454	0.00084	0.00189	-0.00047	0.00145	2.07599
A2	1.89850	0.00026	0.00028	-0.00015	0.00006	1.89856
A3	2.31015	-0.00110	-0.00217	0.00062	-0.00151	2.30864
A4	2.14352	-0.00045	-0.00125	0.00040	-0.00089	2.14263
A5	1.91295	-0.00049	-0.00126	0.00024	-0.00095	1.91200
A6	2.22671	0.00094	0.00252	-0.00063	0.00184	2.22855
A7	2.05951	-0.00016	-0.00038	0.00004	-0.00032	2.05919
A8	2.08925	0.00000	0.00027	-0.00015	0.00012	2.08937
A9	2.13442	0.00016	0.00010	0.00011	0.00020	2.13463
A10	2.09438	0.00024	0.00112	-0.00033	0.00079	2.09518
A11	2.09819	-0.00011	-0.00065	0.00024	-0.00042	2.09778
A12	2.09061	-0.00014	-0.00047	0.00010	-0.00038	2.09023
A13	2.12501	-0.00015	-0.00034	0.00012	-0.00022	2.12478
A14	2.08458	0.00011	0.00017	-0.00010	0.00007	2.08465
A15	2.07360	0.00004	0.00017	-0.00002	0.00015	2.07375
A16	2.06942	-0.00033	-0.00104	0.00024	-0.00081	2.06860
A17	2.13167	-0.00014	-0.00040	0.00002	-0.00038	2.13130
A18	2.08210	0.00046	0.00145	-0.00026	0.00119	2.08329
A19	1.86737	0.00120	0.00285	-0.00041	0.00236	1.86973
A20	2.17795	-0.00259	-0.00337	0.00057	-0.00273	2.17522
A21	2.23785	0.00139	0.00051	-0.00020	0.00038	2.23823
A22	1.86291	-0.00001	-0.00025	0.00014	-0.00040	1.86252
A23	2.19198	0.00067	0.00177	-0.00020	0.00105	2.19303
A24	2.22824	-0.00066	-0.00154	0.00049	-0.00156	2.22668
A25	1.88302	-0.00095	-0.00165	0.00032	-0.00132	1.88170
A26	2.20803	0.00080	0.00004	-0.00044	-0.00044	2.20759
A27	2.19213	0.00016	0.00160	0.00016	0.00173	2.19386
A28	2.34858	-0.00120	-0.00485	0.00255	-0.00265	2.34594
A29	2.01381	0.00094	0.00363	-0.00126	0.00203	2.01584
A30	1.92034	0.00028	0.00148	-0.00030	0.00083	1.92117
A31	2.25394	-0.00151	-0.00443	0.00072	-0.00371	2.25023
A32	2.07954	0.00151	0.00412	-0.00093	0.00320	2.08274
A33	1.94971	0.00001	0.00031	0.00021	0.00049	1.95020
A34	1.95694	0.00060	0.00175	-0.00063	0.00107	1.95801
A35	1.85928	-0.00067	-0.00179	0.00048	-0.00130	1.85798
A36	2.46694	0.00007	0.00005	0.00018	0.00025	2.46719
A37	1.98713	-0.00074	-0.00300	0.00114	-0.00181	1.98532
A38	1.91556	0.00058	0.00243	-0.00090	0.00133	1.91688
A39	2.38049	0.00016	0.00051	-0.00022	0.00048	2.38097
A40	1.57388	-0.00059	-0.00155	0.00019	-0.00135	1.57253
A41	1.95704	0.00072	0.00249	-0.00081	0.00164	1.95868
A42	2.12599	-0.00020	0.00000	0.00007	0.00014	2.12613
A43	2.19989	-0.00051	-0.00235	0.00074	-0.00153	2.19836
A44	1.86687	0.00006	-0.00006	0.00001	-0.00005	1.86682
A45	2.45182	-0.00005	-0.00023	0.00030	0.00005	2.45187

A46	1.96442	0.00000	0.00032	-0.00024	0.00005	1.96447
A47	1.92050	0.00005	0.00111	-0.00022	0.00064	1.92113
A48	1.97074	-0.00007	-0.00072	0.00049	-0.00018	1.97056
A49	2.39157	0.00004	-0.00019	-0.00003	-0.00012	2.39145
A50	1.86180	0.00000	-0.00158	0.00127	-0.00004	1.86176
A51	2.20247	0.00010	-0.00369	0.00352	0.00067	2.20314
A52	2.21097	-0.00008	-0.00230	0.00174	0.00030	2.21126
A53	1.56154	0.00007	0.00001	-0.00024	-0.00022	1.56132
A54	1.55976	0.00077	0.00137	-0.00026	0.00111	1.56087
A55	1.98265	-0.00007	-0.00009	0.00019	0.00012	1.98277
A56	2.35464	0.00020	0.00018	-0.00007	0.00013	2.35476
A57	1.94590	-0.00013	-0.00010	-0.00013	-0.00025	1.94565
A58	2.35477	0.00023	-0.00007	0.00003	-0.00003	2.35474
A59	1.94537	0.00007	0.00044	-0.00020	0.00022	1.94560
A60	1.98305	-0.00030	-0.00037	0.00016	-0.00020	1.98285
A61	1.97129	-0.00028	-0.00097	0.00030	-0.00064	1.97066
A62	2.39109	0.00015	0.00043	-0.00027	0.00025	2.39134
A63	1.92076	0.00013	0.00051	-0.00002	0.00036	1.92113
A64	1.96465	-0.00006	0.00011	-0.00004	0.00004	1.96469
A65	2.45145	0.00007	-0.00004	0.00017	0.00014	2.45159
A66	1.86698	-0.00001	-0.00001	-0.00010	-0.00009	1.86689
A67	1.85708	0.00011	0.00019	0.00005	0.00027	1.85735
A68	2.46780	-0.00021	-0.00025	-0.00015	-0.00039	2.46741
A69	1.95822	0.00011	0.00009	0.00014	0.00020	1.95842
A70	1.98458	-0.00003	-0.00015	0.00017	0.00006	1.98465
A71	1.91694	0.00023	0.00066	-0.00016	0.00037	1.91732
A72	2.38166	-0.00020	-0.00056	-0.00001	-0.00048	2.38118
A73	1.95957	-0.00016	-0.00011	-0.00017	-0.00031	1.95926
A74	2.19806	0.00008	-0.00034	0.00026	-0.00008	2.19798
A75	2.12550	0.00008	0.00044	0.00001	0.00045	2.12595
A76	1.94993	0.00024	-0.00009	0.00056	0.00050	1.95042
A77	2.08248	0.00059	0.00137	-0.00043	0.00099	2.08347
A78	2.25061	-0.00083	-0.00118	-0.00020	-0.00134	2.24927
A79	1.57229	-0.00015	0.00031	-0.00059	-0.00029	1.57199
A80	1.86285	-0.00046	-0.00162	0.00024	-0.00114	1.86172
A81	2.21065	0.00030	-0.00120	0.00121	0.00062	2.21126
A82	2.20366	0.00016	-0.00294	0.00257	0.00022	2.20388
A83	2.34651	-0.00148	-0.00296	0.00058	-0.00237	2.34414
A84	1.92029	0.00046	0.00186	-0.00076	0.00110	1.92139
A85	2.01637	0.00102	0.00111	0.00018	0.00130	2.01766
A86	2.19341	-0.00156	0.00002	-0.00016	-0.00013	2.19328
A87	2.20776	0.00185	0.00078	-0.00006	0.00073	2.20849
A88	1.88201	-0.00030	-0.00080	0.00022	-0.00059	1.88141
A89	1.86264	0.00003	-0.00005	-0.00013	0.00004	1.86268
A90	2.22690	-0.00041	-0.00096	0.00032	-0.00031	2.22659
A91	2.19265	0.00045	0.00092	-0.00001	0.00124	2.19389
A92	1.87053	-0.00028	-0.00019	0.00001	-0.00011	1.87042
A93	2.23456	0.00324	0.00374	-0.00100	0.00271	2.23727
A94	2.17810	-0.00296	-0.00356	0.00099	-0.00260	2.17550
A95	1.91150	0.00004	-0.00001	0.00011	0.00006	1.91156
A96	2.22791	0.00043	0.00134	-0.00047	0.00089	2.22880
A97	2.14377	-0.00046	-0.00133	0.00036	-0.00094	2.14282
A98	1.89792	0.00053	0.00101	-0.00030	0.00075	1.89867
A99	2.30976	-0.00082	-0.00200	0.00068	-0.00134	2.30842
A100	2.07550	0.00030	0.00099	-0.00038	0.00060	2.07610
A101	2.05848	0.00023	0.00045	-0.00003	0.00041	2.05889
A102	2.08940	-0.00015	0.00003	-0.00014	-0.00011	2.08929
A103	2.13531	-0.00009	-0.00048	0.00017	-0.00030	2.13501
A104	2.06927	-0.00029	-0.00095	0.00025	-0.00069	2.06857
A105	2.13074	0.00012	0.00024	0.00004	0.00028	2.13102

A106	2.08318	0.00016	0.00071	-0.00030	0.00041	2.08359
A107	2.09386	0.00048	0.00157	-0.00038	0.00119	2.09505
A108	2.09858	-0.00023	-0.00091	0.00032	-0.00059	2.09799
A109	2.09074	-0.00025	-0.00066	0.00006	-0.00060	2.09014
A110	2.12550	-0.00025	-0.00073	0.00017	-0.00056	2.12494
A111	2.07326	0.00012	0.00057	-0.00004	0.00052	2.07379
A112	2.08442	0.00013	0.00016	-0.00012	0.00004	2.08446
A113	2.16452	0.00201	0.00277	-0.00094	0.00183	2.16635
A114	2.15839	-0.00170	-0.00229	0.00044	-0.00184	2.15654
A115	1.96028	-0.00031	-0.00048	0.00050	0.00001	1.96029
A116	2.15976	-0.00200	-0.00356	0.00058	-0.00297	2.15679
A117	2.16764	0.00049	-0.00026	-0.00015	-0.00041	2.16723
A118	1.95578	0.00151	0.00381	-0.00043	0.00338	1.95917
A119	1.91319	-0.00014	-0.00050	0.00011	-0.00038	1.91281
A120	1.94929	-0.00007	-0.00038	0.00015	-0.00022	1.94907
A121	1.90461	-0.00001	0.00029	-0.00008	0.00020	1.90481
A122	1.90568	0.00010	0.00039	-0.00022	0.00017	1.90585
A123	1.88586	0.00008	0.00006	0.00013	0.00019	1.88605
A124	1.90411	0.00005	0.00015	-0.00009	0.00006	1.90417
A125	1.94868	0.00010	0.00122	-0.00060	0.00063	1.94931
A126	1.91215	0.00004	0.00086	-0.00042	0.00044	1.91259
A127	1.90342	0.00014	0.00214	-0.00095	0.00120	1.90462
A128	1.90676	-0.00009	-0.00131	0.00048	-0.00083	1.90593
A129	1.90489	-0.00011	-0.00131	0.00045	-0.00085	1.90403
A130	1.88690	-0.00009	-0.00172	0.00109	-0.00063	1.88627
A131	3.16720	0.00037	0.00149	-0.00168	-0.00019	3.16701
A132	3.19113	-0.00131	-0.00876	-0.00028	-0.00904	3.18209
A133	3.19725	-0.00191	-0.01454	-0.00031	-0.01484	3.18240
A134	3.16152	0.00054	0.00550	-0.00183	0.00368	3.16520
A135	3.13970	0.00008	0.00132	-0.00016	0.00116	3.14087
A136	3.14180	-0.00003	-0.00024	0.00008	-0.00015	3.14165
A137	3.14044	0.00012	0.00112	0.00007	0.00119	3.14164
A138	3.14460	-0.00037	-0.00203	-0.00085	-0.00288	3.14172
D1	-0.00155	0.00007	0.00032	0.00116	0.00148	-0.00007
D2	3.13939	0.00013	0.00022	0.00313	0.00335	-3.14045
D3	3.14084	0.00006	-0.00065	0.00200	0.00136	-3.14099
D4	-0.00141	0.00011	-0.00075	0.00397	0.00323	0.00182
D5	0.00126	-0.00005	-0.00043	-0.00066	-0.00109	0.00017
D6	-3.13973	-0.00006	-0.00078	-0.00039	-0.00117	-3.14091
D7	-3.14135	-0.00003	0.00081	-0.00173	-0.00093	3.14090
D8	0.00084	-0.00004	0.00046	-0.00147	-0.00101	-0.00017
D9	-0.00227	0.00004	0.00593	0.00823	0.01417	0.01189
D10	3.13332	0.00008	0.01344	0.00173	0.01517	-3.13470
D11	3.14026	0.00002	0.00478	0.00923	0.01402	-3.12891
D12	-0.00733	0.00006	0.01229	0.00273	0.01502	0.00769
D13	0.00075	-0.00004	-0.00008	-0.00077	-0.00086	-0.00011
D14	-3.14140	0.00000	0.00053	-0.00022	0.00031	-3.14109
D15	-3.14007	-0.00011	0.00004	-0.00311	-0.00308	3.14003
D16	0.00096	-0.00007	0.00065	-0.00257	-0.00192	-0.00095
D17	0.00451	-0.00022	-0.00466	-0.01452	-0.01918	-0.01467
D18	3.13612	0.00014	0.00552	0.02944	0.03498	-3.11208
D19	-3.13777	-0.00016	-0.00477	-0.01243	-0.01719	3.12822
D20	-0.00616	0.00020	0.00541	0.03153	0.03697	0.03081
D21	0.00031	-0.00001	-0.00003	-0.00010	-0.00013	0.00018
D22	-3.14156	0.00002	-0.00018	0.00054	0.00036	-3.14120
D23	-3.14071	-0.00004	-0.00066	-0.00066	-0.00132	3.14115
D24	0.00061	-0.00002	-0.00082	-0.00002	-0.00083	-0.00023
D25	-0.00056	0.00002	-0.00010	0.00057	0.00047	-0.00009
D26	3.14078	0.00003	-0.00006	0.00055	0.00048	3.14126
D27	3.14131	0.00000	0.00006	-0.00007	-0.00002	3.14130

D28	-0.00054	0.00000	0.00009	-0.00010	-0.00001	-0.00054
D29	-0.00025	0.00001	0.00033	-0.00018	0.00016	-0.00010
D30	3.14076	0.00001	0.00067	-0.00043	0.00023	3.14100
D31	-3.14159	0.00000	0.00030	-0.00015	0.00014	-3.14145
D32	-0.00058	0.00001	0.00063	-0.00041	0.00022	-0.00035
D33	0.00503	-0.00018	-0.00872	-0.01709	-0.02581	-0.02079
D34	-3.14020	-0.00002	-0.00900	-0.00428	-0.01330	3.12969
D35	-3.13029	-0.00020	-0.01658	-0.01030	-0.02685	3.12604
D36	0.00767	-0.00004	-0.01686	0.00251	-0.01434	-0.00667
D37	0.00057	0.00004	-0.00565	0.00579	0.00013	0.00070
D38	-3.13995	0.00000	-0.00661	0.00610	-0.00052	-3.14047
D39	3.13486	0.00009	0.00348	-0.00213	0.00136	3.13622
D40	-0.00567	0.00005	0.00252	-0.00182	0.00071	-0.00496
D41	-0.00584	0.00024	0.00826	0.01938	0.02764	0.02179
D42	3.13934	0.00009	0.00855	0.00673	0.01526	-3.12859
D43	-3.13718	-0.00014	-0.00219	-0.02577	-0.02792	3.11809
D44	0.00800	-0.00029	-0.00190	-0.03843	-0.04030	-0.03230
D45	-3.11173	-0.00056	-0.01959	-0.02259	-0.04218	3.12927
D46	-0.00648	0.00031	0.00390	0.01666	0.02055	0.01407
D47	0.02561	-0.00038	-0.01993	-0.00760	-0.02752	-0.00191
D48	3.13086	0.00049	0.00356	0.03165	0.03521	-3.11712
D49	-0.03644	0.00047	0.02893	0.02527	0.05419	0.01775
D50	3.10481	0.00067	0.03161	0.02923	0.06084	-3.11753
D51	3.14010	-0.00037	0.00635	-0.01246	-0.00611	3.13399
D52	-0.00184	-0.00017	0.00904	-0.00849	0.00054	-0.00129
D53	-3.13107	-0.00016	-0.00108	-0.00329	-0.00436	-3.13543
D54	0.01084	-0.00035	-0.00359	-0.00702	-0.01061	0.00024
D55	3.13214	0.00030	0.00420	0.00435	0.00854	3.14068
D56	0.01386	-0.00021	-0.01419	0.00433	-0.00985	0.00401
D57	-0.00974	0.00047	0.00646	0.00766	0.01411	0.00437
D58	-3.12802	-0.00005	-0.01194	0.00764	-0.00428	-3.13229
D59	0.00556	0.00011	0.00392	-0.00120	0.00272	0.00829
D60	-3.13178	0.00006	0.00864	-0.00465	0.00399	-3.12779
D61	-3.13055	0.00002	-0.00104	-0.00371	-0.00474	-3.13529
D62	0.01529	-0.00003	0.00368	-0.00715	-0.00347	0.01182
D63	-0.00918	0.00013	-0.00015	0.00463	0.00448	-0.00470
D64	3.12400	0.00027	0.00746	0.00847	0.01594	3.13994
D65	0.00809	-0.00022	-0.00621	-0.00240	-0.00862	-0.00053
D66	3.13454	0.00023	0.01077	0.00438	0.01516	-3.13348
D67	-3.12538	-0.00036	-0.01357	-0.00611	-0.01968	3.13812
D68	0.00108	0.00009	0.00342	0.00067	0.00409	0.00517
D69	0.00286	-0.00038	-0.00670	-0.00425	-0.01095	-0.00809
D70	3.11995	0.00017	0.01262	-0.00425	0.00838	3.12833
D71	3.13866	-0.00031	-0.01313	0.00045	-0.01268	3.12598
D72	-0.02744	0.00023	0.00619	0.00045	0.00666	-0.02078
D73	-0.03291	0.00027	0.00045	0.01395	0.01442	-0.01849
D74	-3.04617	0.00013	0.04527	-0.03862	0.00669	-3.03948
D75	3.11432	0.00020	0.00674	0.00938	0.01611	3.13042
D76	0.10106	0.00007	0.05156	-0.04320	0.00837	0.10943
D77	-0.02907	0.00040	0.00677	0.01126	0.01803	-0.01104
D78	3.13675	0.00004	-0.00178	0.00343	0.00167	3.13842
D79	3.12295	0.00009	-0.00494	0.00659	0.00165	3.12460
D80	0.00559	-0.00027	-0.01348	-0.00124	-0.01471	-0.00913
D81	-3.12593	-0.00033	-0.00934	-0.00590	-0.01526	-3.14119
D82	-0.00001	0.00014	0.00826	0.00112	0.00936	0.00935
D83	0.03817	-0.00042	-0.00449	-0.01551	-0.02000	0.01817
D84	3.05062	-0.00027	-0.04982	0.03757	-0.01219	3.03843
D85	-3.13616	0.00007	0.00705	-0.00492	0.00212	-3.13405
D86	-0.12371	0.00022	-0.03828	0.04816	0.00993	-0.11378
D87	3.13415	0.00032	0.01197	0.00246	0.01443	-3.13461

D88	-0.00974	0.00029	0.01242	0.00066	0.01307	0.00333
D89	0.02595	-0.00018	0.00019	-0.00833	-0.00813	0.01782
D90	-3.11794	-0.00020	0.00064	-0.01013	-0.00950	-3.12743
D91	1.51219	0.00011	-0.03215	0.03768	0.00548	1.51767
D92	-2.65634	0.00009	-0.03242	0.03761	0.00515	-2.65118
D93	-0.59426	0.00009	-0.03273	0.03813	0.00536	-0.58890
D94	-1.47593	-0.00005	0.02141	-0.02520	-0.00375	-1.47968
D95	0.63873	-0.00007	0.02115	-0.02527	-0.00408	0.63465
D96	2.70081	-0.00007	0.02083	-0.02475	-0.00387	2.69693
D97	-0.00562	0.00003	-0.00121	-0.00076	-0.00196	-0.00758
D98	3.13882	0.00009	-0.00089	0.00001	-0.00087	3.13794
D99	-3.14084	0.00011	0.00326	-0.00090	0.00235	-3.13848
D100	0.00309	0.00013	0.00281	0.00093	0.00374	0.00683
D101	-0.01127	0.00001	0.00110	0.00016	0.00126	-0.01001
D102	-3.13420	-0.00019	-0.00861	-0.00146	-0.01006	3.13893
D103	0.00980	-0.00019	-0.00611	0.00021	-0.00590	0.00390
D104	-3.13357	-0.00020	-0.00576	-0.00119	-0.00695	-3.14052
D105	-3.13396	-0.00023	-0.00635	-0.00038	-0.00673	-3.14069
D106	0.00586	-0.00025	-0.00601	-0.00177	-0.00778	-0.00192
D107	3.12429	0.00020	0.00651	0.00112	0.00763	3.13192
D108	-0.02782	0.00008	0.00300	0.00195	0.00495	-0.02288
D109	-0.01451	0.00026	0.00682	0.00188	0.00870	-0.00580
D110	3.11657	0.00014	0.00332	0.00271	0.00602	3.12259
D111	0.01703	-0.00016	-0.00478	-0.00119	-0.00597	0.01106
D112	-3.13699	-0.00003	0.00169	-0.00011	0.00156	-3.13543
D113	-3.11693	-0.00008	-0.00223	-0.00179	-0.00403	-3.12095
D114	0.01224	0.00006	0.00423	-0.00071	0.00351	0.01575
D115	3.13500	-0.00001	-0.00515	-0.00052	-0.00566	3.12934
D116	0.10583	-0.00001	0.03502	-0.03794	-0.00296	0.10287
D117	-0.01690	-0.00014	-0.00859	0.00030	-0.00829	-0.02519
D118	-3.04607	-0.00013	0.03157	-0.03713	-0.00560	-3.05167
D119	3.12097	0.00024	0.01119	0.00238	0.01357	3.13454
D120	-0.00412	-0.00013	-0.00145	-0.00098	-0.00243	-0.00655
D121	-0.00260	0.00004	0.00181	0.00082	0.00264	0.00004
D122	-3.12769	-0.00032	-0.01082	-0.00254	-0.01336	-3.14105
D123	3.13222	0.00009	-0.00062	0.00211	0.00149	3.13371
D124	-0.00778	-0.00013	-0.00723	-0.00067	-0.00789	-0.01567
D125	-0.02049	0.00033	0.00790	0.00438	0.01227	-0.00822
D126	3.12270	0.00011	0.00129	0.00160	0.00289	3.12559
D127	3.14049	0.00004	0.00863	-0.00388	0.00475	-3.13794
D128	0.01599	-0.00034	-0.00446	-0.00737	-0.01183	0.00417
D129	0.01398	-0.00012	-0.00772	0.00243	-0.00528	0.00869
D130	-3.11612	-0.00040	-0.00996	-0.00727	-0.01722	-3.13334
D131	-3.12979	0.00018	0.00129	0.00623	0.00751	-3.12227
D132	0.02330	-0.00010	-0.00095	-0.00347	-0.00442	0.01888
D133	0.01521	0.00016	0.00975	0.00023	0.00999	0.02520
D134	3.04496	0.00017	-0.02996	0.03735	0.00734	3.05231
D135	-3.12427	-0.00013	0.00098	-0.00346	-0.00247	-3.12674
D136	-0.09452	-0.00012	-0.03874	0.03366	-0.00512	-0.09963
D137	-0.00160	-0.00014	0.00419	-0.00796	-0.00377	-0.00537
D138	-3.12492	-0.00040	-0.01073	-0.00447	-0.01520	-3.14012
D139	3.12905	0.00013	0.00632	0.00128	0.00760	3.13664
D140	0.00573	-0.00013	-0.00860	0.00476	-0.00383	0.00190
D141	-0.00833	0.00027	0.00021	0.00876	0.00897	0.00063
D142	3.11277	0.00059	0.01692	0.00485	0.02179	3.13457
D143	3.13586	0.00032	-0.00449	0.01545	0.01096	-3.13637
D144	-0.01280	0.00052	0.00101	0.01698	0.01800	0.00519
D145	0.01609	-0.00001	-0.02230	0.01960	-0.00270	0.01339
D146	-3.13257	0.00019	-0.01680	0.02114	0.00434	-3.12823
D147	-0.62963	-0.00003	-0.02148	0.01921	-0.00229	-0.63192

Stoichiometry C42H18N6O2S4
 Framework group C1[X(C42H18N6O2S4)]
 Deg. of freedom 210
 Full point group C1 NOp 1
 Largest Abelian subgroup C1 NOp 1
 Largest concise Abelian subgroup C1 NOp 1
 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.803435	-0.634181	0.009121
2	6	0	-9.996505	-1.786390	0.018493
3	6	0	-10.521345	-3.070366	0.025750
4	6	0	-11.910499	-3.210274	0.023691
5	6	0	-12.729546	-2.074477	0.014304
6	6	0	-12.195103	-0.781911	0.006887
7	1	0	-9.852392	-3.924850	0.033329
8	1	0	-12.359737	-4.198607	0.029551
9	1	0	-13.808563	-2.194640	0.012469
10	1	0	-12.863060	0.067706	-0.000820
11	6	0	-9.924641	0.565792	0.002365
12	6	0	-8.571770	-1.392475	0.020795
13	6	0	-8.539133	0.086261	-0.008563
14	6	0	-7.403461	0.864611	-0.030565
15	6	0	-6.013172	0.590438	-0.031364
16	6	0	-3.642413	-0.188071	-0.020829
17	6	0	-3.778110	1.224589	-0.028989
18	16	0	-5.178833	-0.993832	-0.026330
19	6	0	-5.099496	1.660670	-0.029001
20	6	0	-2.265755	-0.454829	-0.013456
21	6	0	-1.603216	0.794974	-0.018013
22	7	0	-2.524078	1.817748	-0.042177
23	16	0	-1.148838	-1.809001	-0.010433
24	16	0	1.150444	1.805588	0.002590
25	6	0	0.199582	-0.675168	0.001126
26	6	0	-0.198079	0.671512	-0.007239
27	6	0	1.604245	-0.798655	0.013085
28	6	0	2.266915	0.450899	0.006204
29	6	0	3.644568	0.183812	0.011052
30	6	0	3.779213	-1.228576	0.020740
31	6	0	5.100233	-1.664646	0.016550
32	6	0	6.014578	-0.595047	0.014828
33	16	0	5.181892	0.989388	0.009668
34	7	0	2.524847	-1.821417	0.042329
35	6	0	7.404060	-0.868949	0.008760
36	6	0	8.539277	-0.087616	0.010779
37	6	0	8.568395	1.391774	0.019950
38	6	0	9.925338	-0.562795	0.002213
39	6	0	9.992102	1.789307	0.005656
40	6	0	10.801295	0.638920	-0.003918
41	6	0	10.513963	3.074477	0.002257
42	6	0	12.192024	0.789348	-0.017302
43	6	0	11.902742	3.217146	-0.011326
44	6	0	12.723804	2.082931	-0.020971
45	6	0	10.381899	-1.869211	-0.000108
46	6	0	9.530015	-3.015725	0.006304
47	6	0	11.764939	-2.221679	-0.008720
48	7	0	8.858796	-3.968767	0.010880

49	7	0	12.881256	-2.554845	-0.015756
50	6	0	-10.378938	1.873868	0.000391
51	6	0	-11.761826	2.229530	0.005499
52	6	0	-9.525663	3.019685	-0.007438
53	7	0	-12.877332	2.565501	0.009332
54	7	0	-8.851708	3.970773	-0.013644
55	8	0	-7.617445	-2.162100	-0.001000
56	8	0	7.611493	2.158412	0.030332
57	6	0	2.245001	-3.243960	-0.046795
58	1	0	1.312320	-3.467247	0.475812
59	1	0	2.163060	-3.575740	-1.087604
60	1	0	3.048385	-3.798176	0.442686
61	6	0	-2.245618	3.238921	0.065937
62	1	0	-2.169131	3.558112	1.111159
63	1	0	-1.310451	3.468961	-0.449260
64	1	0	-3.047049	3.798565	-0.420689
65	1	0	5.429145	-2.697342	0.015101
66	1	0	12.861463	-0.059229	-0.025183
67	1	0	13.802519	2.205305	-0.031602
68	1	0	12.350211	4.206310	-0.014442
69	1	0	9.843019	3.927398	0.010110
70	1	0	7.572273	-1.938884	0.000857
71	1	0	-7.571382	1.934582	-0.026758
72	1	0	-5.428918	2.693285	-0.022882

Rotational constants (GHZ): 0.1750166 0.0104081 0.0098252

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis func-
tions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6570.6621583944 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T

Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6570.5772271161 Har-
trees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.24D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Initial guess from the checkpoint file: "PBDB.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000021 -0.000001 -0.000101 Ang= -0.01 deg.

ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1

AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for in-
itial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-
yADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 IlCent= 200000004 NGrid=

0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0=

0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 Integral accuracy reduced to 1.0D-05 until final iterations.
 Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
 SCF Done: E(RB3LYP) = -3683.01996386 A.U. after 13 cycles
 NFock= 13 Conv=0.35D-08 -V/T= 2.0068
 Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1
 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	0.000145376	-0.000079501	-0.000409386
2	6	0.001011342	0.000396198	-0.001443446
3	6	0.000090752	0.000120543	-0.000059048
4	6	-0.000072637	0.000018333	0.000063864
5	6	-0.000017838	0.000047829	0.000003295
6	6	-0.000110786	-0.000075124	-0.000025235
7	1	-0.000002111	-0.000033756	-0.000022296
8	1	-0.000023848	-0.000030135	0.000010796
9	1	-0.000000040	-0.000019747	-0.000012637
10	1	-0.000004120	-0.000031048	0.000015579
11	6	-0.000481354	0.000077127	0.000560804
12	6	-0.003565652	-0.000337221	0.004850029
13	6	0.000697204	0.001119517	-0.001754532
14	6	0.001658247	-0.001168259	-0.001402303
15	6	0.000006257	0.000087626	-0.000094982
16	6	-0.000607595	-0.000124260	-0.000155201
17	6	0.000336232	-0.000031037	-0.000099453
18	16	-0.000482033	0.000523697	-0.000189229
19	6	0.000099228	0.000033835	0.000333938
20	6	0.000129517	-0.000341203	0.000186742
21	6	-0.000116327	0.000184376	-0.000331518
22	7	0.000048944	0.000017386	0.000025899
23	16	0.000038460	0.000151690	0.000027676
24	16	-0.000021923	0.000053400	0.000069241
25	6	-0.000333218	0.000348515	-0.000109895
26	6	0.000122665	-0.000273497	-0.000220281
27	6	0.000627547	-0.000333491	0.000130267
28	6	0.000283101	-0.000250305	0.000251966
29	6	-0.000397689	0.000148101	-0.000020913
30	6	-0.000060729	0.000321107	-0.000358095
31	6	0.000246395	0.000135088	-0.000200504
32	6	-0.000471063	-0.000003775	0.000205077
33	16	0.000178037	-0.000038556	-0.000396652
34	7	-0.000168232	-0.000024179	0.000514659
35	6	0.000097190	0.000364386	0.000017301
36	6	0.000037585	-0.000323523	-0.000307084
37	6	-0.000584664	-0.000065977	0.000603435
38	6	-0.000256613	-0.000319854	-0.000082536
39	6	0.000106140	-0.000072515	-0.000372035
40	6	-0.000010885	0.000248889	-0.000051452
41	6	-0.000025619	-0.000041055	-0.000074627
42	6	0.000374357	-0.000096202	0.000320880
43	6	-0.000017785	-0.000091695	0.000011527
44	6	0.000083411	-0.000193129	0.000031944
45	6	-0.000217042	0.000190860	-0.000143417

46	6	0.000077924	0.000484813	0.000126525
47	6	0.000588683	-0.000138071	0.000452028
48	7	0.000041944	-0.000121373	-0.000009077
49	7	0.000077364	-0.000160482	0.000034988
50	6	0.000283792	0.000115157	0.000318780
51	6	-0.000234448	0.000119542	-0.000218551
52	6	0.000209942	-0.000224826	0.000069756
53	7	-0.000027428	0.000154225	-0.000011523
54	7	-0.000060734	0.000095170	-0.000055314
55	8	0.001426392	-0.000066959	-0.001450793
56	8	0.000013659	0.000045373	-0.000189255
57	6	-0.000044882	0.000008421	0.000040490
58	1	-0.000008758	-0.000058435	-0.000032612
59	1	0.000019006	-0.000015303	-0.000060363
60	1	-0.000015091	-0.000044167	0.000014563
61	6	-0.000144274	-0.000218302	0.000069277
62	1	-0.000005316	0.000062960	0.000112261
63	1	-0.000031122	0.000015258	-0.000021577
64	1	0.000043367	-0.000010786	0.000000019
65	1	-0.000005957	-0.000035701	0.000019357
66	1	-0.000056071	-0.000053872	-0.000045706
67	1	0.000015332	0.000023085	0.000011337
68	1	-0.000007325	0.000040876	0.000008985
69	1	0.000027848	0.000009971	0.000004420
70	1	0.000049772	0.000021411	-0.000047832
71	1	-0.000534156	-0.000281163	0.000755272
72	1	-0.000067646	0.000043725	0.000206385

Cartesian Forces: Max 0.004850029 RMS 0.000543398

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001461948 RMS 0.000233680

Search for a local minimum.

Step number 22 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 16 18 17 19 20
21 22

DE= -3.18D-04 DEPred=-4.66D-04 R= 6.82D-01

TightC=F SS= 1.41D+00 RLast= 1.84D-01 DXNew= 6.9622D-01 5.5313D-01

Trust test= 6.82D-01 RLast= 1.84D-01 DXMaxT set to 5.53D-01

ITU= 1 1 -1 0 -1 0 -1 1 1 1 1 1 1 0 0 0 1 0 0 0

ITU= 1 0

Eigenvalues ---	0.00169	0.00235	0.00241	0.00274	0.00377
Eigenvalues ---	0.00386	0.00422	0.00448	0.00481	0.00503
Eigenvalues ---	0.00534	0.00578	0.00586	0.00599	0.00624
Eigenvalues ---	0.00645	0.00671	0.00680	0.00711	0.00721
Eigenvalues ---	0.00744	0.00759	0.00768	0.00771	0.00777
Eigenvalues ---	0.00793	0.00819	0.00830	0.00844	0.01000
Eigenvalues ---	0.01084	0.01122	0.01135	0.01172	0.01188
Eigenvalues ---	0.01249	0.01320	0.01348	0.01361	0.01380
Eigenvalues ---	0.01413	0.01457	0.01463	0.01550	0.01623
Eigenvalues ---	0.01647	0.01744	0.01753	0.01794	0.01811
Eigenvalues ---	0.01929	0.01953	0.02006	0.02021	0.02065
Eigenvalues ---	0.02075	0.02198	0.02206	0.03446	0.03628
Eigenvalues ---	0.03940	0.04829	0.04838	0.04905	0.04982

```

Eigenvalues --- 0.04999 0.05023 0.05060 0.05330 0.07049
Eigenvalues --- 0.07231 0.07386 0.07564 0.15507 0.15811
Eigenvalues --- 0.15934 0.15986 0.15999 0.16000 0.16000
Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16001
Eigenvalues --- 0.16001 0.16003 0.16006 0.16021 0.16034
Eigenvalues --- 0.16066 0.17849 0.18999 0.19339 0.19797
Eigenvalues --- 0.20600 0.21309 0.21354 0.21877 0.21998
Eigenvalues --- 0.22010 0.22165 0.22462 0.22579 0.22630
Eigenvalues --- 0.22642 0.22686 0.22849 0.23049 0.23187
Eigenvalues --- 0.23356 0.23496 0.23765 0.23808 0.24010
Eigenvalues --- 0.24189 0.24280 0.24316 0.24357 0.24518
Eigenvalues --- 0.24543 0.24604 0.24674 0.24746 0.24857
Eigenvalues --- 0.24919 0.24936 0.24961 0.24969 0.24991
Eigenvalues --- 0.24994 0.24997 0.24998 0.24998 0.24999
Eigenvalues --- 0.24999 0.25000 0.25000 0.25000 0.25003
Eigenvalues --- 0.25011 0.25158 0.25592 0.25870 0.26016
Eigenvalues --- 0.26243 0.26544 0.26798 0.26829 0.27082
Eigenvalues --- 0.27230 0.27721 0.27847 0.28259 0.28470
Eigenvalues --- 0.28535 0.28856 0.29907 0.30262 0.31948
Eigenvalues --- 0.32535 0.34430 0.35495 0.36273 0.36315
Eigenvalues --- 0.36346 0.36475 0.36621 0.36652 0.36790
Eigenvalues --- 0.36830 0.37074 0.37082 0.37097 0.37253
Eigenvalues --- 0.37264 0.37348 0.37440 0.37568 0.37676
Eigenvalues --- 0.37759 0.38007 0.38969 0.40307 0.40697
Eigenvalues --- 0.41630 0.42103 0.42648 0.44423 0.44780
Eigenvalues --- 0.45557 0.46026 0.46573 0.47821 0.47916
Eigenvalues --- 0.48225 0.52166 0.53451 0.55344 0.57321
Eigenvalues --- 0.61912 0.68550 0.73151 0.80242 0.81989
Eigenvalues --- 0.91556 1.25854 1.26327 1.29348 1.35387
En-DIIS/RFO-DIIS IScMMF= 0 using points: 22 21 20 19
RFO step: Lambda=-7.34323477D-05.
DidBck=T Rises=F RFO-DIIS coefs: 0.42540 0.21758 0.09667 0.26035
Iteration 1 RMS(Cart)= 0.03219001 RMS(Int)= 0.00026669
Iteration 2 RMS(Cart)= 0.00076975 RMS(Int)= 0.00010274
Iteration 3 RMS(Cart)= 0.00000019 RMS(Int)= 0.00010274
Variable Old X -DE/DX Delta X Delta X Delta X New X
(Linear) (Quad) (Total)
R1 2.65828 0.00007 0.00002 0.00017 0.00019 2.65847
R2 2.64465 -0.00002 0.00007 -0.00011 -0.00005 2.64460
R3 2.81072 -0.00017 -0.00020 0.00078 0.00037 2.81108
R4 2.62128 0.00007 0.00011 -0.00024 -0.00012 2.62116
R5 2.79337 0.00034 0.00031 -0.00032 0.00018 2.79355
R6 2.63840 0.00008 0.00000 0.00000 0.00001 2.63841
R7 2.05077 -0.00002 -0.00004 0.00007 0.00003 2.05080
R8 2.64627 0.00005 -0.00008 0.00025 0.00016 2.64643
R9 2.05159 -0.00003 -0.00001 0.00000 -0.00002 2.05158
R10 2.64319 0.00002 0.00006 -0.00015 -0.00011 2.64308
R11 2.05166 -0.00001 -0.00002 0.00005 0.00003 2.05169
R12 2.04237 0.00000 -0.00019 0.00039 0.00021 2.04258
R13 2.77069 0.00004 0.00003 -0.00094 -0.00102 2.76967
R14 2.61674 -0.00031 -0.00004 -0.00033 -0.00038 2.61637
R15 2.79564 0.00030 0.00024 -0.00032 0.00007 2.79570
R16 2.31716 0.00018 -0.00013 0.00048 0.00036 2.31751
R17 2.60211 0.00146 0.00091 0.00031 0.00122 2.60333
R18 2.67786 -0.00021 -0.00179 0.00641 0.00462 2.68248
R19 2.04671 0.00009 0.00005 0.00023 0.00028 2.04699
R20 3.38364 -0.00031 -0.00048 0.00050 0.00002 3.38366
R21 2.65922 0.00007 0.00012 -0.00012 -0.00001 2.65921
R22 2.68187 -0.00018 -0.00044 0.00099 0.00055 2.68242
R23 3.27848 0.00045 0.00060 -0.00058 0.00002 3.27850

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R24	2.64993	0.00046	0.00049	-0.00011	0.00037	2.65031
R25	2.62952	-0.00004	0.00050	-0.00225	-0.00175	2.62777
R26	2.62162	0.00015	0.00066	-0.00132	-0.00065	2.62097
R27	2.04829	-0.00010	-0.00005	-0.00001	-0.00006	2.04822
R28	2.67314	0.00000	-0.00008	0.00010	0.00003	2.67316
R29	3.31715	0.00014	0.00017	-0.00032	-0.00015	3.31700
R30	2.60113	-0.00003	0.00065	-0.00169	-0.00103	2.60010
R31	2.66563	0.00035	0.00100	-0.00291	-0.00190	2.66373
R32	2.74431	0.00010	-0.00027	0.00133	0.00106	2.74537
R33	3.32932	0.00013	0.00020	-0.00037	-0.00018	3.32914
R34	3.32975	0.00004	0.00009	-0.00034	-0.00025	3.32950
R35	3.31737	0.00009	0.00026	-0.00071	-0.00045	3.31692
R36	2.65354	0.00020	0.00001	0.00024	0.00026	2.65379
R37	2.66476	0.00072	0.00068	-0.00024	0.00044	2.66521
R38	2.67285	0.00003	-0.00007	0.00011	0.00004	2.67289
R39	2.60097	0.00002	0.00081	-0.00260	-0.00180	2.59917
R40	2.65188	-0.00030	0.00089	-0.00442	-0.00353	2.64835
R41	2.68119	0.00007	-0.00003	0.00001	-0.00001	2.68118
R42	3.27981	0.00011	0.00021	-0.00068	-0.00047	3.27935
R43	2.62887	0.00021	0.00102	-0.00361	-0.00259	2.62628
R44	2.62213	-0.00013	0.00068	-0.00257	-0.00189	2.62024
R45	2.65913	0.00020	0.00035	-0.00090	-0.00055	2.65858
R46	2.04811	-0.00001	0.00000	-0.00003	-0.00003	2.04807
R47	3.38247	0.00013	0.00027	-0.00055	-0.00028	3.38218
R48	2.67629	0.00057	0.00191	-0.00442	-0.00251	2.67379
R49	2.74491	-0.00012	-0.00029	0.00079	0.00050	2.74541
R50	2.60426	0.00072	0.00041	0.00021	0.00062	2.60489
R51	2.04678	0.00002	0.00000	0.00022	0.00022	2.04699
R52	2.79624	0.00017	0.00003	0.00091	0.00092	2.79716
R53	2.76897	0.00065	0.00062	-0.00059	0.00005	2.76902
R54	2.79346	0.00024	0.00032	-0.00009	0.00021	2.79367
R55	2.31713	0.00011	-0.00008	0.00029	0.00021	2.31734
R56	2.81021	0.00005	-0.00025	0.00062	0.00041	2.81062
R57	2.61519	0.00075	0.00058	-0.00086	-0.00029	2.61490
R58	2.65792	0.00019	0.00011	-0.00007	0.00005	2.65797
R59	2.62122	0.00011	0.00024	-0.00068	-0.00044	2.62078
R60	2.64355	0.00048	0.00029	0.00023	0.00052	2.64407
R61	2.63835	0.00015	-0.00004	0.00024	0.00020	2.63855
R62	2.05077	-0.00003	-0.00002	0.00002	-0.00001	2.05076
R63	2.64302	0.00013	0.00011	-0.00019	-0.00008	2.64294
R64	2.04256	-0.00008	-0.00030	0.00070	0.00040	2.04296
R65	2.64607	0.00011	0.00018	-0.00040	-0.00022	2.64586
R66	2.05162	-0.00004	-0.00002	0.00000	-0.00002	2.05160
R67	2.05165	0.00000	-0.00001	0.00004	0.00003	2.05168
R68	2.69923	0.00036	0.00019	0.00011	0.00030	2.69953
R69	2.69716	0.00088	0.00044	0.00100	0.00144	2.69859
R70	2.20284	-0.00012	-0.00006	0.00011	0.00005	2.20290
R71	2.20152	0.00013	0.00003	-0.00001	0.00003	2.20155
R72	2.69834	0.00042	0.00025	0.00026	0.00051	2.69885
R73	2.69976	0.00014	0.00008	-0.00015	-0.00007	2.69969
R74	2.20155	0.00008	0.00003	-0.00003	0.00000	2.20154
R75	2.20282	-0.00009	-0.00003	0.00007	0.00003	2.20286
R76	2.06393	-0.00002	-0.00005	0.00014	0.00008	2.06401
R77	2.07016	-0.00006	0.00004	-0.00019	-0.00015	2.07001
R78	2.06333	-0.00001	0.00001	-0.00005	-0.00004	2.06329
R79	2.07028	-0.00011	0.00013	-0.00053	-0.00040	2.06989
R80	2.06394	-0.00003	0.00000	-0.00005	-0.00005	2.06389
R81	2.06344	-0.00004	0.00004	-0.00019	-0.00015	2.06329
A1	2.07599	0.00009	0.00020	-0.00066	-0.00038	2.07561
A2	1.89856	0.00008	0.00012	-0.00023	-0.00024	1.89832

A3	2.30864	-0.00017	-0.00032	0.00088	0.00063	2.30926
A4	2.14263	-0.00006	-0.00017	0.00059	0.00033	2.14295
A5	1.91200	-0.00012	-0.00015	-0.00013	-0.00004	1.91197
A6	2.22855	0.00018	0.00032	-0.00046	-0.00029	2.22827
A7	2.05919	-0.00003	-0.00002	-0.00004	-0.00003	2.05916
A8	2.08937	-0.00002	0.00008	-0.00029	-0.00022	2.08914
A9	2.13463	0.00004	-0.00006	0.00033	0.00025	2.13488
A10	2.09518	0.00004	0.00016	-0.00039	-0.00022	2.09495
A11	2.09778	-0.00001	-0.00012	0.00031	0.00019	2.09797
A12	2.09023	-0.00002	-0.00004	0.00008	0.00004	2.09027
A13	2.12478	-0.00001	-0.00006	0.00023	0.00016	2.12494
A14	2.08465	0.00002	0.00005	-0.00012	-0.00006	2.08459
A15	2.07375	-0.00002	0.00001	-0.00011	-0.00010	2.07366
A16	2.06860	-0.00003	-0.00010	0.00027	0.00015	2.06876
A17	2.13130	-0.00001	0.00000	0.00003	0.00003	2.13133
A18	2.08329	0.00005	0.00011	-0.00030	-0.00019	2.08310
A19	1.86973	0.00018	0.00020	0.00025	0.00025	1.86997
A20	2.17522	-0.00045	-0.00027	0.00106	0.00090	2.17611
A21	2.23823	0.00027	0.00006	-0.00130	-0.00113	2.23710
A22	1.86252	0.00002	0.00009	0.00051	-0.00007	1.86244
A23	2.19303	0.00033	0.00036	0.00154	0.00059	2.19362
A24	2.22668	-0.00028	0.00006	0.00070	-0.00055	2.22613
A25	1.88170	-0.00014	-0.00014	0.00024	0.00024	1.88194
A26	2.20759	0.00062	0.00027	-0.00003	0.00020	2.20779
A27	2.19386	-0.00047	-0.00012	-0.00028	-0.00044	2.19342
A28	2.34594	-0.00090	-0.00113	0.00064	-0.00040	2.34554
A29	2.01584	0.00064	0.00082	-0.00115	-0.00023	2.01560
A30	1.92117	0.00028	0.00033	-0.00023	0.00019	1.92137
A31	2.25023	-0.00060	-0.00029	-0.00102	-0.00130	2.24893
A32	2.08274	0.00053	0.00041	0.00031	0.00073	2.08346
A33	1.95020	0.00008	-0.00011	0.00069	0.00057	1.95078
A34	1.95801	0.00016	0.00034	-0.00052	-0.00018	1.95783
A35	1.85798	-0.00017	-0.00023	0.00016	-0.00009	1.85789
A36	2.46719	0.00002	-0.00011	0.00035	0.00024	2.46743
A37	1.98532	-0.00023	-0.00060	0.00116	0.00056	1.98588
A38	1.91688	0.00016	0.00056	-0.00105	-0.00048	1.91641
A39	2.38097	0.00007	0.00001	-0.00008	-0.00007	2.38089
A40	1.57253	-0.00016	-0.00007	-0.00047	-0.00054	1.57199
A41	1.95868	0.00015	0.00042	-0.00089	-0.00046	1.95822
A42	2.12613	-0.00009	-0.00008	0.00001	-0.00005	2.12608
A43	2.19836	-0.00006	-0.00040	0.00090	0.00052	2.19888
A44	1.86682	0.00005	-0.00001	-0.00004	-0.00006	1.86676
A45	2.45187	-0.00006	-0.00016	0.00021	0.00004	2.45191
A46	1.96447	0.00002	0.00014	-0.00027	-0.00012	1.96435
A47	1.92113	-0.00002	0.00024	-0.00038	-0.00016	1.92098
A48	1.97056	-0.00001	-0.00029	0.00075	0.00046	1.97102
A49	2.39145	0.00003	-0.00004	-0.00021	-0.00027	2.39118
A50	1.86176	-0.00001	-0.00084	0.00188	0.00097	1.86273
A51	2.20314	0.00008	-0.00240	0.00565	0.00316	2.20631
A52	2.21126	-0.00006	-0.00142	0.00240	0.00088	2.21215
A53	1.56132	0.00007	0.00013	-0.00052	-0.00039	1.56094
A54	1.56087	0.00022	0.00011	0.00014	0.00025	1.56112
A55	1.98277	-0.00005	-0.00012	0.00031	0.00020	1.98297
A56	2.35476	0.00009	0.00003	0.00006	0.00009	2.35485
A57	1.94565	-0.00003	0.00009	-0.00038	-0.00029	1.94536
A58	2.35474	0.00012	-0.00002	0.00023	0.00020	2.35494
A59	1.94560	-0.00002	0.00011	-0.00033	-0.00021	1.94539
A60	1.98285	-0.00010	-0.00009	0.00009	0.00000	1.98285
A61	1.97066	-0.00004	-0.00016	0.00027	0.00011	1.97077
A62	2.39134	0.00004	0.00009	-0.00038	-0.00028	2.39106

A63	1.92113	0.00000	0.00007	0.00012	0.00018	1.92131
A64	1.96469	-0.00005	0.00004	-0.00010	-0.00006	1.96462
A65	2.45159	0.00003	-0.00010	0.00022	0.00013	2.45172
A66	1.86689	0.00002	0.00004	-0.00010	-0.00006	1.86684
A67	1.85735	0.00001	-0.00005	0.00014	0.00009	1.85744
A68	2.46741	-0.00003	0.00009	-0.00050	-0.00041	2.46701
A69	1.95842	0.00002	-0.00007	0.00037	0.00031	1.95873
A70	1.98465	-0.00006	-0.00012	0.00013	0.00002	1.98466
A71	1.91732	0.00003	0.00015	-0.00003	0.00011	1.91743
A72	2.38118	0.00003	-0.00003	-0.00014	-0.00016	2.38102
A73	1.95926	0.00007	0.00012	0.00002	0.00014	1.95941
A74	2.19798	0.00000	-0.00014	0.00025	0.00013	2.19810
A75	2.12595	-0.00007	-0.00002	-0.00028	-0.00029	2.12566
A76	1.95042	-0.00011	-0.00034	0.00068	0.00035	1.95078
A77	2.08347	0.00000	0.00018	-0.00141	-0.00122	2.08225
A78	2.24927	0.00011	0.00012	0.00074	0.00087	2.25014
A79	1.57199	0.00007	0.00034	-0.00116	-0.00081	1.57118
A80	1.86172	-0.00006	-0.00023	-0.00009	-0.00030	1.86142
A81	2.21126	0.00000	-0.00101	0.00200	0.00104	2.21230
A82	2.20388	0.00007	-0.00173	0.00428	0.00260	2.20648
A83	2.34414	0.00009	-0.00025	0.00278	0.00253	2.34666
A84	1.92139	-0.00005	0.00038	-0.00213	-0.00175	1.91964
A85	2.01766	-0.00004	-0.00014	-0.00064	-0.00078	2.01688
A86	2.19328	-0.00012	0.00009	0.00122	0.00131	2.19459
A87	2.20849	0.00024	0.00001	-0.00094	-0.00092	2.20757
A88	1.88141	-0.00012	-0.00010	-0.00028	-0.00040	1.88101
A89	1.86268	0.00006	-0.00005	-0.00005	0.00003	1.86271
A90	2.22659	-0.00006	-0.00035	0.00049	0.00037	2.22697
A91	2.19389	0.00001	-0.00021	-0.00041	-0.00039	2.19350
A92	1.87042	-0.00001	-0.00004	0.00044	0.00044	1.87085
A93	2.23727	0.00060	0.00049	-0.00076	-0.00029	2.23698
A94	2.17550	-0.00059	-0.00046	0.00032	-0.00015	2.17535
A95	1.91156	0.00002	-0.00004	0.00028	0.00020	1.91176
A96	2.22880	0.00008	0.00022	-0.00046	-0.00021	2.22859
A97	2.14282	-0.00010	-0.00018	0.00018	0.00001	2.14283
A98	1.89867	0.00005	0.00012	-0.00039	-0.00025	1.89842
A99	2.30842	-0.00007	-0.00032	0.00080	0.00047	2.30889
A100	2.07610	0.00003	0.00020	-0.00041	-0.00022	2.07588
A101	2.05889	0.00007	0.00001	0.00021	0.00021	2.05910
A102	2.08929	-0.00004	0.00008	-0.00032	-0.00024	2.08905
A103	2.13501	-0.00003	-0.00009	0.00011	0.00003	2.13504
A104	2.06857	-0.00003	-0.00012	0.00022	0.00010	2.06867
A105	2.13102	0.00005	-0.00003	0.00027	0.00024	2.13126
A106	2.08359	-0.00002	0.00015	-0.00049	-0.00034	2.08325
A107	2.09505	0.00008	0.00017	-0.00023	-0.00006	2.09499
A108	2.09799	-0.00005	-0.00016	0.00029	0.00013	2.09813
A109	2.09014	-0.00003	-0.00001	-0.00006	-0.00007	2.09007
A110	2.12494	-0.00005	-0.00008	0.00003	-0.00004	2.12489
A111	2.07379	-0.00001	0.00001	-0.00001	0.00000	2.07379
A112	2.08446	0.00005	0.00007	-0.00002	0.00004	2.08450
A113	2.16635	0.00040	0.00046	-0.00088	-0.00042	2.16593
A114	2.15654	-0.00028	-0.00019	-0.00009	-0.00028	2.15626
A115	1.96029	-0.00012	-0.00027	0.00097	0.00070	1.96100
A116	2.15679	-0.00036	-0.00024	0.00063	0.00040	2.15718
A117	2.16723	0.00010	0.00010	-0.00113	-0.00103	2.16620
A118	1.95917	0.00026	0.00014	0.00050	0.00064	1.95981
A119	1.91281	-0.00008	-0.00005	-0.00015	-0.00020	1.91261
A120	1.94907	0.00001	-0.00008	0.00024	0.00016	1.94923
A121	1.90481	-0.00004	0.00004	-0.00023	-0.00019	1.90462
A122	1.90585	0.00004	0.00012	-0.00019	-0.00007	1.90578

A123	1.88605	0.00006	-0.00008	0.00034	0.00027	1.88631
A124	1.90417	0.00002	0.00005	-0.00001	0.00004	1.90421
A125	1.94931	-0.00010	0.00031	-0.00118	-0.00087	1.94844
A126	1.91259	0.00003	0.00021	-0.00067	-0.00046	1.91213
A127	1.90462	0.00004	0.00048	-0.00137	-0.00088	1.90374
A128	1.90593	0.00002	-0.00024	0.00079	0.00055	1.90648
A129	1.90403	0.00003	-0.00023	0.00087	0.00064	1.90467
A130	1.88627	-0.00002	-0.00058	0.00166	0.00108	1.88736
A131	3.16701	0.00007	0.00093	-0.00309	-0.00216	3.16485
A132	3.18209	-0.00027	0.00042	-0.00566	-0.00524	3.17684
A133	3.18240	-0.00030	0.00059	-0.00514	-0.00455	3.17786
A134	3.16520	0.00019	0.00089	-0.00207	-0.00118	3.16402
A135	3.14087	0.00004	0.00005	0.00044	0.00049	3.14136
A136	3.14165	-0.00001	-0.00004	0.00008	0.00003	3.14168
A137	3.14164	-0.00001	-0.00007	0.00042	0.00035	3.14198
A138	3.14172	0.00003	0.00055	-0.00224	-0.00169	3.14002
D1	-0.00007	-0.00012	-0.00068	0.00045	-0.00023	-0.00030
D2	-3.14045	-0.00030	-0.00181	-0.00021	-0.00201	3.14073
D3	-3.14099	-0.00020	-0.00113	-0.00029	-0.00143	3.14076
D4	0.00182	-0.00038	-0.00226	-0.00095	-0.00321	-0.00139
D5	0.00017	0.00006	0.00039	-0.00039	0.00001	0.00018
D6	-3.14091	0.00001	0.00025	-0.00102	-0.00077	3.14151
D7	3.14090	0.00016	0.00098	0.00056	0.00154	-3.14074
D8	-0.00017	0.00011	0.00083	-0.00007	0.00076	0.00059
D9	0.01189	-0.00022	-0.00490	-0.01539	-0.02028	-0.00839
D10	-3.13470	0.00013	-0.00138	-0.01402	-0.01540	3.13309
D11	-3.12891	-0.00031	-0.00543	-0.01626	-0.02170	3.13258
D12	0.00769	0.00004	-0.00192	-0.01489	-0.01681	-0.00912
D13	-0.00011	0.00011	0.00044	-0.00004	0.00040	0.00030
D14	-3.14109	-0.00001	0.00011	-0.00110	-0.00099	3.14110
D15	3.14003	0.00032	0.00179	0.00074	0.00253	-3.14062
D16	-0.00095	0.00020	0.00146	-0.00032	0.00114	0.00018
D17	-0.01467	0.00083	0.00847	0.01673	0.02519	0.01052
D18	-3.11208	-0.00084	-0.01708	-0.04681	-0.06391	3.10720
D19	3.12822	0.00064	0.00727	0.01603	0.02329	-3.13167
D20	0.03081	-0.00103	-0.01828	-0.04751	-0.06580	-0.03499
D21	0.00018	-0.00003	0.00006	-0.00041	-0.00036	-0.00017
D22	-3.14120	-0.00006	-0.00031	0.00004	-0.00027	-3.14146
D23	3.14115	0.00010	0.00040	0.00067	0.00107	-3.14096
D24	-0.00023	0.00006	0.00003	0.00113	0.00116	0.00094
D25	-0.00009	-0.00003	-0.00033	0.00047	0.00015	0.00006
D26	3.14126	0.00000	-0.00031	0.00098	0.00066	-3.14126
D27	3.14130	0.00001	0.00004	0.00002	0.00006	3.14135
D28	-0.00054	0.00003	0.00005	0.00052	0.00057	0.00003
D29	-0.00010	0.00001	0.00009	-0.00006	0.00003	-0.00006
D30	3.14100	0.00006	0.00023	0.00055	0.00078	-3.14141
D31	-3.14145	-0.00001	0.00008	-0.00056	-0.00048	3.14126
D32	-0.00035	0.00003	0.00022	0.00005	0.00027	-0.00008
D33	-0.02079	0.00073	0.01006	0.02550	0.03555	0.01477
D34	3.12969	0.00042	0.00272	0.03256	0.03526	-3.11824
D35	3.12604	0.00036	0.00637	0.02406	0.03044	-3.12671
D36	-0.00667	0.00005	-0.00097	0.03112	0.03015	0.02347
D37	0.00070	-0.00016	-0.00316	0.00321	0.00005	0.00076
D38	-3.14047	-0.00030	-0.00330	0.00203	-0.00127	3.14144
D39	3.13622	0.00028	0.00111	0.00488	0.00600	-3.14097
D40	-0.00496	0.00013	0.00097	0.00370	0.00467	-0.00029
D41	0.02179	-0.00095	-0.01136	-0.02599	-0.03733	-0.01554
D42	-3.12859	-0.00063	-0.00409	-0.03297	-0.03704	3.11755
D43	3.11809	0.00078	0.01484	0.03919	0.05398	-3.11112
D44	-0.03230	0.00109	0.02211	0.03221	0.05427	0.02197

D45	3.12927	0.00027	0.01356	-0.02657	-0.01301	3.11627
D46	0.01407	-0.00048	-0.00967	0.01449	0.00482	0.01889
D47	-0.00191	-0.00010	0.00495	-0.01830	-0.01335	-0.01526
D48	-3.11712	-0.00085	-0.01828	0.02276	0.00448	-3.11264
D49	0.01775	-0.00041	-0.01531	0.04131	0.02601	0.04376
D50	-3.11753	-0.00061	-0.01766	0.04476	0.02710	-3.09043
D51	3.13399	0.00032	0.00702	0.00185	0.00887	-3.14033
D52	-0.00129	0.00012	0.00467	0.00529	0.00996	0.00867
D53	-3.13543	-0.00008	0.00192	-0.00656	-0.00464	-3.14007
D54	0.00024	0.00011	0.00413	-0.00980	-0.00566	-0.00543
D55	3.14068	0.00001	-0.00261	0.00827	0.00565	-3.13686
D56	0.00401	0.00000	-0.00208	0.00463	0.00255	0.00657
D57	0.00437	-0.00015	-0.00458	0.01116	0.00658	0.01095
D58	-3.13229	-0.00017	-0.00405	0.00753	0.00348	-3.12881
D59	0.00829	-0.00003	0.00058	-0.00085	-0.00028	0.00801
D60	-3.12779	0.00004	0.00242	-0.00548	-0.00306	-3.13085
D61	-3.13529	-0.00001	0.00216	-0.00669	-0.00453	-3.13982
D62	0.01182	0.00006	0.00400	-0.01132	-0.00732	0.00450
D63	-0.00470	-0.00005	-0.00266	0.00601	0.00335	-0.00134
D64	3.13994	-0.00008	-0.00508	0.01497	0.00990	-3.13334
D65	-0.00053	0.00002	0.00156	-0.00614	-0.00458	-0.00511
D66	-3.13348	-0.00001	-0.00283	0.01186	0.00903	-3.12445
D67	3.13812	0.00005	0.00390	-0.01480	-0.01090	3.12722
D68	0.00517	0.00002	-0.00049	0.00321	0.00271	0.00788
D69	-0.00809	0.00012	0.00263	-0.00675	-0.00412	-0.01221
D70	3.12833	0.00013	0.00206	-0.00294	-0.00087	3.12746
D71	3.12598	0.00002	0.00012	-0.00044	-0.00032	3.12566
D72	-0.02078	0.00004	-0.00045	0.00337	0.00293	-0.01785
D73	-0.01849	-0.00012	-0.00803	0.02451	0.01649	-0.00200
D74	-3.03948	-0.00012	0.02085	-0.06042	-0.03959	-3.07907
D75	3.13042	-0.00002	-0.00557	0.01836	0.01279	-3.13997
D76	0.10943	-0.00003	0.02330	-0.06657	-0.04329	0.06614
D77	-0.01104	-0.00010	-0.00666	0.02179	0.01512	0.00409
D78	3.13842	-0.00005	-0.00193	0.00579	0.00385	-3.14091
D79	3.12460	-0.00008	-0.00365	0.00939	0.00574	3.13035
D80	-0.00913	-0.00003	0.00109	-0.00662	-0.00553	-0.01465
D81	-3.14119	0.00003	0.00367	-0.01442	-0.01076	3.13124
D82	0.00935	0.00000	-0.00087	0.00422	0.00335	0.01270
D83	0.01817	0.00013	0.00903	-0.02849	-0.01946	-0.00129
D84	3.03843	0.00015	-0.02017	0.05725	0.03707	3.07550
D85	-3.13405	0.00006	0.00263	-0.00686	-0.00424	-3.13828
D86	-0.11378	0.00008	-0.02658	0.07888	0.05229	-0.06149
D87	-3.13461	-0.00002	-0.00176	0.00823	0.00648	-3.12813
D88	0.00333	0.00004	-0.00073	0.00585	0.00513	0.00845
D89	0.01782	0.00005	0.00477	-0.01381	-0.00904	0.00877
D90	-3.12743	0.00011	0.00580	-0.01620	-0.01040	-3.13783
D91	1.51767	0.00003	-0.02069	0.06237	0.04168	1.55936
D92	-2.65118	0.00001	-0.02064	0.06214	0.04150	-2.60968
D93	-0.58890	0.00003	-0.02093	0.06296	0.04203	-0.54687
D94	-1.47968	0.00002	0.01382	-0.03925	-0.02542	-1.50510
D95	0.63465	0.00000	0.01387	-0.03948	-0.02560	0.60905
D96	2.69693	0.00002	0.01358	-0.03866	-0.02508	2.67186
D97	-0.00758	0.00002	0.00047	-0.00091	-0.00044	-0.00803
D98	3.13794	0.00001	0.00002	-0.00004	-0.00002	3.13792
D99	-3.13848	0.00003	0.00043	0.00002	0.00045	-3.13803
D100	0.00683	-0.00003	-0.00061	0.00244	0.00183	0.00865
D101	-0.01001	0.00003	-0.00012	0.00088	0.00075	-0.00926
D102	3.13893	0.00005	0.00108	-0.00342	-0.00234	3.13659
D103	0.00390	-0.00004	0.00005	-0.00262	-0.00256	0.00134
D104	-3.14052	0.00001	0.00085	-0.00446	-0.00361	3.13906

D105	-3.14069	-0.00003	0.00040	-0.00328	-0.00288	3.13961
D106	-0.00192	0.00001	0.00119	-0.00512	-0.00393	-0.00585
D107	3.13192	0.00002	-0.00083	0.00490	0.00407	3.13598
D108	-0.02288	0.00006	-0.00120	0.00679	0.00559	-0.01729
D109	-0.00580	0.00001	-0.00128	0.00576	0.00448	-0.00132
D110	3.12259	0.00005	-0.00165	0.00765	0.00600	3.12860
D111	0.01106	-0.00004	0.00082	-0.00397	-0.00315	0.00791
D112	-3.13543	-0.00005	0.00002	-0.00112	-0.00109	-3.13652
D113	-3.12095	-0.00006	0.00109	-0.00534	-0.00425	-3.12521
D114	0.01575	-0.00008	0.00029	-0.00249	-0.00219	0.01355
D115	3.12934	0.00008	0.00045	-0.00008	0.00036	3.12970
D116	0.10287	0.00001	0.02080	-0.05651	-0.03570	0.06717
D117	-0.02519	0.00012	0.00008	0.00177	0.00185	-0.02334
D118	-3.05167	0.00005	0.02044	-0.05465	-0.03421	-3.08588
D119	3.13454	-0.00002	-0.00169	0.00629	0.00460	3.13914
D120	-0.00655	0.00005	0.00061	0.00063	0.00124	-0.00531
D121	0.00004	0.00000	-0.00053	0.00215	0.00162	0.00166
D122	-3.14105	0.00006	0.00177	-0.00352	-0.00175	3.14039
D123	3.13371	0.00002	-0.00119	0.00346	0.00227	3.13598
D124	-0.01567	0.00007	0.00059	-0.00113	-0.00053	-0.01620
D125	-0.00822	-0.00002	-0.00274	0.00728	0.00454	-0.00368
D126	3.12559	0.00003	-0.00096	0.00269	0.00174	3.12733
D127	-3.13794	0.00004	0.00198	-0.00259	-0.00060	-3.13855
D128	0.00417	0.00011	0.00437	-0.00846	-0.00409	0.00008
D129	0.00869	-0.00012	-0.00118	-0.00117	-0.00235	0.00634
D130	-3.13334	0.00004	0.00447	-0.01244	-0.00797	-3.14132
D131	-3.12227	-0.00017	-0.00363	0.00510	0.00147	-3.12080
D132	0.01888	-0.00002	0.00202	-0.00618	-0.00415	0.01473
D133	0.02520	-0.00012	-0.00042	-0.00039	-0.00081	0.02439
D134	3.05231	-0.00005	-0.02056	0.05553	0.03497	3.08727
D135	-3.12674	-0.00006	0.00195	-0.00649	-0.00453	-3.13127
D136	-0.09963	0.00000	-0.01819	0.04944	0.03125	-0.06839
D137	-0.00537	0.00019	0.00446	-0.00526	-0.00079	-0.00616
D138	-3.14012	0.00010	0.00288	-0.00517	-0.00228	3.14079
D139	3.13664	0.00004	-0.00092	0.00548	0.00456	3.14121
D140	0.00190	-0.00005	-0.00250	0.00557	0.00308	0.00498
D141	0.00063	-0.00017	-0.00505	0.00786	0.00281	0.00344
D142	3.13457	-0.00006	-0.00329	0.00775	0.00446	3.13903
D143	-3.13637	-0.00011	-0.00879	-0.01483	-0.02362	3.12319
D144	0.00519	-0.00012	-0.00983	-0.01166	-0.02149	-0.01630
D145	0.01339	-0.00022	-0.01067	-0.01472	-0.02539	-0.01200
D146	-3.12823	-0.00024	-0.01171	-0.01155	-0.02326	3.13170
D147	-0.63192	0.00002	-0.01040	0.02777	0.01737	-0.61455
D148	1.48230	0.00002	-0.01034	0.02759	0.01725	1.49955
D149	-2.69417	0.00002	-0.01030	0.02757	0.01728	-2.67689
D150	2.64659	-0.00005	0.01366	-0.03903	-0.02538	2.62121
D151	-1.52238	-0.00006	0.01372	-0.03921	-0.02549	-1.54787
D152	0.58434	-0.00005	0.01375	-0.03922	-0.02547	0.55887
D153	-0.00084	-0.00015	-0.00204	0.00293	0.00089	0.00004
D154	-3.14065	-0.00009	-0.00270	0.00682	0.00412	-3.13653
D155	3.14078	-0.00013	-0.00096	-0.00038	-0.00134	3.13944
D156	0.00097	-0.00008	-0.00162	0.00351	0.00190	0.00287
D157	-3.13228	-0.00013	-0.00294	0.00311	0.00017	-3.13210
D158	0.00327	0.00009	-0.00627	0.00764	0.00138	0.00465
D159	0.00781	-0.00018	-0.00238	-0.00017	-0.00256	0.00525
D160	-3.13983	0.00004	-0.00571	0.00436	-0.00135	-3.14118
D161	3.13293	0.00008	0.00283	-0.00369	-0.00086	3.13207
D162	-0.00862	0.00001	0.00292	-0.00588	-0.00295	-0.01157
D163	-0.00714	0.00013	0.00227	-0.00037	0.00189	-0.00525
D164	3.13450	0.00006	0.00236	-0.00256	-0.00020	3.13430

D165	-0.00558	0.00016	0.00161	0.00069	0.00230	-0.00328
D166	3.13659	0.00011	0.00116	0.00018	0.00134	3.13793
D167	-3.14128	-0.00006	0.00485	-0.00374	0.00112	-3.14015
D168	0.00090	-0.00011	0.00440	-0.00425	0.00016	0.00106
D169	0.00375	-0.00003	-0.00129	0.00081	-0.00048	0.00327
D170	-3.13726	-0.00005	-0.00114	0.00046	-0.00068	-3.13794
D171	-3.13789	0.00004	-0.00138	0.00290	0.00152	-3.13637
D172	0.00429	0.00002	-0.00123	0.00255	0.00132	0.00561
D173	-0.00044	0.00000	0.00032	-0.00042	-0.00010	-0.00054
D174	3.14158	0.00005	0.00028	0.00048	0.00076	-3.14084
D175	3.14120	-0.00008	0.00043	-0.00296	-0.00253	3.13867
D176	0.00004	-0.00004	0.00040	-0.00207	-0.00167	-0.00162
D177	0.00118	-0.00008	-0.00021	-0.00093	-0.00114	0.00003
D178	-3.14091	-0.00007	-0.00034	-0.00063	-0.00097	3.14130
D179	-3.14097	-0.00003	0.00021	-0.00045	-0.00024	-3.14121
D180	0.00013	-0.00002	0.00008	-0.00015	-0.00007	0.00006
D181	3.14098	0.00008	0.00041	0.00094	0.00134	-3.14086
D182	-0.00060	0.00005	0.00037	0.00088	0.00124	0.00064
D183	0.00004	0.00002	-0.00010	0.00036	0.00027	0.00031
D184	-3.14154	0.00000	-0.00014	0.00031	0.00016	-3.14137
D185	3.14068	0.00003	-0.00017	0.00029	0.00012	3.14080
D186	-0.00052	0.00002	-0.00029	0.00066	0.00037	-0.00014
D187	-0.00027	0.00001	0.00000	-0.00010	-0.00010	-0.00038
D188	-3.14147	0.00000	-0.00013	0.00028	0.00015	-3.14132
D189	-0.00006	-0.00001	0.00004	-0.00034	-0.00030	-0.00035
D190	3.14154	-0.00001	0.00009	-0.00052	-0.00043	3.14111
D191	3.14152	0.00001	0.00008	-0.00027	-0.00019	3.14132
D192	-0.00007	0.00001	0.00013	-0.00045	-0.00033	-0.00039
D193	0.00026	0.00000	-0.00005	0.00012	0.00007	0.00033
D194	-3.14132	0.00000	-0.00011	0.00034	0.00023	-3.14109
D195	3.14147	0.00001	0.00007	-0.00025	-0.00018	3.14129
D196	-0.00011	0.00001	0.00001	-0.00003	-0.00002	-0.00013
D197	-0.00009	0.00000	0.00003	0.00010	0.00014	0.00004
D198	3.14149	0.00000	0.00009	-0.00012	-0.00003	3.14146
D199	3.14149	0.00000	-0.00001	0.00028	0.00027	-3.14143
D200	-0.00011	0.00001	0.00005	0.00006	0.00011	0.00000

Item	Value	Threshold	Converged?

Maximum Force	0.001462	0.000450	NO
RMS Force	0.000234	0.000300	YES
Maximum Displacement	0.209919	0.001800	NO
RMS Displacement	0.032181	0.001200	NO

Predicted change in Energy=-1.836706D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.803022	-0.635498	0.018072
2	6	0	-9.994925	-1.787034	0.023811
3	6	0	-10.517674	-3.071172	0.064446
4	6	0	-11.906238	-3.212342	0.100548
5	6	0	-12.726511	-2.077295	0.095317

6	6	0	-12.194044	-0.784603	0.054403
7	1	0	-9.847448	-3.924712	0.066527
8	1	0	-12.354079	-4.200784	0.133029
9	1	0	-13.805078	-2.198252	0.123922
10	1	0	-12.863218	0.064226	0.051996
11	6	0	-9.925447	0.564738	-0.028093
12	6	0	-8.570996	-1.392264	-0.019837
13	6	0	-8.539986	0.086716	-0.038490
14	6	0	-7.404284	0.866357	-0.051986
15	6	0	-6.011534	0.592406	-0.037626
16	6	0	-3.641901	-0.187219	-0.016132
17	6	0	-3.777794	1.225560	0.006215
18	16	0	-5.178210	-0.992330	-0.054346
19	6	0	-5.098068	1.662036	0.003136
20	6	0	-2.265044	-0.453943	-0.007417
21	6	0	-1.602807	0.795879	0.012923
22	7	0	-2.523843	1.818009	0.022263
23	16	0	-1.147707	-1.807310	-0.038524
24	16	0	1.149170	1.807351	0.063909
25	6	0	0.199823	-0.673119	-0.001390
26	6	0	-0.198599	0.673288	0.022680
27	6	0	1.604835	-0.795686	0.005775
28	6	0	2.266586	0.454090	0.033451
29	6	0	3.642590	0.188272	0.030956
30	6	0	3.778342	-1.223685	-0.000594
31	6	0	5.098405	-1.658078	-0.014180
32	6	0	6.011875	-0.588510	0.014896
33	16	0	5.178818	0.995182	0.049996
34	7	0	2.525414	-1.817603	0.003925
35	6	0	7.399910	-0.862836	0.006726
36	6	0	8.537766	-0.084768	0.009558
37	6	0	8.573339	1.394931	0.023530
38	6	0	9.921924	-0.565347	-0.006519
39	6	0	9.998827	1.786397	0.008080
40	6	0	10.803240	0.632725	-0.009715
41	6	0	10.525882	3.069200	0.009466
42	6	0	12.194775	0.777822	-0.026721
43	6	0	11.915262	3.206532	-0.008016
44	6	0	12.731712	2.069232	-0.025795
45	6	0	10.372909	-1.873513	-0.014922
46	6	0	9.515659	-3.016219	-0.008281
47	6	0	11.755248	-2.231562	-0.029749
48	7	0	8.837990	-3.964715	-0.003069
49	7	0	12.871980	-2.563229	-0.042037
50	6	0	-10.379776	1.872313	-0.055115
51	6	0	-11.762637	2.228912	-0.040810
52	6	0	-9.525577	3.016572	-0.099239
53	7	0	-12.879417	2.560489	-0.030687
54	7	0	-8.849719	3.965579	-0.137489
55	8	0	-7.614720	-2.159568	0.008024
56	8	0	7.620007	2.166089	0.039251
57	6	0	2.244883	-3.240249	-0.085687
58	1	0	1.317609	-3.464765	0.446026
59	1	0	2.152164	-3.569709	-1.126244
60	1	0	3.053490	-3.795258	0.394150
61	6	0	-2.243141	3.240071	0.119940
62	1	0	-2.154523	3.563569	1.162656
63	1	0	-1.313740	3.466322	-0.407176
64	1	0	-3.050364	3.796932	-0.360082
65	1	0	5.428267	-2.690176	-0.038182

66	1	0	12.861190	-0.073315	-0.041037
67	1	0	13.810882	2.187347	-0.039424
68	1	0	12.366708	4.193881	-0.008003
69	1	0	9.858286	3.924657	0.023790
70	1	0	7.565716	-1.933215	-0.006253
71	1	0	-7.573168	1.936222	-0.036543
72	1	0	-5.427675	2.694226	0.030058

Rotational constants (GHZ): 0.1750908 0.0104098 0.0098276

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6571.0788892757 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T
Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6570.9939577535 Hartrees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.24D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Initial guess from the checkpoint file: "PBDB.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000012 -0.000002 0.000073 Ang= 0.01 deg.

ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1

AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-yADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOPCl= 0 IICent= 200000004 NGrid=

0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0=

0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Integral accuracy reduced to 1.0D-05 until final iterations.

Initial convergence to 1.0D-05 achieved. Increase integral accuracy.

SCF Done: E(RB3LYP) = -3683.01985375 A.U. after 12 cycles

NFock= 12 Conv=0.72D-08 -V/T= 2.0068

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IICent= 0 IOPClX= 0 NMat=1

NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-0.000203290	-0.000170278	0.000255940
2	6	-0.000932464	-0.000045011	0.001170324

3	6	-0.000006747	0.000146443	0.000073136
4	6	0.000006927	-0.000020138	-0.000152122
5	6	0.000055752	0.000144693	0.000018781
6	6	-0.000161804	-0.000181936	-0.000226492
7	1	-0.000019640	-0.000015518	-0.000027101
8	1	-0.000014689	-0.000027367	0.000003188
9	1	-0.000010241	-0.000027182	0.000014665
10	1	0.000081379	-0.000042822	-0.000004580
11	6	-0.000234823	0.000326386	0.000002887
12	6	0.003492494	0.000579502	-0.003801084
13	6	-0.001539321	0.000082052	0.002107585
14	6	0.003349043	-0.001371557	-0.001515520
15	6	-0.001241611	0.001149853	-0.001109793
16	6	-0.000739784	-0.000348523	0.000367392
17	6	0.001592363	-0.000180203	-0.000328274
18	16	-0.000332374	0.000317597	-0.000485161
19	6	-0.000894164	0.000475869	0.000302575
20	6	-0.000620981	-0.000154396	0.000695390
21	6	0.000536220	0.000734773	-0.002001944
22	7	-0.001074154	-0.000625250	0.001098663
23	16	0.000063297	0.000137960	0.000011565
24	16	-0.000202072	-0.000124660	0.000021481
25	6	-0.000254401	0.000073521	0.000151379
26	6	0.000749513	-0.000402419	0.000121830
27	6	0.000000369	0.000139943	-0.000473267
28	6	-0.000681108	0.000183306	-0.000244640
29	6	0.000007968	-0.000534760	0.000463732
30	6	0.000021805	0.000332061	-0.000714158
31	6	0.001275100	0.000223526	-0.000152182
32	6	-0.000878089	-0.000174114	-0.000007509
33	16	0.000170565	-0.000270203	0.000125019
34	7	0.000005232	0.000575255	0.000382325
35	6	0.000810093	-0.000112049	0.000662478
36	6	0.000008850	-0.000454851	-0.000483579
37	6	-0.000632553	0.000176262	0.000287412
38	6	-0.000157373	-0.000453632	-0.000363372
39	6	0.000058899	0.000120501	-0.000142225
40	6	-0.000005313	0.000179826	0.000012447
41	6	-0.000052905	-0.000267505	-0.000103746
42	6	0.000402947	0.000131081	0.000392376
43	6	-0.000085373	-0.000057593	-0.000066989
44	6	0.000086810	-0.000187483	0.000049349
45	6	0.000358399	0.000373230	0.000345581
46	6	0.000092289	0.000387450	0.000110418
47	6	0.000131760	-0.000224842	0.000107294
48	7	0.000117627	-0.000163354	0.000084434
49	7	0.000065414	0.000072683	0.000055228
50	6	0.000138625	0.000014276	-0.000192531
51	6	-0.000008183	0.000386746	0.000010383
52	6	-0.000127386	-0.000344661	0.000346415
53	7	-0.000042028	0.000000851	-0.000034881
54	7	-0.000059643	0.000150146	-0.000214343
55	8	-0.001570255	-0.000300165	0.001798464
56	8	0.000137962	0.000332286	-0.000191869
57	6	-0.000214000	-0.000173893	0.000191810
58	1	-0.000009264	-0.000068180	-0.000023263
59	1	0.000022442	-0.000038303	-0.000054431
60	1	-0.000016523	-0.000031723	0.000035376
61	6	0.000038566	0.000373664	0.000111851
62	1	-0.000016949	0.000007673	0.000060015

63	1	-0.000063858	-0.000094384	-0.000059995
64	1	0.000022700	-0.000149118	-0.000056735
65	1	-0.000085618	-0.000046425	0.000147167
66	1	-0.000196004	-0.000072042	-0.000167342
67	1	0.000014025	0.000032867	0.000007483
68	1	-0.000014931	0.000039103	-0.000018373
69	1	0.000012707	-0.000010972	0.000017017
70	1	-0.000148094	-0.000207551	0.000147495
71	1	-0.000214688	-0.000232045	0.000745641
72	1	-0.000165443	0.000005723	0.000303511

Cartesian Forces: Max 0.003801084 RMS 0.000634423

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.002077557 RMS 0.000338539

Search for a local minimum.

Step number 23 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 16 18 19 20 21
22 23

DE= 1.10D-04 DEPred=-1.84D-04 R=-6.00D-01

Trust test=-6.00D-01 RLast= 2.31D-01 DXMaxT set to 2.77D-01

ITU= -1 1 1 -1 0 -1 0 -1 1 1 1 1 1 0 0 0 1 0 0

ITU= 0 1 0

Eigenvalues ---	0.00138	0.00238	0.00260	0.00276	0.00373
Eigenvalues ---	0.00387	0.00448	0.00480	0.00502	0.00534
Eigenvalues ---	0.00564	0.00578	0.00600	0.00618	0.00634
Eigenvalues ---	0.00668	0.00678	0.00696	0.00717	0.00744
Eigenvalues ---	0.00748	0.00759	0.00769	0.00775	0.00786
Eigenvalues ---	0.00802	0.00820	0.00829	0.00967	0.01083
Eigenvalues ---	0.01121	0.01131	0.01149	0.01169	0.01245
Eigenvalues ---	0.01316	0.01325	0.01355	0.01361	0.01380
Eigenvalues ---	0.01457	0.01462	0.01546	0.01606	0.01646
Eigenvalues ---	0.01743	0.01746	0.01767	0.01794	0.01929
Eigenvalues ---	0.01953	0.02006	0.02021	0.02065	0.02074
Eigenvalues ---	0.02193	0.02200	0.02437	0.03507	0.03744
Eigenvalues ---	0.03956	0.04829	0.04838	0.04906	0.04980
Eigenvalues ---	0.04991	0.05019	0.05102	0.05326	0.07059
Eigenvalues ---	0.07231	0.07393	0.07565	0.15357	0.15696
Eigenvalues ---	0.15935	0.15986	0.15999	0.16000	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16001
Eigenvalues ---	0.16001	0.16003	0.16009	0.16024	0.16042
Eigenvalues ---	0.16066	0.18416	0.18993	0.19461	0.19826
Eigenvalues ---	0.20646	0.21264	0.21386	0.21713	0.21995
Eigenvalues ---	0.22014	0.22098	0.22440	0.22569	0.22626
Eigenvalues ---	0.22642	0.22682	0.22826	0.23031	0.23185
Eigenvalues ---	0.23358	0.23496	0.23740	0.23874	0.24012
Eigenvalues ---	0.24159	0.24216	0.24298	0.24339	0.24531
Eigenvalues ---	0.24586	0.24632	0.24741	0.24860	0.24871
Eigenvalues ---	0.24904	0.24953	0.24966	0.24989	0.24991
Eigenvalues ---	0.24995	0.24997	0.24998	0.24999	0.24999
Eigenvalues ---	0.25000	0.25000	0.25000	0.25001	0.25011
Eigenvalues ---	0.25027	0.25168	0.25564	0.25625	0.25960
Eigenvalues ---	0.26227	0.26537	0.26783	0.26825	0.27085

```

Eigenvalues ---      0.27229    0.27700    0.27846    0.28265    0.28435
Eigenvalues ---      0.28532    0.28754    0.29887    0.30222    0.31820
Eigenvalues ---      0.32401    0.34328    0.35366    0.35984    0.36279
Eigenvalues ---      0.36338    0.36474    0.36602    0.36649    0.36779
Eigenvalues ---      0.36827    0.37002    0.37069    0.37090    0.37175
Eigenvalues ---      0.37253    0.37268    0.37419    0.37567    0.37674
Eigenvalues ---      0.37758    0.37973    0.38926    0.40307    0.40664
Eigenvalues ---      0.41621    0.42048    0.42643    0.44424    0.44695
Eigenvalues ---      0.45251    0.45663    0.46482    0.47791    0.47841
Eigenvalues ---      0.48118    0.52144    0.53325    0.55356    0.57082
Eigenvalues ---      0.59306    0.68376    0.73279    0.80245    0.81968
Eigenvalues ---      0.90945    1.25843    1.26321    1.29349    1.35390
En-DIIS/RFO-DIIS IScMMF=          0 using points:      23      22      21      20      19
RFO step:  Lambda=-1.28126372D-04.
DidBck=T Rises=F RFO-DIIS coefs:      0.27815      0.33091      0.14970      0.06363
0.17762
Iteration  1 RMS(Cart)=  0.04479056 RMS(Int)=  0.00032570
Iteration  2 RMS(Cart)=  0.00096638 RMS(Int)=  0.00010179
Iteration  3 RMS(Cart)=  0.00000023 RMS(Int)=  0.00010179
Variable      Old X      -DE/DX      Delta X      Delta X      Delta X      New X
(Linear)      (Quad)      (Total)
R1      2.65847    -0.00004    -0.00012    0.00013    0.00000    2.65847
R2      2.64460    -0.00002     0.00008   -0.00002    0.00006    2.64466
R3      2.81108    -0.00035    -0.00040    0.00039    0.00000    2.81108
R4      2.62116     0.00013     0.00016    0.00001    0.00017    2.62133
R5      2.79355     0.00022     0.00008    0.00048    0.00054    2.79409
R6      2.63841     0.00009    -0.00001    0.00001    0.00000    2.63841
R7      2.05080    -0.00003    -0.00005     0.00000   -0.00005    2.05075
R8      2.64643    -0.00002    -0.00017     0.00012   -0.00005    2.64638
R9      2.05158    -0.00003     0.00000   -0.00004   -0.00004    2.05154
R10     2.64308     0.00006     0.00012   -0.00005     0.00007    2.64315
R11     2.05169    -0.00002    -0.00004     0.00001   -0.00003    2.05166
R12     2.04258    -0.00005    -0.00027     0.00007   -0.00021    2.04237
R13     2.76967     0.00054     0.00076   -0.00028     0.00051    2.77017
R14     2.61637    -0.00001     0.00024   -0.00035   -0.00011    2.61626
R15     2.79570     0.00036     0.00011     0.00055     0.00067    2.79637
R16     2.31751    -0.00019    -0.00034     0.00023   -0.00011    2.31740
R17     2.60333     0.00084    -0.00028     0.00202     0.00174    2.60507
R18     2.68248    -0.00208    -0.00455     0.00280   -0.00175    2.68073
R19     2.04699    -0.00011    -0.00017     0.00025     0.00008    2.04707
R20     3.38366    -0.00038    -0.00033     0.00016   -0.00014    3.38352
R21     2.65921    -0.00006     0.00008   -0.00014   -0.00005    2.65915
R22     2.68242    -0.00025    -0.00070     0.00017   -0.00050    2.68192
R23     3.27850     0.00049     0.00038     0.00094     0.00133    3.27983
R24     2.65031     0.00024     0.00006     0.00096     0.00120    2.65150
R25     2.62777     0.00081     0.00160   -0.00081     0.00077    2.62854
R26     2.62097     0.00021     0.00092   -0.00030     0.00048    2.62144
R27     2.04822    -0.00008     0.00001   -0.00007   -0.00006    2.04816
R28     2.67316     0.00010    -0.00008   -0.00011   -0.00016    2.67300
R29     3.31700     0.00022     0.00022     0.00025     0.00047    3.31747
R30     2.60010     0.00016     0.00118   -0.00053     0.00051    2.60061
R31     2.66373     0.00112     0.00204   -0.00050     0.00152    2.66525
R32     2.74537    -0.00014    -0.00095     0.00070   -0.00025    2.74512
R33     3.32914     0.00020     0.00026     0.00021     0.00050    3.32964
R34     3.32950     0.00017     0.00024     0.00001     0.00026    3.32976
R35     3.31692     0.00026     0.00050   -0.00009     0.00042    3.31734
R36     2.65379     0.00017    -0.00018     0.00014   -0.00003    2.65377
R37     2.66521     0.00052     0.00013     0.00140     0.00152    2.66673
R38     2.67289     0.00023    -0.00008   -0.00008   -0.00014    2.67275
R39     2.59917     0.00069     0.00184   -0.00089     0.00088    2.60005

```

R40	2.64835	0.00111	0.00314	-0.00219	0.00104	2.64939
R41	2.68118	0.00037	-0.00001	-0.00013	-0.00013	2.68105
R42	3.27935	0.00031	0.00048	0.00006	0.00054	3.27989
R43	2.62628	0.00143	0.00255	-0.00098	0.00156	2.62784
R44	2.62024	0.00062	0.00183	-0.00111	0.00064	2.62088
R45	2.65858	0.00060	0.00063	-0.00038	0.00025	2.65882
R46	2.04807	0.00001	0.00002	-0.00004	-0.00002	2.04805
R47	3.38218	0.00016	0.00039	-0.00006	0.00034	3.38252
R48	2.67379	0.00128	0.00309	-0.00068	0.00240	2.67619
R49	2.74541	-0.00027	-0.00055	0.00028	-0.00027	2.74514
R50	2.60489	0.00015	-0.00017	0.00063	0.00045	2.60534
R51	2.04699	-0.00014	-0.00016	0.00022	0.00006	2.04706
R52	2.79716	-0.00031	-0.00065	0.00074	0.00008	2.79724
R53	2.76902	0.00068	0.00038	0.00081	0.00120	2.77022
R54	2.79367	0.00014	0.00006	0.00037	0.00042	2.79408
R55	2.31734	0.00000	-0.00021	0.00020	-0.00001	2.31733
R56	2.81062	0.00006	-0.00046	0.00071	0.00027	2.81089
R57	2.61490	0.00111	0.00059	0.00023	0.00082	2.61572
R58	2.65797	0.00026	0.00004	0.00006	0.00011	2.65808
R59	2.62078	0.00028	0.00048	0.00009	0.00056	2.62134
R60	2.64407	0.00025	-0.00018	0.00100	0.00082	2.64489
R61	2.63855	0.00004	-0.00017	0.00002	-0.00016	2.63839
R62	2.05076	-0.00002	-0.00001	-0.00003	-0.00004	2.05072
R63	2.64294	0.00019	0.00013	-0.00012	0.00001	2.64296
R64	2.04296	-0.00027	-0.00049	0.00010	-0.00039	2.04257
R65	2.64586	0.00018	0.00027	0.00010	0.00037	2.64623
R66	2.05160	-0.00003	0.00000	-0.00006	-0.00006	2.05155
R67	2.05168	-0.00001	-0.00003	0.00001	-0.00002	2.05166
R68	2.69953	0.00022	-0.00009	0.00065	0.00056	2.70010
R69	2.69859	0.00029	-0.00075	0.00190	0.00116	2.69975
R70	2.20290	-0.00016	-0.00007	-0.00003	-0.00010	2.20279
R71	2.20155	0.00005	0.00000	0.00003	0.00003	2.20158
R72	2.69885	0.00020	-0.00020	0.00091	0.00071	2.69956
R73	2.69969	0.00018	0.00011	0.00024	0.00035	2.70004
R74	2.20154	0.00005	0.00002	0.00001	0.00003	2.20157
R75	2.20286	-0.00014	-0.00005	-0.00001	-0.00006	2.20280
R76	2.06401	-0.00003	-0.00009	0.00003	-0.00006	2.06395
R77	2.07001	-0.00006	0.00013	-0.00018	-0.00004	2.06996
R78	2.06329	-0.00001	0.00004	-0.00005	-0.00001	2.06328
R79	2.06989	-0.00006	0.00037	-0.00039	-0.00001	2.06987
R80	2.06389	0.00002	0.00003	-0.00007	-0.00004	2.06386
R81	2.06329	-0.00001	0.00014	-0.00015	-0.00001	2.06327
A1	2.07561	0.00018	0.00041	-0.00027	0.00013	2.07574
A2	1.89832	0.00022	0.00025	-0.00010	0.00020	1.89851
A3	2.30926	-0.00041	-0.00066	0.00036	-0.00033	2.30894
A4	2.14295	-0.00013	-0.00035	0.00021	-0.00014	2.14281
A5	1.91197	-0.00008	-0.00007	-0.00011	-0.00017	1.91180
A6	2.22827	0.00022	0.00042	-0.00010	0.00031	2.22857
A7	2.05916	-0.00002	0.00001	-0.00002	-0.00001	2.05915
A8	2.08914	0.00000	0.00022	-0.00013	0.00008	2.08922
A9	2.13488	0.00002	-0.00022	0.00016	-0.00007	2.13481
A10	2.09495	0.00007	0.00027	-0.00014	0.00012	2.09508
A11	2.09797	-0.00003	-0.00021	0.00012	-0.00009	2.09787
A12	2.09027	-0.00004	-0.00005	0.00002	-0.00003	2.09024
A13	2.12494	-0.00004	-0.00015	0.00009	-0.00006	2.12488
A14	2.08459	0.00004	0.00008	0.00002	0.00010	2.08469
A15	2.07366	0.00000	0.00007	-0.00011	-0.00003	2.07362
A16	2.06876	-0.00007	-0.00018	0.00013	-0.00004	2.06872
A17	2.13133	-0.00003	-0.00003	0.00002	-0.00001	2.13132
A18	2.08310	0.00009	0.00020	-0.00015	0.00005	2.08315

A19	1.86997	0.00008	-0.00004	0.00023	0.00027	1.87024
A20	2.17611	-0.00108	-0.00082	0.00070	-0.00016	2.17596
A21	2.23710	0.00101	0.00085	-0.00093	-0.00011	2.23699
A22	1.86244	0.00006	0.00012	-0.00002	0.00022	1.86266
A23	2.19362	0.00012	-0.00018	0.00073	0.00062	2.19424
A24	2.22613	-0.00011	0.00044	-0.00040	0.00011	2.22624
A25	1.88194	-0.00027	-0.00027	-0.00023	-0.00042	1.88152
A26	2.20779	0.00076	0.00004	0.00046	0.00047	2.20826
A27	2.19342	-0.00049	0.00023	-0.00021	-0.00001	2.19341
A28	2.34554	-0.00069	-0.00048	-0.00061	-0.00120	2.34434
A29	2.01560	0.00069	0.00072	0.00085	0.00145	2.01705
A30	1.92137	0.00003	0.00008	0.00044	0.00040	1.92177
A31	2.24893	-0.00019	0.00075	-0.00084	-0.00010	2.24883
A32	2.08346	0.00022	-0.00025	0.00064	0.00037	2.08384
A33	1.95078	-0.00003	-0.00049	0.00024	-0.00025	1.95052
A34	1.95783	0.00009	0.00036	0.00003	0.00034	1.95817
A35	1.85789	-0.00011	-0.00009	-0.00031	-0.00033	1.85756
A36	2.46743	0.00002	-0.00025	0.00028	0.00002	2.46745
A37	1.98588	-0.00037	-0.00081	-0.00001	-0.00075	1.98513
A38	1.91641	0.00022	0.00073	-0.00008	0.00043	1.91684
A39	2.38089	0.00015	0.00005	0.00009	0.00031	2.38121
A40	1.57199	0.00010	0.00034	-0.00046	-0.00009	1.57191
A41	1.95822	0.00021	0.00061	0.00023	0.00082	1.95904
A42	2.12608	-0.00011	-0.00002	-0.00022	-0.00020	2.12588
A43	2.19888	-0.00010	-0.00065	0.00000	-0.00061	2.19827
A44	1.86676	0.00007	0.00004	-0.00004	0.00009	1.86685
A45	2.45191	-0.00002	-0.00014	0.00000	-0.00010	2.45181
A46	1.96435	-0.00004	0.00018	-0.00003	0.00011	1.96446
A47	1.92098	-0.00004	0.00027	-0.00007	0.00000	1.92098
A48	1.97102	-0.00010	-0.00053	0.00026	-0.00018	1.97084
A49	2.39118	0.00014	0.00017	-0.00020	0.00018	2.39135
A50	1.86273	-0.00013	-0.00127	0.00049	-0.00026	1.86247
A51	2.20631	0.00003	-0.00392	0.00196	-0.00078	2.20553
A52	2.21215	0.00009	-0.00161	0.00019	-0.00022	2.21193
A53	1.56094	0.00027	0.00036	-0.00022	0.00016	1.56110
A54	1.56112	0.00016	-0.00011	0.00035	0.00024	1.56136
A55	1.98297	-0.00011	-0.00022	0.00013	-0.00008	1.98289
A56	2.35485	0.00008	-0.00005	0.00014	0.00010	2.35495
A57	1.94536	0.00003	0.00027	-0.00026	-0.00002	1.94534
A58	2.35494	0.00009	-0.00016	0.00017	0.00004	2.35498
A59	1.94539	-0.00002	0.00022	-0.00015	0.00003	1.94542
A60	1.98285	-0.00007	-0.00006	-0.00002	-0.00006	1.98279
A61	1.97077	-0.00003	-0.00019	-0.00001	-0.00015	1.97061
A62	2.39106	0.00015	0.00026	-0.00015	0.00020	2.39126
A63	1.92131	-0.00012	-0.00008	0.00018	-0.00003	1.92128
A64	1.96462	-0.00009	0.00007	-0.00005	0.00000	1.96463
A65	2.45172	0.00008	-0.00016	0.00006	-0.00009	2.45163
A66	1.86684	0.00001	0.00007	-0.00001	0.00008	1.86692
A67	1.85744	0.00005	-0.00010	0.00009	0.00001	1.85745
A68	2.46701	0.00012	0.00035	-0.00027	0.00009	2.46710
A69	1.95873	-0.00018	-0.00027	0.00018	-0.00010	1.95863
A70	1.98466	-0.00004	-0.00009	-0.00004	-0.00009	1.98457
A71	1.91743	-0.00018	0.00002	0.00020	0.00009	1.91752
A72	2.38102	0.00023	0.00009	-0.00015	0.00004	2.38106
A73	1.95941	-0.00009	-0.00002	0.00009	0.00006	1.95946
A74	2.19810	0.00008	-0.00018	0.00004	-0.00012	2.19798
A75	2.12566	0.00001	0.00019	-0.00014	0.00008	2.12574
A76	1.95078	-0.00018	-0.00048	0.00023	-0.00024	1.95053
A77	2.08225	0.00093	0.00100	-0.00054	0.00046	2.08272
A78	2.25014	-0.00075	-0.00055	0.00033	-0.00021	2.24994

A79	1.57118	0.00049	0.00081	-0.00045	0.00038	1.57156
A80	1.86142	0.00025	0.00006	-0.00029	-0.00002	1.86141
A81	2.21230	-0.00008	-0.00144	0.00059	-0.00028	2.21202
A82	2.20648	-0.00016	-0.00305	0.00168	-0.00081	2.20567
A83	2.34666	-0.00139	-0.00199	0.00099	-0.00100	2.34566
A84	1.91964	0.00081	0.00152	-0.00078	0.00074	1.92038
A85	2.01688	0.00058	0.00048	-0.00021	0.00027	2.01714
A86	2.19459	-0.00133	-0.00089	0.00052	-0.00036	2.19424
A87	2.20757	0.00112	0.00067	-0.00029	0.00040	2.20797
A88	1.88101	0.00021	0.00022	-0.00025	-0.00004	1.88097
A89	1.86271	0.00000	-0.00005	0.00002	0.00005	1.86276
A90	2.22697	-0.00035	-0.00050	0.00009	-0.00026	2.22670
A91	2.19350	0.00035	0.00014	-0.00007	0.00022	2.19372
A92	1.87085	-0.00033	-0.00034	0.00009	-0.00023	1.87062
A93	2.23698	0.00093	0.00053	-0.00052	0.00000	2.23698
A94	2.17535	-0.00061	-0.00019	0.00042	0.00023	2.17558
A95	1.91176	-0.00002	-0.00017	0.00027	0.00008	1.91184
A96	2.22859	0.00007	0.00030	-0.00029	0.00003	2.22862
A97	2.14283	-0.00004	-0.00013	0.00001	-0.00011	2.14273
A98	1.89842	0.00014	0.00026	-0.00011	0.00016	1.89858
A99	2.30889	-0.00014	-0.00055	0.00046	-0.00009	2.30879
A100	2.07588	0.00000	0.00029	-0.00035	-0.00007	2.07581
A101	2.05910	0.00000	-0.00015	0.00024	0.00009	2.05919
A102	2.08905	0.00001	0.00022	-0.00022	0.00001	2.08906
A103	2.13504	-0.00002	-0.00008	-0.00003	-0.00010	2.13493
A104	2.06867	-0.00002	-0.00015	0.00019	0.00004	2.06871
A105	2.13126	0.00002	-0.00019	0.00020	0.00001	2.13127
A106	2.08325	0.00001	0.00034	-0.00039	-0.00004	2.08321
A107	2.09499	0.00006	0.00016	-0.00003	0.00013	2.09512
A108	2.09813	-0.00006	-0.00020	0.00011	-0.00009	2.09803
A109	2.09007	0.00000	0.00004	-0.00008	-0.00003	2.09003
A110	2.12489	0.00000	-0.00002	-0.00006	-0.00008	2.12482
A111	2.07379	-0.00003	0.00000	-0.00002	-0.00001	2.07378
A112	2.08450	0.00003	0.00002	0.00008	0.00009	2.08459
A113	2.16593	0.00070	0.00061	-0.00014	0.00046	2.16639
A114	2.15626	-0.00030	0.00009	0.00074	0.00083	2.15709
A115	1.96100	-0.00040	-0.00070	-0.00060	-0.00129	1.95971
A116	2.15718	-0.00078	-0.00043	0.00064	0.00021	2.15739
A117	2.16620	0.00068	0.00081	-0.00059	0.00022	2.16642
A118	1.95981	0.00010	-0.00038	-0.00006	-0.00043	1.95937
A119	1.91261	-0.00008	0.00011	-0.00029	-0.00018	1.91243
A120	1.94923	-0.00003	-0.00017	0.00019	0.00002	1.94925
A121	1.90462	0.00000	0.00017	-0.00022	-0.00006	1.90456
A122	1.90578	0.00005	0.00013	-0.00002	0.00011	1.90589
A123	1.88631	0.00005	-0.00024	0.00037	0.00012	1.88644
A124	1.90421	0.00001	0.00000	-0.00001	-0.00001	1.90420
A125	1.94844	-0.00008	0.00083	-0.00088	-0.00005	1.94839
A126	1.91213	0.00015	0.00048	-0.00023	0.00024	1.91238
A127	1.90374	0.00022	0.00096	-0.00057	0.00039	1.90413
A128	1.90648	-0.00006	-0.00056	0.00040	-0.00016	1.90633
A129	1.90467	-0.00008	-0.00061	0.00050	-0.00011	1.90456
A130	1.88736	-0.00015	-0.00117	0.00085	-0.00032	1.88703
A131	3.16485	0.00033	0.00218	-0.00116	0.00102	3.16586
A132	3.17684	0.00021	0.00407	-0.00346	0.00061	3.17746
A133	3.17786	0.00004	0.00370	-0.00372	-0.00002	3.17784
A134	3.16402	0.00040	0.00145	0.00045	0.00190	3.16593
A135	3.14136	-0.00002	-0.00032	0.00041	0.00010	3.14145
A136	3.14168	-0.00001	-0.00005	0.00000	-0.00005	3.14163
A137	3.14198	0.00000	-0.00030	0.00025	-0.00006	3.14192
A138	3.14002	0.00032	0.00160	-0.00051	0.00108	3.14111

D1	-0.00030	0.00015	-0.00030	0.00096	0.00067	0.00037
D2	3.14073	0.00024	0.00022	0.00115	0.00137	-3.14109
D3	3.14076	0.00025	0.00026	0.00125	0.00151	-3.14091
D4	-0.00139	0.00034	0.00077	0.00144	0.00221	0.00082
D5	0.00018	-0.00006	0.00026	-0.00062	-0.00036	-0.00019
D6	3.14151	-0.00002	0.00073	-0.00073	-0.00001	3.14151
D7	-3.14074	-0.00020	-0.00045	-0.00099	-0.00144	3.14100
D8	0.00059	-0.00015	0.00002	-0.00110	-0.00108	-0.00049
D9	-0.00839	-0.00001	0.01128	-0.00922	0.00206	-0.00633
D10	3.13309	-0.00017	0.01015	-0.00834	0.00181	3.13490
D11	3.13258	0.00012	0.01194	-0.00888	0.00305	3.13564
D12	-0.00912	-0.00004	0.01081	-0.00801	0.00280	-0.00632
D13	0.00030	-0.00013	0.00001	-0.00055	-0.00054	-0.00024
D14	3.14110	-0.00002	0.00079	-0.00059	0.00019	3.14130
D15	-3.14062	-0.00024	-0.00060	-0.00078	-0.00138	3.14118
D16	0.00018	-0.00012	0.00017	-0.00082	-0.00064	-0.00046
D17	0.01052	-0.00054	-0.01239	0.00681	-0.00558	0.00494
D18	3.10720	0.00107	0.03448	0.01399	0.04849	-3.12750
D19	-3.13167	-0.00045	-0.01184	0.00701	-0.00483	-3.13650
D20	-0.03499	0.00117	0.03503	0.01419	0.04924	0.01424
D21	-0.00017	0.00004	0.00030	-0.00018	0.00012	-0.00005
D22	-3.14146	0.00005	-0.00002	0.00009	0.00008	-3.14139
D23	-3.14096	-0.00008	-0.00050	-0.00013	-0.00063	-3.14159
D24	0.00094	-0.00007	-0.00082	0.00014	-0.00068	0.00026
D25	0.00006	0.00004	-0.00033	0.00049	0.00016	0.00022
D26	-3.14126	-0.00001	-0.00069	0.00050	-0.00019	-3.14145
D27	3.14135	0.00003	-0.00001	0.00022	0.00021	3.14156
D28	0.00003	-0.00002	-0.00038	0.00023	-0.00015	-0.00011
D29	-0.00006	-0.00003	0.00004	-0.00007	-0.00004	-0.00010
D30	-3.14141	-0.00007	-0.00041	0.00003	-0.00038	3.14140
D31	3.14126	0.00002	0.00040	-0.00009	0.00032	3.14157
D32	-0.00008	-0.00002	-0.00005	0.00002	-0.00003	-0.00012
D33	0.01477	-0.00033	-0.01878	0.01330	-0.00548	0.00929
D34	-3.11824	-0.00036	-0.02357	0.00971	-0.01385	-3.13209
D35	-3.12671	-0.00016	-0.01759	0.01238	-0.00521	-3.13192
D36	0.02347	-0.00019	-0.02239	0.00879	-0.01359	0.00988
D37	0.00076	0.00012	-0.00219	0.00225	0.00006	0.00081
D38	3.14144	0.00023	-0.00134	0.00179	0.00045	-3.14130
D39	-3.14097	-0.00008	-0.00356	0.00331	-0.00025	-3.14122
D40	-0.00029	0.00003	-0.00272	0.00285	0.00014	-0.00014
D41	-0.01554	0.00053	0.01918	-0.01242	0.00675	-0.00879
D42	3.11755	0.00057	0.02392	-0.00887	0.01504	3.13260
D43	-3.11112	-0.00113	-0.02885	-0.01982	-0.04863	3.12343
D44	0.02197	-0.00109	-0.02410	-0.01626	-0.04034	-0.01837
D45	3.11627	0.00034	0.01859	0.00478	0.02338	3.13965
D46	0.01889	-0.00068	-0.01009	-0.01771	-0.02781	-0.00892
D47	-0.01526	0.00030	0.01297	0.00058	0.01356	-0.00170
D48	-3.11264	-0.00072	-0.01571	-0.02192	-0.03762	3.13292
D49	0.04376	-0.00080	-0.02934	-0.02442	-0.05376	-0.01000
D50	-3.09043	-0.00123	-0.03175	-0.03211	-0.06385	3.12891
D51	-3.14033	0.00019	-0.00176	-0.00279	-0.00456	3.13829
D52	0.00867	-0.00023	-0.00417	-0.01048	-0.01466	-0.00599
D53	-3.14007	-0.00021	0.00465	-0.00807	-0.00342	3.13970
D54	-0.00543	0.00019	0.00691	-0.00085	0.00605	0.00063
D55	-3.13686	0.00005	-0.00586	0.00534	-0.00052	-3.13738
D56	0.00657	0.00006	-0.00326	0.00258	-0.00067	0.00590
D57	0.01095	-0.00030	-0.00788	-0.00111	-0.00899	0.00196
D58	-3.12881	-0.00030	-0.00528	-0.00386	-0.00914	-3.13795
D59	0.00801	-0.00015	0.00058	-0.00378	-0.00320	0.00482
D60	-3.13085	0.00003	0.00385	-0.00445	-0.00061	-3.13146

D61	-3.13982	-0.00001	0.00474	-0.00274	0.00200	-3.13782
D62	0.00450	0.00017	0.00801	-0.00341	0.00459	0.00909
D63	-0.00134	-0.00003	-0.00423	0.00256	-0.00166	-0.00301
D64	-3.13334	-0.00024	-0.01062	0.00097	-0.00965	3.14019
D65	-0.00511	0.00014	0.00438	-0.00144	0.00293	-0.00218
D66	-3.12445	-0.00016	-0.00846	0.00282	-0.00563	-3.13008
D67	3.12722	0.00035	0.01055	0.00010	0.01064	3.13786
D68	0.00788	0.00004	-0.00229	0.00435	0.00207	0.00996
D69	-0.01221	0.00029	0.00478	0.00311	0.00789	-0.00432
D70	3.12746	0.00029	0.00204	0.00600	0.00804	3.13551
D71	3.12566	0.00005	0.00032	0.00402	0.00435	3.13002
D72	-0.01785	0.00004	-0.00242	0.00692	0.00451	-0.01334
D73	-0.00200	-0.00042	-0.01739	0.00698	-0.01040	-0.01241
D74	-3.07907	-0.00019	0.04277	-0.03544	0.00740	-3.07167
D75	-3.13997	-0.00018	-0.01304	0.00609	-0.00696	3.13625
D76	0.06614	0.00005	0.04712	-0.03633	0.01084	0.07698
D77	0.00409	-0.00041	-0.01547	0.00588	-0.00958	-0.00549
D78	-3.14091	-0.00014	-0.00410	0.00157	-0.00249	3.13978
D79	3.13035	-0.00020	-0.00663	0.00295	-0.00368	3.12667
D80	-0.01465	0.00007	0.00475	-0.00136	0.00341	-0.01125
D81	3.13124	0.00026	0.01028	-0.00465	0.00560	3.13684
D82	0.01270	-0.00006	-0.00302	-0.00024	-0.00326	0.00943
D83	-0.00129	0.00051	0.02022	-0.00792	0.01230	0.01101
D84	3.07550	0.00028	-0.04049	0.03477	-0.00562	3.06988
D85	-3.13828	0.00015	0.00485	-0.00211	0.00273	-3.13555
D86	-0.06149	-0.00009	-0.05586	0.04058	-0.01519	-0.07668
D87	-3.12813	-0.00019	-0.00588	0.00171	-0.00418	-3.13231
D88	0.00845	-0.00004	-0.00421	0.00269	-0.00154	0.00691
D89	0.00877	0.00018	0.00979	-0.00422	0.00558	0.01435
D90	-3.13783	0.00033	0.01146	-0.00324	0.00822	-3.12961
D91	1.55936	-0.00012	-0.04418	0.03318	-0.01105	1.54831
D92	-2.60968	-0.00015	-0.04402	0.03294	-0.01112	-2.62080
D93	-0.54687	-0.00011	-0.04459	0.03350	-0.01114	-0.55801
D94	-1.50510	0.00016	0.02777	-0.01757	0.01025	-1.49485
D95	0.60905	0.00013	0.02794	-0.01781	0.01018	0.61923
D96	2.67186	0.00017	0.02736	-0.01725	0.01016	2.68202
D97	-0.00803	0.00003	0.00064	0.00179	0.00243	-0.00559
D98	3.13792	-0.00004	0.00003	0.00003	0.00006	3.13798
D99	-3.13803	0.00001	-0.00004	0.00098	0.00093	-3.13710
D100	0.00865	-0.00014	-0.00174	-0.00001	-0.00176	0.00690
D101	-0.00926	0.00008	-0.00063	0.00082	0.00019	-0.00907
D102	3.13659	0.00012	0.00243	0.00135	0.00379	3.14038
D103	0.00134	0.00000	0.00190	-0.00289	-0.00098	0.00035
D104	3.13906	0.00011	0.00319	-0.00213	0.00106	3.14012
D105	3.13961	0.00006	0.00236	-0.00154	0.00082	3.14044
D106	-0.00585	0.00017	0.00365	-0.00079	0.00286	-0.00299
D107	3.13598	-0.00003	-0.00351	0.00315	-0.00036	3.13562
D108	-0.01729	0.00006	-0.00486	0.00643	0.00157	-0.01572
D109	-0.00132	-0.00011	-0.00411	0.00141	-0.00270	-0.00401
D110	3.12860	-0.00001	-0.00546	0.00469	-0.00077	3.12783
D111	0.00791	0.00000	0.00284	-0.00144	0.00139	0.00930
D112	-3.13652	-0.00003	0.00081	-0.00180	-0.00100	-3.13752
D113	-3.12521	-0.00007	0.00382	-0.00382	-0.00001	-3.12521
D114	0.01355	-0.00010	0.00178	-0.00418	-0.00240	0.01115
D115	3.12970	0.00012	0.00004	0.00296	0.00301	3.13271
D116	0.06717	0.00012	0.03993	-0.02333	0.01655	0.08372
D117	-0.02334	0.00021	-0.00128	0.00618	0.00490	-0.01844
D118	-3.08588	0.00022	0.03861	-0.02011	0.01844	-3.06744
D119	3.13914	-0.00010	-0.00448	-0.00003	-0.00451	3.13463
D120	-0.00531	0.00001	-0.00049	0.00023	-0.00026	-0.00558

D121	0.00166	-0.00006	-0.00153	0.00048	-0.00104	0.00062
D122	3.14039	0.00006	0.00247	0.00074	0.00321	-3.13959
D123	3.13598	0.00007	-0.00245	0.00290	0.00045	3.13643
D124	-0.01620	0.00020	0.00078	0.00333	0.00412	-0.01208
D125	-0.00368	-0.00001	-0.00514	0.00272	-0.00242	-0.00609
D126	3.12733	0.00012	-0.00191	0.00315	0.00125	3.12858
D127	-3.13855	-0.00004	0.00177	-0.00124	0.00052	-3.13803
D128	0.00008	0.00008	0.00590	-0.00098	0.00492	0.00500
D129	0.00634	-0.00009	0.00091	-0.00344	-0.00252	0.00382
D130	-3.14132	0.00011	0.00878	-0.00477	0.00402	-3.13730
D131	-3.12080	-0.00026	-0.00350	-0.00403	-0.00753	-3.12833
D132	0.01473	-0.00005	0.00437	-0.00536	-0.00099	0.01374
D133	0.02439	-0.00025	0.00030	-0.00586	-0.00557	0.01883
D134	3.08727	-0.00025	-0.03924	0.02025	-0.01901	3.06826
D135	-3.13127	-0.00009	0.00459	-0.00529	-0.00069	-3.13196
D136	-0.06839	-0.00009	-0.03494	0.02082	-0.01414	-0.08252
D137	-0.00616	0.00015	0.00358	0.00263	0.00620	0.00004
D138	3.14079	0.00001	0.00359	-0.00190	0.00169	-3.14070
D139	3.14121	-0.00005	-0.00392	0.00390	-0.00003	3.14118
D140	0.00498	-0.00019	-0.00391	-0.00063	-0.00454	0.00044
D141	0.00344	-0.00013	-0.00543	-0.00092	-0.00636	-0.00291
D142	3.13903	0.00003	-0.00545	0.00415	-0.00130	3.13773
D143	3.12319	0.00036	0.01120	-0.00597	0.00523	3.12843
D144	-0.01630	0.00034	0.00895	-0.00455	0.00440	-0.01190
D145	-0.01200	0.00020	0.01122	-0.01137	-0.00015	-0.01215
D146	3.13170	0.00017	0.00897	-0.00996	-0.00099	3.13071
D147	-0.61455	0.00000	-0.01962	0.01179	-0.00786	-0.62241
D148	1.49955	-0.00001	-0.01949	0.01169	-0.00783	1.49172
D149	-2.67689	-0.00002	-0.01948	0.01165	-0.00787	-2.68476
D150	2.62121	-0.00001	0.02761	-0.01943	0.00822	2.62943
D151	-1.54787	-0.00002	0.02774	-0.01953	0.00824	-1.53963
D152	0.55887	-0.00003	0.02775	-0.01957	0.00821	0.56708
D153	0.00004	0.00002	-0.00200	0.00081	-0.00119	-0.00115
D154	-3.13653	0.00000	-0.00480	0.00312	-0.00168	-3.13821
D155	3.13944	0.00004	0.00034	-0.00066	-0.00032	3.13912
D156	0.00287	0.00002	-0.00246	0.00165	-0.00081	0.00206
D157	-3.13210	-0.00008	-0.00202	-0.00386	-0.00588	-3.13799
D158	0.00465	0.00012	-0.00543	0.00708	0.00165	0.00630
D159	0.00525	-0.00006	0.00034	-0.00581	-0.00547	-0.00022
D160	-3.14118	0.00014	-0.00307	0.00513	0.00206	-3.13911
D161	3.13207	0.00005	0.00246	0.00264	0.00509	3.13716
D162	-0.01157	0.00005	0.00406	0.00030	0.00436	-0.00721
D163	-0.00525	0.00003	0.00008	0.00460	0.00468	-0.00057
D164	3.13430	0.00003	0.00168	0.00226	0.00394	3.13824
D165	-0.00328	0.00007	-0.00066	0.00492	0.00426	0.00098
D166	3.13793	0.00006	-0.00025	0.00348	0.00324	3.14117
D167	-3.14015	-0.00012	0.00267	-0.00576	-0.00309	3.13994
D168	0.00106	-0.00013	0.00308	-0.00719	-0.00411	-0.00305
D169	0.00327	0.00001	-0.00049	-0.00159	-0.00207	0.00120
D170	-3.13794	-0.00001	-0.00023	-0.00212	-0.00235	-3.14029
D171	-3.13637	0.00001	-0.00202	0.00065	-0.00137	-3.13774
D172	0.00561	-0.00001	-0.00176	0.00011	-0.00165	0.00396
D173	-0.00054	0.00001	0.00028	0.00021	0.00049	-0.00005
D174	-3.14084	-0.00002	-0.00037	0.00083	0.00046	-3.14039
D175	3.13867	0.00001	0.00214	-0.00251	-0.00036	3.13831
D176	-0.00162	-0.00002	0.00149	-0.00189	-0.00040	-0.00202
D177	0.00003	-0.00005	0.00071	-0.00209	-0.00138	-0.00135
D178	3.14130	-0.00004	0.00049	-0.00164	-0.00115	3.14015
D179	-3.14121	-0.00005	0.00033	-0.00074	-0.00042	3.14156
D180	0.00006	-0.00003	0.00011	-0.00029	-0.00019	-0.00012

D181	-3.14086	0.00002	-0.00072	0.00196	0.00124	-3.13962
D182	0.00064	0.00001	-0.00067	0.00181	0.00114	0.00178
D183	0.00031	0.00002	-0.00026	0.00035	0.00009	0.00040
D184	-3.14137	0.00000	-0.00022	0.00020	-0.00001	-3.14138
D185	3.14080	0.00004	-0.00021	0.00069	0.00048	3.14128
D186	-0.00014	0.00002	-0.00048	0.00079	0.00031	0.00017
D187	-0.00038	0.00002	0.00007	0.00011	0.00018	-0.00020
D188	-3.14132	0.00000	-0.00020	0.00021	0.00002	-3.14131
D189	-0.00035	0.00000	0.00024	-0.00024	0.00000	-0.00035
D190	3.14111	0.00000	0.00037	-0.00037	0.00000	3.14111
D191	3.14132	0.00001	0.00019	-0.00009	0.00011	3.14143
D192	-0.00039	0.00001	0.00032	-0.00022	0.00010	-0.00029
D193	0.00033	0.00000	-0.00008	-0.00001	-0.00009	0.00024
D194	-3.14109	-0.00001	-0.00024	0.00009	-0.00014	-3.14124
D195	3.14129	0.00002	0.00018	-0.00011	0.00007	3.14136
D196	-0.00013	0.00001	0.00002	0.00000	0.00002	-0.00011
D197	0.00004	-0.00001	-0.00008	0.00007	0.00000	0.00004
D198	3.14146	0.00000	0.00008	-0.00003	0.00005	3.14152
D199	-3.14143	-0.00001	-0.00020	0.00020	0.00000	-3.14142
D200	0.00000	0.00000	-0.00005	0.00010	0.00005	0.00005

Item	Value	Threshold	Converged?

Maximum Force	0.002078	0.000450	NO

RMS Force	0.000339	0.000300	NO

Maximum Displacement	0.241496	0.001800	NO

RMS Displacement	0.044838	0.001200	NO

Predicted change in Energy=-2.670750D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.803936	-0.638227	-0.019693
2	6	0	-9.994417	-1.788730	-0.030435
3	6	0	-10.516200	-3.073971	-0.039152
4	6	0	-11.905026	-3.217147	-0.036761
5	6	0	-12.726655	-2.083157	-0.025766
6	6	0	-12.195243	-0.789372	-0.017208
7	1	0	-9.845091	-3.926746	-0.047555
8	1	0	-12.352023	-4.206459	-0.043163
9	1	0	-13.805405	-2.205705	-0.023863
10	1	0	-12.865302	0.058584	-0.009019
11	6	0	-9.927617	0.563794	-0.013396
12	6	0	-8.570264	-1.391302	-0.030451
13	6	0	-8.541045	0.088070	-0.011978
14	6	0	-7.405539	0.869574	0.003920
15	6	0	-6.013704	0.595464	0.009879
16	6	0	-3.643730	-0.184452	0.016374
17	6	0	-3.778470	1.228345	0.012451
18	16	0	-5.181220	-0.989717	0.011780
19	6	0	-5.099149	1.664900	0.011961
20	6	0	-2.266319	-0.451749	0.021428
21	6	0	-1.603444	0.797799	0.017497

22	7	0	-2.524078	1.820594	0.003128
23	16	0	-1.149714	-1.806387	0.015482
24	16	0	1.150350	1.807998	0.035598
25	6	0	0.198975	-0.672590	0.024379
26	6	0	-0.198489	0.674301	0.024316
27	6	0	1.604725	-0.796043	0.029682
28	6	0	2.267134	0.453605	0.028384
29	6	0	3.643558	0.187037	0.028536
30	6	0	3.778642	-1.225266	0.029090
31	6	0	5.099317	-1.660614	0.022736
32	6	0	6.013333	-0.590946	0.022105
33	16	0	5.180496	0.993432	0.029779
34	7	0	2.525158	-1.818605	0.045035
35	6	0	7.402608	-0.865584	0.014828
36	6	0	8.539815	-0.086297	-0.000761
37	6	0	8.573282	1.393475	-0.016571
38	6	0	9.925248	-0.565314	-0.010037
39	6	0	9.998464	1.786757	-0.035067
40	6	0	10.804659	0.634128	-0.032454
41	6	0	10.523849	3.070423	-0.054255
42	6	0	12.196418	0.781174	-0.050030
43	6	0	11.912966	3.209526	-0.072058
44	6	0	12.731381	2.073259	-0.069798
45	6	0	10.378242	-1.873210	0.002612
46	6	0	9.522976	-3.017512	0.028018
47	6	0	11.761381	-2.230788	-0.006855
48	7	0	8.848101	-3.967714	0.049029
49	7	0	12.878120	-2.562638	-0.014052
50	6	0	-10.383686	1.870980	-0.010138
51	6	0	-11.767500	2.225671	-0.011497
52	6	0	-9.531005	3.017439	-0.004441
53	7	0	-12.884816	2.555637	-0.012676
54	7	0	-8.858318	3.969418	-0.000428
55	8	0	-7.613098	-2.157588	-0.052552
56	8	0	7.618699	2.163226	-0.012364
57	6	0	2.244493	-3.241644	-0.035108
58	1	0	1.316360	-3.462073	0.496749
59	1	0	2.153338	-3.578335	-1.073462
60	1	0	3.052271	-3.793407	0.449833
61	6	0	-2.242895	3.243782	0.078459
62	1	0	-2.150865	3.582879	1.115903
63	1	0	-1.315183	3.462140	-0.454883
64	1	0	-3.051348	3.793860	-0.407265
65	1	0	5.428643	-2.693141	0.018196
66	1	0	12.864063	-0.068855	-0.049207
67	1	0	13.810379	2.192790	-0.083821
68	1	0	12.362846	4.197431	-0.087811
69	1	0	9.855067	3.925046	-0.055182
70	1	0	7.569267	-1.935914	0.022612
71	1	0	-7.574424	1.939585	0.007767
72	1	0	-5.427951	2.697661	0.014564

Rotational constants (GHZ): 0.1749910 0.0104055 0.0098230

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis func-

tions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6569.9337144266 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T
 Big=T
 Integral buffers will be 131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 Nuclear repulsion after empirical dispersion term = 6569.8487969890 Har-
 trees.
 One-electron integrals computed using PRISM.
 NBasis= 916 RedAO= T EigKep= 3.24D-04 NBF= 916
 NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916
 Initial guess from the checkpoint file: "PBDB.chk"
 B after Tr= 0.000000 0.000000 0.000000
 Rot= 1.000000 0.000018 -0.000001 -0.000050 Ang= 0.01 deg.
 ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1
 AccDes= 0.00D+00
 Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for in-
 itial guess.
 HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-
 yADJ=14
 ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
 FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlgl= 2001
 NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
 wScrn= 0.000000 ICntrl= 500 IOPCl= 0 IlCent= 200000004 NGrid=
 0
 NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0=
 0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 Integral accuracy reduced to 1.0D-05 until final iterations.
 Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
 SCF Done: E(RB3LYP) = -3683.02007204 A.U. after 12 cycles
 NFock= 12 Conv=0.77D-08 -V/T= 2.0068
 Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOPClX= 0 NMat=1
 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-0.000041641	-0.000149518	0.000031612
2	6	0.000132938	-0.000026792	-0.000065393
3	6	-0.000023237	0.000044497	0.000063788
4	6	-0.000048472	-0.000013172	-0.000060587
5	6	0.000031917	0.000085412	0.000030243
6	6	-0.000121253	-0.000151482	-0.000064224
7	1	-0.000014022	-0.000014391	-0.000005603
8	1	-0.000003843	-0.000011062	-0.000002830
9	1	0.000006009	-0.000013505	-0.000007651
10	1	0.000000419	-0.000056759	-0.000010170
11	6	0.000123932	0.000229519	-0.000178645
12	6	-0.000331430	-0.000083399	0.000721801
13	6	0.000304608	-0.000005028	-0.000203776
14	6	0.000578120	-0.000742508	0.001007644
15	6	-0.001013949	0.000732304	-0.000392893
16	6	0.000298542	-0.000162493	-0.000308506
17	6	0.000747977	-0.000145617	0.000164327
18	16	-0.000487783	-0.000057708	0.000257474

19	6	-0.000169991	0.000266877	-0.000344325
20	6	-0.000432851	0.000094646	0.000108782
21	6	0.000050667	0.000355798	-0.000869207
22	7	-0.000590073	-0.000298323	0.000580260
23	16	-0.000002333	0.000008495	0.000013818
24	16	-0.000108393	-0.000067368	-0.000019901
25	6	0.000118439	-0.000073025	0.000172974
26	6	0.000338984	-0.000204960	0.000124663
27	6	-0.000390965	0.000284269	-0.000172225
28	6	-0.000401970	0.000156634	-0.000317636
29	6	0.000229111	-0.000361686	0.000063308
30	6	-0.000074550	0.000179999	-0.000105272
31	6	0.000517133	0.000100376	0.000079569
32	6	-0.000119526	-0.000181438	-0.000100358
33	16	-0.000070233	-0.000193935	0.000341804
34	7	0.000138286	0.000318849	-0.000049579
35	6	0.000319612	-0.000073303	0.000241556
36	6	-0.000120857	-0.000291668	-0.000021759
37	6	0.000094733	0.000223972	-0.000434446
38	6	-0.000028778	-0.000208200	-0.000338878
39	6	-0.000187343	0.000007220	0.000109138
40	6	0.000093788	0.000066920	0.000143072
41	6	-0.000043155	-0.000052991	-0.000031951
42	6	0.000123037	0.000260667	0.000143824
43	6	0.000024324	-0.000015387	-0.000011065
44	6	-0.000013761	-0.000113375	-0.000007596
45	6	0.000379977	0.000231862	0.000327292
46	6	0.000023246	0.000059986	0.000032578
47	6	-0.000190581	-0.000220093	-0.000148143
48	7	0.000064833	-0.000054609	0.000063131
49	7	0.000012950	0.000055636	0.000015329
50	6	-0.000090296	-0.000063638	-0.000233449
51	6	0.000112057	0.000299344	0.000202047
52	6	-0.000033934	-0.000110728	0.000071745
53	7	-0.000002980	-0.000020000	-0.000021195
54	7	-0.000060501	0.000071834	-0.000063059
55	8	0.000285678	0.000088743	-0.000656782
56	8	0.000012615	0.000199249	0.000090994
57	6	-0.000061635	-0.000106821	-0.000001231
58	1	0.000014715	-0.000018478	-0.000004269
59	1	-0.000011857	-0.000052693	-0.000040038
60	1	-0.000014523	0.000001883	0.000024596
61	6	0.000075358	0.000250076	0.000042686
62	1	-0.000019135	-0.000022847	0.000019625
63	1	-0.000039640	-0.000062294	-0.000011534
64	1	0.000028326	-0.000088884	-0.000038623
65	1	-0.000037308	-0.000029951	0.000092753
66	1	-0.000070523	0.000011990	-0.000059146
67	1	0.000009285	0.000023138	0.000007418
68	1	-0.000009909	0.000017727	-0.000020449
69	1	-0.000005272	-0.000005107	0.000016969
70	1	-0.000132353	-0.000141674	0.000092827
71	1	0.000294424	-0.000005434	-0.000057095
72	1	0.000034816	0.000044420	-0.000020160

Cartesian Forces: Max 0.001013949 RMS 0.000234295

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.

```

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD:  received Info=          1 from GESDD.
Internal Forces:  Max          0.001352490  RMS          0.000193823
Search for a local minimum.
Step number 24 out of a maximum of 429
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 16 18 17 19 20
21 22 23 24
DE= -2.18D-04 DEPred=-2.67D-04 R= 8.17D-01
TightC=F SS= 1.41D+00 RLast= 1.56D-01 DXNew= 4.6512D-01 4.6826D-01
Trust test= 8.17D-01 RLast= 1.56D-01 DXMaxT set to 4.65D-01
ITU= 1 -1 1 1 -1 0 -1 0 -1 1 1 1 1 1 0 0 0 1 0
ITU= 0 0 1 0
Eigenvalues --- 0.00157 0.00243 0.00268 0.00348 0.00379
Eigenvalues --- 0.00406 0.00450 0.00480 0.00502 0.00549
Eigenvalues --- 0.00577 0.00590 0.00609 0.00619 0.00635
Eigenvalues --- 0.00668 0.00681 0.00713 0.00744 0.00747
Eigenvalues --- 0.00759 0.00769 0.00775 0.00783 0.00794
Eigenvalues --- 0.00818 0.00825 0.00842 0.01024 0.01087
Eigenvalues --- 0.01119 0.01134 0.01168 0.01237 0.01292
Eigenvalues --- 0.01316 0.01333 0.01361 0.01380 0.01447
Eigenvalues --- 0.01457 0.01462 0.01603 0.01640 0.01649
Eigenvalues --- 0.01745 0.01748 0.01794 0.01820 0.01929
Eigenvalues --- 0.01953 0.02006 0.02021 0.02068 0.02075
Eigenvalues --- 0.02188 0.02201 0.03016 0.03468 0.03902
Eigenvalues --- 0.03988 0.04829 0.04838 0.04905 0.04973
Eigenvalues --- 0.05011 0.05038 0.05120 0.05333 0.07058
Eigenvalues --- 0.07231 0.07390 0.07568 0.15514 0.15789
Eigenvalues --- 0.15941 0.15989 0.16000 0.16000 0.16000
Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16001
Eigenvalues --- 0.16002 0.16004 0.16011 0.16022 0.16037
Eigenvalues --- 0.16069 0.18668 0.19032 0.19472 0.19974
Eigenvalues --- 0.20731 0.21314 0.21617 0.21939 0.21996
Eigenvalues --- 0.22013 0.22289 0.22506 0.22593 0.22632
Eigenvalues --- 0.22646 0.22696 0.22849 0.23055 0.23245
Eigenvalues --- 0.23348 0.23495 0.23775 0.23976 0.24048
Eigenvalues --- 0.24222 0.24272 0.24328 0.24386 0.24539
Eigenvalues --- 0.24579 0.24643 0.24705 0.24809 0.24874
Eigenvalues --- 0.24925 0.24950 0.24987 0.24987 0.24994
Eigenvalues --- 0.24998 0.24998 0.24999 0.24999 0.25000
Eigenvalues --- 0.25000 0.25000 0.25000 0.25001 0.25011
Eigenvalues --- 0.25029 0.25273 0.25593 0.25891 0.26017
Eigenvalues --- 0.26270 0.26530 0.26791 0.26836 0.27125
Eigenvalues --- 0.27226 0.27731 0.27849 0.28318 0.28480
Eigenvalues --- 0.28576 0.28867 0.29951 0.30365 0.31897
Eigenvalues --- 0.32771 0.34805 0.35501 0.36286 0.36335
Eigenvalues --- 0.36408 0.36474 0.36649 0.36693 0.36756
Eigenvalues --- 0.36822 0.36882 0.37080 0.37094 0.37161
Eigenvalues --- 0.37259 0.37273 0.37418 0.37569 0.37676
Eigenvalues --- 0.37758 0.38017 0.38979 0.40304 0.40813
Eigenvalues --- 0.41655 0.42079 0.42654 0.44425 0.44792
Eigenvalues --- 0.45572 0.46128 0.46620 0.47796 0.47926
Eigenvalues --- 0.48467 0.52173 0.53569 0.55310 0.57272
Eigenvalues --- 0.62029 0.70818 0.73185 0.80305 0.81930
Eigenvalues --- 0.93390 1.25855 1.26329 1.29347 1.35384
En-DIIS/RFO-DIIS IScMMF= 0 using points: 24 23 22 21 20
RFO step: Lambda=-3.11778284D-05.

```

DidBck=F Rises=F RFO-DIIS coefs: 0.58955 0.14026 0.18764 0.04768
0.03487

Iteration 1 RMS(Cart)= 0.05031341 RMS(Int)= 0.00022191

Iteration 2 RMS(Cart)= 0.00074003 RMS(Int)= 0.00001384

Iteration 3 RMS(Cart)= 0.00000013 RMS(Int)= 0.00001384

Variable (Linear)	Old X (Quad)	-DE/DX (Total)	Delta X	Delta X	Delta X	New X
R1	2.65847	-0.00009	-0.00005	-0.00002	-0.00006	2.65841
R2	2.64466	-0.00006	0.00000	-0.00001	-0.00001	2.64466
R3	2.81108	-0.00038	-0.00002	-0.00072	-0.00073	2.81035
R4	2.62133	0.00004	-0.00003	0.00018	0.00015	2.62148
R5	2.79409	0.00002	-0.00034	0.00099	0.00064	2.79473
R6	2.63841	0.00008	-0.00001	0.00011	0.00011	2.63852
R7	2.05075	-0.00002	0.00001	-0.00005	-0.00005	2.05071
R8	2.64638	-0.00001	-0.00004	0.00008	0.00004	2.64642
R9	2.05154	-0.00001	0.00002	-0.00007	-0.00005	2.05149
R10	2.64315	0.00003	0.00000	0.00003	0.00004	2.64319
R11	2.05166	-0.00001	0.00000	-0.00002	-0.00002	2.05164
R12	2.04237	0.00002	0.00001	-0.00005	-0.00004	2.04232
R13	2.77017	0.00027	0.00014	-0.00027	-0.00012	2.77005
R14	2.61626	-0.00003	0.00025	-0.00055	-0.00029	2.61597
R15	2.79637	0.00012	-0.00039	0.00125	0.00084	2.79721
R16	2.31740	-0.00019	-0.00004	0.00004	-0.00001	2.31739
R17	2.60507	0.00008	-0.00157	0.00377	0.00220	2.60727
R18	2.68073	-0.00135	-0.00114	-0.00107	-0.00222	2.67852
R19	2.04707	-0.00012	-0.00014	0.00026	0.00012	2.04719
R20	3.38352	-0.00021	0.00008	-0.00069	-0.00060	3.38292
R21	2.65915	-0.00003	0.00001	0.00011	0.00012	2.65927
R22	2.68192	-0.00014	0.00008	-0.00025	-0.00017	2.68175
R23	3.27983	0.00014	-0.00062	0.00168	0.00106	3.28089
R24	2.65150	-0.00022	-0.00070	0.00104	0.00035	2.65186
R25	2.62854	0.00043	0.00042	-0.00003	0.00039	2.62893
R26	2.62144	0.00001	-0.00001	0.00014	0.00012	2.62156
R27	2.04816	-0.00004	0.00004	-0.00018	-0.00014	2.04803
R28	2.67300	0.00003	0.00007	0.00002	0.00009	2.67309
R29	3.31747	0.00007	-0.00015	0.00049	0.00034	3.31781
R30	2.60061	-0.00003	0.00014	-0.00026	-0.00013	2.60048
R31	2.66525	0.00050	0.00011	0.00102	0.00113	2.66638
R32	2.74512	-0.00008	-0.00019	0.00019	0.00000	2.74512
R33	3.32964	0.00005	-0.00015	0.00044	0.00029	3.32993
R34	3.32976	0.00006	-0.00001	0.00015	0.00014	3.32990
R35	3.31734	0.00011	-0.00002	0.00030	0.00027	3.31761
R36	2.65377	0.00008	-0.00005	0.00025	0.00020	2.65397
R37	2.66673	-0.00007	-0.00082	0.00178	0.00096	2.66769
R38	2.67275	0.00015	0.00009	0.00004	0.00013	2.67288
R39	2.60005	0.00034	0.00031	0.00002	0.00033	2.60038
R40	2.64939	0.00070	0.00097	-0.00058	0.00039	2.64978
R41	2.68105	0.00026	0.00008	0.00006	0.00015	2.68119
R42	3.27989	0.00014	-0.00003	0.00038	0.00035	3.28024
R43	2.62784	0.00075	0.00033	0.00083	0.00116	2.62900
R44	2.62088	0.00035	0.00047	-0.00028	0.00018	2.62107
R45	2.65882	0.00032	0.00015	0.00026	0.00042	2.65924
R46	2.04805	0.00001	0.00002	-0.00004	-0.00002	2.04803
R47	3.38252	0.00005	0.00004	0.00022	0.00027	3.38279
R48	2.67619	0.00038	0.00033	0.00166	0.00199	2.67818
R49	2.74514	-0.00018	-0.00001	-0.00027	-0.00028	2.74486
R50	2.60534	-0.00014	-0.00033	0.00102	0.00069	2.60603
R51	2.04706	-0.00012	-0.00011	0.00028	0.00018	2.04723
R52	2.79724	-0.00028	-0.00034	0.00055	0.00020	2.79744
R53	2.77022	0.00022	-0.00072	0.00094	0.00022	2.77044

R54	2.79408	0.00002	-0.00027	0.00092	0.00064	2.79472
R55	2.31733	-0.00007	-0.00006	0.00012	0.00006	2.31739
R56	2.81089	-0.00021	-0.00032	-0.00010	-0.00040	2.81048
R57	2.61572	0.00038	-0.00035	0.00093	0.00058	2.61630
R58	2.65808	0.00011	-0.00009	0.00022	0.00013	2.65821
R59	2.62134	0.00005	-0.00003	0.00032	0.00029	2.62163
R60	2.64489	-0.00011	-0.00064	0.00122	0.00058	2.64547
R61	2.63839	0.00005	0.00001	0.00006	0.00007	2.63846
R62	2.05072	0.00000	0.00002	-0.00006	-0.00004	2.05068
R63	2.64296	0.00011	0.00002	0.00009	0.00011	2.64306
R64	2.04257	-0.00009	0.00006	-0.00028	-0.00022	2.04234
R65	2.64623	0.00007	-0.00004	0.00033	0.00029	2.64652
R66	2.05155	-0.00001	0.00003	-0.00009	-0.00006	2.05149
R67	2.05166	-0.00001	0.00000	-0.00001	-0.00001	2.05164
R68	2.70010	0.00001	-0.00042	0.00070	0.00028	2.70037
R69	2.69975	-0.00014	-0.00118	0.00217	0.00099	2.70074
R70	2.20279	-0.00005	0.00003	-0.00012	-0.00009	2.20270
R71	2.20158	0.00000	-0.00003	0.00005	0.00002	2.20160
R72	2.69956	-0.00007	-0.00054	0.00103	0.00049	2.70005
R73	2.70004	0.00003	-0.00014	0.00025	0.00011	2.70015
R74	2.20157	0.00001	-0.00002	0.00003	0.00002	2.20159
R75	2.20280	-0.00007	0.00001	-0.00009	-0.00007	2.20272
R76	2.06395	-0.00001	0.00000	-0.00002	-0.00003	2.06392
R77	2.06996	-0.00004	0.00006	-0.00018	-0.00013	2.06984
R78	2.06328	-0.00001	0.00001	-0.00004	-0.00003	2.06325
R79	2.06987	-0.00002	0.00012	-0.00028	-0.00017	2.06971
R80	2.06386	0.00003	0.00003	-0.00003	0.00000	2.06385
R81	2.06327	-0.00002	0.00004	-0.00012	-0.00008	2.06320
A1	2.07574	0.00017	0.00002	0.00038	0.00039	2.07613
A2	1.89851	0.00014	0.00000	0.00019	0.00020	1.89871
A3	2.30894	-0.00031	-0.00001	-0.00057	-0.00059	2.30835
A4	2.14281	-0.00010	-0.00002	-0.00022	-0.00023	2.14258
A5	1.91180	-0.00005	0.00009	-0.00036	-0.00029	1.91151
A6	2.22857	0.00015	-0.00007	0.00058	0.00052	2.22909
A7	2.05915	-0.00002	0.00002	-0.00009	-0.00008	2.05908
A8	2.08922	0.00000	0.00004	-0.00005	-0.00001	2.08921
A9	2.13481	0.00002	-0.00006	0.00014	0.00009	2.13489
A10	2.09508	0.00004	0.00000	0.00017	0.00017	2.09524
A11	2.09787	-0.00002	-0.00001	-0.00007	-0.00008	2.09779
A12	2.09024	-0.00002	0.00001	-0.00010	-0.00009	2.09015
A13	2.12488	-0.00003	-0.00001	-0.00004	-0.00004	2.12483
A14	2.08469	0.00003	-0.00004	0.00010	0.00006	2.08475
A15	2.07362	0.00001	0.00005	-0.00007	-0.00002	2.07361
A16	2.06872	-0.00006	-0.00001	-0.00020	-0.00021	2.06851
A17	2.13132	-0.00002	-0.00001	-0.00008	-0.00008	2.13124
A18	2.08315	0.00009	0.00001	0.00028	0.00029	2.08344
A19	1.87024	0.00005	-0.00027	0.00086	0.00062	1.87086
A20	2.17596	-0.00090	-0.00016	-0.00140	-0.00157	2.17439
A21	2.23699	0.00086	0.00042	0.00054	0.00095	2.23794
A22	1.86266	0.00004	-0.00005	0.00007	0.00007	1.86273
A23	2.19424	-0.00003	-0.00043	0.00054	0.00022	2.19446
A24	2.22624	0.00000	0.00017	-0.00053	-0.00025	2.22599
A25	1.88152	-0.00017	0.00017	-0.00072	-0.00055	1.88097
A26	2.20826	0.00041	-0.00024	0.00052	0.00029	2.20854
A27	2.19341	-0.00024	0.00005	0.00021	0.00027	2.19368
A28	2.34434	-0.00019	0.00062	-0.00115	-0.00047	2.34387
A29	2.01705	0.00026	-0.00061	0.00126	0.00072	2.01777
A30	1.92177	-0.00007	-0.00018	-0.00022	-0.00034	1.92144
A31	2.24883	0.00006	0.00047	-0.00074	-0.00027	2.24856
A32	2.08384	-0.00005	-0.00039	0.00065	0.00027	2.08410

A33	1.95052	-0.00002	-0.00008	0.00008	-0.00001	1.95052
A34	1.95817	0.00006	-0.00017	0.00040	0.00023	1.95840
A35	1.85756	-0.00003	0.00022	-0.00058	-0.00035	1.85721
A36	2.46745	-0.00003	-0.00006	0.00018	0.00012	2.46758
A37	1.98513	-0.00018	0.00021	-0.00083	-0.00062	1.98451
A38	1.91684	0.00013	-0.00010	0.00045	0.00032	1.91716
A39	2.38121	0.00006	-0.00011	0.00038	0.00029	2.38150
A40	1.57191	0.00006	0.00030	-0.00041	-0.00011	1.57179
A41	1.95904	0.00007	-0.00027	0.00077	0.00049	1.95953
A42	2.12588	-0.00006	0.00009	-0.00037	-0.00028	2.12560
A43	2.19827	-0.00001	0.00017	-0.00039	-0.00022	2.19805
A44	1.86685	0.00004	-0.00003	0.00011	0.00009	1.86694
A45	2.45181	-0.00002	0.00007	-0.00009	-0.00002	2.45179
A46	1.96446	-0.00002	-0.00005	0.00004	-0.00001	1.96445
A47	1.92098	0.00002	0.00001	0.00000	-0.00002	1.92097
A48	1.97084	-0.00005	-0.00006	-0.00002	-0.00007	1.97077
A49	2.39135	0.00003	0.00002	0.00000	0.00004	2.39140
A50	1.86247	-0.00015	-0.00016	-0.00009	-0.00022	1.86225
A51	2.20553	0.00011	-0.00060	0.00113	0.00063	2.20616
A52	2.21193	0.00003	-0.00018	0.00006	-0.00001	2.21192
A53	1.56110	0.00013	0.00012	0.00010	0.00021	1.56132
A54	1.56136	-0.00001	-0.00017	0.00043	0.00026	1.56162
A55	1.98289	-0.00005	-0.00006	-0.00001	-0.00006	1.98283
A56	2.35495	0.00002	-0.00005	0.00015	0.00010	2.35506
A57	1.94534	0.00003	0.00010	-0.00014	-0.00004	1.94530
A58	2.35498	0.00001	-0.00006	0.00018	0.00013	2.35510
A59	1.94542	-0.00001	0.00004	-0.00008	-0.00004	1.94538
A60	1.98279	0.00000	0.00001	-0.00010	-0.00008	1.98270
A61	1.97061	0.00000	0.00005	-0.00009	-0.00003	1.97058
A62	2.39126	0.00006	0.00002	0.00008	0.00010	2.39136
A63	1.92128	-0.00006	-0.00008	0.00003	-0.00006	1.92122
A64	1.96463	-0.00003	-0.00001	-0.00009	-0.00010	1.96452
A65	2.45163	0.00004	0.00002	0.00008	0.00010	2.45173
A66	1.86692	-0.00001	-0.00002	0.00001	-0.00001	1.86691
A67	1.85745	0.00002	-0.00003	0.00010	0.00008	1.85753
A68	2.46710	0.00007	0.00011	-0.00010	0.00001	2.46711
A69	1.95863	-0.00009	-0.00009	0.00000	-0.00009	1.95854
A70	1.98457	-0.00002	0.00003	-0.00014	-0.00011	1.98446
A71	1.91752	-0.00013	-0.00010	0.00004	-0.00007	1.91745
A72	2.38106	0.00015	0.00007	0.00011	0.00019	2.38126
A73	1.95946	-0.00008	-0.00003	0.00013	0.00010	1.95956
A74	2.19798	0.00007	0.00001	0.00003	0.00004	2.19802
A75	2.12574	0.00001	0.00001	-0.00016	-0.00014	2.12560
A76	1.95053	-0.00005	-0.00010	-0.00018	-0.00028	1.95026
A77	2.08272	0.00059	0.00015	0.00042	0.00057	2.08329
A78	2.24994	-0.00054	-0.00007	-0.00024	-0.00030	2.24964
A79	1.57156	0.00025	0.00017	0.00021	0.00038	1.57195
A80	1.86141	0.00018	0.00018	-0.00004	0.00015	1.86155
A81	2.21202	-0.00009	-0.00022	0.00008	-0.00011	2.21191
A82	2.20567	-0.00009	-0.00043	0.00058	0.00018	2.20585
A83	2.34566	-0.00098	-0.00012	-0.00046	-0.00058	2.34508
A84	1.92038	0.00055	0.00019	0.00051	0.00069	1.92107
A85	2.01714	0.00043	-0.00007	-0.00005	-0.00012	2.01703
A86	2.19424	-0.00091	-0.00015	0.00019	0.00005	2.19429
A87	2.20797	0.00077	0.00002	0.00008	0.00011	2.20807
A88	1.88097	0.00014	0.00013	-0.00027	-0.00015	1.88082
A89	1.86276	-0.00003	-0.00005	-0.00004	-0.00005	1.86271
A90	2.22670	-0.00022	-0.00004	-0.00027	-0.00024	2.22646
A91	2.19372	0.00025	-0.00009	0.00031	0.00029	2.19401
A92	1.87062	-0.00016	0.00001	0.00021	0.00023	1.87085

A93	2.23698	0.00082	0.00015	0.00082	0.00096	2.23794
A94	2.17558	-0.00067	-0.00016	-0.00102	-0.00118	2.17439
A95	1.91184	-0.00006	-0.00013	-0.00002	-0.00015	1.91169
A96	2.22862	0.00010	0.00008	0.00035	0.00044	2.22905
A97	2.14273	-0.00004	0.00005	-0.00033	-0.00028	2.14244
A98	1.89858	0.00011	-0.00001	0.00012	0.00011	1.89869
A99	2.30879	-0.00021	-0.00012	-0.00032	-0.00044	2.30835
A100	2.07581	0.00011	0.00013	0.00021	0.00033	2.07614
A101	2.05919	-0.00004	-0.00013	0.00016	0.00003	2.05922
A102	2.08906	0.00002	0.00010	-0.00006	0.00004	2.08910
A103	2.13493	0.00001	0.00003	-0.00010	-0.00007	2.13487
A104	2.06871	-0.00006	-0.00004	-0.00018	-0.00022	2.06849
A105	2.13127	-0.00001	-0.00011	0.00017	0.00006	2.13133
A106	2.08321	0.00006	0.00015	0.00001	0.00015	2.08336
A107	2.09512	0.00003	-0.00006	0.00030	0.00024	2.09535
A108	2.09803	-0.00004	0.00001	-0.00018	-0.00018	2.09785
A109	2.09003	0.00001	0.00006	-0.00011	-0.00006	2.08998
A110	2.12482	0.00000	0.00006	-0.00016	-0.00010	2.12472
A111	2.07378	-0.00002	0.00000	-0.00001	-0.00001	2.07376
A112	2.08459	0.00003	-0.00006	0.00017	0.00011	2.08470
A113	2.16639	0.00053	0.00001	0.00075	0.00076	2.16714
A114	2.15709	-0.00052	-0.00041	-0.00065	-0.00106	2.15604
A115	1.95971	-0.00001	0.00040	-0.00010	0.00030	1.96001
A116	2.15739	-0.00070	-0.00021	-0.00129	-0.00150	2.15589
A117	2.16642	0.00054	0.00027	0.00032	0.00058	2.16700
A118	1.95937	0.00016	-0.00005	0.00097	0.00092	1.96029
A119	1.91243	0.00000	0.00016	-0.00033	-0.00017	1.91226
A120	1.94925	-0.00009	-0.00007	-0.00008	-0.00015	1.94910
A121	1.90456	0.00003	0.00009	-0.00008	0.00001	1.90457
A122	1.90589	0.00004	-0.00003	0.00014	0.00011	1.90600
A123	1.88644	0.00000	-0.00014	0.00033	0.00019	1.88663
A124	1.90420	0.00002	-0.00001	0.00003	0.00002	1.90423
A125	1.94839	0.00000	0.00027	-0.00054	-0.00027	1.94812
A126	1.91238	0.00007	0.00003	0.00013	0.00016	1.91254
A127	1.90413	0.00013	0.00008	0.00023	0.00031	1.90444
A128	1.90633	-0.00004	-0.00009	0.00002	-0.00007	1.90626
A129	1.90456	-0.00007	-0.00014	0.00008	-0.00007	1.90449
A130	1.88703	-0.00008	-0.00017	0.00011	-0.00006	1.88697
A131	3.16586	0.00020	0.00045	-0.00012	0.00033	3.16619
A132	3.17746	0.00013	0.00169	-0.00213	-0.00044	3.17702
A133	3.17784	0.00005	0.00201	-0.00346	-0.00146	3.17638
A134	3.16593	0.00019	-0.00062	0.00245	0.00183	3.16776
A135	3.14145	-0.00003	-0.00022	0.00028	0.00007	3.14152
A136	3.14163	0.00000	0.00001	-0.00007	-0.00006	3.14157
A137	3.14192	-0.00002	-0.00012	0.00015	0.00003	3.14195
A138	3.14111	0.00004	0.00020	0.00024	0.00044	3.14155
D1	0.00037	-0.00003	-0.00032	0.00062	0.00029	0.00066
D2	-3.14109	-0.00001	-0.00024	0.00180	0.00157	-3.13952
D3	-3.14091	-0.00007	-0.00034	0.00025	-0.00009	-3.14100
D4	0.00082	-0.00004	-0.00026	0.00144	0.00118	0.00200
D5	-0.00019	0.00002	0.00024	-0.00044	-0.00020	-0.00039
D6	3.14151	-0.00001	0.00028	-0.00082	-0.00053	3.14097
D7	3.14100	0.00007	0.00027	0.00003	0.00030	3.14130
D8	-0.00049	0.00004	0.00031	-0.00035	-0.00003	-0.00053
D9	-0.00633	0.00008	0.00393	0.00051	0.00444	-0.00189
D10	3.13490	0.00002	0.00268	-0.00038	0.00230	3.13720
D11	3.13564	0.00004	0.00390	0.00007	0.00398	3.13961
D12	-0.00632	-0.00002	0.00266	-0.00082	0.00184	-0.00448
D13	-0.00024	0.00002	0.00016	-0.00031	-0.00015	-0.00040
D14	3.14130	0.00001	0.00019	-0.00001	0.00018	3.14148

D15	3.14118	-0.00001	0.00006	-0.00173	-0.00167	3.13952
D16	-0.00046	-0.00001	0.00009	-0.00142	-0.00133	-0.00179
D17	0.00494	-0.00001	-0.00347	-0.00280	-0.00627	-0.00133
D18	-3.12750	-0.00032	-0.00490	-0.01161	-0.01651	3.13918
D19	-3.13650	0.00002	-0.00338	-0.00154	-0.00492	-3.14142
D20	0.01424	-0.00029	-0.00481	-0.01034	-0.01516	-0.00091
D21	-0.00005	0.00000	0.00007	-0.00015	-0.00008	-0.00013
D22	-3.14139	0.00000	0.00002	0.00005	0.00007	-3.14132
D23	-3.14159	0.00001	0.00005	-0.00047	-0.00042	3.14117
D24	0.00026	0.00000	0.00000	-0.00027	-0.00028	-0.00002
D25	0.00022	-0.00001	-0.00015	0.00031	0.00017	0.00039
D26	-3.14145	0.00000	-0.00014	0.00043	0.00028	-3.14117
D27	3.14156	-0.00001	-0.00010	0.00012	0.00002	3.14158
D28	-0.00011	0.00001	-0.00009	0.00023	0.00014	0.00002
D29	-0.00010	0.00000	-0.00002	-0.00001	-0.00002	-0.00012
D30	3.14140	0.00003	-0.00006	0.00036	0.00030	-3.14149
D31	3.14157	-0.00001	-0.00002	-0.00012	-0.00014	3.14143
D32	-0.00012	0.00001	-0.00006	0.00024	0.00018	0.00007
D33	0.00929	-0.00009	-0.00602	-0.00223	-0.00825	0.00104
D34	-3.13209	-0.00002	-0.00341	-0.00290	-0.00631	-3.13840
D35	-3.13192	-0.00003	-0.00471	-0.00130	-0.00601	-3.13793
D36	0.00988	0.00004	-0.00210	-0.00197	-0.00407	0.00581
D37	0.00081	0.00000	-0.00013	0.00190	0.00176	0.00258
D38	-3.14130	0.00009	0.00021	0.00324	0.00345	-3.13785
D39	-3.14122	-0.00007	-0.00165	0.00082	-0.00084	3.14113
D40	-0.00014	0.00003	-0.00131	0.00216	0.00085	0.00070
D41	-0.00879	0.00006	0.00585	0.00307	0.00891	0.00013
D42	3.13260	-0.00001	0.00327	0.00373	0.00700	3.13959
D43	3.12343	0.00038	0.00731	0.01209	0.01940	-3.14036
D44	-0.01837	0.00031	0.00473	0.01275	0.01748	-0.00089
D45	3.13965	0.00012	-0.00259	0.01519	0.01260	-3.13094
D46	-0.00892	0.00033	0.00888	-0.00719	0.00169	-0.00722
D47	-0.00170	0.00021	0.00046	0.01441	0.01487	0.01318
D48	3.13292	0.00041	0.01193	-0.00797	0.00396	3.13689
D49	-0.01000	0.00032	0.01323	0.00558	0.01880	0.00881
D50	3.12891	0.00043	0.01681	-0.00019	0.01663	-3.13765
D51	3.13829	0.00012	0.00220	0.02707	0.02928	-3.11562
D52	-0.00599	0.00023	0.00579	0.02131	0.02710	0.02111
D53	3.13970	0.00025	0.00310	0.00108	0.00418	-3.13931
D54	0.00063	0.00015	-0.00026	0.00648	0.00622	0.00685
D55	-3.13738	-0.00020	-0.00188	-0.00288	-0.00477	3.14104
D56	0.00590	-0.00012	0.00013	-0.00141	-0.00128	0.00462
D57	0.00196	-0.00011	0.00112	-0.00772	-0.00660	-0.00464
D58	-3.13795	-0.00003	0.00314	-0.00624	-0.00310	-3.14105
D59	0.00482	0.00012	0.00144	-0.00001	0.00143	0.00624
D60	-3.13146	0.00014	0.00096	0.00125	0.00221	-3.12925
D61	-3.13782	0.00008	0.00077	0.00220	0.00297	-3.13485
D62	0.00909	0.00009	0.00029	0.00347	0.00376	0.01285
D63	-0.00301	-0.00015	-0.00064	-0.00366	-0.00430	-0.00731
D64	3.14019	-0.00009	0.00038	-0.00706	-0.00668	3.13351
D65	-0.00218	0.00002	0.00053	0.00192	0.00245	0.00027
D66	-3.13008	-0.00004	-0.00096	-0.00379	-0.00475	-3.13483
D67	3.13786	-0.00004	-0.00046	0.00520	0.00475	-3.14058
D68	0.00996	-0.00010	-0.00195	-0.00050	-0.00245	0.00751
D69	-0.00432	0.00000	-0.00164	0.00505	0.00341	-0.00091
D70	3.13551	-0.00009	-0.00376	0.00350	-0.00026	3.13525
D71	3.13002	-0.00002	-0.00098	0.00332	0.00233	3.13235
D72	-0.01334	-0.00011	-0.00310	0.00177	-0.00133	-0.01468
D73	-0.01241	-0.00017	-0.00101	-0.00756	-0.00858	-0.02098
D74	-3.07167	-0.00006	0.00767	-0.02151	-0.01383	-3.08550

D75	3.13625	-0.00016	-0.00165	-0.00587	-0.00753	3.12872
D76	0.07698	-0.00004	0.00703	-0.01982	-0.01279	0.06420
D77	-0.00549	-0.00013	-0.00119	-0.00674	-0.00793	-0.01342
D78	3.13978	-0.00004	-0.00012	-0.00244	-0.00256	3.13722
D79	3.12667	-0.00009	-0.00016	-0.00281	-0.00297	3.12370
D80	-0.01125	0.00001	0.00091	0.00149	0.00240	-0.00885
D81	3.13684	0.00007	0.00141	0.00340	0.00481	-3.14153
D82	0.00943	0.00000	-0.00013	-0.00251	-0.00264	0.00679
D83	0.01101	0.00019	0.00136	0.00880	0.01016	0.02117
D84	3.06988	0.00007	-0.00740	0.02288	0.01548	3.08536
D85	-3.13555	0.00006	-0.00009	0.00300	0.00291	-3.13265
D86	-0.07668	-0.00006	-0.00885	0.01707	0.00823	-0.06845
D87	-3.13231	-0.00007	-0.00086	-0.00301	-0.00388	-3.13619
D88	0.00691	-0.00002	-0.00141	0.00079	-0.00062	0.00629
D89	0.01435	0.00006	0.00061	0.00291	0.00352	0.01787
D90	-3.12961	0.00012	0.00007	0.00671	0.00677	-3.12284
D91	1.54831	-0.00006	-0.00741	0.01441	0.00700	1.55530
D92	-2.62080	-0.00007	-0.00732	0.01417	0.00684	-2.61396
D93	-0.55801	-0.00006	-0.00746	0.01451	0.00705	-0.55096
D94	-1.49485	0.00009	0.00297	-0.00227	0.00071	-1.49414
D95	0.61923	0.00008	0.00306	-0.00251	0.00056	0.61978
D96	2.68202	0.00009	0.00293	-0.00217	0.00076	2.68278
D97	-0.00559	-0.00001	-0.00068	0.00301	0.00233	-0.00327
D98	3.13798	-0.00002	0.00006	0.00032	0.00038	3.13836
D99	-3.13710	0.00000	-0.00056	0.00166	0.00111	-3.13599
D100	0.00690	-0.00005	-0.00001	-0.00219	-0.00220	0.00470
D101	-0.00907	0.00003	-0.00032	0.00159	0.00126	-0.00780
D102	3.14038	0.00000	-0.00028	0.00310	0.00282	-3.13998
D103	0.00035	0.00002	0.00132	-0.00274	-0.00142	-0.00107
D104	3.14012	0.00006	0.00090	0.00020	0.00110	3.14121
D105	3.14044	0.00003	0.00075	-0.00069	0.00006	3.14049
D106	-0.00299	0.00007	0.00033	0.00224	0.00257	-0.00041
D107	3.13562	-0.00004	-0.00131	0.00164	0.00033	3.13596
D108	-0.01572	-0.00003	-0.00239	0.00427	0.00187	-0.01385
D109	-0.00401	-0.00005	-0.00058	-0.00100	-0.00158	-0.00560
D110	3.12783	-0.00004	-0.00166	0.00162	-0.00004	3.12779
D111	0.00930	0.00001	0.00058	-0.00065	-0.00007	0.00923
D112	-3.13752	0.00003	0.00055	-0.00166	-0.00111	-3.13863
D113	-3.12521	0.00000	0.00137	-0.00256	-0.00119	-3.12640
D114	0.01115	0.00002	0.00134	-0.00357	-0.00223	0.00893
D115	3.13271	-0.00001	-0.00084	0.00365	0.00281	3.13552
D116	0.08372	0.00003	0.00359	-0.00333	0.00026	0.08397
D117	-0.01844	0.00000	-0.00191	0.00622	0.00432	-0.01412
D118	-3.06744	0.00004	0.00253	-0.00076	0.00177	-3.06567
D119	3.13463	0.00000	-0.00027	-0.00198	-0.00225	3.13238
D120	-0.00558	-0.00003	0.00006	-0.00208	-0.00201	-0.00759
D121	0.00062	-0.00003	-0.00023	-0.00051	-0.00074	-0.00013
D122	-3.13959	-0.00006	0.00011	-0.00061	-0.00051	-3.14009
D123	3.13643	0.00002	-0.00100	0.00294	0.00194	3.13837
D124	-0.01208	0.00003	-0.00094	0.00439	0.00345	-0.00863
D125	-0.00609	0.00003	-0.00122	0.00300	0.00178	-0.00432
D126	3.12858	0.00005	-0.00117	0.00446	0.00329	3.13187
D127	-3.13803	-0.00003	-0.00003	-0.00138	-0.00141	-3.13944
D128	0.00500	-0.00006	0.00032	-0.00148	-0.00116	0.00384
D129	0.00382	0.00002	0.00172	-0.00323	-0.00152	0.00230
D130	-3.13730	0.00003	0.00196	-0.00283	-0.00088	-3.13817
D131	-3.12833	0.00000	0.00164	-0.00522	-0.00358	-3.13191
D132	0.01374	0.00000	0.00188	-0.00482	-0.00294	0.01080
D133	0.01883	-0.00002	0.00175	-0.00655	-0.00479	0.01403
D134	3.06826	-0.00006	-0.00264	0.00036	-0.00228	3.06599

D135	-3.13196	0.00000	0.00183	-0.00462	-0.00279	-3.13475
D136	-0.08252	-0.00004	-0.00256	0.00229	-0.00027	-0.08279
D137	0.00004	-0.00006	-0.00144	0.00205	0.00061	0.00065
D138	-3.14070	-0.00007	0.00125	-0.00439	-0.00314	3.13934
D139	3.14118	-0.00007	-0.00168	0.00167	0.00000	3.14118
D140	0.00044	-0.00007	0.00101	-0.00477	-0.00375	-0.00332
D141	-0.00291	0.00007	0.00063	-0.00030	0.00033	-0.00258
D142	3.13773	0.00008	-0.00238	0.00691	0.00453	-3.14093
D143	3.12843	0.00022	0.00131	0.03359	0.03490	-3.11986
D144	-0.01190	0.00023	0.00058	0.03533	0.03591	0.02402
D145	-0.01215	0.00021	0.00452	0.02590	0.03043	0.01827
D146	3.13071	0.00022	0.00379	0.02765	0.03144	-3.12104
D147	-0.62241	-0.00002	-0.00152	0.00099	-0.00053	-0.62294
D148	1.49172	-0.00003	-0.00149	0.00089	-0.00061	1.49111
D149	-2.68476	-0.00004	-0.00149	0.00083	-0.00067	-2.68543
D150	2.62943	0.00001	0.00372	-0.00728	-0.00356	2.62587
D151	-1.53963	0.00000	0.00374	-0.00738	-0.00364	-1.54326
D152	0.56708	-0.00001	0.00374	-0.00744	-0.00370	0.56338
D153	-0.00115	0.00010	-0.00074	0.00428	0.00353	0.00239
D154	-3.13821	0.00005	-0.00149	0.00393	0.00245	-3.13576
D155	3.13912	0.00009	0.00002	0.00246	0.00248	-3.14158
D156	0.00206	0.00004	-0.00072	0.00212	0.00139	0.00345
D157	-3.13799	0.00007	0.00116	0.00364	0.00480	-3.13319
D158	0.00630	-0.00003	-0.00087	0.00230	0.00143	0.00773
D159	-0.00022	0.00011	0.00179	0.00393	0.00571	0.00550
D160	-3.13911	0.00001	-0.00025	0.00259	0.00234	-3.13677
D161	3.13716	-0.00006	-0.00078	-0.00373	-0.00451	3.13265
D162	-0.00721	0.00001	-0.00026	-0.00204	-0.00230	-0.00951
D163	-0.00057	-0.00010	-0.00141	-0.00402	-0.00543	-0.00601
D164	3.13824	-0.00002	-0.00089	-0.00233	-0.00322	3.13502
D165	0.00098	-0.00009	-0.00152	-0.00235	-0.00387	-0.00288
D166	3.14117	-0.00006	-0.00107	-0.00178	-0.00285	3.13832
D167	3.13994	0.00001	0.00047	-0.00104	-0.00058	3.13937
D168	-0.00305	0.00004	0.00091	-0.00047	0.00044	-0.00261
D169	0.00120	0.00004	0.00048	0.00261	0.00309	0.00429
D170	-3.14029	0.00005	0.00063	0.00234	0.00297	-3.13732
D171	-3.13774	-0.00003	-0.00002	0.00100	0.00098	-3.13676
D172	0.00396	-0.00002	0.00013	0.00072	0.00085	0.00481
D173	-0.00005	-0.00001	-0.00002	-0.00105	-0.00107	-0.00113
D174	-3.14039	-0.00006	-0.00018	-0.00164	-0.00182	3.14098
D175	3.13831	0.00008	0.00059	0.00091	0.00150	3.13981
D176	-0.00202	0.00002	0.00043	0.00033	0.00075	-0.00127
D177	-0.00135	0.00003	0.00065	-0.00015	0.00051	-0.00085
D178	3.14015	0.00003	0.00053	0.00009	0.00061	3.14076
D179	3.14156	0.00000	0.00023	-0.00068	-0.00045	3.14111
D180	-0.00012	0.00000	0.00010	-0.00045	-0.00035	-0.00047
D181	-3.13962	-0.00004	-0.00059	-0.00057	-0.00116	-3.14078
D182	0.00178	-0.00003	-0.00054	-0.00054	-0.00108	0.00070
D183	0.00040	0.00000	-0.00009	0.00007	-0.00002	0.00038
D184	-3.14138	0.00000	-0.00003	0.00010	0.00006	-3.14132
D185	3.14128	0.00000	-0.00024	0.00079	0.00055	-3.14135
D186	0.00017	-0.00001	-0.00023	0.00059	0.00037	0.00054
D187	-0.00020	0.00001	-0.00007	0.00049	0.00041	0.00022
D188	-3.14131	0.00000	-0.00007	0.00030	0.00023	-3.14108
D189	-0.00035	0.00001	0.00005	0.00025	0.00030	-0.00005
D190	3.14111	0.00001	0.00012	-0.00003	0.00010	3.14121
D191	3.14143	0.00000	-0.00001	0.00023	0.00022	-3.14153
D192	-0.00029	0.00000	0.00007	-0.00005	0.00001	-0.00027
D193	0.00024	0.00000	0.00004	-0.00017	-0.00014	0.00010
D194	-3.14124	-0.00001	0.00000	-0.00013	-0.00013	-3.14137

D195	3.14136	0.00000	0.00003	0.00001	0.00004	3.14140
D196	-0.00011	0.00000	-0.00001	0.00005	0.00004	-0.00007
D197	0.00004	-0.00001	-0.00003	-0.00021	-0.00023	-0.00019
D198	3.14152	0.00000	0.00001	-0.00025	-0.00023	3.14128
D199	-3.14142	-0.00001	-0.00010	0.00007	-0.00003	-3.14145
D200	0.00005	0.00000	-0.00006	0.00003	-0.00003	0.00002

Item	Value	Threshold	Converged?

Maximum Force	0.001352	0.000450	NO
RMS Force	0.000194	0.000300	YES
Maximum Displacement	0.225296	0.001800	NO
RMS Displacement	0.050392	0.001200	NO

Predicted change in Energy=-5.924392D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.804658	-0.637873	0.027273
2	6	0	-9.995427	-1.788457	0.044559
3	6	0	-10.517834	-3.073348	0.067920
4	6	0	-11.906790	-3.215662	0.074783
5	6	0	-12.728008	-2.081414	0.058438
6	6	0	-12.196053	-0.788021	0.034599
7	1	0	-9.847127	-3.926358	0.080428
8	1	0	-12.354230	-4.204597	0.093167
9	1	0	-13.806797	-2.203395	0.064364
10	1	0	-12.865492	0.060349	0.022667
11	6	0	-9.928524	0.563590	0.003496
12	6	0	-8.570967	-1.390964	0.035705
13	6	0	-8.541735	0.088741	0.009777
14	6	0	-7.405457	0.871235	-0.003190
15	6	0	-6.014840	0.597050	-0.010827
16	6	0	-3.645002	-0.183305	-0.020489
17	6	0	-3.778897	1.229477	-0.025414
18	16	0	-5.183297	-0.988249	-0.018174
19	6	0	-5.099761	1.666088	-0.019372
20	6	0	-2.267465	-0.450979	-0.018470
21	6	0	-1.604164	0.798399	-0.021836
22	7	0	-2.524359	1.821371	-0.043188
23	16	0	-1.151145	-1.806098	-0.020508
24	16	0	1.150839	1.807347	-0.007344
25	6	0	0.198238	-0.672872	-0.013908
26	6	0	-0.198666	0.674295	-0.014560
27	6	0	1.604443	-0.796929	-0.008073
28	6	0	2.267350	0.452529	-0.011623
29	6	0	3.643872	0.185404	-0.009188
30	6	0	3.778532	-1.227008	-0.004025
31	6	0	5.099718	-1.662808	-0.005156
32	6	0	6.014187	-0.593241	-0.008228
33	16	0	5.181291	0.991285	-0.008628
34	7	0	2.524682	-1.819889	0.007984
35	6	0	7.404591	-0.867697	-0.006940

36	6	0	8.541457	-0.087349	0.012389
37	6	0	8.573748	1.392338	0.042316
38	6	0	9.927529	-0.564872	0.003094
39	6	0	9.999014	1.787020	0.042879
40	6	0	10.805995	0.635102	0.019047
41	6	0	10.524062	3.070978	0.062657
42	6	0	12.198094	0.782846	0.014404
43	6	0	11.913244	3.210861	0.058000
44	6	0	12.732466	2.075239	0.033998
45	6	0	10.383114	-1.872113	-0.016066
46	6	0	9.530731	-3.018954	-0.029187
47	6	0	11.767875	-2.225512	-0.024347
48	7	0	8.858662	-3.971250	-0.040262
49	7	0	12.885795	-2.553393	-0.031690
50	6	0	-10.386555	1.869668	-0.022667
51	6	0	-11.771689	2.220196	-0.026899
52	6	0	-9.536278	3.017680	-0.049814
53	7	0	-12.890487	2.545109	-0.031445
54	7	0	-8.867385	3.972027	-0.072215
55	8	0	-7.613533	-2.157113	0.048910
56	8	0	7.618270	2.160782	0.062296
57	6	0	2.243514	-3.242687	-0.072014
58	1	0	1.315287	-3.462534	0.459890
59	1	0	2.152201	-3.579259	-1.110323
60	1	0	3.051134	-3.794712	0.412857
61	6	0	-2.242040	3.245244	0.012396
62	1	0	-2.142545	3.596890	1.044869
63	1	0	-1.317989	3.456612	-0.530037
64	1	0	-3.053532	3.789918	-0.474256
65	1	0	5.428899	-2.695379	-0.004873
66	1	0	12.865995	-0.066634	-0.004017
67	1	0	13.811459	2.195514	0.030290
68	1	0	12.362609	4.198983	0.072632
69	1	0	9.855006	3.925165	0.080924
70	1	0	7.572316	-1.937776	-0.027970
71	1	0	-7.573929	1.941124	-0.026661
72	1	0	-5.428308	2.698852	-0.016039

Rotational constants (GHZ): 0.1750509 0.0104002 0.0098185

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6569.0531925302 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T
Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6568.9682953803 Hartrees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.25D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Initial guess from the checkpoint file: "PBDB.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000012 -0.000001 -0.000036 Ang= 0.00 deg.


```

ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn=      1
AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn=      1 diagonalized for in-
itial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn=      1 IDoV= 1 UseB2=F IT-
yADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag=      0 FMFlag=      100000 FMFlgl=      2001
NFxFlg=      0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl=      500 IOpCl= 0 IlCent= 200000004 NGrid=
0
NMat0=      1 NMatS0=      1 NMatT0=      0 NMatD0=      1 NMtDS0=      0 NMtDT0=
0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on      energy=1.00D-06.
No special actions if energy rises.
Integral accuracy reduced to 1.0D-05 until final iterations.
Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
SCF Done: E(RB3LYP) = -3683.02005105 A.U. after 12 cycles
NFock= 12 Conv=0.77D-08 -V/T= 2.0068
Calling FoFJK, ICntrl=      2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1
NMatS=1 NMatT=0.
***** Axes restored to original set *****

```

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	0.000059136	-0.000000830	0.000008696
2	6	0.000187619	-0.000112964	-0.000024108
3	6	0.000004649	-0.000037885	-0.000016884
4	6	-0.000046589	-0.000031618	-0.000043551
5	6	0.000062226	0.000049078	0.000049771
6	6	-0.000057831	-0.000004802	-0.000014604
7	1	0.000002241	0.000007674	-0.000007371
8	1	-0.000002089	0.000006421	0.000010710
9	1	0.000000073	-0.000002786	0.000000792
10	1	0.000058353	0.000064739	0.000050575
11	6	-0.000008676	0.000045934	0.000076667
12	6	0.000092952	-0.000148180	-0.000008437
13	6	0.000352852	-0.000594394	0.000079626
14	6	-0.000757296	0.000384933	0.001172479
15	6	-0.000379586	0.000378663	-0.000133169
16	6	0.000149215	-0.000141379	0.000192185
17	6	0.000114715	-0.000079598	0.000409879
18	16	0.000575042	-0.000130116	-0.000590176
19	6	-0.000117870	0.000075918	-0.000198715
20	6	-0.000139074	0.000176252	-0.000254620
21	6	-0.000192305	0.000105880	0.000158472
22	7	-0.000192120	-0.000119502	-0.000005441
23	16	-0.000033277	-0.000049848	0.000027770
24	16	-0.000041409	-0.000063447	-0.000091257
25	6	0.000321739	-0.000226187	0.000114129
26	6	-0.000007839	0.000011421	0.000281670
27	6	-0.000666841	0.000331715	-0.000052737
28	6	-0.000402149	0.000233158	-0.000268871
29	6	0.000042344	-0.000355821	0.000422995
30	6	-0.000027056	-0.000024699	0.000231218
31	6	-0.000130431	-0.000100396	0.000455879

32	6	0.000585846	-0.000136650	-0.000324460
33	16	0.000503485	-0.000038751	-0.000389716
34	7	0.000370420	0.000199810	-0.000514309
35	6	-0.000141581	-0.000147072	0.000106333
36	6	-0.000302816	0.000030353	0.000140355
37	6	-0.000247072	0.000073434	-0.000000012
38	6	0.000010139	-0.000018112	0.000081527
39	6	0.000024323	0.000064392	-0.000181345
40	6	0.000213667	-0.000102509	0.000085602
41	6	0.000014787	0.000055138	-0.000015418
42	6	-0.000124117	0.000210419	-0.000065905
43	6	0.000036348	0.000031714	0.000059343
44	6	-0.000097035	-0.000020502	-0.000076158
45	6	0.000397999	0.000067815	0.000363207
46	6	-0.000008003	-0.000223600	-0.000055412
47	6	-0.000370192	0.000049571	-0.000311643
48	7	0.000033644	0.000054988	0.000015621
49	7	-0.000017007	0.000132453	0.000008863
50	6	-0.000297810	-0.000175170	-0.000252986
51	6	0.000190952	0.000035564	0.000179416
52	6	-0.000031594	0.000102685	-0.000092436
53	7	0.000002565	-0.000150639	-0.000034811
54	7	0.000019820	-0.000021957	0.000029392
55	8	-0.000291626	0.000045625	0.000017221
56	8	0.000019476	0.000107696	0.000313185
57	6	0.000012239	-0.000063313	-0.000087975
58	1	0.000033709	0.000034228	0.000012542
59	1	-0.000028504	-0.000049112	-0.000009404
60	1	-0.000014523	0.000028641	0.000024588
61	6	0.000272236	0.000272419	-0.000199872
62	1	-0.000024934	-0.000098944	-0.000046384
63	1	-0.000005273	-0.000032302	0.000036962
64	1	0.000015017	-0.000023677	-0.000024415
65	1	-0.000074790	-0.000016130	0.000132587
66	1	-0.000057832	-0.000030950	-0.000062516
67	1	0.000002923	0.000013221	0.000003713
68	1	-0.000011010	-0.000005891	-0.000019404
69	1	-0.000004140	-0.000011892	-0.000004063
70	1	0.000114406	-0.000047434	-0.000261458
71	1	0.000449833	0.000156574	-0.000562972
72	1	0.000005306	0.000000537	-0.000050956

Cartesian Forces: Max 0.001172479 RMS 0.000212034

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.000958255 RMS 0.000154709

Search for a local minimum.

Step number 25 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 16 18 17 19 20

21 22 23 24 25

DE= 2.10D-05 DEPred=-5.92D-05 R=-3.54D-01

Trust test=-3.54D-01 RLast= 1.04D-01 DXMaxT set to 2.33D-01

ITU= -1 1 -1 1 1 -1 0 -1 0 -1 1 1 1 1 1 1 0 0 0 1

ITU= 0 0 0 1 0

Eigenvalues	---	0.00144	0.00247	0.00268	0.00374	0.00386
Eigenvalues	---	0.00449	0.00480	0.00501	0.00504	0.00566
Eigenvalues	---	0.00580	0.00593	0.00611	0.00630	0.00642
Eigenvalues	---	0.00681	0.00694	0.00735	0.00744	0.00747
Eigenvalues	---	0.00759	0.00770	0.00775	0.00783	0.00795
Eigenvalues	---	0.00823	0.00832	0.00892	0.01050	0.01094
Eigenvalues	---	0.01133	0.01152	0.01189	0.01275	0.01315
Eigenvalues	---	0.01328	0.01333	0.01361	0.01380	0.01457
Eigenvalues	---	0.01460	0.01472	0.01603	0.01646	0.01743
Eigenvalues	---	0.01747	0.01776	0.01794	0.01928	0.01953
Eigenvalues	---	0.02006	0.02021	0.02061	0.02074	0.02179
Eigenvalues	---	0.02200	0.02799	0.03181	0.03522	0.03885
Eigenvalues	---	0.04003	0.04830	0.04838	0.04909	0.04979
Eigenvalues	---	0.05013	0.05045	0.05119	0.05342	0.07059
Eigenvalues	---	0.07233	0.07390	0.07570	0.15500	0.15786
Eigenvalues	---	0.15941	0.15991	0.15999	0.16000	0.16000
Eigenvalues	---	0.16000	0.16000	0.16000	0.16000	0.16001
Eigenvalues	---	0.16002	0.16009	0.16011	0.16030	0.16041
Eigenvalues	---	0.16069	0.18573	0.19032	0.19467	0.19950
Eigenvalues	---	0.20706	0.21314	0.21609	0.21935	0.21996
Eigenvalues	---	0.22011	0.22297	0.22495	0.22594	0.22632
Eigenvalues	---	0.22646	0.22695	0.22848	0.23057	0.23262
Eigenvalues	---	0.23337	0.23493	0.23771	0.23958	0.24057
Eigenvalues	---	0.24184	0.24271	0.24345	0.24387	0.24528
Eigenvalues	---	0.24577	0.24649	0.24664	0.24820	0.24884
Eigenvalues	---	0.24920	0.24950	0.24986	0.24988	0.24994
Eigenvalues	---	0.24997	0.24999	0.24999	0.25000	0.25000
Eigenvalues	---	0.25000	0.25000	0.25000	0.25003	0.25010
Eigenvalues	---	0.25012	0.25256	0.25600	0.25895	0.26091
Eigenvalues	---	0.26267	0.26543	0.26798	0.26853	0.27151
Eigenvalues	---	0.27229	0.27731	0.27847	0.28318	0.28493
Eigenvalues	---	0.28590	0.28871	0.29956	0.30357	0.31876
Eigenvalues	---	0.32817	0.35346	0.35508	0.36276	0.36336
Eigenvalues	---	0.36451	0.36474	0.36606	0.36662	0.36812
Eigenvalues	---	0.36849	0.37006	0.37082	0.37114	0.37170
Eigenvalues	---	0.37261	0.37291	0.37425	0.37569	0.37677
Eigenvalues	---	0.37758	0.38022	0.38978	0.40302	0.40986
Eigenvalues	---	0.41673	0.42074	0.42657	0.44432	0.44788
Eigenvalues	---	0.45585	0.46080	0.46686	0.47787	0.47923
Eigenvalues	---	0.48459	0.52197	0.53564	0.55338	0.57232
Eigenvalues	---	0.63109	0.71116	0.73028	0.80388	0.81951
Eigenvalues	---	0.93626	1.25856	1.26331	1.29346	1.35379

En-DIIS/RFO-DIIS IScMMF= 0 using points: 25 24 23 22 21

RFO step: Lambda=-2.97019211D-05.

DidBck=T Rises=F RFO-DIIS coefs: 0.33608 0.38886 0.08985 0.13343 0.05178

Iteration 1 RMS(Cart)= 0.03259817 RMS(Int)= 0.00013445

Iteration 2 RMS(Cart)= 0.00036988 RMS(Int)= 0.00000783

Iteration 3 RMS(Cart)= 0.00000004 RMS(Int)= 0.00000783

Variable	Old X	-DE/DX	Delta X	Delta X	Delta X	New X
(Linear)	(Quad)	(Total)				
R1	2.65841	0.00005	0.00001	0.00004	0.00005	2.65845
R2	2.64466	0.00006	0.00000	0.00006	0.00006	2.64472
R3	2.81035	0.00012	0.00052	-0.00036	0.00018	2.81053
R4	2.62148	-0.00003	-0.00015	0.00012	-0.00003	2.62145
R5	2.79473	-0.00022	-0.00075	0.00037	-0.00039	2.79434
R6	2.63852	-0.00003	-0.00008	0.00004	-0.00003	2.63849
R7	2.05071	0.00000	0.00004	-0.00005	0.00000	2.05070
R8	2.64642	-0.00009	-0.00005	-0.00008	-0.00013	2.64629

R9	2.05149	0.00001	0.00005	-0.00003	0.00002	2.05151
R10	2.64319	0.00003	-0.00002	0.00006	0.00004	2.64323
R11	2.05164	0.00000	0.00002	-0.00002	-0.00001	2.05163
R12	2.04232	-0.00009	0.00006	-0.00019	-0.00013	2.04219
R13	2.77005	0.00003	0.00026	0.00003	0.00030	2.77035
R14	2.61597	0.00028	0.00038	-0.00010	0.00028	2.61625
R15	2.79721	-0.00025	-0.00088	0.00051	-0.00038	2.79683
R16	2.31739	-0.00022	-0.00002	-0.00015	-0.00017	2.31722
R17	2.60727	-0.00096	-0.00277	0.00170	-0.00107	2.60620
R18	2.67852	-0.00048	0.00069	-0.00236	-0.00167	2.67684
R19	2.04719	-0.00008	-0.00021	0.00007	-0.00013	2.04706
R20	3.38292	-0.00001	0.00057	-0.00066	-0.00009	3.38283
R21	2.65927	-0.00001	-0.00012	0.00011	-0.00001	2.65926
R22	2.68175	-0.00005	0.00015	-0.00031	-0.00016	2.68159
R23	3.28089	-0.00015	-0.00125	0.00094	-0.00032	3.28057
R24	2.65186	-0.00037	-0.00081	0.00012	-0.00070	2.65116
R25	2.62893	0.00022	-0.00001	0.00042	0.00041	2.62934
R26	2.62156	-0.00010	-0.00013	0.00016	0.00003	2.62160
R27	2.04803	0.00002	0.00014	-0.00011	0.00003	2.04806
R28	2.67309	-0.00006	-0.00007	0.00003	-0.00004	2.67305
R29	3.31781	-0.00003	-0.00037	0.00029	-0.00008	3.31773
R30	2.60048	-0.00001	0.00017	0.00000	0.00018	2.60066
R31	2.66638	0.00001	-0.00082	0.00104	0.00022	2.66660
R32	2.74512	-0.00008	-0.00011	-0.00032	-0.00043	2.74469
R33	3.32993	-0.00004	-0.00033	0.00024	-0.00009	3.32984
R34	3.32990	-0.00001	-0.00013	0.00011	-0.00002	3.32988
R35	3.31761	0.00001	-0.00024	0.00029	0.00005	3.31767
R36	2.65397	-0.00006	-0.00019	0.00009	-0.00010	2.65387
R37	2.66769	-0.00048	-0.00141	0.00043	-0.00098	2.66670
R38	2.67288	0.00006	-0.00005	0.00006	0.00001	2.67289
R39	2.60038	0.00016	-0.00006	0.00049	0.00043	2.60081
R40	2.64978	0.00053	0.00038	0.00080	0.00118	2.65096
R41	2.68119	0.00015	-0.00006	0.00015	0.00009	2.68129
R42	3.28024	0.00001	-0.00027	0.00032	0.00005	3.28030
R43	2.62900	0.00025	-0.00067	0.00120	0.00053	2.62953
R44	2.62107	0.00022	0.00018	0.00035	0.00053	2.62160
R45	2.65924	0.00000	-0.00024	0.00035	0.00011	2.65935
R46	2.04803	0.00002	0.00003	0.00000	0.00002	2.04806
R47	3.38279	-0.00006	-0.00017	0.00023	0.00006	3.38284
R48	2.67818	-0.00044	-0.00134	0.00125	-0.00008	2.67810
R49	2.74486	-0.00007	0.00022	-0.00045	-0.00023	2.74464
R50	2.60603	-0.00057	-0.00076	0.00040	-0.00036	2.60567
R51	2.04723	-0.00011	-0.00019	0.00002	-0.00017	2.04707
R52	2.79744	-0.00035	-0.00041	-0.00012	-0.00053	2.79691
R53	2.77044	-0.00004	-0.00069	0.00083	0.00014	2.77058
R54	2.79472	-0.00020	-0.00070	0.00037	-0.00033	2.79439
R55	2.31739	-0.00022	-0.00008	-0.00007	-0.00015	2.31725
R56	2.81048	0.00005	0.00011	-0.00010	0.00002	2.81050
R57	2.61630	0.00008	-0.00073	0.00084	0.00012	2.61642
R58	2.65821	0.00012	-0.00016	0.00026	0.00010	2.65831
R59	2.62163	-0.00007	-0.00027	0.00016	-0.00011	2.62152
R60	2.64547	-0.00028	-0.00090	0.00044	-0.00046	2.64502
R61	2.63846	-0.00007	-0.00003	-0.00001	-0.00004	2.63842
R62	2.05068	0.00001	0.00004	-0.00003	0.00001	2.05069
R63	2.64306	0.00004	-0.00007	0.00013	0.00006	2.64313
R64	2.04234	-0.00009	0.00024	-0.00036	-0.00013	2.04222
R65	2.64652	-0.00008	-0.00027	0.00014	-0.00013	2.64639
R66	2.05149	0.00001	0.00006	-0.00005	0.00002	2.05151
R67	2.05164	-0.00001	0.00001	-0.00002	-0.00001	2.05163
R68	2.70037	-0.00017	-0.00048	0.00029	-0.00019	2.70018

R69	2.70074	-0.00052	-0.00155	0.00075	-0.00080	2.69993
R70	2.20270	0.00005	0.00009	-0.00006	0.00003	2.20273
R71	2.20160	-0.00005	-0.00004	0.00004	0.00000	2.20159
R72	2.70005	-0.00027	-0.00075	0.00034	-0.00041	2.69964
R73	2.70015	-0.00008	-0.00016	0.00009	-0.00008	2.70008
R74	2.20159	-0.00004	-0.00003	0.00003	0.00000	2.20159
R75	2.20272	0.00002	0.00006	-0.00005	0.00001	2.20274
R76	2.06392	0.00001	0.00002	-0.00004	-0.00002	2.06391
R77	2.06984	0.00000	0.00013	-0.00006	0.00006	2.06990
R78	2.06325	-0.00001	0.00003	-0.00001	0.00001	2.06326
R79	2.06971	0.00005	0.00018	-0.00002	0.00016	2.06987
R80	2.06385	0.00005	0.00002	0.00002	0.00004	2.06389
R81	2.06320	-0.00001	0.00008	-0.00003	0.00005	2.06325
A1	2.07613	-0.00009	-0.00030	0.00020	-0.00010	2.07603
A2	1.89871	-0.00004	-0.00014	0.00009	-0.00004	1.89866
A3	2.30835	0.00013	0.00044	-0.00029	0.00015	2.30850
A4	2.14258	0.00003	0.00018	-0.00017	0.00001	2.14259
A5	1.91151	0.00006	0.00029	-0.00016	0.00012	1.91164
A6	2.22909	-0.00009	-0.00047	0.00033	-0.00013	2.22896
A7	2.05908	0.00002	0.00007	-0.00002	0.00005	2.05913
A8	2.08921	0.00000	0.00002	0.00001	0.00003	2.08924
A9	2.13489	-0.00002	-0.00010	0.00001	-0.00008	2.13481
A10	2.09524	-0.00001	-0.00014	0.00014	-0.00001	2.09524
A11	2.09779	0.00000	0.00006	-0.00008	-0.00002	2.09777
A12	2.09015	0.00001	0.00008	-0.00005	0.00003	2.09017
A13	2.12483	0.00002	0.00003	-0.00004	-0.00001	2.12482
A14	2.08475	-0.00001	-0.00006	0.00007	0.00001	2.08476
A15	2.07361	-0.00001	0.00003	-0.00003	0.00000	2.07361
A16	2.06851	0.00002	0.00016	-0.00011	0.00006	2.06856
A17	2.13124	0.00003	0.00007	0.00001	0.00008	2.13132
A18	2.08344	-0.00006	-0.00024	0.00010	-0.00014	2.08330
A19	1.87086	-0.00016	-0.00065	0.00036	-0.00027	1.87058
A20	2.17439	0.00032	0.00106	-0.00056	0.00050	2.17488
A21	2.23794	-0.00016	-0.00041	0.00020	-0.00022	2.23772
A22	1.86273	0.00000	-0.00007	0.00006	0.00004	1.86278
A23	2.19446	-0.00008	-0.00048	0.00010	-0.00028	2.19418
A24	2.22599	0.00008	0.00032	-0.00017	0.00024	2.22623
A25	1.88097	0.00015	0.00051	-0.00035	0.00015	1.88112
A26	2.20854	-0.00001	-0.00033	0.00029	-0.00004	2.20850
A27	2.19368	-0.00014	-0.00018	0.00006	-0.00012	2.19356
A28	2.34387	-0.00001	0.00085	-0.00067	0.00020	2.34406
A29	2.01777	-0.00005	-0.00094	0.00082	-0.00010	2.01767
A30	1.92144	0.00007	0.00003	-0.00004	0.00001	1.92144
A31	2.24856	0.00015	0.00064	-0.00010	0.00053	2.24909
A32	2.08410	-0.00011	-0.00058	0.00021	-0.00037	2.08373
A33	1.95052	-0.00005	-0.00006	-0.00010	-0.00015	1.95036
A34	1.95840	-0.00001	-0.00026	0.00033	0.00007	1.95846
A35	1.85721	0.00007	0.00041	-0.00032	0.00009	1.85730
A36	2.46758	-0.00007	-0.00015	-0.00001	-0.00015	2.46742
A37	1.98451	-0.00001	0.00061	-0.00074	-0.00014	1.98437
A38	1.91716	0.00001	-0.00031	0.00046	0.00017	1.91732
A39	2.38150	0.00000	-0.00029	0.00026	-0.00004	2.38146
A40	1.57179	0.00009	0.00027	-0.00009	0.00019	1.57198
A41	1.95953	-0.00003	-0.00055	0.00059	0.00005	1.95958
A42	2.12560	0.00000	0.00024	-0.00028	-0.00003	2.12557
A43	2.19805	0.00003	0.00030	-0.00031	-0.00001	2.19803
A44	1.86694	-0.00001	-0.00007	0.00007	0.00001	1.86694
A45	2.45179	0.00001	0.00003	-0.00011	-0.00007	2.45171
A46	1.96445	0.00000	0.00000	0.00007	0.00007	1.96452
A47	1.92097	0.00004	0.00001	0.00009	0.00012	1.92108

A48	1.97077	0.00000	0.00002	-0.00017	-0.00015	1.97062
A49	2.39140	-0.00004	-0.00002	0.00004	0.00002	2.39142
A50	1.86225	-0.00010	0.00004	-0.00048	-0.00044	1.86181
A51	2.20616	0.00009	-0.00083	-0.00024	-0.00109	2.20507
A52	2.21192	0.00001	-0.00011	-0.00020	-0.00033	2.21159
A53	1.56132	0.00000	-0.00011	0.00014	0.00003	1.56135
A54	1.56162	-0.00015	-0.00035	0.00007	-0.00028	1.56135
A55	1.98283	0.00000	0.00002	-0.00005	-0.00002	1.98280
A56	2.35506	-0.00003	-0.00012	0.00001	-0.00011	2.35495
A57	1.94530	0.00002	0.00010	0.00003	0.00013	1.94543
A58	2.35510	-0.00008	-0.00013	0.00000	-0.00013	2.35498
A59	1.94538	0.00000	0.00005	0.00002	0.00007	1.94544
A60	1.98270	0.00008	0.00008	-0.00002	0.00006	1.98277
A61	1.97058	0.00002	0.00008	-0.00005	0.00002	1.97060
A62	2.39136	0.00000	-0.00008	0.00011	0.00002	2.39138
A63	1.92122	-0.00002	-0.00001	-0.00006	-0.00006	1.92116
A64	1.96452	0.00003	0.00008	-0.00002	0.00006	1.96458
A65	2.45173	0.00000	-0.00007	0.00003	-0.00005	2.45168
A66	1.86691	-0.00002	0.00000	-0.00001	-0.00001	1.86690
A67	1.85753	0.00000	-0.00008	0.00000	-0.00008	1.85745
A68	2.46711	0.00005	0.00006	0.00008	0.00014	2.46726
A69	1.95854	-0.00004	0.00002	-0.00008	-0.00006	1.95848
A70	1.98446	0.00000	0.00009	-0.00011	-0.00002	1.98444
A71	1.91745	-0.00009	-0.00002	-0.00006	-0.00008	1.91738
A72	2.38126	0.00009	-0.00008	0.00018	0.00009	2.38135
A73	1.95956	-0.00010	-0.00009	0.00004	-0.00005	1.95952
A74	2.19802	0.00006	-0.00001	0.00004	0.00003	2.19805
A75	2.12560	0.00004	0.00010	-0.00009	0.00002	2.12561
A76	1.95026	0.00010	0.00016	-0.00020	-0.00004	1.95022
A77	2.08329	0.00035	-0.00033	0.00060	0.00027	2.08356
A78	2.24964	-0.00045	0.00016	-0.00040	-0.00023	2.24941
A79	1.57195	0.00004	-0.00019	0.00035	0.00016	1.57210
A80	1.86155	0.00014	0.00002	0.00011	0.00013	1.86169
A81	2.21191	-0.00008	-0.00008	-0.00031	-0.00039	2.21152
A82	2.20585	-0.00007	-0.00039	-0.00049	-0.00089	2.20496
A83	2.34508	-0.00078	0.00031	-0.00109	-0.00078	2.34431
A84	1.92107	0.00040	-0.00040	0.00083	0.00043	1.92151
A85	2.01703	0.00038	0.00008	0.00026	0.00035	2.01737
A86	2.19429	-0.00066	-0.00017	-0.00054	-0.00071	2.19358
A87	2.20807	0.00042	-0.00005	0.00051	0.00047	2.20854
A88	1.88082	0.00024	0.00022	0.00003	0.00024	1.88106
A89	1.86271	-0.00003	0.00001	0.00002	0.00004	1.86275
A90	2.22646	-0.00013	0.00018	-0.00031	-0.00010	2.22636
A91	2.19401	0.00016	-0.00025	0.00029	0.00006	2.19408
A92	1.87085	-0.00021	-0.00016	-0.00013	-0.00029	1.87056
A93	2.23794	-0.00002	-0.00072	0.00070	-0.00003	2.23792
A94	2.17439	0.00023	0.00088	-0.00057	0.00031	2.17471
A95	1.91169	0.00001	0.00004	-0.00003	0.00001	1.91170
A96	2.22905	-0.00007	-0.00030	0.00020	-0.00010	2.22895
A97	2.14244	0.00007	0.00026	-0.00017	0.00009	2.14254
A98	1.89869	0.00000	-0.00011	0.00013	0.00002	1.89871
A99	2.30835	0.00007	0.00030	-0.00026	0.00005	2.30840
A100	2.07614	-0.00007	-0.00019	0.00013	-0.00006	2.07608
A101	2.05922	-0.00004	-0.00011	0.00004	-0.00006	2.05916
A102	2.08910	0.00003	0.00002	0.00005	0.00008	2.08917
A103	2.13487	0.00001	0.00008	-0.00010	-0.00001	2.13485
A104	2.06849	0.00002	0.00015	-0.00012	0.00004	2.06853
A105	2.13133	0.00000	-0.00010	0.00008	-0.00003	2.13130
A106	2.08336	-0.00002	-0.00005	0.00004	-0.00001	2.08335
A107	2.09535	-0.00004	-0.00024	0.00018	-0.00006	2.09529

A108	2.09785	0.00000	0.00015	-0.00019	-0.00004	2.09781
A109	2.08998	0.00004	0.00009	0.00001	0.00010	2.09008
A110	2.12472	0.00005	0.00012	-0.00007	0.00006	2.12478
A111	2.07376	-0.00004	-0.00002	-0.00006	-0.00008	2.07369
A112	2.08470	-0.00001	-0.00011	0.00013	0.00002	2.08472
A113	2.16714	-0.00003	-0.00065	0.00057	-0.00007	2.16707
A114	2.15604	0.00011	0.00062	-0.00036	0.00026	2.15629
A115	1.96001	-0.00009	0.00003	-0.00021	-0.00019	1.95982
A116	2.15589	0.00022	0.00102	-0.00056	0.00046	2.15635
A117	2.16700	-0.00008	-0.00024	0.00013	-0.00010	2.16690
A118	1.96029	-0.00014	-0.00078	0.00043	-0.00035	1.95994
A119	1.91226	0.00008	0.00022	-0.00005	0.00017	1.91243
A120	1.94910	-0.00011	0.00007	-0.00027	-0.00020	1.94890
A121	1.90457	0.00006	0.00004	0.00009	0.00013	1.90470
A122	1.90600	0.00001	-0.00010	0.00014	0.00004	1.90604
A123	1.88663	-0.00004	-0.00022	0.00008	-0.00014	1.88649
A124	1.90423	0.00000	-0.00002	0.00002	0.00000	1.90422
A125	1.94812	0.00015	0.00032	0.00016	0.00048	1.94860
A126	1.91254	-0.00003	-0.00011	0.00020	0.00009	1.91262
A127	1.90444	0.00002	-0.00021	0.00048	0.00026	1.90470
A128	1.90626	-0.00005	0.00003	-0.00021	-0.00019	1.90607
A129	1.90449	-0.00007	0.00000	-0.00024	-0.00024	1.90426
A130	1.88697	-0.00002	-0.00004	-0.00040	-0.00044	1.88654
A131	3.16619	0.00008	-0.00009	0.00066	0.00058	3.16677
A132	3.17702	0.00027	0.00156	0.00033	0.00189	3.17891
A133	3.17638	0.00033	0.00258	0.00050	0.00308	3.17946
A134	3.16776	-0.00008	-0.00171	0.00139	-0.00032	3.16744
A135	3.14152	0.00003	-0.00022	0.00012	-0.00010	3.14142
A136	3.14157	0.00000	0.00005	-0.00005	0.00001	3.14158
A137	3.14195	-0.00003	-0.00013	-0.00012	-0.00025	3.14170
A138	3.14155	-0.00003	-0.00013	0.00030	0.00017	3.14172
D1	0.00066	0.00001	-0.00041	0.00007	-0.00034	0.00032
D2	-3.13952	-0.00002	-0.00122	0.00029	-0.00093	-3.14045
D3	-3.14100	0.00000	-0.00016	-0.00039	-0.00055	-3.14155
D4	0.00200	-0.00002	-0.00096	-0.00017	-0.00114	0.00086
D5	-0.00039	0.00000	0.00029	-0.00003	0.00026	-0.00013
D6	3.14097	0.00000	0.00056	-0.00029	0.00027	3.14124
D7	3.14130	0.00000	-0.00004	0.00057	0.00053	-3.14136
D8	-0.00053	0.00000	0.00023	0.00031	0.00054	0.00001
D9	-0.00189	-0.00001	-0.00049	0.00282	0.00233	0.00044
D10	3.13720	0.00004	0.00004	0.00325	0.00329	3.14049
D11	3.13961	-0.00001	-0.00019	0.00227	0.00208	-3.14149
D12	-0.00448	0.00004	0.00034	0.00270	0.00304	-0.00144
D13	-0.00040	-0.00001	0.00022	-0.00008	0.00014	-0.00025
D14	3.14148	-0.00001	-0.00001	0.00009	0.00008	3.14156
D15	3.13952	0.00003	0.00118	-0.00034	0.00084	3.14036
D16	-0.00179	0.00003	0.00095	-0.00017	0.00078	-0.00101
D17	-0.00133	0.00005	0.00203	-0.00250	-0.00048	-0.00181
D18	3.13918	0.00009	0.00765	-0.00877	-0.00112	3.13806
D19	-3.14142	0.00002	0.00117	-0.00227	-0.00110	3.14066
D20	-0.00091	0.00006	0.00679	-0.00853	-0.00174	-0.00265
D21	-0.00013	0.00000	0.00009	0.00004	0.00013	0.00000
D22	-3.14132	0.00000	-0.00004	-0.00004	-0.00008	-3.14140
D23	3.14117	0.00000	0.00032	-0.00013	0.00019	3.14136
D24	-0.00002	0.00000	0.00020	-0.00022	-0.00002	-0.00004
D25	0.00039	0.00000	-0.00021	0.00000	-0.00021	0.00018
D26	-3.14117	0.00000	-0.00028	0.00005	-0.00023	-3.14140
D27	3.14158	0.00001	-0.00008	0.00008	0.00000	3.14158
D28	0.00002	0.00000	-0.00016	0.00014	-0.00002	0.00000
D29	-0.00012	0.00000	0.00001	-0.00001	0.00001	-0.00012

D30	-3.14149	0.00000	-0.00025	0.00024	-0.00001	-3.14150
D31	3.14143	0.00000	0.00009	-0.00006	0.00003	3.14146
D32	0.00007	0.00000	-0.00018	0.00019	0.00002	0.00009
D33	0.00104	0.00004	0.00174	-0.00432	-0.00259	-0.00155
D34	-3.13840	0.00006	0.00216	-0.00299	-0.00083	-3.13924
D35	-3.13793	-0.00001	0.00118	-0.00478	-0.00360	-3.14153
D36	0.00581	0.00001	0.00160	-0.00345	-0.00185	0.00397
D37	0.00258	-0.00002	-0.00120	-0.00043	-0.00164	0.00094
D38	-3.13785	-0.00007	-0.00215	0.00029	-0.00186	-3.13970
D39	3.14113	0.00003	-0.00056	0.00009	-0.00046	3.14067
D40	0.00070	-0.00001	-0.00150	0.00082	-0.00068	0.00002
D41	0.00013	-0.00005	-0.00229	0.00421	0.00192	0.00204
D42	3.13959	-0.00007	-0.00271	0.00290	0.00018	3.13978
D43	-3.14036	-0.00009	-0.00805	0.01062	0.00257	-3.13779
D44	-0.00089	-0.00011	-0.00847	0.00931	0.00083	-0.00006
D45	-3.13094	-0.00042	-0.01021	-0.00386	-0.01407	3.13818
D46	-0.00722	0.00009	0.00457	0.00530	0.00987	0.00264
D47	0.01318	-0.00039	-0.00971	-0.00230	-0.01201	0.00116
D48	3.13689	0.00012	0.00506	0.00686	0.01192	-3.13438
D49	0.00881	-0.00018	-0.00532	-0.00793	-0.01325	-0.00445
D50	-3.13765	-0.00003	-0.00165	-0.00653	-0.00818	3.13735
D51	-3.11562	-0.00067	-0.01951	-0.01673	-0.03623	3.13133
D52	0.02111	-0.00052	-0.01583	-0.01533	-0.03116	-0.01006
D53	-3.13931	-0.00015	-0.00075	0.00177	0.00102	-3.13829
D54	0.00685	-0.00029	-0.00420	0.00046	-0.00373	0.00311
D55	3.14104	0.00018	0.00182	-0.00152	0.00030	3.14134
D56	0.00462	0.00002	0.00107	-0.00297	-0.00190	0.00272
D57	-0.00464	0.00030	0.00490	-0.00035	0.00455	-0.00009
D58	-3.14105	0.00015	0.00415	-0.00180	0.00235	-3.13870
D59	0.00624	-0.00008	-0.00016	0.00035	0.00020	0.00644
D60	-3.12925	-0.00013	-0.00094	0.00202	0.00108	-3.12817
D61	-3.13485	-0.00005	-0.00144	0.00159	0.00015	-3.13470
D62	0.01285	-0.00010	-0.00222	0.00326	0.00103	0.01388
D63	-0.00731	0.00021	0.00246	-0.00046	0.00200	-0.00531
D64	3.13351	0.00017	0.00443	-0.00236	0.00207	3.13558
D65	0.00027	0.00001	-0.00114	0.00160	0.00046	0.00073
D66	-3.13483	0.00002	0.00224	-0.00301	-0.00077	-3.13560
D67	-3.14058	0.00005	-0.00304	0.00344	0.00040	-3.14018
D68	0.00751	0.00006	0.00034	-0.00117	-0.00083	0.00668
D69	-0.00091	-0.00015	-0.00310	0.00001	-0.00309	-0.00401
D70	3.13525	0.00002	-0.00231	0.00153	-0.00078	3.13446
D71	3.13235	-0.00008	-0.00203	-0.00227	-0.00430	3.12805
D72	-0.01468	0.00008	-0.00124	-0.00074	-0.00198	-0.01666
D73	-0.02098	0.00016	0.00475	-0.00689	-0.00213	-0.02311
D74	-3.08550	0.00019	0.01413	0.00562	0.01975	-3.06575
D75	3.12872	0.00010	0.00371	-0.00467	-0.00096	3.12776
D76	0.06420	0.00013	0.01309	0.00783	0.02092	0.08512
D77	-0.01342	0.00009	0.00416	-0.00599	-0.00182	-0.01524
D78	3.13722	0.00002	0.00159	-0.00250	-0.00092	3.13630
D79	3.12370	0.00008	0.00184	-0.00281	-0.00098	3.12272
D80	-0.00885	0.00001	-0.00074	0.00067	-0.00007	-0.00892
D81	-3.14153	0.00000	-0.00196	0.00422	0.00226	-3.13927
D82	0.00679	0.00001	0.00155	-0.00056	0.00099	0.00778
D83	0.02117	-0.00015	-0.00549	0.00792	0.00243	0.02360
D84	3.08536	-0.00018	-0.01497	-0.00464	-0.01960	3.06576
D85	-3.13265	-0.00005	-0.00201	0.00321	0.00120	-3.13144
D86	-0.06845	-0.00008	-0.01148	-0.00935	-0.02083	-0.08928
D87	-3.13619	0.00006	0.00178	-0.00148	0.00029	-3.13590
D88	0.00629	-0.00003	-0.00079	-0.00042	-0.00121	0.00508
D89	0.01787	-0.00005	-0.00177	0.00332	0.00154	0.01941

D90	-3.12284	-0.00013	-0.00434	0.00438	0.00004	-3.12280
D91	1.55530	-0.00001	-0.00961	-0.00631	-0.01593	1.53938
D92	-2.61396	0.00001	-0.00944	-0.00635	-0.01579	-2.62975
D93	-0.55096	-0.00003	-0.00968	-0.00643	-0.01611	-0.56707
D94	-1.49414	0.00003	0.00161	0.00865	0.01026	-1.48388
D95	0.61978	0.00005	0.00178	0.00861	0.01040	0.63018
D96	2.68278	0.00002	0.00155	0.00853	0.01007	2.69285
D97	-0.00327	-0.00003	-0.00203	0.00033	-0.00170	-0.00497
D98	3.13836	-0.00003	-0.00022	-0.00063	-0.00085	3.13751
D99	-3.13599	-0.00005	-0.00120	-0.00028	-0.00148	-3.13747
D100	0.00470	0.00004	0.00141	-0.00136	0.00005	0.00475
D101	-0.00780	-0.00004	-0.00110	0.00083	-0.00026	-0.00807
D102	-3.13998	-0.00001	-0.00196	0.00054	-0.00143	-3.14141
D103	-0.00107	0.00003	0.00199	-0.00001	0.00198	0.00091
D104	3.14121	-0.00003	0.00001	0.00081	0.00082	-3.14115
D105	3.14049	0.00004	0.00062	0.00072	0.00134	-3.14136
D106	-0.00041	-0.00003	-0.00137	0.00154	0.00017	-0.00024
D107	3.13596	0.00000	-0.00127	0.00006	-0.00121	3.13474
D108	-0.01385	-0.00005	-0.00297	-0.00077	-0.00373	-0.01758
D109	-0.00560	0.00000	0.00051	-0.00089	-0.00038	-0.00597
D110	3.12779	-0.00006	-0.00118	-0.00171	-0.00290	3.12489
D111	0.00923	0.00003	0.00056	-0.00014	0.00042	0.00965
D112	-3.13863	0.00001	0.00113	0.00006	0.00119	-3.13743
D113	-3.12640	0.00007	0.00179	0.00046	0.00225	-3.12416
D114	0.00893	0.00005	0.00236	0.00066	0.00302	0.01195
D115	3.13552	-0.00008	-0.00246	0.00011	-0.00236	3.13316
D116	0.08397	0.00002	0.00204	0.00812	0.01016	0.09413
D117	-0.01412	-0.00013	-0.00413	-0.00070	-0.00483	-0.01895
D118	-3.06567	-0.00003	0.00038	0.00731	0.00769	-3.05798
D119	3.13238	0.00002	0.00118	-0.00006	0.00113	3.13350
D120	-0.00759	0.00008	0.00131	0.00017	0.00148	-0.00611
D121	-0.00013	0.00005	0.00034	-0.00034	0.00000	-0.00013
D122	-3.14009	0.00010	0.00047	-0.00011	0.00035	-3.13974
D123	3.13837	-0.00013	-0.00191	-0.00063	-0.00254	3.13583
D124	-0.00863	-0.00013	-0.00292	-0.00008	-0.00300	-0.01163
D125	-0.00432	-0.00017	-0.00199	-0.00079	-0.00278	-0.00709
D126	3.13187	-0.00017	-0.00300	-0.00023	-0.00323	3.12863
D127	-3.13944	0.00009	0.00066	0.00057	0.00123	-3.13821
D128	0.00384	0.00015	0.00079	0.00081	0.00159	0.00543
D129	0.00230	0.00009	0.00241	0.00027	0.00268	0.00498
D130	-3.13817	0.00015	0.00184	0.00316	0.00501	-3.13317
D131	-3.13191	0.00009	0.00379	-0.00048	0.00331	-3.12860
D132	0.01080	0.00015	0.00322	0.00241	0.00563	0.01643
D133	0.01403	0.00016	0.00435	0.00048	0.00483	0.01886
D134	3.06599	0.00006	-0.00012	-0.00748	-0.00760	3.05839
D135	-3.13475	0.00016	0.00301	0.00121	0.00422	-3.13053
D136	-0.08279	0.00006	-0.00146	-0.00675	-0.00821	-0.09100
D137	0.00065	0.00003	-0.00177	0.00034	-0.00142	-0.00078
D138	3.13934	0.00015	0.00283	0.00026	0.00310	-3.14075
D139	3.14118	-0.00003	-0.00123	-0.00241	-0.00364	3.13754
D140	-0.00332	0.00009	0.00337	-0.00249	0.00088	-0.00244
D141	-0.00258	-0.00010	0.00055	-0.00066	-0.00012	-0.00270
D142	-3.14093	-0.00024	-0.00460	-0.00057	-0.00518	3.13708
D143	-3.11986	-0.00050	-0.02080	-0.00272	-0.02352	3.13980
D144	0.02402	-0.00058	-0.02201	-0.00334	-0.02534	-0.00132
D145	0.01827	-0.00035	-0.01532	-0.00282	-0.01813	0.00014
D146	-3.12104	-0.00043	-0.01652	-0.00343	-0.01995	-3.14099
D147	-0.62294	-0.00006	-0.00059	-0.00556	-0.00615	-0.62908
D148	1.49111	-0.00006	-0.00051	-0.00560	-0.00611	1.48500
D149	-2.68543	-0.00009	-0.00047	-0.00569	-0.00615	-2.69158

D150	2.62587	0.00005	0.00475	0.00394	0.00870	2.63457
D151	-1.54326	0.00005	0.00483	0.00390	0.00873	-1.53453
D152	0.56338	0.00002	0.00487	0.00382	0.00869	0.57207
D153	0.00239	-0.00033	-0.00264	-0.00129	-0.00393	-0.00155
D154	-3.13576	-0.00032	-0.00259	-0.00248	-0.00507	-3.14084
D155	-3.14158	-0.00025	-0.00139	-0.00065	-0.00204	3.13956
D156	0.00345	-0.00024	-0.00134	-0.00184	-0.00318	0.00027
D157	-3.13319	-0.00010	-0.00124	-0.00408	-0.00532	-3.13851
D158	0.00773	-0.00012	-0.00337	-0.00026	-0.00362	0.00411
D159	0.00550	-0.00011	-0.00128	-0.00308	-0.00436	0.00114
D160	-3.13677	-0.00013	-0.00341	0.00075	-0.00266	-3.13943
D161	3.13265	0.00009	0.00150	0.00362	0.00512	3.13777
D162	-0.00951	0.00002	0.00067	0.00369	0.00437	-0.00514
D163	-0.00601	0.00010	0.00154	0.00261	0.00415	-0.00185
D164	3.13502	0.00002	0.00072	0.00268	0.00340	3.13842
D165	-0.00288	0.00008	0.00053	0.00242	0.00294	0.00006
D166	3.13832	0.00004	0.00038	0.00190	0.00228	3.14061
D167	3.13937	0.00010	0.00260	-0.00132	0.00128	3.14065
D168	-0.00261	0.00006	0.00246	-0.00184	0.00062	-0.00199
D169	0.00429	-0.00005	-0.00124	-0.00113	-0.00237	0.00192
D170	-3.13732	-0.00005	-0.00097	-0.00123	-0.00220	-3.13952
D171	-3.13676	0.00002	-0.00045	-0.00120	-0.00165	-3.13841
D172	0.00481	0.00002	-0.00018	-0.00130	-0.00148	0.00334
D173	-0.00113	0.00000	0.00057	0.00002	0.00059	-0.00053
D174	3.14098	0.00006	0.00090	-0.00016	0.00074	-3.14146
D175	3.13981	-0.00009	-0.00039	0.00011	-0.00028	3.13952
D176	-0.00127	-0.00003	-0.00007	-0.00007	-0.00014	-0.00141
D177	-0.00085	-0.00002	0.00044	-0.00081	-0.00037	-0.00122
D178	3.14076	-0.00002	0.00021	-0.00073	-0.00052	3.14024
D179	3.14111	0.00002	0.00057	-0.00032	0.00025	3.14136
D180	-0.00047	0.00001	0.00034	-0.00024	0.00010	-0.00037
D181	-3.14078	0.00003	0.00006	0.00062	0.00068	-3.14011
D182	0.00070	0.00003	0.00008	0.00055	0.00062	0.00133
D183	0.00038	-0.00001	-0.00010	0.00004	-0.00006	0.00031
D184	-3.14132	-0.00001	-0.00008	-0.00004	-0.00012	-3.14144
D185	-3.14135	-0.00001	-0.00063	0.00036	-0.00027	3.14156
D186	0.00054	-0.00001	-0.00050	0.00018	-0.00032	0.00021
D187	0.00022	-0.00001	-0.00034	0.00026	-0.00008	0.00013
D188	-3.14108	-0.00001	-0.00021	0.00008	-0.00014	-3.14121
D189	-0.00005	0.00000	-0.00014	0.00015	0.00001	-0.00003
D190	3.14121	0.00000	0.00004	0.00011	0.00015	3.14136
D191	-3.14153	0.00001	-0.00015	0.00022	0.00007	-3.14146
D192	-0.00027	0.00001	0.00002	0.00018	0.00020	-0.00007
D193	0.00010	0.00000	0.00011	-0.00008	0.00004	0.00014
D194	-3.14137	0.00000	0.00009	-0.00014	-0.00005	-3.14142
D195	3.14140	0.00000	-0.00001	0.00010	0.00009	3.14149
D196	-0.00007	0.00000	-0.00003	0.00003	0.00000	-0.00007
D197	-0.00019	0.00000	0.00013	-0.00013	0.00000	-0.00019
D198	3.14128	0.00000	0.00015	-0.00006	0.00009	3.14137
D199	-3.14145	0.00000	-0.00005	-0.00009	-0.00013	-3.14158
D200	0.00002	0.00000	-0.00002	-0.00002	-0.00005	-0.00002

Item	Value	Threshold	Converged?

Maximum Force	0.000958	0.000450	NO
RMS Force	0.000155	0.000300	YES
Maximum Displacement	0.132736	0.001800	NO
RMS Displacement	0.032618	0.001200	NO

Predicted change in Energy=-7.150070D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.803822	-0.637691	0.005344
2	6	0	-9.994766	-1.788528	-0.003045
3	6	0	-10.517350	-3.073540	-0.004388
4	6	0	-11.906286	-3.215844	0.003267
5	6	0	-12.727341	-2.081476	0.011970
6	6	0	-12.195241	-0.787900	0.013067
7	1	0	-9.846802	-3.926738	-0.011034
8	1	0	-12.353799	-4.204927	0.002682
9	1	0	-13.806127	-2.203441	0.018062
10	1	0	-12.864652	0.060460	0.020000
11	6	0	-9.927399	0.563911	0.004365
12	6	0	-8.570408	-1.391375	-0.008588
13	6	0	-8.540711	0.088344	-0.005666
14	6	0	-7.404565	0.870133	-0.007093
15	6	0	-6.014849	0.595901	-0.012512
16	6	0	-3.644716	-0.183869	-0.015585
17	6	0	-3.778788	1.228805	-0.022163
18	16	0	-5.182702	-0.989044	-0.013800
19	6	0	-5.099982	1.665134	-0.017549
20	6	0	-2.267531	-0.451403	-0.012077
21	6	0	-1.604286	0.797980	-0.015599
22	7	0	-2.524411	1.821056	-0.040837
23	16	0	-1.151274	-1.806519	-0.010814
24	16	0	1.150757	1.806808	0.003056
25	6	0	0.198121	-0.673403	-0.001341
26	6	0	-0.198700	0.673727	-0.005707
27	6	0	1.603763	-0.797646	0.008863
28	6	0	2.266935	0.451673	0.004413
29	6	0	3.644007	0.184143	0.009860
30	6	0	3.778243	-1.228347	0.017678
31	6	0	5.099569	-1.664614	0.016508
32	6	0	6.014333	-0.595221	0.014233
33	16	0	5.181736	0.989493	0.012282
34	7	0	2.523926	-1.820839	0.032280
35	6	0	7.404700	-0.869632	0.011764
36	6	0	8.540825	-0.088314	0.007457
37	6	0	8.570949	1.391428	0.002159
38	6	0	9.927542	-0.564274	0.004564
39	6	0	9.995460	1.788104	-0.005534
40	6	0	10.804194	0.637102	-0.005176
41	6	0	10.518444	3.072969	-0.013418
42	6	0	12.195817	0.786857	-0.013532
43	6	0	11.907384	3.214837	-0.021664
44	6	0	12.728231	2.080217	-0.021770
45	6	0	10.384713	-1.871150	0.011106
46	6	0	9.533693	-3.018892	0.022896
47	6	0	11.769388	-2.223248	0.007569
48	7	0	8.863248	-3.972366	0.032538
49	7	0	12.886989	-2.552282	0.004948
50	6	0	-10.384559	1.870701	0.010026

51	6	0	-11.769060	2.222768	0.018688
52	6	0	-9.533399	3.018325	0.006788
53	7	0	-12.886454	2.552425	0.025706
54	7	0	-8.863442	3.972195	0.004393
55	8	0	-7.613473	-2.158107	-0.012733
56	8	0	7.614336	2.158590	0.004716
57	6	0	2.243037	-3.243234	-0.053498
58	1	0	1.312596	-3.464911	0.473738
59	1	0	2.156141	-3.576249	-1.093367
60	1	0	3.048523	-3.797009	0.432940
61	6	0	-2.243170	3.243914	0.036133
62	1	0	-2.151038	3.582001	1.073894
63	1	0	-1.315465	3.463093	-0.496921
64	1	0	-3.051235	3.795141	-0.448901
65	1	0	5.428485	-2.697281	0.014182
66	1	0	12.864977	-0.061746	-0.014020
67	1	0	13.807042	2.201947	-0.028433
68	1	0	12.355201	4.203760	-0.028203
69	1	0	9.848095	3.926344	-0.013164
70	1	0	7.572845	-1.939762	0.013352
71	1	0	-7.572647	1.940228	0.002573
72	1	0	-5.428799	2.697830	-0.014902

Rotational constants (GHZ): 0.1750010 0.0104029 0.0098205

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis func-
tions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6569.4716810395 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T

Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6569.3867743085 Har-
trees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.25D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Initial guess from the checkpoint file: "PBDB.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000017 0.000001 -0.000018 Ang= 0.00 deg.

ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1

AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for in-
itial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-
yADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 IlCent= 200000004 NGrid=

0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0=

0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 Integral accuracy reduced to 1.0D-05 until final iterations.
 Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
 SCF Done: E(RB3LYP) = -3683.02011395 A.U. after 12 cycles
 NFock= 12 Conv=0.37D-08 -V/T= 2.0068
 Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1
 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	0.000025375	-0.000014410	-0.000030485
2	6	0.000032227	-0.000038177	0.000017189
3	6	0.000013919	-0.000019841	-0.000017785
4	6	-0.000022254	-0.000006291	-0.000017482
5	6	0.000013126	0.000021270	0.000023319
6	6	0.000014196	-0.000038476	-0.000005596
7	1	0.000005006	-0.000001335	-0.000004318
8	1	-0.000002817	0.000001440	0.000005717
9	1	-0.000003532	-0.000003154	-0.000000363
10	1	-0.000013360	-0.000007258	-0.000007389
11	6	-0.000063932	-0.000010021	0.000200865
12	6	-0.000026558	-0.000102550	-0.000011688
13	6	0.000171370	-0.000160350	-0.000129361
14	6	0.000068519	0.000400734	-0.000506273
15	6	-0.000021259	0.000004762	0.000300001
16	6	0.000076900	-0.000010589	-0.000113610
17	6	-0.000152488	0.000022699	0.000255597
18	16	0.000032147	-0.000080390	0.000105612
19	6	0.000077918	-0.000069795	-0.000081333
20	6	0.000118233	0.000031110	-0.000198753
21	6	-0.000144095	-0.000006681	0.000342384
22	7	0.000038818	0.000012015	-0.000206979
23	16	0.000000228	-0.000007228	-0.000008683
24	16	0.000015304	0.000006020	-0.000047477
25	6	0.000094718	-0.000014984	-0.000019342
26	6	-0.000096680	-0.000001330	0.000077494
27	6	-0.000139926	0.000052684	0.000027725
28	6	-0.000048723	0.000015813	-0.000029856
29	6	0.000073940	-0.000056727	-0.000024331
30	6	0.000022925	0.000000576	0.000104336
31	6	-0.000029639	-0.000008736	-0.000003341
32	6	0.000139793	-0.000103631	0.000120878
33	16	0.000005987	-0.000048944	0.000024170
34	7	0.000083899	-0.000005934	-0.000078595
35	6	-0.000103565	-0.000006361	-0.000071389
36	6	-0.000040357	0.000014961	0.000030247
37	6	0.000097335	0.000061052	-0.000167006
38	6	0.000016986	0.000027094	-0.000025109
39	6	-0.000103206	0.000006416	0.000025111
40	6	0.000080306	-0.000017274	0.000079998
41	6	-0.000010722	0.000039496	-0.000003261
42	6	-0.000054129	0.000112765	-0.000037910
43	6	0.000045768	-0.000002849	0.000030211
44	6	-0.000049172	-0.000032357	-0.000039730
45	6	0.000138393	0.000011585	0.000113156
46	6	-0.000028023	-0.000096986	-0.000020536
47	6	-0.000152469	0.000009796	-0.000124133

48	7	0.000003448	0.000013634	0.000003724
49	7	-0.000015037	0.000037171	-0.000003888
50	6	-0.000113282	-0.000028100	-0.000070084
51	6	0.000088668	-0.000013750	0.000054447
52	6	-0.000036084	0.000044768	-0.000042111
53	7	0.000006414	-0.000000076	-0.000000431
54	7	0.000009443	-0.000006361	0.000014718
55	8	-0.000068668	0.000009853	0.000042465
56	8	0.000019405	0.000032530	0.000087095
57	6	-0.000008102	0.000001316	-0.000022275
58	1	0.000019067	0.000014970	-0.000002678
59	1	-0.000013622	-0.000002009	-0.000004014
60	1	-0.000010332	0.000000746	0.000013324
61	6	0.000116637	0.000038511	-0.000100384
62	1	-0.000008964	-0.000044126	-0.000015781
63	1	-0.000000264	-0.000007046	0.000031569
64	1	0.000018577	0.000015676	-0.000009324
65	1	0.000013286	0.000001738	-0.000002475
66	1	-0.000003981	-0.000003691	-0.000006779
67	1	0.000003582	0.000007596	0.000003219
68	1	-0.000003240	-0.000001116	-0.000009614
69	1	-0.000006810	-0.000004797	0.000003628
70	1	-0.000020195	-0.000019685	-0.000008761
71	1	-0.000193906	0.000030962	0.000223074
72	1	0.000007524	0.000001657	-0.000030558

Cartesian Forces: Max 0.000506273 RMS 0.000084321

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000357856 RMS 0.000049796

Search for a local minimum.

Step number 26 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 16 18 17 19 20

21 22 23 24 25

26

DE= -6.29D-05 DEPred=-7.15D-05 R= 8.80D-01

TightC=F SS= 1.41D+00 RLast= 9.56D-02 DXNew= 3.9112D-01 2.8675D-01

Trust test= 8.80D-01 RLast= 9.56D-02 DXMaxT set to 2.87D-01

ITU= 1 -1 1 -1 1 1 -1 0 -1 0 -1 1 1 1 1 1 1 0 0 0

ITU= 1 0 0 0 1 0

Eigenvalues ---	0.00237	0.00262	0.00268	0.00385	0.00393
Eigenvalues ---	0.00438	0.00480	0.00497	0.00514	0.00567
Eigenvalues ---	0.00580	0.00601	0.00618	0.00635	0.00648
Eigenvalues ---	0.00681	0.00713	0.00744	0.00745	0.00749
Eigenvalues ---	0.00767	0.00772	0.00775	0.00784	0.00810
Eigenvalues ---	0.00827	0.00863	0.01037	0.01059	0.01095
Eigenvalues ---	0.01133	0.01160	0.01226	0.01288	0.01315
Eigenvalues ---	0.01332	0.01361	0.01380	0.01457	0.01460
Eigenvalues ---	0.01466	0.01602	0.01630	0.01647	0.01744
Eigenvalues ---	0.01748	0.01794	0.01923	0.01948	0.01993
Eigenvalues ---	0.02009	0.02021	0.02061	0.02074	0.02180
Eigenvalues ---	0.02210	0.02850	0.03475	0.03582	0.03923
Eigenvalues ---	0.03949	0.04829	0.04838	0.04909	0.04983
Eigenvalues ---	0.05011	0.05043	0.05115	0.05343	0.07054

Eigenvalues	---	0.07234	0.07388	0.07567	0.15465	0.15739
Eigenvalues	---	0.15930	0.15986	0.15993	0.16000	0.16000
Eigenvalues	---	0.16000	0.16000	0.16000	0.16000	0.16001
Eigenvalues	---	0.16001	0.16007	0.16010	0.16025	0.16051
Eigenvalues	---	0.16080	0.18768	0.19046	0.19560	0.20047
Eigenvalues	---	0.20675	0.21297	0.21644	0.21970	0.21995
Eigenvalues	---	0.22016	0.22289	0.22440	0.22580	0.22634
Eigenvalues	---	0.22648	0.22710	0.22832	0.23051	0.23245
Eigenvalues	---	0.23331	0.23490	0.23736	0.23895	0.24016
Eigenvalues	---	0.24127	0.24269	0.24304	0.24404	0.24498
Eigenvalues	---	0.24564	0.24601	0.24647	0.24752	0.24862
Eigenvalues	---	0.24913	0.24948	0.24968	0.24984	0.24993
Eigenvalues	---	0.24995	0.24997	0.24999	0.24999	0.25000
Eigenvalues	---	0.25000	0.25000	0.25000	0.25001	0.25011
Eigenvalues	---	0.25030	0.25259	0.25593	0.25902	0.26142
Eigenvalues	---	0.26224	0.26562	0.26801	0.26864	0.27120
Eigenvalues	---	0.27231	0.27729	0.27839	0.28324	0.28497
Eigenvalues	---	0.28537	0.28849	0.29951	0.30324	0.31862
Eigenvalues	---	0.32904	0.35137	0.35468	0.36259	0.36305
Eigenvalues	---	0.36342	0.36474	0.36648	0.36695	0.36775
Eigenvalues	---	0.36829	0.37048	0.37086	0.37118	0.37252
Eigenvalues	---	0.37263	0.37406	0.37493	0.37568	0.37677
Eigenvalues	---	0.37758	0.38037	0.39005	0.40303	0.40847
Eigenvalues	---	0.41636	0.42037	0.42646	0.44419	0.44773
Eigenvalues	---	0.45596	0.46272	0.46646	0.47793	0.47973
Eigenvalues	---	0.48438	0.52223	0.53425	0.55369	0.57043
Eigenvalues	---	0.62754	0.66251	0.73139	0.80292	0.82018
Eigenvalues	---	0.90224	1.25853	1.26334	1.29347	1.35378
En-DIIS/RFO-DIIS IScMMF= 0 using points: 26 25 24 23 22						
RFO step: Lambda=-3.34784972D-06.						
DidBck=F Rises=F RFO-DIIS coefs: 0.66427 0.10894 0.13876 0.02828 0.05975						
Iteration 1	RMS (Cart)=	0.01117527	RMS (Int)=	0.00001959		
Iteration 2	RMS (Cart)=	0.00005095	RMS (Int)=	0.00000319		
Iteration 3	RMS (Cart)=	0.00000000	RMS (Int)=	0.00000319		
Variable	Old X	-DE/DX	Delta X	Delta X	Delta X	New X
(Linear)	(Quad)	(Total)				
R1	2.65845	-0.00002	-0.00001	0.00005	0.00003	2.65849
R2	2.64472	-0.00003	-0.00002	0.00005	0.00003	2.64474
R3	2.81053	-0.00007	0.00008	-0.00033	-0.00024	2.81029
R4	2.62145	-0.00002	-0.00003	0.00002	-0.00001	2.62144
R5	2.79434	-0.00006	-0.00007	-0.00011	-0.00019	2.79415
R6	2.63849	0.00001	-0.00001	0.00005	0.00003	2.63852
R7	2.05070	0.00000	0.00001	-0.00003	-0.00002	2.05069
R8	2.64629	-0.00002	0.00003	-0.00013	-0.00010	2.64619
R9	2.05151	0.00000	0.00001	-0.00001	0.00000	2.05151
R10	2.64323	0.00001	-0.00002	0.00007	0.00005	2.64328
R11	2.05163	0.00000	0.00001	-0.00002	-0.00001	2.05162
R12	2.04219	0.00002	0.00006	-0.00015	-0.00009	2.04210
R13	2.77035	-0.00002	-0.00006	0.00006	0.00001	2.77036
R14	2.61625	0.00005	0.00000	0.00017	0.00018	2.61643
R15	2.79683	-0.00011	-0.00013	-0.00012	-0.00025	2.79658
R16	2.31722	-0.00003	0.00005	-0.00017	-0.00012	2.31710
R17	2.60620	-0.00036	-0.00037	0.00015	-0.00021	2.60598
R18	2.67684	0.00023	0.00094	-0.00176	-0.00082	2.67602
R19	2.04706	-0.00004	-0.00001	-0.00007	-0.00008	2.04699
R20	3.38283	0.00004	0.00018	-0.00056	-0.00038	3.38245
R21	2.65926	0.00007	-0.00002	0.00024	0.00022	2.65948
R22	2.68159	-0.00002	0.00010	-0.00023	-0.00013	2.68146
R23	3.28057	-0.00007	-0.00025	0.00013	-0.00013	3.28045

R24	2.65116	-0.00005	0.00003	-0.00054	-0.00051	2.65065
R25	2.62934	0.00001	-0.00019	0.00038	0.00019	2.62953
R26	2.62160	-0.00001	-0.00004	0.00014	0.00010	2.62169
R27	2.04806	0.00001	0.00003	-0.00007	-0.00004	2.04802
R28	2.67305	-0.00005	0.00001	0.00000	0.00001	2.67306
R29	3.31773	-0.00001	-0.00008	0.00004	-0.00004	3.31769
R30	2.60066	0.00003	-0.00001	0.00008	0.00007	2.60073
R31	2.66660	-0.00006	-0.00035	0.00051	0.00016	2.66676
R32	2.74469	0.00000	0.00010	-0.00020	-0.00010	2.74459
R33	3.32984	-0.00001	-0.00007	0.00002	-0.00005	3.32979
R34	3.32988	-0.00001	-0.00003	-0.00002	-0.00005	3.32982
R35	3.31767	0.00000	-0.00009	0.00015	0.00006	3.31773
R36	2.65387	-0.00001	-0.00003	0.00010	0.00008	2.65395
R37	2.66670	-0.00008	-0.00005	-0.00059	-0.00063	2.66607
R38	2.67289	0.00002	-0.00002	0.00014	0.00012	2.67300
R39	2.60081	0.00002	-0.00019	0.00045	0.00026	2.60107
R40	2.65096	0.00006	-0.00037	0.00112	0.00076	2.65172
R41	2.68129	0.00005	-0.00005	0.00028	0.00023	2.68151
R42	3.28030	-0.00001	-0.00012	0.00013	0.00001	3.28031
R43	2.62953	-0.00004	-0.00042	0.00084	0.00041	2.62994
R44	2.62160	0.00002	-0.00016	0.00045	0.00028	2.62188
R45	2.65935	-0.00003	-0.00012	0.00033	0.00021	2.65956
R46	2.04806	0.00001	0.00000	0.00002	0.00002	2.04808
R47	3.38284	-0.00002	-0.00009	0.00013	0.00004	3.38288
R48	2.67810	-0.00029	-0.00049	-0.00018	-0.00067	2.67744
R49	2.74464	0.00000	0.00013	-0.00035	-0.00022	2.74442
R50	2.60567	-0.00022	-0.00011	-0.00013	-0.00024	2.60543
R51	2.04707	-0.00003	0.00000	-0.00010	-0.00010	2.04696
R52	2.79691	-0.00013	0.00007	-0.00064	-0.00057	2.79634
R53	2.77058	-0.00009	-0.00021	0.00023	0.00002	2.77060
R54	2.79439	-0.00008	-0.00008	-0.00008	-0.00016	2.79423
R55	2.31725	-0.00007	0.00002	-0.00016	-0.00014	2.31711
R56	2.81050	-0.00004	0.00004	-0.00014	-0.00010	2.81040
R57	2.61642	-0.00007	-0.00023	0.00059	0.00037	2.61679
R58	2.65831	0.00005	-0.00008	0.00033	0.00026	2.65857
R59	2.62152	-0.00003	-0.00005	-0.00011	-0.00016	2.62136
R60	2.64502	-0.00012	-0.00008	-0.00021	-0.00029	2.64472
R61	2.63842	0.00000	0.00000	0.00005	0.00005	2.63847
R62	2.05069	0.00000	0.00001	-0.00001	0.00000	2.05069
R63	2.64313	0.00003	-0.00004	0.00020	0.00016	2.64329
R64	2.04222	-0.00001	0.00010	-0.00030	-0.00020	2.04202
R65	2.64639	-0.00004	-0.00004	-0.00012	-0.00017	2.64623
R66	2.05151	0.00000	0.00001	-0.00001	0.00000	2.05151
R67	2.05163	0.00000	0.00001	-0.00002	-0.00001	2.05162
R68	2.70018	-0.00008	-0.00007	-0.00014	-0.00021	2.69998
R69	2.69993	-0.00021	-0.00014	-0.00039	-0.00053	2.69940
R70	2.20273	0.00001	0.00002	-0.00001	0.00001	2.20274
R71	2.20159	-0.00003	-0.00001	0.00002	0.00001	2.20160
R72	2.69964	-0.00011	-0.00007	-0.00026	-0.00033	2.69931
R73	2.70008	-0.00004	-0.00003	-0.00013	-0.00015	2.69992
R74	2.20159	0.00000	-0.00001	0.00001	0.00001	2.20160
R75	2.20274	0.00000	0.00001	-0.00002	0.00000	2.20274
R76	2.06391	0.00001	0.00001	-0.00001	0.00000	2.06391
R77	2.06990	0.00000	0.00002	-0.00002	0.00000	2.06990
R78	2.06326	-0.00001	0.00001	-0.00002	-0.00001	2.06325
R79	2.06987	0.00002	0.00001	0.00006	0.00007	2.06993
R80	2.06389	0.00003	-0.00001	0.00008	0.00007	2.06397
R81	2.06325	-0.00002	0.00001	-0.00003	-0.00002	2.06323
A1	2.07603	0.00002	-0.00004	0.00012	0.00008	2.07610
A2	1.89866	0.00001	-0.00003	0.00003	0.00000	1.89866

A3	2.30850	-0.00003	0.00008	-0.00015	-0.00008	2.30842
A4	2.14259	-0.00001	0.00004	-0.00012	-0.00007	2.14252
A5	1.91164	0.00000	0.00004	-0.00006	-0.00003	1.91160
A6	2.22896	0.00001	-0.00008	0.00018	0.00010	2.22906
A7	2.05913	0.00000	0.00000	0.00000	0.00000	2.05913
A8	2.08924	0.00000	0.00000	-0.00002	-0.00002	2.08922
A9	2.13481	0.00000	0.00000	0.00002	0.00002	2.13483
A10	2.09524	0.00000	-0.00003	0.00009	0.00006	2.09529
A11	2.09777	0.00000	0.00002	-0.00006	-0.00003	2.09774
A12	2.09017	0.00000	0.00001	-0.00004	-0.00002	2.09015
A13	2.12482	0.00000	0.00001	-0.00002	-0.00001	2.12481
A14	2.08476	0.00001	-0.00002	0.00004	0.00002	2.08478
A15	2.07361	0.00000	0.00001	-0.00002	-0.00001	2.07360
A16	2.06856	-0.00001	0.00002	-0.00008	-0.00006	2.06851
A17	2.13132	0.00000	-0.00001	0.00004	0.00003	2.13135
A18	2.08330	0.00001	-0.00001	0.00004	0.00003	2.08333
A19	1.87058	-0.00003	-0.00009	0.00006	-0.00002	1.87056
A20	2.17488	-0.00010	0.00015	-0.00056	-0.00042	2.17447
A21	2.23772	0.00013	-0.00006	0.00051	0.00044	2.23816
A22	1.86278	-0.00001	-0.00005	0.00007	0.00004	1.86282
A23	2.19418	-0.00002	-0.00004	-0.00015	-0.00015	2.19403
A24	2.22623	0.00003	0.00000	0.00007	0.00011	2.22634
A25	1.88112	0.00004	0.00010	-0.00008	0.00000	1.88112
A26	2.20850	0.00006	-0.00010	0.00031	0.00020	2.20871
A27	2.19356	-0.00010	0.00001	-0.00020	-0.00020	2.19335
A28	2.34406	-0.00002	0.00017	-0.00010	0.00007	2.34414
A29	2.01767	-0.00005	-0.00024	0.00014	-0.00009	2.01757
A30	1.92144	0.00006	0.00003	-0.00001	0.00003	1.92147
A31	2.24909	0.00005	-0.00003	0.00023	0.00020	2.24929
A32	2.08373	-0.00001	-0.00001	-0.00007	-0.00008	2.08365
A33	1.95036	-0.00004	0.00004	-0.00016	-0.00012	1.95024
A34	1.95846	0.00001	-0.00009	0.00021	0.00012	1.95858
A35	1.85730	0.00003	0.00008	-0.00006	0.00003	1.85733
A36	2.46742	-0.00004	0.00001	-0.00015	-0.00015	2.46727
A37	1.98437	0.00002	0.00022	-0.00045	-0.00023	1.98414
A38	1.91732	-0.00002	-0.00014	0.00036	0.00022	1.91755
A39	2.38146	0.00000	-0.00008	0.00010	0.00002	2.38148
A40	1.57198	0.00002	0.00000	0.00012	0.00012	1.57210
A41	1.95958	-0.00001	-0.00017	0.00028	0.00010	1.95968
A42	2.12557	0.00000	0.00009	-0.00023	-0.00013	2.12543
A43	2.19803	0.00001	0.00008	-0.00004	0.00004	2.19807
A44	1.86694	-0.00001	-0.00003	0.00005	0.00003	1.86697
A45	2.45171	0.00001	0.00004	-0.00008	-0.00005	2.45166
A46	1.96452	0.00000	-0.00002	0.00002	0.00000	1.96452
A47	1.92108	0.00001	-0.00003	0.00021	0.00019	1.92127
A48	1.97062	0.00002	0.00005	-0.00011	-0.00006	1.97057
A49	2.39142	-0.00003	-0.00002	-0.00008	-0.00010	2.39132
A50	1.86181	-0.00001	0.00016	-0.00051	-0.00035	1.86146
A51	2.20507	0.00007	0.00010	-0.00039	-0.00029	2.20478
A52	2.21159	-0.00005	0.00008	-0.00051	-0.00042	2.21117
A53	1.56135	-0.00001	-0.00005	0.00012	0.00007	1.56142
A54	1.56135	-0.00003	0.00000	-0.00013	-0.00013	1.56122
A55	1.98280	0.00000	0.00002	-0.00008	-0.00006	1.98274
A56	2.35495	0.00001	0.00000	0.00000	-0.00001	2.35494
A57	1.94543	0.00000	-0.00002	0.00008	0.00006	1.94550
A58	2.35498	-0.00002	0.00000	-0.00005	-0.00005	2.35493
A59	1.94544	0.00000	0.00000	0.00002	0.00002	1.94546
A60	1.98277	0.00002	0.00000	0.00002	0.00003	1.98279
A61	1.97060	0.00001	0.00001	0.00004	0.00004	1.97065
A62	2.39138	-0.00001	-0.00003	0.00004	0.00002	2.39140

A63	1.92116	0.00000	0.00003	-0.00009	-0.00007	1.92109
A64	1.96458	0.00000	0.00001	-0.00001	-0.00001	1.96458
A65	2.45168	0.00000	-0.00001	0.00006	0.00005	2.45173
A66	1.86690	0.00000	0.00000	-0.00004	-0.00004	1.86686
A67	1.85745	-0.00001	0.00000	-0.00003	-0.00002	1.85742
A68	2.46726	-0.00001	-0.00004	0.00008	0.00004	2.46730
A69	1.95848	0.00001	0.00003	-0.00005	-0.00002	1.95846
A70	1.98444	0.00000	0.00004	-0.00009	-0.00005	1.98439
A71	1.91738	-0.00001	0.00003	-0.00016	-0.00014	1.91724
A72	2.38135	0.00002	-0.00007	0.00024	0.00017	2.38152
A73	1.95952	-0.00003	-0.00002	-0.00004	-0.00006	1.95946
A74	2.19805	0.00002	-0.00002	0.00015	0.00013	2.19819
A75	2.12561	0.00001	0.00004	-0.00011	-0.00007	2.12554
A76	1.95022	0.00006	0.00008	-0.00008	-0.00001	1.95021
A77	2.08356	0.00006	-0.00019	0.00067	0.00048	2.08404
A78	2.24941	-0.00011	0.00011	-0.00059	-0.00048	2.24893
A79	1.57210	-0.00004	-0.00013	0.00025	0.00013	1.57223
A80	1.86169	0.00002	-0.00006	0.00023	0.00017	1.86186
A81	2.21152	-0.00004	0.00012	-0.00048	-0.00036	2.21117
A82	2.20496	0.00001	0.00017	-0.00054	-0.00036	2.20460
A83	2.34431	-0.00022	0.00033	-0.00140	-0.00107	2.34324
A84	1.92151	0.00011	-0.00026	0.00093	0.00067	1.92218
A85	2.01737	0.00011	-0.00007	0.00046	0.00040	2.01777
A86	2.19358	-0.00017	0.00018	-0.00100	-0.00082	2.19276
A87	2.20854	0.00009	-0.00016	0.00070	0.00053	2.20907
A88	1.88106	0.00008	-0.00002	0.00031	0.00029	1.88135
A89	1.86275	-0.00001	-0.00001	-0.00001	-0.00002	1.86273
A90	2.22636	-0.00003	0.00009	-0.00031	-0.00022	2.22614
A91	2.19408	0.00005	-0.00008	0.00032	0.00023	2.19431
A92	1.87056	-0.00004	0.00004	-0.00026	-0.00022	1.87034
A93	2.23792	-0.00001	-0.00019	0.00051	0.00032	2.23824
A94	2.17471	0.00005	0.00015	-0.00025	-0.00010	2.17461
A95	1.91170	-0.00001	0.00001	-0.00006	-0.00005	1.91165
A96	2.22895	0.00000	-0.00005	0.00009	0.00004	2.22899
A97	2.14254	0.00002	0.00004	-0.00003	0.00001	2.14255
A98	1.89871	-0.00001	-0.00003	0.00002	-0.00001	1.89870
A99	2.30840	0.00002	0.00006	-0.00008	-0.00001	2.30838
A100	2.07608	-0.00001	-0.00003	0.00006	0.00002	2.07610
A101	2.05916	-0.00002	-0.00001	-0.00004	-0.00005	2.05911
A102	2.08917	0.00001	-0.00002	0.00011	0.00008	2.08926
A103	2.13485	0.00000	0.00003	-0.00007	-0.00004	2.13481
A104	2.06853	0.00000	0.00003	-0.00008	-0.00005	2.06847
A105	2.13130	0.00000	-0.00002	0.00009	0.00007	2.13137
A106	2.08335	0.00000	-0.00001	-0.00001	-0.00001	2.08334
A107	2.09529	-0.00001	-0.00004	0.00006	0.00002	2.09531
A108	2.09781	0.00000	0.00005	-0.00018	-0.00012	2.09769
A109	2.09008	0.00001	-0.00001	0.00011	0.00010	2.09018
A110	2.12478	0.00002	0.00001	0.00004	0.00005	2.12483
A111	2.07369	-0.00002	0.00003	-0.00013	-0.00010	2.07359
A112	2.08472	0.00000	-0.00004	0.00010	0.00006	2.08478
A113	2.16707	-0.00003	-0.00016	0.00020	0.00003	2.16711
A114	2.15629	0.00000	0.00010	-0.00046	-0.00036	2.15593
A115	1.95982	0.00004	0.00007	0.00027	0.00033	1.96015
A116	2.15635	-0.00008	0.00014	-0.00065	-0.00051	2.15584
A117	2.16690	0.00007	-0.00006	0.00021	0.00015	2.16705
A118	1.95994	0.00001	-0.00009	0.00045	0.00036	1.96029
A119	1.91243	0.00002	0.00001	0.00013	0.00014	1.91257
A120	1.94890	-0.00002	0.00009	-0.00040	-0.00031	1.94859
A121	1.90470	0.00001	-0.00003	0.00015	0.00013	1.90482
A122	1.90604	0.00000	-0.00004	0.00013	0.00008	1.90612

A123	1.88649	-0.00001	-0.00002	-0.00004	-0.00006	1.88643
A124	1.90422	0.00000	-0.00001	0.00003	0.00002	1.90424
A125	1.94860	0.00008	-0.00004	0.00054	0.00050	1.94910
A126	1.91262	-0.00003	-0.00006	0.00004	-0.00002	1.91260
A127	1.90470	-0.00003	-0.00014	0.00033	0.00019	1.90489
A128	1.90607	-0.00001	0.00006	-0.00021	-0.00015	1.90592
A129	1.90426	-0.00002	0.00007	-0.00031	-0.00024	1.90401
A130	1.88654	0.00001	0.00012	-0.00042	-0.00030	1.88624
A131	3.16677	0.00001	-0.00023	0.00047	0.00024	3.16701
A132	3.17891	0.00007	-0.00028	0.00158	0.00131	3.18022
A133	3.17946	0.00000	-0.00043	0.00159	0.00116	3.18063
A134	3.16744	-0.00004	-0.00040	0.00039	-0.00001	3.16742
A135	3.14142	0.00000	-0.00002	0.00003	0.00001	3.14143
A136	3.14158	0.00000	0.00001	0.00001	0.00003	3.14160
A137	3.14170	-0.00001	0.00006	-0.00027	-0.00021	3.14149
A138	3.14172	-0.00001	-0.00015	0.00016	0.00001	3.14174
D1	0.00032	0.00000	0.00000	-0.00023	-0.00023	0.00009
D2	-3.14045	-0.00001	-0.00004	-0.00095	-0.00099	-3.14144
D3	-3.14155	0.00001	0.00016	-0.00026	-0.00010	3.14153
D4	0.00086	0.00000	0.00011	-0.00098	-0.00087	-0.00001
D5	-0.00013	0.00000	-0.00001	0.00019	0.00018	0.00005
D6	3.14124	0.00001	0.00008	0.00014	0.00021	3.14146
D7	-3.14136	-0.00002	-0.00021	0.00023	0.00002	-3.14134
D8	0.00001	-0.00001	-0.00012	0.00018	0.00005	0.00007
D9	0.00044	-0.00003	-0.00076	-0.00286	-0.00362	-0.00319
D10	3.14049	-0.00001	-0.00087	-0.00052	-0.00138	3.13911
D11	-3.14149	-0.00002	-0.00057	-0.00290	-0.00347	3.13822
D12	-0.00144	0.00001	-0.00068	-0.00055	-0.00123	-0.00267
D13	-0.00025	0.00000	0.00001	0.00008	0.00009	-0.00017
D14	3.14156	0.00000	-0.00003	-0.00002	-0.00005	3.14151
D15	3.14036	0.00002	0.00007	0.00094	0.00100	3.14136
D16	-0.00101	0.00001	0.00003	0.00084	0.00086	-0.00015
D17	-0.00181	0.00003	0.00057	0.00440	0.00497	0.00316
D18	3.13806	0.00004	0.00367	0.00226	0.00593	-3.13919
D19	3.14066	0.00002	0.00052	0.00363	0.00415	-3.13837
D20	-0.00265	0.00003	0.00362	0.00149	0.00511	0.00246
D21	0.00000	0.00000	-0.00002	0.00011	0.00010	0.00010
D22	-3.14140	-0.00001	0.00002	-0.00021	-0.00019	-3.14158
D23	3.14136	0.00000	0.00002	0.00021	0.00024	-3.14159
D24	-0.00004	0.00000	0.00006	-0.00010	-0.00005	-0.00008
D25	0.00018	0.00000	0.00001	-0.00015	-0.00014	0.00004
D26	-3.14140	0.00000	-0.00001	-0.00016	-0.00017	-3.14157
D27	3.14158	0.00000	-0.00003	0.00017	0.00014	-3.14146
D28	0.00000	0.00000	-0.00005	0.00016	0.00011	0.00011
D29	-0.00012	0.00000	0.00000	-0.00001	0.00000	-0.00012
D30	-3.14150	0.00000	-0.00008	0.00004	-0.00003	-3.14153
D31	3.14146	0.00000	0.00002	0.00001	0.00003	3.14149
D32	0.00009	0.00000	-0.00006	0.00006	-0.00001	0.00008
D33	-0.00155	0.00005	0.00110	0.00554	0.00664	0.00509
D34	-3.13924	-0.00001	0.00082	-0.00127	-0.00045	-3.13968
D35	-3.14153	0.00003	0.00121	0.00308	0.00429	-3.13724
D36	0.00397	-0.00003	0.00094	-0.00373	-0.00279	0.00117
D37	0.00094	0.00001	0.00014	-0.00130	-0.00116	-0.00021
D38	-3.13970	-0.00002	-0.00012	-0.00155	-0.00167	-3.14137
D39	3.14067	0.00004	0.00001	0.00156	0.00156	-3.14095
D40	0.00002	0.00001	-0.00025	0.00131	0.00105	0.00108
D41	0.00204	-0.00005	-0.00103	-0.00610	-0.00713	-0.00508
D42	3.13978	0.00001	-0.00076	0.00064	-0.00012	3.13966
D43	-3.13779	-0.00006	-0.00421	-0.00390	-0.00811	3.13729
D44	-0.00006	0.00000	-0.00394	0.00283	-0.00110	-0.00116

D45	3.13818	0.00014	0.00058	0.00897	0.00956	-3.13545
D46	0.00264	-0.00005	-0.00154	0.00014	-0.00139	0.00125
D47	0.00116	0.00007	0.00026	0.00099	0.00125	0.00242
D48	-3.13438	-0.00012	-0.00186	-0.00784	-0.00970	3.13911
D49	-0.00445	-0.00001	0.00336	-0.00373	-0.00037	-0.00481
D50	3.13735	0.00003	0.00298	0.00060	0.00358	3.14093
D51	3.13133	0.00017	0.00540	0.00475	0.01015	3.14148
D52	-0.01006	0.00021	0.00501	0.00908	0.01409	0.00403
D53	-3.13829	0.00002	-0.00071	0.00205	0.00134	-3.13695
D54	0.00311	-0.00002	-0.00035	-0.00201	-0.00236	0.00075
D55	3.14134	0.00000	0.00069	0.00007	0.00076	-3.14109
D56	0.00272	0.00001	0.00083	-0.00202	-0.00118	0.00154
D57	-0.00009	0.00003	0.00037	0.00370	0.00407	0.00398
D58	-3.13870	0.00004	0.00051	0.00161	0.00212	-3.13658
D59	0.00644	0.00002	-0.00009	0.00233	0.00224	0.00867
D60	-3.12817	-0.00003	-0.00063	0.00142	0.00080	-3.12738
D61	-3.13470	0.00000	-0.00063	0.00012	-0.00051	-3.13521
D62	0.01388	-0.00005	-0.00117	-0.00079	-0.00195	0.01193
D63	-0.00531	0.00000	0.00025	-0.00015	0.00010	-0.00520
D64	3.13558	0.00003	0.00108	0.00325	0.00433	3.13991
D65	0.00073	-0.00003	-0.00070	-0.00067	-0.00137	-0.00064
D66	-3.13560	0.00003	0.00129	0.00167	0.00296	-3.13264
D67	-3.14018	-0.00007	-0.00150	-0.00395	-0.00544	3.13756
D68	0.00668	0.00000	0.00049	-0.00161	-0.00112	0.00556
D69	-0.00401	-0.00004	-0.00018	-0.00389	-0.00407	-0.00808
D70	3.13446	-0.00004	-0.00033	-0.00169	-0.00203	3.13244
D71	3.12805	0.00003	0.00055	-0.00265	-0.00210	3.12595
D72	-0.01666	0.00003	0.00040	-0.00046	-0.00006	-0.01672
D73	-0.02311	0.00011	0.00259	0.00196	0.00455	-0.01856
D74	-3.06575	0.00010	-0.00178	0.01680	0.01502	-3.05073
D75	3.12776	0.00005	0.00188	0.00076	0.00264	3.13040
D76	0.08512	0.00004	-0.00249	0.01560	0.01311	0.09823
D77	-0.01524	0.00010	0.00235	0.00192	0.00428	-0.01097
D78	3.13630	0.00004	0.00088	0.00006	0.00093	3.13724
D79	3.12272	0.00006	0.00098	0.00031	0.00130	3.12402
D80	-0.00892	0.00000	-0.00049	-0.00156	-0.00204	-0.01096
D81	-3.13927	-0.00006	-0.00170	-0.00047	-0.00217	-3.14143
D82	0.00778	0.00000	0.00035	0.00196	0.00231	0.01009
D83	0.02360	-0.00013	-0.00304	-0.00240	-0.00544	0.01816
D84	3.06576	-0.00011	0.00135	-0.01730	-0.01594	3.04981
D85	-3.13144	-0.00005	-0.00105	0.00013	-0.00092	-3.13236
D86	-0.08928	-0.00003	0.00334	-0.01477	-0.01143	-0.10071
D87	-3.13590	0.00004	0.00076	0.00177	0.00253	-3.13336
D88	0.00508	0.00000	0.00038	0.00008	0.00046	0.00554
D89	0.01941	-0.00005	-0.00127	-0.00081	-0.00207	0.01734
D90	-3.12280	-0.00009	-0.00165	-0.00250	-0.00415	-3.12695
D91	1.53938	0.00002	0.00224	-0.00759	-0.00535	1.53403
D92	-2.62975	0.00003	0.00225	-0.00748	-0.00523	-2.63497
D93	-0.56707	0.00001	0.00228	-0.00777	-0.00549	-0.57257
D94	-1.48388	0.00000	-0.00299	0.01015	0.00716	-1.47672
D95	0.63018	0.00001	-0.00298	0.01026	0.00728	0.63746
D96	2.69285	-0.00001	-0.00295	0.00997	0.00702	2.69987
D97	-0.00497	0.00000	-0.00014	-0.00194	-0.00208	-0.00705
D98	3.13751	0.00001	0.00020	-0.00073	-0.00054	3.13698
D99	-3.13747	-0.00001	0.00014	-0.00111	-0.00098	-3.13845
D100	0.00475	0.00003	0.00053	0.00060	0.00113	0.00587
D101	-0.00807	-0.00002	-0.00026	-0.00025	-0.00051	-0.00858
D102	-3.14141	-0.00002	-0.00036	-0.00175	-0.00210	3.13967
D103	0.00091	0.00000	-0.00010	0.00143	0.00133	0.00224
D104	-3.14115	-0.00003	-0.00040	0.00013	-0.00027	-3.14143

D105	-3.14136	-0.00001	-0.00036	0.00051	0.00015	-3.14120
D106	-0.00024	-0.00004	-0.00066	-0.00079	-0.00145	-0.00169
D107	3.13474	0.00000	0.00012	-0.00060	-0.00048	3.13426
D108	-0.01758	-0.00001	0.00036	-0.00250	-0.00214	-0.01972
D109	-0.00597	0.00002	0.00045	0.00059	0.00104	-0.00493
D110	3.12489	0.00001	0.00069	-0.00131	-0.00062	3.12427
D111	0.00965	0.00001	-0.00006	-0.00014	-0.00020	0.00945
D112	-3.13743	0.00001	0.00000	0.00085	0.00086	-3.13657
D113	-3.12416	0.00002	-0.00023	0.00124	0.00101	-3.12315
D114	0.01195	0.00002	-0.00017	0.00223	0.00207	0.01401
D115	3.13316	-0.00002	-0.00013	-0.00200	-0.00213	3.13103
D116	0.09413	0.00000	-0.00279	0.00608	0.00329	0.09742
D117	-0.01895	-0.00003	0.00010	-0.00386	-0.00376	-0.02271
D118	-3.05798	-0.00001	-0.00256	0.00422	0.00166	-3.05633
D119	3.13350	0.00001	0.00026	0.00173	0.00198	3.13548
D120	-0.00611	-0.00001	-0.00009	0.00026	0.00017	-0.00594
D121	-0.00013	0.00001	0.00016	0.00028	0.00045	0.00032
D122	-3.13974	-0.00001	-0.00018	-0.00118	-0.00136	-3.14111
D123	3.13583	-0.00001	0.00024	-0.00169	-0.00145	3.13438
D124	-0.01163	-0.00003	-0.00011	-0.00269	-0.00279	-0.01442
D125	-0.00709	0.00000	0.00047	-0.00070	-0.00023	-0.00733
D126	3.12863	-0.00002	0.00013	-0.00170	-0.00157	3.12706
D127	-3.13821	0.00001	-0.00010	0.00150	0.00140	-3.13681
D128	0.00543	0.00000	-0.00046	-0.00002	-0.00048	0.00495
D129	0.00498	0.00001	-0.00019	0.00126	0.00106	0.00605
D130	-3.13317	-0.00001	-0.00136	0.00221	0.00085	-3.13232
D131	-3.12860	0.00002	0.00028	0.00262	0.00290	-3.12571
D132	0.01643	0.00001	-0.00089	0.00357	0.00268	0.01911
D133	0.01886	0.00003	0.00001	0.00404	0.00404	0.02290
D134	3.05839	0.00001	0.00265	-0.00400	-0.00134	3.05704
D135	-3.13053	0.00002	-0.00045	0.00271	0.00226	-3.12827
D136	-0.09100	0.00000	0.00219	-0.00532	-0.00313	-0.09413
D137	-0.00078	-0.00001	-0.00016	-0.00125	-0.00141	-0.00218
D138	-3.14075	-0.00002	-0.00034	-0.00060	-0.00094	3.14149
D139	3.13754	0.00001	0.00095	-0.00215	-0.00120	3.13634
D140	-0.00244	0.00000	0.00077	-0.00151	-0.00074	-0.00317
D141	-0.00270	0.00001	0.00036	0.00072	0.00107	-0.00163
D142	3.13708	0.00002	0.00056	0.00000	0.00056	3.13764
D143	3.13980	0.00003	0.00093	0.00222	0.00316	-3.14023
D144	-0.00132	0.00003	0.00126	0.00094	0.00220	0.00088
D145	0.00014	0.00002	0.00072	0.00299	0.00371	0.00385
D146	-3.14099	0.00002	0.00104	0.00171	0.00275	-3.13823
D147	-0.62908	-0.00002	0.00184	-0.00603	-0.00419	-0.63328
D148	1.48500	-0.00002	0.00185	-0.00604	-0.00419	1.48081
D149	-2.69158	-0.00003	0.00188	-0.00615	-0.00428	-2.69586
D150	2.63457	0.00000	-0.00132	0.00354	0.00222	2.63679
D151	-1.53453	0.00000	-0.00131	0.00353	0.00222	-1.53231
D152	0.57207	-0.00001	-0.00128	0.00342	0.00214	0.57421
D153	-0.00155	0.00001	0.00057	-0.00148	-0.00091	-0.00246
D154	-3.14084	0.00000	0.00105	-0.00323	-0.00218	3.14017
D155	3.13956	0.00002	0.00023	-0.00014	0.00009	3.13965
D156	0.00027	0.00001	0.00071	-0.00189	-0.00118	-0.00091
D157	-3.13851	0.00003	0.00121	-0.00142	-0.00022	-3.13873
D158	0.00411	-0.00003	0.00066	-0.00243	-0.00177	0.00234
D159	0.00114	0.00003	0.00080	0.00005	0.00086	0.00199
D160	-3.13943	-0.00002	0.00026	-0.00096	-0.00070	-3.14012
D161	3.13777	-0.00002	-0.00109	0.00164	0.00054	3.13832
D162	-0.00514	0.00000	-0.00115	0.00250	0.00135	-0.00380
D163	-0.00185	-0.00002	-0.00069	0.00015	-0.00054	-0.00240
D164	3.13842	-0.00001	-0.00075	0.00101	0.00026	3.13868

D165	0.000006	-0.000003	-0.000062	-0.000025	-0.000087	-0.000081
D166	3.14061	-0.000002	-0.000049	0.00017	-0.00032	3.14029
D167	3.14065	0.000002	-0.00010	0.00074	0.00064	3.14129
D168	-0.00199	0.000003	0.000004	0.00115	0.00120	-0.00079
D169	0.00192	0.000000	0.00031	-0.00030	0.00000	0.00192
D170	-3.13952	0.000001	0.00031	-0.00021	0.00010	-3.13942
D171	-3.13841	-0.000001	0.00036	-0.00113	-0.00076	-3.13917
D172	0.00334	-0.000001	0.00037	-0.00103	-0.00066	0.00267
D173	-0.00053	0.000000	0.000001	-0.00015	-0.00014	-0.00067
D174	-3.14146	-0.000001	0.000008	-0.00049	-0.00042	3.14131
D175	3.13952	0.000002	-0.000006	0.00085	0.00079	3.14032
D176	-0.00141	0.000001	0.000001	0.00051	0.00052	-0.00089
D177	-0.00122	0.000002	0.000020	0.00034	0.00054	-0.00068
D178	3.14024	0.000002	0.000020	0.00026	0.00046	3.14070
D179	3.14136	0.000001	0.000007	-0.00005	0.00002	3.14138
D180	-0.00037	0.000000	0.000007	-0.00013	-0.00006	-0.00043
D181	-3.14011	-0.000002	-0.00015	-0.00058	-0.00073	-3.14084
D182	0.00133	-0.000001	-0.00014	-0.00060	-0.00074	0.00059
D183	0.00031	-0.000001	0.000000	-0.00011	-0.00011	0.00020
D184	-3.14144	0.000000	0.000002	-0.00014	-0.00012	-3.14156
D185	3.14156	-0.000001	-0.000008	0.00012	0.00003	3.14159
D186	0.00021	-0.000001	-0.000002	-0.00009	-0.00012	0.00010
D187	0.00013	0.000000	-0.000008	0.00022	0.00014	0.00028
D188	-3.14121	0.000000	-0.000002	0.00001	-0.00001	-3.14122
D189	-0.00003	0.000000	-0.000006	0.00026	0.00020	0.00017
D190	3.14136	0.000000	-0.000005	0.00027	0.00022	3.14158
D191	-3.14146	0.000000	-0.000007	0.00028	0.00021	-3.14125
D192	-0.00007	0.000000	-0.000006	0.00030	0.00024	0.00016
D193	0.00014	0.000000	0.000002	-0.00007	-0.00005	0.00009
D194	-3.14142	0.000000	0.000005	-0.00015	-0.00011	-3.14153
D195	3.14149	0.000000	-0.000003	0.00013	0.00009	3.14159
D196	-0.00007	0.000000	-0.000001	0.00005	0.00004	-0.00003
D197	-0.00019	0.000000	0.000005	-0.00017	-0.00012	-0.00032
D198	3.14137	0.000000	0.000002	-0.00009	-0.00007	3.14130
D199	-3.14158	0.000000	0.000003	-0.00018	-0.00015	3.14146
D200	-0.00002	0.000000	0.000001	-0.00010	-0.00009	-0.00011

Item	Value	Threshold	Converged?

Maximum Force	0.000358	0.000450	YES

RMS Force	0.000050	0.000300	YES

Maximum Displacement	0.065010	0.001800	NO

RMS Displacement	0.011172	0.001200	NO

Predicted change in Energy=-1.051581D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.802843	-0.637121	-0.000601
2	6	0	-9.993743	-1.787977	0.000843
3	6	0	-10.516403	-3.072948	0.004998
4	6	0	-11.905385	-3.215149	0.008037
5	6	0	-12.726429	-2.080804	0.006738

6	6	0	-12.194306	-0.787215	0.002373
7	1	0	-9.845877	-3.926178	0.005867
8	1	0	-12.352923	-4.204216	0.011331
9	1	0	-13.805231	-2.202728	0.009154
10	1	0	-12.863673	0.061144	0.001569
11	6	0	-9.926505	0.564377	-0.005088
12	6	0	-8.569488	-1.390808	-0.002615
13	6	0	-8.539788	0.088780	-0.001852
14	6	0	-7.403570	0.870268	-0.002177
15	6	0	-6.014313	0.595926	-0.005672
16	6	0	-3.644183	-0.183729	-0.002892
17	6	0	-3.777985	1.228900	-0.009946
18	16	0	-5.182157	-0.988784	-0.004637
19	6	0	-5.099295	1.665199	-0.005642
20	6	0	-2.267321	-0.451509	0.000190
21	6	0	-1.603769	0.797704	-0.005898
22	7	0	-2.523561	1.821227	-0.026773
23	16	0	-1.151429	-1.806898	-0.001772
24	16	0	1.151597	1.805748	0.010588
25	6	0	0.198332	-0.674256	0.006995
26	6	0	-0.198122	0.673022	0.002092
27	6	0	1.603609	-0.798953	0.015494
28	6	0	2.267286	0.450166	0.010586
29	6	0	3.644647	0.181973	0.013177
30	6	0	3.778274	-1.230705	0.019185
31	6	0	5.099617	-1.667578	0.013223
32	6	0	6.014823	-0.598418	0.010344
33	16	0	5.182761	0.986602	0.011665
34	7	0	2.523549	-1.822526	0.039112
35	6	0	7.404871	-0.872575	0.004365
36	6	0	8.539958	-0.089965	0.001685
37	6	0	8.567098	1.389544	0.001860
38	6	0	9.927504	-0.563522	-0.003042
39	6	0	9.990723	1.789066	-0.005653
40	6	0	10.801781	0.639541	-0.009154
41	6	0	10.511150	3.074897	-0.009587
42	6	0	12.192955	0.791993	-0.017457
43	6	0	11.899840	3.219456	-0.017592
44	6	0	12.722830	2.086506	-0.021618
45	6	0	10.387407	-1.869662	-0.001644
46	6	0	9.538835	-3.019116	0.005754
47	6	0	11.772649	-2.218343	-0.007025
48	7	0	8.870594	-3.974173	0.011734
49	7	0	12.890614	-2.546138	-0.011309
50	6	0	-10.384265	1.871058	-0.010357
51	6	0	-11.768948	2.221799	-0.012374
52	6	0	-9.533800	3.019092	-0.014903
53	7	0	-12.886290	2.551721	-0.014046
54	7	0	-8.864368	3.973326	-0.018514
55	8	0	-7.612691	-2.157616	-0.004767
56	8	0	7.608829	2.154510	0.006630
57	6	0	2.241872	-3.244558	-0.048148
58	1	0	1.312954	-3.466897	0.481489
59	1	0	2.151775	-3.575518	-1.088400
60	1	0	3.048580	-3.799560	0.434842
61	6	0	-2.242110	3.242923	0.067904
62	1	0	-2.150245	3.568655	1.109670
63	1	0	-1.314178	3.468519	-0.462149
64	1	0	-3.049706	3.800420	-0.410680
65	1	0	5.428237	-2.700341	0.008067

66	1	0	12.863745	-0.055180	-0.020804
67	1	0	13.801404	2.210286	-0.028120
68	1	0	12.345641	4.209307	-0.020888
69	1	0	9.839199	3.927005	-0.006571
70	1	0	7.573855	-1.942515	0.001869
71	1	0	-7.571558	1.940379	-0.003924
72	1	0	-5.428189	2.697845	-0.001592

Rotational constants (GHZ): 0.1749887 0.0104046 0.0098219

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6569.8426746969 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T

Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6569.7577638534 Hartrees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.24D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Initial guess from the checkpoint file: "PBDB.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000018 0.000000 -0.000039 Ang= 0.00 deg.

ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1

AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-yADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 2001

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 IlCent= 200000004 NGrid=

0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0=

0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Integral accuracy reduced to 1.0D-05 until final iterations.

Initial convergence to 1.0D-05 achieved. Increase integral accuracy.

SCF Done: E(RB3LYP) = -3683.02011453 A.U. after 10 cycles

NFock= 10 Conv=0.78D-08 -V/T= 2.0068

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1

NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-0.000022597	0.000043444	0.000032627
2	6	-0.000071911	0.000019167	0.000031976

3	6	-0.000009082	-0.000028289	0.000003772
4	6	0.000007239	0.000010375	0.000013788
5	6	-0.000004412	-0.000011525	-0.000005691
6	6	0.000050441	0.000002322	0.000049138
7	1	0.000001258	0.000003467	0.000008273
8	1	0.000005596	0.000002527	-0.000002231
9	1	-0.000002372	0.000000136	-0.000005019
10	1	-0.000023774	0.000003526	-0.000019402
11	6	0.000207998	-0.000037999	-0.000216046
12	6	0.000061636	-0.000019068	-0.000219226
13	6	-0.000209917	-0.000159222	0.000236413
14	6	-0.000639068	0.000341310	-0.000044041
15	6	0.000587270	-0.000197750	-0.000077627
16	6	-0.000187868	0.000050056	-0.000013166
17	6	-0.000023779	0.000121626	-0.000276082
18	16	0.000070953	-0.000004317	0.000166682
19	6	-0.000063254	-0.000103075	0.000222276
20	6	0.000039417	-0.000141860	0.000220091
21	6	0.000336848	-0.000015718	-0.000080306
22	7	-0.000111155	0.000059291	0.000031538
23	16	0.000031327	0.000030515	-0.000031235
24	16	0.000020972	0.000034038	0.000027697
25	6	-0.000149948	0.000072561	-0.000046963
26	6	-0.000054347	0.000045951	-0.000117480
27	6	0.000261886	-0.000154831	-0.000016170
28	6	0.000145659	-0.000082824	0.000192970
29	6	-0.000143349	0.000122642	0.000040230
30	6	0.000178079	-0.000019161	-0.000130364
31	6	-0.000120898	0.000002767	-0.000155314
32	6	-0.000144484	0.000085319	0.000064904
33	16	-0.000073886	0.000067858	-0.000154327
34	7	-0.000096222	-0.000124497	0.000178561
35	6	0.000013301	0.000015464	-0.000004462
36	6	0.000136885	0.000020935	0.000049200
37	6	0.000143456	-0.000036530	0.000124574
38	6	-0.000008351	0.000109699	0.000092223
39	6	0.000006174	0.000019799	-0.000006164
40	6	-0.000006680	0.000003795	-0.000000264
41	6	-0.000006430	0.000010037	-0.000003609
42	6	-0.000072947	-0.000016294	-0.000077849
43	6	0.000006897	-0.000033806	0.000012880
44	6	0.000002285	0.000001700	-0.000003690
45	6	-0.000140261	-0.000141730	-0.000127084
46	6	-0.000036324	-0.000024483	-0.000028666
47	6	0.000027094	0.000070864	0.000017140
48	7	-0.000018969	-0.000002029	-0.000018045
49	7	-0.000020954	-0.000014354	-0.000016296
50	6	0.000045079	0.000065670	0.000076403
51	6	-0.000057795	-0.000126964	-0.000050186
52	6	-0.000019232	0.000015152	-0.000033353
53	7	0.000009754	0.000030879	0.000014603
54	7	0.000023349	-0.000011457	0.000028769
55	8	0.000087776	-0.000001888	0.000059849
56	8	-0.000024947	-0.000124958	-0.000030726
57	6	-0.000045362	0.000047944	0.000051446
58	1	0.000006474	0.000007669	-0.000012971
59	1	0.000003692	0.000050445	0.000013999
60	1	-0.000008303	-0.000019358	0.000007830
61	6	-0.000046032	-0.000094031	0.000070622
62	1	0.000026962	0.000034909	0.000010140

63	1	-0.000004562	0.000000164	0.000010656
64	1	0.000005607	0.000036524	0.000001792
65	1	0.000019820	0.000010783	-0.000038899
66	1	0.000049704	0.000010976	0.000041148
67	1	0.000003000	-0.000000254	0.000001049
68	1	0.000002279	-0.000004002	0.000003128
69	1	-0.000000392	-0.000000991	-0.000005615
70	1	0.000038904	0.000037631	0.000014798
71	1	0.000028272	0.000049953	-0.000153881
72	1	-0.000023480	-0.000016622	-0.000000732

 Cartesian Forces: Max 0.000639068 RMS 0.000105223

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000599517 RMS 0.000082633

Search for a local minimum.

Step number 27 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 16 18 17 19 20

21 22 23 24 25

26 27

DE= -5.73D-07 DEPred=-1.05D-05 R= 5.45D-02

Trust test= 5.45D-02 RLast= 4.88D-02 DXMaxT set to 1.43D-01

ITU= -1 1 -1 1 -1 1 1 -1 0 -1 0 -1 1 1 1 1 1 0 0

ITU= 0 1 0 0 0 1 0

Eigenvalues ---	0.00224	0.00262	0.00269	0.00386	0.00410
Eigenvalues ---	0.00414	0.00480	0.00508	0.00516	0.00567
Eigenvalues ---	0.00580	0.00605	0.00617	0.00646	0.00677
Eigenvalues ---	0.00680	0.00720	0.00738	0.00744	0.00753
Eigenvalues ---	0.00770	0.00775	0.00779	0.00784	0.00824
Eigenvalues ---	0.00826	0.00863	0.01048	0.01095	0.01133
Eigenvalues ---	0.01134	0.01181	0.01262	0.01290	0.01319
Eigenvalues ---	0.01332	0.01361	0.01380	0.01457	0.01461
Eigenvalues ---	0.01462	0.01603	0.01646	0.01743	0.01747
Eigenvalues ---	0.01763	0.01794	0.01927	0.01952	0.02006
Eigenvalues ---	0.02021	0.02061	0.02074	0.02170	0.02190
Eigenvalues ---	0.02531	0.02887	0.03443	0.03679	0.03939
Eigenvalues ---	0.03984	0.04828	0.04838	0.04908	0.04980
Eigenvalues ---	0.05012	0.05049	0.05148	0.05347	0.07050
Eigenvalues ---	0.07235	0.07390	0.07568	0.15457	0.15737
Eigenvalues ---	0.15950	0.15986	0.15996	0.16000	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16001
Eigenvalues ---	0.16003	0.16009	0.16022	0.16041	0.16071
Eigenvalues ---	0.16079	0.18986	0.19041	0.19556	0.20170
Eigenvalues ---	0.20833	0.21278	0.21733	0.21996	0.22001
Eigenvalues ---	0.22025	0.22390	0.22557	0.22611	0.22635
Eigenvalues ---	0.22647	0.22783	0.22932	0.23065	0.23302
Eigenvalues ---	0.23367	0.23437	0.23720	0.23975	0.24046
Eigenvalues ---	0.24164	0.24274	0.24323	0.24393	0.24507
Eigenvalues ---	0.24564	0.24643	0.24693	0.24723	0.24862
Eigenvalues ---	0.24916	0.24948	0.24973	0.24984	0.24989
Eigenvalues ---	0.24995	0.24998	0.24999	0.24999	0.25000
Eigenvalues ---	0.25000	0.25000	0.25000	0.25001	0.25012
Eigenvalues ---	0.25096	0.25570	0.25729	0.26010	0.26157
Eigenvalues ---	0.26365	0.26558	0.26799	0.26882	0.27219

```

Eigenvalues ---      0.27270    0.27729    0.27845    0.28429    0.28487
Eigenvalues ---      0.28744    0.28827    0.30000    0.30485    0.31832
Eigenvalues ---      0.32924    0.35423    0.35516    0.36273    0.36308
Eigenvalues ---      0.36341    0.36474    0.36648    0.36762    0.36826
Eigenvalues ---      0.36874    0.37046    0.37086    0.37116    0.37248
Eigenvalues ---      0.37264    0.37396    0.37438    0.37567    0.37676
Eigenvalues ---      0.37758    0.38060    0.39019    0.40309    0.40989
Eigenvalues ---      0.41700    0.42022    0.42639    0.44396    0.44743
Eigenvalues ---      0.45558    0.46258    0.46657    0.47763    0.47973
Eigenvalues ---      0.48505    0.52211    0.53284    0.55350    0.57001
Eigenvalues ---      0.62303    0.71773    0.74221    0.80427    0.82031
Eigenvalues ---      0.90350    1.25853    1.26332    1.29344    1.35375
En-DIIS/RFO-DIIS IScMMF=          0 using points:      27      26      25      24      23
RFO step:  Lambda=-4.70810320D-06.
DidBck=T Rises=F RFO-DIIS coefs:      0.46596      0.41455      0.04803      0.05790
0.01355
Iteration  1 RMS(Cart)=  0.00601808 RMS(Int)=  0.00000538
Iteration  2 RMS(Cart)=  0.00001796 RMS(Int)=  0.00000254
Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000254
Variable      Old X      -DE/DX      Delta X      Delta X      Delta X      New X
(Linear)      (Quad)      (Total)
R1      2.65849      0.00001      -0.00002      0.00000      -0.00002      2.65847
R2      2.64474     -0.00002     -0.00002     -0.00004     -0.00006      2.64469
R3      2.81029      0.00007      0.00016     -0.00011      0.00005      2.81034
R4      2.62144     -0.00002      0.00000     -0.00003     -0.00003      2.62141
R5      2.79415      0.00001      0.00010     -0.00010      0.00000      2.79415
R6      2.63852     -0.00001     -0.00002      0.00003      0.00001      2.63853
R7      2.05069      0.00001      0.00001      0.00000      0.00001      2.05070
R8      2.64619      0.00001      0.00007     -0.00003      0.00003      2.64622
R9      2.05151      0.00000      0.00000      0.00000      0.00000      2.05151
R10     2.64328      0.00000     -0.00004      0.00004      0.00000      2.64329
R11     2.05162      0.00000      0.00001      0.00000      0.00001      2.05163
R12     2.04210      0.00003      0.00007      0.00002      0.00009      2.04219
R13     2.77036     -0.00010     -0.00004     -0.00008     -0.00012      2.77024
R14     2.61643     -0.00001     -0.00011      0.00007     -0.00004      2.61639
R15     2.79658     -0.00005      0.00011     -0.00023     -0.00012      2.79646
R16     2.31710      0.00011      0.00009      0.00000      0.00008      2.31718
R17     2.60598     -0.00021      0.00006     -0.00063     -0.00057      2.60541
R18     2.67602      0.00057      0.00082      0.00081      0.00163      2.67766
R19     2.04699      0.00003      0.00005     -0.00005      0.00000      2.04698
R20     3.38245      0.00014      0.00026      0.00014      0.00040      3.38285
R21     2.65948      0.00002     -0.00013      0.00011     -0.00002      2.65947
R22     2.68146      0.00001      0.00011     -0.00011      0.00000      2.68146
R23     3.28045     -0.00005      0.00001     -0.00017     -0.00016      3.28029
R24     2.65065      0.00018      0.00032      0.00009      0.00041      2.65106
R25     2.62953     -0.00010     -0.00019      0.00010     -0.00009      2.62944
R26     2.62169      0.00002     -0.00007      0.00009      0.00001      2.62171
R27     2.04802      0.00002      0.00003      0.00001      0.00004      2.04806
R28     2.67306     -0.00006      0.00000     -0.00011     -0.00011      2.67295
R29     3.31769      0.00000      0.00000      0.00000      0.00000      3.31769
R30     2.60073      0.00007     -0.00006      0.00019      0.00013      2.60086
R31     2.66676     -0.00013     -0.00021     -0.00001     -0.00023      2.66653
R32     2.74459     -0.00001      0.00011     -0.00004      0.00007      2.74466
R33     3.32979      0.00001      0.00001      0.00003      0.00004      3.32983
R34     3.32982     -0.00001      0.00002     -0.00003     -0.00001      3.32981
R35     3.31773     -0.00002     -0.00006      0.00003     -0.00004      3.31769
R36     2.65395     -0.00002     -0.00004      0.00003     -0.00002      2.65393
R37     2.66607      0.00015      0.00037      0.00003      0.00040      2.66647
R38     2.67300     -0.00005     -0.00007      0.00001     -0.00006      2.67294
R39     2.60107     -0.00009     -0.00022      0.00012     -0.00011      2.60096

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R40	2.65172	-0.00026	-0.00059	0.00015	-0.00043	2.65129
R41	2.68151	-0.00008	-0.00014	0.00007	-0.00007	2.68144
R42	3.28031	-0.00002	-0.00005	0.00003	-0.00002	3.28029
R43	2.62994	-0.00029	-0.00039	-0.00006	-0.00045	2.62949
R44	2.62188	-0.00010	-0.00024	0.00010	-0.00013	2.62174
R45	2.65956	-0.00006	-0.00016	0.00004	-0.00012	2.65944
R46	2.04808	0.00000	-0.00001	0.00001	0.00000	2.04808
R47	3.38288	0.00006	-0.00005	0.00011	0.00006	3.38294
R48	2.67744	0.00013	0.00019	-0.00026	-0.00007	2.67736
R49	2.74442	0.00009	0.00017	0.00001	0.00018	2.74460
R50	2.60543	0.00016	0.00012	-0.00013	-0.00001	2.60542
R51	2.04696	0.00005	0.00006	-0.00005	0.00001	2.04698
R52	2.79634	0.00011	0.00035	-0.00026	0.00009	2.79643
R53	2.77060	-0.00018	-0.00006	-0.00021	-0.00027	2.77033
R54	2.79423	-0.00001	0.00008	-0.00017	-0.00009	2.79414
R55	2.31711	0.00004	0.00009	-0.00004	0.00004	2.31715
R56	2.81040	-0.00002	0.00008	-0.00011	-0.00003	2.81037
R57	2.61679	-0.00028	-0.00026	-0.00008	-0.00034	2.61645
R58	2.65857	-0.00006	-0.00016	0.00007	-0.00009	2.65848
R59	2.62136	0.00002	0.00007	-0.00002	0.00005	2.62141
R60	2.64472	-0.00001	0.00016	-0.00024	-0.00008	2.64464
R61	2.63847	0.00002	-0.00002	0.00006	0.00003	2.63850
R62	2.05069	0.00000	0.00000	0.00001	0.00001	2.05070
R63	2.64329	0.00000	-0.00010	0.00009	-0.00001	2.64327
R64	2.04202	0.00006	0.00014	0.00000	0.00014	2.04216
R65	2.64623	-0.00001	0.00008	-0.00007	0.00001	2.64624
R66	2.05151	0.00000	0.00000	0.00000	0.00000	2.05151
R67	2.05162	0.00000	0.00001	0.00000	0.00000	2.05163
R68	2.69998	-0.00003	0.00011	-0.00015	-0.00004	2.69993
R69	2.69940	-0.00002	0.00029	-0.00043	-0.00013	2.69927
R70	2.20274	0.00000	0.00000	0.00000	0.00000	2.20274
R71	2.20160	-0.00002	-0.00001	-0.00001	-0.00002	2.20158
R72	2.69931	0.00002	0.00018	-0.00018	0.00000	2.69931
R73	2.69992	0.00000	0.00008	-0.00005	0.00002	2.69995
R74	2.20160	0.00000	-0.00001	0.00000	-0.00001	2.20159
R75	2.20274	0.00001	0.00001	0.00000	0.00000	2.20274
R76	2.06391	0.00001	0.00001	0.00001	0.00002	2.06392
R77	2.06990	0.00002	0.00000	0.00001	0.00001	2.06991
R78	2.06325	-0.00001	0.00001	-0.00002	-0.00001	2.06324
R79	2.06993	0.00000	-0.00004	0.00002	-0.00002	2.06991
R80	2.06397	0.00001	-0.00004	0.00004	0.00000	2.06397
R81	2.06323	-0.00001	0.00001	-0.00003	-0.00002	2.06320
A1	2.07610	-0.00003	-0.00006	0.00003	-0.00003	2.07608
A2	1.89866	-0.00003	-0.00001	0.00000	-0.00001	1.89865
A3	2.30842	0.00005	0.00007	-0.00003	0.00004	2.30846
A4	2.14252	0.00002	0.00006	-0.00001	0.00004	2.14256
A5	1.91160	0.00001	0.00002	-0.00001	0.00001	1.91162
A6	2.22906	-0.00003	-0.00008	0.00003	-0.00005	2.22901
A7	2.05913	0.00000	0.00000	0.00000	0.00000	2.05913
A8	2.08922	0.00000	0.00001	-0.00001	0.00000	2.08922
A9	2.13483	0.00000	-0.00001	0.00001	0.00001	2.13484
A10	2.09529	-0.00001	-0.00004	0.00000	-0.00004	2.09525
A11	2.09774	0.00000	0.00003	-0.00001	0.00002	2.09776
A12	2.09015	0.00001	0.00002	0.00001	0.00003	2.09018
A13	2.12481	0.00001	0.00001	0.00000	0.00001	2.12482
A14	2.08478	0.00000	-0.00002	0.00003	0.00002	2.08479
A15	2.07360	-0.00001	0.00001	-0.00003	-0.00002	2.07357
A16	2.06851	0.00001	0.00004	-0.00002	0.00002	2.06853
A17	2.13135	0.00001	-0.00002	0.00003	0.00001	2.13136
A18	2.08333	-0.00002	-0.00002	-0.00001	-0.00003	2.08330

A19	1.87056	-0.00001	0.00000	-0.00006	-0.00006	1.87050
A20	2.17447	0.00020	0.00028	-0.00012	0.00016	2.17463
A21	2.23816	-0.00019	-0.00027	0.00018	-0.00010	2.23806
A22	1.86282	-0.00002	-0.00004	-0.00002	-0.00005	1.86277
A23	2.19403	0.00002	0.00009	-0.00004	0.00006	2.19409
A24	2.22634	0.00001	-0.00007	0.00005	-0.00001	2.22633
A25	1.88112	0.00006	0.00003	0.00009	0.00012	1.88124
A26	2.20871	-0.00009	-0.00013	0.00017	0.00004	2.20874
A27	2.19335	0.00003	0.00010	-0.00026	-0.00015	2.19320
A28	2.34414	0.00002	-0.00001	-0.00011	-0.00011	2.34402
A29	2.01757	-0.00009	-0.00001	-0.00016	-0.00016	2.01742
A30	1.92147	0.00007	0.00000	0.00027	0.00028	1.92175
A31	2.24929	0.00004	-0.00015	0.00021	0.00006	2.24936
A32	2.08365	-0.00002	0.00007	-0.00008	-0.00001	2.08363
A33	1.95024	-0.00002	0.00009	-0.00013	-0.00004	1.95020
A34	1.95858	-0.00001	-0.00009	0.00007	-0.00002	1.95856
A35	1.85733	0.00003	0.00000	0.00006	0.00007	1.85739
A36	2.46727	-0.00002	0.00009	-0.00013	-0.00004	2.46723
A37	1.98414	0.00007	0.00020	-0.00002	0.00018	1.98432
A38	1.91755	-0.00006	-0.00017	0.00000	-0.00017	1.91738
A39	2.38148	0.00000	-0.00003	0.00002	-0.00001	2.38147
A40	1.57210	-0.00002	-0.00008	0.00005	-0.00002	1.57208
A41	1.95968	-0.00002	-0.00011	0.00003	-0.00008	1.95960
A42	2.12543	0.00001	0.00010	-0.00008	0.00002	2.12546
A43	2.19807	0.00001	0.00001	0.00004	0.00005	2.19812
A44	1.86697	-0.00002	-0.00002	-0.00002	-0.00004	1.86693
A45	2.45166	0.00001	0.00004	-0.00001	0.00003	2.45170
A46	1.96452	0.00001	-0.00001	0.00003	0.00002	1.96454
A47	1.92127	-0.00002	-0.00011	0.00003	-0.00009	1.92118
A48	1.97057	0.00003	0.00006	0.00002	0.00008	1.97064
A49	2.39132	-0.00001	0.00004	-0.00005	0.00000	2.39132
A50	1.86146	0.00007	0.00026	-0.00006	0.00021	1.86167
A51	2.20478	0.00000	0.00025	-0.00008	0.00020	2.20498
A52	2.21117	-0.00007	0.00027	-0.00035	-0.00006	2.21111
A53	1.56142	-0.00004	-0.00006	-0.00001	-0.00007	1.56135
A54	1.56122	0.00004	0.00008	0.00002	0.00010	1.56132
A55	1.98274	0.00001	0.00004	-0.00002	0.00002	1.98276
A56	2.35494	0.00001	0.00001	0.00004	0.00005	2.35499
A57	1.94550	-0.00002	-0.00005	-0.00002	-0.00006	1.94543
A58	2.35493	0.00001	0.00003	0.00000	0.00004	2.35496
A59	1.94546	0.00000	-0.00002	0.00000	-0.00002	1.94544
A60	1.98279	-0.00001	-0.00002	0.00000	-0.00001	1.98278
A61	1.97065	0.00000	-0.00002	0.00002	0.00000	1.97064
A62	2.39140	-0.00002	-0.00002	-0.00001	-0.00003	2.39137
A63	1.92109	0.00002	0.00005	0.00000	0.00005	1.92114
A64	1.96458	-0.00001	0.00000	-0.00003	-0.00003	1.96455
A65	2.45173	-0.00001	-0.00003	-0.00001	-0.00004	2.45169
A66	1.86686	0.00002	0.00002	0.00003	0.00005	1.86692
A67	1.85742	-0.00002	0.00002	-0.00002	0.00000	1.85742
A68	2.46730	-0.00004	-0.00004	-0.00004	-0.00008	2.46722
A69	1.95846	0.00005	0.00002	0.00006	0.00009	1.95855
A70	1.98439	-0.00001	0.00004	-0.00005	-0.00001	1.98438
A71	1.91724	0.00006	0.00009	0.00001	0.00010	1.91734
A72	2.38152	-0.00004	-0.00012	0.00004	-0.00007	2.38145
A73	1.95946	0.00008	0.00003	0.00004	0.00007	1.95952
A74	2.19819	-0.00005	-0.00008	0.00002	-0.00005	2.19813
A75	2.12554	-0.00003	0.00005	-0.00006	-0.00002	2.12552
A76	1.95021	-0.00003	0.00003	0.00001	0.00004	1.95025
A77	2.08404	-0.00035	-0.00034	-0.00009	-0.00042	2.08362
A78	2.24893	0.00039	0.00031	0.00008	0.00039	2.24932

A79	1.57223	-0.00009	-0.00012	-0.00006	-0.00018	1.57205
A80	1.86186	-0.00008	-0.00012	0.00002	-0.00010	1.86176
A81	2.21117	0.00000	0.00025	-0.00022	0.00004	2.21121
A82	2.20460	0.00008	0.00030	-0.00007	0.00024	2.20484
A83	2.34324	0.00060	0.00072	-0.00007	0.00065	2.34389
A84	1.92218	-0.00030	-0.00047	0.00007	-0.00040	1.92178
A85	2.01777	-0.00030	-0.00025	0.00000	-0.00025	2.01752
A86	2.19276	0.00052	0.00052	-0.00013	0.00039	2.19315
A87	2.20907	-0.00042	-0.00035	0.00005	-0.00031	2.20877
A88	1.88135	-0.00010	-0.00017	0.00009	-0.00008	1.88126
A89	1.86273	0.00003	0.00001	0.00002	0.00003	1.86276
A90	2.22614	0.00013	0.00015	-0.00001	0.00014	2.22629
A91	2.19431	-0.00016	-0.00016	-0.00002	-0.00017	2.19414
A92	1.87034	0.00013	0.00014	-0.00002	0.00012	1.87046
A93	2.23824	-0.00030	-0.00024	0.00001	-0.00023	2.23801
A94	2.17461	0.00017	0.00010	0.00002	0.00011	2.17472
A95	1.91165	-0.00001	0.00003	-0.00005	-0.00001	1.91164
A96	2.22899	0.00000	-0.00004	0.00002	-0.00002	2.22897
A97	2.14255	0.00001	0.00001	0.00003	0.00003	2.14258
A98	1.89870	-0.00005	-0.00001	-0.00004	-0.00005	1.89866
A99	2.30838	0.00005	0.00004	0.00004	0.00008	2.30846
A100	2.07610	-0.00001	-0.00003	-0.00001	-0.00003	2.07607
A101	2.05911	0.00001	0.00003	-0.00003	0.00000	2.05912
A102	2.08926	0.00000	-0.00006	0.00004	-0.00002	2.08924
A103	2.13481	0.00000	0.00003	-0.00001	0.00002	2.13483
A104	2.06847	0.00002	0.00004	0.00001	0.00005	2.06852
A105	2.13137	0.00000	-0.00004	0.00003	-0.00001	2.13136
A106	2.08334	-0.00002	0.00000	-0.00004	-0.00004	2.08330
A107	2.09531	-0.00002	-0.00002	-0.00005	-0.00007	2.09525
A108	2.09769	0.00002	0.00008	-0.00003	0.00005	2.09774
A109	2.09018	0.00001	-0.00006	0.00008	0.00001	2.09019
A110	2.12483	0.00000	-0.00002	0.00004	0.00001	2.12484
A111	2.07359	0.00000	0.00007	-0.00009	-0.00002	2.07356
A112	2.08478	0.00000	-0.00004	0.00005	0.00001	2.08478
A113	2.16711	-0.00020	-0.00007	-0.00008	-0.00015	2.16696
A114	2.15593	0.00014	0.00023	-0.00004	0.00018	2.15611
A115	1.96015	0.00005	-0.00016	0.00012	-0.00004	1.96012
A116	2.15584	0.00017	0.00032	-0.00009	0.00023	2.15607
A117	2.16705	-0.00013	-0.00011	0.00004	-0.00007	2.16698
A118	1.96029	-0.00005	-0.00021	0.00004	-0.00016	1.96013
A119	1.91257	-0.00001	-0.00008	0.00006	-0.00003	1.91255
A120	1.94859	0.00008	0.00020	0.00003	0.00022	1.94882
A121	1.90482	-0.00004	-0.00008	-0.00005	-0.00013	1.90469
A122	1.90612	-0.00002	-0.00006	0.00002	-0.00004	1.90609
A123	1.88643	0.00001	0.00003	-0.00003	0.00000	1.88643
A124	1.90424	-0.00002	-0.00001	-0.00003	-0.00004	1.90420
A125	1.94910	-0.00006	-0.00031	0.00013	-0.00017	1.94892
A126	1.91260	0.00001	-0.00001	0.00000	-0.00002	1.91259
A127	1.90489	-0.00004	-0.00016	-0.00007	-0.00023	1.90467
A128	1.90592	0.00003	0.00011	0.00002	0.00013	1.90605
A129	1.90401	0.00004	0.00016	-0.00003	0.00013	1.90414
A130	1.88624	0.00002	0.00022	-0.00006	0.00017	1.88640
A131	3.16701	-0.00006	-0.00023	0.00022	-0.00001	3.16699
A132	3.18022	-0.00005	-0.00090	0.00057	-0.00033	3.17989
A133	3.18063	-0.00008	-0.00089	-0.00007	-0.00096	3.17967
A134	3.16742	-0.00008	-0.00011	-0.00055	-0.00066	3.16676
A135	3.14143	0.00001	0.00000	0.00004	0.00004	3.14147
A136	3.14160	0.00000	-0.00001	0.00005	0.00004	3.14164
A137	3.14149	0.00000	0.00014	-0.00013	0.00002	3.14151
A138	3.14174	-0.00002	-0.00007	-0.00014	-0.00021	3.14152

D1	0.00009	0.00000	0.00013	-0.00011	0.00002	0.00011
D2	-3.14144	0.00002	0.00051	-0.00023	0.00028	-3.14116
D3	3.14153	0.00000	0.00011	-0.00010	0.00001	3.14154
D4	-0.00001	0.00001	0.00049	-0.00022	0.00027	0.00026
D5	0.00005	0.00000	-0.00011	0.00005	-0.00006	-0.00001
D6	3.14146	0.00000	-0.00011	0.00006	-0.00005	3.14141
D7	-3.14134	0.00001	-0.00007	0.00003	-0.00004	-3.14139
D8	0.00007	0.00000	-0.00007	0.00004	-0.00003	0.00003
D9	-0.00319	0.00004	0.00131	0.00081	0.00212	-0.00107
D10	3.13911	0.00000	0.00016	0.00074	0.00089	3.14000
D11	3.13822	0.00004	0.00128	0.00082	0.00210	3.14032
D12	-0.00267	-0.00001	0.00013	0.00075	0.00088	-0.00179
D13	-0.00017	0.00000	-0.00005	0.00011	0.00006	-0.00011
D14	3.14151	0.00000	0.00000	0.00004	0.00004	3.14155
D15	3.14136	-0.00002	-0.00050	0.00024	-0.00025	3.14110
D16	-0.00015	-0.00002	-0.00045	0.00018	-0.00027	-0.00042
D17	0.00316	-0.00006	-0.00207	-0.00045	-0.00253	0.00063
D18	-3.13919	-0.00002	-0.00251	-0.00007	-0.00258	3.14142
D19	-3.13837	-0.00004	-0.00167	-0.00058	-0.00224	-3.14062
D20	0.00246	0.00000	-0.00211	-0.00019	-0.00229	0.00016
D21	0.00010	0.00000	-0.00006	-0.00003	-0.00010	0.00000
D22	-3.14158	0.00000	0.00010	-0.00008	0.00003	-3.14156
D23	-3.14159	0.00000	-0.00011	0.00003	-0.00008	3.14152
D24	-0.00008	0.00000	0.00006	-0.00001	0.00004	-0.00004
D25	0.00004	0.00000	0.00009	-0.00003	0.00006	0.00010
D26	-3.14157	0.00000	0.00010	0.00000	0.00010	-3.14147
D27	-3.14146	0.00000	-0.00008	0.00001	-0.00007	-3.14153
D28	0.00011	0.00000	-0.00007	0.00004	-0.00002	0.00009
D29	-0.00012	0.00000	0.00000	0.00002	0.00003	-0.00009
D30	-3.14153	0.00000	0.00000	0.00001	0.00001	-3.14152
D31	3.14149	0.00000	-0.00001	-0.00001	-0.00002	3.14147
D32	0.00008	0.00000	-0.00001	-0.00002	-0.00003	0.00005
D33	0.00509	-0.00008	-0.00257	-0.00107	-0.00365	0.00144
D34	-3.13968	0.00000	0.00098	0.00118	0.00216	-3.13753
D35	-3.13724	-0.00003	-0.00136	-0.00100	-0.00236	-3.13960
D36	0.00117	0.00005	0.00219	0.00125	0.00344	0.00461
D37	-0.00021	0.00001	0.00069	0.00006	0.00075	0.00053
D38	-3.14137	0.00003	0.00086	-0.00002	0.00084	-3.14053
D39	-3.14095	-0.00004	-0.00072	-0.00002	-0.00074	3.14149
D40	0.00108	-0.00002	-0.00054	-0.00011	-0.00065	0.00042
D41	-0.00508	0.00009	0.00285	0.00095	0.00379	-0.00129
D42	3.13966	0.00000	-0.00066	-0.00128	-0.00194	3.13771
D43	3.13729	0.00004	0.00330	0.00055	0.00384	3.14114
D44	-0.00116	-0.00004	-0.00021	-0.00168	-0.00189	-0.00305
D45	-3.13545	-0.00013	-0.00464	-0.00309	-0.00773	3.14001
D46	0.00125	0.00000	-0.00018	-0.00220	-0.00238	-0.00113
D47	0.00242	-0.00003	-0.00048	-0.00045	-0.00093	0.00149
D48	3.13911	0.00010	0.00398	0.00044	0.00442	-3.13965
D49	-0.00481	0.00008	0.00116	0.00205	0.00322	-0.00159
D50	3.14093	0.00001	-0.00126	0.00107	-0.00019	3.14074
D51	3.14148	-0.00005	-0.00312	0.00120	-0.00192	3.13956
D52	0.00403	-0.00012	-0.00554	0.00021	-0.00533	-0.00129
D53	-3.13695	0.00001	-0.00109	0.00054	-0.00054	-3.13750
D54	0.00075	0.00008	0.00118	0.00147	0.00265	0.00340
D55	-3.14109	-0.00004	-0.00010	-0.00066	-0.00076	3.14134
D56	0.00154	0.00001	0.00096	0.00043	0.00139	0.00292
D57	0.00398	-0.00010	-0.00212	-0.00149	-0.00361	0.00037
D58	-3.13658	-0.00005	-0.00107	-0.00040	-0.00147	-3.13805
D59	0.00867	-0.00002	-0.00128	0.00046	-0.00082	0.00786
D60	-3.12738	0.00002	-0.00070	0.00012	-0.00058	-3.12795

D61	-3.13521	0.00000	0.00002	0.00007	0.00009	-3.13512
D62	0.01193	0.00003	0.00059	-0.00026	0.00033	0.01225
D63	-0.00520	-0.00003	0.00004	-0.00108	-0.00105	-0.00625
D64	3.13991	-0.00006	-0.00195	-0.00049	-0.00244	3.13747
D65	-0.00064	0.00002	0.00046	-0.00006	0.00040	-0.00023
D66	-3.13264	-0.00003	-0.00107	0.00000	-0.00107	-3.13371
D67	3.13756	0.00004	0.00237	-0.00063	0.00174	3.13930
D68	0.00556	-0.00001	0.00084	-0.00057	0.00027	0.00583
D69	-0.00808	0.00008	0.00219	0.00068	0.00287	-0.00520
D70	3.13244	0.00002	0.00109	-0.00046	0.00062	3.13306
D71	3.12595	0.00003	0.00141	0.00114	0.00255	3.12850
D72	-0.01672	-0.00003	0.00030	-0.00001	0.00030	-0.01642
D73	-0.01856	-0.00007	-0.00142	0.00048	-0.00094	-0.01950
D74	-3.05073	-0.00006	-0.00949	0.00518	-0.00432	-3.05505
D75	3.13040	-0.00002	-0.00066	0.00004	-0.00063	3.12977
D76	0.09823	-0.00001	-0.00873	0.00473	-0.00400	0.09422
D77	-0.01097	-0.00006	-0.00137	0.00036	-0.00101	-0.01197
D78	3.13724	-0.00001	-0.00017	0.00051	0.00034	3.13758
D79	3.12402	-0.00003	-0.00031	0.00032	0.00001	3.12403
D80	-0.01096	0.00002	0.00088	0.00047	0.00136	-0.00961
D81	-3.14143	0.00002	0.00047	-0.00051	-0.00005	-3.14148
D82	0.01009	-0.00002	-0.00112	-0.00045	-0.00157	0.00852
D83	0.01816	0.00008	0.00172	-0.00052	0.00120	0.01936
D84	3.04981	0.00008	0.00983	-0.00521	0.00461	3.05443
D85	-3.13236	0.00002	0.00010	-0.00072	-0.00062	-3.13298
D86	-0.10071	0.00001	0.00821	-0.00542	0.00279	-0.09792
D87	-3.13336	-0.00003	-0.00105	-0.00017	-0.00122	-3.13458
D88	0.00554	0.00000	-0.00003	-0.00021	-0.00025	0.00529
D89	0.01734	0.00003	0.00060	0.00004	0.00064	0.01797
D90	-3.12695	0.00006	0.00161	-0.00001	0.00161	-3.12534
D91	1.53403	0.00000	0.00441	-0.00082	0.00359	1.53761
D92	-2.63497	0.00001	0.00434	-0.00071	0.00363	-2.63135
D93	-0.57257	0.00002	0.00451	-0.00082	0.00368	-0.56888
D94	-1.47672	0.00000	-0.00524	0.00477	-0.00047	-1.47719
D95	0.63746	0.00001	-0.00531	0.00488	-0.00043	0.63703
D96	2.69987	0.00002	-0.00514	0.00477	-0.00037	2.69950
D97	-0.00705	0.00002	0.00112	0.00034	0.00145	-0.00560
D98	3.13698	0.00002	0.00036	0.00068	0.00104	3.13802
D99	-3.13845	0.00002	0.00061	0.00063	0.00124	-3.13721
D100	0.00587	-0.00001	-0.00043	0.00068	0.00026	0.00613
D101	-0.00858	0.00000	0.00021	-0.00076	-0.00054	-0.00912
D102	3.13967	0.00003	0.00104	0.00070	0.00175	3.14142
D103	0.00224	-0.00002	-0.00083	-0.00014	-0.00097	0.00128
D104	-3.14143	0.00001	-0.00005	-0.00017	-0.00022	3.14154
D105	-3.14120	-0.00001	-0.00026	-0.00040	-0.00065	3.14133
D106	-0.00169	0.00001	0.00053	-0.00044	0.00009	-0.00159
D107	3.13426	0.00000	0.00038	-0.00049	-0.00011	3.13415
D108	-0.01972	0.00003	0.00144	0.00052	0.00196	-0.01777
D109	-0.00493	-0.00001	-0.00036	-0.00015	-0.00051	-0.00544
D110	3.12427	0.00002	0.00069	0.00086	0.00155	3.12582
D111	0.00945	0.00000	0.00004	0.00067	0.00071	0.01016
D112	-3.13657	-0.00001	-0.00051	-0.00030	-0.00081	-3.13738
D113	-3.12315	-0.00002	-0.00072	-0.00006	-0.00079	-3.12393
D114	0.01401	-0.00004	-0.00127	-0.00104	-0.00231	0.01170
D115	3.13103	0.00004	0.00118	0.00063	0.00181	3.13284
D116	0.09742	0.00000	-0.00321	0.00322	0.00000	0.09742
D117	-0.02271	0.00007	0.00221	0.00162	0.00383	-0.01888
D118	-3.05633	0.00003	-0.00218	0.00421	0.00203	-3.05430
D119	3.13548	-0.00003	-0.00097	-0.00138	-0.00235	3.13313
D120	-0.00594	0.00000	-0.00012	-0.00022	-0.00034	-0.00628

D121	0.00032	-0.00001	-0.00017	0.00003	-0.00014	0.00018
D122	-3.14111	0.00003	0.00068	0.00119	0.00187	-3.13924
D123	3.13438	0.00002	0.00093	-0.00004	0.00089	3.13527
D124	-0.01442	0.00005	0.00155	0.00097	0.00252	-0.01190
D125	-0.00733	0.00000	0.00036	-0.00082	-0.00046	-0.00779
D126	3.12706	0.00003	0.00097	0.00019	0.00117	3.12823
D127	-3.13681	-0.00001	-0.00080	0.00027	-0.00053	-3.13734
D128	0.00495	0.00002	0.00008	0.00147	0.00155	0.00651
D129	0.00605	-0.00003	-0.00075	-0.00058	-0.00132	0.00472
D130	-3.13232	-0.00001	-0.00104	0.00020	-0.00084	-3.13316
D131	-3.12571	-0.00007	-0.00158	-0.00196	-0.00355	-3.12925
D132	0.01911	-0.00004	-0.00188	-0.00118	-0.00306	0.01605
D133	0.02290	-0.00007	-0.00232	-0.00160	-0.00392	0.01898
D134	3.05704	-0.00005	0.00205	-0.00419	-0.00214	3.05490
D135	-3.12827	-0.00004	-0.00150	-0.00025	-0.00176	-3.13002
D136	-0.09413	-0.00001	0.00286	-0.00284	0.00002	-0.09410
D137	-0.00218	0.00005	0.00079	0.00168	0.00247	0.00029
D138	3.14149	0.00002	0.00033	-0.00012	0.00021	-3.14148
D139	3.13634	0.00002	0.00108	0.00094	0.00201	3.13835
D140	-0.00317	0.00000	0.00062	-0.00087	-0.00025	-0.00342
D141	-0.00163	-0.00004	-0.00050	-0.00180	-0.00230	-0.00392
D142	3.13764	-0.00001	0.00002	0.00021	0.00023	3.13787
D143	-3.14023	-0.00001	-0.00144	0.00195	0.00051	-3.13971
D144	0.00088	0.00000	-0.00077	0.00154	0.00076	0.00164
D145	0.00385	-0.00004	-0.00199	-0.00020	-0.00218	0.00167
D146	-3.13823	-0.00003	-0.00132	-0.00061	-0.00193	-3.14017
D147	-0.63328	-0.00001	0.00312	-0.00314	-0.00002	-0.63330
D148	1.48081	0.00001	0.00312	-0.00306	0.00006	1.48087
D149	-2.69586	0.00001	0.00317	-0.00311	0.00006	-2.69580
D150	2.63679	-0.00004	-0.00208	-0.00007	-0.00215	2.63464
D151	-1.53231	-0.00002	-0.00208	0.00002	-0.00207	-1.53437
D152	0.57421	-0.00002	-0.00203	-0.00004	-0.00206	0.57215
D153	-0.00246	0.00000	0.00072	-0.00068	0.00004	-0.00242
D154	3.14017	0.00001	0.00162	-0.00066	0.00096	3.14112
D155	3.13965	-0.00001	0.00002	-0.00025	-0.00023	3.13942
D156	-0.00091	0.00001	0.00092	-0.00023	0.00070	-0.00022
D157	-3.13873	0.00000	0.00049	-0.00012	0.00037	-3.13836
D158	0.00234	0.00000	0.00125	-0.00063	0.00062	0.00296
D159	0.00199	-0.00001	-0.00027	-0.00014	-0.00041	0.00159
D160	-3.14012	-0.00001	0.00049	-0.00065	-0.00016	-3.14028
D161	3.13832	0.00000	-0.00065	0.00032	-0.00033	3.13799
D162	-0.00380	-0.00001	-0.00114	0.00040	-0.00074	-0.00454
D163	-0.00240	0.00001	0.00012	0.00034	0.00046	-0.00194
D164	3.13868	0.00000	-0.00037	0.00042	0.00005	3.13872
D165	-0.00081	0.00000	0.00033	-0.00013	0.00020	-0.00061
D166	3.14029	0.00000	0.00006	0.00012	0.00018	3.14046
D167	3.14129	0.00000	-0.00041	0.00037	-0.00004	3.14125
D168	-0.00079	0.00000	-0.00069	0.00062	-0.00006	-0.00086
D169	0.00192	-0.00001	0.00009	-0.00043	-0.00034	0.00158
D170	-3.13942	-0.00001	0.00003	-0.00042	-0.00040	-3.13981
D171	-3.13917	0.00000	0.00055	-0.00050	0.00005	-3.13912
D172	0.00267	0.00000	0.00049	-0.00050	0.00000	0.00267
D173	-0.00067	0.00000	0.00007	0.00009	0.00017	-0.00051
D174	3.14131	0.00002	0.00026	0.00011	0.00037	-3.14151
D175	3.14032	-0.00001	-0.00049	0.00018	-0.00031	3.14001
D176	-0.00089	0.00000	-0.00031	0.00020	-0.00011	-0.00100
D177	-0.00068	0.00000	-0.00026	0.00035	0.00009	-0.00059
D178	3.14070	0.00000	-0.00021	0.00034	0.00013	3.14083
D179	3.14138	0.00000	0.00000	0.00011	0.00010	3.14148
D180	-0.00043	0.00001	0.00005	0.00010	0.00015	-0.00028

D181	-3.14084	0.00000	0.00038	-0.00036	0.00002	-3.14082
D182	0.00059	0.00000	0.00038	-0.00042	-0.00003	0.00055
D183	0.00020	0.00000	0.00007	-0.00007	-0.00001	0.00019
D184	-3.14156	0.00000	0.00008	-0.00013	-0.00006	3.14157
D185	3.14159	0.00000	-0.00003	-0.00005	-0.00009	3.14151
D186	0.00010	0.00000	0.00007	-0.00013	-0.00006	0.00004
D187	0.00028	-0.00001	-0.00010	-0.00005	-0.00015	0.00013
D188	-3.14122	0.00000	0.00000	-0.00012	-0.00012	-3.14134
D189	0.00017	0.00000	-0.00013	-0.00001	-0.00014	0.00003
D190	3.14158	0.00000	-0.00014	0.00008	-0.00006	3.14152
D191	-3.14125	0.00000	-0.00014	0.00005	-0.00009	-3.14134
D192	0.00016	0.00000	-0.00015	0.00014	-0.00001	0.00015
D193	0.00009	0.00000	0.00003	-0.00003	0.00000	0.00009
D194	-3.14153	0.00000	0.00008	-0.00006	0.00002	-3.14151
D195	3.14159	0.00000	-0.00006	0.00004	-0.00003	3.14156
D196	-0.00003	0.00000	-0.00002	0.00001	-0.00001	-0.00004
D197	-0.00032	0.00000	0.00008	0.00006	0.00014	-0.00017
D198	3.14130	0.00000	0.00004	0.00009	0.00013	3.14143
D199	3.14146	0.00000	0.00010	-0.00003	0.00006	3.14152
D200	-0.00011	0.00000	0.00005	-0.00001	0.00005	-0.00006

Item	Value	Threshold	Converged?

Maximum Force	0.000600	0.000450	NO
RMS Force	0.000083	0.000300	YES
Maximum Displacement	0.033650	0.001800	NO
RMS Displacement	0.006020	0.001200	NO

Predicted change in Energy=-6.444617D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.803232	-0.637563	0.005068
2	6	0	-9.993833	-1.788191	0.001977
3	6	0	-10.516070	-3.073315	0.006431
4	6	0	-11.904992	-3.215952	0.014435
5	6	0	-12.726347	-2.081816	0.017739
6	6	0	-12.194600	-0.788073	0.013103
7	1	0	-9.845275	-3.926338	0.003710
8	1	0	-12.352227	-4.205157	0.018150
9	1	0	-13.805104	-2.204020	0.024089
10	1	0	-12.864254	0.060116	0.015964
11	6	0	-9.927211	0.564192	-0.001165
12	6	0	-8.569701	-1.390649	-0.005953
13	6	0	-8.540469	0.088887	-0.006730
14	6	0	-7.404626	0.870384	-0.008904
15	6	0	-6.014509	0.595935	-0.012462
16	6	0	-3.644292	-0.183670	-0.011158
17	6	0	-3.778305	1.228939	-0.017981
18	16	0	-5.182092	-0.988879	-0.013406
19	6	0	-5.099563	1.665253	-0.014940
20	6	0	-2.267198	-0.451370	-0.006590
21	6	0	-1.603830	0.797880	-0.011046

22	7	0	-2.523852	1.821253	-0.033654
23	16	0	-1.151146	-1.806630	-0.006460
24	16	0	1.151241	1.806429	0.007248
25	6	0	0.198408	-0.673712	0.002592
26	6	0	-0.198285	0.673489	-0.001886
27	6	0	1.603922	-0.798089	0.011404
28	6	0	2.267281	0.451163	0.006488
29	6	0	3.644494	0.183429	0.010488
30	6	0	3.778528	-1.229167	0.017516
31	6	0	5.099791	-1.665559	0.014159
32	6	0	6.014693	-0.596226	0.010603
33	16	0	5.182287	0.988649	0.012026
34	7	0	2.524045	-1.821456	0.033401
35	6	0	7.404660	-0.870625	0.006766
36	6	0	8.540386	-0.088954	0.004657
37	6	0	8.569320	1.390569	0.003179
38	6	0	9.927263	-0.564032	0.001175
39	6	0	9.993376	1.788385	-0.003478
40	6	0	10.803033	0.637924	-0.005193
41	6	0	10.515316	3.073631	-0.008195
42	6	0	12.194348	0.788743	-0.012272
43	6	0	11.904198	3.216569	-0.015149
44	6	0	12.725800	2.082600	-0.017218
45	6	0	10.385335	-1.870622	0.004230
46	6	0	9.535046	-3.018774	0.012227
47	6	0	11.769976	-2.221420	0.000401
48	7	0	8.865354	-3.972810	0.018749
49	7	0	12.887538	-2.550566	-0.002627
50	6	0	-10.385105	1.870816	-0.002004
51	6	0	-11.769731	2.221744	0.003719
52	6	0	-9.534694	3.018891	-0.009271
53	7	0	-12.887331	2.550747	0.008352
54	7	0	-8.864681	3.972705	-0.015291
55	8	0	-7.612626	-2.157174	-0.010044
56	8	0	7.612069	2.156853	0.006441
57	6	0	2.242760	-3.243481	-0.056734
58	1	0	1.313692	-3.467070	0.472133
59	1	0	2.153179	-3.572691	-1.097593
60	1	0	3.049451	-3.799078	0.425585
61	6	0	-2.242408	3.243280	0.056544
62	1	0	-2.149687	3.571937	1.097300
63	1	0	-1.314975	3.467343	-0.475033
64	1	0	-3.050614	3.799082	-0.422953
65	1	0	5.428688	-2.698240	0.010898
66	1	0	12.864189	-0.059281	-0.014126
67	1	0	13.804534	2.205038	-0.022795
68	1	0	12.351206	4.205875	-0.019064
69	1	0	9.844338	3.926516	-0.006617
70	1	0	7.573034	-1.940671	0.005489
71	1	0	-7.572950	1.940442	-0.007269
72	1	0	-5.428496	2.697910	-0.011509

Rotational constants (GHZ): 0.1750072 0.0104039 0.0098214

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6569.7416199172 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T
 Big=T
 Integral buffers will be 131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 Nuclear repulsion after empirical dispersion term = 6569.6567082334 Har-
 trees.
 One-electron integrals computed using PRISM.
 NBasis= 916 RedAO= T EigKep= 3.24D-04 NBF= 916
 NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916
 Initial guess from the checkpoint file: "PBDB.chk"
 B after Tr= 0.000000 0.000000 0.000000
 Rot= 1.000000 0.000003 0.000000 0.000019 Ang= 0.00 deg.
 ExpMin= 1.17D-01 ExpMax= 2.19D+04 ExpMxC= 3.30D+03 IAcc=1 IRadAn= 1
 AccDes= 0.00D+00
 Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for in-
 itial guess.
 HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 IDoV= 1 UseB2=F IT-
 yADJ=14
 ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
 FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlgl= 2001
 NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
 wScrn= 0.000000 ICntrl= 500 IOPCl= 0 IlCent= 200000004 NGrid=
 0
 NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0=
 0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 Integral accuracy reduced to 1.0D-05 until final iterations.
 Initial convergence to 1.0D-05 achieved. Increase integral accuracy.
 SCF Done: E(RB3LYP) = -3683.02012020 A.U. after 10 cycles
 NFock= 10 Conv=0.69D-08 -V/T= 2.0068
 Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOPClX= 0 NMat=1
 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-0.000004644	0.000013782	0.000002384
2	6	-0.000018186	0.000013952	0.000018958
3	6	-0.000006464	-0.000004228	0.000000299
4	6	0.000005446	-0.000000051	0.000002959
5	6	-0.000000439	-0.000004677	-0.000002160
6	6	0.000011572	0.000006543	0.000005241
7	1	0.000000662	0.000002516	0.000001225
8	1	0.000001942	0.000000708	-0.000000364
9	1	-0.000002454	-0.000000284	0.000000657
10	1	-0.000002358	0.000005321	-0.000000090
11	6	-0.000036397	-0.000015173	0.000005328
12	6	0.000023621	0.000023753	-0.000044537
13	6	0.000039884	-0.000001928	-0.000044176
14	6	0.000053448	-0.000060753	0.000019629
15	6	-0.000087200	-0.000013721	0.000036602
16	6	-0.000057753	-0.000017070	0.000013872
17	6	0.000019033	0.000035172	-0.000053830
18	16	0.000046732	0.000005977	-0.000007246

19	6	0.000027533	0.000029043	-0.000043425
20	6	0.000000989	-0.000026401	0.000031882
21	6	0.000073324	0.000010613	-0.000036931
22	7	-0.000064851	0.000020090	0.000021694
23	16	-0.000012387	-0.000003277	0.000013323
24	16	-0.000008218	0.000001328	0.000014491
25	6	-0.000023457	0.000001649	0.000007035
26	6	0.000006375	0.000012262	-0.000027139
27	6	-0.000038388	-0.000045290	0.000120204
28	6	0.000093614	-0.000006702	-0.000015704
29	6	0.000017616	0.000048032	-0.000079510
30	6	-0.000055331	-0.000008228	0.000061577
31	6	-0.000108390	-0.000013539	0.000065116
32	6	0.000038946	0.000045684	-0.000120301
33	16	-0.000073520	0.000015478	0.000035024
34	7	0.000077889	-0.000026753	-0.000094692
35	6	0.000032771	0.000008939	0.000000427
36	6	0.000018741	-0.000001560	0.000043833
37	6	0.000057171	-0.000004437	0.000015650
38	6	-0.000000669	0.000029840	0.000008463
39	6	-0.000006314	-0.000021348	0.000001276
40	6	-0.000013325	0.000005172	0.000000677
41	6	-0.000002475	0.000012507	0.000007186
42	6	-0.000004585	-0.000011181	-0.000015982
43	6	0.000006117	-0.000005301	0.000004595
44	6	0.000002044	-0.000008047	-0.000002771
45	6	-0.000053983	-0.000038104	-0.000051089
46	6	-0.000005846	0.000006698	0.000002263
47	6	0.000031783	0.000020710	0.000028722
48	7	-0.000007413	0.000003486	-0.000007219
49	7	0.000001604	-0.000013612	-0.000001169
50	6	0.000016295	0.000011912	0.000020998
51	6	-0.000018641	-0.000017490	-0.000028932
52	6	0.000006426	-0.000003900	0.000022680
53	7	-0.000000474	-0.000000915	0.000002873
54	7	0.000004412	-0.000002693	-0.000004742
55	8	-0.000005317	0.000002288	0.000031208
56	8	-0.000030547	-0.000028707	-0.000024279
57	6	0.000010238	0.000015785	-0.000026738
58	1	0.000012083	0.000012365	-0.000004850
59	1	-0.000010138	0.000006103	-0.000002745
60	1	-0.000007745	-0.000002633	0.000012008
61	6	-0.000003944	-0.000021541	0.000041769
62	1	0.000012956	0.000007739	0.000001202
63	1	-0.000006542	-0.000008318	0.000007574
64	1	0.000007383	0.000011706	-0.000007492
65	1	-0.000001455	0.000000648	-0.000000602
66	1	0.000014133	0.000002589	0.000013049
67	1	0.000001205	-0.000000773	0.000000981
68	1	0.000001124	-0.000001066	0.000001451
69	1	0.000002392	0.000000912	-0.000003728
70	1	0.000011772	0.000010662	0.000004409
71	1	-0.000004055	-0.000015819	0.000005628
72	1	-0.000005365	-0.000006443	-0.000003981

Cartesian Forces: Max 0.000120301 RMS 0.000029381

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.

```

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD:  received Info=          1 from GESDD.
Internal Forces:  Max          0.000133630 RMS          0.000022324
Search for a local minimum.
Step number 28 out of a maximum of 429
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 16 18 17 19 20
21 22 23 24 25
26 27 28
DE= -5.67D-06 DEPred=-6.44D-06 R= 8.80D-01
TightC=F SS= 1.41D+00 RLast= 2.39D-02 DXNew= 2.4113D-01 7.1609D-02
Trust test= 8.80D-01 RLast= 2.39D-02 DXMaxT set to 1.43D-01
ITU= 1 -1 1 -1 1 -1 1 1 -1 0 -1 0 -1 1 1 1 1 1 1 0
ITU= 0 0 1 0 0 0 1 0
Eigenvalues --- 0.00252 0.00268 0.00274 0.00362 0.00388
Eigenvalues --- 0.00419 0.00480 0.00505 0.00513 0.00567
Eigenvalues --- 0.00581 0.00604 0.00619 0.00648 0.00679
Eigenvalues --- 0.00688 0.00702 0.00744 0.00748 0.00766
Eigenvalues --- 0.00770 0.00774 0.00783 0.00808 0.00827
Eigenvalues --- 0.00863 0.01002 0.01060 0.01095 0.01133
Eigenvalues --- 0.01150 0.01238 0.01280 0.01314 0.01327
Eigenvalues --- 0.01360 0.01379 0.01404 0.01457 0.01463
Eigenvalues --- 0.01541 0.01603 0.01646 0.01744 0.01747
Eigenvalues --- 0.01793 0.01895 0.01927 0.01953 0.02006
Eigenvalues --- 0.02021 0.02061 0.02075 0.02168 0.02189
Eigenvalues --- 0.02563 0.02937 0.03493 0.03669 0.03939
Eigenvalues --- 0.04008 0.04829 0.04838 0.04909 0.05011
Eigenvalues --- 0.05018 0.05049 0.05135 0.05354 0.07050
Eigenvalues --- 0.07232 0.07392 0.07570 0.15440 0.15800
Eigenvalues --- 0.15951 0.15984 0.15997 0.15999 0.16000
Eigenvalues --- 0.16000 0.16000 0.16000 0.16000 0.16002
Eigenvalues --- 0.16002 0.16010 0.16024 0.16048 0.16068
Eigenvalues --- 0.16083 0.19030 0.19147 0.19657 0.20362
Eigenvalues --- 0.20927 0.21324 0.21775 0.21975 0.22002
Eigenvalues --- 0.22096 0.22362 0.22559 0.22598 0.22632
Eigenvalues --- 0.22648 0.22781 0.22832 0.23051 0.23235
Eigenvalues --- 0.23372 0.23410 0.23733 0.23908 0.24046
Eigenvalues --- 0.24220 0.24272 0.24311 0.24350 0.24524
Eigenvalues --- 0.24579 0.24650 0.24712 0.24733 0.24871
Eigenvalues --- 0.24923 0.24954 0.24972 0.24979 0.24987
Eigenvalues --- 0.24995 0.24998 0.24999 0.25000 0.25000
Eigenvalues --- 0.25000 0.25000 0.25000 0.25001 0.25012
Eigenvalues --- 0.25067 0.25600 0.25820 0.26005 0.26201
Eigenvalues --- 0.26509 0.26564 0.26809 0.26882 0.27207
Eigenvalues --- 0.27253 0.27736 0.27845 0.28436 0.28507
Eigenvalues --- 0.28644 0.28877 0.29994 0.30435 0.31865
Eigenvalues --- 0.32984 0.35386 0.35508 0.36279 0.36335
Eigenvalues --- 0.36405 0.36474 0.36648 0.36778 0.36817
Eigenvalues --- 0.36870 0.37053 0.37086 0.37096 0.37253
Eigenvalues --- 0.37259 0.37384 0.37429 0.37569 0.37678
Eigenvalues --- 0.37758 0.38044 0.39014 0.40304 0.40992
Eigenvalues --- 0.41678 0.42006 0.42647 0.44409 0.44846
Eigenvalues --- 0.45589 0.46375 0.46677 0.47773 0.47956
Eigenvalues --- 0.48602 0.52232 0.53442 0.55346 0.56937
Eigenvalues --- 0.63770 0.70755 0.73161 0.80395 0.82059
Eigenvalues --- 0.91411 1.25856 1.26335 1.29346 1.35376
En-DIIS/RFO-DIIS IScMMF= 0 using points: 28 27 26 25 24
RFO step: Lambda=-5.01350542D-07.

```

DidBck=T Rises=F RFO-DIIS coefs: 0.48871 0.20782 0.22625 0.03301
0.04421

Iteration 1 RMS(Cart)= 0.00135288 RMS(Int)= 0.00000135
Iteration 2 RMS(Cart)= 0.00000259 RMS(Int)= 0.00000109
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000109

Variable (Linear)	Old X (Quad)	-DE/DX (Total)	Delta X	Delta X	Delta X	New X
R1	2.65847	0.00001	0.00000	0.00000	0.00000	2.65847
R2	2.64469	0.00000	0.00002	-0.00004	-0.00002	2.64466
R3	2.81034	0.00004	0.00007	-0.00005	0.00001	2.81035
R4	2.62141	0.00000	0.00001	-0.00002	-0.00001	2.62140
R5	2.79415	0.00001	0.00006	-0.00003	0.00004	2.79418
R6	2.63853	-0.00001	-0.00002	0.00002	0.00000	2.63854
R7	2.05070	0.00000	0.00000	0.00000	0.00000	2.05070
R8	2.64622	0.00000	0.00002	-0.00002	0.00001	2.64623
R9	2.05151	0.00000	0.00000	0.00000	0.00000	2.05151
R10	2.64329	0.00000	-0.00002	0.00003	0.00001	2.64330
R11	2.05163	0.00000	0.00000	0.00000	0.00000	2.05163
R12	2.04219	0.00000	-0.00001	0.00004	0.00003	2.04222
R13	2.77024	0.00000	0.00004	-0.00008	-0.00004	2.77020
R14	2.61639	-0.00001	-0.00004	0.00004	0.00000	2.61639
R15	2.79646	0.00002	0.00013	-0.00012	0.00000	2.79647
R16	2.31718	0.00002	0.00001	0.00003	0.00004	2.31722
R17	2.60541	0.00003	0.00034	-0.00052	-0.00018	2.60523
R18	2.67766	-0.00008	-0.00036	0.00061	0.00025	2.67791
R19	2.04698	0.00001	0.00003	-0.00003	0.00000	2.04699
R20	3.38285	0.00002	-0.00006	0.00022	0.00016	3.38301
R21	2.65947	-0.00004	-0.00006	0.00004	-0.00002	2.65945
R22	2.68146	-0.00001	0.00006	-0.00010	-0.00004	2.68143
R23	3.28029	-0.00001	0.00010	-0.00017	-0.00008	3.28021
R24	2.65106	0.00002	-0.00002	0.00021	0.00020	2.65126
R25	2.62944	-0.00003	-0.00006	0.00006	0.00000	2.62944
R26	2.62171	-0.00001	-0.00004	0.00008	0.00003	2.62174
R27	2.04806	0.00001	0.00000	0.00002	0.00002	2.04807
R28	2.67295	-0.00003	0.00006	-0.00013	-0.00008	2.67287
R29	3.31769	0.00000	0.00000	0.00001	0.00001	3.31770
R30	2.60086	0.00000	-0.00010	0.00018	0.00008	2.60094
R31	2.66653	-0.00003	0.00000	-0.00004	-0.00004	2.66649
R32	2.74466	-0.00001	0.00003	-0.00001	0.00001	2.74468
R33	3.32983	0.00000	-0.00001	0.00004	0.00003	3.32986
R34	3.32981	-0.00001	0.00002	-0.00002	-0.00001	3.32981
R35	3.31769	-0.00001	-0.00002	0.00001	0.00000	3.31769
R36	2.65393	-0.00002	-0.00002	0.00002	0.00000	2.65393
R37	2.66647	0.00000	0.00002	0.00019	0.00021	2.66668
R38	2.67294	-0.00002	-0.00001	-0.00001	-0.00002	2.67292
R39	2.60096	-0.00004	-0.00007	0.00003	-0.00004	2.60091
R40	2.65129	-0.00008	-0.00012	-0.00008	-0.00019	2.65110
R41	2.68144	-0.00002	-0.00005	0.00003	-0.00001	2.68143
R42	3.28029	-0.00001	-0.00001	0.00001	0.00000	3.28028
R43	2.62949	-0.00006	0.00001	-0.00014	-0.00013	2.62936
R44	2.62174	-0.00003	-0.00007	0.00003	-0.00004	2.62170
R45	2.65944	-0.00001	-0.00003	0.00001	-0.00001	2.65942
R46	2.04808	0.00000	-0.00001	0.00001	0.00000	2.04808
R47	3.38294	0.00001	-0.00006	0.00012	0.00006	3.38300
R48	2.67736	0.00007	0.00016	0.00001	0.00017	2.67753
R49	2.74460	0.00002	0.00001	0.00007	0.00008	2.74468
R50	2.60542	0.00006	0.00008	-0.00004	0.00004	2.60546
R51	2.04698	0.00002	0.00003	-0.00002	0.00001	2.04698
R52	2.79643	0.00004	0.00016	-0.00012	0.00004	2.79647
R53	2.77033	-0.00003	0.00011	-0.00027	-0.00016	2.77017

R54	2.79414	0.00001	0.00010	-0.00010	-0.00001	2.79413
R55	2.31715	0.00004	0.00003	0.00001	0.00004	2.31719
R56	2.81037	0.00001	0.00006	-0.00010	-0.00004	2.81033
R57	2.61645	-0.00005	0.00003	-0.00015	-0.00012	2.61633
R58	2.65848	-0.00001	-0.00005	0.00004	-0.00001	2.65847
R59	2.62141	0.00000	0.00002	0.00002	0.00004	2.62145
R60	2.64464	0.00002	0.00014	-0.00016	-0.00002	2.64462
R61	2.63850	0.00001	-0.00003	0.00007	0.00004	2.63854
R62	2.05070	0.00000	0.00000	0.00001	0.00000	2.05071
R63	2.64327	0.00001	-0.00005	0.00008	0.00003	2.64330
R64	2.04216	0.00002	0.00001	0.00005	0.00006	2.04221
R65	2.64624	0.00000	0.00004	-0.00004	0.00001	2.64624
R66	2.05151	0.00000	0.00000	0.00000	0.00000	2.05151
R67	2.05163	0.00000	0.00000	0.00000	0.00000	2.05163
R68	2.69993	0.00001	0.00009	-0.00011	-0.00002	2.69991
R69	2.69927	0.00004	0.00025	-0.00029	-0.00004	2.69923
R70	2.20274	0.00000	0.00000	0.00000	0.00000	2.20273
R71	2.20158	0.00001	0.00001	-0.00001	-0.00001	2.20158
R72	2.69931	0.00002	0.00011	-0.00009	0.00002	2.69933
R73	2.69995	0.00000	0.00004	-0.00002	0.00001	2.69996
R74	2.20159	0.00000	0.00000	0.00000	0.00000	2.20158
R75	2.20274	0.00000	0.00000	-0.00001	0.00000	2.20274
R76	2.06392	0.00001	-0.00001	0.00003	0.00002	2.06394
R77	2.06991	0.00000	-0.00001	0.00001	0.00000	2.06991
R78	2.06324	0.00000	0.00001	-0.00003	-0.00002	2.06322
R79	2.06991	0.00000	-0.00001	0.00001	-0.00001	2.06990
R80	2.06397	0.00001	-0.00003	0.00005	0.00002	2.06399
R81	2.06320	-0.00001	0.00002	-0.00004	-0.00003	2.06318
A1	2.07608	-0.00002	-0.00002	0.00001	-0.00001	2.07607
A2	1.89865	-0.00001	0.00000	0.00000	0.00000	1.89866
A3	2.30846	0.00002	0.00002	-0.00002	0.00000	2.30846
A4	2.14256	0.00001	0.00001	0.00000	0.00001	2.14257
A5	1.91162	0.00000	0.00001	-0.00002	-0.00001	1.91161
A6	2.22901	-0.00001	-0.00002	0.00001	0.00000	2.22900
A7	2.05913	0.00000	0.00000	0.00000	0.00000	2.05913
A8	2.08922	0.00000	0.00001	-0.00001	0.00000	2.08922
A9	2.13484	0.00000	-0.00001	0.00001	0.00000	2.13484
A10	2.09525	0.00000	0.00000	-0.00001	-0.00001	2.09524
A11	2.09776	0.00000	0.00001	-0.00001	0.00000	2.09775
A12	2.09018	0.00000	0.00000	0.00002	0.00001	2.09019
A13	2.12482	0.00000	0.00000	0.00001	0.00001	2.12483
A14	2.08479	0.00000	-0.00002	0.00003	0.00001	2.08480
A15	2.07357	0.00000	0.00002	-0.00003	-0.00002	2.07355
A16	2.06853	0.00001	0.00001	-0.00001	0.00000	2.06853
A17	2.13136	0.00000	-0.00002	0.00003	0.00001	2.13137
A18	2.08330	-0.00001	0.00001	-0.00002	-0.00001	2.08329
A19	1.87050	0.00000	0.00003	-0.00004	0.00000	1.87050
A20	2.17463	0.00009	0.00008	-0.00002	0.00006	2.17468
A21	2.23806	-0.00009	-0.00011	0.00006	-0.00005	2.23800
A22	1.86277	0.00000	0.00001	-0.00002	-0.00002	1.86275
A23	2.19409	-0.00001	0.00003	-0.00001	0.00002	2.19411
A24	2.22633	0.00001	-0.00003	0.00003	0.00000	2.22633
A25	1.88124	0.00000	-0.00005	0.00007	0.00002	1.88126
A26	2.20874	-0.00005	-0.00009	0.00009	0.00000	2.20875
A27	2.19320	0.00005	0.00014	-0.00016	-0.00002	2.19318
A28	2.34402	0.00004	0.00004	-0.00008	-0.00003	2.34399
A29	2.01742	-0.00001	0.00008	-0.00011	-0.00002	2.01739
A30	1.92175	-0.00003	-0.00014	0.00019	0.00005	1.92180
A31	2.24936	0.00004	-0.00012	0.00023	0.00011	2.24947
A32	2.08363	-0.00006	0.00005	-0.00015	-0.00010	2.08354

A33	1.95020	0.00002	0.00007	-0.00008	-0.00001	1.95018
A34	1.95856	0.00000	-0.00004	0.00006	0.00002	1.95858
A35	1.85739	0.00001	-0.00003	0.00006	0.00003	1.85742
A36	2.46723	-0.00001	0.00007	-0.00012	-0.00005	2.46718
A37	1.98432	0.00001	0.00002	0.00003	0.00005	1.98437
A38	1.91738	-0.00001	-0.00001	-0.00006	-0.00007	1.91730
A39	2.38147	0.00000	-0.00001	0.00003	0.00002	2.38149
A40	1.57208	-0.00002	-0.00003	0.00001	-0.00002	1.57206
A41	1.95960	-0.00001	-0.00002	-0.00002	-0.00003	1.95957
A42	2.12546	0.00001	0.00004	-0.00004	0.00000	2.12546
A43	2.19812	0.00000	-0.00003	0.00006	0.00003	2.19815
A44	1.86693	-0.00001	0.00001	-0.00003	-0.00002	1.86691
A45	2.45170	0.00001	0.00001	0.00003	0.00003	2.45173
A46	1.96454	0.00000	-0.00001	0.00001	0.00000	1.96453
A47	1.92118	0.00000	-0.00002	-0.00001	-0.00004	1.92114
A48	1.97064	0.00001	-0.00001	0.00005	0.00004	1.97069
A49	2.39132	-0.00001	0.00002	-0.00004	-0.00002	2.39131
A50	1.86167	0.00001	0.00004	0.00001	0.00006	1.86173
A51	2.20498	0.00003	0.00004	0.00009	0.00015	2.20513
A52	2.21111	-0.00004	0.00018	-0.00037	-0.00017	2.21094
A53	1.56135	-0.00001	0.00000	-0.00002	-0.00001	1.56134
A54	1.56132	-0.00001	0.00000	0.00006	0.00005	1.56137
A55	1.98276	0.00000	0.00001	-0.00002	-0.00001	1.98275
A56	2.35499	0.00000	-0.00002	0.00006	0.00004	2.35503
A57	1.94543	-0.00001	0.00000	-0.00004	-0.00003	1.94540
A58	2.35496	0.00000	0.00000	0.00002	0.00002	2.35498
A59	1.94544	0.00000	0.00000	-0.00002	-0.00002	1.94543
A60	1.98278	0.00001	0.00000	0.00000	0.00000	1.98278
A61	1.97064	0.00000	-0.00001	0.00001	0.00000	1.97065
A62	2.39137	-0.00001	0.00000	-0.00002	-0.00001	2.39136
A63	1.92114	0.00001	0.00000	0.00000	0.00000	1.92113
A64	1.96455	0.00000	0.00002	-0.00003	-0.00001	1.96453
A65	2.45169	0.00000	0.00000	0.00000	0.00000	2.45170
A66	1.86692	0.00000	-0.00002	0.00003	0.00002	1.86694
A67	1.85742	0.00000	0.00001	-0.00002	-0.00001	1.85741
A68	2.46722	-0.00001	0.00002	-0.00006	-0.00004	2.46718
A69	1.95855	0.00001	-0.00003	0.00008	0.00005	1.95860
A70	1.98438	0.00000	0.00003	-0.00005	-0.00002	1.98436
A71	1.91734	0.00001	0.00000	0.00001	0.00001	1.91735
A72	2.38145	-0.00001	-0.00003	0.00003	0.00000	2.38145
A73	1.95952	0.00002	-0.00002	0.00007	0.00005	1.95957
A74	2.19813	-0.00001	-0.00002	0.00000	-0.00001	2.19812
A75	2.12552	-0.00001	0.00004	-0.00007	-0.00003	2.12549
A76	1.95025	-0.00001	0.00000	-0.00002	-0.00002	1.95023
A77	2.08362	-0.00007	0.00002	-0.00019	-0.00016	2.08345
A78	2.24932	0.00009	-0.00002	0.00020	0.00018	2.24950
A79	1.57205	-0.00001	0.00003	-0.00007	-0.00005	1.57200
A80	1.86176	-0.00002	-0.00002	-0.00005	-0.00007	1.86169
A81	2.21121	-0.00001	0.00012	-0.00018	-0.00005	2.21115
A82	2.20484	0.00004	0.00005	0.00010	0.00015	2.20499
A83	2.34389	0.00013	0.00008	0.00017	0.00025	2.34413
A84	1.92178	-0.00007	-0.00006	-0.00006	-0.00013	1.92165
A85	2.01752	-0.00007	-0.00002	-0.00011	-0.00012	2.01740
A86	2.19315	0.00012	0.00010	0.00004	0.00015	2.19330
A87	2.20877	-0.00009	-0.00005	-0.00007	-0.00011	2.20865
A88	1.88126	-0.00002	-0.00006	0.00002	-0.00003	1.88123
A89	1.86276	0.00001	-0.00001	0.00003	0.00001	1.86278
A90	2.22629	0.00003	0.00001	0.00004	0.00005	2.22634
A91	2.19414	-0.00003	0.00000	-0.00007	-0.00007	2.19407
A92	1.87046	0.00003	0.00002	0.00005	0.00007	1.87052

A93	2.23801	-0.00007	-0.00002	-0.00001	-0.00003	2.23797
A94	2.17472	0.00004	0.00000	-0.00003	-0.00003	2.17469
A95	1.91164	0.00000	0.00003	-0.00006	-0.00004	1.91160
A96	2.22897	0.00000	-0.00001	0.00005	0.00004	2.22900
A97	2.14258	0.00000	-0.00001	0.00001	0.00000	2.14258
A98	1.89866	-0.00001	0.00002	-0.00003	-0.00001	1.89864
A99	2.30846	0.00001	-0.00002	0.00003	0.00001	2.30848
A100	2.07607	0.00000	0.00000	0.00000	0.00000	2.07607
A101	2.05912	0.00001	0.00002	-0.00001	0.00000	2.05912
A102	2.08924	0.00000	-0.00002	0.00002	0.00000	2.08924
A103	2.13483	0.00000	0.00001	-0.00001	0.00000	2.13483
A104	2.06852	0.00000	0.00000	0.00002	0.00002	2.06854
A105	2.13136	0.00000	-0.00002	0.00002	0.00000	2.13136
A106	2.08330	0.00000	0.00002	-0.00004	-0.00002	2.08328
A107	2.09525	0.00000	0.00002	-0.00004	-0.00002	2.09523
A108	2.09774	0.00000	0.00002	-0.00001	0.00001	2.09775
A109	2.09019	0.00000	-0.00004	0.00006	0.00001	2.09021
A110	2.12484	0.00000	-0.00002	0.00002	0.00000	2.12484
A111	2.07356	0.00000	0.00005	-0.00007	-0.00002	2.07354
A112	2.08478	0.00000	-0.00003	0.00005	0.00002	2.08480
A113	2.16696	-0.00005	0.00004	-0.00007	-0.00003	2.16693
A114	2.15611	0.00004	0.00004	-0.00002	0.00002	2.15613
A115	1.96012	0.00001	-0.00008	0.00009	0.00001	1.96012
A116	2.15607	0.00007	0.00007	0.00001	0.00008	2.15615
A117	2.16698	-0.00006	-0.00003	-0.00002	-0.00005	2.16693
A118	1.96013	-0.00001	-0.00004	0.00002	-0.00002	1.96011
A119	1.91255	0.00001	-0.00004	0.00009	0.00005	1.91260
A120	1.94882	0.00000	0.00000	0.00004	0.00004	1.94885
A121	1.90469	0.00000	0.00002	-0.00006	-0.00004	1.90465
A122	1.90609	0.00000	-0.00001	0.00000	-0.00001	1.90608
A123	1.88643	0.00000	0.00002	-0.00003	-0.00001	1.88642
A124	1.90420	0.00000	0.00001	-0.00005	-0.00003	1.90417
A125	1.94892	-0.00002	-0.00009	-0.00001	-0.00010	1.94883
A126	1.91259	0.00001	0.00000	0.00003	0.00003	1.91262
A127	1.90467	-0.00001	0.00002	-0.00014	-0.00011	1.90455
A128	1.90605	0.00001	0.00000	0.00008	0.00007	1.90612
A129	1.90414	0.00001	0.00003	0.00001	0.00004	1.90418
A130	1.88640	0.00000	0.00004	0.00003	0.00007	1.88647
A131	3.16699	-0.00002	-0.00012	0.00016	0.00003	3.16703
A132	3.17989	-0.00003	-0.00035	0.00010	-0.00026	3.17963
A133	3.17967	0.00000	-0.00004	-0.00039	-0.00043	3.17924
A134	3.16676	0.00000	0.00029	-0.00047	-0.00018	3.16658
A135	3.14147	0.00000	-0.00002	0.00008	0.00006	3.14152
A136	3.14164	0.00000	-0.00003	0.00003	0.00000	3.14164
A137	3.14151	0.00001	0.00007	-0.00004	0.00004	3.14154
A138	3.14152	0.00001	0.00007	-0.00001	0.00007	3.14159
D1	0.00011	0.00000	0.00007	-0.00007	0.00000	0.00011
D2	-3.14116	0.00000	0.00016	-0.00013	0.00002	-3.14113
D3	3.14154	0.00001	0.00007	0.00002	0.00010	-3.14155
D4	0.00026	0.00001	0.00016	-0.00004	0.00013	0.00039
D5	-0.00001	0.00000	-0.00003	0.00005	0.00002	0.00001
D6	3.14141	0.00000	-0.00004	0.00007	0.00003	3.14144
D7	-3.14139	0.00000	-0.00004	-0.00007	-0.00011	-3.14150
D8	0.00003	0.00000	-0.00004	-0.00006	-0.00010	-0.00007
D9	-0.00107	-0.00001	-0.00036	-0.00013	-0.00049	-0.00156
D10	3.14000	-0.00001	-0.00039	-0.00040	-0.00079	3.13921
D11	3.14032	0.00000	-0.00036	-0.00001	-0.00037	3.13995
D12	-0.00179	0.00000	-0.00039	-0.00028	-0.00067	-0.00247
D13	-0.00011	0.00000	-0.00006	0.00004	-0.00002	-0.00013
D14	3.14155	0.00000	-0.00002	0.00003	0.00001	3.14156

D15	3.14110	0.00000	-0.00017	0.00011	-0.00005	3.14105
D16	-0.00042	0.00000	-0.00012	0.00010	-0.00002	-0.00044
D17	0.00063	0.00000	0.00010	0.00018	0.00028	0.00091
D18	3.14142	0.00001	0.00033	0.00048	0.00081	-3.14096
D19	-3.14062	0.00000	0.00019	0.00012	0.00031	-3.14031
D20	0.00016	0.00002	0.00043	0.00041	0.00084	0.00100
D21	0.00000	0.00000	0.00001	0.00001	0.00002	0.00002
D22	-3.14156	0.00000	0.00005	-0.00002	0.00003	-3.14153
D23	3.14152	0.00000	-0.00003	0.00002	-0.00001	3.14151
D24	-0.00004	0.00000	0.00000	0.00000	0.00000	-0.00004
D25	0.00010	0.00000	0.00002	-0.00003	0.00000	0.00009
D26	-3.14147	0.00000	0.00001	-0.00002	-0.00002	-3.14148
D27	-3.14153	0.00000	-0.00001	0.00000	-0.00001	-3.14154
D28	0.00009	0.00000	-0.00003	0.00000	-0.00003	0.00007
D29	-0.00009	0.00000	-0.00001	-0.00001	-0.00002	-0.00011
D30	-3.14152	0.00000	-0.00001	-0.00002	-0.00003	-3.14154
D31	3.14147	0.00000	0.00000	-0.00001	-0.00001	3.14147
D32	0.00005	0.00000	0.00001	-0.00002	-0.00002	0.00003
D33	0.00144	0.00000	0.00041	0.00024	0.00065	0.00210
D34	-3.13753	-0.00001	-0.00062	0.00039	-0.00023	-3.13776
D35	-3.13960	0.00001	0.00045	0.00052	0.00097	-3.13863
D36	0.00461	-0.00001	-0.00059	0.00068	0.00009	0.00470
D37	0.00053	0.00001	0.00002	0.00036	0.00038	0.00091
D38	-3.14053	0.00001	0.00007	0.00028	0.00035	-3.14018
D39	3.14149	0.00000	-0.00002	0.00003	0.00001	3.14150
D40	0.00042	0.00000	0.00003	-0.00005	-0.00002	0.00040
D41	-0.00129	0.00000	-0.00032	-0.00026	-0.00058	-0.00187
D42	3.13771	0.00002	0.00071	-0.00041	0.00030	3.13801
D43	3.14114	-0.00002	-0.00056	-0.00056	-0.00112	3.14002
D44	-0.00305	0.00000	0.00046	-0.00071	-0.00025	-0.00329
D45	3.14001	0.00003	0.00158	-0.00086	0.00072	3.14072
D46	-0.00113	0.00002	0.00080	-0.00035	0.00045	-0.00068
D47	0.00149	0.00001	0.00037	-0.00069	-0.00032	0.00117
D48	-3.13965	0.00000	-0.00041	-0.00017	-0.00059	-3.14023
D49	-0.00159	0.00000	-0.00134	0.00229	0.00095	-0.00065
D50	3.14074	0.00001	-0.00109	0.00236	0.00127	-3.14118
D51	3.13956	0.00001	-0.00059	0.00180	0.00120	3.14076
D52	-0.00129	0.00002	-0.00034	0.00187	0.00153	0.00023
D53	-3.13750	0.00000	-0.00039	-0.00009	-0.00048	-3.13797
D54	0.00340	-0.00002	-0.00062	-0.00016	-0.00078	0.00262
D55	3.14134	0.00001	0.00034	-0.00024	0.00010	3.14145
D56	0.00292	-0.00001	-0.00015	-0.00011	-0.00025	0.00267
D57	0.00037	0.00002	0.00055	-0.00018	0.00038	0.00075
D58	-3.13805	0.00001	0.00006	-0.00005	0.00002	-3.13803
D59	0.00786	-0.00001	-0.00034	-0.00065	-0.00099	0.00687
D60	-3.12795	0.00000	-0.00013	0.00004	-0.00009	-3.12804
D61	-3.13512	0.00000	-0.00003	0.00007	0.00004	-3.13508
D62	0.01225	0.00001	0.00018	0.00076	0.00094	0.01319
D63	-0.00625	0.00002	0.00054	0.00044	0.00098	-0.00527
D64	3.13747	0.00000	0.00007	-0.00066	-0.00059	3.13688
D65	-0.00023	0.00000	0.00007	0.00019	0.00025	0.00002
D66	-3.13371	-0.00001	-0.00008	-0.00093	-0.00101	-3.13472
D67	3.13930	0.00002	0.00052	0.00125	0.00177	3.14107
D68	0.00583	0.00001	0.00037	0.00013	0.00051	0.00633
D69	-0.00520	-0.00001	-0.00015	0.00052	0.00038	-0.00482
D70	3.13306	0.00001	0.00037	0.00039	0.00075	3.13381
D71	3.12850	-0.00002	-0.00044	-0.00041	-0.00085	3.12765
D72	-0.01642	-0.00001	0.00008	-0.00055	-0.00047	-0.01690
D73	-0.01950	-0.00003	-0.00036	-0.00141	-0.00177	-0.02127
D74	-3.05505	-0.00002	-0.00326	0.00118	-0.00208	-3.05713

D75	3.12977	-0.00001	-0.00007	-0.00050	-0.00057	3.12920
D76	0.09422	0.00000	-0.00298	0.00209	-0.00089	0.09334
D77	-0.01197	-0.00002	-0.00029	-0.00108	-0.00137	-0.01334
D78	3.13758	-0.00001	-0.00027	-0.00025	-0.00053	3.13705
D79	3.12403	-0.00001	-0.00019	-0.00031	-0.00050	3.12353
D80	-0.00961	-0.00001	-0.00017	0.00052	0.00034	-0.00926
D81	-3.14148	0.00001	0.00029	0.00065	0.00095	-3.14054
D82	0.00852	0.00000	0.00014	-0.00051	-0.00036	0.00816
D83	0.01936	0.00003	0.00040	0.00153	0.00193	0.02129
D84	3.05443	0.00003	0.00331	-0.00104	0.00227	3.05670
D85	-3.13298	0.00002	0.00038	0.00042	0.00079	-3.13219
D86	-0.09792	0.00001	0.00329	-0.00215	0.00113	-0.09678
D87	-3.13458	0.00000	0.00000	-0.00040	-0.00039	-3.13498
D88	0.00529	0.00000	0.00011	-0.00022	-0.00011	0.00518
D89	0.01797	0.00001	0.00003	0.00074	0.00077	0.01874
D90	-3.12534	0.00001	0.00013	0.00091	0.00105	-3.12429
D91	1.53761	0.00000	0.00071	0.00157	0.00228	1.53989
D92	-2.63135	0.00000	0.00065	0.00168	0.00233	-2.62902
D93	-0.56888	0.00001	0.00072	0.00165	0.00237	-0.56652
D94	-1.47719	0.00001	-0.00276	0.00464	0.00188	-1.47531
D95	0.63703	0.00001	-0.00282	0.00475	0.00193	0.63896
D96	2.69950	0.00002	-0.00275	0.00472	0.00197	2.70147
D97	-0.00560	0.00000	-0.00008	0.00039	0.00030	-0.00530
D98	3.13802	-0.00001	-0.00032	0.00013	-0.00019	3.13783
D99	-3.13721	-0.00001	-0.00027	-0.00004	-0.00031	-3.13752
D100	0.00613	-0.00001	-0.00038	-0.00021	-0.00059	0.00553
D101	-0.00912	0.00001	0.00040	0.00021	0.00061	-0.00851
D102	3.14142	-0.00001	-0.00027	-0.00059	-0.00086	3.14056
D103	0.00128	0.00000	0.00000	-0.00017	-0.00017	0.00111
D104	3.14154	0.00000	0.00008	-0.00003	0.00005	3.14159
D105	3.14133	0.00001	0.00018	0.00003	0.00021	3.14154
D106	-0.00159	0.00001	0.00026	0.00016	0.00043	-0.00117
D107	3.13415	0.00000	0.00028	0.00025	0.00053	3.13469
D108	-0.01777	-0.00002	-0.00014	-0.00072	-0.00086	-0.01863
D109	-0.00544	0.00000	0.00004	0.00000	0.00005	-0.00540
D110	3.12582	-0.00002	-0.00038	-0.00097	-0.00135	3.12448
D111	0.01016	-0.00001	-0.00033	-0.00017	-0.00050	0.00966
D112	-3.13738	0.00001	0.00011	0.00037	0.00048	-3.13691
D113	-3.12393	0.00001	-0.00003	0.00054	0.00051	-3.12342
D114	0.01170	0.00002	0.00042	0.00107	0.00149	0.01319
D115	3.13284	-0.00002	-0.00022	-0.00060	-0.00082	3.13202
D116	0.09742	-0.00001	-0.00180	0.00072	-0.00108	0.09635
D117	-0.01888	-0.00004	-0.00064	-0.00155	-0.00219	-0.02107
D118	-3.05430	-0.00003	-0.00221	-0.00023	-0.00244	-3.05674
D119	3.13313	0.00002	0.00061	0.00062	0.00123	3.13437
D120	-0.00628	0.00000	0.00010	-0.00022	-0.00012	-0.00641
D121	0.00018	0.00000	-0.00003	-0.00015	-0.00018	0.00000
D122	-3.13924	-0.00002	-0.00055	-0.00100	-0.00154	-3.14078
D123	3.13527	-0.00001	0.00009	-0.00025	-0.00016	3.13512
D124	-0.01190	-0.00003	-0.00036	-0.00081	-0.00117	-0.01307
D125	-0.00779	0.00001	0.00044	0.00032	0.00076	-0.00703
D126	3.12823	-0.00001	-0.00001	-0.00024	-0.00025	3.12798
D127	-3.13734	0.00000	-0.00019	-0.00009	-0.00028	-3.13761
D128	0.00651	-0.00003	-0.00072	-0.00096	-0.00168	0.00482
D129	0.00472	0.00003	0.00021	0.00076	0.00098	0.00570
D130	-3.13316	-0.00001	-0.00018	-0.00065	-0.00082	-3.13398
D131	-3.12925	0.00005	0.00084	0.00152	0.00236	-3.12689
D132	0.01605	0.00001	0.00045	0.00011	0.00056	0.01661
D133	0.01898	0.00004	0.00062	0.00145	0.00207	0.02105
D134	3.05490	0.00003	0.00219	0.00012	0.00231	3.05721

D135	-3.13002	0.00002	0.00001	0.00072	0.00072	-3.12930
D136	-0.09410	0.00001	0.00158	-0.00062	0.00096	-0.09314
D137	0.00029	-0.00005	-0.00075	-0.00148	-0.00223	-0.00194
D138	-3.14148	-0.00002	0.00008	-0.00087	-0.00079	3.14092
D139	3.13835	-0.00001	-0.00038	-0.00013	-0.00052	3.13783
D140	-0.00342	0.00002	0.00045	0.00048	0.00093	-0.00249
D141	-0.00392	0.00004	0.00084	0.00139	0.00224	-0.00169
D142	3.13787	0.00001	-0.00009	0.00071	0.00062	3.13849
D143	-3.13971	-0.00003	-0.00095	-0.00159	-0.00254	3.14094
D144	0.00164	-0.00002	-0.00069	-0.00131	-0.00200	-0.00036
D145	0.00167	0.00001	0.00004	-0.00086	-0.00081	0.00085
D146	-3.14017	0.00002	0.00030	-0.00058	-0.00028	-3.14044
D147	-0.63330	-0.00002	0.00178	-0.00320	-0.00142	-0.63472
D148	1.48087	-0.00002	0.00174	-0.00311	-0.00137	1.47950
D149	-2.69580	-0.00002	0.00177	-0.00319	-0.00142	-2.69721
D150	2.63464	0.00000	-0.00009	-0.00161	-0.00170	2.63294
D151	-1.53437	0.00000	-0.00013	-0.00153	-0.00166	-1.53603
D152	0.57215	-0.00001	-0.00010	-0.00160	-0.00170	0.57044
D153	-0.00242	0.00001	0.00041	0.00004	0.00045	-0.00197
D154	3.14112	0.00001	0.00046	0.00018	0.00064	-3.14142
D155	3.13942	0.00000	0.00014	-0.00025	-0.00011	3.13931
D156	-0.00022	0.00000	0.00019	-0.00011	0.00008	-0.00014
D157	-3.13836	0.00000	0.00008	0.00025	0.00032	-3.13804
D158	0.00296	0.00000	0.00044	-0.00031	0.00013	0.00308
D159	0.00159	0.00000	0.00003	0.00013	0.00016	0.00175
D160	-3.14028	0.00000	0.00039	-0.00043	-0.00003	-3.14032
D161	3.13799	0.00000	-0.00019	-0.00004	-0.00024	3.13775
D162	-0.00454	0.00000	-0.00027	0.00000	-0.00027	-0.00480
D163	-0.00194	0.00000	-0.00015	0.00008	-0.00008	-0.00201
D164	3.13872	0.00000	-0.00022	0.00012	-0.00010	3.13862
D165	-0.00061	0.00000	0.00011	-0.00030	-0.00019	-0.00081
D166	3.14046	0.00000	-0.00004	-0.00002	-0.00006	3.14040
D167	3.14125	0.00000	-0.00025	0.00024	0.00000	3.14125
D168	-0.00086	0.00000	-0.00040	0.00053	0.00013	-0.00073
D169	0.00158	0.00000	0.00022	-0.00026	-0.00005	0.00154
D170	-3.13981	0.00000	0.00021	-0.00035	-0.00014	-3.13995
D171	-3.13912	0.00000	0.00029	-0.00031	-0.00002	-3.13914
D172	0.00267	0.00000	0.00028	-0.00039	-0.00011	0.00256
D173	-0.00051	0.00000	-0.00004	0.00009	0.00004	-0.00046
D174	-3.14151	0.00000	-0.00004	0.00011	0.00007	-3.14144
D175	3.14001	0.00000	-0.00013	0.00014	0.00001	3.14002
D176	-0.00100	0.00000	-0.00012	0.00016	0.00003	-0.00097
D177	-0.00059	0.00000	-0.00020	0.00035	0.00015	-0.00044
D178	3.14083	0.00000	-0.00019	0.00042	0.00023	3.14106
D179	3.14148	0.00000	-0.00006	0.00008	0.00002	3.14151
D180	-0.00028	0.00000	-0.00005	0.00015	0.00010	-0.00018
D181	-3.14082	0.00000	0.00021	-0.00039	-0.00018	-3.14100
D182	0.00055	0.00000	0.00024	-0.00038	-0.00013	0.00042
D183	0.00019	0.00000	0.00004	-0.00008	-0.00003	0.00016
D184	3.14157	0.00000	0.00007	-0.00006	0.00001	3.14158
D185	3.14151	0.00000	0.00003	-0.00002	0.00001	3.14152
D186	0.00004	0.00000	0.00007	-0.00003	0.00004	0.00008
D187	0.00013	0.00000	0.00002	-0.00010	-0.00008	0.00004
D188	-3.14134	0.00000	0.00006	-0.00012	-0.00006	-3.14139
D189	0.00003	0.00000	0.00000	-0.00005	-0.00005	-0.00002
D190	3.14152	0.00000	-0.00005	0.00007	0.00001	3.14154
D191	-3.14134	0.00000	-0.00004	-0.00006	-0.00010	-3.14144
D192	0.00015	0.00000	-0.00008	0.00005	-0.00003	0.00012
D193	0.00009	0.00000	0.00002	-0.00002	0.00000	0.00009
D194	-3.14151	0.00000	0.00003	-0.00002	0.00002	-3.14150

D195	3.14156	0.00000	-0.00002	0.00000	-0.00003	3.14154
D196	-0.00004	0.00000	-0.00001	0.00000	-0.00001	-0.00005
D197	-0.00017	0.00000	-0.00002	0.00009	0.00007	-0.00011
D198	3.14143	0.00000	-0.00004	0.00010	0.00005	3.14148
D199	3.14152	0.00000	0.00002	-0.00002	0.00000	3.14152
D200	-0.00006	0.00000	0.00001	-0.00002	-0.00001	-0.00008

Item	Value	Threshold	Converged?

Maximum Force	0.000134	0.000450	YES
RMS Force	0.000022	0.000300	YES
Maximum Displacement	0.006524	0.001800	NO
RMS Displacement	0.001353	0.001200	NO

Predicted change in Energy=-1.278513D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.803458	-0.637553	0.006640
2	6	0	-9.994077	-1.788196	0.003403
3	6	0	-10.516316	-3.073314	0.008143
4	6	0	-11.905239	-3.215944	0.016623
5	6	0	-12.726575	-2.081791	0.020073
6	6	0	-12.194813	-0.788050	0.015124
7	1	0	-9.845524	-3.926343	0.005303
8	1	0	-12.352476	-4.205147	0.020603
9	1	0	-13.805334	-2.203963	0.026778
10	1	0	-12.864480	0.060151	0.018086
11	6	0	-9.927423	0.564196	-0.000124
12	6	0	-8.569926	-1.390659	-0.004977
13	6	0	-8.540708	0.088879	-0.005483
14	6	0	-7.404934	0.870304	-0.008258
15	6	0	-6.014701	0.595766	-0.012470
16	6	0	-3.644448	-0.183759	-0.013381
17	6	0	-3.778551	1.228832	-0.017907
18	16	0	-5.182148	-0.989072	-0.015033
19	6	0	-5.099814	1.665123	-0.013903
20	6	0	-2.267243	-0.451440	-0.009464
21	6	0	-1.603967	0.797819	-0.011676
22	7	0	-2.524093	1.821160	-0.034051
23	16	0	-1.151101	-1.806632	-0.010564
24	16	0	1.150996	1.806597	0.008720
25	6	0	0.198377	-0.673612	0.000375
26	6	0	-0.198433	0.673560	-0.002221
27	6	0	1.604011	-0.797842	0.009757
28	6	0	2.267218	0.451484	0.007206
29	6	0	3.644367	0.183949	0.010888
30	6	0	3.778579	-1.228632	0.015602
31	6	0	5.099841	-1.664798	0.011447
32	6	0	6.014634	-0.595375	0.010849
33	16	0	5.182021	0.989428	0.012416
34	7	0	2.524211	-1.821105	0.031924
35	6	0	7.404673	-0.869873	0.007618

36	6	0	8.540657	-0.088540	0.005559
37	6	0	8.570262	1.390988	0.003976
38	6	0	9.927252	-0.564176	0.002018
39	6	0	9.994489	1.788178	-0.003032
40	6	0	10.803595	0.637336	-0.004598
41	6	0	10.517046	3.073194	-0.008021
42	6	0	12.194971	0.787495	-0.011683
43	6	0	11.906013	3.215479	-0.015063
44	6	0	12.727061	2.081104	-0.016886
45	6	0	10.384709	-1.870914	0.005247
46	6	0	9.533871	-3.018644	0.013468
47	6	0	11.769158	-2.222370	0.001416
48	7	0	8.863751	-3.972375	0.020235
49	7	0	12.886643	-2.551765	-0.001610
50	6	0	-10.385235	1.870848	-0.001885
51	6	0	-11.769822	2.221974	0.003731
52	6	0	-9.534687	3.018825	-0.010067
53	7	0	-12.887516	2.550655	0.008229
54	7	0	-8.864389	3.972432	-0.016754
55	8	0	-7.612833	-2.157188	-0.010094
56	8	0	7.613385	2.157771	0.007215
57	6	0	2.242924	-3.243224	-0.057393
58	1	0	1.314815	-3.466859	0.473157
59	1	0	2.151580	-3.572726	-1.098008
60	1	0	3.050544	-3.798576	0.423630
61	6	0	-2.242434	3.243187	0.055563
62	1	0	-2.147189	3.571670	1.096143
63	1	0	-1.316325	3.467339	-0.478303
64	1	0	-3.051903	3.798910	-0.421857
65	1	0	5.428880	-2.697430	0.007200
66	1	0	12.864431	-0.060868	-0.013375
67	1	0	13.805858	2.202990	-0.022482
68	1	0	12.353495	4.204570	-0.019177
69	1	0	9.846468	3.926397	-0.006535
70	1	0	7.572849	-1.939954	0.006325
71	1	0	-7.573267	1.940362	-0.006874
72	1	0	-5.428798	2.697771	-0.009410

Rotational constants (GHZ): 0.1750179 0.0104034 0.0098210

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6569.6757336065 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=T
Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6569.5908217081 Hartrees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.24D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Initial guess from the checkpoint file: "PBDB.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000001 0.000000 0.000009 Ang= 0.00 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3683.02012070 A.U. after 8 cycles

NFock= 8 Conv=0.49D-08 -V/T= 2.0068

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1

NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-0.000002168	0.000004567	0.000001500
2	6	0.000005139	0.000003260	0.000010342
3	6	-0.000005975	-0.000000879	0.000000258
4	6	0.000003676	-0.000003989	0.000001736
5	6	-0.000000914	-0.000005702	-0.000002726
6	6	-0.000004254	0.000012788	-0.000003900
7	1	-0.000001541	0.000001734	0.000001134
8	1	0.000000646	0.000000468	-0.000000477
9	1	-0.000000576	0.000000474	0.000001055
10	1	0.000007507	0.000006329	0.000005427
11	6	-0.000046769	0.000000259	-0.000013331
12	6	0.000021978	0.000035965	0.000002302
13	6	0.000000900	0.000050403	0.000009539
14	6	0.000136235	-0.000151564	0.000085068
15	6	-0.000101791	0.000025172	-0.000043218
16	6	0.000061508	-0.000031388	-0.000022158
17	6	-0.000044464	-0.000016269	0.000092466
18	16	-0.000019692	0.000007152	-0.000009353
19	6	-0.000008339	0.000036663	0.000001618
20	6	0.000009851	0.000031706	-0.000073836
21	6	-0.000081723	-0.000007624	0.000062122
22	7	0.000046830	0.000019727	-0.000079285
23	16	-0.000009507	-0.000009477	0.000015874
24	16	-0.000007508	-0.000010911	-0.000010297
25	6	0.000063182	-0.000034143	-0.000003937
26	6	-0.000003507	0.000006775	0.000031465
27	6	-0.000002762	0.000039712	-0.000071561
28	6	-0.000043343	0.000011289	0.000027179
29	6	-0.000023135	-0.000001004	0.000026913
30	6	0.000026425	0.000007733	-0.000052853
31	6	0.000068462	-0.000000162	-0.000074064
32	6	-0.000029252	-0.000012951	0.000060942
33	16	0.000046857	0.000011284	-0.000019153
34	7	-0.000049445	-0.000017881	0.000066472
35	6	-0.000037944	0.000007221	0.000012032
36	6	-0.000010560	0.000026320	-0.000019549
37	6	-0.000023197	-0.000010063	-0.000003893
38	6	0.000019543	-0.000001999	-0.000001506
39	6	0.000004829	-0.000032178	-0.000007755
40	6	-0.000015217	-0.000007630	-0.000009040
41	6	0.000006133	0.000018051	0.000012663
42	6	0.000013467	-0.000023513	0.000005964
43	6	0.000000979	0.000013187	-0.000000288
44	6	0.000000164	0.000002206	0.000000219
45	6	-0.000025244	0.000002648	-0.000020711
46	6	0.000009875	0.000013711	0.000006960
47	6	0.000033432	0.000002216	0.000032249
48	7	-0.000007964	0.000011344	-0.000001825

49	7	0.000010145	-0.000005086	0.000005897
50	6	0.000006798	-0.000006622	-0.000000766
51	6	-0.000005042	0.000018250	-0.000005125
52	6	0.000020327	0.000000944	0.000020138
53	7	-0.000003434	-0.000015697	-0.000003445
54	7	-0.000006328	-0.000006165	-0.000008370
55	8	-0.000018945	0.000004042	-0.000016524
56	8	-0.000012700	0.000013282	-0.000015435
57	6	-0.000016935	-0.000003580	0.000003624
58	1	0.000003830	0.000001456	-0.000013453
59	1	-0.000007330	0.000007909	-0.000001666
60	1	-0.000006044	-0.000010481	0.000009867
61	6	0.000023698	0.000005545	0.000008600
62	1	0.000003108	-0.000011285	-0.000004987
63	1	-0.000003020	-0.000006269	0.000008674
64	1	0.000005893	0.000005387	-0.000009340
65	1	-0.000003968	0.000000384	0.000004790
66	1	-0.000003120	-0.000004913	-0.000001795
67	1	0.000000045	-0.000001585	-0.000000557
68	1	0.000000351	-0.000000641	0.000001865
69	1	0.000003261	0.000001671	-0.000002384
70	1	-0.000003201	0.000005295	0.000001764
71	1	0.000027939	-0.000020256	-0.000006196
72	1	0.000003843	-0.000002622	-0.000003959

 Cartesian Forces: Max 0.000151564 RMS 0.000028553

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.000173217 RMS 0.000018380

Search for a local minimum.

Step number 29 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 16 18 17 19 20

21 22 23 24 25

26 27 28 29

DE= -5.06D-07 DEPred=-1.28D-06 R= 3.96D-01

Trust test= 3.96D-01 RLast= 1.28D-02 DXMaxT set to 1.43D-01

ITU= 0 1 -1 1 -1 1 -1 1 1 -1 0 -1 0 -1 1 1 1 1 1 1

ITU= 0 0 0 1 0 0 0 1 0

Eigenvalues --- 0.00234 0.00267 0.00270 0.00291 0.00389

Eigenvalues --- 0.00419 0.00480 0.00509 0.00530 0.00577

Eigenvalues --- 0.00582 0.00617 0.00628 0.00641 0.00654

Eigenvalues --- 0.00680 0.00709 0.00744 0.00749 0.00769

Eigenvalues --- 0.00770 0.00777 0.00785 0.00823 0.00827

Eigenvalues --- 0.00865 0.01029 0.01093 0.01131 0.01135

Eigenvalues --- 0.01167 0.01246 0.01279 0.01322 0.01332

Eigenvalues --- 0.01360 0.01380 0.01438 0.01457 0.01464

Eigenvalues --- 0.01603 0.01646 0.01743 0.01747 0.01768

Eigenvalues --- 0.01794 0.01927 0.01953 0.02006 0.02021

Eigenvalues --- 0.02060 0.02075 0.02155 0.02187 0.02516

Eigenvalues --- 0.02896 0.02929 0.03543 0.03617 0.03935

Eigenvalues --- 0.03992 0.04829 0.04839 0.04909 0.05013

Eigenvalues --- 0.05028 0.05062 0.05168 0.05354 0.07046

Eigenvalues --- 0.07230 0.07394 0.07570 0.15433 0.15768

Eigenvalues	---	0.15953	0.15986	0.15992	0.15997	0.16000
Eigenvalues	---	0.16000	0.16000	0.16000	0.16000	0.16001
Eigenvalues	---	0.16009	0.16015	0.16037	0.16051	0.16081
Eigenvalues	---	0.16086	0.19027	0.19162	0.19646	0.20365
Eigenvalues	---	0.20952	0.21270	0.21802	0.21953	0.22004
Eigenvalues	---	0.22045	0.22341	0.22530	0.22598	0.22636
Eigenvalues	---	0.22647	0.22807	0.22932	0.23039	0.23186
Eigenvalues	---	0.23385	0.23447	0.23728	0.23799	0.24031
Eigenvalues	---	0.24192	0.24265	0.24290	0.24343	0.24524
Eigenvalues	---	0.24587	0.24647	0.24731	0.24776	0.24872
Eigenvalues	---	0.24917	0.24952	0.24962	0.24976	0.24986
Eigenvalues	---	0.24995	0.24998	0.24998	0.24999	0.25000
Eigenvalues	---	0.25000	0.25000	0.25000	0.25001	0.25009
Eigenvalues	---	0.25101	0.25591	0.25864	0.26113	0.26222
Eigenvalues	---	0.26554	0.26784	0.26888	0.27059	0.27231
Eigenvalues	---	0.27721	0.27813	0.27891	0.28502	0.28532
Eigenvalues	---	0.28830	0.29745	0.30188	0.31789	0.31947
Eigenvalues	---	0.32957	0.35424	0.35490	0.36279	0.36305
Eigenvalues	---	0.36344	0.36474	0.36643	0.36748	0.36830
Eigenvalues	---	0.36852	0.37059	0.37088	0.37099	0.37248
Eigenvalues	---	0.37257	0.37416	0.37559	0.37671	0.37757
Eigenvalues	---	0.37885	0.38324	0.39096	0.40309	0.40966
Eigenvalues	---	0.41690	0.42011	0.42645	0.44422	0.44868
Eigenvalues	---	0.45690	0.46247	0.46789	0.47765	0.47972
Eigenvalues	---	0.48366	0.52226	0.53376	0.55346	0.56872
Eigenvalues	---	0.62741	0.71478	0.73537	0.80503	0.82116
Eigenvalues	---	0.90317	1.25854	1.26349	1.29352	1.35375
En-DIIS/RFO-DIIS IScMMF= 0 using points: 29 28 27 26 25						
RFO step: Lambda=-3.07745056D-07.						
DidBck=T Rises=F RFO-DIIS coefs: 0.58167 0.32559 0.03364 0.04792 0.01118						
Iteration 1	RMS (Cart)=	0.00113430	RMS (Int)=	0.00000094		
Iteration 2	RMS (Cart)=	0.00000142	RMS (Int)=	0.00000018		
Iteration 3	RMS (Cart)=	0.00000000	RMS (Int)=	0.00000018		
Variable	Old X	-DE/DX	Delta X	Delta X	Delta X	New X
(Linear)	(Quad)	(Total)				
R1	2.65847	0.00001	0.00000	0.00002	0.00002	2.65849
R2	2.64466	0.00001	0.00001	-0.00003	-0.00001	2.64465
R3	2.81035	0.00003	0.00000	0.00004	0.00004	2.81039
R4	2.62140	0.00000	0.00001	-0.00003	-0.00002	2.62138
R5	2.79418	-0.00001	0.00000	-0.00001	-0.00001	2.79417
R6	2.63854	-0.00001	0.00000	0.00000	-0.00001	2.63853
R7	2.05070	0.00000	0.00000	0.00001	0.00001	2.05071
R8	2.64623	0.00000	0.00000	-0.00001	0.00000	2.64623
R9	2.05151	0.00000	0.00000	0.00000	0.00000	2.05152
R10	2.64330	0.00000	-0.00001	0.00001	0.00000	2.64330
R11	2.05163	0.00000	0.00000	0.00000	0.00000	2.05163
R12	2.04222	-0.00001	-0.00001	0.00003	0.00001	2.04224
R13	2.77020	0.00003	0.00002	0.00007	0.00009	2.77029
R14	2.61639	-0.00001	-0.00001	-0.00002	-0.00003	2.61636
R15	2.79647	0.00003	0.00003	0.00003	0.00006	2.79652
R16	2.31722	-0.00002	-0.00002	0.00001	-0.00001	2.31722
R17	2.60523	0.00011	0.00015	-0.00006	0.00009	2.60532
R18	2.67791	-0.00017	-0.00019	-0.00022	-0.00041	2.67749
R19	2.04699	0.00000	0.00001	-0.00001	0.00000	2.04698
R20	3.38301	-0.00003	-0.00008	0.00011	0.00003	3.38304
R21	2.65945	-0.00004	0.00000	-0.00007	-0.00007	2.65938
R22	2.68143	-0.00001	0.00002	-0.00006	-0.00003	2.68139
R23	3.28021	0.00001	0.00006	-0.00005	0.00001	3.28022
R24	2.65126	-0.00006	-0.00008	0.00005	-0.00003	2.65122

R25	2.62944	-0.00002	-0.00001	-0.00008	-0.00009	2.62935
R26	2.62174	-0.00002	-0.00002	-0.00003	-0.00005	2.62169
R27	2.04807	0.00000	-0.00001	0.00003	0.00002	2.04809
R28	2.67287	-0.00001	0.00004	-0.00012	-0.00007	2.67279
R29	3.31770	-0.00001	0.00000	-0.00001	-0.00001	3.31769
R30	2.60094	-0.00005	-0.00005	-0.00001	-0.00006	2.60088
R31	2.66649	-0.00003	0.00002	-0.00014	-0.00012	2.66637
R32	2.74468	0.00000	0.00000	0.00001	0.00001	2.74468
R33	3.32986	-0.00001	-0.00001	0.00001	0.00000	3.32986
R34	3.32981	0.00000	0.00001	-0.00003	-0.00003	3.32978
R35	3.31769	0.00000	0.00000	-0.00001	-0.00001	3.31768
R36	2.65393	-0.00002	0.00000	-0.00002	-0.00002	2.65391
R37	2.66668	-0.00009	-0.00008	-0.00007	-0.00015	2.66653
R38	2.67292	-0.00001	0.00001	-0.00004	-0.00003	2.67289
R39	2.60091	-0.00003	0.00001	-0.00013	-0.00012	2.60080
R40	2.65110	0.00000	0.00006	-0.00023	-0.00017	2.65093
R41	2.68143	0.00000	0.00000	0.00001	0.00001	2.68143
R42	3.28028	-0.00001	0.00000	-0.00002	-0.00002	3.28026
R43	2.62936	0.00001	0.00007	-0.00016	-0.00010	2.62927
R44	2.62170	-0.00001	0.00001	-0.00009	-0.00009	2.62162
R45	2.65942	-0.00001	0.00000	-0.00004	-0.00004	2.65938
R46	2.04808	0.00000	0.00000	0.00000	0.00000	2.04808
R47	3.38300	-0.00002	-0.00003	0.00004	0.00000	3.38300
R48	2.67753	-0.00005	-0.00002	-0.00007	-0.00009	2.67744
R49	2.74468	-0.00001	-0.00003	0.00006	0.00002	2.74470
R50	2.60546	-0.00001	0.00000	0.00000	0.00000	2.60545
R51	2.04698	0.00000	0.00000	-0.00001	0.00000	2.04698
R52	2.79647	0.00001	0.00002	-0.00001	0.00000	2.79647
R53	2.77017	0.00003	0.00009	-0.00003	0.00006	2.77022
R54	2.79413	0.00001	0.00002	-0.00003	0.00000	2.79413
R55	2.31719	0.00002	-0.00001	0.00003	0.00002	2.31722
R56	2.81033	0.00004	0.00002	0.00006	0.00008	2.81041
R57	2.61633	0.00004	0.00006	-0.00007	-0.00001	2.61631
R58	2.65847	0.00002	0.00000	0.00004	0.00004	2.65851
R59	2.62145	-0.00003	-0.00001	-0.00005	-0.00006	2.62139
R60	2.64462	0.00003	0.00004	-0.00001	0.00003	2.64465
R61	2.63854	-0.00001	-0.00002	0.00004	0.00002	2.63856
R62	2.05071	0.00000	0.00000	0.00001	0.00000	2.05071
R63	2.64330	-0.00001	-0.00002	0.00004	0.00002	2.64332
R64	2.04221	-0.00001	-0.00002	0.00005	0.00003	2.04224
R65	2.64624	-0.00001	0.00001	-0.00005	-0.00004	2.64620
R66	2.05151	0.00000	0.00000	0.00000	0.00000	2.05151
R67	2.05163	0.00000	0.00000	0.00000	0.00000	2.05163
R68	2.69991	0.00002	0.00003	0.00003	0.00006	2.69997
R69	2.69923	0.00005	0.00007	0.00005	0.00012	2.69935
R70	2.20273	0.00001	0.00000	0.00001	0.00001	2.20274
R71	2.20158	0.00001	0.00000	0.00000	0.00001	2.20158
R72	2.69933	0.00001	0.00002	0.00002	0.00004	2.69937
R73	2.69996	0.00000	0.00000	0.00002	0.00002	2.69998
R74	2.20158	0.00000	0.00000	0.00000	0.00000	2.20158
R75	2.20274	0.00001	0.00000	0.00000	0.00000	2.20274
R76	2.06394	0.00001	-0.00001	0.00004	0.00003	2.06398
R77	2.06991	0.00000	0.00000	0.00001	0.00001	2.06992
R78	2.06322	0.00000	0.00001	-0.00003	-0.00002	2.06320
R79	2.06990	0.00001	0.00000	0.00000	0.00000	2.06990
R80	2.06399	0.00001	-0.00001	0.00005	0.00004	2.06403
R81	2.06318	0.00000	0.00001	-0.00004	-0.00003	2.06315
A1	2.07607	-0.00001	0.00000	-0.00004	-0.00003	2.07604
A2	1.89866	0.00000	0.00000	0.00000	0.00000	1.89866
A3	2.30846	0.00002	0.00000	0.00004	0.00003	2.30849

A4	2.14257	0.00000	0.00000	0.00002	0.00002	2.14259
A5	1.91161	0.00001	0.00000	0.00001	0.00002	1.91163
A6	2.22900	-0.00001	0.00000	-0.00004	-0.00004	2.22897
A7	2.05913	0.00000	0.00000	0.00001	0.00001	2.05914
A8	2.08922	0.00000	0.00000	-0.00001	-0.00001	2.08921
A9	2.13484	0.00000	0.00000	0.00000	0.00000	2.13484
A10	2.09524	0.00000	0.00001	-0.00002	-0.00002	2.09523
A11	2.09775	0.00000	0.00000	0.00000	0.00000	2.09776
A12	2.09019	0.00000	-0.00001	0.00002	0.00001	2.09020
A13	2.12483	0.00000	0.00000	0.00001	0.00001	2.12483
A14	2.08480	0.00000	-0.00001	0.00002	0.00001	2.08481
A15	2.07355	0.00000	0.00001	-0.00003	-0.00002	2.07354
A16	2.06853	0.00000	0.00000	0.00002	0.00002	2.06855
A17	2.13137	0.00000	-0.00001	0.00003	0.00002	2.13139
A18	2.08329	-0.00001	0.00001	-0.00005	-0.00004	2.08325
A19	1.87050	0.00000	0.00001	-0.00002	-0.00001	1.87049
A20	2.17468	0.00005	-0.00002	0.00014	0.00012	2.17481
A21	2.23800	-0.00005	0.00001	-0.00013	-0.00012	2.23789
A22	1.86275	0.00001	0.00001	0.00001	0.00002	1.86277
A23	2.19411	-0.00001	0.00000	-0.00001	-0.00001	2.19409
A24	2.22633	0.00000	-0.00001	0.00000	0.00000	2.22632
A25	1.88126	-0.00001	-0.00002	0.00000	-0.00003	1.88123
A26	2.20875	-0.00003	-0.00002	0.00005	0.00003	2.20878
A27	2.19318	0.00004	0.00004	-0.00004	0.00000	2.19317
A28	2.34399	0.00003	0.00002	0.00000	0.00002	2.34401
A29	2.01739	0.00001	0.00003	0.00006	0.00009	2.01749
A30	1.92180	-0.00004	-0.00005	-0.00006	-0.00011	1.92169
A31	2.24947	0.00001	-0.00007	0.00017	0.00010	2.24957
A32	2.08354	-0.00004	0.00005	-0.00022	-0.00016	2.08337
A33	1.95018	0.00002	0.00002	0.00004	0.00006	1.95024
A34	1.95858	0.00001	-0.00001	0.00007	0.00005	1.95863
A35	1.85742	0.00000	-0.00002	0.00003	0.00001	1.85744
A36	2.46718	0.00000	0.00004	-0.00010	-0.00006	2.46712
A37	1.98437	-0.00001	-0.00002	0.00001	-0.00001	1.98436
A38	1.91730	0.00001	0.00003	-0.00003	0.00000	1.91730
A39	2.38149	0.00000	-0.00001	0.00002	0.00001	2.38150
A40	1.57206	-0.00002	0.00000	-0.00009	-0.00009	1.57197
A41	1.95957	0.00000	0.00002	-0.00003	-0.00001	1.95955
A42	2.12546	0.00000	0.00001	-0.00001	-0.00001	2.12545
A43	2.19815	0.00000	-0.00002	0.00004	0.00002	2.19817
A44	1.86691	0.00000	0.00001	-0.00004	-0.00003	1.86688
A45	2.45173	0.00000	-0.00001	0.00003	0.00001	2.45174
A46	1.96453	0.00000	0.00000	0.00001	0.00001	1.96454
A47	1.92114	0.00002	0.00001	0.00004	0.00005	1.92119
A48	1.97069	0.00000	-0.00002	0.00006	0.00004	1.97073
A49	2.39131	-0.00002	0.00001	-0.00009	-0.00008	2.39122
A50	1.86173	-0.00002	-0.00002	0.00001	-0.00001	1.86173
A51	2.20513	0.00004	-0.00005	0.00034	0.00029	2.20542
A52	2.21094	-0.00002	0.00011	-0.00028	-0.00017	2.21077
A53	1.56134	-0.00001	0.00001	-0.00006	-0.00005	1.56129
A54	1.56137	-0.00003	-0.00002	-0.00004	-0.00006	1.56131
A55	1.98275	0.00001	0.00001	0.00002	0.00003	1.98278
A56	2.35503	-0.00001	-0.00002	0.00002	0.00000	2.35503
A57	1.94540	0.00000	0.00001	-0.00004	-0.00003	1.94537
A58	2.35498	-0.00001	-0.00001	-0.00001	-0.00002	2.35497
A59	1.94543	0.00000	0.00001	-0.00004	-0.00003	1.94539
A60	1.98278	0.00002	0.00000	0.00005	0.00005	1.98282
A61	1.97065	0.00001	0.00000	0.00003	0.00003	1.97067
A62	2.39136	-0.00002	0.00001	-0.00008	-0.00008	2.39128
A63	1.92113	0.00001	0.00000	0.00005	0.00005	1.92119

A64	1.96453	0.00001	0.00001	0.00001	0.00002	1.96455
A65	2.45170	0.00000	0.00000	0.00000	0.00000	2.45170
A66	1.86694	-0.00001	-0.00001	-0.00001	-0.00002	1.86692
A67	1.85741	0.00000	0.00001	0.00000	0.00001	1.85741
A68	2.46718	0.00000	0.00002	-0.00006	-0.00004	2.46714
A69	1.95860	-0.00001	-0.00003	0.00006	0.00003	1.95863
A70	1.98436	0.00000	0.00001	-0.00003	-0.00002	1.98434
A71	1.91735	-0.00001	-0.00001	0.00001	0.00001	1.91736
A72	2.38145	0.00000	-0.00001	0.00002	0.00001	2.38146
A73	1.95957	-0.00001	-0.00002	0.00003	0.00001	1.95958
A74	2.19812	0.00000	0.00000	0.00001	0.00001	2.19813
A75	2.12549	0.00001	0.00002	-0.00004	-0.00002	2.12547
A76	1.95023	0.00001	0.00001	0.00002	0.00003	1.95025
A77	2.08345	0.00003	0.00008	-0.00013	-0.00005	2.08340
A78	2.24950	-0.00004	-0.00008	0.00011	0.00003	2.24953
A79	1.57200	0.00000	0.00003	-0.00008	-0.00005	1.57195
A80	1.86169	0.00000	0.00003	-0.00005	-0.00002	1.86167
A81	2.21115	-0.00003	0.00004	-0.00015	-0.00010	2.21105
A82	2.20499	0.00002	-0.00005	0.00026	0.00021	2.20519
A83	2.34413	-0.00006	-0.00009	0.00008	-0.00001	2.34412
A84	1.92165	0.00003	0.00005	-0.00007	-0.00003	1.92163
A85	2.01740	0.00004	0.00005	-0.00001	0.00004	2.01744
A86	2.19330	-0.00004	-0.00004	-0.00002	-0.00006	2.19324
A87	2.20865	0.00003	0.00004	0.00000	0.00004	2.20870
A88	1.88123	0.00001	0.00000	0.00002	0.00002	1.88125
A89	1.86278	-0.00001	-0.00001	0.00001	0.00000	1.86278
A90	2.22634	-0.00001	-0.00002	0.00002	0.00000	2.22634
A91	2.19407	0.00002	0.00003	-0.00004	-0.00001	2.19406
A92	1.87052	-0.00002	-0.00002	0.00000	-0.00003	1.87050
A93	2.23797	-0.00002	0.00002	-0.00011	-0.00010	2.23788
A94	2.17469	0.00004	0.00001	0.00012	0.00012	2.17481
A95	1.91160	0.00001	0.00002	0.00000	0.00002	1.91162
A96	2.22900	-0.00001	-0.00001	-0.00002	-0.00004	2.22897
A97	2.14258	0.00000	0.00000	0.00002	0.00002	2.14259
A98	1.89864	0.00000	0.00001	-0.00002	-0.00001	1.89863
A99	2.30848	0.00001	-0.00001	0.00008	0.00007	2.30854
A100	2.07607	-0.00001	0.00000	-0.00005	-0.00005	2.07601
A101	2.05912	0.00001	0.00000	0.00003	0.00003	2.05915
A102	2.08924	0.00000	0.00000	-0.00002	-0.00002	2.08922
A103	2.13483	0.00000	0.00000	-0.00001	-0.00001	2.13482
A104	2.06854	0.00000	-0.00001	0.00004	0.00003	2.06857
A105	2.13136	0.00000	0.00000	0.00004	0.00003	2.13140
A106	2.08328	0.00000	0.00001	-0.00007	-0.00006	2.08322
A107	2.09523	0.00001	0.00001	-0.00003	-0.00001	2.09521
A108	2.09775	0.00000	0.00000	0.00000	0.00000	2.09775
A109	2.09021	0.00000	-0.00001	0.00003	0.00001	2.09022
A110	2.12484	0.00000	-0.00001	0.00000	-0.00001	2.12483
A111	2.07354	0.00000	0.00002	-0.00004	-0.00002	2.07352
A112	2.08480	0.00000	-0.00001	0.00004	0.00003	2.08483
A113	2.16693	-0.00002	0.00002	-0.00013	-0.00011	2.16682
A114	2.15613	0.00003	-0.00001	0.00016	0.00015	2.15629
A115	1.96012	-0.00001	-0.00002	-0.00003	-0.00004	1.96008
A116	2.15615	0.00003	-0.00003	0.00016	0.00013	2.15628
A117	2.16693	-0.00003	0.00002	-0.00013	-0.00011	2.16682
A118	1.96011	0.00000	0.00001	-0.00003	-0.00002	1.96008
A119	1.91260	-0.00001	-0.00003	0.00004	0.00001	1.91261
A120	1.94885	0.00001	-0.00002	0.00006	0.00004	1.94890
A121	1.90465	-0.00001	0.00002	-0.00008	-0.00006	1.90459
A122	1.90608	0.00000	0.00000	0.00001	0.00001	1.90608
A123	1.88642	0.00001	0.00001	0.00003	0.00003	1.88646

A124	1.90417	0.00000	0.00002	-0.00004	-0.00003	1.90414
A125	1.94883	0.00001	0.00002	-0.00004	-0.00002	1.94881
A126	1.91262	0.00000	-0.00001	0.00004	0.00003	1.91265
A127	1.90455	-0.00001	0.00005	-0.00015	-0.00010	1.90446
A128	1.90612	0.00000	-0.00003	0.00007	0.00004	1.90616
A129	1.90418	-0.00001	-0.00001	0.00000	-0.00001	1.90417
A130	1.88647	0.00000	-0.00002	0.00008	0.00006	1.88653
A131	3.16703	-0.00002	-0.00003	-0.00016	-0.00020	3.16683
A132	3.17963	0.00000	0.00004	-0.00028	-0.00024	3.17939
A133	3.17924	0.00003	0.00017	-0.00012	0.00005	3.17929
A134	3.16658	0.00002	0.00014	0.00007	0.00021	3.16678
A135	3.14152	0.00000	-0.00003	0.00004	0.00002	3.14154
A136	3.14164	0.00000	-0.00001	-0.00001	-0.00002	3.14162
A137	3.14154	0.00000	0.00000	0.00003	0.00003	3.14157
A138	3.14159	0.00000	-0.00001	0.00009	0.00008	3.14167
D1	0.00011	0.00000	0.00002	0.00005	0.00007	0.00018
D2	-3.14113	0.00000	0.00003	0.00014	0.00017	-3.14096
D3	-3.14155	0.00000	-0.00003	0.00013	0.00010	-3.14145
D4	0.00039	0.00000	-0.00001	0.00022	0.00020	0.00059
D5	0.00001	0.00000	-0.00002	0.00000	-0.00002	-0.00001
D6	3.14144	0.00000	-0.00002	-0.00001	-0.00004	3.14140
D7	-3.14150	0.00000	0.00004	-0.00010	-0.00005	-3.14155
D8	-0.00007	0.00000	0.00004	-0.00011	-0.00008	-0.00014
D9	-0.00156	0.00000	0.00020	-0.00029	-0.00010	-0.00165
D10	3.13921	0.00000	0.00029	-0.00057	-0.00028	3.13893
D11	3.13995	0.00000	0.00014	-0.00020	-0.00006	3.13989
D12	-0.00247	0.00000	0.00024	-0.00048	-0.00024	-0.00271
D13	-0.00013	0.00000	0.00000	-0.00007	-0.00008	-0.00020
D14	3.14156	0.00000	-0.00001	0.00000	-0.00001	3.14156
D15	3.14105	0.00000	-0.00002	-0.00018	-0.00021	3.14085
D16	-0.00044	0.00000	-0.00003	-0.00011	-0.00014	-0.00058
D17	0.00091	0.00000	-0.00017	-0.00006	-0.00023	0.00068
D18	-3.14096	0.00000	-0.00044	0.00028	-0.00015	-3.14111
D19	-3.14031	0.00000	-0.00015	0.00004	-0.00012	-3.14043
D20	0.00100	0.00000	-0.00042	0.00038	-0.00004	0.00096
D21	0.00002	0.00000	-0.00001	0.00004	0.00004	0.00006
D22	-3.14153	0.00000	0.00000	0.00007	0.00006	-3.14146
D23	3.14151	0.00000	-0.00001	-0.00003	-0.00004	3.14148
D24	-0.00004	0.00000	0.00000	-0.00001	-0.00001	-0.00004
D25	0.00009	0.00000	0.00001	0.00000	0.00001	0.00011
D26	-3.14148	0.00000	0.00001	-0.00001	0.00000	-3.14148
D27	-3.14154	0.00000	0.00000	-0.00002	-0.00001	-3.14155
D28	0.00007	0.00000	0.00001	-0.00003	-0.00002	0.00004
D29	-0.00011	0.00000	0.00000	-0.00003	-0.00002	-0.00013
D30	-3.14154	0.00000	0.00001	-0.00001	0.00000	-3.14154
D31	3.14147	0.00000	0.00000	-0.00001	-0.00001	3.14146
D32	0.00003	0.00000	0.00001	0.00000	0.00001	0.00004
D33	0.00210	0.00000	-0.00030	0.00025	-0.00005	0.00205
D34	-3.13776	0.00000	-0.00007	-0.00048	-0.00055	-3.13831
D35	-3.13863	0.00000	-0.00040	0.00054	0.00014	-3.13848
D36	0.00470	0.00000	-0.00017	-0.00019	-0.00036	0.00434
D37	0.00091	0.00000	-0.00014	0.00046	0.00032	0.00123
D38	-3.14018	0.00000	-0.00010	0.00040	0.00030	-3.13988
D39	3.14150	0.00000	-0.00002	0.00012	0.00010	-3.14159
D40	0.00040	0.00000	0.00002	0.00006	0.00008	0.00048
D41	-0.00187	0.00000	0.00029	-0.00012	0.00017	-0.00170
D42	3.13801	0.00000	0.00006	0.00060	0.00066	3.13867
D43	3.14002	0.00000	0.00056	-0.00048	0.00009	3.14010
D44	-0.00329	0.00000	0.00033	0.00025	0.00058	-0.00271
D45	3.14072	0.00001	0.00001	0.00114	0.00115	-3.14131

D46	-0.00068	0.00001	0.00000	0.00137	0.00138	0.00070
D47	0.00117	0.00001	0.00028	0.00028	0.00056	0.00173
D48	-3.14023	0.00001	0.00027	0.00052	0.00079	-3.13944
D49	-0.00065	-0.00001	-0.00053	-0.00009	-0.00062	-0.00126
D50	-3.14118	0.00000	-0.00063	0.00048	-0.00016	-3.14133
D51	3.14076	-0.00001	-0.00052	-0.00032	-0.00084	3.13992
D52	0.00023	0.00000	-0.00063	0.00025	-0.00038	-0.00014
D53	-3.13797	0.00001	0.00016	0.00010	0.00026	-3.13772
D54	0.00262	0.00000	0.00026	-0.00044	-0.00017	0.00245
D55	3.14145	0.00000	-0.00002	-0.00010	-0.00012	3.14132
D56	0.00267	0.00000	0.00007	-0.00025	-0.00018	0.00249
D57	0.00075	0.00000	-0.00011	0.00038	0.00026	0.00101
D58	-3.13803	0.00001	-0.00002	0.00023	0.00021	-3.13782
D59	0.00687	0.00001	0.00035	-0.00025	0.00010	0.00697
D60	-3.12804	0.00000	0.00003	-0.00012	-0.00009	-3.12813
D61	-3.13508	0.00000	0.00000	-0.00026	-0.00025	-3.13533
D62	0.01319	-0.00002	-0.00032	-0.00013	-0.00044	0.01275
D63	-0.00527	-0.00001	-0.00034	0.00039	0.00004	-0.00522
D64	3.13688	0.00001	0.00019	0.00039	0.00058	3.13746
D65	0.00002	0.00000	-0.00007	-0.00011	-0.00018	-0.00016
D66	-3.13472	0.00002	0.00036	0.00041	0.00076	-3.13396
D67	3.14107	-0.00002	-0.00058	-0.00012	-0.00070	3.14037
D68	0.00633	0.00000	-0.00016	0.00041	0.00025	0.00658
D69	-0.00482	-0.00001	-0.00015	-0.00008	-0.00023	-0.00506
D70	3.13381	-0.00001	-0.00024	0.00007	-0.00018	3.13363
D71	3.12765	0.00001	0.00029	-0.00026	0.00003	3.12768
D72	-0.01690	0.00001	0.00020	-0.00011	0.00009	-0.01681
D73	-0.02127	0.00003	0.00058	0.00032	0.00090	-0.02037
D74	-3.05713	0.00002	0.00016	-0.00038	-0.00022	-3.05735
D75	3.12920	0.00001	0.00015	0.00049	0.00064	3.12985
D76	0.09334	0.00000	-0.00027	-0.00021	-0.00047	0.09286
D77	-0.01334	0.00002	0.00043	0.00032	0.00075	-0.01259
D78	3.13705	0.00001	0.00014	-0.00015	0.00000	3.13705
D79	3.12353	0.00001	0.00014	-0.00004	0.00010	3.12363
D80	-0.00926	-0.00001	-0.00015	-0.00051	-0.00066	-0.00992
D81	-3.14054	-0.00001	-0.00029	0.00003	-0.00026	-3.14080
D82	0.00816	0.00001	0.00015	0.00057	0.00072	0.00887
D83	0.02129	-0.00003	-0.00063	-0.00039	-0.00102	0.02028
D84	3.05670	-0.00002	-0.00022	0.00036	0.00014	3.05684
D85	-3.13219	-0.00001	-0.00023	0.00024	0.00001	-3.13218
D86	-0.09678	0.00000	0.00017	0.00099	0.00117	-0.09562
D87	-3.13498	0.00001	0.00013	0.00052	0.00064	-3.13434
D88	0.00518	0.00000	0.00006	0.00012	0.00018	0.00535
D89	0.01874	-0.00001	-0.00027	-0.00013	-0.00040	0.01834
D90	-3.12429	-0.00002	-0.00034	-0.00053	-0.00087	-3.12516
D91	1.53989	0.00001	-0.00079	0.00426	0.00346	1.54335
D92	-2.62902	0.00001	-0.00082	0.00435	0.00352	-2.62549
D93	-0.56652	0.00001	-0.00083	0.00438	0.00355	-0.56296
D94	-1.47531	0.00000	-0.00128	0.00339	0.00211	-1.47320
D95	0.63896	0.00000	-0.00131	0.00348	0.00217	0.64113
D96	2.70147	0.00000	-0.00132	0.00352	0.00220	2.70367
D97	-0.00530	-0.00001	-0.00012	-0.00051	-0.00063	-0.00593
D98	3.13783	0.00000	0.00002	-0.00051	-0.00048	3.13735
D99	-3.13752	-0.00001	0.00009	-0.00053	-0.00044	-3.13796
D100	0.00553	0.00000	0.00016	-0.00012	0.00003	0.00557
D101	-0.00851	0.00000	-0.00017	0.00021	0.00004	-0.00848
D102	3.14056	0.00001	0.00034	0.00027	0.00061	3.14117
D103	0.00111	0.00001	0.00006	0.00032	0.00038	0.00149
D104	3.14159	0.00000	0.00001	0.00001	0.00002	-3.14157
D105	3.14154	0.00000	-0.00005	0.00032	0.00027	-3.14138

D106	-0.00117	-0.00001	-0.00010	0.00001	-0.00009	-0.00126
D107	3.13469	0.00000	-0.00017	0.00014	-0.00003	3.13466
D108	-0.01863	0.00001	0.00035	0.00013	0.00048	-0.01815
D109	-0.00540	0.00000	-0.00003	0.00015	0.00012	-0.00528
D110	3.12448	0.00002	0.00049	0.00014	0.00063	3.12510
D111	0.00966	0.00000	0.00015	-0.00024	-0.00009	0.00957
D112	-3.13691	-0.00001	-0.00019	-0.00029	-0.00048	-3.13738
D113	-3.12342	-0.00001	-0.00023	-0.00024	-0.00046	-3.12388
D114	0.01319	-0.00002	-0.00057	-0.00028	-0.00084	0.01235
D115	3.13202	0.00001	0.00033	0.00031	0.00064	3.13265
D116	0.09635	0.00000	0.00014	-0.00030	-0.00015	0.09619
D117	-0.02107	0.00003	0.00084	0.00030	0.00113	-0.01994
D118	-3.05674	0.00002	0.00065	-0.00031	0.00034	-3.05640
D119	3.13437	-0.00001	-0.00043	0.00008	-0.00035	3.13402
D120	-0.00641	0.00000	0.00006	0.00007	0.00013	-0.00628
D121	0.00000	0.00000	0.00006	0.00014	0.00021	0.00021
D122	-3.14078	0.00002	0.00055	0.00013	0.00068	-3.14010
D123	3.13512	0.00000	0.00010	-0.00006	0.00004	3.13516
D124	-0.01307	0.00001	0.00045	0.00003	0.00049	-0.01258
D125	-0.00703	0.00000	-0.00023	-0.00005	-0.00028	-0.00731
D126	3.12798	0.00000	0.00013	0.00004	0.00017	3.12814
D127	-3.13761	0.00001	0.00007	0.00030	0.00037	-3.13724
D128	0.00482	0.00002	0.00057	0.00029	0.00086	0.00568
D129	0.00570	-0.00002	-0.00038	-0.00031	-0.00069	0.00501
D130	-3.13398	0.00001	0.00032	0.00016	0.00048	-3.13350
D131	-3.12689	-0.00003	-0.00087	-0.00044	-0.00130	-3.12820
D132	0.01661	0.00000	-0.00017	0.00004	-0.00013	0.01648
D133	0.02105	-0.00002	-0.00080	-0.00020	-0.00100	0.02005
D134	3.05721	-0.00002	-0.00060	0.00037	-0.00023	3.05697
D135	-3.12930	-0.00001	-0.00032	-0.00008	-0.00041	-3.12970
D136	-0.09314	0.00000	-0.00013	0.00049	0.00036	-0.09278
D137	-0.00194	0.00004	0.00080	0.00053	0.00133	-0.00061
D138	3.14092	0.00002	0.00033	0.00045	0.00078	-3.14149
D139	3.13783	0.00001	0.00014	0.00007	0.00021	3.13805
D140	-0.00249	-0.00001	-0.00033	0.00000	-0.00033	-0.00283
D141	-0.00169	-0.00003	-0.00078	-0.00047	-0.00125	-0.00294
D142	3.13849	-0.00002	-0.00026	-0.00038	-0.00064	3.13785
D143	3.14094	0.00002	0.00109	-0.00005	0.00104	-3.14121
D144	-0.00036	0.00001	0.00092	-0.00007	0.00085	0.00049
D145	0.00085	0.00000	0.00053	-0.00014	0.00039	0.00124
D146	-3.14044	0.00000	0.00035	-0.00016	0.00020	-3.14024
D147	-0.63472	-0.00001	0.00091	-0.00263	-0.00172	-0.63644
D148	1.47950	0.00000	0.00088	-0.00256	-0.00168	1.47782
D149	-2.69721	0.00000	0.00091	-0.00264	-0.00173	-2.69894
D150	2.63294	-0.00002	0.00068	-0.00333	-0.00265	2.63029
D151	-1.53603	-0.00002	0.00066	-0.00326	-0.00260	-1.53863
D152	0.57044	-0.00002	0.00068	-0.00333	-0.00265	0.56779
D153	-0.00197	0.00000	-0.00009	-0.00003	-0.00012	-0.00209
D154	-3.14142	0.00000	-0.00017	0.00006	-0.00011	-3.14153
D155	3.13931	0.00000	0.00009	0.00000	0.00008	3.13939
D156	-0.00014	0.00000	0.00001	0.00008	0.00009	-0.00005
D157	-3.13804	0.00000	-0.00010	0.00013	0.00003	-3.13800
D158	0.00308	0.00000	0.00004	-0.00001	0.00002	0.00311
D159	0.00175	0.00000	-0.00003	0.00006	0.00003	0.00178
D160	-3.14032	0.00000	0.00010	-0.00008	0.00002	-3.14030
D161	3.13775	0.00000	0.00004	-0.00005	-0.00001	3.13774
D162	-0.00480	0.00000	0.00005	0.00004	0.00010	-0.00471
D163	-0.00201	0.00000	-0.00003	0.00002	-0.00001	-0.00202
D164	3.13862	0.00000	-0.00001	0.00012	0.00010	3.13872
D165	-0.00081	0.00000	0.00008	-0.00012	-0.00004	-0.00085

D166	3.14040	0.00000	0.00000	-0.00001	-0.00001	3.14039
D167	3.14125	0.00000	-0.00005	0.00002	-0.00003	3.14122
D168	-0.00073	0.00000	-0.00013	0.00013	0.00000	-0.00073
D169	0.00154	0.00000	0.00008	-0.00009	-0.00002	0.00152
D170	-3.13995	0.00000	0.00011	-0.00019	-0.00008	-3.14003
D171	-3.13914	0.00000	0.00007	-0.00019	-0.00012	-3.13926
D172	0.00256	0.00000	0.00010	-0.00029	-0.00018	0.00238
D173	-0.00046	0.00000	-0.00003	0.00003	0.00000	-0.00047
D174	-3.14144	0.00000	-0.00005	-0.00005	-0.00010	-3.14154
D175	3.14002	0.00000	-0.00002	0.00014	0.00012	3.14014
D176	-0.00097	0.00000	-0.00003	0.00006	0.00003	-0.00094
D177	-0.00044	0.00000	-0.00010	0.00013	0.00004	-0.00041
D178	3.14106	0.00000	-0.00013	0.00022	0.00009	3.14115
D179	3.14151	0.00000	-0.00002	0.00003	0.00001	3.14151
D180	-0.00018	0.00000	-0.00005	0.00011	0.00006	-0.00012
D181	-3.14100	0.00000	0.00011	-0.00015	-0.00004	-3.14104
D182	0.00042	0.00000	0.00010	-0.00005	0.00004	0.00046
D183	0.00016	0.00000	0.00002	-0.00003	0.00000	0.00016
D184	3.14158	0.00000	0.00001	0.00007	0.00008	-3.14153
D185	3.14152	0.00000	0.00000	0.00000	0.00000	3.14152
D186	0.00008	0.00000	0.00000	0.00005	0.00005	0.00013
D187	0.00004	0.00000	0.00004	-0.00011	-0.00007	-0.00002
D188	-3.14139	0.00000	0.00004	-0.00005	-0.00002	-3.14141
D189	-0.00002	0.00000	0.00002	-0.00006	-0.00004	-0.00006
D190	3.14154	0.00000	-0.00002	0.00003	0.00001	3.14155
D191	-3.14144	0.00000	0.00004	-0.00016	-0.00012	-3.14156
D192	0.00012	0.00000	0.00000	-0.00007	-0.00007	0.00005
D193	0.00009	0.00000	0.00000	0.00002	0.00003	0.00012
D194	-3.14150	0.00000	0.00000	0.00002	0.00002	-3.14147
D195	3.14154	0.00000	0.00001	-0.00003	-0.00002	3.14151
D196	-0.00005	0.00000	0.00000	-0.00003	-0.00003	-0.00008
D197	-0.00011	0.00000	-0.00003	0.00006	0.00003	-0.00008
D198	3.14148	0.00000	-0.00003	0.00006	0.00003	3.14151
D199	3.14152	0.00000	0.00000	-0.00002	-0.00002	3.14150
D200	-0.00008	0.00000	0.00001	-0.00002	-0.00002	-0.00009

Item	Value	Threshold	Converged?

Maximum Force	0.000173	0.000450	YES

RMS Force	0.000018	0.000300	YES

Maximum Displacement	0.005338	0.001800	NO

RMS Displacement	0.001134	0.001200	YES

Predicted change in Energy=-6.003769D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.803309	-0.637306	0.006390
2	6	0	-9.994052	-1.788054	0.004105
3	6	0	-10.516415	-3.073110	0.008858
4	6	0	-11.905352	-3.215613	0.016452
5	6	0	-12.726569	-2.081373	0.018993
6	6	0	-12.194674	-0.787685	0.013977

7	1	0	-9.845697	-3.926204	0.006769
8	1	0	-12.352683	-4.204774	0.020471
9	1	0	-13.805348	-2.203416	0.025015
10	1	0	-12.864294	0.060564	0.016222
11	6	0	-9.927114	0.564357	-0.000236
12	6	0	-8.569848	-1.390711	-0.003198
13	6	0	-8.540407	0.088851	-0.004374
14	6	0	-7.404474	0.870130	-0.007250
15	6	0	-6.014493	0.595445	-0.011590
16	6	0	-3.644328	-0.184030	-0.012084
17	6	0	-3.778435	1.228541	-0.017232
18	16	0	-5.181984	-0.989434	-0.013377
19	6	0	-5.099661	1.664800	-0.013291
20	6	0	-2.267140	-0.451717	-0.008523
21	6	0	-1.603905	0.797516	-0.011804
22	7	0	-2.524000	1.820854	-0.033517
23	16	0	-1.150990	-1.806895	-0.010226
24	16	0	1.150907	1.806491	0.007681
25	6	0	0.198424	-0.673794	0.000291
26	6	0	-0.198423	0.673354	-0.002805
27	6	0	1.603987	-0.797933	0.009568
28	6	0	2.267148	0.451399	0.006596
29	6	0	3.644212	0.183902	0.010858
30	6	0	3.778453	-1.228678	0.016049
31	6	0	5.099685	-1.664776	0.012554
32	6	0	6.014431	-0.595341	0.011102
33	16	0	5.181811	0.989459	0.013210
34	7	0	2.524133	-1.821167	0.031459
35	6	0	7.404416	-0.869861	0.007425
36	6	0	8.540408	-0.088541	0.005580
37	6	0	8.569939	1.390992	0.004700
38	6	0	9.927048	-0.564139	0.001609
39	6	0	9.994141	1.788260	-0.002365
40	6	0	10.803344	0.637464	-0.004571
41	6	0	10.516569	3.073294	-0.006840
42	6	0	12.194717	0.787802	-0.011709
43	6	0	11.905531	3.215746	-0.014008
44	6	0	12.726683	2.081475	-0.016410
45	6	0	10.384420	-1.870900	0.004036
46	6	0	9.533367	-3.018514	0.011701
47	6	0	11.768856	-2.222671	-0.000267
48	7	0	8.862892	-3.972004	0.018015
49	7	0	12.886350	-2.552042	-0.003676
50	6	0	-10.384605	1.871100	-0.003092
51	6	0	-11.769084	2.222749	0.001492
52	6	0	-9.533647	3.018784	-0.011484
53	7	0	-12.886643	2.551898	0.005110
54	7	0	-8.863211	3.972296	-0.018262
55	8	0	-7.612865	-2.157380	-0.007183
56	8	0	7.613016	2.157736	0.008463
57	6	0	2.242660	-3.243254	-0.057987
58	1	0	1.315521	-3.467131	0.474191
59	1	0	2.149412	-3.572329	-1.098570
60	1	0	3.051193	-3.798770	0.421285
61	6	0	-2.241949	3.242863	0.055230
62	1	0	-2.143325	3.571292	1.095513
63	1	0	-1.317570	3.467008	-0.481671
64	1	0	-3.052997	3.798565	-0.419493
65	1	0	5.428775	-2.697394	0.008328
66	1	0	12.864319	-0.060466	-0.013864

67	1	0	13.805472	2.203450	-0.022067
68	1	0	12.352898	4.204891	-0.017722
69	1	0	9.845899	3.926424	-0.004799
70	1	0	7.572539	-1.939949	0.005677
71	1	0	-7.572543	1.940227	-0.005620
72	1	0	-5.428684	2.697446	-0.009074

 Rotational constants (GHZ): 0.1750143 0.0104042 0.0098217
 Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.
 There are 916 symmetry adapted basis functions of A symmetry.
 916 basis functions, 1734 primitive gaussians, 916 cartesian basis func-
 tions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6569.7918750987 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T
 Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6569.7069606789 Har-
 trees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.24D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Initial guess from the checkpoint file: "PBDB.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000004 Ang= 0.00 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3683.02012130 A.U. after 7 cycles

NFock= 7 Conv=0.99D-08 -V/T= 2.0068

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1

NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	0.000009074	-0.000002453	0.000001720
2	6	0.000007982	-0.000006778	-0.000009533
3	6	0.000002588	0.000005600	-0.000002494
4	6	-0.000001361	-0.000003535	0.000001520
5	6	-0.000003609	-0.000002557	-0.000002993
6	6	-0.000013488	0.000004642	-0.000009309
7	1	-0.000002385	0.000000843	-0.000000349
8	1	-0.000001472	-0.000000284	0.000000167
9	1	0.000001134	0.000001159	0.000001371
10	1	0.000006263	-0.000003152	0.000003487
11	6	-0.000001676	0.000001826	0.000005178
12	6	-0.000010120	0.000003411	0.000017059
13	6	-0.000029688	0.000056557	0.000022995
14	6	0.000042292	-0.000039891	-0.000012211
15	6	0.000011108	0.000004020	-0.000017554
16	6	0.000055768	-0.000012370	0.000021210
17	6	-0.000006546	-0.000029196	0.000043104
18	16	-0.000033102	-0.000005779	-0.000014106
19	6	-0.000010410	0.000004508	-0.000002308

20	6	-0.000034752	0.000053942	-0.000014613
21	6	-0.000038060	-0.000010391	-0.000031646
22	7	0.000009294	-0.000004103	-0.000011732
23	16	0.000010229	-0.000009556	-0.000011943
24	16	-0.000000977	-0.000007105	-0.000013270
25	6	0.000013118	-0.000018689	0.000018197
26	6	0.000019303	-0.000001111	0.000018765
27	6	-0.000053444	0.000033656	-0.000008223
28	6	-0.000048104	0.000017967	-0.000036508
29	6	0.000030326	-0.000024655	0.000017455
30	6	-0.000001873	-0.000007441	-0.000011354
31	6	0.000015933	-0.000006887	0.000044430
32	6	0.000023447	-0.000011875	-0.000025283
33	16	0.000009391	0.000007865	0.000036372
34	7	0.000019722	0.000019386	-0.000001993
35	6	0.000001859	0.000001630	0.000000345
36	6	-0.000013075	0.000006038	-0.000006461
37	6	-0.000026158	-0.000004867	-0.000002922
38	6	-0.000002663	-0.000020069	-0.000004950
39	6	0.000016092	-0.000005480	0.000003747
40	6	-0.000008621	-0.000005509	-0.000013278
41	6	0.000006492	-0.000009956	0.000003172
42	6	0.000013347	-0.000003626	0.000015022
43	6	-0.000008548	0.000012732	-0.000011685
44	6	0.000008372	0.000012061	0.000009416
45	6	0.000013404	0.000024282	0.000017010
46	6	0.000009424	0.000006507	0.000001844
47	6	-0.000004842	-0.000021560	-0.000006034
48	7	0.000001362	-0.000000581	0.000004349
49	7	0.000003126	0.000002279	0.000002758
50	6	-0.000004154	-0.000015363	-0.000011428
51	6	0.000009209	0.000023791	0.000015443
52	6	0.000005569	0.000000276	-0.000007742
53	7	-0.000001957	-0.000008167	-0.000003632
54	7	-0.000004824	-0.000002035	0.000000051
55	8	-0.000008067	0.000001924	-0.000010483
56	8	0.000003097	0.000011026	-0.000006419
57	6	-0.000002407	-0.000005285	-0.000012724
58	1	0.000006849	0.000002471	-0.000007149
59	1	-0.000008564	-0.000002447	-0.000005415
60	1	-0.000006763	-0.000004239	0.000008986
61	6	0.000014190	0.000016326	0.000013147
62	1	0.000000906	-0.000009192	-0.000002668
63	1	-0.000004432	-0.000007176	0.000002232
64	1	0.000004560	-0.000003618	-0.000009810
65	1	-0.000001305	-0.000000464	0.000001212
66	1	-0.000005985	0.000005800	-0.000004856
67	1	-0.000001499	-0.000001562	-0.000001608
68	1	-0.000000193	-0.000000079	0.000002211
69	1	0.000001304	0.000000420	0.000000877
70	1	-0.000002777	-0.000001380	-0.000003046
71	1	-0.000003421	-0.000003739	0.000011240
72	1	0.000005188	0.000001254	0.000003642

Cartesian Forces: Max 0.000056557 RMS 0.000015442

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

```

GSVD:  received Info=                      1 from GESDD.
Internal Forces: Max      0.000069991 RMS      0.000012093
Search for a local minimum.
Step number 30 out of a maximum of 429
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 16 18 17 19 20
21 22 23 24 25
26 27 28 29 30
DE= -5.98D-07 DEPred=-6.00D-07 R= 9.97D-01
Trust test= 9.97D-01 RLast= 1.07D-02 DXMaxT set to 1.43D-01
ITU= 0 0 1 -1 1 -1 1 -1 1 1 -1 0 -1 0 -1 1 1 1 1 1
ITU= 1 0 0 0 1 0 0 0 0 1 0
Eigenvalues --- 0.00118 0.00256 0.00267 0.00282 0.00396
Eigenvalues --- 0.00433 0.00480 0.00509 0.00530 0.00576
Eigenvalues --- 0.00593 0.00610 0.00620 0.00632 0.00650
Eigenvalues --- 0.00680 0.00707 0.00744 0.00749 0.00769
Eigenvalues --- 0.00775 0.00777 0.00795 0.00825 0.00851
Eigenvalues --- 0.00928 0.01033 0.01093 0.01131 0.01135
Eigenvalues --- 0.01234 0.01246 0.01291 0.01323 0.01360
Eigenvalues --- 0.01378 0.01380 0.01439 0.01457 0.01528
Eigenvalues --- 0.01603 0.01646 0.01744 0.01747 0.01791
Eigenvalues --- 0.01796 0.01927 0.01953 0.02006 0.02021
Eigenvalues --- 0.02062 0.02075 0.02172 0.02193 0.02544
Eigenvalues --- 0.02896 0.02938 0.03610 0.03878 0.03953
Eigenvalues --- 0.04043 0.04830 0.04839 0.04910 0.05013
Eigenvalues --- 0.05026 0.05081 0.05189 0.05404 0.07043
Eigenvalues --- 0.07228 0.07395 0.07574 0.15448 0.15849
Eigenvalues --- 0.15973 0.15985 0.15989 0.15998 0.16000
Eigenvalues --- 0.16000 0.16000 0.16000 0.16001 0.16004
Eigenvalues --- 0.16012 0.16023 0.16039 0.16071 0.16079
Eigenvalues --- 0.16087 0.19024 0.19210 0.19844 0.20599
Eigenvalues --- 0.21125 0.21466 0.21874 0.22000 0.22005
Eigenvalues --- 0.22314 0.22373 0.22572 0.22599 0.22636
Eigenvalues --- 0.22672 0.22884 0.22991 0.23127 0.23212
Eigenvalues --- 0.23377 0.23457 0.23613 0.23839 0.24048
Eigenvalues --- 0.24181 0.24262 0.24333 0.24432 0.24529
Eigenvalues --- 0.24591 0.24704 0.24739 0.24840 0.24877
Eigenvalues --- 0.24932 0.24957 0.24974 0.24983 0.24989
Eigenvalues --- 0.24996 0.24998 0.24999 0.24999 0.25000
Eigenvalues --- 0.25000 0.25000 0.25001 0.25006 0.25100
Eigenvalues --- 0.25313 0.25620 0.25975 0.26123 0.26206
Eigenvalues --- 0.26559 0.26781 0.26899 0.27162 0.27232
Eigenvalues --- 0.27734 0.27816 0.28037 0.28498 0.28580
Eigenvalues --- 0.28896 0.29583 0.30166 0.31143 0.31875
Eigenvalues --- 0.33183 0.35421 0.35598 0.36272 0.36337
Eigenvalues --- 0.36471 0.36481 0.36640 0.36803 0.36830
Eigenvalues --- 0.37049 0.37064 0.37096 0.37148 0.37253
Eigenvalues --- 0.37269 0.37416 0.37562 0.37670 0.37757
Eigenvalues --- 0.38008 0.38222 0.39091 0.40311 0.41058
Eigenvalues --- 0.41751 0.42036 0.42645 0.44416 0.44957
Eigenvalues --- 0.45660 0.46476 0.46989 0.47759 0.47973
Eigenvalues --- 0.48650 0.52251 0.53376 0.55364 0.57017
Eigenvalues --- 0.65825 0.72494 0.77677 0.80609 0.82206
Eigenvalues --- 0.91392 1.25854 1.26345 1.29351 1.35374
En-DIIS/RFO-DIIS IScMMF= 0 using points: 30 29 28 27 26
RFO step: Lambda=-1.05146457D-07.
DidBck=F Rises=F RFO-DIIS coefs: 0.99707 0.02492 0.01907 -0.01242
-0.02864

```

```

Iteration 1 RMS(Cart)= 0.00144006 RMS(Int)= 0.00000317
Iteration 2 RMS(Cart)= 0.00000333 RMS(Int)= 0.00000006
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000006
Variable      Old X      -DE/DX      Delta X      Delta X      Delta X      New X
(Linear)      (Quad)      (Total)
R1            2.65849    -0.00001    0.00000    0.00002    0.00002    2.65851
R2            2.64465     0.00001    0.00000    0.00000   -0.00001    2.64464
R3            2.81039   -0.00001    0.00000   -0.00001   -0.00002    2.81038
R4            2.62138     0.00001    0.00000   -0.00001   -0.00001    2.62137
R5            2.79417     0.00000    0.00000     0.00001     0.00000    2.79417
R6            2.63853     0.00000    0.00000     0.00000     0.00001    2.63853
R7            2.05071     0.00000    0.00000     0.00000     0.00000    2.05071
R8            2.64623     0.00000    0.00000   -0.00001   -0.00001    2.64622
R9            2.05152     0.00000    0.00000     0.00000     0.00000    2.05152
R10           2.64330     0.00000    0.00000     0.00001     0.00001    2.64331
R11           2.05163     0.00000    0.00000     0.00000     0.00000    2.05163
R12           2.04224   -0.00001    0.00000     0.00000     0.00000    2.04224
R13           2.77029     0.00000   -0.00001   -0.00001   -0.00002    2.77027
R14           2.61636     0.00000    0.00000   -0.00001     0.00000    2.61635
R15           2.79652     0.00001   -0.00001     0.00004     0.00003    2.79655
R16           2.31722   -0.00001     0.00000     0.00000     0.00000    2.31722
R17           2.60532     0.00007   -0.00003     0.00015     0.00012    2.60544
R18           2.67749     0.00000     0.00005   -0.00021   -0.00016    2.67734
R19           2.04698     0.00000     0.00000     0.00000   -0.00001    2.04698
R20           3.38304   -0.00003     0.00001   -0.00005   -0.00004    3.38300
R21           2.65938     0.00001     0.00001     0.00000     0.00000    2.65938
R22           2.68139     0.00001     0.00000   -0.00004   -0.00004    2.68135
R23           3.28022     0.00001   -0.00001   -0.00002   -0.00003    3.28019
R24           2.65122   -0.00004     0.00001   -0.00015   -0.00014    2.65108
R25           2.62935     0.00002     0.00000   -0.00002   -0.00002    2.62934
R26           2.62169     0.00000     0.00000   -0.00002   -0.00002    2.62167
R27           2.04809   -0.00001     0.00000     0.00000     0.00000    2.04810
R28           2.67279     0.00002   -0.00001   -0.00006   -0.00007    2.67272
R29           3.31769     0.00000     0.00000   -0.00001   -0.00001    3.31769
R30           2.60088   -0.00002     0.00001   -0.00010   -0.00009    2.60078
R31           2.66637     0.00002   -0.00001   -0.00007   -0.00008    2.66630
R32           2.74468     0.00000     0.00000     0.00001     0.00001    2.74470
R33           3.32986     0.00000     0.00000     0.00000     0.00000    3.32986
R34           3.32978     0.00001     0.00000   -0.00002   -0.00002    3.32976
R35           3.31768     0.00001     0.00000     0.00001     0.00001    3.31769
R36           2.65391   -0.00001     0.00000   -0.00001   -0.00001    2.65390
R37           2.66653   -0.00003     0.00000   -0.00024   -0.00023    2.66629
R38           2.67289     0.00001     0.00000   -0.00001     0.00000    2.67289
R39           2.60080     0.00002     0.00000   -0.00007   -0.00006    2.60073
R40           2.65093     0.00007     0.00000     0.00003     0.00003    2.65096
R41           2.68143     0.00001     0.00000     0.00004     0.00005    2.68148
R42           3.28026     0.00000     0.00000   -0.00003   -0.00003    3.28023
R43           2.62927     0.00006   -0.00001     0.00001     0.00000    2.62927
R44           2.62162     0.00003     0.00000     0.00000     0.00000    2.62162
R45           2.65938     0.00001     0.00000     0.00001     0.00001    2.65940
R46           2.04808     0.00000     0.00000     0.00000     0.00000    2.04808
R47           3.38300   -0.00002     0.00000   -0.00001   -0.00001    3.38300
R48           2.67744     0.00000   -0.00002   -0.00006   -0.00008    2.67736
R49           2.74470   -0.00002     0.00000     0.00000     0.00001    2.74470
R50           2.60545     0.00000   -0.00001     0.00005     0.00004    2.60549
R51           2.04698     0.00000     0.00000     0.00001     0.00001    2.04699
R52           2.79647     0.00001   -0.00001     0.00005     0.00003    2.79650
R53           2.77022     0.00003   -0.00001   -0.00005   -0.00007    2.77016
R54           2.79413     0.00002   -0.00001     0.00006     0.00005    2.79418
R55           2.31722     0.00000     0.00000     0.00004     0.00004    2.31726

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R56	2.81041	-0.00001	-0.00001	-0.00003	-0.00003	2.81038
R57	2.61631	0.00003	-0.00001	-0.00001	-0.00001	2.61630
R58	2.65851	-0.00001	0.00000	0.00005	0.00005	2.65856
R59	2.62139	0.00000	0.00000	-0.00006	-0.00007	2.62132
R60	2.64465	0.00000	-0.00001	-0.00001	-0.00002	2.64463
R61	2.63856	-0.00001	0.00000	0.00004	0.00004	2.63860
R62	2.05071	0.00000	0.00000	0.00000	0.00000	2.05071
R63	2.64332	-0.00001	0.00000	0.00004	0.00005	2.64337
R64	2.04224	-0.00001	0.00000	0.00002	0.00002	2.04226
R65	2.64620	0.00001	0.00000	-0.00003	-0.00003	2.64617
R66	2.05151	0.00000	0.00000	0.00000	0.00000	2.05152
R67	2.05163	0.00000	0.00000	0.00000	0.00000	2.05163
R68	2.69997	0.00000	-0.00001	0.00002	0.00001	2.69998
R69	2.69935	0.00000	-0.00002	0.00006	0.00003	2.69938
R70	2.20274	0.00000	0.00000	0.00000	0.00000	2.20274
R71	2.20158	0.00000	0.00000	0.00000	0.00000	2.20159
R72	2.69937	-0.00001	-0.00001	-0.00001	-0.00002	2.69935
R73	2.69998	0.00000	0.00000	0.00000	-0.00001	2.69997
R74	2.20158	0.00000	0.00000	0.00000	0.00000	2.20158
R75	2.20274	0.00000	0.00000	0.00000	0.00000	2.20274
R76	2.06398	0.00001	0.00000	0.00006	0.00006	2.06404
R77	2.06992	0.00000	0.00000	0.00000	0.00000	2.06992
R78	2.06320	0.00000	0.00000	-0.00005	-0.00005	2.06315
R79	2.06990	0.00000	0.00000	0.00001	0.00001	2.06991
R80	2.06403	0.00001	0.00000	0.00008	0.00008	2.06411
R81	2.06315	0.00000	0.00000	-0.00006	-0.00006	2.06309
A1	2.07604	0.00001	0.00000	0.00000	0.00000	2.07604
A2	1.89866	0.00000	0.00000	0.00001	0.00000	1.89866
A3	2.30849	-0.00001	0.00000	-0.00001	-0.00001	2.30849
A4	2.14259	-0.00001	0.00000	0.00000	0.00000	2.14259
A5	1.91163	0.00000	0.00000	-0.00002	-0.00002	1.91161
A6	2.22897	0.00001	0.00000	0.00002	0.00002	2.22898
A7	2.05914	0.00000	0.00000	0.00000	0.00000	2.05914
A8	2.08921	0.00000	0.00000	0.00000	0.00000	2.08921
A9	2.13484	0.00000	0.00000	0.00000	0.00000	2.13484
A10	2.09523	0.00000	0.00000	0.00000	0.00000	2.09523
A11	2.09776	0.00000	0.00000	-0.00001	-0.00001	2.09775
A12	2.09020	0.00000	0.00000	0.00001	0.00001	2.09021
A13	2.12483	0.00000	0.00000	0.00000	0.00000	2.12484
A14	2.08481	0.00000	0.00000	0.00001	0.00001	2.08482
A15	2.07354	0.00000	0.00000	-0.00001	-0.00001	2.07353
A16	2.06855	0.00000	0.00000	0.00000	-0.00001	2.06854
A17	2.13139	0.00000	0.00000	0.00001	0.00001	2.13140
A18	2.08325	0.00001	0.00000	-0.00001	-0.00001	2.08324
A19	1.87049	0.00000	0.00000	0.00002	0.00002	1.87051
A20	2.17481	-0.00003	0.00000	0.00000	0.00000	2.17480
A21	2.23789	0.00003	0.00001	-0.00002	-0.00001	2.23787
A22	1.86277	0.00000	0.00000	0.00001	0.00001	1.86278
A23	2.19409	0.00000	0.00000	0.00000	0.00000	2.19410
A24	2.22632	0.00000	0.00000	-0.00001	-0.00001	2.22631
A25	1.88123	-0.00001	0.00001	-0.00002	-0.00002	1.88122
A26	2.20878	-0.00001	0.00001	0.00002	0.00003	2.20881
A27	2.19317	0.00002	-0.00001	-0.00001	-0.00002	2.19316
A28	2.34401	0.00001	0.00000	-0.00001	-0.00001	2.34399
A29	2.01749	0.00000	-0.00001	0.00007	0.00006	2.01754
A30	1.92169	-0.00001	0.00001	-0.00006	-0.00004	1.92165
A31	2.24957	-0.00002	0.00001	0.00005	0.00006	2.24963
A32	2.08337	0.00002	0.00000	-0.00008	-0.00009	2.08328
A33	1.95024	0.00000	-0.00001	0.00003	0.00003	1.95027
A34	1.95863	-0.00001	0.00000	0.00006	0.00006	1.95869

A35	1.85744	0.00000	0.00000	0.00004	0.00005	1.85748
A36	2.46712	0.00001	-0.00001	-0.00010	-0.00011	2.46701
A37	1.98436	-0.00001	0.00000	-0.00004	-0.00004	1.98432
A38	1.91730	0.00001	0.00000	-0.00002	-0.00002	1.91728
A39	2.38150	0.00001	0.00000	0.00006	0.00006	2.38156
A40	1.57197	0.00001	0.00000	-0.00005	-0.00004	1.57192
A41	1.95955	0.00001	0.00000	-0.00001	-0.00001	1.95955
A42	2.12545	0.00000	0.00000	-0.00002	-0.00003	2.12543
A43	2.19817	-0.00001	0.00000	0.00003	0.00003	2.19821
A44	1.86688	0.00000	0.00000	-0.00004	-0.00004	1.86684
A45	2.45174	0.00001	0.00000	0.00006	0.00006	2.45181
A46	1.96454	-0.00001	0.00000	-0.00003	-0.00003	1.96451
A47	1.92119	0.00001	0.00000	0.00007	0.00007	1.92126
A48	1.97073	0.00000	0.00000	0.00007	0.00007	1.97080
A49	2.39122	-0.00001	0.00000	-0.00014	-0.00014	2.39108
A50	1.86173	-0.00001	0.00000	-0.00004	-0.00005	1.86168
A51	2.20542	0.00003	0.00000	0.00052	0.00052	2.20594
A52	2.21077	-0.00001	-0.00002	-0.00038	-0.00040	2.21037
A53	1.56129	0.00001	0.00000	-0.00001	-0.00001	1.56127
A54	1.56131	-0.00001	0.00000	-0.00007	-0.00007	1.56124
A55	1.98278	0.00000	0.00000	0.00001	0.00001	1.98279
A56	2.35503	0.00000	0.00000	0.00002	0.00002	2.35505
A57	1.94537	0.00000	0.00000	-0.00003	-0.00003	1.94534
A58	2.35497	0.00000	0.00000	-0.00001	-0.00001	2.35496
A59	1.94539	0.00000	0.00000	-0.00004	-0.00004	1.94535
A60	1.98282	0.00000	0.00000	0.00005	0.00005	1.98288
A61	1.97067	0.00000	0.00000	0.00006	0.00006	1.97073
A62	2.39128	0.00000	0.00000	-0.00009	-0.00010	2.39119
A63	1.92119	0.00000	0.00000	0.00004	0.00004	1.92122
A64	1.96455	0.00000	0.00000	-0.00001	-0.00001	1.96454
A65	2.45170	0.00001	0.00000	0.00005	0.00005	2.45175
A66	1.86692	-0.00001	0.00000	-0.00005	-0.00004	1.86687
A67	1.85741	0.00001	0.00000	0.00003	0.00003	1.85744
A68	2.46714	0.00001	0.00000	-0.00003	-0.00004	2.46710
A69	1.95863	-0.00002	0.00000	0.00001	0.00001	1.95864
A70	1.98434	0.00000	0.00000	-0.00003	-0.00003	1.98431
A71	1.91736	-0.00002	0.00000	-0.00005	-0.00005	1.91731
A72	2.38146	0.00001	0.00000	0.00008	0.00008	2.38154
A73	1.95958	-0.00001	0.00000	0.00002	0.00003	1.95961
A74	2.19813	0.00000	0.00000	0.00003	0.00003	2.19816
A75	2.12547	0.00000	0.00000	-0.00005	-0.00005	2.12542
A76	1.95025	0.00000	0.00000	-0.00002	-0.00002	1.95024
A77	2.08340	0.00004	-0.00001	-0.00001	-0.00001	2.08339
A78	2.24953	-0.00004	0.00001	0.00002	0.00003	2.24956
A79	1.57195	0.00003	0.00000	0.00002	0.00002	1.57197
A80	1.86167	0.00002	0.00000	0.00003	0.00003	1.86170
A81	2.21105	-0.00003	-0.00001	-0.00029	-0.00030	2.21075
A82	2.20519	0.00001	0.00000	0.00033	0.00033	2.20553
A83	2.34412	-0.00005	0.00000	-0.00002	-0.00001	2.34411
A84	1.92163	0.00002	0.00000	0.00001	0.00001	1.92164
A85	2.01744	0.00003	0.00000	0.00001	0.00001	2.01744
A86	2.19324	-0.00003	0.00000	0.00000	-0.00001	2.19323
A87	2.20870	0.00004	0.00000	0.00001	0.00001	2.20871
A88	1.88125	0.00000	0.00000	-0.00001	0.00000	1.88124
A89	1.86278	0.00000	0.00000	0.00000	0.00000	1.86278
A90	2.22634	-0.00001	0.00000	0.00000	0.00000	2.22634
A91	2.19406	0.00001	0.00000	0.00000	0.00000	2.19406
A92	1.87050	0.00000	0.00000	0.00004	0.00004	1.87053
A93	2.23788	0.00006	0.00000	0.00006	0.00006	2.23794
A94	2.17481	-0.00005	0.00000	-0.00010	-0.00010	2.17471

A95	1.91162	0.00000	0.00000	-0.00003	-0.00004	1.91159
A96	2.22897	0.00001	0.00000	0.00006	0.00006	2.22902
A97	2.14259	-0.00001	0.00000	-0.00002	-0.00002	2.14258
A98	1.89863	0.00001	0.00000	0.00000	0.00000	1.89863
A99	2.30854	-0.00003	0.00000	-0.00003	-0.00002	2.30852
A100	2.07601	0.00001	0.00000	0.00002	0.00002	2.07604
A101	2.05915	0.00000	0.00000	0.00001	0.00001	2.05916
A102	2.08922	0.00000	0.00000	0.00000	0.00000	2.08922
A103	2.13482	0.00000	0.00000	-0.00001	-0.00001	2.13481
A104	2.06857	-0.00001	0.00000	-0.00001	-0.00001	2.06855
A105	2.13140	0.00000	0.00000	0.00002	0.00002	2.13142
A106	2.08322	0.00001	0.00000	-0.00001	-0.00001	2.08321
A107	2.09521	0.00001	0.00000	0.00001	0.00001	2.09523
A108	2.09775	0.00000	0.00000	-0.00002	-0.00003	2.09773
A109	2.09022	0.00000	0.00000	0.00001	0.00001	2.09023
A110	2.12483	0.00000	0.00000	-0.00001	-0.00001	2.12482
A111	2.07352	0.00001	0.00000	-0.00002	-0.00002	2.07350
A112	2.08483	0.00000	0.00000	0.00003	0.00003	2.08486
A113	2.16682	0.00004	-0.00001	-0.00002	-0.00002	2.16680
A114	2.15629	-0.00005	0.00000	-0.00009	-0.00010	2.15619
A115	1.96008	0.00000	0.00001	0.00011	0.00012	1.96020
A116	2.15628	-0.00003	0.00000	-0.00004	-0.00005	2.15623
A117	2.16682	0.00002	0.00000	-0.00005	-0.00005	2.16677
A118	1.96008	0.00001	0.00000	0.00010	0.00010	1.96019
A119	1.91261	0.00000	0.00000	0.00005	0.00006	1.91266
A120	1.94890	-0.00001	0.00000	-0.00001	-0.00001	1.94888
A121	1.90459	0.00000	0.00000	-0.00008	-0.00009	1.90450
A122	1.90608	0.00000	0.00000	0.00004	0.00004	1.90612
A123	1.88646	0.00000	0.00000	0.00005	0.00005	1.88651
A124	1.90414	0.00000	0.00000	-0.00004	-0.00004	1.90410
A125	1.94881	0.00001	0.00001	0.00000	0.00001	1.94882
A126	1.91265	0.00000	0.00000	0.00008	0.00008	1.91272
A127	1.90446	0.00001	-0.00001	-0.00011	-0.00012	1.90434
A128	1.90616	-0.00001	0.00000	0.00004	0.00005	1.90621
A129	1.90417	-0.00001	0.00000	-0.00007	-0.00007	1.90410
A130	1.88653	0.00000	0.00000	0.00006	0.00006	1.88659
A131	3.16683	0.00001	0.00001	-0.00019	-0.00018	3.16665
A132	3.17939	0.00001	0.00002	-0.00014	-0.00012	3.17927
A133	3.17929	0.00002	-0.00002	0.00021	0.00019	3.17948
A134	3.16678	0.00001	-0.00003	0.00012	0.00009	3.16688
A135	3.14154	0.00000	0.00000	-0.00002	-0.00002	3.14152
A136	3.14162	0.00000	0.00000	-0.00002	-0.00001	3.14161
A137	3.14157	0.00000	0.00000	0.00001	0.00000	3.14157
A138	3.14167	-0.00001	-0.00001	-0.00008	-0.00009	3.14158
D1	0.00018	0.00000	-0.00001	0.00010	0.00009	0.00027
D2	-3.14096	0.00000	-0.00002	0.00020	0.00019	-3.14077
D3	-3.14145	0.00000	0.00000	0.00007	0.00007	-3.14139
D4	0.00059	0.00000	-0.00001	0.00017	0.00016	0.00075
D5	-0.00001	0.00000	0.00000	-0.00007	-0.00007	-0.00008
D6	3.14140	0.00000	0.00000	-0.00011	-0.00010	3.14130
D7	-3.14155	0.00000	0.00000	-0.00003	-0.00003	-3.14158
D8	-0.00014	0.00000	0.00000	-0.00007	-0.00007	-0.00021
D9	-0.00165	0.00000	-0.00003	0.00028	0.00026	-0.00140
D10	3.13893	0.00000	-0.00002	0.00024	0.00022	3.13915
D11	3.13989	0.00000	-0.00002	0.00025	0.00022	3.14012
D12	-0.00271	0.00000	-0.00001	0.00020	0.00018	-0.00253
D13	-0.00020	0.00000	0.00000	-0.00005	-0.00004	-0.00025
D14	3.14156	0.00000	0.00000	-0.00004	-0.00004	3.14152
D15	3.14085	0.00000	0.00002	-0.00017	-0.00016	3.14069
D16	-0.00058	0.00000	0.00001	-0.00017	-0.00015	-0.00073

D17	0.00068	0.00000	0.00005	-0.00056	-0.00051	0.00017
D18	-3.14111	0.00000	0.00008	-0.00058	-0.00049	3.14158
D19	-3.14043	0.00000	0.00003	-0.00044	-0.00041	-3.14084
D20	0.00096	0.00000	0.00007	-0.00047	-0.00039	0.00057
D21	0.00006	0.00000	0.00000	-0.00003	-0.00003	0.00003
D22	-3.14146	0.00000	0.00000	0.00003	0.00002	-3.14144
D23	3.14148	0.00000	0.00000	-0.00003	-0.00003	3.14145
D24	-0.00004	0.00000	0.00000	0.00002	0.00002	-0.00002
D25	0.00011	0.00000	0.00000	0.00005	0.00005	0.00015
D26	-3.14148	0.00000	0.00000	0.00005	0.00005	-3.14143
D27	-3.14155	0.00000	0.00000	0.00000	0.00000	-3.14156
D28	0.00004	0.00000	0.00000	0.00000	0.00000	0.00005
D29	-0.00013	0.00000	0.00000	0.00000	0.00000	-0.00013
D30	-3.14154	0.00000	0.00000	0.00004	0.00003	-3.14151
D31	3.14146	0.00000	0.00000	0.00000	0.00000	3.14145
D32	0.00004	0.00000	0.00000	0.00003	0.00003	0.00007
D33	0.00205	0.00000	0.00005	-0.00062	-0.00057	0.00148
D34	-3.13831	0.00001	0.00007	0.00087	0.00094	-3.13736
D35	-3.13848	0.00000	0.00005	-0.00057	-0.00052	-3.13901
D36	0.00434	0.00000	0.00006	0.00092	0.00099	0.00533
D37	0.00123	-0.00001	0.00000	0.00022	0.00022	0.00145
D38	-3.13988	-0.00001	-0.00001	0.00025	0.00025	-3.13964
D39	-3.14159	0.00000	0.00001	0.00016	0.00017	-3.14142
D40	0.00048	0.00000	0.00000	0.00019	0.00020	0.00068
D41	-0.00170	0.00000	-0.00006	0.00072	0.00066	-0.00104
D42	3.13867	-0.00001	-0.00008	-0.00076	-0.00084	3.13784
D43	3.14010	0.00000	-0.00010	0.00074	0.00064	3.14075
D44	-0.00271	0.00000	-0.00012	-0.00073	-0.00085	-0.00356
D45	-3.14131	-0.00001	-0.00003	-0.00052	-0.00055	3.14132
D46	0.00070	-0.00002	-0.00013	-0.00130	-0.00143	-0.00073
D47	0.00173	0.00000	-0.00001	0.00123	0.00122	0.00295
D48	-3.13944	-0.00001	-0.00011	0.00045	0.00034	-3.13910
D49	-0.00126	-0.00001	0.00014	-0.00076	-0.00061	-0.00188
D50	-3.14133	-0.00001	0.00012	-0.00130	-0.00118	3.14068
D51	3.13992	0.00000	0.00024	-0.00001	0.00023	3.14015
D52	-0.00014	-0.00001	0.00022	-0.00056	-0.00034	-0.00048
D53	-3.13772	0.00000	0.00000	0.00020	0.00021	-3.13751
D54	0.00245	0.00000	0.00002	0.00072	0.00074	0.00319
D55	3.14132	0.00000	-0.00001	-0.00009	-0.00010	3.14122
D56	0.00249	0.00000	0.00002	0.00026	0.00027	0.00277
D57	0.00101	0.00000	-0.00002	-0.00055	-0.00058	0.00043
D58	-3.13782	0.00000	0.00000	-0.00020	-0.00020	-3.13802
D59	0.00697	0.00001	0.00001	0.00054	0.00054	0.00752
D60	-3.12813	0.00000	0.00000	0.00012	0.00012	-3.12802
D61	-3.13533	0.00000	-0.00001	0.00004	0.00003	-3.13530
D62	0.01275	0.00000	-0.00002	-0.00037	-0.00040	0.01235
D63	-0.00522	-0.00001	-0.00002	-0.00070	-0.00072	-0.00594
D64	3.13746	0.00000	0.00001	0.00006	0.00007	3.13753
D65	-0.00016	0.00000	-0.00002	-0.00003	-0.00005	-0.00021
D66	-3.13396	0.00000	0.00002	0.00025	0.00027	-3.13369
D67	3.14037	-0.00001	-0.00004	-0.00077	-0.00081	3.13956
D68	0.00658	-0.00001	-0.00001	-0.00048	-0.00049	0.00609
D69	-0.00506	0.00000	0.00001	0.00002	0.00003	-0.00503
D70	3.13363	0.00000	-0.00002	-0.00035	-0.00036	3.13327
D71	3.12768	0.00000	0.00003	0.00059	0.00061	3.12829
D72	-0.01681	0.00000	0.00000	0.00022	0.00022	-0.01659
D73	-0.02037	0.00001	0.00005	0.00064	0.00069	-0.01968
D74	-3.05735	0.00001	0.00021	-0.00028	-0.00007	-3.05742
D75	3.12985	0.00000	0.00004	0.00009	0.00012	3.12997
D76	0.09286	0.00000	0.00019	-0.00083	-0.00064	0.09222

D77	-0.01259	0.00001	0.00005	0.00043	0.00048	-0.01211
D78	3.13705	0.00001	0.00003	0.00033	0.00036	3.13741
D79	3.12363	0.00001	0.00003	0.00024	0.00026	3.12389
D80	-0.00992	0.00001	0.00001	0.00013	0.00014	-0.00978
D81	-3.14080	-0.00001	-0.00004	-0.00052	-0.00057	-3.14136
D82	0.00887	-0.00001	-0.00001	-0.00023	-0.00023	0.00864
D83	0.02028	-0.00001	-0.00006	-0.00066	-0.00072	0.01956
D84	3.05684	0.00000	-0.00022	0.00033	0.00012	3.05696
D85	-3.13218	-0.00001	-0.00003	-0.00051	-0.00055	-3.13273
D86	-0.09562	0.00000	-0.00019	0.00048	0.00029	-0.09533
D87	-3.13434	0.00000	0.00001	-0.00010	-0.00009	-3.13443
D88	0.00535	0.00000	0.00000	0.00008	0.00008	0.00543
D89	0.01834	0.00000	-0.00002	-0.00025	-0.00027	0.01807
D90	-3.12516	0.00000	-0.00003	-0.00007	-0.00010	-3.12526
D91	1.54335	0.00000	0.00003	0.00612	0.00615	1.54950
D92	-2.62549	0.00001	0.00004	0.00622	0.00626	-2.61923
D93	-0.56296	0.00001	0.00004	0.00628	0.00631	-0.55665
D94	-1.47320	0.00000	0.00022	0.00498	0.00520	-1.46800
D95	0.64113	0.00000	0.00023	0.00509	0.00532	0.64645
D96	2.70367	0.00001	0.00022	0.00514	0.00536	2.70903
D97	-0.00593	0.00001	0.00001	0.00027	0.00028	-0.00565
D98	3.13735	0.00001	0.00002	0.00036	0.00038	3.13773
D99	-3.13796	0.00001	0.00002	0.00038	0.00040	-3.13756
D100	0.00557	0.00000	0.00003	0.00020	0.00023	0.00579
D101	-0.00848	0.00000	-0.00002	-0.00017	-0.00019	-0.00867
D102	3.14117	0.00000	-0.00001	-0.00001	-0.00002	3.14115
D103	0.00149	0.00000	-0.00001	-0.00025	-0.00026	0.00123
D104	-3.14157	0.00000	-0.00002	-0.00011	-0.00013	-3.14148
D105	-3.14138	0.00000	-0.00002	-0.00032	-0.00033	-3.14147
D106	-0.00126	0.00000	-0.00003	-0.00018	-0.00020	-0.00146
D107	3.13466	0.00000	-0.00001	-0.00004	-0.00005	3.13462
D108	-0.01815	0.00000	0.00000	0.00012	0.00012	-0.01802
D109	-0.00528	0.00000	0.00001	0.00004	0.00005	-0.00522
D110	3.12510	0.00000	0.00001	0.00021	0.00022	3.12532
D111	0.00957	0.00000	0.00001	0.00011	0.00012	0.00969
D112	-3.13738	0.00000	0.00000	0.00000	0.00000	-3.13738
D113	-3.12388	0.00000	0.00001	-0.00001	0.00000	-3.12388
D114	0.01235	0.00000	0.00000	-0.00012	-0.00012	0.01223
D115	3.13265	0.00000	-0.00001	-0.00009	-0.00009	3.13256
D116	0.09619	0.00000	0.00007	-0.00085	-0.00077	0.09542
D117	-0.01994	-0.00001	0.00000	0.00007	0.00007	-0.01987
D118	-3.05640	0.00000	0.00008	-0.00069	-0.00061	-3.05701
D119	3.13402	0.00000	-0.00001	-0.00004	-0.00005	3.13397
D120	-0.00628	0.00000	-0.00001	-0.00004	-0.00006	-0.00634
D121	0.00021	0.00000	0.00000	0.00011	0.00011	0.00032
D122	-3.14010	0.00000	0.00000	0.00011	0.00011	-3.13999
D123	3.13516	0.00000	-0.00001	0.00009	0.00008	3.13524
D124	-0.01258	0.00000	0.00000	-0.00007	-0.00007	-0.01265
D125	-0.00731	0.00000	-0.00001	0.00009	0.00008	-0.00722
D126	3.12814	0.00000	0.00000	-0.00007	-0.00007	3.12807
D127	-3.13724	-0.00001	0.00001	-0.00054	-0.00053	-3.13777
D128	0.00568	-0.00001	0.00001	-0.00054	-0.00053	0.00516
D129	0.00501	0.00001	0.00000	0.00058	0.00058	0.00559
D130	-3.13350	0.00000	-0.00003	0.00013	0.00010	-3.13340
D131	-3.12820	0.00001	-0.00001	0.00080	0.00079	-3.12741
D132	0.01648	0.00000	-0.00004	0.00035	0.00031	0.01679
D133	0.02005	0.00000	0.00000	0.00000	0.00000	0.02005
D134	3.05697	0.00000	-0.00008	0.00070	0.00063	3.05760
D135	-3.12970	0.00000	0.00001	-0.00021	-0.00020	-3.12991
D136	-0.09278	0.00000	-0.00007	0.00049	0.00043	-0.09236

D137	-0.00061	-0.00001	0.00001	-0.00098	-0.00097	-0.00158
D138	-3.14149	-0.00001	-0.00004	0.00001	-0.00003	-3.14152
D139	3.13805	0.00000	0.00004	-0.00055	-0.00051	3.13753
D140	-0.00283	0.00000	-0.00001	0.00044	0.00043	-0.00240
D141	-0.00294	0.00001	-0.00001	0.00086	0.00085	-0.00208
D142	3.13785	0.00000	0.00004	-0.00024	-0.00020	3.13765
D143	-3.14121	0.00000	0.00005	-0.00072	-0.00067	3.14131
D144	0.00049	0.00000	0.00005	-0.00081	-0.00077	-0.00027
D145	0.00124	0.00001	0.00000	0.00045	0.00045	0.00169
D146	-3.14024	0.00001	-0.00001	0.00036	0.00036	-3.13989
D147	-0.63644	-0.00001	-0.00015	-0.00411	-0.00426	-0.64070
D148	1.47782	-0.00001	-0.00014	-0.00404	-0.00418	1.47364
D149	-2.69894	-0.00001	-0.00015	-0.00415	-0.00430	-2.70324
D150	2.63029	-0.00001	-0.00005	-0.00499	-0.00504	2.62525
D151	-1.53863	-0.00001	-0.00005	-0.00491	-0.00496	-1.54360
D152	0.56779	-0.00001	-0.00005	-0.00503	-0.00508	0.56271
D153	-0.00209	0.00000	-0.00001	0.00024	0.00022	-0.00187
D154	-3.14153	0.00000	-0.00001	-0.00003	-0.00003	-3.14157
D155	3.13939	0.00000	-0.00001	0.00033	0.00032	3.13971
D156	-0.00005	0.00000	0.00000	0.00007	0.00006	0.00001
D157	-3.13800	0.00000	0.00002	-0.00032	-0.00031	-3.13831
D158	0.00311	0.00000	-0.00002	-0.00025	-0.00027	0.00283
D159	0.00178	0.00000	0.00001	-0.00010	-0.00009	0.00169
D160	-3.14030	0.00000	-0.00003	-0.00003	-0.00006	-3.14036
D161	3.13774	0.00000	0.00000	0.00036	0.00035	3.13809
D162	-0.00471	0.00000	0.00000	0.00041	0.00041	-0.00429
D163	-0.00202	0.00000	0.00000	0.00013	0.00014	-0.00188
D164	3.13872	0.00000	0.00001	0.00019	0.00019	3.13892
D165	-0.00085	0.00000	-0.00002	0.00003	0.00001	-0.00084
D166	3.14039	0.00000	0.00000	0.00006	0.00006	3.14045
D167	3.14122	0.00000	0.00002	-0.00004	-0.00002	3.14119
D168	-0.00073	0.00000	0.00003	-0.00001	0.00003	-0.00070
D169	0.00152	0.00000	-0.00001	-0.00012	-0.00013	0.00138
D170	-3.14003	0.00000	-0.00002	-0.00017	-0.00019	-3.14022
D171	-3.13926	0.00000	-0.00002	-0.00017	-0.00019	-3.13945
D172	0.00238	0.00000	-0.00002	-0.00022	-0.00025	0.00213
D173	-0.00047	0.00000	0.00000	0.00000	0.00000	-0.00046
D174	-3.14154	0.00000	0.00001	-0.00002	-0.00002	-3.14156
D175	3.14014	0.00000	0.00001	0.00006	0.00007	3.14021
D176	-0.00094	0.00000	0.00001	0.00004	0.00005	-0.00089
D177	-0.00041	0.00000	0.00002	0.00006	0.00008	-0.00033
D178	3.14115	0.00000	0.00002	0.00010	0.00013	3.14127
D179	3.14151	0.00000	0.00001	0.00003	0.00003	3.14155
D180	-0.00012	0.00000	0.00001	0.00007	0.00008	-0.00004
D181	-3.14104	0.00000	-0.00002	-0.00005	-0.00008	-3.14112
D182	0.00046	0.00000	-0.00003	-0.00001	-0.00004	0.00042
D183	0.00016	0.00000	0.00000	-0.00002	-0.00002	0.00013
D184	-3.14153	0.00000	-0.00001	0.00002	0.00002	-3.14151
D185	3.14152	0.00000	0.00000	-0.00002	-0.00002	3.14150
D186	0.00013	0.00000	0.00000	0.00001	0.00001	0.00014
D187	-0.00002	0.00000	0.00000	-0.00007	-0.00008	-0.00010
D188	-3.14141	0.00000	-0.00001	-0.00005	-0.00005	-3.14147
D189	-0.00006	0.00000	0.00000	-0.00003	-0.00003	-0.00009
D190	3.14155	0.00000	0.00000	-0.00007	-0.00006	3.14148
D191	-3.14156	0.00000	0.00000	-0.00007	-0.00007	3.14155
D192	0.00005	0.00000	0.00001	-0.00011	-0.00011	-0.00006
D193	0.00012	0.00000	0.00000	0.00003	0.00003	0.00014
D194	-3.14147	0.00000	0.00000	0.00001	0.00001	-3.14146
D195	3.14151	0.00000	0.00000	0.00000	0.00000	3.14151
D196	-0.00008	0.00000	0.00000	-0.00001	-0.00001	-0.00009

D197	-0.00008	0.00000	0.00000	0.00003	0.00003	-0.00005
D198	3.14151	0.00000	0.00000	0.00004	0.00004	3.14156
D199	3.14150	0.00000	0.00000	0.00006	0.00006	3.14156
D200	-0.00009	0.00000	0.00000	0.00008	0.00008	-0.00002

Item	Value	Threshold	Converged?

Maximum Force	0.000070	0.000450	YES
RMS Force	0.000012	0.000300	YES
Maximum Displacement	0.009992	0.001800	NO
RMS Displacement	0.001440	0.001200	NO

Predicted change in Energy=-3.388322D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.803171	-0.637277	0.005486
2	6	0	-9.993938	-1.788053	0.002995
3	6	0	-10.516333	-3.073091	0.007472
4	6	0	-11.905278	-3.215557	0.015048
5	6	0	-12.726462	-2.081301	0.017876
6	6	0	-12.194537	-0.787618	0.013112
7	1	0	-9.845639	-3.926203	0.005194
8	1	0	-12.352626	-4.204711	0.018877
9	1	0	-13.805246	-2.203309	0.023931
10	1	0	-12.864146	0.060641	0.015606
11	6	0	-9.926958	0.564362	-0.000962
12	6	0	-8.569729	-1.390722	-0.004051
13	6	0	-8.540262	0.088856	-0.005568
14	6	0	-7.404248	0.870131	-0.007412
15	6	0	-6.014361	0.595394	-0.011416
16	6	0	-3.644246	-0.183977	-0.011021
17	6	0	-3.778339	1.228569	-0.016822
18	16	0	-5.181843	-0.989457	-0.013218
19	6	0	-5.099571	1.664786	-0.013401
20	6	0	-2.267150	-0.451723	-0.006959
21	6	0	-1.603911	0.797465	-0.010666
22	7	0	-2.523887	1.820843	-0.032499
23	16	0	-1.150989	-1.806888	-0.008061
24	16	0	1.150786	1.806609	0.008257
25	6	0	0.198400	-0.673750	0.001714
26	6	0	-0.198463	0.673388	-0.001691
27	6	0	1.603849	-0.797813	0.010527
28	6	0	2.267025	0.451506	0.006967
29	6	0	3.644089	0.183927	0.010811
30	6	0	3.778290	-1.228680	0.016198
31	6	0	5.099523	-1.664776	0.012438
32	6	0	6.014300	-0.595358	0.011334
33	16	0	5.181692	0.989445	0.012506
34	7	0	2.523928	-1.821066	0.032225
35	6	0	7.404233	-0.869922	0.007486
36	6	0	8.540259	-0.088615	0.005209
37	6	0	8.569812	1.390935	0.004161

38	6	0	9.926859	-0.564216	0.001166
39	6	0	9.994045	1.788190	-0.002950
40	6	0	10.803206	0.637329	-0.005034
41	6	0	10.516551	3.073155	-0.007509
42	6	0	12.194579	0.787564	-0.012038
43	6	0	11.905544	3.215524	-0.014608
44	6	0	12.726631	2.081228	-0.016825
45	6	0	10.384292	-1.870951	0.003485
46	6	0	9.533264	-3.018590	0.011087
47	6	0	11.768795	-2.222526	-0.000905
48	7	0	8.862637	-3.971974	0.017331
49	7	0	12.886377	-2.551603	-0.004370
50	6	0	-10.384425	1.871111	-0.003348
51	6	0	-11.768904	2.222714	0.001874
52	6	0	-9.533393	3.018735	-0.011864
53	7	0	-12.886407	2.552044	0.006015
54	7	0	-8.862981	3.972262	-0.018857
55	8	0	-7.612748	-2.157400	-0.007635
56	8	0	7.612884	2.157704	0.007869
57	6	0	2.241861	-3.243108	-0.056091
58	1	0	1.317403	-3.467075	0.480759
59	1	0	2.143356	-3.571955	-1.096263
60	1	0	3.052818	-3.798714	0.418906
61	6	0	-2.241120	3.242748	0.055741
62	1	0	-2.136870	3.570433	1.095714
63	1	0	-1.319624	3.467225	-0.486042
64	1	0	-3.054717	3.798802	-0.414108
65	1	0	5.428645	-2.697385	0.008206
66	1	0	12.864146	-0.060746	-0.014046
67	1	0	13.805432	2.203114	-0.022390
68	1	0	12.352945	4.204654	-0.018444
69	1	0	9.845942	3.926334	-0.005543
70	1	0	7.572328	-1.940018	0.006113
71	1	0	-7.572220	1.940240	-0.005901
72	1	0	-5.428663	2.697413	-0.009401

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Rotational constants (GHZ):      0.1750219      0.0104045      0.0098220
Standard basis: 6-31G(d,p) (6D, 7F)
There are 916 symmetry adapted cartesian basis functions of A symmetry.
There are 916 symmetry adapted basis functions of A symmetry.
916 basis functions, 1734 primitive gaussians, 916 cartesian basis func-
tions
196 alpha electrons      196 beta electrons
nuclear repulsion energy      6569.8690212006 Hartrees.
NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T
Big=T
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
Nuclear repulsion after empirical dispersion term = 6569.7841050102 Har-
trees.
One-electron integrals computed using PRISM.
NBasis= 916 RedAO= T EigKep= 3.24D-04 NBF= 916
NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916
Initial guess from the checkpoint file: "PBDB.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 -0.000001 -0.000001 0.000003 Ang= 0.00 deg.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.

```

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3683.02012154 A.U. after 7 cycles

NFock= 7 Conv=0.71D-08 -V/T= 2.0068

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1

NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	0.000015875	0.000004508	0.000002815
2	6	0.000005702	-0.000014348	-0.000021687
3	6	0.000004404	0.000007576	-0.000002180
4	6	0.000001260	-0.000002312	0.000002313
5	6	-0.000006587	-0.000004950	-0.000005255
6	6	-0.000012659	0.000009409	-0.000007555
7	1	-0.000001479	0.000001172	-0.000002791
8	1	-0.000002945	-0.000000559	0.000000482
9	1	0.000001658	0.000001633	0.000002339
10	1	0.000005848	-0.000003700	0.000006897
11	6	-0.000013369	-0.000010133	0.000032413
12	6	-0.000033816	-0.000013799	0.000047951
13	6	0.000058253	0.000040981	-0.000061691
14	6	-0.000058569	0.000026150	0.000024220
15	6	0.000001640	-0.000023963	0.000039617
16	6	0.000011257	0.000023916	0.000055811
17	6	0.000002420	-0.000042771	-0.000035281
18	16	-0.000007475	0.000006713	-0.000058144
19	6	0.000024660	0.000005296	-0.000039458
20	6	-0.000009239	0.000046039	0.000028678
21	6	-0.000003196	-0.000030487	-0.000062033
22	7	-0.000018000	-0.000020113	0.000036178
23	16	0.000003455	-0.000004019	0.000005935
24	16	-0.000002951	-0.000004378	0.000005633
25	6	-0.000031545	0.000012264	-0.000020499
26	6	0.000020448	0.000002448	0.000008993
27	6	-0.000006004	-0.000006612	0.000024631
28	6	-0.000023008	0.000001414	-0.000032803
29	6	0.000014485	-0.000014608	0.000026594
30	6	-0.000007469	-0.000018152	-0.000011325
31	6	0.000059058	0.000004428	-0.000011207
32	6	-0.000060184	-0.000004006	0.000036400
33	16	0.000042082	0.000001900	-0.000002371
34	7	0.000023766	0.000029760	0.000012312
35	6	0.000025527	-0.000022180	0.000013337
36	6	-0.000023663	0.000011055	-0.000028473
37	6	-0.000044703	-0.000011161	-0.000011043
38	6	0.000009721	-0.000025134	0.000000017
39	6	0.000029715	0.000033696	0.000018479
40	6	-0.000022594	-0.000013476	-0.000028158
41	6	0.000007983	-0.000035561	-0.000002453
42	6	0.000013772	-0.000025932	0.000018338
43	6	-0.000022196	0.000014327	-0.000017739
44	6	0.000014520	0.000029710	0.000014990
45	6	0.000027760	0.000031555	0.000028008
46	6	0.000005941	-0.000000015	0.000001371
47	6	-0.000008838	-0.000003934	-0.000007794
48	7	0.000006310	-0.000002339	0.000007165
49	7	0.000001210	0.000011891	0.000003214
50	6	0.000007615	-0.000006372	-0.000002011


```

Eigenvalues --- 0.16000 0.16000 0.16000 0.16001 0.16009
Eigenvalues --- 0.16011 0.16025 0.16046 0.16068 0.16085
Eigenvalues --- 0.16098 0.19070 0.19274 0.19916 0.20714
Eigenvalues --- 0.21177 0.21473 0.21878 0.22000 0.22007
Eigenvalues --- 0.22365 0.22501 0.22588 0.22624 0.22684
Eigenvalues --- 0.22780 0.22836 0.22977 0.23102 0.23205
Eigenvalues --- 0.23382 0.23465 0.23587 0.23829 0.24035
Eigenvalues --- 0.24200 0.24263 0.24321 0.24412 0.24541
Eigenvalues --- 0.24591 0.24689 0.24751 0.24846 0.24877
Eigenvalues --- 0.24932 0.24958 0.24979 0.24982 0.24990
Eigenvalues --- 0.24996 0.24998 0.24999 0.25000 0.25000
Eigenvalues --- 0.25000 0.25001 0.25003 0.25011 0.25101
Eigenvalues --- 0.25377 0.25658 0.26002 0.26112 0.26229
Eigenvalues --- 0.26567 0.26781 0.26923 0.27219 0.27245
Eigenvalues --- 0.27739 0.27839 0.28268 0.28500 0.28631
Eigenvalues --- 0.28850 0.29866 0.30358 0.31532 0.32124
Eigenvalues --- 0.33571 0.35431 0.35640 0.36272 0.36337
Eigenvalues --- 0.36473 0.36504 0.36637 0.36818 0.36834
Eigenvalues --- 0.37035 0.37082 0.37101 0.37224 0.37250
Eigenvalues --- 0.37276 0.37416 0.37556 0.37670 0.37757
Eigenvalues --- 0.38062 0.38249 0.39042 0.40318 0.41138
Eigenvalues --- 0.41749 0.42051 0.42648 0.44421 0.45127
Eigenvalues --- 0.45731 0.46604 0.46985 0.47797 0.47979
Eigenvalues --- 0.49304 0.52240 0.53422 0.55596 0.57543
Eigenvalues --- 0.64418 0.72880 0.77368 0.80644 0.82172
Eigenvalues --- 0.91025 1.25855 1.26349 1.29351 1.35374
En-DIIS/RFO-DIIS IScMMF= 0 using points: 31 30 29 28 27
RFO step: Lambda=-1.38861661D-07.
DidBck=T Rises=F RFO-DIIS coefs: 0.75691 0.52983 -0.15334 -0.13882
0.00541
Iteration 1 RMS(Cart)= 0.00167020 RMS(Int)= 0.00000288
Iteration 2 RMS(Cart)= 0.00000311 RMS(Int)= 0.00000003
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000003
Variable Old X -DE/DX Delta X Delta X Delta X New X
(Linear) (Quad) (Total)
R1 2.65851 -0.00001 0.00000 -0.00001 0.00000 2.65851
R2 2.64464 0.00001 0.00000 0.00001 0.00000 2.64465
R3 2.81038 0.00000 0.00002 -0.00001 0.00001 2.81039
R4 2.62137 0.00001 0.00000 0.00000 0.00000 2.62137
R5 2.79417 0.00000 0.00000 -0.00001 -0.00001 2.79416
R6 2.63853 0.00000 0.00000 0.00001 0.00001 2.63854
R7 2.05071 0.00000 0.00000 0.00000 0.00000 2.05071
R8 2.64622 0.00000 0.00000 -0.00001 -0.00001 2.64621
R9 2.05152 0.00000 0.00000 0.00000 0.00000 2.05152
R10 2.64331 -0.00001 0.00000 0.00001 0.00001 2.64331
R11 2.05163 0.00000 0.00000 0.00000 0.00000 2.05163
R12 2.04224 -0.00001 0.00001 -0.00002 -0.00001 2.04223
R13 2.77027 0.00000 0.00003 0.00000 0.00002 2.77029
R14 2.61635 0.00001 -0.00001 0.00001 0.00000 2.61635
R15 2.79655 -0.00001 0.00001 -0.00001 0.00000 2.79655
R16 2.31722 -0.00001 0.00000 -0.00001 -0.00001 2.31721
R17 2.60544 0.00002 -0.00002 0.00007 0.00004 2.60548
R18 2.67734 0.00006 -0.00006 0.00025 0.00020 2.67753
R19 2.04698 0.00000 0.00000 -0.00001 -0.00001 2.04697
R20 3.38300 -0.00002 0.00004 -0.00005 -0.00001 3.38299
R21 2.65938 0.00003 -0.00002 0.00003 0.00001 2.65939
R22 2.68135 0.00004 0.00000 -0.00002 -0.00003 2.68132
R23 3.28019 0.00002 0.00000 0.00008 0.00008 3.28026
R24 2.65108 0.00002 0.00005 -0.00005 0.00000 2.65108
R25 2.62934 0.00003 -0.00002 0.00007 0.00005 2.62939

```

R26	2.62167	0.00002	-0.00001	0.00003	0.00002	2.62170
R27	2.04810	-0.00001	0.00001	-0.00001	0.00000	2.04809
R28	2.67272	0.00005	-0.00001	-0.00002	-0.00004	2.67269
R29	3.31769	0.00001	0.00000	0.00005	0.00005	3.31774
R30	2.60078	0.00001	0.00001	-0.00004	-0.00002	2.60076
R31	2.66630	0.00005	-0.00002	0.00004	0.00002	2.66632
R32	2.74470	-0.00001	0.00000	-0.00003	-0.00003	2.74467
R33	3.32986	0.00001	0.00000	0.00003	0.00004	3.32990
R34	3.32976	0.00002	0.00000	0.00003	0.00003	3.32979
R35	3.31769	0.00001	-0.00001	0.00006	0.00005	3.31774
R36	2.65390	0.00000	0.00000	-0.00003	-0.00003	2.65387
R37	2.66629	0.00006	0.00004	-0.00005	-0.00001	2.66628
R38	2.67289	0.00001	-0.00001	-0.00001	-0.00002	2.67287
R39	2.60073	0.00004	-0.00002	0.00005	0.00002	2.60076
R40	2.65096	0.00006	-0.00008	0.00022	0.00014	2.65109
R41	2.68148	0.00000	-0.00001	0.00003	0.00001	2.68149
R42	3.28023	0.00001	0.00000	0.00002	0.00002	3.28025
R43	2.62927	0.00005	-0.00004	0.00010	0.00006	2.62933
R44	2.62162	0.00003	-0.00003	0.00009	0.00006	2.62168
R45	2.65940	0.00001	-0.00002	0.00002	0.00000	2.65940
R46	2.04808	0.00000	0.00000	0.00000	0.00000	2.04808
R47	3.38300	-0.00002	0.00001	-0.00002	-0.00001	3.38299
R48	2.67736	0.00003	0.00002	0.00000	0.00002	2.67738
R49	2.74470	-0.00002	0.00001	-0.00003	-0.00002	2.74469
R50	2.60549	-0.00001	0.00000	0.00002	0.00001	2.60551
R51	2.04699	-0.00001	0.00000	0.00000	-0.00001	2.04698
R52	2.79650	-0.00001	0.00000	0.00002	0.00001	2.79652
R53	2.77016	0.00004	0.00001	0.00006	0.00007	2.77023
R54	2.79418	0.00000	-0.00001	0.00002	0.00001	2.79419
R55	2.31726	-0.00003	0.00000	0.00000	0.00000	2.31726
R56	2.81038	0.00002	0.00003	0.00001	0.00003	2.81042
R57	2.61630	0.00006	-0.00002	0.00004	0.00002	2.61633
R58	2.65856	-0.00002	0.00000	0.00002	0.00002	2.65858
R59	2.62132	0.00002	0.00000	0.00000	0.00000	2.62132
R60	2.64463	0.00001	0.00001	-0.00001	0.00000	2.64463
R61	2.63860	-0.00003	0.00000	-0.00001	-0.00001	2.63860
R62	2.05071	0.00000	0.00000	0.00000	0.00000	2.05071
R63	2.64337	-0.00002	0.00000	0.00001	0.00001	2.64337
R64	2.04226	-0.00002	0.00001	-0.00003	-0.00002	2.04224
R65	2.64617	0.00001	0.00000	0.00001	0.00000	2.64617
R66	2.05152	0.00000	0.00000	0.00000	0.00000	2.05151
R67	2.05163	0.00000	0.00000	0.00000	0.00000	2.05163
R68	2.69998	0.00000	0.00001	0.00001	0.00002	2.70001
R69	2.69938	-0.00001	0.00002	-0.00001	0.00001	2.69939
R70	2.20274	0.00000	0.00000	0.00000	0.00000	2.20274
R71	2.20159	0.00000	0.00000	0.00000	0.00000	2.20159
R72	2.69935	0.00000	0.00002	-0.00002	0.00000	2.69935
R73	2.69997	0.00000	0.00001	0.00001	0.00001	2.69999
R74	2.20158	0.00000	0.00000	0.00000	0.00000	2.20158
R75	2.20274	0.00000	0.00000	0.00000	0.00000	2.20274
R76	2.06404	0.00000	0.00000	0.00006	0.00006	2.06410
R77	2.06992	0.00000	0.00000	0.00000	0.00000	2.06992
R78	2.06315	0.00000	0.00000	-0.00005	-0.00005	2.06311
R79	2.06991	0.00000	0.00000	0.00001	0.00001	2.06992
R80	2.06411	0.00000	-0.00001	0.00008	0.00007	2.06418
R81	2.06309	0.00000	0.00000	-0.00006	-0.00006	2.06303
A1	2.07604	0.00001	-0.00001	0.00002	0.00001	2.07605
A2	1.89866	0.00000	0.00000	0.00000	0.00000	1.89867
A3	2.30849	-0.00001	0.00001	-0.00002	-0.00001	2.30847
A4	2.14259	-0.00001	0.00001	-0.00002	-0.00001	2.14258

A5	1.91161	0.00000	0.00001	-0.00001	0.00000	1.91161
A6	2.22898	0.00000	-0.00001	0.00003	0.00001	2.22900
A7	2.05914	0.00000	0.00000	0.00000	0.00000	2.05914
A8	2.08921	0.00000	0.00000	0.00001	0.00001	2.08922
A9	2.13484	0.00000	0.00000	-0.00002	-0.00002	2.13482
A10	2.09523	0.00000	-0.00001	0.00001	0.00001	2.09523
A11	2.09775	0.00000	0.00000	-0.00001	-0.00001	2.09774
A12	2.09021	0.00000	0.00000	0.00000	0.00000	2.09021
A13	2.12484	0.00000	0.00000	-0.00001	-0.00001	2.12483
A14	2.08482	0.00000	0.00000	0.00000	0.00001	2.08483
A15	2.07353	0.00001	0.00000	0.00001	0.00000	2.07353
A16	2.06854	0.00000	0.00001	0.00000	0.00000	2.06854
A17	2.13140	-0.00001	0.00000	0.00000	0.00000	2.13141
A18	2.08324	0.00001	-0.00001	0.00001	0.00000	2.08324
A19	1.87051	0.00000	-0.00001	0.00000	-0.00001	1.87050
A20	2.17480	-0.00003	0.00004	-0.00002	0.00002	2.17483
A21	2.23787	0.00003	-0.00004	0.00002	-0.00001	2.23786
A22	1.86278	0.00000	0.00000	0.00001	0.00001	1.86278
A23	2.19410	0.00000	0.00000	-0.00001	-0.00001	2.19408
A24	2.22631	0.00000	0.00000	0.00000	0.00000	2.22632
A25	1.88122	0.00000	0.00000	0.00000	0.00000	1.88121
A26	2.20881	-0.00001	0.00000	0.00001	0.00001	2.20882
A27	2.19316	0.00001	0.00000	0.00000	0.00000	2.19315
A28	2.34399	0.00001	0.00000	-0.00004	-0.00003	2.34396
A29	2.01754	-0.00001	0.00001	-0.00001	0.00000	2.01754
A30	1.92165	0.00000	-0.00002	0.00005	0.00003	1.92168
A31	2.24963	-0.00003	0.00003	0.00001	0.00004	2.24967
A32	2.08328	0.00004	-0.00004	0.00004	0.00000	2.08328
A33	1.95027	-0.00001	0.00001	-0.00005	-0.00004	1.95023
A34	1.95869	-0.00002	0.00000	0.00002	0.00003	1.95872
A35	1.85748	0.00000	0.00000	0.00004	0.00004	1.85752
A36	2.46701	0.00002	0.00000	-0.00006	-0.00006	2.46695
A37	1.98432	-0.00001	0.00001	-0.00008	-0.00007	1.98425
A38	1.91728	0.00000	-0.00001	-0.00001	-0.00001	1.91727
A39	2.38156	0.00001	-0.00001	0.00009	0.00008	2.38164
A40	1.57192	0.00003	-0.00002	0.00003	0.00001	1.57193
A41	1.95955	0.00001	-0.00001	0.00008	0.00007	1.95962
A42	2.12543	0.00000	0.00000	-0.00004	-0.00004	2.12539
A43	2.19821	-0.00001	0.00000	-0.00004	-0.00003	2.19817
A44	1.86684	0.00000	0.00000	-0.00005	-0.00006	1.86679
A45	2.45181	0.00001	-0.00001	0.00009	0.00009	2.45189
A46	1.96451	-0.00001	0.00001	-0.00003	-0.00003	1.96449
A47	1.92126	0.00000	-0.00001	0.00007	0.00006	1.92132
A48	1.97080	-0.00001	0.00000	0.00004	0.00005	1.97085
A49	2.39108	0.00001	0.00001	-0.00012	-0.00011	2.39097
A50	1.86168	0.00001	0.00002	-0.00006	-0.00004	1.86164
A51	2.20594	-0.00001	-0.00002	0.00043	0.00040	2.20634
A52	2.21037	0.00000	0.00003	-0.00041	-0.00039	2.20998
A53	1.56127	0.00002	-0.00001	0.00001	0.00000	1.56127
A54	1.56124	0.00002	0.00001	-0.00003	-0.00002	1.56122
A55	1.98279	0.00000	0.00000	0.00001	0.00001	1.98280
A56	2.35505	0.00000	0.00000	0.00002	0.00002	2.35507
A57	1.94534	0.00000	0.00000	-0.00002	-0.00003	1.94531
A58	2.35496	0.00001	0.00000	-0.00001	-0.00001	2.35495
A59	1.94535	0.00001	0.00000	-0.00002	-0.00002	1.94533
A60	1.98288	-0.00001	0.00000	0.00003	0.00003	1.98291
A61	1.97073	0.00000	-0.00001	0.00004	0.00004	1.97077
A62	2.39119	0.00001	0.00000	-0.00007	-0.00007	2.39112
A63	1.92122	-0.00001	0.00001	0.00002	0.00003	1.92125
A64	1.96454	-0.00001	0.00001	-0.00002	-0.00002	1.96452

A65	2.45175	0.00001	-0.00001	0.00007	0.00006	2.45181
A66	1.86687	0.00000	0.00001	-0.00005	-0.00004	1.86684
A67	1.85744	0.00001	-0.00001	0.00003	0.00002	1.85746
A68	2.46710	0.00001	-0.00001	-0.00001	-0.00002	2.46709
A69	1.95864	-0.00001	0.00001	-0.00001	0.00000	1.95864
A70	1.98431	0.00000	0.00000	-0.00002	-0.00003	1.98428
A71	1.91731	-0.00001	0.00002	-0.00005	-0.00003	1.91728
A72	2.38154	0.00000	-0.00002	0.00007	0.00006	2.38160
A73	1.95961	-0.00001	0.00000	0.00002	0.00002	1.95963
A74	2.19816	0.00000	-0.00001	0.00001	0.00000	2.19816
A75	2.12542	0.00001	0.00000	-0.00002	-0.00002	2.12540
A76	1.95024	0.00000	0.00001	-0.00002	-0.00001	1.95023
A77	2.08339	0.00004	-0.00003	0.00002	-0.00002	2.08337
A78	2.24956	-0.00004	0.00002	0.00000	0.00003	2.24959
A79	1.57197	0.00002	-0.00002	0.00004	0.00002	1.57198
A80	1.86170	0.00001	-0.00002	0.00004	0.00002	1.86171
A81	2.21075	-0.00001	0.00004	-0.00034	-0.00031	2.21044
A82	2.20553	0.00000	0.00000	0.00028	0.00028	2.20581
A83	2.34411	-0.00004	0.00003	-0.00006	-0.00003	2.34408
A84	1.92164	0.00002	-0.00002	0.00004	0.00001	1.92165
A85	2.01744	0.00002	-0.00001	0.00002	0.00001	2.01746
A86	2.19323	-0.00004	0.00000	-0.00001	-0.00001	2.19322
A87	2.20871	0.00003	0.00000	0.00002	0.00001	2.20873
A88	1.88124	0.00000	0.00000	-0.00001	-0.00001	1.88124
A89	1.86278	0.00000	0.00000	0.00001	0.00001	1.86279
A90	2.22634	-0.00001	0.00001	-0.00001	0.00000	2.22634
A91	2.19406	0.00001	-0.00001	0.00000	-0.00001	2.19406
A92	1.87053	-0.00002	-0.00001	-0.00001	-0.00002	1.87052
A93	2.23794	0.00002	-0.00004	0.00000	-0.00004	2.23789
A94	2.17471	0.00000	0.00005	0.00000	0.00006	2.17477
A95	1.91159	0.00001	0.00001	-0.00001	0.00000	1.91159
A96	2.22902	-0.00001	-0.00002	0.00002	0.00000	2.22902
A97	2.14258	0.00000	0.00001	-0.00001	0.00000	2.14257
A98	1.89863	0.00001	-0.00001	0.00001	0.00001	1.89864
A99	2.30852	-0.00001	0.00003	-0.00003	0.00000	2.30852
A100	2.07604	0.00000	-0.00002	0.00001	-0.00001	2.07603
A101	2.05916	0.00000	0.00001	0.00000	0.00001	2.05916
A102	2.08922	0.00000	-0.00001	0.00002	0.00001	2.08923
A103	2.13481	0.00000	0.00000	-0.00002	-0.00002	2.13479
A104	2.06855	0.00000	0.00001	0.00000	0.00001	2.06856
A105	2.13142	0.00000	0.00000	0.00000	0.00000	2.13142
A106	2.08321	0.00000	-0.00002	0.00000	-0.00001	2.08320
A107	2.09523	0.00000	-0.00001	0.00001	0.00000	2.09523
A108	2.09773	0.00000	0.00001	-0.00002	-0.00001	2.09772
A109	2.09023	0.00000	0.00000	0.00001	0.00001	2.09024
A110	2.12482	0.00000	0.00000	-0.00001	-0.00001	2.12482
A111	2.07350	0.00000	0.00000	0.00000	-0.00001	2.07350
A112	2.08486	-0.00001	0.00000	0.00001	0.00001	2.08487
A113	2.16680	0.00003	-0.00003	0.00001	-0.00002	2.16678
A114	2.15619	0.00000	0.00007	0.00002	0.00009	2.15629
A115	1.96020	-0.00003	-0.00004	-0.00003	-0.00007	1.96012
A116	2.15623	-0.00002	0.00006	-0.00001	0.00005	2.15628
A117	2.16677	0.00003	-0.00002	0.00003	0.00000	2.16677
A118	1.96019	-0.00002	-0.00003	-0.00002	-0.00005	1.96013
A119	1.91266	0.00000	0.00000	0.00008	0.00008	1.91274
A120	1.94888	-0.00001	0.00002	-0.00004	-0.00002	1.94886
A121	1.90450	0.00000	0.00000	-0.00008	-0.00008	1.90442
A122	1.90612	0.00000	-0.00001	0.00004	0.00003	1.90615
A123	1.88651	0.00000	0.00000	0.00005	0.00005	1.88656
A124	1.90410	0.00000	0.00000	-0.00005	-0.00005	1.90405

A125	1.94882	0.00000	-0.00002	0.00002	0.00000	1.94882
A126	1.91272	0.00001	-0.00001	0.00012	0.00011	1.91284
A127	1.90434	0.00001	-0.00001	-0.00005	-0.00006	1.90428
A128	1.90621	-0.00001	0.00001	0.00001	0.00002	1.90623
A129	1.90410	-0.00001	0.00002	-0.00012	-0.00011	1.90399
A130	1.88659	-0.00001	0.00001	0.00002	0.00003	1.88662
A131	3.16665	0.00002	-0.00001	0.00004	0.00003	3.16668
A132	3.17927	0.00003	-0.00007	0.00031	0.00024	3.17952
A133	3.17948	0.00000	-0.00009	0.00027	0.00019	3.17967
A134	3.16688	0.00000	0.00002	-0.00004	-0.00003	3.16685
A135	3.14152	0.00000	0.00002	-0.00006	-0.00004	3.14148
A136	3.14161	0.00000	0.00000	0.00001	0.00001	3.14162
A137	3.14157	0.00000	0.00001	-0.00006	-0.00005	3.14152
A138	3.14158	0.00000	0.00006	-0.00011	-0.00005	3.14152
D1	0.00027	0.00000	0.00000	0.00000	-0.00001	0.00026
D2	-3.14077	-0.00001	0.00001	-0.00011	-0.00010	-3.14087
D3	-3.14139	0.00000	0.00002	0.00000	0.00002	-3.14136
D4	0.00075	-0.00001	0.00004	-0.00011	-0.00007	0.00068
D5	-0.00008	0.00000	0.00002	-0.00003	-0.00001	-0.00009
D6	3.14130	0.00000	0.00002	-0.00003	-0.00001	3.14129
D7	-3.14158	0.00000	-0.00002	-0.00003	-0.00005	3.14155
D8	-0.00021	0.00000	-0.00002	-0.00003	-0.00005	-0.00026
D9	-0.00140	-0.00001	-0.00017	-0.00049	-0.00065	-0.00205
D10	3.13915	0.00000	-0.00024	-0.00026	-0.00051	3.13864
D11	3.14012	0.00000	-0.00013	-0.00048	-0.00062	3.13950
D12	-0.00253	0.00000	-0.00021	-0.00026	-0.00047	-0.00299
D13	-0.00025	0.00000	-0.00001	0.00004	0.00003	-0.00022
D14	3.14152	0.00000	0.00001	-0.00004	-0.00003	3.14149
D15	3.14069	0.00001	-0.00003	0.00017	0.00014	3.14083
D16	-0.00073	0.00001	0.00000	0.00009	0.00008	-0.00065
D17	0.00017	0.00001	0.00011	0.00065	0.00076	0.00093
D18	3.14158	0.00000	0.00020	0.00063	0.00083	-3.14078
D19	-3.14084	0.00001	0.00012	0.00054	0.00066	-3.14018
D20	0.00057	0.00000	0.00021	0.00052	0.00073	0.00130
D21	0.00003	0.00000	0.00002	-0.00005	-0.00003	0.00001
D22	-3.14144	0.00000	0.00002	-0.00006	-0.00004	-3.14148
D23	3.14145	0.00000	0.00000	0.00003	0.00003	3.14148
D24	-0.00002	0.00000	-0.00001	0.00002	0.00001	-0.00001
D25	0.00015	0.00000	-0.00001	0.00002	0.00001	0.00016
D26	-3.14143	0.00000	-0.00002	0.00002	0.00000	-3.14143
D27	-3.14156	0.00000	-0.00001	0.00003	0.00003	-3.14153
D28	0.00005	0.00000	-0.00001	0.00003	0.00002	0.00006
D29	-0.00013	0.00000	-0.00001	0.00002	0.00001	-0.00012
D30	-3.14151	0.00000	-0.00001	0.00002	0.00001	-3.14150
D31	3.14145	0.00000	0.00000	0.00002	0.00002	3.14147
D32	0.00007	0.00000	-0.00001	0.00002	0.00002	0.00009
D33	0.00148	0.00001	0.00023	0.00088	0.00111	0.00259
D34	-3.13736	0.00000	-0.00043	0.00053	0.00010	-3.13726
D35	-3.13901	0.00001	0.00031	0.00065	0.00096	-3.13805
D36	0.00533	-0.00001	-0.00035	0.00029	-0.00006	0.00528
D37	0.00145	-0.00001	0.00008	-0.00009	-0.00001	0.00144
D38	-3.13964	-0.00001	0.00007	-0.00003	0.00004	-3.13960
D39	-3.14142	0.00000	-0.00001	0.00018	0.00017	-3.14125
D40	0.00068	0.00000	-0.00002	0.00024	0.00021	0.00089
D41	-0.00104	-0.00002	-0.00021	-0.00094	-0.00115	-0.00219
D42	3.13784	0.00000	0.00044	-0.00059	-0.00015	3.13769
D43	3.14075	-0.00001	-0.00030	-0.00092	-0.00122	3.13952
D44	-0.00356	0.00001	0.00035	-0.00057	-0.00022	-0.00378
D45	3.14132	0.00000	0.00060	-0.00069	-0.00009	3.14123
D46	-0.00073	0.00001	0.00082	0.00007	0.00088	0.00015

D47	0.00295	-0.00002	-0.00017	-0.00110	-0.00128	0.00167
D48	-3.13910	-0.00001	0.00004	-0.00035	-0.00031	-3.13941
D49	-0.00188	0.00000	0.00008	0.00090	0.00098	-0.00090
D50	3.14068	0.00001	0.00041	0.00112	0.00153	-3.14098
D51	3.14015	-0.00001	-0.00013	0.00017	0.00005	3.14020
D52	-0.00048	0.00000	0.00021	0.00040	0.00060	0.00012
D53	-3.13751	-0.00001	-0.00004	-0.00014	-0.00018	-3.13769
D54	0.00319	-0.00002	-0.00035	-0.00035	-0.00070	0.00249
D55	3.14122	0.00001	0.00001	0.00026	0.00026	3.14149
D56	0.00277	0.00000	-0.00016	-0.00017	-0.00033	0.00243
D57	0.00043	0.00002	0.00028	0.00044	0.00073	0.00116
D58	-3.13802	0.00001	0.00012	0.00002	0.00013	-3.13789
D59	0.00752	-0.00001	-0.00023	0.00004	-0.00019	0.00733
D60	-3.12802	0.00000	-0.00006	0.00016	0.00010	-3.12792
D61	-3.13530	0.00000	-0.00007	0.00014	0.00006	-3.13524
D62	0.01235	0.00001	0.00009	0.00025	0.00034	0.01269
D63	-0.00594	0.00002	0.00032	0.00017	0.00050	-0.00544
D64	3.13753	0.00000	0.00008	0.00003	0.00012	3.13765
D65	-0.00021	0.00000	-0.00001	0.00005	0.00004	-0.00017
D66	-3.13369	-0.00001	0.00002	-0.00066	-0.00063	-3.13432
D67	3.13956	0.00001	0.00022	0.00019	0.00041	3.13997
D68	0.00609	0.00000	0.00026	-0.00052	-0.00027	0.00582
D69	-0.00503	-0.00001	-0.00004	-0.00032	-0.00036	-0.00539
D70	3.13327	0.00001	0.00013	0.00013	0.00027	3.13354
D71	3.12829	-0.00002	-0.00027	-0.00048	-0.00074	3.12755
D72	-0.01659	0.00000	-0.00009	-0.00003	-0.00012	-0.01671
D73	-0.01968	-0.00001	-0.00014	-0.00046	-0.00060	-0.02028
D74	-3.05742	-0.00001	-0.00030	0.00004	-0.00026	-3.05768
D75	3.12997	0.00000	0.00008	-0.00030	-0.00022	3.12975
D76	0.09222	0.00000	-0.00008	0.00019	0.00011	0.09234
D77	-0.01211	-0.00001	-0.00008	-0.00034	-0.00042	-0.01253
D78	3.13741	0.00000	-0.00016	0.00013	-0.00003	3.13737
D79	3.12389	0.00000	-0.00010	0.00015	0.00005	3.12394
D80	-0.00978	0.00000	-0.00018	0.00062	0.00043	-0.00935
D81	-3.14136	0.00001	0.00019	0.00015	0.00034	-3.14102
D82	0.00864	0.00000	0.00022	-0.00058	-0.00036	0.00828
D83	0.01956	0.00001	0.00013	0.00049	0.00063	0.02018
D84	3.05696	0.00001	0.00029	0.00006	0.00035	3.05731
D85	-3.13273	0.00001	0.00024	-0.00014	0.00011	-3.13263
D86	-0.09533	0.00000	0.00040	-0.00057	-0.00017	-0.09550
D87	-3.13443	0.00000	0.00016	-0.00061	-0.00045	-3.13488
D88	0.00543	0.00000	0.00002	-0.00029	-0.00027	0.00516
D89	0.01807	0.00000	0.00005	0.00003	0.00008	0.01815
D90	-3.12526	0.00000	-0.00009	0.00036	0.00026	-3.12500
D91	1.54950	0.00000	-0.00022	0.00543	0.00522	1.55472
D92	-2.61923	0.00000	-0.00022	0.00554	0.00532	-2.61392
D93	-0.55665	0.00000	-0.00022	0.00561	0.00539	-0.55127
D94	-1.46800	0.00000	-0.00041	0.00599	0.00558	-1.46242
D95	0.64645	0.00000	-0.00041	0.00609	0.00568	0.65213
D96	2.70903	0.00001	-0.00041	0.00616	0.00575	2.71478
D97	-0.00565	0.00000	-0.00022	0.00043	0.00021	-0.00543
D98	3.13773	0.00000	-0.00026	0.00049	0.00022	3.13795
D99	-3.13756	0.00000	-0.00027	0.00038	0.00011	-3.13745
D100	0.00579	0.00000	-0.00013	0.00005	-0.00008	0.00572
D101	-0.00867	0.00000	0.00014	-0.00013	0.00001	-0.00866
D102	3.14115	0.00000	0.00006	-0.00012	-0.00006	3.14109
D103	0.00123	0.00000	0.00015	-0.00016	-0.00001	0.00122
D104	3.14148	0.00000	0.00004	0.00009	0.00013	-3.14157
D105	3.14147	0.00000	0.00019	-0.00021	-0.00002	3.14145
D106	-0.00146	0.00000	0.00008	0.00005	0.00012	-0.00134

D107	3.13462	0.00000	0.00008	-0.00020	-0.00013	3.13449
D108	-0.01802	0.00000	-0.00002	-0.00027	-0.00028	-0.01831
D109	-0.00522	0.00000	0.00003	-0.00015	-0.00012	-0.00534
D110	3.12532	-0.00001	-0.00006	-0.00021	-0.00027	3.12505
D111	0.00969	0.00000	-0.00013	0.00018	0.00006	0.00974
D112	-3.13738	0.00000	-0.00007	0.00018	0.00011	-3.13727
D113	-3.12388	0.00000	-0.00006	0.00023	0.00017	-3.12371
D114	0.01223	0.00000	0.00000	0.00022	0.00022	0.01245
D115	3.13256	0.00000	0.00009	-0.00009	-0.00001	3.13255
D116	0.09542	0.00000	0.00000	0.00006	0.00006	0.09548
D117	-0.01987	0.00000	0.00000	-0.00016	-0.00016	-0.02003
D118	-3.05701	0.00000	-0.00009	0.00000	-0.00009	-3.05710
D119	3.13397	0.00000	0.00009	-0.00021	-0.00012	3.13385
D120	-0.00634	0.00000	0.00004	0.00002	0.00006	-0.00628
D121	0.00032	0.00000	0.00001	-0.00020	-0.00019	0.00013
D122	-3.13999	0.00000	-0.00005	0.00004	-0.00001	-3.14000
D123	3.13524	0.00000	-0.00003	-0.00005	-0.00008	3.13516
D124	-0.01265	0.00000	-0.00001	0.00011	0.00010	-0.01255
D125	-0.00722	0.00000	0.00000	-0.00020	-0.00020	-0.00742
D126	3.12807	0.00000	0.00003	-0.00005	-0.00002	3.12805
D127	-3.13777	0.00001	0.00020	0.00027	0.00047	-3.13730
D128	0.00516	0.00001	0.00014	0.00051	0.00065	0.00581
D129	0.00559	-0.00001	-0.00020	-0.00034	-0.00055	0.00505
D130	-3.13340	0.00000	0.00001	0.00006	0.00007	-3.13333
D131	-3.12741	-0.00001	-0.00023	-0.00055	-0.00079	-3.12819
D132	0.01679	0.00000	-0.00002	-0.00015	-0.00017	0.01662
D133	0.02005	0.00000	0.00001	0.00003	0.00004	0.02009
D134	3.05760	0.00000	0.00010	-0.00018	-0.00008	3.05753
D135	-3.12991	0.00000	0.00004	0.00023	0.00027	-3.12963
D136	-0.09236	0.00000	0.00013	0.00003	0.00016	-0.09220
D137	-0.00158	0.00002	0.00031	0.00072	0.00103	-0.00055
D138	-3.14152	0.00001	0.00013	0.00011	0.00023	-3.14128
D139	3.13753	0.00001	0.00011	0.00033	0.00044	3.13797
D140	-0.00240	-0.00001	-0.00007	-0.00028	-0.00036	-0.00276
D141	-0.00208	-0.00002	-0.00026	-0.00070	-0.00096	-0.00304
D142	3.13765	0.00000	-0.00005	-0.00002	-0.00007	3.13759
D143	3.14131	0.00002	0.00012	0.00091	0.00103	-3.14085
D144	-0.00027	0.00001	0.00016	0.00070	0.00086	0.00059
D145	0.00169	0.00000	-0.00009	0.00018	0.00008	0.00177
D146	-3.13989	0.00000	-0.00006	-0.00003	-0.00009	-3.13997
D147	-0.64070	-0.00001	0.00035	-0.00511	-0.00476	-0.64546
D148	1.47364	-0.00001	0.00035	-0.00503	-0.00468	1.46896
D149	-2.70324	-0.00001	0.00036	-0.00517	-0.00481	-2.70805
D150	2.62525	0.00000	0.00025	-0.00490	-0.00465	2.62060
D151	-1.54360	0.00000	0.00025	-0.00482	-0.00457	-1.54817
D152	0.56271	-0.00001	0.00026	-0.00496	-0.00471	0.55800
D153	-0.00187	0.00000	-0.00003	0.00016	0.00013	-0.00174
D154	-3.14157	0.00000	0.00006	-0.00011	-0.00005	3.14156
D155	3.13971	0.00000	-0.00007	0.00037	0.00031	3.14002
D156	0.00001	0.00000	0.00002	0.00010	0.00012	0.00013
D157	-3.13831	0.00000	0.00013	-0.00047	-0.00034	-3.13865
D158	0.00283	0.00000	0.00009	-0.00035	-0.00026	0.00257
D159	0.00169	0.00000	0.00005	-0.00024	-0.00018	0.00150
D160	-3.14036	0.00000	0.00002	-0.00012	-0.00011	-3.14047
D161	3.13809	0.00000	-0.00012	0.00048	0.00036	3.13846
D162	-0.00429	0.00000	-0.00010	0.00057	0.00047	-0.00383
D163	-0.00188	0.00000	-0.00005	0.00025	0.00021	-0.00168
D164	3.13892	0.00000	-0.00003	0.00034	0.00031	3.13923
D165	-0.00084	0.00000	-0.00004	0.00013	0.00009	-0.00075
D166	3.14045	0.00000	-0.00003	0.00012	0.00009	3.14055

D167	3.14119	0.00000	0.00000	0.00002	0.00002	3.14121
D168	-0.00070	0.00000	0.00001	0.00001	0.00002	-0.00068
D169	0.00138	0.00000	0.00002	-0.00017	-0.00015	0.00123
D170	-3.14022	0.00000	0.00001	-0.00014	-0.00013	-3.14035
D171	-3.13945	0.00000	0.00001	-0.00026	-0.00025	-3.13970
D172	0.00213	0.00000	-0.00001	-0.00022	-0.00023	0.00190
D173	-0.00046	0.00000	0.00000	0.00001	0.00002	-0.00045
D174	-3.14156	0.00000	-0.00002	-0.00002	-0.00004	3.14159
D175	3.14021	0.00000	0.00002	0.00011	0.00014	3.14034
D176	-0.00089	0.00000	0.00000	0.00008	0.00008	-0.00080
D177	-0.00033	0.00000	0.00001	0.00002	0.00004	-0.00030
D178	3.14127	0.00000	0.00002	-0.00001	0.00002	3.14129
D179	3.14155	0.00000	0.00000	0.00004	0.00003	3.14158
D180	-0.00004	0.00000	0.00001	0.00000	0.00002	-0.00002
D181	-3.14112	0.00000	-0.00002	0.00000	-0.00002	-3.14114
D182	0.00042	0.00000	0.00000	-0.00001	0.00000	0.00042
D183	0.00013	0.00000	0.00000	-0.00002	-0.00001	0.00012
D184	-3.14151	0.00000	0.00002	-0.00002	0.00000	-3.14151
D185	3.14150	0.00000	0.00001	-0.00004	-0.00003	3.14147
D186	0.00014	0.00000	0.00002	-0.00006	-0.00004	0.00010
D187	-0.00010	0.00000	-0.00001	0.00000	-0.00001	-0.00011
D188	-3.14147	0.00000	0.00000	-0.00002	-0.00002	-3.14148
D189	-0.00009	0.00000	-0.00001	0.00002	0.00001	-0.00008
D190	3.14148	0.00000	0.00002	-0.00006	-0.00004	3.14145
D191	3.14155	0.00000	-0.00003	0.00002	-0.00001	3.14155
D192	-0.00006	0.00000	0.00000	-0.00005	-0.00005	-0.00011
D193	0.00014	0.00000	0.00000	0.00000	0.00000	0.00014
D194	-3.14146	0.00000	0.00001	0.00000	0.00000	-3.14146
D195	3.14151	0.00000	-0.00001	0.00002	0.00001	3.14152
D196	-0.00009	0.00000	-0.00001	0.00002	0.00001	-0.00008
D197	-0.00005	0.00000	0.00001	-0.00001	0.00000	-0.00005
D198	3.14156	0.00000	0.00001	-0.00001	0.00000	3.14155
D199	3.14156	0.00000	-0.00002	0.00006	0.00004	-3.14158
D200	-0.00002	0.00000	-0.00003	0.00007	0.00004	0.00002

Item	Value	Threshold	Converged?

Maximum Force	0.000062	0.000450	YES

RMS Force	0.000013	0.000300	YES

Maximum Displacement	0.009480	0.001800	NO

RMS Displacement	0.001670	0.001200	NO

Predicted change in Energy=-3.350173D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.803311	-0.637292	0.006006
2	6	0	-9.994060	-1.788054	0.003803
3	6	0	-10.516447	-3.073092	0.009323
4	6	0	-11.905389	-3.215567	0.017655
5	6	0	-12.726588	-2.081325	0.020213
6	6	0	-12.194672	-0.787640	0.014419
7	1	0	-9.845762	-3.926210	0.007194

8	1	0	-12.352718	-4.204727	0.022268
9	1	0	-13.805366	-2.203340	0.026863
10	1	0	-12.864284	0.060609	0.016745
11	6	0	-9.927123	0.564365	-0.001648
12	6	0	-8.569866	-1.390706	-0.004337
13	6	0	-8.540409	0.088870	-0.005775
14	6	0	-7.404381	0.870162	-0.008296
15	6	0	-6.014399	0.595364	-0.011915
16	6	0	-3.644236	-0.183967	-0.011165
17	6	0	-3.778296	1.228570	-0.016481
18	16	0	-5.181864	-0.989472	-0.013449
19	6	0	-5.099575	1.664735	-0.012997
20	6	0	-2.267154	-0.451793	-0.007021
21	6	0	-1.603923	0.797378	-0.010140
22	7	0	-2.523816	1.820809	-0.032234
23	16	0	-1.150942	-1.806949	-0.007753
24	16	0	1.150741	1.806657	0.009061
25	6	0	0.198425	-0.673756	0.002329
26	6	0	-0.198459	0.673358	-0.000979
27	6	0	1.603873	-0.797753	0.011305
28	6	0	2.267035	0.451565	0.007815
29	6	0	3.644162	0.183930	0.011678
30	6	0	3.778351	-1.228685	0.017260
31	6	0	5.099621	-1.664771	0.013439
32	6	0	6.014399	-0.595353	0.011381
33	16	0	5.181784	0.989437	0.013430
34	7	0	2.523935	-1.821033	0.033263
35	6	0	7.404336	-0.869945	0.007058
36	6	0	8.540359	-0.088623	0.004895
37	6	0	8.569886	1.390935	0.004734
38	6	0	9.927004	-0.564201	0.000341
39	6	0	9.994112	1.788239	-0.002106
40	6	0	10.803315	0.637398	-0.004984
41	6	0	10.516580	3.073223	-0.005779
42	6	0	12.194681	0.787693	-0.011865
43	6	0	11.905564	3.215647	-0.012762
44	6	0	12.726695	2.081380	-0.015752
45	6	0	10.384416	-1.870958	0.001463
46	6	0	9.533335	-3.018579	0.008072
47	6	0	11.768886	-2.222687	-0.003367
48	7	0	8.862698	-3.971961	0.013445
49	7	0	12.886350	-2.552159	-0.007227
50	6	0	-10.384589	1.871114	-0.005181
51	6	0	-11.769049	2.222788	-0.000133
52	6	0	-9.533557	3.018737	-0.014893
53	7	0	-12.886474	2.552385	0.003881
54	7	0	-8.863125	3.972241	-0.022937
55	8	0	-7.612893	-2.157379	-0.008799
56	8	0	7.612941	2.157683	0.008953
57	6	0	2.241417	-3.242982	-0.054955
58	1	0	1.319369	-3.467446	0.485879
59	1	0	2.138279	-3.570956	-1.094952
60	1	0	3.054542	-3.798922	0.415867
61	6	0	-2.240426	3.242570	0.056065
62	1	0	-2.130691	3.569118	1.095835
63	1	0	-1.321786	3.467674	-0.490366
64	1	0	-3.056496	3.799161	-0.408761
65	1	0	5.428760	-2.697374	0.009265
66	1	0	12.864279	-0.060578	-0.014442
67	1	0	13.805490	2.203298	-0.021223

68	1	0	12.352920	4.204799	-0.015950
69	1	0	9.845955	3.926387	-0.003226
70	1	0	7.572425	-1.940038	0.005283
71	1	0	-7.572354	1.940267	-0.006905
72	1	0	-5.428678	2.697356	-0.008891

Rotational constants (GHZ): 0.1750168 0.0104043 0.0098218

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6569.8187408699 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T
Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6569.7338233945 Hartrees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.24D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Initial guess from the checkpoint file: "PBDB.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000002 -0.000001 0.000001 Ang= 0.00 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3683.02012169 A.U. after 7 cycles

NFock= 7 Conv=0.85D-08 -V/T= 2.0068

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1

NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	0.000008014	-0.000001084	0.000003602
2	6	-0.000005105	-0.000012864	-0.000013982
3	6	-0.000001492	0.000009179	0.000002985
4	6	0.000006677	-0.000002059	0.000003857
5	6	-0.000008038	-0.000009819	-0.000008496
6	6	-0.000009315	0.000010509	-0.000003038
7	1	-0.000001089	-0.000000131	-0.000001421
8	1	-0.000002267	-0.000000323	-0.000000830
9	1	0.000001852	0.000002006	0.000001740
10	1	0.000000980	-0.000007642	0.000001928
11	6	0.000020201	-0.000009181	-0.000005570
12	6	-0.000013528	-0.000008944	0.000022166
13	6	-0.000007159	0.000002563	0.000028464
14	6	0.000034447	0.000032517	0.000002430
15	6	-0.000004269	-0.000009435	-0.000030475
16	6	0.000034388	0.000056500	0.000029769
17	6	-0.000045921	-0.000036259	-0.000029511
18	16	-0.000032672	-0.000004328	-0.000026127
19	6	-0.000024840	-0.000006358	0.000017288
20	6	0.000025715	0.000046420	-0.000002013

21	6	-0.000028616	-0.000054159	0.000004906
22	7	0.000032078	-0.000003466	-0.000002020
23	16	-0.000005322	-0.000008496	0.000011437
24	16	0.000002938	0.000001489	0.000013144
25	6	-0.000021496	0.000016600	-0.000025949
26	6	-0.000002405	0.000006038	0.000004883
27	6	0.000028229	-0.000010802	0.000018929
28	6	0.000006495	-0.000018510	-0.000005928
29	6	0.000001896	0.000007701	-0.000013229
30	6	-0.000010187	-0.000013030	-0.000011439
31	6	-0.000004924	0.000002720	0.000037989
32	6	-0.000001070	0.000016664	-0.000040839
33	16	0.000006895	-0.000004684	0.000034737
34	7	0.000012660	0.000012222	0.000004839
35	6	0.000029708	-0.000031550	-0.000001135
36	6	-0.000021008	0.000004294	-0.000010663
37	6	-0.000040178	-0.000008738	-0.000014842
38	6	0.000000711	-0.000018409	-0.000003615
39	6	0.000032508	0.000039947	0.000024749
40	6	-0.000025585	-0.000005604	-0.000028022
41	6	0.000008222	-0.000033111	-0.000004094
42	6	0.000008254	-0.000025048	0.000013186
43	6	-0.000021045	0.000013471	-0.000012807
44	6	0.000013951	0.000032946	0.000014201
45	6	0.000021333	0.000026367	0.000019710
46	6	0.000004459	-0.000007450	0.000003909
47	6	-0.000012755	-0.000001696	-0.000011258
48	7	0.000007314	-0.000002061	0.000004904
49	7	-0.000001132	-0.000000156	-0.000000371
50	6	0.000010075	-0.000005446	0.000000518
51	6	-0.000001378	-0.000004759	0.000005111
52	6	-0.000014258	0.000005178	-0.000006295
53	7	-0.000001369	0.000008583	0.000000133
54	7	0.000002831	-0.000001684	-0.000003497
55	8	0.000005268	0.000000896	-0.000013775
56	8	0.000030607	0.000010782	0.000018125
57	6	-0.000003957	-0.000006097	-0.000000517
58	1	0.000002919	0.000001171	-0.000000017
59	1	-0.000001712	-0.000001529	-0.000001942
60	1	-0.000002426	0.000001018	0.000001947
61	6	-0.000004652	0.000011293	-0.000006757
62	1	-0.000003708	-0.000001022	0.000000185
63	1	0.000000506	0.000001257	-0.000006803
64	1	-0.000003445	-0.000006877	0.000000449
65	1	-0.000002142	0.000000929	-0.000000222
66	1	-0.000007556	0.000006747	-0.000006253
67	1	-0.000003548	-0.000004074	-0.000002948
68	1	0.000004480	-0.000000342	-0.000000090
69	1	-0.000000983	0.000000254	0.000002418
70	1	-0.000005321	-0.000004965	-0.000000294
71	1	-0.000003197	0.000001612	-0.000000457
72	1	0.000004452	0.000002321	0.000002900

Cartesian Forces: Max 0.000056500 RMS 0.000015869

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.

```

Internal Forces: Max      0.000055702 RMS      0.000011727
Search for a local minimum.
Step number 32 out of a maximum of 429
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 16 18 17 19 20
21 22 23 24 25
26 27 28 29 30
31 32
DE= -1.53D-07 DEPred=-3.35D-07 R= 4.56D-01
Trust test= 4.56D-01 RLast= 1.85D-02 DXMaxT set to 1.43D-01
ITU= 0 0 0 0 1 -1 1 -1 1 -1 1 1 -1 0 -1 0 -1 1 1 1
ITU= 1 1 1 0 0 0 1 0 0 0 1 0
Eigenvalues --- 0.00055 0.00264 0.00270 0.00293 0.00401
Eigenvalues --- 0.00462 0.00490 0.00509 0.00539 0.00581
Eigenvalues --- 0.00591 0.00608 0.00625 0.00632 0.00677
Eigenvalues --- 0.00696 0.00723 0.00744 0.00756 0.00771
Eigenvalues --- 0.00778 0.00784 0.00799 0.00835 0.00861
Eigenvalues --- 0.01025 0.01093 0.01116 0.01134 0.01152
Eigenvalues --- 0.01263 0.01301 0.01322 0.01356 0.01363
Eigenvalues --- 0.01381 0.01429 0.01457 0.01535 0.01599
Eigenvalues --- 0.01637 0.01653 0.01747 0.01755 0.01794
Eigenvalues --- 0.01927 0.01953 0.02006 0.02021 0.02053
Eigenvalues --- 0.02073 0.02121 0.02190 0.02423 0.02788
Eigenvalues --- 0.02899 0.02972 0.03714 0.03898 0.03989
Eigenvalues --- 0.04030 0.04830 0.04839 0.04911 0.05015
Eigenvalues --- 0.05086 0.05107 0.05218 0.05439 0.07043
Eigenvalues --- 0.07228 0.07394 0.07573 0.15439 0.15839
Eigenvalues --- 0.15981 0.15983 0.15997 0.15999 0.16000
Eigenvalues --- 0.16000 0.16000 0.16001 0.16002 0.16009
Eigenvalues --- 0.16012 0.16021 0.16049 0.16068 0.16090
Eigenvalues --- 0.16099 0.19053 0.19391 0.19928 0.20717
Eigenvalues --- 0.21194 0.21538 0.21894 0.21999 0.22007
Eigenvalues --- 0.22402 0.22500 0.22600 0.22626 0.22679
Eigenvalues --- 0.22771 0.22976 0.23113 0.23182 0.23232
Eigenvalues --- 0.23376 0.23477 0.23570 0.23831 0.24149
Eigenvalues --- 0.24202 0.24265 0.24324 0.24416 0.24549
Eigenvalues --- 0.24602 0.24673 0.24775 0.24850 0.24905
Eigenvalues --- 0.24931 0.24966 0.24980 0.24987 0.24994
Eigenvalues --- 0.24997 0.24998 0.24999 0.25000 0.25000
Eigenvalues --- 0.25000 0.25001 0.25007 0.25096 0.25149
Eigenvalues --- 0.25304 0.25653 0.25943 0.26155 0.26311
Eigenvalues --- 0.26557 0.26790 0.26936 0.27234 0.27329
Eigenvalues --- 0.27744 0.27853 0.28313 0.28521 0.28735
Eigenvalues --- 0.28866 0.29861 0.30333 0.31696 0.32304
Eigenvalues --- 0.33377 0.35461 0.35633 0.36276 0.36336
Eigenvalues --- 0.36473 0.36497 0.36638 0.36820 0.36840
Eigenvalues --- 0.36959 0.37074 0.37087 0.37139 0.37250
Eigenvalues --- 0.37257 0.37417 0.37552 0.37669 0.37757
Eigenvalues --- 0.38040 0.38348 0.39016 0.40316 0.41106
Eigenvalues --- 0.41720 0.42021 0.42653 0.44427 0.45122
Eigenvalues --- 0.45764 0.46383 0.46985 0.47888 0.47973
Eigenvalues --- 0.48820 0.52271 0.53522 0.55645 0.57819
Eigenvalues --- 0.66226 0.72871 0.75928 0.80554 0.82356
Eigenvalues --- 0.92813 1.25858 1.26355 1.29352 1.35374
En-DIIS/RFO-DIIS IScMMF= 0 using points: 32 31 30 29 28
RFO step: Lambda=-9.01434488D-08.
DidBck=T Rises=F RFO-DIIS coefs: 0.68897 0.28739 -0.04142 0.03452
0.03054

```

```

Iteration 1 RMS(Cart)= 0.00125652 RMS(Int)= 0.00000016
Iteration 2 RMS(Cart)= 0.00000078 RMS(Int)= 0.00000001
Variable      Old X      -DE/DX      Delta X      Delta X      Delta X      New X
(Linear)      (Quad)      (Total)
R1      2.65851    -0.00001    0.00000    -0.00002    -0.00002    2.65849
R2      2.64465     0.00000    0.00000     0.00001     0.00002    2.64466
R3      2.81039    -0.00001    -0.00001     0.00000    -0.00001    2.81038
R4      2.62137     0.00001    0.00000     0.00002     0.00002    2.62139
R5      2.79416     0.00000    0.00000     0.00000     0.00000    2.79417
R6      2.63854     0.00000    0.00000     0.00000     0.00000    2.63854
R7      2.05071     0.00000    0.00000     0.00000     0.00000    2.05071
R8      2.64621     0.00001    0.00000     0.00000     0.00001    2.64622
R9      2.05152     0.00000    0.00000     0.00000     0.00000    2.05152
R10     2.64331    -0.00001     0.00000    -0.00001    -0.00001    2.64330
R11     2.05163     0.00000     0.00000     0.00000     0.00000    2.05163
R12     2.04223     0.00000     0.00000    -0.00002    -0.00001    2.04221
R13     2.77029     0.00000    -0.00001    -0.00002    -0.00004    2.77026
R14     2.61635     0.00000     0.00000     0.00002     0.00002    2.61637
R15     2.79655     0.00000     0.00000    -0.00002    -0.00003    2.79652
R16     2.31721     0.00000     0.00000    -0.00001    -0.00001    2.31720
R17     2.60548    -0.00002    -0.00002    -0.00003    -0.00004    2.60544
R18     2.67753    -0.00002    -0.00004     0.00003    -0.00001    2.67752
R19     2.04697     0.00000     0.00000     0.00000     0.00001    2.04697
R20     3.38299    -0.00002     0.00000    -0.00008    -0.00008    3.38291
R21     2.65939     0.00001     0.00000     0.00001     0.00002    2.65941
R22     2.68132     0.00006     0.00001     0.00006     0.00007    2.68139
R23     3.28026     0.00000    -0.00002     0.00004     0.00002    3.28028
R24     2.65108     0.00002     0.00000     0.00008     0.00008    2.65116
R25     2.62939     0.00001    -0.00001     0.00004     0.00003    2.62942
R26     2.62170     0.00002     0.00000     0.00004     0.00004    2.62173
R27     2.04809    -0.00001     0.00000    -0.00001    -0.00001    2.04808
R28     2.67269     0.00005     0.00002     0.00007     0.00009    2.67278
R29     3.31774     0.00000    -0.00001     0.00003     0.00002    3.31775
R30     2.60076     0.00002     0.00001     0.00002     0.00003    2.60080
R31     2.66632     0.00003     0.00000     0.00006     0.00007    2.66639
R32     2.74467     0.00000     0.00001    -0.00002    -0.00001    2.74466
R33     3.32990     0.00000    -0.00001     0.00001     0.00000    3.32990
R34     3.32979     0.00001    -0.00001     0.00004     0.00004    3.32982
R35     3.31774     0.00000    -0.00002     0.00003     0.00001    3.31775
R36     2.65387     0.00001     0.00001    -0.00001     0.00000    2.65387
R37     2.66628     0.00005     0.00001     0.00015     0.00016    2.66644
R38     2.67287     0.00001     0.00001     0.00000     0.00001    2.67288
R39     2.60076     0.00001     0.00000     0.00003     0.00004    2.60079
R40     2.65109     0.00000    -0.00003     0.00005     0.00002    2.65112
R41     2.68149     0.00000    -0.00001     0.00000    -0.00001    2.68149
R42     3.28025     0.00000     0.00000     0.00001     0.00000    3.28026
R43     2.62933     0.00002    -0.00001     0.00005     0.00004    2.62937
R44     2.62168     0.00001    -0.00001     0.00004     0.00003    2.62171
R45     2.65940     0.00001     0.00000     0.00001     0.00001    2.65941
R46     2.04808     0.00000     0.00000     0.00000     0.00000    2.04808
R47     3.38299    -0.00002     0.00000    -0.00006    -0.00005    3.38293
R48     2.67738     0.00002     0.00000     0.00008     0.00008    2.67746
R49     2.74469    -0.00001     0.00000    -0.00002    -0.00002    2.74466
R50     2.60551    -0.00002    -0.00001    -0.00002    -0.00003    2.60548
R51     2.04698    -0.00001     0.00000     0.00000     0.00000    2.04698
R52     2.79652    -0.00001    -0.00001     0.00001     0.00000    2.79652
R53     2.77023     0.00002    -0.00002     0.00005     0.00003    2.77026
R54     2.79419    -0.00001     0.00000    -0.00001    -0.00001    2.79417
R55     2.31726    -0.00004     0.00000    -0.00003    -0.00004    2.31722
R56     2.81042    -0.00001    -0.00001     0.00000    -0.00002    2.81040

```

R57	2.61633	0.00003	0.00000	0.00005	0.00004	2.61637
R58	2.65858	-0.00003	-0.00001	-0.00003	-0.00004	2.65854
R59	2.62132	0.00002	0.00000	0.00005	0.00005	2.62137
R60	2.64463	0.00000	0.00000	0.00001	0.00001	2.64464
R61	2.63860	-0.00002	0.00000	-0.00004	-0.00004	2.63856
R62	2.05071	0.00000	0.00000	0.00000	0.00000	2.05071
R63	2.64337	-0.00003	-0.00001	-0.00003	-0.00004	2.64334
R64	2.04224	-0.00001	0.00000	-0.00003	-0.00003	2.04221
R65	2.64617	0.00001	0.00000	0.00003	0.00003	2.64620
R66	2.05151	0.00000	0.00000	0.00000	0.00000	2.05152
R67	2.05163	0.00000	0.00000	0.00000	0.00000	2.05163
R68	2.70001	-0.00001	-0.00001	-0.00002	-0.00004	2.69997
R69	2.69939	-0.00002	-0.00001	-0.00004	-0.00005	2.69934
R70	2.20274	0.00000	0.00000	0.00000	0.00000	2.20274
R71	2.20159	0.00000	0.00000	0.00000	0.00000	2.20159
R72	2.69935	0.00000	0.00000	0.00000	0.00000	2.69935
R73	2.69999	0.00000	-0.00001	-0.00001	-0.00002	2.69997
R74	2.20158	0.00000	0.00000	0.00000	0.00000	2.20159
R75	2.20274	0.00000	0.00000	0.00000	0.00000	2.20274
R76	2.06410	0.00000	-0.00002	0.00002	0.00000	2.06409
R77	2.06992	0.00000	0.00000	0.00000	0.00000	2.06992
R78	2.06311	0.00000	0.00002	-0.00002	0.00000	2.06310
R79	2.06992	0.00000	0.00000	0.00001	0.00000	2.06992
R80	2.06418	-0.00001	-0.00003	0.00002	-0.00001	2.06417
R81	2.06303	0.00000	0.00002	-0.00001	0.00001	2.06304
A1	2.07605	0.00001	0.00000	0.00002	0.00002	2.07607
A2	1.89867	0.00000	0.00000	0.00000	0.00000	1.89866
A3	2.30847	-0.00001	0.00000	-0.00002	-0.00002	2.30845
A4	2.14258	-0.00001	0.00000	-0.00002	-0.00002	2.14256
A5	1.91161	0.00000	0.00000	0.00000	0.00000	1.91161
A6	2.22900	0.00001	0.00000	0.00002	0.00001	2.22901
A7	2.05914	0.00000	0.00000	0.00000	0.00000	2.05914
A8	2.08922	0.00000	0.00000	0.00001	0.00001	2.08923
A9	2.13482	0.00000	0.00001	-0.00001	-0.00001	2.13481
A10	2.09523	0.00000	0.00000	0.00001	0.00001	2.09525
A11	2.09774	0.00000	0.00000	0.00000	0.00000	2.09774
A12	2.09021	0.00000	0.00000	-0.00001	-0.00001	2.09020
A13	2.12483	0.00000	0.00000	-0.00001	-0.00001	2.12482
A14	2.08483	0.00000	0.00000	-0.00002	-0.00002	2.08481
A15	2.07353	0.00001	0.00000	0.00003	0.00003	2.07356
A16	2.06854	0.00000	0.00000	-0.00001	-0.00001	2.06854
A17	2.13141	-0.00001	0.00000	-0.00002	-0.00003	2.13138
A18	2.08324	0.00001	0.00000	0.00003	0.00003	2.08327
A19	1.87050	0.00000	0.00000	-0.00001	0.00000	1.87050
A20	2.17483	-0.00004	-0.00002	-0.00005	-0.00006	2.17476
A21	2.23786	0.00004	0.00001	0.00005	0.00007	2.23792
A22	1.86278	0.00000	0.00000	-0.00001	-0.00001	1.86277
A23	2.19408	0.00000	0.00000	0.00000	0.00000	2.19408
A24	2.22632	0.00000	0.00000	0.00001	0.00001	2.22633
A25	1.88121	0.00000	0.00000	0.00001	0.00002	1.88123
A26	2.20882	-0.00001	-0.00001	-0.00007	-0.00007	2.20874
A27	2.19315	0.00001	0.00000	0.00006	0.00006	2.19321
A28	2.34396	0.00000	0.00001	0.00002	0.00004	2.34400
A29	2.01754	0.00000	-0.00001	-0.00005	-0.00006	2.01749
A30	1.92168	0.00000	0.00000	0.00003	0.00002	1.92170
A31	2.24967	-0.00004	-0.00002	-0.00010	-0.00012	2.24955
A32	2.08328	0.00004	0.00002	0.00011	0.00012	2.08340
A33	1.95023	0.00001	0.00001	-0.00001	0.00000	1.95023
A34	1.95872	-0.00002	-0.00001	-0.00005	-0.00006	1.95866
A35	1.85752	0.00000	-0.00001	0.00001	0.00000	1.85752

A36	2.46695	0.00003	0.00003	0.00003	0.00006	2.46701
A37	1.98425	0.00000	0.00002	-0.00001	0.00001	1.98426
A38	1.91727	0.00000	0.00001	-0.00002	-0.00001	1.91726
A39	2.38164	0.00000	-0.00003	0.00003	0.00000	2.38164
A40	1.57193	0.00002	0.00000	0.00005	0.00006	1.57199
A41	1.95962	0.00000	-0.00002	0.00002	0.00000	1.95961
A42	2.12539	0.00000	0.00001	0.00000	0.00002	2.12541
A43	2.19817	0.00000	0.00001	-0.00002	-0.00001	2.19816
A44	1.86679	0.00000	0.00002	-0.00003	0.00000	1.86678
A45	2.45189	0.00001	-0.00003	0.00006	0.00003	2.45192
A46	1.96449	-0.00001	0.00001	-0.00003	-0.00002	1.96447
A47	1.92132	-0.00001	-0.00002	0.00001	-0.00001	1.92131
A48	1.97085	-0.00001	-0.00002	-0.00001	-0.00003	1.97082
A49	2.39097	0.00002	0.00004	0.00000	0.00005	2.39102
A50	1.86164	0.00001	0.00001	0.00002	0.00003	1.86167
A51	2.20634	-0.00003	-0.00016	0.00005	-0.00011	2.20624
A52	2.20998	0.00002	0.00015	-0.00010	0.00005	2.21003
A53	1.56127	0.00001	0.00001	0.00003	0.00003	1.56130
A54	1.56122	0.00002	0.00001	0.00005	0.00006	1.56128
A55	1.98280	0.00000	-0.00001	0.00000	-0.00001	1.98279
A56	2.35507	0.00000	-0.00001	0.00000	-0.00001	2.35506
A57	1.94531	0.00001	0.00001	0.00001	0.00002	1.94533
A58	2.35495	0.00001	0.00000	0.00001	0.00002	2.35497
A59	1.94533	0.00001	0.00001	0.00001	0.00002	1.94535
A60	1.98291	-0.00002	-0.00001	-0.00003	-0.00004	1.98287
A61	1.97077	0.00000	-0.00002	0.00000	-0.00002	1.97075
A62	2.39112	0.00001	0.00003	-0.00001	0.00002	2.39114
A63	1.92125	0.00000	-0.00001	0.00001	0.00000	1.92125
A64	1.96452	-0.00001	0.00001	-0.00002	-0.00002	1.96450
A65	2.45181	0.00001	-0.00002	0.00004	0.00002	2.45183
A66	1.86684	0.00000	0.00001	-0.00001	0.00000	1.86683
A67	1.85746	0.00000	-0.00001	0.00002	0.00001	1.85747
A68	2.46709	0.00000	0.00001	0.00000	0.00001	2.46710
A69	1.95864	-0.00001	0.00000	-0.00002	-0.00003	1.95861
A70	1.98428	0.00000	0.00001	0.00001	0.00002	1.98430
A71	1.91728	0.00000	0.00001	-0.00001	0.00000	1.91728
A72	2.38160	0.00000	-0.00002	0.00001	-0.00002	2.38159
A73	1.95963	-0.00001	-0.00001	-0.00001	-0.00002	1.95960
A74	2.19816	0.00000	0.00000	0.00000	-0.00001	2.19815
A75	2.12540	0.00001	0.00001	0.00002	0.00003	2.12542
A76	1.95023	0.00000	0.00000	0.00000	0.00000	1.95023
A77	2.08337	0.00004	0.00001	0.00006	0.00007	2.08345
A78	2.24959	-0.00004	-0.00002	-0.00006	-0.00008	2.24951
A79	1.57198	0.00001	0.00000	0.00003	0.00003	1.57201
A80	1.86171	0.00000	0.00000	0.00000	0.00000	1.86171
A81	2.21044	0.00000	0.00011	-0.00013	-0.00002	2.21043
A82	2.20581	0.00000	-0.00011	0.00009	-0.00003	2.20578
A83	2.34408	-0.00004	0.00000	-0.00003	-0.00003	2.34405
A84	1.92165	0.00002	0.00000	0.00003	0.00003	1.92168
A85	2.01746	0.00002	0.00000	0.00000	0.00000	2.01746
A86	2.19322	-0.00003	0.00000	0.00001	0.00001	2.19323
A87	2.20873	0.00003	0.00000	0.00000	-0.00001	2.20872
A88	1.88124	0.00000	0.00000	-0.00001	0.00000	1.88123
A89	1.86279	0.00000	0.00000	0.00000	-0.00001	1.86279
A90	2.22634	-0.00001	0.00000	-0.00001	-0.00001	2.22633
A91	2.19406	0.00001	0.00001	0.00001	0.00002	2.19407
A92	1.87052	-0.00001	0.00000	-0.00002	-0.00002	1.87050
A93	2.23789	0.00005	0.00002	0.00003	0.00005	2.23794
A94	2.17477	-0.00004	-0.00002	-0.00001	-0.00003	2.17474
A95	1.91159	0.00001	0.00000	0.00001	0.00001	1.91160

A96	2.22902	0.00000	0.00000	0.00000	0.00000	2.22902
A97	2.14257	0.00000	0.00000	-0.00001	-0.00001	2.14257
A98	1.89864	0.00001	0.00000	0.00002	0.00002	1.89866
A99	2.30852	-0.00002	0.00000	-0.00004	-0.00004	2.30848
A100	2.07603	0.00001	0.00001	0.00002	0.00002	2.07605
A101	2.05916	-0.00001	0.00000	-0.00001	-0.00002	2.05914
A102	2.08923	0.00000	0.00000	0.00001	0.00001	2.08924
A103	2.13479	0.00000	0.00001	0.00000	0.00001	2.13480
A104	2.06856	0.00000	0.00000	-0.00001	-0.00001	2.06855
A105	2.13142	-0.00001	0.00000	-0.00003	-0.00003	2.13139
A106	2.08320	0.00001	0.00001	0.00004	0.00005	2.08325
A107	2.09523	0.00000	0.00000	0.00001	0.00001	2.09524
A108	2.09772	0.00000	0.00000	0.00001	0.00001	2.09773
A109	2.09024	0.00000	0.00000	-0.00002	-0.00002	2.09022
A110	2.12482	0.00000	0.00000	0.00000	0.00000	2.12482
A111	2.07350	0.00001	0.00000	0.00003	0.00004	2.07353
A112	2.08487	-0.00001	-0.00001	-0.00003	-0.00004	2.08483
A113	2.16678	0.00005	0.00002	0.00006	0.00008	2.16685
A114	2.15629	-0.00004	-0.00004	-0.00002	-0.00006	2.15623
A115	1.96012	-0.00001	0.00002	-0.00004	-0.00002	1.96010
A116	2.15628	-0.00004	-0.00002	-0.00004	-0.00006	2.15622
A117	2.16677	0.00004	0.00001	0.00007	0.00008	2.16685
A118	1.96013	0.00000	0.00002	-0.00003	-0.00002	1.96012
A119	1.91274	0.00000	-0.00003	0.00004	0.00002	1.91275
A120	1.94886	0.00000	0.00000	-0.00002	-0.00002	1.94885
A121	1.90442	0.00000	0.00003	-0.00002	0.00001	1.90443
A122	1.90615	0.00000	-0.00001	0.00001	0.00000	1.90615
A123	1.88656	0.00000	-0.00002	0.00001	-0.00001	1.88655
A124	1.90405	0.00000	0.00002	-0.00002	0.00000	1.90404
A125	1.94882	0.00000	0.00000	0.00001	0.00002	1.94884
A126	1.91284	0.00000	-0.00004	0.00006	0.00002	1.91286
A127	1.90428	0.00001	0.00003	0.00002	0.00005	1.90433
A128	1.90623	0.00000	-0.00001	-0.00002	-0.00003	1.90620
A129	1.90399	0.00000	0.00003	-0.00006	-0.00003	1.90397
A130	1.88662	0.00000	-0.00002	-0.00001	-0.00003	1.88659
A131	3.16668	0.00002	0.00001	0.00016	0.00017	3.16685
A132	3.17952	0.00000	-0.00005	0.00012	0.00007	3.17959
A133	3.17967	-0.00002	-0.00005	-0.00010	-0.00015	3.17951
A134	3.16685	0.00000	0.00000	-0.00008	-0.00009	3.16676
A135	3.14148	0.00000	0.00001	-0.00001	0.00000	3.14148
A136	3.14162	0.00000	0.00000	0.00001	0.00001	3.14163
A137	3.14152	0.00000	0.00001	-0.00001	0.00000	3.14153
A138	3.14152	0.00001	0.00001	0.00010	0.00011	3.14164
D1	0.00026	0.00000	0.00000	-0.00006	-0.00006	0.00020
D2	-3.14087	0.00000	0.00002	-0.00009	-0.00008	-3.14095
D3	-3.14136	0.00000	-0.00002	-0.00006	-0.00008	-3.14144
D4	0.00068	0.00000	0.00000	-0.00009	-0.00009	0.00059
D5	-0.00009	0.00000	0.00001	0.00005	0.00005	-0.00003
D6	3.14129	0.00000	0.00001	0.00005	0.00005	3.14134
D7	3.14155	0.00000	0.00002	0.00005	0.00007	-3.14156
D8	-0.00026	0.00000	0.00002	0.00005	0.00007	-0.00018
D9	-0.00205	0.00000	0.00022	0.00018	0.00040	-0.00165
D10	3.13864	0.00000	0.00019	0.00008	0.00027	3.13891
D11	3.13950	0.00000	0.00020	0.00018	0.00038	3.13988
D12	-0.00299	0.00000	0.00018	0.00008	0.00025	-0.00274
D13	-0.00022	0.00000	0.00000	0.00002	0.00002	-0.00020
D14	3.14149	0.00000	0.00001	0.00002	0.00003	3.14152
D15	3.14083	0.00000	-0.00002	0.00007	0.00004	3.14087
D16	-0.00065	0.00000	-0.00001	0.00007	0.00005	-0.00060
D17	0.00093	0.00000	-0.00022	-0.00003	-0.00025	0.00068

D18	-3.14078	-0.00001	-0.00026	-0.00021	-0.00047	-3.14124
D19	-3.14018	0.00000	-0.00020	-0.00007	-0.00027	-3.14044
D20	0.00130	-0.00001	-0.00024	-0.00024	-0.00048	0.00081
D21	0.00001	0.00000	0.00001	0.00002	0.00002	0.00003
D22	-3.14148	0.00000	0.00001	-0.00002	-0.00001	-3.14149
D23	3.14148	0.00000	-0.00001	0.00002	0.00001	3.14149
D24	-0.00001	0.00000	0.00000	-0.00002	-0.00002	-0.00003
D25	0.00016	0.00000	0.00000	-0.00002	-0.00003	0.00014
D26	-3.14143	0.00000	0.00000	-0.00003	-0.00003	-3.14146
D27	-3.14153	0.00000	-0.00001	0.00001	0.00000	-3.14153
D28	0.00006	0.00000	0.00000	0.00000	0.00000	0.00006
D29	-0.00012	0.00000	0.00000	-0.00001	-0.00001	-0.00013
D30	-3.14150	0.00000	0.00000	-0.00001	-0.00001	-3.14152
D31	3.14147	0.00000	-0.00001	0.00000	-0.00001	3.14146
D32	0.00009	0.00000	-0.00001	0.00000	-0.00001	0.00008
D33	0.00259	0.00000	-0.00035	-0.00020	-0.00055	0.00205
D34	-3.13726	0.00000	-0.00001	-0.00080	-0.00081	-3.13808
D35	-3.13805	0.00000	-0.00032	-0.00009	-0.00041	-3.13847
D36	0.00528	0.00000	0.00001	-0.00069	-0.00068	0.00460
D37	0.00144	-0.00001	-0.00003	-0.00013	-0.00016	0.00128
D38	-3.13960	0.00000	-0.00005	-0.00003	-0.00008	-3.13968
D39	-3.14125	-0.00001	-0.00006	-0.00025	-0.00032	-3.14157
D40	0.00089	-0.00001	-0.00008	-0.00016	-0.00024	0.00065
D41	-0.00219	0.00000	0.00035	0.00014	0.00049	-0.00170
D42	3.13769	0.00000	0.00001	0.00074	0.00076	3.13845
D43	3.13952	0.00001	0.00039	0.00032	0.00072	3.14024
D44	-0.00378	0.00001	0.00006	0.00092	0.00098	-0.00281
D45	3.14123	0.00000	-0.00006	0.00056	0.00051	-3.14145
D46	0.00015	-0.00001	-0.00034	0.00041	0.00006	0.00022
D47	0.00167	0.00000	0.00034	-0.00015	0.00019	0.00186
D48	-3.13941	0.00000	0.00005	-0.00030	-0.00025	-3.13966
D49	-0.00090	-0.00001	-0.00028	-0.00046	-0.00074	-0.00164
D50	-3.14098	-0.00002	-0.00048	-0.00055	-0.00103	3.14118
D51	3.14020	0.00000	0.00000	-0.00031	-0.00032	3.13988
D52	0.00012	-0.00001	-0.00020	-0.00040	-0.00060	-0.00048
D53	-3.13769	0.00000	0.00005	-0.00015	-0.00010	-3.13779
D54	0.00249	0.00001	0.00024	-0.00007	0.00017	0.00265
D55	3.14149	0.00000	-0.00007	0.00011	0.00003	3.14152
D56	0.00243	0.00001	0.00012	0.00008	0.00019	0.00263
D57	0.00116	-0.00001	-0.00024	0.00003	-0.00021	0.00096
D58	-3.13789	0.00000	-0.00005	0.00000	-0.00005	-3.13794
D59	0.00733	0.00000	0.00007	-0.00008	-0.00002	0.00731
D60	-3.12792	0.00000	-0.00002	-0.00013	-0.00015	-3.12807
D61	-3.13524	0.00000	0.00000	0.00000	-0.00001	-3.13525
D62	0.01269	-0.00001	-0.00010	-0.00004	-0.00014	0.01255
D63	-0.00544	0.00000	-0.00017	0.00009	-0.00009	-0.00553
D64	3.13765	0.00000	-0.00006	-0.00004	-0.00010	3.13755
D65	-0.00017	0.00000	-0.00001	-0.00002	-0.00003	-0.00020
D66	-3.13432	0.00001	0.00017	0.00020	0.00037	-3.13395
D67	3.13997	0.00000	-0.00012	0.00010	-0.00001	3.13996
D68	0.00582	0.00000	0.00006	0.00032	0.00038	0.00621
D69	-0.00539	0.00001	0.00011	0.00003	0.00015	-0.00524
D70	3.13354	0.00000	-0.00009	0.00006	-0.00002	3.13352
D71	3.12755	0.00001	0.00024	0.00009	0.00033	3.12788
D72	-0.01671	0.00000	0.00004	0.00012	0.00016	-0.01655
D73	-0.02028	0.00001	0.00016	0.00009	0.00026	-0.02002
D74	-3.05768	0.00000	0.00016	0.00037	0.00053	-3.05715
D75	3.12975	0.00000	0.00004	0.00003	0.00008	3.12982
D76	0.09234	0.00000	0.00004	0.00031	0.00035	0.09269
D77	-0.01253	0.00000	0.00011	0.00008	0.00019	-0.01234

D78	3.13737	0.00000	0.00002	-0.00019	-0.00017	3.13720
D79	3.12394	0.00000	-0.00001	-0.00007	-0.00008	3.12385
D80	-0.00935	-0.00001	-0.00011	-0.00033	-0.00044	-0.00979
D81	-3.14102	0.00000	-0.00010	0.00024	0.00014	-3.14088
D82	0.00828	0.00001	0.00008	0.00047	0.00055	0.00883
D83	0.02018	-0.00001	-0.00017	-0.00010	-0.00027	0.01991
D84	3.05731	-0.00001	-0.00019	-0.00037	-0.00056	3.05675
D85	-3.13263	0.00000	-0.00004	0.00025	0.00021	-3.13242
D86	-0.09550	0.00000	-0.00006	-0.00002	-0.00008	-0.09558
D87	-3.13488	0.00000	0.00011	0.00029	0.00040	-3.13448
D88	0.00516	0.00000	0.00007	-0.00005	0.00003	0.00519
D89	0.01815	0.00000	-0.00001	-0.00008	-0.00009	0.01806
D90	-3.12500	-0.00001	-0.00005	-0.00041	-0.00046	-3.12546
D91	1.55472	0.00000	-0.00206	0.00131	-0.00075	1.55397
D92	-2.61392	0.00000	-0.00210	0.00134	-0.00076	-2.61468
D93	-0.55127	0.00000	-0.00213	0.00137	-0.00076	-0.55203
D94	-1.46242	0.00000	-0.00205	0.00164	-0.00041	-1.46283
D95	0.65213	0.00000	-0.00209	0.00166	-0.00043	0.65170
D96	2.71478	0.00000	-0.00212	0.00169	-0.00043	2.71436
D97	-0.00543	-0.00001	-0.00004	-0.00050	-0.00054	-0.00598
D98	3.13795	0.00000	-0.00004	-0.00045	-0.00050	3.13746
D99	-3.13745	-0.00001	-0.00001	-0.00055	-0.00056	-3.13801
D100	0.00572	0.00000	0.00003	-0.00021	-0.00018	0.00554
D101	-0.00866	0.00000	-0.00002	0.00026	0.00024	-0.00842
D102	3.14109	0.00000	0.00001	0.00014	0.00015	3.14124
D103	0.00122	0.00000	-0.00001	0.00041	0.00040	0.00162
D104	-3.14157	0.00000	-0.00004	0.00015	0.00011	-3.14146
D105	3.14145	0.00000	-0.00001	0.00037	0.00036	-3.14137
D106	-0.00134	0.00000	-0.00004	0.00012	0.00008	-0.00126
D107	3.13449	0.00000	0.00003	0.00003	0.00006	3.13455
D108	-0.01831	0.00000	0.00008	0.00000	0.00008	-0.01823
D109	-0.00534	0.00000	0.00003	0.00008	0.00011	-0.00523
D110	3.12505	0.00000	0.00008	0.00005	0.00013	3.12518
D111	0.00974	0.00000	0.00000	-0.00025	-0.00025	0.00950
D112	-3.13727	0.00000	-0.00002	-0.00017	-0.00019	-3.13746
D113	-3.12371	0.00000	-0.00004	-0.00022	-0.00026	-3.12397
D114	0.01245	0.00000	-0.00006	-0.00014	-0.00020	0.01226
D115	3.13255	0.00000	-0.00001	0.00018	0.00017	3.13272
D116	0.09548	0.00000	0.00004	0.00058	0.00062	0.09610
D117	-0.02003	0.00000	0.00004	0.00015	0.00019	-0.01984
D118	-3.05710	0.00000	0.00009	0.00055	0.00064	-3.05646
D119	3.13385	0.00000	0.00002	0.00019	0.00022	3.13407
D120	-0.00628	0.00000	-0.00002	0.00026	0.00024	-0.00604
D121	0.00013	0.00000	0.00005	0.00008	0.00013	0.00026
D122	-3.14000	0.00000	0.00000	0.00015	0.00015	-3.13985
D123	3.13516	0.00000	0.00003	0.00006	0.00009	3.13524
D124	-0.01255	0.00000	-0.00002	0.00001	-0.00002	-0.01257
D125	-0.00742	0.00000	0.00006	0.00002	0.00007	-0.00735
D126	3.12805	0.00000	0.00001	-0.00004	-0.00003	3.12802
D127	-3.13730	-0.00001	-0.00015	-0.00023	-0.00038	-3.13768
D128	0.00581	-0.00001	-0.00019	-0.00016	-0.00035	0.00545
D129	0.00505	0.00001	0.00017	0.00019	0.00036	0.00540
D130	-3.13333	0.00000	-0.00003	-0.00010	-0.00013	-3.13346
D131	-3.12819	0.00001	0.00024	0.00026	0.00050	-3.12769
D132	0.01662	0.00000	0.00004	-0.00003	0.00001	0.01663
D133	0.02009	0.00000	-0.00001	-0.00009	-0.00010	0.01999
D134	3.05753	0.00000	-0.00005	-0.00051	-0.00055	3.05697
D135	-3.12963	0.00000	-0.00008	-0.00017	-0.00024	-3.12988
D136	-0.09220	0.00000	-0.00011	-0.00058	-0.00069	-0.09289
D137	-0.00055	-0.00002	-0.00032	-0.00030	-0.00062	-0.00117

D138	-3.14128	-0.00001	-0.00010	-0.00019	-0.00029	-3.14157
D139	3.13797	-0.00001	-0.00012	-0.00003	-0.00015	3.13782
D140	-0.00276	0.00000	0.00009	0.00009	0.00018	-0.00258
D141	-0.00304	0.00002	0.00029	0.00026	0.00055	-0.00249
D142	3.13759	0.00001	0.00005	0.00013	0.00018	3.13777
D143	-3.14085	-0.00001	-0.00030	-0.00029	-0.00058	-3.14143
D144	0.00059	0.00000	-0.00024	-0.00004	-0.00029	0.00030
D145	0.00177	0.00000	-0.00004	-0.00015	-0.00019	0.00159
D146	-3.13997	0.00001	0.00001	0.00010	0.00011	-3.13986
D147	-0.64546	0.00000	0.00174	-0.00209	-0.00036	-0.64581
D148	1.46896	0.00000	0.00171	-0.00206	-0.00036	1.46860
D149	-2.70805	0.00000	0.00175	-0.00212	-0.00036	-2.70842
D150	2.62060	0.00000	0.00179	-0.00161	0.00018	2.62078
D151	-1.54817	0.00000	0.00176	-0.00158	0.00018	-1.54799
D152	0.55800	0.00000	0.00181	-0.00163	0.00017	0.55818
D153	-0.00174	0.00000	-0.00005	0.00026	0.00020	-0.00154
D154	3.14156	0.00000	0.00001	0.00018	0.00019	-3.14144
D155	3.14002	0.00000	-0.00010	0.00000	-0.00011	3.13991
D156	0.00013	0.00000	-0.00005	-0.00008	-0.00013	0.00001
D157	-3.13865	0.00000	0.00010	-0.00008	0.00002	-3.13863
D158	0.00257	0.00000	0.00008	0.00001	0.00009	0.00267
D159	0.00150	0.00000	0.00005	-0.00002	0.00003	0.00153
D160	-3.14047	0.00000	0.00003	0.00008	0.00011	-3.14036
D161	3.13846	0.00000	-0.00011	0.00005	-0.00006	3.13839
D162	-0.00383	0.00000	-0.00015	0.00011	-0.00004	-0.00387
D163	-0.00168	0.00000	-0.00006	-0.00002	-0.00008	-0.00176
D164	3.13923	0.00000	-0.00010	0.00004	-0.00006	3.13917
D165	-0.00075	0.00000	-0.00002	0.00005	0.00003	-0.00072
D166	3.14055	0.00000	-0.00003	0.00001	-0.00002	3.14053
D167	3.14121	0.00000	0.00000	-0.00004	-0.00005	3.14116
D168	-0.00068	0.00000	-0.00001	-0.00008	-0.00009	-0.00077
D169	0.00123	0.00000	0.00005	0.00005	0.00010	0.00133
D170	-3.14035	0.00000	0.00005	0.00010	0.00016	-3.14019
D171	-3.13970	0.00000	0.00009	-0.00001	0.00008	-3.13962
D172	0.00190	0.00000	0.00009	0.00004	0.00014	0.00204
D173	-0.00045	0.00000	-0.00001	0.00000	0.00000	-0.00045
D174	3.14159	0.00000	0.00002	-0.00001	0.00001	-3.14159
D175	3.14034	0.00000	-0.00005	0.00007	0.00002	3.14036
D176	-0.00080	0.00000	-0.00003	0.00006	0.00003	-0.00077
D177	-0.00030	0.00000	-0.00002	-0.00006	-0.00008	-0.00037
D178	3.14129	0.00000	-0.00002	-0.00011	-0.00013	3.14116
D179	3.14158	0.00000	-0.00001	-0.00002	-0.00004	3.14154
D180	-0.00002	0.00000	-0.00001	-0.00007	-0.00009	-0.00011
D181	-3.14114	0.00000	0.00002	0.00005	0.00007	-3.14107
D182	0.00042	0.00000	0.00000	0.00003	0.00004	0.00046
D183	0.00012	0.00000	0.00001	0.00001	0.00002	0.00014
D184	-3.14151	0.00000	-0.00001	-0.00001	-0.00001	-3.14152
D185	3.14147	0.00000	0.00001	0.00002	0.00003	3.14150
D186	0.00010	0.00000	0.00001	-0.00003	-0.00002	0.00008
D187	-0.00011	0.00000	0.00001	0.00008	0.00009	-0.00002
D188	-3.14148	0.00000	0.00001	0.00004	0.00005	-3.14144
D189	-0.00008	0.00000	0.00000	0.00004	0.00004	-0.00004
D190	3.14145	0.00000	0.00001	0.00003	0.00004	3.14149
D191	3.14155	0.00000	0.00001	0.00006	0.00008	-3.14156
D192	-0.00011	0.00000	0.00002	0.00005	0.00007	-0.00003
D193	0.00014	0.00000	0.00000	-0.00003	-0.00003	0.00011
D194	-3.14146	0.00000	0.00000	-0.00001	-0.00001	-3.14147
D195	3.14152	0.00000	0.00000	0.00001	0.00001	3.14154
D196	-0.00008	0.00000	0.00000	0.00003	0.00003	-0.00004
D197	-0.00005	0.00000	0.00000	-0.00003	-0.00004	-0.00008

D198	3.14155	0.00000	0.00000	-0.00005	-0.00006	3.14150
D199	-3.14158	0.00000	-0.00001	-0.00002	-0.00004	3.14157
D200	0.00002	0.00000	-0.00001	-0.00004	-0.00006	-0.00003

Item	Value	Threshold	Converged?

Maximum Force	0.000056	0.000450	YES
RMS Force	0.000012	0.000300	YES
Maximum Displacement	0.007056	0.001800	NO
RMS Displacement	0.001257	0.001200	NO

Predicted change in Energy=-1.378410D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4
Framework group C1[X(C42H18N6O2S4)]
Deg. of freedom 210
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.803374	-0.637280	0.006303
2	6	0	-9.994144	-1.788045	0.003908
3	6	0	-10.516575	-3.073078	0.008516
4	6	0	-11.905523	-3.215512	0.016069
5	6	0	-12.726704	-2.081253	0.018752
6	6	0	-12.194752	-0.787585	0.013884
7	1	0	-9.845922	-3.926220	0.006311
8	1	0	-12.352887	-4.204659	0.019950
9	1	0	-13.805485	-2.203269	0.024763
10	1	0	-12.864310	0.060698	0.016263
11	6	0	-9.927164	0.564363	-0.000202
12	6	0	-8.569938	-1.390713	-0.003354
13	6	0	-8.540477	0.088850	-0.004388
14	6	0	-7.404512	0.870191	-0.006934
15	6	0	-6.014514	0.595520	-0.011121
16	6	0	-3.644340	-0.183927	-0.011427
17	6	0	-3.778373	1.228649	-0.017256
18	16	0	-5.182048	-0.989306	-0.012584
19	6	0	-5.099651	1.664868	-0.013289
20	6	0	-2.267223	-0.451793	-0.007871
21	6	0	-1.603946	0.797405	-0.011877
22	7	0	-2.523860	1.820847	-0.033704
23	16	0	-1.151003	-1.806953	-0.009024
24	16	0	1.150841	1.806545	0.006297
25	6	0	0.198401	-0.673803	0.000660
26	6	0	-0.198449	0.673318	-0.003164
27	6	0	1.603928	-0.797865	0.009665
28	6	0	2.267128	0.451438	0.005823
29	6	0	3.644259	0.183765	0.010003
30	6	0	3.778422	-1.228848	0.015950
31	6	0	5.099700	-1.664984	0.012587
32	6	0	6.014495	-0.595571	0.010995
33	16	0	5.181915	0.989207	0.011868
34	7	0	2.523979	-1.821175	0.031887
35	6	0	7.404494	-0.870082	0.007530
36	6	0	8.540431	-0.088661	0.005411
37	6	0	8.569836	1.390899	0.004544
38	6	0	9.927135	-0.564127	0.001625

39	6	0	9.994029	1.788305	-0.001984
40	6	0	10.803319	0.637552	-0.004056
41	6	0	10.516407	3.073354	-0.006111
42	6	0	12.194682	0.787932	-0.010679
43	6	0	11.905364	3.215858	-0.012751
44	6	0	12.726589	2.081639	-0.015013
45	6	0	10.384730	-1.870844	0.003621
46	6	0	9.533902	-3.018626	0.010542
47	6	0	11.769242	-2.222302	-0.000503
48	7	0	8.863630	-3.972262	0.016183
49	7	0	12.886747	-2.551643	-0.003779
50	6	0	-10.384695	1.871102	-0.002952
51	6	0	-11.769192	2.222620	0.001698
52	6	0	-9.533808	3.018831	-0.011466
53	7	0	-12.886707	2.551923	0.005417
54	7	0	-8.863408	3.972368	-0.018382
55	8	0	-7.612975	-2.157396	-0.007280
56	8	0	7.612834	2.157549	0.008128
57	6	0	2.241459	-3.243090	-0.056681
58	1	0	1.319352	-3.467685	0.483998
59	1	0	2.138433	-3.570811	-1.096769
60	1	0	3.054522	-3.799157	0.414094
61	6	0	-2.240517	3.242614	0.054553
62	1	0	-2.130940	3.569242	1.094317
63	1	0	-1.321799	3.467724	-0.491734
64	1	0	-3.056502	3.799213	-0.410425
65	1	0	5.428800	-2.697600	0.008859
66	1	0	12.864297	-0.060307	-0.012684
67	1	0	13.805371	2.203679	-0.020275
68	1	0	12.352669	4.205032	-0.016236
69	1	0	9.845725	3.926474	-0.004191
70	1	0	7.572684	-1.940159	0.006230
71	1	0	-7.572607	1.940280	-0.005451
72	1	0	-5.428699	2.697501	-0.009423

Rotational constants (GHZ): 0.1750171 0.0104040 0.0098215

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6569.7722453942 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T
Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6569.6873287728 Hartrees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.24D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Initial guess from the checkpoint file: "PBDB.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 -0.000003 Ang= 0.00 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3683.02012181 A.U. after 7 cycles
 NFock= 7 Conv=0.82D-08 -V/T= 2.0068
 Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1
 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	0.000004880	0.000001214	-0.000004869
2	6	-0.000003300	-0.000003008	-0.000007968
3	6	-0.000000874	0.000003937	-0.000000422
4	6	0.000004346	-0.000000772	0.000004580
5	6	-0.000005007	-0.000007589	-0.000003563
6	6	-0.000000507	0.000008881	-0.000001535
7	1	-0.000000254	-0.000000549	-0.000000375
8	1	-0.000001203	-0.000000341	-0.000000609
9	1	0.000000204	0.000000532	0.000000676
10	1	0.000000245	-0.000001561	0.000000988
11	6	-0.000010610	-0.000004951	0.000005820
12	6	-0.000000037	0.000004835	0.000003331
13	6	-0.000001827	0.000004658	0.000011356
14	6	0.000023211	-0.000001703	0.000010399
15	6	-0.000008908	-0.000016136	-0.000010234
16	6	0.000025558	0.000025522	0.000030842
17	6	-0.000016543	-0.000021822	-0.000024810
18	16	-0.000008793	0.000000542	-0.000007507
19	6	0.000001975	0.000000240	-0.000000301
20	6	-0.000015115	0.000017849	0.000006905
21	6	-0.000003775	-0.000024189	-0.000015029
22	7	0.000012406	0.000005013	0.000019350
23	16	0.000011439	-0.000001672	-0.000013349
24	16	0.000008772	-0.000001229	-0.000005802
25	6	-0.000002857	-0.000009898	0.000017096
26	6	0.000003698	0.000007615	-0.000004656
27	6	-0.000017327	0.000004807	0.000012716
28	6	0.000000206	0.000001577	-0.000004835
29	6	-0.000004559	0.000007640	0.000001113
30	6	-0.000015194	-0.000005894	-0.000000848
31	6	0.000018106	-0.000001005	-0.000007486
32	6	-0.000011589	0.000009225	0.000010216
33	16	0.000012928	-0.000003678	-0.000000936
34	7	0.000008126	0.000000896	-0.000007315
35	6	-0.000007408	-0.000011924	0.000007230
36	6	-0.000001730	0.000004817	-0.000008351
37	6	-0.000013672	-0.000006313	-0.000008349
38	6	0.000002531	-0.000004039	0.000004274
39	6	0.000019079	0.000015020	0.000014098
40	6	-0.000017305	-0.000001324	-0.000016490
41	6	0.000005505	-0.000009562	-0.000000782
42	6	0.000003422	-0.000021186	0.000002599
43	6	-0.000010197	0.000006213	-0.000006300
44	6	0.000006792	0.000018991	0.000008747
45	6	-0.000007606	0.000003924	-0.000007310
46	6	0.000003089	0.000001586	0.000003195
47	6	0.000004643	0.000000508	0.000003975
48	7	-0.000000257	0.000001169	-0.000000167
49	7	0.000000204	-0.000001745	-0.000000160
50	6	0.000003461	-0.000002816	0.000005587
51	6	-0.000002731	0.000002833	-0.000002815

52	6	0.000007356	0.000001048	-0.000007786
53	7	-0.000001164	-0.000001465	-0.000000040
54	7	-0.000003693	-0.000002529	-0.000000245
55	8	-0.000001050	-0.000001257	-0.000000479
56	8	0.000008812	0.000004119	0.000007021
57	6	0.000001218	0.000001388	-0.000004610
58	1	0.000002159	0.000001186	-0.000000689
59	1	-0.000001832	-0.000000855	-0.000001259
60	1	-0.000001367	0.000000352	0.000001681
61	6	-0.000006509	-0.000001083	-0.000005642
62	1	-0.000001247	0.000002164	0.000000977
63	1	0.000001789	0.000001565	-0.000003502
64	1	-0.000002405	-0.000002131	0.000002636
65	1	-0.000001211	0.000000124	0.000000905
66	1	-0.000000423	0.000003096	-0.000000218
67	1	-0.000000689	-0.000001907	-0.000001720
68	1	0.000002819	-0.000000099	0.000000642
69	1	-0.000000506	0.000001496	0.000001064
70	1	0.000001685	0.000002019	-0.000001088
71	1	-0.000000987	-0.000003352	0.000001690
72	1	0.000001602	0.000000985	-0.000001256

Cartesian Forces: Max 0.000030842 RMS 0.000008169

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000028688 RMS 0.000004208

Search for a local minimum.

Step number 33 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 16 18 17 19 20

21 22 23 24 25

26 27 28 29 30

31 32 33

DE= -1.17D-07 DEPred=-1.38D-07 R= 8.51D-01

Trust test= 8.51D-01 RLast= 4.34D-03 DXMaxT set to 1.43D-01

ITU= 0 0 0 0 0 1 -1 1 -1 1 -1 1 1 -1 0 -1 0 -1 1 1

ITU= 1 1 1 1 0 0 0 1 0 0 0 0 1 0

Eigenvalues --- 0.00069 0.00256 0.00269 0.00294 0.00411

Eigenvalues --- 0.00467 0.00492 0.00512 0.00534 0.00553

Eigenvalues --- 0.00583 0.00609 0.00625 0.00633 0.00677

Eigenvalues --- 0.00701 0.00727 0.00744 0.00760 0.00773

Eigenvalues --- 0.00777 0.00787 0.00805 0.00848 0.00890

Eigenvalues --- 0.01025 0.01093 0.01127 0.01134 0.01174

Eigenvalues --- 0.01279 0.01314 0.01328 0.01360 0.01379

Eigenvalues --- 0.01419 0.01440 0.01457 0.01598 0.01637

Eigenvalues --- 0.01653 0.01739 0.01744 0.01794 0.01926

Eigenvalues --- 0.01947 0.01994 0.02006 0.02021 0.02064

Eigenvalues --- 0.02075 0.02147 0.02261 0.02499 0.02814

Eigenvalues --- 0.02918 0.02994 0.03735 0.03947 0.03956

Eigenvalues --- 0.04050 0.04832 0.04839 0.04912 0.05025

Eigenvalues --- 0.05088 0.05157 0.05291 0.05447 0.07044

Eigenvalues --- 0.07227 0.07393 0.07572 0.15334 0.15806

Eigenvalues --- 0.15956 0.15984 0.15992 0.15999 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16001 0.16010

Eigenvalues --- 0.16012 0.16023 0.16033 0.16064 0.16088

```

Eigenvalues --- 0.16096 0.19078 0.19412 0.19943 0.20707
Eigenvalues --- 0.21183 0.21366 0.21761 0.21915 0.22004
Eigenvalues --- 0.22078 0.22444 0.22598 0.22614 0.22644
Eigenvalues --- 0.22805 0.22959 0.23019 0.23158 0.23265
Eigenvalues --- 0.23370 0.23425 0.23536 0.23820 0.23902
Eigenvalues --- 0.24220 0.24266 0.24321 0.24428 0.24549
Eigenvalues --- 0.24578 0.24644 0.24719 0.24852 0.24880
Eigenvalues --- 0.24937 0.24957 0.24974 0.24989 0.24991
Eigenvalues --- 0.24995 0.24997 0.24999 0.25000 0.25000
Eigenvalues --- 0.25000 0.25001 0.25002 0.25017 0.25100
Eigenvalues --- 0.25387 0.25590 0.25908 0.26156 0.26301
Eigenvalues --- 0.26566 0.26795 0.26922 0.27236 0.27300
Eigenvalues --- 0.27721 0.27842 0.28314 0.28530 0.28743
Eigenvalues --- 0.28902 0.29868 0.30328 0.31785 0.32824
Eigenvalues --- 0.33761 0.35460 0.35638 0.36279 0.36336
Eigenvalues --- 0.36470 0.36479 0.36637 0.36822 0.36845
Eigenvalues --- 0.37021 0.37070 0.37091 0.37187 0.37249
Eigenvalues --- 0.37260 0.37416 0.37546 0.37672 0.37758
Eigenvalues --- 0.38016 0.38676 0.39169 0.40317 0.41095
Eigenvalues --- 0.41728 0.41924 0.42661 0.44411 0.45145
Eigenvalues --- 0.45731 0.46648 0.47019 0.47766 0.47982
Eigenvalues --- 0.49019 0.52278 0.53700 0.55190 0.56423
Eigenvalues --- 0.66632 0.72735 0.75449 0.80524 0.82305
Eigenvalues --- 0.91785 1.25857 1.26358 1.29353 1.35372
En-DIIS/RFO-DIIS IScMMF= 0 using points: 33 32 31 30 29
RFO step: Lambda=-1.80654238D-08.
DidBck=F Rises=F RFO-DIIS coefs: 0.78526 0.17418 0.03845 -0.06901
0.07113
Iteration 1 RMS(Cart)= 0.00110756 RMS(Int)= 0.00000009
Iteration 2 RMS(Cart)= 0.00000036 RMS(Int)= 0.00000001
Variable Old X -DE/DX Delta X Delta X Delta X New X
(Linear) (Quad) (Total)
R1 2.65849 0.00000 0.00000 -0.00001 -0.00001 2.65848
R2 2.64466 0.00000 0.00000 0.00001 0.00001 2.64467
R3 2.81038 0.00000 0.00000 0.00002 0.00001 2.81040
R4 2.62139 0.00000 0.00000 0.00001 0.00001 2.62140
R5 2.79417 0.00000 0.00000 0.00001 0.00001 2.79417
R6 2.63854 0.00000 0.00000 -0.00001 -0.00001 2.63853
R7 2.05071 0.00000 0.00000 0.00000 0.00000 2.05070
R8 2.64622 0.00000 0.00000 0.00001 0.00001 2.64622
R9 2.05152 0.00000 0.00000 0.00000 0.00000 2.05152
R10 2.64330 0.00000 0.00000 -0.00001 -0.00001 2.64329
R11 2.05163 0.00000 0.00000 0.00000 0.00000 2.05163
R12 2.04221 0.00000 0.00000 -0.00001 -0.00001 2.04221
R13 2.77026 0.00001 0.00000 0.00001 0.00001 2.77027
R14 2.61637 0.00000 0.00000 0.00001 0.00001 2.61638
R15 2.79652 0.00000 0.00000 0.00000 0.00000 2.79652
R16 2.31720 0.00000 0.00000 -0.00001 0.00000 2.31720
R17 2.60544 0.00001 0.00000 0.00000 0.00000 2.60544
R18 2.67752 -0.00002 0.00002 -0.00013 -0.00010 2.67742
R19 2.04697 0.00000 0.00000 0.00001 0.00001 2.04698
R20 3.38291 0.00000 0.00002 -0.00006 -0.00005 3.38287
R21 2.65941 -0.00001 0.00000 -0.00001 -0.00001 2.65940
R22 2.68139 0.00003 -0.00001 0.00008 0.00006 2.68146
R23 3.28028 0.00000 -0.00001 0.00000 0.00000 3.28028
R24 2.65116 -0.00001 -0.00001 0.00001 0.00000 2.65116
R25 2.62942 -0.00001 0.00000 -0.00001 -0.00001 2.62941
R26 2.62173 -0.00001 -0.00001 0.00001 0.00000 2.62173
R27 2.04808 0.00000 0.00000 -0.00001 0.00000 2.04808
R28 2.67278 0.00002 -0.00001 0.00007 0.00006 2.67284

```


R29	3.31775	0.00000	0.00000	0.00000	0.00000	3.31775
R30	2.60080	-0.00001	0.00000	-0.00001	-0.00001	2.60079
R31	2.66639	0.00000	-0.00001	0.00001	0.00001	2.66639
R32	2.74466	0.00000	0.00000	-0.00001	0.00000	2.74465
R33	3.32990	0.00000	0.00000	-0.00001	-0.00002	3.32988
R34	3.32982	0.00000	-0.00001	0.00002	0.00002	3.32984
R35	3.31775	0.00000	0.00000	0.00000	-0.00001	3.31775
R36	2.65387	0.00000	0.00000	-0.00001	0.00000	2.65386
R37	2.66644	-0.00002	-0.00002	0.00003	0.00001	2.66645
R38	2.67288	0.00000	0.00000	0.00000	0.00000	2.67288
R39	2.60079	0.00000	0.00000	-0.00001	-0.00001	2.60079
R40	2.65112	0.00000	0.00000	-0.00003	-0.00003	2.65109
R41	2.68149	0.00000	0.00000	-0.00001	-0.00001	2.68148
R42	3.28026	0.00000	0.00000	0.00000	0.00000	3.28026
R43	2.62937	0.00001	0.00000	0.00002	0.00002	2.62939
R44	2.62171	0.00000	0.00000	0.00000	0.00000	2.62170
R45	2.65941	0.00000	0.00000	0.00000	0.00000	2.65941
R46	2.04808	0.00000	0.00000	0.00000	0.00000	2.04808
R47	3.38293	-0.00001	0.00001	-0.00005	-0.00004	3.38289
R48	2.67746	0.00000	-0.00001	0.00004	0.00002	2.67748
R49	2.74466	0.00000	0.00000	-0.00001	-0.00001	2.74466
R50	2.60548	-0.00001	0.00001	-0.00003	-0.00002	2.60546
R51	2.04698	0.00000	0.00000	0.00000	0.00000	2.04698
R52	2.79652	0.00000	0.00000	0.00000	0.00000	2.79652
R53	2.77026	0.00000	-0.00001	0.00003	0.00002	2.77027
R54	2.79417	0.00000	0.00000	-0.00001	-0.00001	2.79417
R55	2.31722	-0.00001	0.00001	-0.00003	-0.00002	2.31720
R56	2.81040	0.00000	0.00000	0.00000	-0.00001	2.81039
R57	2.61637	0.00000	-0.00001	0.00003	0.00002	2.61639
R58	2.65854	-0.00002	0.00001	-0.00004	-0.00004	2.65850
R59	2.62137	0.00000	-0.00001	0.00003	0.00002	2.62140
R60	2.64464	0.00001	0.00000	0.00003	0.00002	2.64466
R61	2.63856	-0.00001	0.00001	-0.00003	-0.00003	2.63853
R62	2.05071	0.00000	0.00000	0.00000	0.00000	2.05071
R63	2.64334	-0.00002	0.00001	-0.00004	-0.00003	2.64330
R64	2.04221	0.00000	0.00001	-0.00002	-0.00001	2.04220
R65	2.64620	0.00000	0.00000	0.00002	0.00002	2.64622
R66	2.05152	0.00000	0.00000	0.00000	0.00000	2.05152
R67	2.05163	0.00000	0.00000	0.00000	0.00000	2.05163
R68	2.69997	0.00000	0.00000	-0.00001	-0.00001	2.69996
R69	2.69934	0.00001	0.00000	0.00000	0.00000	2.69934
R70	2.20274	0.00000	0.00000	0.00000	0.00000	2.20274
R71	2.20159	0.00000	0.00000	0.00000	0.00000	2.20159
R72	2.69935	0.00000	0.00000	0.00001	0.00001	2.69936
R73	2.69997	0.00000	0.00000	-0.00001	0.00000	2.69997
R74	2.20159	0.00000	0.00000	0.00000	0.00000	2.20159
R75	2.20274	0.00000	0.00000	0.00000	0.00000	2.20274
R76	2.06409	0.00000	0.00000	0.00001	0.00000	2.06410
R77	2.06992	0.00000	0.00000	0.00000	0.00000	2.06992
R78	2.06310	0.00000	0.00000	-0.00001	0.00000	2.06310
R79	2.06992	0.00000	0.00000	0.00000	0.00000	2.06992
R80	2.06417	0.00000	0.00000	0.00000	-0.00001	2.06416
R81	2.06304	0.00000	0.00000	0.00001	0.00001	2.06305
A1	2.07607	0.00000	0.00000	0.00000	0.00000	2.07607
A2	1.89866	0.00000	0.00000	0.00000	0.00000	1.89866
A3	2.30845	0.00000	0.00000	0.00000	0.00000	2.30846
A4	2.14256	0.00000	0.00000	0.00000	0.00000	2.14256
A5	1.91161	0.00000	0.00000	0.00001	0.00001	1.91162
A6	2.22901	0.00000	0.00000	-0.00001	-0.00001	2.22900
A7	2.05914	0.00000	0.00000	0.00000	0.00000	2.05914

A8	2.08923	0.00000	0.00000	0.00001	0.00000	2.08924
A9	2.13481	0.00000	0.00000	0.00000	0.00000	2.13481
A10	2.09525	0.00000	0.00000	0.00000	0.00000	2.09525
A11	2.09774	0.00000	0.00000	0.00000	0.00000	2.09774
A12	2.09020	0.00000	0.00000	-0.00001	-0.00001	2.09019
A13	2.12482	0.00000	0.00000	0.00000	0.00000	2.12482
A14	2.08481	0.00000	0.00000	-0.00002	-0.00001	2.08480
A15	2.07356	0.00000	0.00000	0.00002	0.00002	2.07357
A16	2.06854	0.00000	0.00000	0.00000	0.00000	2.06854
A17	2.13138	0.00000	0.00000	-0.00002	-0.00002	2.13136
A18	2.08327	0.00000	0.00000	0.00002	0.00001	2.08328
A19	1.87050	0.00000	0.00000	-0.00001	0.00000	1.87049
A20	2.17476	0.00000	0.00000	-0.00002	-0.00002	2.17475
A21	2.23792	0.00000	-0.00001	0.00003	0.00002	2.23794
A22	1.86277	0.00000	0.00000	-0.00001	0.00000	1.86277
A23	2.19408	0.00000	0.00000	0.00000	0.00000	2.19408
A24	2.22633	0.00000	0.00000	0.00001	0.00000	2.22633
A25	1.88123	0.00000	0.00000	0.00001	0.00000	1.88124
A26	2.20874	-0.00001	0.00001	-0.00007	-0.00006	2.20869
A27	2.19321	0.00001	-0.00001	0.00006	0.00005	2.19326
A28	2.34400	0.00001	-0.00001	0.00006	0.00005	2.34405
A29	2.01749	0.00000	0.00001	-0.00003	-0.00003	2.01746
A30	1.92170	-0.00001	0.00000	-0.00003	-0.00002	1.92168
A31	2.24955	-0.00002	0.00002	-0.00010	-0.00008	2.24947
A32	2.08340	0.00001	-0.00001	0.00007	0.00006	2.08346
A33	1.95023	0.00001	0.00000	0.00003	0.00002	1.95026
A34	1.95866	-0.00001	0.00001	-0.00005	-0.00004	1.95862
A35	1.85752	-0.00001	0.00000	0.00000	-0.00001	1.85751
A36	2.46701	0.00001	-0.00001	0.00005	0.00005	2.46706
A37	1.98426	0.00000	0.00000	0.00002	0.00002	1.98428
A38	1.91726	0.00000	0.00000	-0.00001	-0.00001	1.91725
A39	2.38164	0.00000	0.00000	-0.00001	-0.00001	2.38163
A40	1.57199	0.00000	-0.00001	0.00002	0.00002	1.57201
A41	1.95961	0.00000	0.00000	-0.00002	-0.00002	1.95959
A42	2.12541	0.00000	0.00000	0.00002	0.00002	2.12542
A43	2.19816	0.00000	0.00000	0.00000	0.00000	2.19817
A44	1.86678	0.00000	0.00001	0.00000	0.00000	1.86679
A45	2.45192	0.00000	-0.00001	0.00002	0.00001	2.45192
A46	1.96447	0.00000	0.00001	-0.00001	-0.00001	1.96446
A47	1.92131	0.00000	0.00000	-0.00001	-0.00001	1.92130
A48	1.97082	0.00000	0.00000	-0.00002	-0.00002	1.97080
A49	2.39102	0.00000	0.00000	0.00002	0.00003	2.39104
A50	1.86167	0.00000	-0.00001	0.00003	0.00002	1.86169
A51	2.20624	-0.00001	-0.00001	-0.00006	-0.00008	2.20616
A52	2.21003	0.00001	0.00002	0.00003	0.00005	2.21007
A53	1.56130	0.00000	0.00000	0.00002	0.00001	1.56131
A54	1.56128	0.00000	-0.00001	0.00002	0.00001	1.56129
A55	1.98279	0.00000	0.00000	0.00001	0.00000	1.98280
A56	2.35506	-0.00001	0.00000	-0.00002	-0.00002	2.35504
A57	1.94533	0.00000	0.00000	0.00002	0.00002	1.94535
A58	2.35497	0.00000	0.00000	0.00001	0.00001	2.35497
A59	1.94535	0.00000	0.00000	0.00001	0.00001	1.94536
A60	1.98287	0.00000	0.00000	-0.00002	-0.00002	1.98285
A61	1.97075	0.00000	0.00000	-0.00001	-0.00001	1.97075
A62	2.39114	0.00000	0.00000	0.00000	0.00000	2.39114
A63	1.92125	0.00000	0.00000	0.00001	0.00000	1.92126
A64	1.96450	0.00000	0.00000	-0.00001	0.00000	1.96450
A65	2.45183	0.00000	-0.00001	0.00002	0.00001	2.45184
A66	1.86683	0.00000	0.00000	-0.00001	-0.00001	1.86683
A67	1.85747	0.00000	0.00000	0.00001	0.00001	1.85748

A68	2.46710	0.00000	0.00000	0.00001	0.00001	2.46711
A69	1.95861	0.00000	0.00000	-0.00002	-0.00001	1.95860
A70	1.98430	0.00000	0.00000	0.00001	0.00001	1.98431
A71	1.91728	0.00000	0.00000	0.00000	0.00000	1.91728
A72	2.38159	0.00000	0.00000	-0.00001	-0.00001	2.38157
A73	1.95960	0.00000	0.00000	-0.00002	-0.00002	1.95958
A74	2.19815	0.00000	0.00000	0.00000	0.00000	2.19815
A75	2.12542	0.00000	0.00000	0.00002	0.00002	2.12544
A76	1.95023	0.00001	0.00000	0.00002	0.00002	1.95025
A77	2.08345	0.00001	-0.00001	0.00005	0.00004	2.08349
A78	2.24951	-0.00001	0.00001	-0.00007	-0.00006	2.24945
A79	1.57201	0.00000	0.00000	0.00001	0.00001	1.57202
A80	1.86171	0.00000	0.00000	-0.00002	-0.00001	1.86170
A81	2.21043	0.00000	0.00002	-0.00004	-0.00001	2.21041
A82	2.20578	0.00000	-0.00002	0.00003	0.00001	2.20580
A83	2.34405	-0.00001	0.00001	-0.00002	-0.00001	2.34404
A84	1.92168	0.00000	-0.00001	0.00001	0.00000	1.92168
A85	2.01746	0.00000	0.00000	0.00001	0.00000	2.01746
A86	2.19323	0.00000	0.00000	0.00001	0.00001	2.19325
A87	2.20872	0.00000	0.00000	-0.00001	-0.00001	2.20870
A88	1.88123	0.00000	0.00000	0.00000	0.00000	1.88123
A89	1.86279	0.00000	0.00000	-0.00001	-0.00001	1.86278
A90	2.22633	0.00000	0.00000	-0.00001	0.00000	2.22632
A91	2.19407	0.00001	0.00000	0.00002	0.00001	2.19409
A92	1.87050	0.00000	0.00001	-0.00002	-0.00001	1.87049
A93	2.23794	0.00000	0.00000	0.00001	0.00001	2.23795
A94	2.17474	0.00000	0.00000	0.00000	0.00000	2.17474
A95	1.91160	0.00000	0.00000	0.00002	0.00002	1.91161
A96	2.22902	0.00000	0.00000	-0.00002	-0.00001	2.22901
A97	2.14257	0.00000	0.00000	0.00000	0.00000	2.14256
A98	1.89866	0.00000	0.00000	0.00001	0.00001	1.89866
A99	2.30848	0.00000	0.00000	-0.00002	-0.00002	2.30846
A100	2.07605	0.00000	0.00000	0.00001	0.00001	2.07606
A101	2.05914	0.00000	0.00000	-0.00001	-0.00001	2.05914
A102	2.08924	0.00000	0.00000	0.00000	0.00000	2.08924
A103	2.13480	0.00000	0.00000	0.00001	0.00001	2.13481
A104	2.06855	0.00000	0.00000	-0.00001	-0.00001	2.06854
A105	2.13139	0.00000	0.00000	-0.00003	-0.00002	2.13137
A106	2.08325	0.00000	-0.00001	0.00004	0.00003	2.08328
A107	2.09524	0.00000	0.00000	0.00001	0.00001	2.09525
A108	2.09773	0.00000	0.00000	0.00001	0.00001	2.09774
A109	2.09022	0.00000	0.00000	-0.00002	-0.00002	2.09020
A110	2.12482	0.00000	0.00000	0.00000	0.00000	2.12482
A111	2.07353	0.00000	-0.00001	0.00004	0.00003	2.07356
A112	2.08483	0.00000	0.00001	-0.00004	-0.00003	2.08480
A113	2.16685	0.00001	-0.00001	0.00004	0.00004	2.16689
A114	2.15623	-0.00001	0.00000	-0.00002	-0.00002	2.15620
A115	1.96010	0.00000	0.00001	-0.00002	-0.00001	1.96009
A116	2.15622	0.00000	0.00000	-0.00002	-0.00001	2.15620
A117	2.16685	0.00001	-0.00001	0.00005	0.00004	2.16689
A118	1.96012	0.00000	0.00001	-0.00003	-0.00002	1.96009
A119	1.91275	0.00000	-0.00001	0.00002	0.00002	1.91277
A120	1.94885	0.00000	0.00000	-0.00002	-0.00001	1.94883
A121	1.90443	0.00000	0.00001	0.00000	0.00001	1.90444
A122	1.90615	0.00000	0.00000	0.00000	0.00000	1.90615
A123	1.88655	0.00000	0.00000	-0.00001	-0.00001	1.88654
A124	1.90404	0.00000	0.00000	-0.00001	0.00000	1.90404
A125	1.94884	0.00000	0.00000	0.00000	0.00000	1.94884
A126	1.91286	0.00000	-0.00001	0.00002	0.00001	1.91287
A127	1.90433	0.00000	0.00000	0.00003	0.00003	1.90436

A128	1.90620	0.00000	0.00000	-0.00002	-0.00002	1.90618
A129	1.90397	0.00000	0.00001	-0.00002	-0.00001	1.90396
A130	1.88659	0.00000	0.00000	-0.00002	-0.00001	1.88657
A131	3.16685	0.00000	-0.00002	0.00006	0.00003	3.16688
A132	3.17959	0.00000	-0.00001	-0.00007	-0.00007	3.17952
A133	3.17951	0.00000	0.00002	-0.00006	-0.00004	3.17948
A134	3.16676	0.00001	0.00000	0.00005	0.00005	3.16682
A135	3.14148	0.00000	0.00000	0.00001	0.00001	3.14150
A136	3.14163	0.00000	0.00000	0.00000	0.00000	3.14162
A137	3.14153	0.00000	0.00000	0.00003	0.00003	3.14156
A138	3.14164	-0.00001	-0.00003	0.00001	-0.00002	3.14162
D1	0.00020	0.00000	0.00001	-0.00003	-0.00002	0.00018
D2	-3.14095	0.00000	0.00001	-0.00005	-0.00004	-3.14099
D3	-3.14144	0.00000	0.00001	-0.00006	-0.00005	-3.14149
D4	0.00059	0.00000	0.00001	-0.00007	-0.00007	0.00053
D5	-0.00003	0.00000	-0.00001	0.00001	0.00000	-0.00003
D6	3.14134	0.00000	-0.00001	0.00003	0.00003	3.14137
D7	-3.14156	0.00000	-0.00001	0.00005	0.00004	-3.14152
D8	-0.00018	0.00000	-0.00001	0.00007	0.00006	-0.00012
D9	-0.00165	0.00000	-0.00005	0.00024	0.00019	-0.00146
D10	3.13891	0.00000	-0.00002	0.00043	0.00041	3.13932
D11	3.13988	0.00000	-0.00005	0.00021	0.00015	3.14004
D12	-0.00274	0.00000	-0.00002	0.00039	0.00038	-0.00236
D13	-0.00020	0.00000	0.00000	0.00002	0.00002	-0.00018
D14	3.14152	0.00000	-0.00001	0.00003	0.00002	3.14154
D15	3.14087	0.00000	0.00000	0.00004	0.00004	3.14091
D16	-0.00060	0.00000	0.00000	0.00005	0.00004	-0.00055
D17	0.00068	0.00000	0.00004	-0.00012	-0.00008	0.00060
D18	-3.14124	0.00000	0.00008	-0.00024	-0.00016	-3.14140
D19	-3.14044	0.00000	0.00004	-0.00014	-0.00010	-3.14054
D20	0.00081	0.00000	0.00008	-0.00026	-0.00018	0.00064
D21	0.00003	0.00000	-0.00001	0.00001	0.00000	0.00003
D22	-3.14149	0.00000	0.00000	0.00000	0.00000	-3.14150
D23	3.14149	0.00000	0.00000	0.00000	0.00000	3.14149
D24	-0.00003	0.00000	0.00000	-0.00001	-0.00001	-0.00004
D25	0.00014	0.00000	0.00000	-0.00002	-0.00002	0.00012
D26	-3.14146	0.00000	0.00001	-0.00002	-0.00001	-3.14147
D27	-3.14153	0.00000	0.00000	-0.00001	-0.00001	-3.14154
D28	0.00006	0.00000	0.00000	-0.00001	-0.00001	0.00006
D29	-0.00013	0.00000	0.00000	0.00001	0.00002	-0.00012
D30	-3.14152	0.00000	0.00000	-0.00001	-0.00001	-3.14152
D31	3.14146	0.00000	0.00000	0.00001	0.00001	3.14147
D32	0.00008	0.00000	0.00000	-0.00001	-0.00001	0.00007
D33	0.00205	0.00000	0.00008	-0.00031	-0.00023	0.00181
D34	-3.13808	0.00000	0.00021	-0.00011	0.00010	-3.13798
D35	-3.13847	0.00000	0.00004	-0.00051	-0.00047	-3.13893
D36	0.00460	0.00000	0.00017	-0.00031	-0.00013	0.00446
D37	0.00128	0.00000	0.00001	-0.00028	-0.00027	0.00101
D38	-3.13968	-0.00001	-0.00001	-0.00039	-0.00040	-3.14008
D39	-3.14157	0.00000	0.00005	-0.00005	0.00000	-3.14157
D40	0.00065	0.00000	0.00004	-0.00017	-0.00013	0.00052
D41	-0.00170	0.00000	-0.00007	0.00027	0.00019	-0.00150
D42	3.13845	0.00000	-0.00020	0.00007	-0.00013	3.13831
D43	3.14024	0.00000	-0.00011	0.00039	0.00028	3.14052
D44	-0.00281	0.00000	-0.00024	0.00019	-0.00005	-0.00286
D45	-3.14145	0.00000	-0.00019	0.00008	-0.00010	-3.14155
D46	0.00022	0.00000	-0.00014	-0.00018	-0.00033	-0.00011
D47	0.00186	0.00000	-0.00003	0.00032	0.00029	0.00215
D48	-3.13966	0.00000	0.00001	0.00005	0.00006	-3.13959
D49	-0.00164	0.00000	0.00016	-0.00044	-0.00028	-0.00191

D50	3.14118	0.00000	0.00017	-0.00049	-0.00032	3.14086
D51	3.13988	0.00000	0.00013	-0.00019	-0.00006	3.13982
D52	-0.00048	0.00000	0.00013	-0.00024	-0.00011	-0.00059
D53	-3.13779	0.00000	0.00001	-0.00004	-0.00003	-3.13782
D54	0.00265	0.00000	0.00000	0.00001	0.00001	0.00267
D55	3.14152	0.00000	-0.00001	0.00002	0.00001	3.14153
D56	0.00263	0.00000	-0.00002	0.00010	0.00009	0.00271
D57	0.00096	0.00000	0.00000	-0.00002	-0.00003	0.00093
D58	-3.13794	0.00000	-0.00001	0.00006	0.00005	-3.13789
D59	0.00731	0.00000	0.00000	-0.00002	-0.00002	0.00730
D60	-3.12807	0.00000	0.00004	-0.00007	-0.00004	-3.12811
D61	-3.13525	0.00000	0.00002	0.00003	0.00004	-3.13520
D62	0.01255	0.00000	0.00005	-0.00003	0.00002	0.01257
D63	-0.00553	0.00000	0.00000	0.00000	0.00000	-0.00553
D64	3.13755	0.00000	-0.00002	-0.00007	-0.00009	3.13746
D65	-0.00020	0.00000	0.00002	-0.00002	0.00000	-0.00020
D66	-3.13395	0.00000	-0.00011	0.00006	-0.00005	-3.13400
D67	3.13996	0.00000	0.00004	0.00005	0.00009	3.14005
D68	0.00621	0.00000	-0.00009	0.00013	0.00004	0.00625
D69	-0.00524	0.00000	0.00000	0.00003	0.00003	-0.00521
D70	3.13352	0.00000	0.00001	-0.00006	-0.00005	3.13347
D71	3.12788	0.00000	-0.00004	0.00010	0.00006	3.12794
D72	-0.01655	0.00000	-0.00004	0.00002	-0.00002	-0.01657
D73	-0.02002	0.00000	-0.00010	0.00006	-0.00003	-0.02005
D74	-3.05715	0.00000	-0.00009	0.00017	0.00008	-3.05707
D75	3.12982	0.00000	-0.00005	-0.00001	-0.00006	3.12976
D76	0.09269	0.00000	-0.00005	0.00010	0.00005	0.09274
D77	-0.01234	0.00000	-0.00008	0.00006	-0.00002	-0.01236
D78	3.13720	0.00000	0.00004	0.00008	0.00012	3.13733
D79	3.12385	0.00000	0.00001	0.00000	0.00001	3.12387
D80	-0.00979	0.00000	0.00012	0.00003	0.00015	-0.00964
D81	-3.14088	0.00000	-0.00002	-0.00021	-0.00024	-3.14112
D82	0.00883	-0.00001	-0.00015	-0.00013	-0.00028	0.00854
D83	0.01991	0.00000	0.00011	-0.00007	0.00003	0.01994
D84	3.05675	0.00000	0.00010	-0.00019	-0.00009	3.05666
D85	-3.13242	0.00000	-0.00005	-0.00011	-0.00016	-3.13258
D86	-0.09558	0.00000	-0.00006	-0.00022	-0.00028	-0.09587
D87	-3.13448	0.00000	-0.00011	0.00003	-0.00008	-3.13456
D88	0.00519	0.00000	-0.00001	0.00012	0.00012	0.00530
D89	0.01806	0.00000	0.00005	0.00007	0.00011	0.01817
D90	-3.12546	0.00001	0.00015	0.00016	0.00031	-3.12515
D91	1.55397	0.00000	-0.00031	-0.00031	-0.00062	1.55335
D92	-2.61468	0.00000	-0.00032	-0.00032	-0.00064	-2.61532
D93	-0.55203	0.00000	-0.00032	-0.00031	-0.00063	-0.55266
D94	-1.46283	0.00000	-0.00030	-0.00018	-0.00048	-1.46331
D95	0.65170	0.00000	-0.00030	-0.00019	-0.00049	0.65121
D96	2.71436	0.00000	-0.00031	-0.00018	-0.00049	2.71387
D97	-0.00598	0.00001	0.00015	0.00020	0.00036	-0.00562
D98	3.13746	0.00001	0.00013	0.00009	0.00022	3.13768
D99	-3.13801	0.00001	0.00015	0.00013	0.00028	-3.13773
D100	0.00554	0.00000	0.00004	0.00004	0.00008	0.00561
D101	-0.00842	0.00000	-0.00005	0.00000	-0.00005	-0.00847
D102	3.14124	0.00000	-0.00007	-0.00027	-0.00034	3.14090
D103	0.00162	-0.00001	-0.00011	-0.00023	-0.00034	0.00129
D104	-3.14146	-0.00001	-0.00003	-0.00015	-0.00018	3.14155
D105	-3.14137	-0.00001	-0.00010	-0.00014	-0.00024	3.14158
D106	-0.00126	0.00000	-0.00001	-0.00007	-0.00008	-0.00135
D107	3.13455	0.00000	-0.00001	0.00018	0.00018	3.13473
D108	-0.01823	0.00000	-0.00004	0.00001	-0.00003	-0.01826
D109	-0.00523	0.00000	-0.00003	0.00007	0.00004	-0.00519

D110	3.12518	0.00000	-0.00006	-0.00010	-0.00016	3.12502
D111	0.00950	0.00000	0.00006	-0.00004	0.00001	0.00951
D112	-3.13746	0.00000	0.00007	0.00014	0.00021	-3.13725
D113	-3.12397	0.00001	0.00008	0.00008	0.00016	-3.12381
D114	0.01226	0.00001	0.00009	0.00026	0.00035	0.01261
D115	3.13272	0.00000	-0.00008	-0.00018	-0.00026	3.13246
D116	0.09610	0.00000	-0.00012	0.00002	-0.00011	0.09600
D117	-0.01984	-0.00001	-0.00011	-0.00035	-0.00046	-0.02030
D118	-3.05646	-0.00001	-0.00016	-0.00015	-0.00030	-3.05676
D119	3.13407	0.00000	-0.00002	0.00020	0.00018	3.13425
D120	-0.00604	0.00000	-0.00006	0.00007	0.00000	-0.00604
D121	0.00026	0.00000	-0.00004	-0.00006	-0.00010	0.00016
D122	-3.13985	0.00000	-0.00008	-0.00020	-0.00028	-3.14013
D123	3.13524	0.00000	-0.00002	-0.00008	-0.00010	3.13514
D124	-0.01257	0.00000	-0.00003	-0.00015	-0.00018	-0.01275
D125	-0.00735	0.00000	0.00001	0.00000	0.00002	-0.00733
D126	3.12802	0.00000	0.00000	-0.00006	-0.00006	3.12796
D127	-3.13768	0.00000	0.00004	0.00031	0.00035	-3.13733
D128	0.00545	0.00000	-0.00001	0.00018	0.00016	0.00562
D129	0.00540	0.00000	-0.00001	-0.00025	-0.00025	0.00515
D130	-3.13346	0.00000	-0.00001	0.00004	0.00003	-3.13342
D131	-3.12769	0.00000	0.00002	-0.00016	-0.00015	-3.12784
D132	0.01663	0.00000	0.00001	0.00013	0.00014	0.01677
D133	0.01999	0.00001	0.00009	0.00030	0.00040	0.02038
D134	3.05697	0.00000	0.00014	0.00010	0.00024	3.05721
D135	-3.12988	0.00000	0.00007	0.00022	0.00029	-3.12958
D136	-0.09289	0.00000	0.00012	0.00002	0.00013	-0.09276
D137	-0.00117	0.00001	0.00000	0.00038	0.00037	-0.00080
D138	-3.14157	0.00000	0.00000	0.00014	0.00013	-3.14144
D139	3.13782	0.00000	0.00000	0.00010	0.00010	3.13792
D140	-0.00258	0.00000	0.00000	-0.00014	-0.00014	-0.00272
D141	-0.00249	-0.00001	0.00001	-0.00031	-0.00031	-0.00279
D142	3.13777	0.00000	0.00001	-0.00005	-0.00004	3.13773
D143	-3.14143	0.00001	0.00001	0.00037	0.00038	-3.14105
D144	0.00030	0.00000	-0.00003	0.00024	0.00021	0.00051
D145	0.00159	0.00000	0.00001	0.00009	0.00010	0.00168
D146	-3.13986	0.00000	-0.00004	-0.00004	-0.00008	-3.13994
D147	-0.64581	0.00000	0.00040	-0.00073	-0.00033	-0.64615
D148	1.46860	0.00000	0.00039	-0.00072	-0.00033	1.46827
D149	-2.70842	0.00000	0.00041	-0.00074	-0.00034	-2.70876
D150	2.62078	0.00000	0.00035	-0.00049	-0.00014	2.62064
D151	-1.54799	0.00000	0.00034	-0.00048	-0.00014	-1.54813
D152	0.55818	0.00000	0.00035	-0.00050	-0.00015	0.55803
D153	-0.00154	0.00000	-0.00004	-0.00006	-0.00010	-0.00164
D154	-3.14144	0.00000	-0.00003	-0.00007	-0.00010	-3.14153
D155	3.13991	0.00000	0.00000	0.00008	0.00008	3.13999
D156	0.00001	0.00000	0.00002	0.00007	0.00008	0.00009
D157	-3.13863	0.00000	0.00001	0.00001	0.00001	-3.13862
D158	0.00267	0.00000	-0.00001	0.00006	0.00005	0.00271
D159	0.00153	0.00000	0.00000	0.00001	0.00001	0.00155
D160	-3.14036	0.00000	-0.00002	0.00006	0.00004	-3.14031
D161	3.13839	0.00000	0.00000	-0.00005	-0.00006	3.13834
D162	-0.00387	0.00000	-0.00002	-0.00008	-0.00009	-0.00396
D163	-0.00176	0.00000	0.00001	-0.00006	-0.00005	-0.00181
D164	3.13917	0.00000	-0.00001	-0.00008	-0.00009	3.13908
D165	-0.00072	0.00000	-0.00001	0.00004	0.00004	-0.00068
D166	3.14053	0.00000	0.00000	-0.00001	-0.00001	3.14052
D167	3.14116	0.00000	0.00001	-0.00001	0.00000	3.14117
D168	-0.00077	0.00000	0.00002	-0.00006	-0.00004	-0.00081
D169	0.00133	0.00000	-0.00001	0.00009	0.00008	0.00141

D170	-3.14019	0.00000	-0.00002	0.00012	0.00009	-3.14010
D171	-3.13962	0.00000	0.00000	0.00011	0.00011	-3.13951
D172	0.00204	0.00000	-0.00001	0.00014	0.00013	0.00217
D173	-0.00045	0.00000	0.00000	0.00002	0.00002	-0.00043
D174	-3.14159	0.00000	0.00001	0.00003	0.00004	-3.14155
D175	3.14036	0.00000	-0.00002	-0.00001	-0.00003	3.14034
D176	-0.00077	0.00000	-0.00001	0.00001	-0.00001	-0.00078
D177	-0.00037	0.00000	0.00001	-0.00008	-0.00007	-0.00044
D178	3.14116	0.00000	0.00002	-0.00011	-0.00009	3.14108
D179	3.14154	0.00000	0.00001	-0.00003	-0.00003	3.14152
D180	-0.00011	0.00000	0.00001	-0.00005	-0.00004	-0.00015
D181	-3.14107	0.00000	-0.00001	0.00008	0.00007	-3.14100
D182	0.00046	0.00000	-0.00001	0.00004	0.00003	0.00049
D183	0.00014	0.00000	0.00000	0.00002	0.00002	0.00016
D184	-3.14152	0.00000	0.00000	-0.00002	-0.00002	-3.14155
D185	3.14150	0.00000	0.00000	0.00002	0.00002	3.14152
D186	0.00008	0.00000	0.00000	-0.00001	-0.00001	0.00007
D187	-0.00002	0.00000	-0.00001	0.00005	0.00004	0.00002
D188	-3.14144	0.00000	-0.00001	0.00002	0.00001	-3.14142
D189	-0.00004	0.00000	-0.00001	0.00002	0.00001	-0.00003
D190	3.14149	0.00000	-0.00001	0.00003	0.00002	3.14151
D191	-3.14156	0.00000	-0.00001	0.00006	0.00005	-3.14151
D192	-0.00003	0.00000	-0.00001	0.00007	0.00006	0.00003
D193	0.00011	0.00000	0.00000	-0.00002	-0.00001	0.00010
D194	-3.14147	0.00000	0.00000	-0.00002	-0.00002	-3.14148
D195	3.14154	0.00000	0.00000	0.00001	0.00001	3.14155
D196	-0.00004	0.00000	-0.00001	0.00001	0.00001	-0.00004
D197	-0.00008	0.00000	0.00001	-0.00002	-0.00001	-0.00009
D198	3.14150	0.00000	0.00001	-0.00002	-0.00001	3.14149
D199	3.14157	0.00000	0.00001	-0.00003	-0.00003	3.14155
D200	-0.00003	0.00000	0.00001	-0.00003	-0.00002	-0.00006

Item	Value	Threshold	Converged?

Maximum Force	0.000029	0.000450	YES
RMS Force	0.000004	0.000300	YES
Maximum Displacement	0.004072	0.001800	NO
RMS Displacement	0.001108	0.001200	YES

Predicted change in Energy=-4.590940D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group	C1	NOp	1

Largest Abelian subgroup	C1	NOp	1

Largest concise Abelian subgroup	C1	NOp	1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.803362	-0.637248	0.004854
2	6	0	-9.994182	-1.788042	0.002808
3	6	0	-10.516671	-3.073058	0.007291
4	6	0	-11.905624	-3.215430	0.014329
5	6	0	-12.726762	-2.081134	0.016636
6	6	0	-12.194756	-0.787495	0.011916
7	1	0	-9.846058	-3.926230	0.005390
8	1	0	-12.353036	-4.204556	0.018093
9	1	0	-13.805548	-2.203123	0.022236
10	1	0	-12.864264	0.060823	0.013985

11	6	0	-9.927090	0.564362	-0.001326
12	6	0	-8.569950	-1.390783	-0.003986
13	6	0	-8.540422	0.088777	-0.005209
14	6	0	-7.404460	0.870125	-0.007294
15	6	0	-6.014497	0.595547	-0.011038
16	6	0	-3.644340	-0.183962	-0.010583
17	6	0	-3.778373	1.228647	-0.016710
18	16	0	-5.182078	-0.989277	-0.011989
19	6	0	-5.099637	1.664891	-0.013187
20	6	0	-2.267223	-0.451818	-0.006542
21	6	0	-1.603934	0.797411	-0.010563
22	7	0	-2.523850	1.820833	-0.032894
23	16	0	-1.150986	-1.806964	-0.007043
24	16	0	1.150882	1.806509	0.007965
25	6	0	0.198410	-0.673815	0.002385
26	6	0	-0.198437	0.673305	-0.001538
27	6	0	1.603941	-0.797900	0.011392
28	6	0	2.267154	0.451396	0.007511
29	6	0	3.644267	0.183700	0.011421
30	6	0	3.778413	-1.228910	0.017387
31	6	0	5.099688	-1.665081	0.013640
32	6	0	6.014485	-0.595674	0.011393
33	16	0	5.181947	0.989102	0.012759
34	7	0	2.523970	-1.821219	0.033834
35	6	0	7.404504	-0.870137	0.007306
36	6	0	8.540397	-0.088672	0.004859
37	6	0	8.569759	1.390889	0.004125
38	6	0	9.927122	-0.564099	0.000532
39	6	0	9.993937	1.788321	-0.002890
40	6	0	10.803254	0.637612	-0.005420
41	6	0	10.516277	3.073400	-0.007098
42	6	0	12.194623	0.788026	-0.012655
43	6	0	11.905214	3.215935	-0.014320
44	6	0	12.726480	2.081735	-0.017074
45	6	0	10.384775	-1.870805	0.002337
46	6	0	9.534041	-3.018650	0.009553
47	6	0	11.769308	-2.222173	-0.002279
48	7	0	8.863877	-3.972361	0.015451
49	7	0	12.886858	-2.551359	-0.005955
50	6	0	-10.384581	1.871120	-0.003822
51	6	0	-11.769081	2.222662	0.000492
52	6	0	-9.533700	3.018856	-0.011553
53	7	0	-12.886604	2.551941	0.003912
54	7	0	-8.863354	3.972437	-0.017851
55	8	0	-7.613026	-2.157513	-0.007377
56	8	0	7.612742	2.157500	0.008168
57	6	0	2.241394	-3.243148	-0.054277
58	1	0	1.319514	-3.467620	0.486843
59	1	0	2.137929	-3.571100	-1.094249
60	1	0	3.054647	-3.799121	0.416278
61	6	0	-2.240627	3.242627	0.055290
62	1	0	-2.131973	3.569491	1.095077
63	1	0	-1.321434	3.467650	-0.490226
64	1	0	-3.056206	3.799121	-0.410535
65	1	0	5.428761	-2.697705	0.009826
66	1	0	12.864234	-0.060208	-0.015043
67	1	0	13.805252	2.203842	-0.022794
68	1	0	12.352508	4.205115	-0.017864
69	1	0	9.845567	3.926497	-0.004829
70	1	0	7.572737	-1.940208	0.005922

71	1	0	-7.572593	1.940211	-0.005982
72	1	0	-5.428669	2.697528	-0.009558

Rotational constants (GHZ): 0.1750165 0.0104040 0.0098216

Standard basis: 6-31G(d,p) (6D, 7F)

There are 916 symmetry adapted cartesian basis functions of A symmetry.

There are 916 symmetry adapted basis functions of A symmetry.

916 basis functions, 1734 primitive gaussians, 916 cartesian basis functions

196 alpha electrons 196 beta electrons

nuclear repulsion energy 6569.7762367142 Hartrees.

NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T

Big=T

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

Nuclear repulsion after empirical dispersion term = 6569.6913201836 Hartrees.

One-electron integrals computed using PRISM.

NBasis= 916 RedAO= T EigKep= 3.24D-04 NBF= 916

NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916

Initial guess from the checkpoint file: "PBDB.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3683.02012183 A.U. after 7 cycles

NFock= 7 Conv=0.50D-08 -V/T= 2.0068

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1

NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-0.000000742	-0.000001084	-0.000001697
2	6	-0.000003184	0.000000420	-0.000001723
3	6	0.000000535	0.000000216	-0.000001346
4	6	0.000001049	0.000000510	0.000002348
5	6	-0.000001354	-0.000002966	-0.000000999
6	6	0.000001597	0.000002476	0.000000878
7	1	-0.000000107	-0.000001063	0.000000127
8	1	-0.000000882	-0.000000547	-0.000000244
9	1	-0.000000762	-0.000000612	-0.000000176
10	1	-0.000001414	-0.000000113	-0.000000174
11	6	-0.000007803	-0.000000426	0.000000738
12	6	-0.000001530	0.000004331	-0.000000989
13	6	0.000006993	0.000007397	-0.000015177
14	6	-0.000017498	-0.000000638	0.000003594
15	6	0.000009749	-0.000016410	0.000008348
16	6	0.000017320	0.000006385	0.000013664
17	6	-0.000000880	-0.000011745	-0.000009647
18	16	0.000001662	0.000003998	0.000004269
19	6	0.000010437	-0.000002292	-0.000003635
20	6	-0.000013092	-0.000000109	-0.000005162
21	6	-0.000000545	-0.000003251	-0.000005491
22	7	0.000007561	0.000004681	0.000011900
23	16	-0.000001142	0.000000721	0.000002200

24	16	0.000000404	-0.000002421	-0.000000701
25	6	0.000013272	-0.000007117	0.000004158
26	6	-0.000003146	0.000001873	0.000001780
27	6	-0.000001086	0.000012191	-0.000028980
28	6	-0.000017230	0.000007685	0.000003937
29	6	0.000002116	-0.000000264	0.000010626
30	6	0.000014229	-0.000000029	-0.000019597
31	6	-0.000004315	-0.000005764	0.000010394
32	6	0.000015332	0.000006708	-0.000007041
33	16	-0.000005256	-0.000005562	0.000004620
34	7	-0.000009795	-0.000003878	0.000015951
35	6	-0.000004514	0.000004692	-0.000007817
36	6	0.000001500	0.000000889	0.000003213
37	6	0.000003219	-0.000002264	-0.000001562
38	6	0.000002612	0.000001837	0.000006591
39	6	0.000007298	-0.000000572	0.000006261
40	6	-0.000004808	0.000000410	-0.000006040
41	6	0.000001868	0.000001190	0.000001340
42	6	0.000000141	-0.000009551	-0.000002347
43	6	-0.000002415	0.000000728	-0.000003383
44	6	0.000001953	0.000007231	0.000003671
45	6	-0.000012037	-0.000002850	-0.000010040
46	6	0.000001318	0.000004933	-0.000000042
47	6	0.000005724	-0.000003915	0.000004410
48	7	-0.000002144	0.000000629	-0.000000584
49	7	0.000000138	0.000002156	0.000000266
50	6	0.000003270	0.000001422	0.000002503
51	6	-0.000001735	0.000004162	0.000000523
52	6	0.000003186	-0.000002677	-0.000001480
53	7	0.000000455	-0.000004025	-0.000000378
54	7	-0.000001334	-0.000000597	0.000000073
55	8	-0.000000441	-0.000002899	0.000004873
56	8	-0.000004179	-0.000000136	-0.000001156
57	6	-0.000004622	0.000003418	0.000005010
58	1	0.000000601	-0.000000763	-0.000001825
59	1	-0.000000423	0.000002107	-0.000000574
60	1	-0.000001503	-0.000002025	0.000001081
61	6	-0.000006000	-0.000006249	-0.000006307
62	1	-0.000000551	0.000002469	0.000000745
63	1	0.000002332	0.000002730	-0.000001333
64	1	-0.000001369	0.000000161	0.000003424
65	1	-0.000000366	-0.000000485	0.000000999
66	1	0.000001474	0.000000554	0.000001667
67	1	0.000000657	0.000000098	-0.000000114
68	1	0.000001062	0.000000373	0.000000846
69	1	0.000000344	0.000001541	0.000000061
70	1	0.000000194	0.000002731	0.000002833
71	1	-0.000001291	-0.000001414	-0.000000722
72	1	-0.000000104	0.000000664	-0.000001434

Cartesian Forces: Max 0.000028980 RMS 0.000005757

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.000022057 RMS 0.000003233

Search for a local minimum.

Step number 34 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 16 18 17 19 20

21 22 23 24 25

26 27 28 29 30

31 32 33 34

DE= -2.75D-08 DEPred=-4.59D-08 R= 5.98D-01

Trust test= 5.98D-01 RLast= 2.65D-03 DXMaxT set to 1.43D-01

ITU= 0 0 0 0 0 0 1 -1 1 -1 1 -1 1 1 -1 0 -1 0 -1 1

ITU= 1 1 1 1 1 0 0 0 1 0 0 0 1 0

Eigenvalues --- 0.00073 0.00248 0.00268 0.00297 0.00393

Eigenvalues --- 0.00433 0.00479 0.00501 0.00521 0.00551

Eigenvalues --- 0.00586 0.00609 0.00631 0.00664 0.00693

Eigenvalues --- 0.00714 0.00743 0.00751 0.00765 0.00776

Eigenvalues --- 0.00779 0.00786 0.00808 0.00879 0.01005

Eigenvalues --- 0.01027 0.01095 0.01125 0.01134 0.01174

Eigenvalues --- 0.01290 0.01314 0.01330 0.01358 0.01380

Eigenvalues --- 0.01425 0.01457 0.01508 0.01594 0.01636

Eigenvalues --- 0.01655 0.01743 0.01760 0.01794 0.01924

Eigenvalues --- 0.01952 0.02006 0.02019 0.02035 0.02062

Eigenvalues --- 0.02078 0.02179 0.02357 0.02782 0.02810

Eigenvalues --- 0.02925 0.03022 0.03785 0.03926 0.03971

Eigenvalues --- 0.04100 0.04831 0.04839 0.04913 0.05023

Eigenvalues --- 0.05089 0.05178 0.05302 0.05482 0.07043

Eigenvalues --- 0.07226 0.07396 0.07577 0.15254 0.15791

Eigenvalues --- 0.15895 0.15984 0.15988 0.15998 0.16000

Eigenvalues --- 0.16000 0.16000 0.16000 0.16001 0.16009

Eigenvalues --- 0.16013 0.16025 0.16030 0.16084 0.16094

Eigenvalues --- 0.16124 0.19078 0.19420 0.19892 0.20230

Eigenvalues --- 0.20759 0.21288 0.21658 0.21900 0.22003

Eigenvalues --- 0.22029 0.22453 0.22602 0.22610 0.22638

Eigenvalues --- 0.22868 0.22890 0.23006 0.23136 0.23275

Eigenvalues --- 0.23402 0.23437 0.23588 0.23768 0.23988

Eigenvalues --- 0.24257 0.24271 0.24312 0.24440 0.24519

Eigenvalues --- 0.24568 0.24664 0.24749 0.24850 0.24874

Eigenvalues --- 0.24934 0.24947 0.24969 0.24986 0.24991

Eigenvalues --- 0.24994 0.24997 0.24999 0.24999 0.25000

Eigenvalues --- 0.25000 0.25001 0.25007 0.25061 0.25102

Eigenvalues --- 0.25516 0.25665 0.25968 0.26187 0.26489

Eigenvalues --- 0.26563 0.26789 0.26927 0.27227 0.27459

Eigenvalues --- 0.27726 0.27850 0.28407 0.28527 0.28868

Eigenvalues --- 0.29500 0.29873 0.30308 0.31797 0.32688

Eigenvalues --- 0.33854 0.35456 0.35651 0.36276 0.36336

Eigenvalues --- 0.36455 0.36476 0.36637 0.36823 0.36849

Eigenvalues --- 0.36998 0.37061 0.37087 0.37195 0.37248

Eigenvalues --- 0.37257 0.37417 0.37542 0.37672 0.37758

Eigenvalues --- 0.38020 0.38916 0.39277 0.40317 0.41280

Eigenvalues --- 0.41730 0.41842 0.42649 0.44342 0.45146

Eigenvalues --- 0.45556 0.46578 0.47089 0.47690 0.47943

Eigenvalues --- 0.49142 0.52253 0.53249 0.54172 0.56077

Eigenvalues --- 0.65451 0.72699 0.76717 0.80600 0.82215

Eigenvalues --- 0.91789 1.25861 1.26356 1.29351 1.35369

En-DIIS/RFO-DIIS IScMMF= 0 using points: 34 33 32 31 30

RFO step: Lambda=-9.82114666D-09.

DidBck=T Rises=F RFO-DIIS coefs: 0.75547 0.29018 -0.02701 -0.03357
0.01493

Iteration 1 RMS(Cart)= 0.00032221 RMS(Int)= 0.00000004

Iteration 2 RMS(Cart)= 0.00000006 RMS(Int)= 0.00000000

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear)	(Quad)	(Total)				
R1	2.65848	0.00000	0.00000	-0.00001	-0.00001	2.65847
R2	2.64467	0.00000	0.00000	0.00001	0.00001	2.64468
R3	2.81040	0.00000	0.00000	0.00001	0.00001	2.81041
R4	2.62140	0.00000	0.00000	0.00001	0.00001	2.62141
R5	2.79417	0.00000	0.00000	0.00001	0.00001	2.79418
R6	2.63853	0.00000	0.00000	-0.00001	-0.00001	2.63852
R7	2.05070	0.00000	0.00000	0.00000	0.00000	2.05070
R8	2.64622	0.00000	0.00000	0.00001	0.00001	2.64623
R9	2.05152	0.00000	0.00000	0.00000	0.00000	2.05152
R10	2.64329	0.00000	0.00000	-0.00001	-0.00001	2.64328
R11	2.05163	0.00000	0.00000	0.00000	0.00000	2.05163
R12	2.04221	0.00000	0.00000	0.00000	0.00000	2.04220
R13	2.77027	0.00000	0.00000	0.00002	0.00002	2.77028
R14	2.61638	0.00000	0.00000	0.00000	0.00000	2.61638
R15	2.79652	0.00000	0.00000	0.00001	0.00000	2.79653
R16	2.31720	0.00000	0.00000	0.00000	0.00000	2.31720
R17	2.60544	0.00001	0.00000	0.00003	0.00002	2.60546
R18	2.67742	0.00002	0.00003	-0.00003	0.00000	2.67741
R19	2.04698	0.00000	0.00000	0.00001	0.00001	2.04699
R20	3.38287	0.00001	0.00001	-0.00002	-0.00002	3.38285
R21	2.65940	0.00000	0.00000	-0.00001	-0.00001	2.65939
R22	2.68146	0.00001	-0.00001	0.00007	0.00005	2.68151
R23	3.28028	0.00000	0.00000	0.00001	0.00001	3.28029
R24	2.65116	-0.00002	0.00001	-0.00004	-0.00003	2.65113
R25	2.62941	-0.00001	0.00001	-0.00001	-0.00001	2.62940
R26	2.62173	-0.00001	0.00000	-0.00001	-0.00001	2.62172
R27	2.04808	0.00000	0.00000	0.00000	0.00000	2.04807
R28	2.67284	0.00000	-0.00001	0.00006	0.00005	2.67288
R29	3.31775	0.00000	0.00000	0.00000	0.00000	3.31775
R30	2.60079	-0.00001	0.00001	-0.00003	-0.00002	2.60076
R31	2.66639	-0.00001	0.00000	0.00000	0.00001	2.66640
R32	2.74465	0.00000	0.00000	0.00000	0.00000	2.74465
R33	3.32988	0.00000	0.00000	-0.00002	-0.00001	3.32987
R34	3.32984	0.00000	0.00000	0.00002	0.00001	3.32985
R35	3.31775	0.00000	0.00000	-0.00001	0.00000	3.31774
R36	2.65386	0.00000	0.00000	-0.00001	-0.00001	2.65385
R37	2.66645	-0.00002	0.00001	-0.00003	-0.00003	2.66643
R38	2.67288	0.00000	0.00000	0.00000	0.00000	2.67288
R39	2.60079	0.00000	0.00001	0.00000	0.00000	2.60079
R40	2.65109	0.00001	0.00001	0.00001	0.00002	2.65111
R41	2.68148	0.00000	0.00000	-0.00001	-0.00001	2.68147
R42	3.28026	0.00000	0.00000	0.00002	0.00002	3.28027
R43	2.62939	0.00000	0.00000	0.00003	0.00003	2.62942
R44	2.62170	0.00000	0.00000	0.00001	0.00001	2.62171
R45	2.65941	-0.00001	0.00000	-0.00001	-0.00001	2.65940
R46	2.04808	0.00000	0.00000	0.00000	0.00000	2.04808
R47	3.38289	0.00000	0.00001	-0.00003	-0.00002	3.38287
R48	2.67748	-0.00001	0.00000	0.00002	0.00002	2.67750
R49	2.74466	0.00000	0.00000	0.00000	0.00000	2.74465
R50	2.60546	0.00000	0.00000	-0.00001	-0.00001	2.60544
R51	2.04698	0.00000	0.00000	0.00000	0.00000	2.04698
R52	2.79652	0.00000	0.00000	0.00001	0.00001	2.79652
R53	2.77027	0.00000	0.00000	0.00001	0.00001	2.77028
R54	2.79417	0.00000	0.00000	0.00000	0.00000	2.79417
R55	2.31720	0.00000	0.00000	-0.00002	-0.00001	2.31719
R56	2.81039	0.00000	0.00000	0.00000	0.00000	2.81039
R57	2.61639	-0.00001	0.00000	0.00000	0.00000	2.61639
R58	2.65850	-0.00001	0.00001	-0.00004	-0.00004	2.65846
R59	2.62140	0.00000	0.00000	0.00002	0.00002	2.62142

R60	2.64466	0.00000	0.00000	0.00003	0.00003	2.64469
R61	2.63853	0.00000	0.00000	-0.00003	-0.00002	2.63851
R62	2.05071	0.00000	0.00000	0.00000	0.00000	2.05070
R63	2.64330	-0.00001	0.00001	-0.00004	-0.00003	2.64327
R64	2.04220	0.00000	0.00000	-0.00001	0.00000	2.04220
R65	2.64622	0.00000	0.00000	0.00003	0.00002	2.64624
R66	2.05152	0.00000	0.00000	0.00000	0.00000	2.05152
R67	2.05163	0.00000	0.00000	0.00000	0.00000	2.05163
R68	2.69996	0.00000	0.00000	0.00000	0.00001	2.69997
R69	2.69934	0.00001	0.00000	0.00002	0.00002	2.69936
R70	2.20274	0.00000	0.00000	0.00000	0.00000	2.20274
R71	2.20159	0.00000	0.00000	0.00000	0.00000	2.20159
R72	2.69936	0.00000	0.00000	0.00002	0.00001	2.69937
R73	2.69997	0.00000	0.00000	0.00001	0.00001	2.69997
R74	2.20159	0.00000	0.00000	0.00000	0.00000	2.20159
R75	2.20274	0.00000	0.00000	0.00000	0.00000	2.20274
R76	2.06410	0.00000	0.00000	0.00000	0.00000	2.06410
R77	2.06992	0.00000	0.00000	0.00000	0.00000	2.06992
R78	2.06310	0.00000	0.00000	0.00000	0.00000	2.06310
R79	2.06992	0.00000	0.00000	0.00000	0.00000	2.06992
R80	2.06416	0.00000	0.00000	-0.00001	-0.00001	2.06416
R81	2.06305	0.00000	0.00000	0.00001	0.00001	2.06305
A1	2.07607	0.00000	0.00000	0.00000	0.00000	2.07607
A2	1.89866	0.00000	0.00000	0.00000	0.00000	1.89866
A3	2.30846	0.00000	0.00000	0.00000	0.00000	2.30846
A4	2.14256	0.00000	0.00000	0.00000	0.00000	2.14256
A5	1.91162	0.00000	0.00000	0.00001	0.00001	1.91163
A6	2.22900	0.00000	0.00000	-0.00001	-0.00001	2.22899
A7	2.05914	0.00000	0.00000	0.00000	0.00000	2.05914
A8	2.08924	0.00000	0.00000	0.00000	0.00000	2.08924
A9	2.13481	0.00000	0.00000	0.00000	0.00000	2.13481
A10	2.09525	0.00000	0.00000	0.00000	0.00000	2.09525
A11	2.09774	0.00000	0.00000	0.00001	0.00000	2.09775
A12	2.09019	0.00000	0.00000	-0.00001	-0.00001	2.09019
A13	2.12482	0.00000	0.00000	0.00000	0.00000	2.12482
A14	2.08480	0.00000	0.00000	-0.00001	-0.00001	2.08479
A15	2.07357	0.00000	0.00000	0.00001	0.00001	2.07358
A16	2.06854	0.00000	0.00000	0.00000	0.00000	2.06854
A17	2.13136	0.00000	0.00000	-0.00001	-0.00001	2.13135
A18	2.08328	0.00000	0.00000	0.00001	0.00001	2.08330
A19	1.87049	0.00000	0.00000	0.00000	0.00000	1.87049
A20	2.17475	0.00000	0.00000	-0.00002	-0.00002	2.17473
A21	2.23794	-0.00001	0.00000	0.00002	0.00002	2.23796
A22	1.86277	0.00000	0.00000	0.00000	0.00000	1.86276
A23	2.19408	0.00000	0.00000	0.00001	0.00001	2.19409
A24	2.22633	0.00000	0.00000	0.00000	0.00000	2.22633
A25	1.88124	0.00000	0.00000	0.00000	0.00000	1.88123
A26	2.20869	0.00000	0.00001	-0.00004	-0.00003	2.20865
A27	2.19326	0.00000	-0.00001	0.00005	0.00004	2.19330
A28	2.34405	0.00000	-0.00001	0.00004	0.00003	2.34408
A29	2.01746	0.00000	0.00000	-0.00002	-0.00002	2.01744
A30	1.92168	0.00000	0.00001	-0.00002	-0.00001	1.92166
A31	2.24947	0.00000	0.00001	-0.00008	-0.00006	2.24940
A32	2.08346	0.00000	-0.00001	0.00006	0.00005	2.08351
A33	1.95026	0.00000	-0.00001	0.00002	0.00002	1.95027
A34	1.95862	0.00000	0.00001	-0.00004	-0.00003	1.95859
A35	1.85751	0.00000	0.00000	-0.00001	-0.00001	1.85750
A36	2.46706	0.00000	-0.00001	0.00005	0.00004	2.46710
A37	1.98428	0.00000	0.00000	0.00002	0.00001	1.98429
A38	1.91725	0.00000	0.00000	0.00000	0.00000	1.91725

A39	2.38163	0.00000	0.00000	-0.00001	-0.00001	2.38162
A40	1.57201	0.00000	0.00000	0.00001	0.00001	1.57202
A41	1.95959	0.00000	0.00001	-0.00001	-0.00001	1.95959
A42	2.12542	0.00000	0.00000	0.00001	0.00001	2.12543
A43	2.19817	0.00000	0.00000	0.00001	0.00000	2.19817
A44	1.86679	0.00000	0.00000	0.00001	0.00001	1.86679
A45	2.45192	-0.00001	0.00000	0.00000	0.00000	2.45192
A46	1.96446	0.00000	0.00000	0.00000	0.00000	1.96445
A47	1.92130	0.00000	0.00000	-0.00001	-0.00001	1.92129
A48	1.97080	0.00000	0.00000	-0.00002	-0.00001	1.97079
A49	2.39104	0.00000	0.00000	0.00002	0.00002	2.39106
A50	1.86169	0.00000	0.00000	0.00001	0.00001	1.86171
A51	2.20616	-0.00001	0.00001	-0.00007	-0.00006	2.20610
A52	2.21007	0.00001	-0.00001	0.00006	0.00005	2.21013
A53	1.56131	0.00000	0.00000	0.00001	0.00000	1.56132
A54	1.56129	-0.00001	0.00000	0.00000	0.00000	1.56128
A55	1.98280	0.00000	0.00000	0.00001	0.00001	1.98281
A56	2.35504	0.00000	0.00000	-0.00002	-0.00002	2.35502
A57	1.94535	0.00000	0.00000	0.00001	0.00001	1.94536
A58	2.35497	0.00000	0.00000	0.00001	0.00000	2.35498
A59	1.94536	0.00000	0.00000	0.00001	0.00001	1.94537
A60	1.98285	0.00000	0.00000	-0.00001	-0.00001	1.98284
A61	1.97075	0.00000	0.00000	0.00000	0.00000	1.97075
A62	2.39114	0.00000	0.00000	-0.00001	-0.00001	2.39113
A63	1.92126	0.00000	0.00000	0.00001	0.00001	1.92126
A64	1.96450	0.00000	0.00000	0.00000	0.00000	1.96450
A65	2.45184	0.00000	0.00000	0.00001	0.00001	2.45185
A66	1.86683	0.00000	0.00000	-0.00001	-0.00001	1.86682
A67	1.85748	0.00000	0.00000	0.00001	0.00001	1.85749
A68	2.46711	0.00000	0.00000	0.00001	0.00001	2.46711
A69	1.95860	0.00000	0.00000	-0.00001	-0.00001	1.95859
A70	1.98431	0.00000	0.00000	0.00001	0.00001	1.98432
A71	1.91728	0.00000	0.00000	0.00000	0.00000	1.91728
A72	2.38157	0.00000	0.00000	-0.00001	-0.00001	2.38157
A73	1.95958	0.00000	0.00000	-0.00002	-0.00002	1.95957
A74	2.19815	0.00000	0.00000	0.00000	0.00000	2.19816
A75	2.12544	0.00000	0.00000	0.00002	0.00001	2.12546
A76	1.95025	0.00000	0.00000	0.00002	0.00001	1.95026
A77	2.08349	0.00000	-0.00001	0.00003	0.00003	2.08352
A78	2.24945	0.00000	0.00001	-0.00005	-0.00004	2.24941
A79	1.57202	0.00000	0.00000	0.00001	0.00001	1.57202
A80	1.86170	0.00000	0.00000	0.00000	0.00000	1.86170
A81	2.21041	0.00000	0.00000	-0.00003	-0.00002	2.21039
A82	2.20580	0.00000	0.00000	0.00002	0.00002	2.20581
A83	2.34404	0.00001	0.00000	0.00000	0.00000	2.34404
A84	1.92168	0.00000	0.00000	0.00000	0.00000	1.92169
A85	2.01746	0.00000	0.00000	0.00000	0.00000	2.01746
A86	2.19325	0.00001	0.00000	0.00002	0.00002	2.19326
A87	2.20870	-0.00001	0.00000	-0.00002	-0.00001	2.20869
A88	1.88123	0.00000	0.00000	0.00000	0.00000	1.88123
A89	1.86278	0.00000	0.00000	-0.00001	-0.00001	1.86276
A90	2.22632	0.00000	0.00000	0.00000	0.00000	2.22632
A91	2.19409	0.00000	0.00000	0.00002	0.00001	2.19410
A92	1.87049	0.00000	0.00000	0.00000	0.00000	1.87049
A93	2.23795	-0.00001	0.00000	0.00000	0.00000	2.23795
A94	2.17474	0.00001	0.00000	0.00001	0.00001	2.17475
A95	1.91161	0.00000	0.00000	0.00002	0.00001	1.91163
A96	2.22901	0.00000	0.00000	-0.00002	-0.00001	2.22899
A97	2.14256	0.00000	0.00000	0.00000	0.00000	2.14256
A98	1.89866	0.00000	0.00000	0.00000	0.00000	1.89866

A99	2.30846	0.00000	0.00000	-0.00001	-0.00001	2.30845
A100	2.07606	0.00000	0.00000	0.00001	0.00001	2.07607
A101	2.05914	0.00000	0.00000	-0.00001	-0.00001	2.05913
A102	2.08924	0.00000	0.00000	0.00000	0.00000	2.08924
A103	2.13481	0.00000	0.00000	0.00001	0.00001	2.13482
A104	2.06854	0.00000	0.00000	-0.00001	-0.00001	2.06853
A105	2.13137	0.00000	0.00000	-0.00002	-0.00002	2.13135
A106	2.08328	0.00000	-0.00001	0.00003	0.00002	2.08330
A107	2.09525	0.00000	0.00000	0.00001	0.00000	2.09525
A108	2.09774	0.00000	0.00000	0.00001	0.00001	2.09775
A109	2.09020	0.00000	0.00000	-0.00002	-0.00002	2.09018
A110	2.12482	0.00000	0.00000	0.00000	0.00000	2.12482
A111	2.07356	0.00000	-0.00001	0.00003	0.00002	2.07359
A112	2.08480	0.00000	0.00001	-0.00003	-0.00002	2.08478
A113	2.16689	-0.00001	-0.00001	0.00003	0.00003	2.16692
A114	2.15620	0.00001	0.00001	-0.00002	-0.00001	2.15619
A115	1.96009	0.00000	0.00000	-0.00001	-0.00002	1.96007
A116	2.15620	0.00000	0.00000	-0.00001	-0.00001	2.15619
A117	2.16689	0.00000	0.00000	0.00004	0.00003	2.16692
A118	1.96009	0.00000	0.00000	-0.00002	-0.00002	1.96007
A119	1.91277	0.00000	0.00000	0.00001	0.00000	1.91277
A120	1.94883	0.00000	0.00000	0.00000	0.00000	1.94884
A121	1.90444	0.00000	0.00000	0.00000	-0.00001	1.90443
A122	1.90615	0.00000	0.00000	0.00000	0.00000	1.90616
A123	1.88654	0.00000	0.00000	0.00000	0.00000	1.88654
A124	1.90404	0.00000	0.00000	0.00000	0.00000	1.90404
A125	1.94884	0.00000	0.00000	-0.00001	0.00000	1.94883
A126	1.91287	0.00000	0.00000	0.00000	0.00000	1.91287
A127	1.90436	0.00000	0.00000	0.00002	0.00001	1.90437
A128	1.90618	0.00000	0.00000	-0.00001	-0.00001	1.90617
A129	1.90396	0.00000	0.00000	0.00001	0.00001	1.90397
A130	1.88657	0.00000	0.00000	-0.00001	-0.00001	1.88657
A131	3.16688	0.00000	0.00000	0.00001	0.00001	3.16689
A132	3.17952	0.00000	0.00003	-0.00003	0.00000	3.17952
A133	3.17948	0.00001	0.00000	0.00003	0.00004	3.17951
A134	3.16682	0.00000	-0.00002	0.00008	0.00007	3.16688
A135	3.14150	0.00000	0.00000	0.00000	0.00000	3.14149
A136	3.14162	0.00000	0.00000	-0.00001	-0.00001	3.14162
A137	3.14156	0.00000	-0.00001	0.00003	0.00002	3.14158
A138	3.14162	0.00000	0.00001	-0.00004	-0.00003	3.14160
D1	0.00018	0.00000	0.00000	-0.00003	-0.00003	0.00015
D2	-3.14099	0.00000	0.00000	-0.00008	-0.00008	-3.14107
D3	-3.14149	0.00000	0.00001	-0.00005	-0.00004	-3.14153
D4	0.00053	0.00000	0.00001	-0.00010	-0.00009	0.00044
D5	-0.00003	0.00000	0.00000	0.00001	0.00001	-0.00002
D6	3.14137	0.00000	0.00000	0.00004	0.00003	3.14140
D7	-3.14152	0.00000	-0.00001	0.00003	0.00002	-3.14150
D8	-0.00012	0.00000	-0.00001	0.00006	0.00005	-0.00007
D9	-0.00146	0.00000	-0.00004	-0.00002	-0.00006	-0.00153
D10	3.13932	0.00000	-0.00010	0.00021	0.00011	3.13943
D11	3.14004	0.00000	-0.00004	-0.00004	-0.00008	3.13996
D12	-0.00236	0.00000	-0.00009	0.00019	0.00010	-0.00227
D13	-0.00018	0.00000	0.00000	0.00003	0.00002	-0.00016
D14	3.14154	0.00000	0.00000	0.00001	0.00001	3.14155
D15	3.14091	0.00000	0.00000	0.00008	0.00008	3.14099
D16	-0.00055	0.00000	0.00000	0.00007	0.00007	-0.00048
D17	0.00060	0.00000	0.00003	0.00017	0.00020	0.00081
D18	-3.14140	0.00000	0.00004	0.00019	0.00023	-3.14117
D19	-3.14054	0.00000	0.00003	0.00012	0.00015	-3.14039
D20	0.00064	0.00000	0.00004	0.00014	0.00018	0.00082

D21	0.00003	0.00000	0.00000	0.00000	0.00000	0.00003
D22	-3.14150	0.00000	0.00000	-0.00001	-0.00001	-3.14151
D23	3.14149	0.00000	0.00000	0.00001	0.00001	3.14150
D24	-0.00004	0.00000	0.00000	0.00000	0.00000	-0.00003
D25	0.00012	0.00000	0.00000	-0.00002	-0.00002	0.00010
D26	-3.14147	0.00000	0.00000	-0.00002	-0.00002	-3.14149
D27	-3.14154	0.00000	0.00000	-0.00001	-0.00001	-3.14155
D28	0.00006	0.00000	0.00000	-0.00001	-0.00001	0.00005
D29	-0.00012	0.00000	0.00000	0.00001	0.00001	-0.00011
D30	-3.14152	0.00000	0.00000	-0.00001	-0.00001	-3.14153
D31	3.14147	0.00000	0.00000	0.00001	0.00001	3.14148
D32	0.00007	0.00000	0.00000	-0.00001	-0.00001	0.00005
D33	0.00181	0.00000	0.00006	0.00013	0.00019	0.00200
D34	-3.13798	0.00000	-0.00007	0.00003	-0.00005	-3.13803
D35	-3.13893	0.00000	0.00012	-0.00011	0.00001	-3.13892
D36	0.00446	0.00000	-0.00001	-0.00021	-0.00023	0.00424
D37	0.00101	0.00000	0.00005	-0.00029	-0.00023	0.00078
D38	-3.14008	0.00000	0.00009	-0.00038	-0.00029	-3.14037
D39	-3.14157	0.00000	-0.00001	-0.00001	-0.00002	-3.14159
D40	0.00052	0.00000	0.00002	-0.00010	-0.00008	0.00044
D41	-0.00150	0.00000	-0.00006	-0.00018	-0.00024	-0.00174
D42	3.13831	0.00000	0.00008	-0.00008	-0.00001	3.13830
D43	3.14052	0.00000	-0.00007	-0.00020	-0.00027	3.14024
D44	-0.00286	0.00000	0.00007	-0.00010	-0.00004	-0.00290
D45	-3.14155	0.00000	0.00005	-0.00011	-0.00006	3.14157
D46	-0.00011	0.00000	0.00012	0.00001	0.00013	0.00002
D47	0.00215	0.00000	-0.00010	-0.00023	-0.00033	0.00182
D48	-3.13959	0.00000	-0.00004	-0.00011	-0.00015	-3.13974
D49	-0.00191	0.00000	0.00006	0.00016	0.00022	-0.00169
D50	3.14086	0.00001	0.00008	0.00025	0.00033	3.14119
D51	3.13982	0.00000	0.00000	0.00004	0.00004	3.13986
D52	-0.00059	0.00000	0.00001	0.00013	0.00015	-0.00044
D53	-3.13782	0.00000	0.00000	-0.00001	-0.00002	-3.13783
D54	0.00267	0.00000	-0.00002	-0.00010	-0.00012	0.00255
D55	3.14153	0.00000	0.00000	0.00004	0.00005	3.14158
D56	0.00271	0.00000	-0.00002	0.00003	0.00001	0.00272
D57	0.00093	0.00000	0.00002	0.00012	0.00014	0.00107
D58	-3.13789	0.00000	-0.00001	0.00011	0.00010	-3.13779
D59	0.00730	0.00000	-0.00001	0.00000	-0.00001	0.00729
D60	-3.12811	0.00000	0.00000	0.00002	0.00002	-3.12809
D61	-3.13520	0.00000	-0.00001	0.00005	0.00004	-3.13516
D62	0.01257	0.00000	0.00000	0.00007	0.00007	0.01264
D63	-0.00553	0.00000	0.00002	0.00006	0.00007	-0.00546
D64	3.13746	0.00000	0.00002	-0.00002	0.00000	3.13746
D65	-0.00020	0.00000	0.00000	-0.00002	-0.00002	-0.00022
D66	-3.13400	0.00000	0.00001	-0.00012	-0.00011	-3.13411
D67	3.14005	0.00000	0.00000	0.00006	0.00005	3.14010
D68	0.00625	0.00000	0.00001	-0.00005	-0.00004	0.00621
D69	-0.00521	0.00000	-0.00001	-0.00008	-0.00008	-0.00530
D70	3.13347	0.00000	0.00002	-0.00007	-0.00005	3.13342
D71	3.12794	0.00000	-0.00002	-0.00010	-0.00012	3.12782
D72	-0.01657	0.00000	0.00001	-0.00009	-0.00009	-0.01666
D73	-0.02005	0.00000	0.00000	-0.00009	-0.00009	-0.02015
D74	-3.05707	0.00000	0.00000	-0.00012	-0.00012	-3.05719
D75	3.12976	0.00000	0.00001	-0.00007	-0.00006	3.12970
D76	0.09274	0.00000	0.00001	-0.00010	-0.00009	0.09266
D77	-0.01236	0.00000	0.00000	-0.00004	-0.00004	-0.01240
D78	3.13733	0.00000	-0.00004	0.00010	0.00005	3.13738
D79	3.12387	0.00000	-0.00001	0.00003	0.00002	3.12389
D80	-0.00964	0.00000	-0.00005	0.00017	0.00012	-0.00952

D81	-3.14112	0.00000	0.00008	-0.00010	-0.00002	-3.14114
D82	0.00854	0.00000	0.00009	-0.00020	-0.00011	0.00843
D83	0.01994	0.00000	0.00000	0.00008	0.00008	0.02002
D84	3.05666	0.00000	0.00000	0.00010	0.00010	3.05676
D85	-3.13258	0.00000	0.00006	-0.00010	-0.00004	-3.13262
D86	-0.09587	0.00000	0.00006	-0.00008	-0.00002	-0.09589
D87	-3.13456	0.00000	0.00003	-0.00014	-0.00011	-3.13467
D88	0.00530	0.00000	-0.00003	-0.00002	-0.00005	0.00525
D89	0.01817	0.00000	-0.00003	0.00005	0.00002	0.01819
D90	-3.12515	0.00000	-0.00009	0.00017	0.00008	-3.12507
D91	1.55335	0.00000	0.00012	-0.00067	-0.00055	1.55280
D92	-2.61532	0.00000	0.00013	-0.00069	-0.00056	-2.61588
D93	-0.55266	0.00000	0.00013	-0.00069	-0.00056	-0.55322
D94	-1.46331	0.00000	0.00013	-0.00070	-0.00058	-1.46389
D95	0.65121	0.00000	0.00013	-0.00072	-0.00059	0.65062
D96	2.71387	0.00000	0.00013	-0.00072	-0.00059	2.71327
D97	-0.00562	0.00000	-0.00011	0.00020	0.00009	-0.00554
D98	3.13768	0.00000	-0.00008	0.00021	0.00013	3.13781
D99	-3.13773	0.00000	-0.00010	0.00026	0.00017	-3.13756
D100	0.00561	0.00000	-0.00003	0.00014	0.00011	0.00572
D101	-0.00847	0.00000	0.00003	-0.00019	-0.00016	-0.00863
D102	3.14090	0.00000	0.00009	0.00002	0.00011	3.14101
D103	0.00129	0.00000	0.00010	-0.00014	-0.00004	0.00125
D104	3.14155	0.00000	0.00005	-0.00005	0.00001	3.14155
D105	3.14158	0.00000	0.00008	-0.00015	-0.00007	3.14151
D106	-0.00135	0.00000	0.00003	-0.00006	-0.00003	-0.00138
D107	3.13473	0.00000	-0.00004	-0.00010	-0.00014	3.13458
D108	-0.01826	0.00000	0.00000	0.00017	0.00018	-0.01808
D109	-0.00519	0.00000	-0.00001	-0.00009	-0.00010	-0.00528
D110	3.12502	0.00000	0.00004	0.00019	0.00022	3.12524
D111	0.00951	0.00000	-0.00002	0.00020	0.00018	0.00969
D112	-3.13725	0.00000	-0.00006	0.00005	0.00000	-3.13726
D113	-3.12381	0.00000	-0.00005	0.00000	-0.00005	-3.12386
D114	0.01261	-0.00001	-0.00009	-0.00014	-0.00023	0.01237
D115	3.13246	0.00000	0.00007	-0.00003	0.00005	3.13251
D116	0.09600	0.00000	0.00007	0.00005	0.00011	0.09611
D117	-0.02030	0.00001	0.00012	0.00024	0.00036	-0.01994
D118	-3.05676	0.00000	0.00011	0.00031	0.00043	-3.05634
D119	3.13425	0.00000	-0.00004	-0.00022	-0.00025	3.13399
D120	-0.00604	0.00000	0.00001	-0.00009	-0.00008	-0.00612
D121	0.00016	0.00000	0.00003	-0.00001	0.00001	0.00017
D122	-3.14013	0.00000	0.00007	0.00012	0.00019	-3.13994
D123	3.13514	0.00000	0.00003	0.00007	0.00010	3.13524
D124	-0.01275	0.00000	0.00005	0.00016	0.00021	-0.01255
D125	-0.00733	0.00000	-0.00001	-0.00001	-0.00002	-0.00735
D126	3.12796	0.00000	0.00001	0.00007	0.00009	3.12805
D127	-3.13733	0.00000	-0.00009	-0.00024	-0.00032	-3.13765
D128	0.00562	0.00000	-0.00004	-0.00010	-0.00014	0.00548
D129	0.00515	0.00000	0.00006	0.00016	0.00022	0.00537
D130	-3.13342	0.00000	-0.00001	0.00009	0.00007	-3.13335
D131	-3.12784	0.00000	0.00003	0.00004	0.00008	-3.12776
D132	0.01677	0.00000	-0.00004	-0.00003	-0.00008	0.01670
D133	0.02038	-0.00001	-0.00010	-0.00025	-0.00035	0.02004
D134	3.05721	-0.00001	-0.00009	-0.00032	-0.00042	3.05679
D135	-3.12958	0.00000	-0.00007	-0.00013	-0.00021	-3.12979
D136	-0.09276	0.00000	-0.00007	-0.00021	-0.00028	-0.09304
D137	-0.00080	-0.00001	-0.00009	-0.00024	-0.00033	-0.00112
D138	-3.14144	0.00000	-0.00004	-0.00001	-0.00006	-3.14149
D139	3.13792	0.00000	-0.00002	-0.00017	-0.00018	3.13774
D140	-0.00272	0.00000	0.00003	0.00006	0.00009	-0.00263

D141	-0.00279	0.00001	0.00007	0.00019	0.00026	-0.00253
D142	3.13773	0.00000	0.00002	-0.00006	-0.00004	3.13769
D143	-3.14105	0.00000	-0.00009	-0.00017	-0.00026	-3.14131
D144	0.00051	0.00000	-0.00004	-0.00016	-0.00020	0.00031
D145	0.00168	0.00000	-0.00004	0.00009	0.00006	0.00174
D146	-3.13994	0.00000	0.00002	0.00010	0.00012	-3.13982
D147	-0.64615	0.00000	0.00004	-0.00043	-0.00039	-0.64654
D148	1.46827	0.00000	0.00004	-0.00042	-0.00038	1.46789
D149	-2.70876	0.00000	0.00004	-0.00043	-0.00039	-2.70914
D150	2.62064	0.00000	0.00003	-0.00034	-0.00031	2.62033
D151	-1.54813	0.00000	0.00003	-0.00033	-0.00030	-1.54843
D152	0.55803	0.00000	0.00003	-0.00034	-0.00031	0.55772
D153	-0.00164	0.00000	0.00003	-0.00004	-0.00001	-0.00165
D154	-3.14153	0.00000	0.00003	0.00000	0.00003	-3.14150
D155	3.13999	0.00000	-0.00002	-0.00005	-0.00008	3.13991
D156	0.00009	0.00000	-0.00002	-0.00001	-0.00004	0.00006
D157	-3.13862	0.00000	0.00000	0.00005	0.00005	-3.13857
D158	0.00271	0.00000	-0.00001	0.00005	0.00004	0.00275
D159	0.00155	0.00000	0.00000	0.00002	0.00001	0.00156
D160	-3.14031	0.00000	-0.00001	0.00001	0.00000	-3.14031
D161	3.13834	0.00000	0.00001	-0.00009	-0.00008	3.13826
D162	-0.00396	0.00000	0.00002	-0.00016	-0.00014	-0.00410
D163	-0.00181	0.00000	0.00001	-0.00005	-0.00004	-0.00185
D164	3.13908	0.00000	0.00002	-0.00012	-0.00010	3.13898
D165	-0.00068	0.00000	-0.00001	0.00003	0.00002	-0.00066
D166	3.14052	0.00000	0.00000	-0.00002	-0.00002	3.14050
D167	3.14117	0.00000	0.00000	0.00003	0.00003	3.14120
D168	-0.00081	0.00000	0.00001	-0.00002	-0.00001	-0.00082
D169	0.00141	0.00000	-0.00001	0.00007	0.00005	0.00146
D170	-3.14010	0.00000	-0.00002	0.00010	0.00008	-3.14002
D171	-3.13951	0.00000	-0.00003	0.00014	0.00011	-3.13940
D172	0.00217	0.00000	-0.00003	0.00017	0.00014	0.00231
D173	-0.00043	0.00000	0.00000	0.00002	0.00002	-0.00041
D174	-3.14155	0.00000	-0.00001	0.00006	0.00005	-3.14150
D175	3.14034	0.00000	0.00001	-0.00006	-0.00005	3.14028
D176	-0.00078	0.00000	0.00000	-0.00002	-0.00002	-0.00080
D177	-0.00044	0.00000	0.00001	-0.00006	-0.00005	-0.00049
D178	3.14108	0.00000	0.00001	-0.00008	-0.00007	3.14101
D179	3.14152	0.00000	0.00000	-0.00001	-0.00001	3.14151
D180	-0.00015	0.00000	0.00001	-0.00004	-0.00003	-0.00018
D181	-3.14100	0.00000	-0.00001	0.00007	0.00006	-3.14094
D182	0.00049	0.00000	-0.00001	0.00004	0.00003	0.00052
D183	0.00016	0.00000	0.00000	0.00002	0.00002	0.00017
D184	-3.14155	0.00000	0.00000	-0.00002	-0.00002	-3.14156
D185	3.14152	0.00000	0.00000	0.00000	-0.00001	3.14151
D186	0.00007	0.00000	0.00000	-0.00001	-0.00001	0.00007
D187	0.00002	0.00000	0.00000	0.00003	0.00002	0.00004
D188	-3.14142	0.00000	0.00000	0.00002	0.00002	-3.14140
D189	-0.00003	0.00000	0.00000	0.00001	0.00001	-0.00002
D190	3.14151	0.00000	0.00000	0.00001	0.00000	3.14152
D191	-3.14151	0.00000	-0.00001	0.00005	0.00004	-3.14147
D192	0.00003	0.00000	-0.00001	0.00005	0.00004	0.00007
D193	0.00010	0.00000	0.00000	0.00000	0.00000	0.00010
D194	-3.14148	0.00000	0.00000	-0.00001	-0.00001	-3.14149
D195	3.14155	0.00000	0.00000	0.00000	0.00000	3.14155
D196	-0.00004	0.00000	0.00000	-0.00001	-0.00001	-0.00004
D197	-0.00009	0.00000	0.00000	-0.00002	-0.00002	-0.00011
D198	3.14149	0.00000	0.00000	-0.00001	-0.00001	3.14148
D199	3.14155	0.00000	0.00000	-0.00002	-0.00001	3.14153
D200	-0.00006	0.00000	0.00000	-0.00001	-0.00001	-0.00006

Item	Value	Threshold	Converged?
Maximum Force	0.000022	0.000450	YES
RMS Force	0.000003	0.000300	YES
Maximum Displacement	0.002345	0.001800	NO
RMS Displacement	0.000322	0.001200	YES

Predicted change in Energy=-2.707715D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4

Framework group C1[X(C42H18N6O2S4)]

Deg. of freedom 210

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.803371	-0.637271	0.004930
2	6	0	-9.994209	-1.788073	0.002849
3	6	0	-10.516716	-3.073085	0.007442
4	6	0	-11.905666	-3.215437	0.014603
5	6	0	-12.726792	-2.081126	0.016920
6	6	0	-12.194771	-0.787500	0.012109
7	1	0	-9.846115	-3.926266	0.005518
8	1	0	-12.353097	-4.204554	0.018445
9	1	0	-13.805578	-2.203111	0.022601
10	1	0	-12.864256	0.060834	0.014179
11	6	0	-9.927078	0.564330	-0.001338
12	6	0	-8.569965	-1.390842	-0.004177
13	6	0	-8.540409	0.088720	-0.005222
14	6	0	-7.404450	0.870095	-0.007426
15	6	0	-6.014476	0.595587	-0.011131
16	6	0	-3.644320	-0.183962	-0.010662
17	6	0	-3.778362	1.228676	-0.016614
18	16	0	-5.182083	-0.989241	-0.012157
19	6	0	-5.099620	1.664929	-0.013038
20	6	0	-2.267214	-0.451795	-0.006598
21	6	0	-1.603923	0.797461	-0.010455
22	7	0	-2.523845	1.820863	-0.032759
23	16	0	-1.150964	-1.806928	-0.007105
24	16	0	1.150915	1.806537	0.008055
25	6	0	0.198420	-0.673774	0.002343
26	6	0	-0.198424	0.673343	-0.001459
27	6	0	1.603937	-0.797878	0.011227
28	6	0	2.267166	0.451409	0.007247
29	6	0	3.644283	0.183683	0.011045
30	6	0	3.778409	-1.228925	0.017023
31	6	0	5.099690	-1.665132	0.013298
32	6	0	6.014493	-0.595734	0.011347
33	16	0	5.181990	0.989050	0.012426
34	7	0	2.523952	-1.821220	0.033317
35	6	0	7.404528	-0.870172	0.007388
36	6	0	8.540398	-0.088684	0.004956
37	6	0	8.569748	1.390882	0.004077
38	6	0	9.927133	-0.564098	0.000737
39	6	0	9.993929	1.788309	-0.002930
40	6	0	10.803248	0.637624	-0.005349
41	6	0	10.516258	3.073402	-0.007267

42	6	0	12.194630	0.788043	-0.012643
43	6	0	11.905183	3.215943	-0.014528
44	6	0	12.726468	2.081741	-0.017202
45	6	0	10.384797	-1.870801	0.002801
46	6	0	9.534100	-3.018676	0.010206
47	6	0	11.769344	-2.222147	-0.001672
48	7	0	8.863977	-3.972415	0.016260
49	7	0	12.886900	-2.551315	-0.005220
50	6	0	-10.384568	1.871088	-0.003704
51	6	0	-11.769079	2.222615	0.000569
52	6	0	-9.533722	3.018856	-0.011178
53	7	0	-12.886594	2.551923	0.003937
54	7	0	-8.863471	3.972505	-0.017293
55	8	0	-7.613055	-2.157586	-0.007884
56	8	0	7.612727	2.157478	0.008003
57	6	0	2.241322	-3.243103	-0.055319
58	1	0	1.319634	-3.467804	0.486037
59	1	0	2.137482	-3.570602	-1.095396
60	1	0	3.054737	-3.799289	0.414699
61	6	0	-2.240714	3.242673	0.055455
62	1	0	-2.132659	3.569632	1.095272
63	1	0	-1.321217	3.467670	-0.489549
64	1	0	-3.056035	3.799114	-0.410893
65	1	0	5.428741	-2.697761	0.009432
66	1	0	12.864228	-0.060198	-0.014970
67	1	0	13.805236	2.203884	-0.022963
68	1	0	12.352484	4.205120	-0.018168
69	1	0	9.845536	3.926489	-0.005095
70	1	0	7.572785	-1.940241	0.006048
71	1	0	-7.572622	1.940178	-0.006089
72	1	0	-5.428646	2.697565	-0.009238

```

-----
Rotational constants (GHZ):      0.1750153      0.0104040      0.0098215
Standard basis: 6-31G(d,p) (6D, 7F)
There are 916 symmetry adapted cartesian basis functions of A symmetry.
There are 916 symmetry adapted basis functions of A symmetry.
916 basis functions, 1734 primitive gaussians, 916 cartesian basis func-
tions
196 alpha electrons      196 beta electrons
nuclear repulsion energy      6569.7672646275 Hartrees.
NAtoms= 72 NActive= 72 NUniq= 72 SFac= 1.00D+00 NATFMM= 60 NAOKFM=T
Big=T
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
Nuclear repulsion after empirical dispersion term = 6569.6823482498 Har-
trees.
One-electron integrals computed using PRISM.
NBasis= 916 RedAO= T EigKep= 3.24D-04 NBF= 916
NBsUse= 916 1.00D-06 EigRej= -1.00D+00 NBFU= 916
Initial guess from the checkpoint file: "PBDB.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000000 0.000000 0.000000 Ang= 0.00 deg.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3683.02012185 A.U. after 6 cycles
NFock= 6 Conv=0.62D-08 -V/T= 2.0068

```

Calling FoFJK, ICntrl= 2127 FMM=T ISym2X=0 IlCent= 0 IOpClX= 0 NMat=1
NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr)		
		X	Y	Z
1	6	-0.000004745	-0.000003410	0.000001862
2	6	-0.000002563	0.000001256	0.000005161
3	6	-0.000000093	-0.000002802	-0.000000074
4	6	-0.000001514	0.000000911	-0.000000526
5	6	0.000001748	0.000000939	0.000000993
6	6	0.000002483	-0.000002550	0.000002511
7	1	-0.000000238	-0.000001303	0.000000764
8	1	-0.000000414	-0.000000500	-0.000000164
9	1	-0.000001268	-0.000001268	-0.000000858
10	1	-0.000001811	0.000001197	-0.000001194
11	6	0.000006057	0.000003223	-0.000011589
12	6	0.000003009	0.000002489	-0.000008900
13	6	-0.000009612	-0.000003685	0.000000094
14	6	-0.000014932	0.000003191	-0.000011485
15	6	0.000013282	-0.000003026	0.000002895
16	6	0.000003707	-0.000003259	-0.000008798
17	6	0.000003613	0.000002188	0.000002884
18	16	0.000003802	0.000001740	0.000014449
19	6	0.000003787	-0.000004265	0.000005889
20	6	-0.000003062	-0.000014828	-0.000009157
21	6	0.000003322	0.000009632	0.000010267
22	7	0.000005189	0.000003166	0.000000210
23	16	-0.000004985	0.000002326	0.000005781
24	16	-0.000003313	-0.000000420	0.000003250
25	6	0.000008970	-0.000000559	0.000001521
26	6	-0.000005837	-0.000000789	-0.000002624
27	6	-0.000015490	0.000001913	0.000004061
28	6	0.000000864	0.000007509	-0.000005595
29	6	0.000009019	-0.000000277	0.000000256
30	6	0.000001141	-0.000000336	0.000012332
31	6	-0.000003032	-0.000002253	-0.000012127
32	6	0.000002093	-0.000001800	0.000019835
33	16	-0.000000941	-0.000001130	-0.000013397
34	7	0.000004290	-0.000005963	-0.000005380
35	6	-0.000012376	0.000012673	-0.000006162
36	6	0.000005640	-0.000000919	0.000004839
37	6	0.000012449	0.000001522	0.000003919
38	6	0.000003541	0.000005653	0.000002947
39	6	-0.000003757	-0.000010852	-0.000002301
40	6	0.000006132	0.000000937	0.000005074
41	6	-0.000000933	0.000009132	0.000002603
42	6	-0.000004258	0.000003243	-0.000005246
43	6	0.000005365	-0.000002441	0.000001761
44	6	-0.000003249	-0.000003558	-0.000003189
45	6	-0.000007362	-0.000005861	-0.000006666
46	6	-0.000000895	0.000002885	-0.000001445
47	6	0.000002424	-0.000002119	0.000002532
48	7	-0.000002390	0.000000333	-0.000000690
49	7	-0.000000270	0.000002461	0.000000155
50	6	0.000001583	0.000003114	-0.000000822
51	6	-0.000000153	-0.000000466	0.000002288
52	6	-0.000001365	-0.000001912	0.000003179
53	7	0.000001336	-0.000003210	-0.000000108

54	7	0.000002062	0.000000758	0.000000490
55	8	0.000001752	-0.000002449	0.000002533
56	8	-0.000009165	-0.000003310	-0.000005552
57	6	0.000001105	0.000005283	-0.000001559
58	1	0.000000824	0.000000600	-0.000000778
59	1	-0.000001001	0.000000226	-0.000001152
60	1	-0.000000896	-0.000001130	0.000001189
61	6	-0.000003629	-0.000008091	-0.000007384
62	1	-0.000000133	0.000001750	0.000000091
63	1	0.000002581	0.000003135	0.000000095
64	1	-0.000001038	0.000001227	0.000003293
65	1	0.000001770	-0.000000465	-0.000000992
66	1	0.000002883	-0.000000736	0.000002802
67	1	0.000001520	0.000001543	0.000001000
68	1	-0.000000051	0.000000654	0.000000525
69	1	0.000000847	0.000001219	-0.000000811
70	1	0.000000954	0.000002772	0.000000951
71	1	-0.000002306	-0.000000628	-0.000000321
72	1	-0.000002067	-0.000000228	-0.000000243

Cartesian Forces: Max 0.000019835 RMS 0.000004971

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000018432 RMS 0.000003723

Search for a local minimum.

Step number 35 out of a maximum of 429

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 16 18 17 19 20

21 22 23 24 25

26 27 28 29 30

31 32 33 34 35

DE= -1.54D-08 DEPred=-2.71D-08 R= 5.70D-01

Trust test= 5.70D-01 RLast= 2.40D-03 DXMaxT set to 1.43D-01

ITU= 0 0 0 0 0 0 0 1 -1 1 -1 1 -1 1 1 -1 0 -1 0 -1

ITU= 1 1 1 1 1 1 0 0 0 1 0 0 0 1 0

Eigenvalues	---	0.00073	0.00203	0.00268	0.00296	0.00316
Eigenvalues	---	0.00425	0.00481	0.00501	0.00522	0.00550
Eigenvalues	---	0.00586	0.00614	0.00631	0.00664	0.00692
Eigenvalues	---	0.00712	0.00744	0.00751	0.00773	0.00778
Eigenvalues	---	0.00785	0.00790	0.00814	0.00885	0.01025
Eigenvalues	---	0.01088	0.01123	0.01134	0.01160	0.01259
Eigenvalues	---	0.01308	0.01325	0.01342	0.01365	0.01380
Eigenvalues	---	0.01457	0.01458	0.01589	0.01614	0.01650
Eigenvalues	---	0.01737	0.01745	0.01794	0.01894	0.01935
Eigenvalues	---	0.01961	0.02006	0.02021	0.02061	0.02075
Eigenvalues	---	0.02086	0.02280	0.02407	0.02806	0.02872
Eigenvalues	---	0.02934	0.03111	0.03807	0.03969	0.04060
Eigenvalues	---	0.04235	0.04831	0.04839	0.04913	0.05043
Eigenvalues	---	0.05089	0.05211	0.05315	0.05495	0.07039
Eigenvalues	---	0.07225	0.07400	0.07576	0.15470	0.15825
Eigenvalues	---	0.15865	0.15984	0.15988	0.15998	0.16000
Eigenvalues	---	0.16000	0.16000	0.16001	0.16006	0.16010
Eigenvalues	---	0.16013	0.16026	0.16032	0.16086	0.16113
Eigenvalues	---	0.16118	0.19068	0.19497	0.19892	0.20589
Eigenvalues	---	0.20757	0.21269	0.21696	0.21889	0.22003

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Eigenvalues ---      0.22025      0.22439      0.22600      0.22614      0.22638
Eigenvalues ---      0.22821      0.22874      0.23010      0.23110      0.23297
Eigenvalues ---      0.23404      0.23513      0.23589      0.23761      0.23997
Eigenvalues ---      0.24258      0.24269      0.24317      0.24418      0.24518
Eigenvalues ---      0.24561      0.24665      0.24772      0.24862      0.24902
Eigenvalues ---      0.24929      0.24964      0.24972      0.24986      0.24991
Eigenvalues ---      0.24994      0.24999      0.24999      0.25000      0.25000
Eigenvalues ---      0.25001      0.25002      0.25012      0.25100      0.25169
Eigenvalues ---      0.25524      0.25749      0.26025      0.26187      0.26478
Eigenvalues ---      0.26581      0.26798      0.26939      0.27226      0.27542
Eigenvalues ---      0.27762      0.27922      0.28388      0.28503      0.28820
Eigenvalues ---      0.29838      0.30065      0.30295      0.31831      0.32716
Eigenvalues ---      0.33839      0.35467      0.35663      0.36272      0.36336
Eigenvalues ---      0.36437      0.36475      0.36635      0.36819      0.36845
Eigenvalues ---      0.36940      0.37057      0.37087      0.37165      0.37245
Eigenvalues ---      0.37257      0.37421      0.37540      0.37671      0.37758
Eigenvalues ---      0.38031      0.38961      0.39303      0.40317      0.41302
Eigenvalues ---      0.41736      0.42022      0.42633      0.44382      0.45155
Eigenvalues ---      0.45944      0.46312      0.47095      0.47781      0.47931
Eigenvalues ---      0.49028      0.52267      0.53065      0.54469      0.56111
Eigenvalues ---      0.64783      0.73202      0.77906      0.80675      0.82504
Eigenvalues ---      0.91684      1.25864      1.26356      1.29353      1.35376
En-DIIS/RFO-DIIS IScMMF=          0 using points:      35      34      33      32      31
RFO step:  Lambda=-9.54133194D-09.
DidBck=T Rises=F RFO-DIIS coefs:      0.67658      0.28479      0.02214      0.00377
0.01272
Iteration 1 RMS(Cart)= 0.00029853 RMS(Int)= 0.00000003
Iteration 2 RMS(Cart)= 0.00000005 RMS(Int)= 0.00000000
Variable      Old X      -DE/DX      Delta X      Delta X      Delta X      New X
(Linear)      (Quad)      (Total)
R1      2.65847      0.00000      0.00000      0.00000      0.00000      2.65847
R2      2.64468      0.00000      0.00000      0.00000      0.00000      2.64468
R3      2.81041      0.00000      0.00000      0.00000      0.00000      2.81041
R4      2.62141      0.00000      0.00000      0.00000      0.00000      2.62140
R5      2.79418      0.00000      0.00000      0.00000      0.00000      2.79418
R6      2.63852      0.00000      0.00000      0.00000      0.00000      2.63852
R7      2.05070      0.00000      0.00000      0.00000      0.00000      2.05070
R8      2.64623      0.00000      0.00000      0.00001      0.00000      2.64624
R9      2.05152      0.00000      0.00000      0.00000      0.00000      2.05152
R10     2.64328      0.00000      0.00000      -0.00001      0.00000      2.64328
R11     2.05163      0.00000      0.00000      0.00000      0.00000      2.05163
R12     2.04220      0.00000      0.00000      0.00000      0.00000      2.04221
R13     2.77028      -0.00001      -0.00001      0.00000      -0.00001      2.77028
R14     2.61638      -0.00001      0.00000      -0.00001      -0.00001      2.61637
R15     2.79653      0.00000      0.00000      0.00000      0.00000      2.79652
R16     2.31720      0.00000      0.00000      0.00000      0.00000      2.31720
R17     2.60546      0.00000      -0.00001      0.00002      0.00001      2.60547
R18     2.67741      0.00002      0.00000      0.00005      0.00006      2.67747
R19     2.04699      0.00000      0.00000      0.00001      0.00000      2.04699
R20     3.38285      0.00001      0.00001      0.00001      0.00001      3.38287
R21     2.65939      0.00000      0.00000      0.00000      0.00000      2.65939
R22     2.68151      -0.00001      -0.00002      0.00004      0.00002      2.68153
R23     3.28029      0.00000      0.00000      0.00000      0.00000      3.28029
R24     2.65113      -0.00001      0.00001      -0.00004      -0.00004      2.65109
R25     2.62940      -0.00001      0.00000      -0.00001      -0.00001      2.62939
R26     2.62172      -0.00001      0.00000      -0.00002      -0.00001      2.62171
R27     2.04807      0.00000      0.00000      0.00000      0.00000      2.04807
R28     2.67288      -0.00001      -0.00002      0.00003      0.00001      2.67289
R29     3.31775      0.00000      0.00000      -0.00001      -0.00001      3.31774
R30     2.60076      0.00000      0.00001      -0.00002      -0.00001      2.60075

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R31	2.66640	-0.00001	0.00000	-0.00001	-0.00002	2.66638
R32	2.74465	0.00000	0.00000	0.00001	0.00001	2.74466
R33	3.32987	0.00000	0.00000	-0.00001	-0.00001	3.32986
R34	3.32985	0.00000	-0.00001	0.00001	0.00000	3.32985
R35	3.31774	0.00000	0.00000	-0.00001	-0.00001	3.31774
R36	2.65385	0.00000	0.00000	0.00000	0.00000	2.65386
R37	2.66643	-0.00001	0.00001	-0.00004	-0.00004	2.66639
R38	2.67288	0.00000	0.00000	0.00000	0.00000	2.67288
R39	2.60079	0.00000	0.00000	0.00000	0.00000	2.60079
R40	2.65111	0.00000	-0.00001	0.00003	0.00002	2.65113
R41	2.68147	0.00000	0.00000	-0.00001	0.00000	2.68147
R42	3.28027	0.00000	-0.00001	0.00001	0.00001	3.28028
R43	2.62942	-0.00001	-0.00001	0.00001	0.00000	2.62941
R44	2.62171	0.00000	0.00000	0.00001	0.00000	2.62171
R45	2.65940	-0.00001	0.00000	-0.00001	-0.00001	2.65939
R46	2.04808	0.00000	0.00000	0.00000	0.00000	2.04808
R47	3.38287	0.00001	0.00001	0.00000	0.00000	3.38288
R48	2.67750	-0.00001	-0.00001	-0.00002	-0.00003	2.67748
R49	2.74465	0.00000	0.00000	0.00000	0.00000	2.74466
R50	2.60544	0.00001	0.00000	0.00000	0.00000	2.60545
R51	2.04698	0.00000	0.00000	0.00000	0.00000	2.04699
R52	2.79652	0.00000	0.00000	0.00001	0.00001	2.79653
R53	2.77028	-0.00001	-0.00001	0.00000	0.00000	2.77028
R54	2.79417	0.00000	0.00000	0.00000	0.00000	2.79417
R55	2.31719	0.00001	0.00001	0.00000	0.00000	2.31719
R56	2.81039	0.00000	0.00000	0.00000	0.00000	2.81039
R57	2.61639	-0.00001	0.00000	-0.00001	-0.00001	2.61637
R58	2.65846	0.00000	0.00001	-0.00003	-0.00001	2.65845
R59	2.62142	-0.00001	-0.00001	0.00000	-0.00001	2.62141
R60	2.64469	0.00000	-0.00001	0.00001	0.00000	2.64469
R61	2.63851	0.00000	0.00001	-0.00001	0.00000	2.63851
R62	2.05070	0.00000	0.00000	0.00000	0.00000	2.05070
R63	2.64327	0.00000	0.00001	-0.00002	-0.00001	2.64326
R64	2.04220	0.00000	0.00000	0.00000	0.00001	2.04220
R65	2.64624	0.00000	-0.00001	0.00001	0.00000	2.64625
R66	2.05152	0.00000	0.00000	0.00000	0.00000	2.05152
R67	2.05163	0.00000	0.00000	0.00000	0.00000	2.05163
R68	2.69997	0.00000	0.00000	0.00001	0.00001	2.69997
R69	2.69936	0.00000	0.00000	0.00001	0.00001	2.69937
R70	2.20274	0.00000	0.00000	0.00000	0.00000	2.20274
R71	2.20159	0.00000	0.00000	0.00000	0.00000	2.20159
R72	2.69937	0.00000	0.00000	0.00000	0.00000	2.69937
R73	2.69997	0.00000	0.00000	0.00000	0.00000	2.69997
R74	2.20159	0.00000	0.00000	0.00000	0.00000	2.20159
R75	2.20274	0.00000	0.00000	0.00000	0.00000	2.20274
R76	2.06410	0.00000	0.00000	0.00000	0.00000	2.06410
R77	2.06992	0.00000	0.00000	0.00000	0.00000	2.06992
R78	2.06310	0.00000	0.00000	0.00000	0.00000	2.06310
R79	2.06992	0.00000	0.00000	0.00000	0.00000	2.06991
R80	2.06416	0.00000	0.00000	-0.00001	-0.00001	2.06415
R81	2.06305	0.00000	0.00000	0.00001	0.00000	2.06306
A1	2.07607	0.00000	0.00000	0.00000	0.00000	2.07606
A2	1.89866	0.00000	0.00000	0.00000	0.00000	1.89866
A3	2.30846	0.00000	0.00000	0.00001	0.00001	2.30847
A4	2.14256	0.00000	0.00000	0.00001	0.00001	2.14257
A5	1.91163	0.00000	0.00000	0.00000	0.00000	1.91163
A6	2.22899	0.00000	0.00000	-0.00001	-0.00001	2.22899
A7	2.05914	0.00000	0.00000	0.00000	0.00000	2.05913
A8	2.08924	0.00000	0.00000	0.00000	0.00000	2.08923
A9	2.13481	0.00000	0.00000	0.00001	0.00001	2.13482

A10	2.09525	0.00000	0.00000	0.00000	0.00000	2.09525
A11	2.09775	0.00000	0.00000	0.00001	0.00000	2.09775
A12	2.09019	0.00000	0.00000	0.00000	0.00000	2.09019
A13	2.12482	0.00000	0.00000	0.00000	0.00000	2.12482
A14	2.08479	0.00000	0.00000	-0.00001	0.00000	2.08478
A15	2.07358	0.00000	0.00000	0.00000	0.00000	2.07358
A16	2.06854	0.00000	0.00000	0.00000	0.00000	2.06854
A17	2.13135	0.00000	0.00000	0.00000	0.00000	2.13135
A18	2.08330	0.00000	0.00000	0.00000	0.00000	2.08329
A19	1.87049	0.00000	0.00000	0.00000	0.00000	1.87049
A20	2.17473	0.00001	0.00001	0.00000	0.00001	2.17474
A21	2.23796	-0.00001	-0.00001	0.00000	-0.00001	2.23795
A22	1.86276	0.00000	0.00000	0.00000	0.00000	1.86276
A23	2.19409	0.00000	0.00000	0.00001	0.00001	2.19410
A24	2.22633	0.00000	0.00000	-0.00001	-0.00001	2.22632
A25	1.88123	0.00000	0.00000	0.00000	0.00000	1.88123
A26	2.20865	0.00000	0.00001	-0.00001	0.00000	2.20865
A27	2.19330	-0.00001	-0.00001	0.00001	0.00000	2.19330
A28	2.34408	-0.00001	-0.00001	0.00001	0.00000	2.34408
A29	2.01744	0.00000	0.00001	-0.00001	0.00000	2.01744
A30	1.92166	0.00000	0.00000	0.00000	0.00000	1.92167
A31	2.24940	0.00000	0.00003	-0.00004	-0.00002	2.24938
A32	2.08351	0.00000	-0.00002	0.00003	0.00001	2.08353
A33	1.95027	0.00000	-0.00001	0.00001	0.00000	1.95028
A34	1.95859	0.00000	0.00001	-0.00002	-0.00001	1.95858
A35	1.85750	0.00000	0.00000	-0.00001	-0.00001	1.85749
A36	2.46710	0.00000	-0.00001	0.00003	0.00001	2.46711
A37	1.98429	0.00000	0.00000	0.00001	0.00001	1.98430
A38	1.91725	0.00000	0.00000	0.00000	0.00000	1.91725
A39	2.38162	0.00000	0.00000	-0.00001	-0.00001	2.38161
A40	1.57202	0.00000	-0.00001	0.00000	0.00000	1.57201
A41	1.95959	0.00000	0.00000	-0.00001	-0.00001	1.95958
A42	2.12543	0.00000	0.00000	0.00000	0.00000	2.12543
A43	2.19817	0.00000	0.00000	0.00001	0.00001	2.19818
A44	1.86679	0.00000	0.00000	0.00001	0.00001	1.86681
A45	2.45192	-0.00001	0.00000	-0.00002	-0.00002	2.45190
A46	1.96445	0.00000	0.00000	0.00000	0.00001	1.96446
A47	1.92129	0.00000	0.00000	-0.00001	-0.00001	1.92128
A48	1.97079	0.00000	0.00001	-0.00001	0.00000	1.97078
A49	2.39106	0.00000	-0.00001	0.00002	0.00001	2.39108
A50	1.86171	0.00000	0.00000	0.00001	0.00000	1.86171
A51	2.20610	0.00000	0.00002	-0.00006	-0.00004	2.20606
A52	2.21013	0.00001	-0.00001	0.00006	0.00005	2.21017
A53	1.56132	-0.00001	0.00000	0.00000	-0.00001	1.56131
A54	1.56128	0.00000	0.00000	-0.00001	-0.00001	1.56128
A55	1.98281	0.00000	0.00000	0.00001	0.00001	1.98281
A56	2.35502	0.00000	0.00001	-0.00002	-0.00001	2.35501
A57	1.94536	0.00000	0.00000	0.00001	0.00000	1.94536
A58	2.35498	0.00000	0.00000	0.00000	0.00000	2.35498
A59	1.94537	0.00000	0.00000	0.00000	0.00000	1.94537
A60	1.98284	0.00000	0.00000	-0.00001	0.00000	1.98284
A61	1.97075	0.00000	0.00000	0.00000	0.00000	1.97075
A62	2.39113	0.00000	0.00000	0.00000	0.00000	2.39113
A63	1.92126	0.00000	0.00000	0.00000	0.00000	1.92126
A64	1.96450	0.00000	0.00000	0.00000	0.00000	1.96450
A65	2.45185	0.00000	0.00000	0.00000	0.00000	2.45184
A66	1.86682	0.00000	0.00000	0.00000	0.00000	1.86682
A67	1.85749	0.00000	0.00000	0.00000	0.00000	1.85748
A68	2.46711	0.00000	0.00000	0.00000	0.00000	2.46711
A69	1.95859	0.00000	0.00000	0.00000	0.00000	1.95859

A70	1.98432	0.00000	0.00000	0.00001	0.00000	1.98432
A71	1.91728	0.00000	0.00000	0.00000	0.00000	1.91728
A72	2.38157	0.00000	0.00000	0.00000	0.00000	2.38157
A73	1.95957	0.00000	0.00001	-0.00001	0.00000	1.95957
A74	2.19816	0.00000	0.00000	0.00000	0.00000	2.19816
A75	2.12546	0.00000	-0.00001	0.00000	0.00000	2.12546
A76	1.95026	0.00000	0.00000	0.00001	0.00001	1.95027
A77	2.08352	-0.00001	-0.00001	0.00000	-0.00001	2.08351
A78	2.24941	0.00001	0.00002	-0.00001	0.00000	2.24941
A79	1.57202	-0.00001	0.00000	0.00000	-0.00001	1.57202
A80	1.86170	0.00000	0.00000	0.00000	0.00000	1.86170
A81	2.21039	0.00000	0.00001	-0.00002	0.00000	2.21038
A82	2.20581	0.00000	-0.00001	0.00002	0.00001	2.20582
A83	2.34404	0.00001	0.00000	0.00001	0.00002	2.34405
A84	1.92169	-0.00001	0.00000	-0.00001	-0.00001	1.92167
A85	2.01746	-0.00001	0.00000	0.00000	0.00000	2.01746
A86	2.19326	0.00001	-0.00001	0.00002	0.00001	2.19328
A87	2.20869	-0.00001	0.00000	-0.00001	-0.00001	2.20868
A88	1.88123	0.00000	0.00000	0.00000	0.00000	1.88123
A89	1.86276	0.00000	0.00000	-0.00001	0.00000	1.86276
A90	2.22632	0.00000	0.00000	0.00000	0.00000	2.22632
A91	2.19410	0.00000	-0.00001	0.00001	0.00000	2.19410
A92	1.87049	0.00000	0.00000	0.00000	0.00000	1.87049
A93	2.23795	-0.00002	0.00000	-0.00001	-0.00001	2.23794
A94	2.17475	0.00001	0.00000	0.00001	0.00001	2.17475
A95	1.91163	0.00000	-0.00001	0.00001	0.00001	1.91163
A96	2.22899	0.00000	0.00001	-0.00001	-0.00001	2.22898
A97	2.14256	0.00000	0.00000	0.00000	0.00000	2.14257
A98	1.89866	0.00000	0.00000	0.00000	0.00000	1.89866
A99	2.30845	0.00001	0.00000	0.00000	0.00000	2.30846
A100	2.07607	0.00000	0.00000	0.00000	0.00000	2.07607
A101	2.05913	0.00000	0.00000	0.00000	0.00000	2.05913
A102	2.08924	0.00000	0.00000	-0.00001	-0.00001	2.08923
A103	2.13482	0.00000	0.00000	0.00001	0.00001	2.13483
A104	2.06853	0.00000	0.00000	0.00000	0.00000	2.06853
A105	2.13135	0.00000	0.00001	-0.00001	0.00000	2.13135
A106	2.08330	0.00000	-0.00001	0.00001	0.00000	2.08330
A107	2.09525	0.00000	0.00000	0.00000	0.00000	2.09525
A108	2.09775	0.00000	0.00000	0.00001	0.00001	2.09776
A109	2.09018	0.00000	0.00001	-0.00001	0.00000	2.09018
A110	2.12482	0.00000	0.00000	0.00000	0.00000	2.12482
A111	2.07359	0.00000	-0.00001	0.00001	0.00000	2.07359
A112	2.08478	0.00000	0.00001	-0.00001	0.00000	2.08477
A113	2.16692	-0.00001	-0.00001	0.00001	0.00000	2.16692
A114	2.15619	0.00001	0.00000	-0.00001	0.00000	2.15619
A115	1.96007	0.00000	0.00001	0.00000	0.00000	1.96008
A116	2.15619	0.00001	0.00000	0.00000	0.00000	2.15619
A117	2.16692	-0.00001	-0.00001	0.00001	0.00000	2.16692
A118	1.96007	0.00000	0.00001	-0.00001	0.00000	1.96007
A119	1.91277	0.00000	0.00000	0.00000	0.00000	1.91277
A120	1.94884	0.00000	0.00000	0.00000	0.00000	1.94884
A121	1.90443	0.00000	0.00000	-0.00001	0.00000	1.90443
A122	1.90616	0.00000	0.00000	0.00000	0.00000	1.90616
A123	1.88654	0.00000	0.00000	0.00000	0.00000	1.88654
A124	1.90404	0.00000	0.00000	0.00000	0.00000	1.90404
A125	1.94883	0.00000	0.00000	-0.00001	0.00000	1.94883
A126	1.91287	0.00000	0.00000	-0.00002	-0.00002	1.91285
A127	1.90437	0.00000	-0.00001	0.00000	0.00000	1.90437
A128	1.90617	0.00000	0.00000	0.00000	0.00000	1.90618
A129	1.90397	0.00000	0.00000	0.00002	0.00002	1.90399

A130	1.88657	0.00000	0.00000	0.00000	0.00000	1.88657
A131	3.16689	-0.00001	-0.00001	-0.00002	-0.00003	3.16686
A132	3.17952	0.00000	0.00000	0.00004	0.00004	3.17955
A133	3.17951	0.00000	-0.00001	0.00006	0.00005	3.17956
A134	3.16688	0.00000	-0.00002	0.00001	-0.00001	3.16687
A135	3.14149	0.00000	0.00000	-0.00002	-0.00002	3.14148
A136	3.14162	0.00000	0.00000	-0.00001	0.00000	3.14161
A137	3.14158	0.00000	-0.00001	0.00000	0.00000	3.14157
A138	3.14160	0.00000	0.00001	0.00000	0.00001	3.14160
D1	0.00015	0.00000	0.00001	-0.00002	-0.00001	0.00014
D2	-3.14107	0.00000	0.00003	-0.00004	-0.00001	-3.14108
D3	-3.14153	0.00000	0.00002	-0.00004	-0.00002	-3.14155
D4	0.00044	0.00000	0.00003	-0.00006	-0.00002	0.00042
D5	-0.00002	0.00000	0.00000	0.00001	0.00001	-0.00001
D6	3.14140	0.00000	-0.00001	0.00003	0.00001	3.14142
D7	-3.14150	0.00000	-0.00001	0.00003	0.00002	-3.14148
D8	-0.00007	0.00000	-0.00002	0.00004	0.00002	-0.00005
D9	-0.00153	0.00000	0.00002	0.00009	0.00010	-0.00142
D10	3.13943	0.00000	-0.00005	0.00006	0.00001	3.13944
D11	3.13996	0.00000	0.00002	0.00007	0.00009	3.14005
D12	-0.00227	0.00000	-0.00004	0.00005	0.00000	-0.00226
D13	-0.00016	0.00000	-0.00001	0.00002	0.00001	-0.00015
D14	3.14155	0.00000	0.00000	0.00001	0.00000	3.14155
D15	3.14099	0.00000	-0.00003	0.00004	0.00001	3.14100
D16	-0.00048	0.00000	-0.00003	0.00003	0.00000	-0.00048
D17	0.00081	0.00000	-0.00007	0.00000	-0.00007	0.00074
D18	-3.14117	0.00000	-0.00007	0.00005	-0.00002	-3.14119
D19	-3.14039	0.00000	-0.00005	-0.00002	-0.00007	-3.14046
D20	0.00082	0.00000	-0.00005	0.00003	-0.00003	0.00079
D21	0.00003	0.00000	0.00000	0.00000	0.00000	0.00003
D22	-3.14151	0.00000	0.00000	0.00000	0.00000	-3.14151
D23	3.14150	0.00000	0.00000	0.00001	0.00001	3.14151
D24	-0.00003	0.00000	0.00000	0.00001	0.00001	-0.00003
D25	0.00010	0.00000	0.00001	-0.00001	0.00000	0.00010
D26	-3.14149	0.00000	0.00001	-0.00001	0.00000	-3.14149
D27	-3.14155	0.00000	0.00000	0.00000	0.00000	-3.14155
D28	0.00005	0.00000	0.00000	-0.00001	0.00000	0.00005
D29	-0.00011	0.00000	0.00000	0.00000	0.00000	-0.00011
D30	-3.14153	0.00000	0.00000	-0.00001	-0.00001	-3.14154
D31	3.14148	0.00000	0.00000	0.00000	0.00000	3.14148
D32	0.00005	0.00000	0.00000	-0.00001	0.00000	0.00005
D33	0.00200	0.00000	-0.00006	-0.00008	-0.00014	0.00186
D34	-3.13803	0.00000	0.00002	-0.00021	-0.00019	-3.13821
D35	-3.13892	0.00000	0.00001	-0.00006	-0.00005	-3.13897
D36	0.00424	0.00000	0.00009	-0.00018	-0.00009	0.00414
D37	0.00078	0.00000	0.00009	-0.00012	-0.00003	0.00075
D38	-3.14037	0.00000	0.00011	-0.00008	0.00003	-3.14034
D39	-3.14159	0.00000	0.00001	-0.00015	-0.00014	3.14146
D40	0.00044	0.00000	0.00003	-0.00010	-0.00007	0.00037
D41	-0.00174	0.00000	0.00008	0.00005	0.00013	-0.00161
D42	3.13830	0.00000	0.00000	0.00017	0.00017	3.13848
D43	3.14024	0.00000	0.00008	0.00001	0.00009	3.14033
D44	-0.00290	0.00000	0.00000	0.00013	0.00013	-0.00276
D45	3.14157	0.00000	0.00002	-0.00010	-0.00009	3.14149
D46	0.00002	0.00000	-0.00004	-0.00005	-0.00009	-0.00007
D47	0.00182	0.00000	0.00011	-0.00025	-0.00014	0.00168
D48	-3.13974	0.00000	0.00005	-0.00020	-0.00014	-3.13988
D49	-0.00169	0.00000	-0.00006	0.00012	0.00006	-0.00163
D50	3.14119	0.00000	-0.00010	0.00006	-0.00004	3.14115
D51	3.13986	0.00000	-0.00001	0.00007	0.00006	3.13993

D52	-0.00044	0.00000	-0.00004	0.00001	-0.00003	-0.00047
D53	-3.13783	0.00000	0.00001	0.00001	0.00003	-3.13781
D54	0.00255	0.00000	0.00004	0.00007	0.00012	0.00267
D55	3.14158	0.00000	-0.00002	0.00000	-0.00002	3.14156
D56	0.00272	0.00000	-0.00001	0.00004	0.00004	0.00276
D57	0.00107	0.00000	-0.00005	-0.00006	-0.00010	0.00096
D58	-3.13779	0.00000	-0.00004	-0.00001	-0.00004	-3.13783
D59	0.00729	0.00000	0.00001	0.00006	0.00006	0.00736
D60	-3.12809	0.00000	0.00000	0.00003	0.00003	-3.12806
D61	-3.13516	0.00000	-0.00002	0.00002	0.00001	-3.13515
D62	0.01264	0.00000	-0.00002	0.00000	-0.00003	0.01262
D63	-0.00546	0.00000	-0.00003	-0.00007	-0.00010	-0.00556
D64	3.13746	0.00000	0.00000	-0.00002	-0.00002	3.13744
D65	-0.00022	0.00000	0.00001	0.00000	0.00001	-0.00021
D66	-3.13411	0.00000	0.00004	0.00001	0.00005	-3.13406
D67	3.14010	0.00000	-0.00003	-0.00005	-0.00007	3.14003
D68	0.00621	0.00000	0.00001	-0.00004	-0.00003	0.00618
D69	-0.00530	0.00000	0.00003	0.00000	0.00003	-0.00527
D70	3.13342	0.00000	0.00001	-0.00005	-0.00004	3.13338
D71	3.12782	0.00000	0.00004	0.00003	0.00008	3.12789
D72	-0.01666	0.00000	0.00003	-0.00001	0.00001	-0.01664
D73	-0.02015	0.00000	0.00003	0.00000	0.00003	-0.02012
D74	-3.05719	0.00000	0.00003	-0.00008	-0.00005	-3.05724
D75	3.12970	0.00000	0.00002	-0.00004	-0.00002	3.12969
D76	0.09266	0.00000	0.00002	-0.00011	-0.00009	0.09256
D77	-0.01240	0.00000	0.00002	-0.00001	0.00001	-0.01239
D78	3.13738	0.00000	-0.00002	-0.00001	-0.00003	3.13735
D79	3.12389	0.00000	-0.00001	-0.00001	-0.00002	3.12387
D80	-0.00952	0.00000	-0.00004	-0.00002	-0.00006	-0.00958
D81	-3.14114	0.00000	0.00001	0.00007	0.00008	-3.14106
D82	0.00843	0.00000	0.00004	0.00007	0.00012	0.00855
D83	0.02002	0.00000	-0.00003	0.00001	-0.00002	0.02000
D84	3.05676	0.00000	-0.00002	0.00007	0.00005	3.05680
D85	-3.13262	0.00000	0.00002	0.00001	0.00003	-3.13259
D86	-0.09589	0.00000	0.00002	0.00008	0.00010	-0.09579
D87	-3.13467	0.00000	0.00004	-0.00002	0.00002	-3.13465
D88	0.00525	0.00000	0.00001	-0.00007	-0.00005	0.00520
D89	0.01819	0.00000	-0.00001	-0.00003	-0.00004	0.01815
D90	-3.12507	0.00000	-0.00003	-0.00008	-0.00011	-3.12518
D91	1.55280	0.00000	0.00015	-0.00073	-0.00058	1.55222
D92	-2.61588	0.00000	0.00015	-0.00074	-0.00059	-2.61647
D93	-0.55322	0.00000	0.00015	-0.00076	-0.00061	-0.55382
D94	-1.46389	0.00000	0.00014	-0.00081	-0.00067	-1.46456
D95	0.65062	0.00000	0.00014	-0.00083	-0.00068	0.64994
D96	2.71327	0.00000	0.00014	-0.00084	-0.00069	2.71258
D97	-0.00554	0.00000	-0.00004	-0.00012	-0.00015	-0.00569
D98	3.13781	0.00000	-0.00005	-0.00008	-0.00013	3.13768
D99	-3.13756	0.00000	-0.00006	-0.00011	-0.00017	-3.13773
D100	0.00572	0.00000	-0.00003	-0.00006	-0.00009	0.00563
D101	-0.00863	0.00000	0.00005	0.00004	0.00009	-0.00855
D102	3.14101	0.00000	-0.00003	0.00002	-0.00001	3.14100
D103	0.00125	0.00000	0.00002	0.00013	0.00015	0.00139
D104	3.14155	0.00000	0.00000	0.00009	0.00009	-3.14154
D105	3.14151	0.00000	0.00003	0.00010	0.00013	-3.14155
D106	-0.00138	0.00000	0.00001	0.00006	0.00007	-0.00130
D107	3.13458	0.00000	0.00004	-0.00007	-0.00003	3.13456
D108	-0.01808	0.00000	-0.00005	-0.00010	-0.00016	-0.01823
D109	-0.00528	0.00000	0.00003	-0.00004	-0.00001	-0.00529
D110	3.12524	0.00000	-0.00006	-0.00007	-0.00014	3.12511
D111	0.00969	0.00000	-0.00006	-0.00001	-0.00006	0.00963

D112	-3.13726	0.00000	-0.00001	0.00001	0.00000	-3.13726
D113	-3.12386	0.00000	0.00001	0.00002	0.00003	-3.12383
D114	0.01237	0.00000	0.00006	0.00003	0.00009	0.01247
D115	3.13251	0.00000	-0.00001	-0.00001	-0.00002	3.13249
D116	0.09611	0.00000	-0.00004	-0.00006	-0.00011	0.09600
D117	-0.01994	0.00000	-0.00010	-0.00005	-0.00015	-0.02009
D118	-3.05634	0.00000	-0.00014	-0.00010	-0.00023	-3.05657
D119	3.13399	0.00000	0.00007	0.00002	0.00009	3.13408
D120	-0.00612	0.00000	0.00002	-0.00001	0.00001	-0.00610
D121	0.00017	0.00000	0.00000	0.00000	0.00000	0.00017
D122	-3.13994	0.00000	-0.00005	-0.00003	-0.00008	-3.14002
D123	3.13524	0.00000	-0.00003	-0.00002	-0.00005	3.13520
D124	-0.01255	0.00000	-0.00006	-0.00003	-0.00009	-0.01263
D125	-0.00735	0.00000	0.00001	0.00000	0.00001	-0.00735
D126	3.12805	0.00000	-0.00003	-0.00001	-0.00004	3.12801
D127	-3.13765	0.00000	0.00009	0.00005	0.00014	-3.13751
D128	0.00548	0.00000	0.00004	0.00003	0.00007	0.00555
D129	0.00537	0.00000	-0.00006	-0.00004	-0.00010	0.00527
D130	-3.13335	0.00000	-0.00002	-0.00003	-0.00005	-3.13340
D131	-3.12776	0.00000	-0.00002	-0.00003	-0.00004	-3.12781
D132	0.01670	0.00000	0.00002	-0.00002	0.00001	0.01670
D133	0.02004	0.00000	0.00010	0.00005	0.00014	0.02018
D134	3.05679	0.00000	0.00014	0.00009	0.00023	3.05702
D135	-3.12979	0.00000	0.00006	0.00003	0.00009	-3.12970
D136	-0.09304	0.00000	0.00009	0.00008	0.00017	-0.09286
D137	-0.00112	0.00001	0.00009	0.00006	0.00015	-0.00097
D138	-3.14149	0.00000	0.00001	-0.00001	0.00001	-3.14149
D139	3.13774	0.00000	0.00005	0.00005	0.00010	3.13784
D140	-0.00263	0.00000	-0.00002	-0.00002	-0.00004	-0.00267
D141	-0.00253	-0.00001	-0.00007	-0.00005	-0.00012	-0.00265
D142	3.13769	0.00000	0.00001	0.00003	0.00004	3.13773
D143	-3.14131	0.00000	0.00007	0.00004	0.00011	-3.14120
D144	0.00031	0.00000	0.00005	0.00006	0.00011	0.00042
D145	0.00174	0.00000	-0.00002	-0.00004	-0.00006	0.00168
D146	-3.13982	0.00000	-0.00004	-0.00002	-0.00006	-3.13988
D147	-0.64654	0.00000	0.00021	-0.00024	-0.00003	-0.64657
D148	1.46789	0.00000	0.00020	-0.00023	-0.00003	1.46786
D149	-2.70914	0.00000	0.00021	-0.00024	-0.00003	-2.70918
D150	2.62033	0.00000	0.00016	-0.00030	-0.00014	2.62019
D151	-1.54843	0.00000	0.00016	-0.00029	-0.00013	-1.54856
D152	0.55772	0.00000	0.00016	-0.00030	-0.00013	0.55759
D153	-0.00165	0.00000	0.00000	-0.00005	-0.00005	-0.00170
D154	-3.14150	0.00000	-0.00001	-0.00002	-0.00002	-3.14152
D155	3.13991	0.00000	0.00002	-0.00007	-0.00005	3.13986
D156	0.00006	0.00000	0.00001	-0.00003	-0.00002	0.00004
D157	-3.13857	0.00000	-0.00001	0.00007	0.00006	-3.13851
D158	0.00275	0.00000	-0.00001	0.00005	0.00004	0.00279
D159	0.00156	0.00000	0.00000	0.00004	0.00003	0.00159
D160	-3.14031	0.00000	0.00000	0.00002	0.00002	-3.14029
D161	3.13826	0.00000	0.00002	-0.00008	-0.00006	3.13820
D162	-0.00410	0.00000	0.00004	-0.00013	-0.00008	-0.00418
D163	-0.00185	0.00000	0.00001	-0.00005	-0.00004	-0.00189
D164	3.13898	0.00000	0.00003	-0.00009	-0.00006	3.13892
D165	-0.00066	0.00000	-0.00001	-0.00001	-0.00002	-0.00068
D166	3.14050	0.00000	0.00001	-0.00003	-0.00003	3.14047
D167	3.14120	0.00000	-0.00001	0.00001	0.00000	3.14120
D168	-0.00082	0.00000	0.00001	-0.00002	-0.00001	-0.00083
D169	0.00146	0.00000	-0.00002	0.00005	0.00003	0.00149
D170	-3.14002	0.00000	-0.00003	0.00008	0.00005	-3.13997
D171	-3.13940	0.00000	-0.00004	0.00009	0.00005	-3.13935

D172	0.00231	0.00000	-0.00005	0.00012	0.00007	0.00238
D173	-0.00041	0.00000	-0.00001	0.00001	0.00000	-0.00041
D174	-3.14150	0.00000	-0.00002	0.00002	0.00000	-3.14150
D175	3.14028	0.00000	0.00002	-0.00004	-0.00002	3.14026
D176	-0.00080	0.00000	0.00001	-0.00003	-0.00002	-0.00083
D177	-0.00049	0.00000	0.00002	-0.00003	-0.00001	-0.00050
D178	3.14101	0.00000	0.00003	-0.00005	-0.00002	3.14098
D179	3.14151	0.00000	0.00000	0.00000	0.00000	3.14151
D180	-0.00018	0.00000	0.00001	-0.00002	-0.00001	-0.00019
D181	-3.14094	0.00000	-0.00002	0.00004	0.00001	-3.14092
D182	0.00052	0.00000	-0.00001	0.00003	0.00002	0.00053
D183	0.00017	0.00000	-0.00001	0.00001	0.00000	0.00017
D184	-3.14156	0.00000	0.00001	0.00000	0.00000	-3.14156
D185	3.14151	0.00000	0.00000	-0.00001	-0.00001	3.14150
D186	0.00007	0.00000	0.00000	0.00000	0.00000	0.00007
D187	0.00004	0.00000	-0.00001	0.00002	0.00001	0.00005
D188	-3.14140	0.00000	-0.00001	0.00003	0.00002	-3.14138
D189	-0.00002	0.00000	0.00000	0.00002	0.00001	-0.00001
D190	3.14152	0.00000	0.00000	0.00000	-0.00001	3.14151
D191	-3.14147	0.00000	-0.00002	0.00003	0.00001	-3.14146
D192	0.00007	0.00000	-0.00001	0.00001	-0.00001	0.00006
D193	0.00010	0.00000	0.00000	0.00000	0.00000	0.00011
D194	-3.14149	0.00000	0.00000	0.00000	0.00000	-3.14149
D195	3.14155	0.00000	0.00000	-0.00001	-0.00001	3.14154
D196	-0.00004	0.00000	0.00000	-0.00001	-0.00001	-0.00005
D197	-0.00011	0.00000	0.00001	-0.00002	-0.00001	-0.00013
D198	3.14148	0.00000	0.00000	-0.00002	-0.00001	3.14147
D199	3.14153	0.00000	0.00001	0.00000	0.00000	3.14154
D200	-0.00006	0.00000	0.00000	0.00000	0.00000	-0.00006

Item	Value	Threshold	Converged?

Maximum Force	0.000018	0.000450	YES

RMS Force	0.000004	0.000300	YES

Maximum Displacement	0.001627	0.001800	YES

RMS Displacement	0.000299	0.001200	YES

Predicted change in Energy=-1.517239D-08

Optimization completed.

-- Stationary point found.

! Optimized Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.

! R1	R(1,2)	1.4068	-DE/DX = 0.0

! R2	R(1,6)	1.3995	-DE/DX = 0.0

! R3	R(1,11)	1.4872	-DE/DX = 0.0

! R4	R(2,3)	1.3872	-DE/DX = 0.0

! R5	R(2,12)	1.4786	-DE/DX = 0.0

! R6	R(3,4)	1.3962	-DE/DX = 0.0

! R7	R(3,7)	1.0852	-DE/DX = 0.0

!	R8	R(4,5)	1.4003	-DE/DX =	0.0
!					
!	R9	R(4,8)	1.0856	-DE/DX =	0.0
!					
!	R10	R(5,6)	1.3988	-DE/DX =	0.0
!					
!	R11	R(5,9)	1.0857	-DE/DX =	0.0
!					
!	R12	R(6,10)	1.0807	-DE/DX =	0.0
!					
!	R13	R(11,13)	1.466	-DE/DX =	0.0
!					
!	R14	R(11,50)	1.3845	-DE/DX =	0.0
!					
!	R15	R(12,13)	1.4799	-DE/DX =	0.0
!					
!	R16	R(12,55)	1.2262	-DE/DX =	0.0
!					
!	R17	R(13,14)	1.3788	-DE/DX =	0.0
!					
!	R18	R(14,15)	1.4168	-DE/DX =	0.0
!					
!	R19	R(14,71)	1.0832	-DE/DX =	0.0
!					
!	R20	R(15,18)	1.7901	-DE/DX =	0.0
!					
!	R21	R(15,19)	1.4073	-DE/DX =	0.0
!					
!	R22	R(16,17)	1.419	-DE/DX =	0.0
!					
!	R23	R(16,18)	1.7359	-DE/DX =	0.0
!					
!	R24	R(16,20)	1.4029	-DE/DX =	0.0
!					
!	R25	R(17,19)	1.3914	-DE/DX =	0.0
!					
!	R26	R(17,22)	1.3874	-DE/DX =	0.0
!					
!	R27	R(19,72)	1.0838	-DE/DX =	0.0
!					
!	R28	R(20,21)	1.4144	-DE/DX =	0.0
!					
!	R29	R(20,23)	1.7557	-DE/DX =	0.0
!					
!	R30	R(21,22)	1.3763	-DE/DX =	0.0
!					
!	R31	R(21,26)	1.411	-DE/DX =	0.0
!					
!	R32	R(22,61)	1.4524	-DE/DX =	0.0
!					
!	R33	R(23,25)	1.7621	-DE/DX =	0.0
!					
!	R34	R(24,26)	1.7621	-DE/DX =	0.0
!					
!	R35	R(24,28)	1.7557	-DE/DX =	0.0
!					
!	R36	R(25,26)	1.4044	-DE/DX =	0.0
!					
!	R37	R(25,27)	1.411	-DE/DX =	0.0
!					

!	R38	R(27,28)	1.4144	-DE/DX =	0.0
!					
!	R39	R(27,34)	1.3763	-DE/DX =	0.0
!					
!	R40	R(28,29)	1.4029	-DE/DX =	0.0
!					
!	R41	R(29,30)	1.419	-DE/DX =	0.0
!					
!	R42	R(29,33)	1.7358	-DE/DX =	0.0
!					
!	R43	R(30,31)	1.3914	-DE/DX =	0.0
!					
!	R44	R(30,34)	1.3874	-DE/DX =	0.0
!					
!	R45	R(31,32)	1.4073	-DE/DX =	0.0
!					
!	R46	R(31,65)	1.0838	-DE/DX =	0.0
!					
!	R47	R(32,33)	1.7901	-DE/DX =	0.0
!					
!	R48	R(32,35)	1.4169	-DE/DX =	0.0
!					
!	R49	R(34,57)	1.4524	-DE/DX =	0.0
!					
!	R50	R(35,36)	1.3787	-DE/DX =	0.0
!					
!	R51	R(35,70)	1.0832	-DE/DX =	0.0
!					
!	R52	R(36,37)	1.4799	-DE/DX =	0.0
!					
!	R53	R(36,38)	1.466	-DE/DX =	0.0
!					
!	R54	R(37,39)	1.4786	-DE/DX =	0.0
!					
!	R55	R(37,56)	1.2262	-DE/DX =	0.0
!					
!	R56	R(38,40)	1.4872	-DE/DX =	0.0
!					
!	R57	R(38,45)	1.3845	-DE/DX =	0.0
!					
!	R58	R(39,40)	1.4068	-DE/DX =	0.0
!					
!	R59	R(39,41)	1.3872	-DE/DX =	0.0
!					
!	R60	R(40,42)	1.3995	-DE/DX =	0.0
!					
!	R61	R(41,43)	1.3962	-DE/DX =	0.0
!					
!	R62	R(41,69)	1.0852	-DE/DX =	0.0
!					
!	R63	R(42,44)	1.3988	-DE/DX =	0.0
!					
!	R64	R(42,66)	1.0807	-DE/DX =	0.0
!					
!	R65	R(43,44)	1.4003	-DE/DX =	0.0
!					
!	R66	R(43,68)	1.0856	-DE/DX =	0.0
!					
!	R67	R(44,67)	1.0857	-DE/DX =	0.0
!					

!	R68	R(45,46)	1.4288	-DE/DX =	0.0
!					
!	R69	R(45,47)	1.4284	-DE/DX =	0.0
!					
!	R70	R(46,48)	1.1656	-DE/DX =	0.0
!					
!	R71	R(47,49)	1.165	-DE/DX =	0.0
!					
!	R72	R(50,51)	1.4284	-DE/DX =	0.0
!					
!	R73	R(50,52)	1.4288	-DE/DX =	0.0
!					
!	R74	R(51,53)	1.165	-DE/DX =	0.0
!					
!	R75	R(52,54)	1.1656	-DE/DX =	0.0
!					
!	R76	R(57,58)	1.0923	-DE/DX =	0.0
!					
!	R77	R(57,59)	1.0954	-DE/DX =	0.0
!					
!	R78	R(57,60)	1.0917	-DE/DX =	0.0
!					
!	R79	R(61,62)	1.0954	-DE/DX =	0.0
!					
!	R80	R(61,63)	1.0923	-DE/DX =	0.0
!					
!	R81	R(61,64)	1.0917	-DE/DX =	0.0
!					
!	A1	A(2,1,6)	118.9499	-DE/DX =	0.0
!					
!	A2	A(2,1,11)	108.7851	-DE/DX =	0.0
!					
!	A3	A(6,1,11)	132.2651	-DE/DX =	0.0
!					
!	A4	A(1,2,3)	122.7598	-DE/DX =	0.0
!					
!	A5	A(1,2,12)	109.5282	-DE/DX =	0.0
!					
!	A6	A(3,2,12)	127.712	-DE/DX =	0.0
!					
!	A7	A(2,3,4)	117.9798	-DE/DX =	0.0
!					
!	A8	A(2,3,7)	119.7045	-DE/DX =	0.0
!					
!	A9	A(4,3,7)	122.3157	-DE/DX =	0.0
!					
!	A10	A(3,4,5)	120.049	-DE/DX =	0.0
!					
!	A11	A(3,4,8)	120.1921	-DE/DX =	0.0
!					
!	A12	A(5,4,8)	119.7588	-DE/DX =	0.0
!					
!	A13	A(4,5,6)	121.7431	-DE/DX =	0.0
!					
!	A14	A(4,5,9)	119.4494	-DE/DX =	0.0
!					
!	A15	A(6,5,9)	118.8075	-DE/DX =	0.0
!					
!	A16	A(1,6,5)	118.5185	-DE/DX =	0.0
!					

!	A17	A(1,6,10)	122.1175	-DE/DX =	0.0
!					
!	A18	A(5,6,10)	119.364	-DE/DX =	0.0
!					
!	A19	A(1,11,13)	107.1713	-DE/DX =	0.0
!					
!	A20	A(1,11,50)	124.603	-DE/DX =	0.0
!					
!	A21	A(13,11,50)	128.2257	-DE/DX =	0.0
!					
!	A22	A(2,12,13)	106.7285	-DE/DX =	0.0
!					
!	A23	A(2,12,55)	125.7121	-DE/DX =	0.0
!					
!	A24	A(13,12,55)	127.5594	-DE/DX =	0.0
!					
!	A25	A(11,13,12)	107.7867	-DE/DX =	0.0
!					
!	A26	A(11,13,14)	126.5465	-DE/DX =	0.0
!					
!	A27	A(12,13,14)	125.6667	-DE/DX =	0.0
!					
!	A28	A(13,14,15)	134.3061	-DE/DX =	0.0
!					
!	A29	A(13,14,71)	115.5907	-DE/DX =	0.0
!					
!	A30	A(15,14,71)	110.1032	-DE/DX =	0.0
!					
!	A31	A(14,15,18)	128.8812	-DE/DX =	0.0
!					
!	A32	A(14,15,19)	119.3765	-DE/DX =	0.0
!					
!	A33	A(18,15,19)	111.7423	-DE/DX =	0.0
!					
!	A34	A(17,16,18)	112.2188	-DE/DX =	0.0
!					
!	A35	A(17,16,20)	106.427	-DE/DX =	0.0
!					
!	A36	A(18,16,20)	141.3542	-DE/DX =	0.0
!					
!	A37	A(16,17,19)	113.6916	-DE/DX =	0.0
!					
!	A38	A(16,17,22)	109.8503	-DE/DX =	0.0
!					
!	A39	A(19,17,22)	136.4567	-DE/DX =	0.0
!					
!	A40	A(15,18,16)	90.0699	-DE/DX =	0.0
!					
!	A41	A(15,19,17)	112.276	-DE/DX =	0.0
!					
!	A42	A(15,19,72)	121.7781	-DE/DX =	0.0
!					
!	A43	A(17,19,72)	125.9457	-DE/DX =	0.0
!					
!	A44	A(16,20,21)	106.9594	-DE/DX =	0.0
!					
!	A45	A(16,20,23)	140.4846	-DE/DX =	0.0
!					
!	A46	A(21,20,23)	112.5549	-DE/DX =	0.0
!					

!	A47	A(20,21,22)	110.0819	-DE/DX =	0.0
!					
!	A48	A(20,21,26)	112.9178	-DE/DX =	0.0
!					
!	A49	A(22,21,26)	136.9979	-DE/DX =	0.0
!					
!	A50	A(17,22,21)	106.6679	-DE/DX =	0.0
!					
!	A51	A(17,22,61)	126.4001	-DE/DX =	0.0
!					
!	A52	A(21,22,61)	126.6309	-DE/DX =	0.0
!					
!	A53	A(20,23,25)	89.4568	-DE/DX =	0.0
!					
!	A54	A(26,24,28)	89.455	-DE/DX =	0.0
!					
!	A55	A(23,25,26)	113.6064	-DE/DX =	0.0
!					
!	A56	A(23,25,27)	134.9327	-DE/DX =	0.0
!					
!	A57	A(26,25,27)	111.4608	-DE/DX =	0.0
!					
!	A58	A(21,26,24)	134.9302	-DE/DX =	0.0
!					
!	A59	A(21,26,25)	111.4614	-DE/DX =	0.0
!					
!	A60	A(24,26,25)	113.6083	-DE/DX =	0.0
!					
!	A61	A(25,27,28)	112.9156	-DE/DX =	0.0
!					
!	A62	A(25,27,34)	137.0018	-DE/DX =	0.0
!					
!	A63	A(28,27,34)	110.0803	-DE/DX =	0.0
!					
!	A64	A(24,28,27)	112.5575	-DE/DX =	0.0
!					
!	A65	A(24,28,29)	140.4804	-DE/DX =	0.0
!					
!	A66	A(27,28,29)	106.961	-DE/DX =	0.0
!					
!	A67	A(28,29,30)	106.4261	-DE/DX =	0.0
!					
!	A68	A(28,29,33)	141.3552	-DE/DX =	0.0
!					
!	A69	A(30,29,33)	112.2187	-DE/DX =	0.0
!					
!	A70	A(29,30,31)	113.693	-DE/DX =	0.0
!					
!	A71	A(29,30,34)	109.8519	-DE/DX =	0.0
!					
!	A72	A(31,30,34)	136.4537	-DE/DX =	0.0
!					
!	A73	A(30,31,32)	112.275	-DE/DX =	0.0
!					
!	A74	A(30,31,65)	125.9451	-DE/DX =	0.0
!					
!	A75	A(32,31,65)	121.7798	-DE/DX =	0.0
!					
!	A76	A(31,32,33)	111.7416	-DE/DX =	0.0
!					

!	A77	A(31,32,35)	119.3766	-DE/DX =	0.0
!					
!	A78	A(33,32,35)	128.8817	-DE/DX =	0.0
!					
!	A79	A(29,33,32)	90.0703	-DE/DX =	0.0
!					
!	A80	A(27,34,30)	106.6673	-DE/DX =	0.0
!					
!	A81	A(27,34,57)	126.6459	-DE/DX =	0.0
!					
!	A82	A(30,34,57)	126.3837	-DE/DX =	0.0
!					
!	A83	A(32,35,36)	134.3034	-DE/DX =	0.0
!					
!	A84	A(32,35,70)	110.1045	-DE/DX =	0.0
!					
!	A85	A(36,35,70)	115.5922	-DE/DX =	0.0
!					
!	A86	A(35,36,37)	125.6648	-DE/DX =	0.0
!					
!	A87	A(35,36,38)	126.5485	-DE/DX =	0.0
!					
!	A88	A(37,36,38)	107.7866	-DE/DX =	0.0
!					
!	A89	A(36,37,39)	106.7285	-DE/DX =	0.0
!					
!	A90	A(36,37,56)	127.5587	-DE/DX =	0.0
!					
!	A91	A(39,37,56)	125.7127	-DE/DX =	0.0
!					
!	A92	A(36,38,40)	107.1711	-DE/DX =	0.0
!					
!	A93	A(36,38,45)	128.2251	-DE/DX =	0.0
!					
!	A94	A(40,38,45)	124.6037	-DE/DX =	0.0
!					
!	A95	A(37,39,40)	109.5282	-DE/DX =	0.0
!					
!	A96	A(37,39,41)	127.7119	-DE/DX =	0.0
!					
!	A97	A(40,39,41)	122.7599	-DE/DX =	0.0
!					
!	A98	A(38,40,39)	108.7854	-DE/DX =	0.0
!					
!	A99	A(38,40,42)	132.2645	-DE/DX =	0.0
!					
!	A100	A(39,40,42)	118.9501	-DE/DX =	0.0
!					
!	A101	A(39,41,43)	117.9794	-DE/DX =	0.0
!					
!	A102	A(39,41,69)	119.7045	-DE/DX =	0.0
!					
!	A103	A(43,41,69)	122.3161	-DE/DX =	0.0
!					
!	A104	A(40,42,44)	118.5182	-DE/DX =	0.0
!					
!	A105	A(40,42,66)	122.1175	-DE/DX =	0.0
!					
!	A106	A(44,42,66)	119.3643	-DE/DX =	0.0
!					

!	A107	A(41,43,44)	120.0492	-DE/DX =	0.0
!					
!	A108	A(41,43,68)	120.1923	-DE/DX =	0.0
!					
!	A109	A(44,43,68)	119.7585	-DE/DX =	0.0
!					
!	A110	A(42,44,43)	121.7432	-DE/DX =	0.0
!					
!	A111	A(42,44,67)	118.8078	-DE/DX =	0.0
!					
!	A112	A(43,44,67)	119.449	-DE/DX =	0.0
!					
!	A113	A(38,45,46)	124.1552	-DE/DX =	0.0
!					
!	A114	A(38,45,47)	123.5408	-DE/DX =	0.0
!					
!	A115	A(46,45,47)	112.304	-DE/DX =	0.0
!					
!	A116	A(11,50,51)	123.5407	-DE/DX =	0.0
!					
!	A117	A(11,50,52)	124.1554	-DE/DX =	0.0
!					
!	A118	A(51,50,52)	112.3039	-DE/DX =	0.0
!					
!	A119	A(34,57,58)	109.5939	-DE/DX =	0.0
!					
!	A120	A(34,57,59)	111.6601	-DE/DX =	0.0
!					
!	A121	A(34,57,60)	109.1161	-DE/DX =	0.0
!					
!	A122	A(58,57,59)	109.2147	-DE/DX =	0.0
!					
!	A123	A(58,57,60)	108.0907	-DE/DX =	0.0
!					
!	A124	A(59,57,60)	109.0933	-DE/DX =	0.0
!					
!	A125	A(22,61,62)	111.6598	-DE/DX =	0.0
!					
!	A126	A(22,61,63)	109.5992	-DE/DX =	0.0
!					
!	A127	A(22,61,64)	109.1125	-DE/DX =	0.0
!					
!	A128	A(62,61,63)	109.2156	-DE/DX =	0.0
!					
!	A129	A(62,61,64)	109.0893	-DE/DX =	0.0
!					
!	A130	A(63,61,64)	108.0923	-DE/DX =	0.0
!					
!	A131	L(45,46,48,2,-1)	181.4494	-DE/DX =	0.0
!					
!	A132	L(45,47,49,41,-1)	182.173	-DE/DX =	0.0
!					
!	A133	L(50,51,53,3,-1)	182.1727	-DE/DX =	0.0
!					
!	A134	L(50,52,54,16,-1)	181.4491	-DE/DX =	0.0
!					
!	A135	L(45,46,48,2,-2)	179.9944	-DE/DX =	0.0
!					
!	A136	L(45,47,49,41,-2)	180.0015	-DE/DX =	0.0
!					

!	A137	L(50,51,53,3,-2)	179.9991	-DE/DX =	0.0
!					
!	A138	L(50,52,54,16,-2)	180.0002	-DE/DX =	0.0
!					
!	D1	D(6,1,2,3)	0.0088	-DE/DX =	0.0
!					
!	D2	D(6,1,2,12)	-179.9698	-DE/DX =	0.0
!					
!	D3	D(11,1,2,3)	-179.9962	-DE/DX =	0.0
!					
!	D4	D(11,1,2,12)	0.0251	-DE/DX =	0.0
!					
!	D5	D(2,1,6,5)	-0.0011	-DE/DX =	0.0
!					
!	D6	D(2,1,6,10)	179.9892	-DE/DX =	0.0
!					
!	D7	D(11,1,6,5)	-179.9946	-DE/DX =	0.0
!					
!	D8	D(11,1,6,10)	-0.0043	-DE/DX =	0.0
!					
!	D9	D(2,1,11,13)	-0.0874	-DE/DX =	0.0
!					
!	D10	D(2,1,11,50)	179.876	-DE/DX =	0.0
!					
!	D11	D(6,1,11,13)	179.9066	-DE/DX =	0.0
!					
!	D12	D(6,1,11,50)	-0.13	-DE/DX =	0.0
!					
!	D13	D(1,2,3,4)	-0.0091	-DE/DX =	0.0
!					
!	D14	D(1,2,3,7)	179.9976	-DE/DX =	0.0
!					
!	D15	D(12,2,3,4)	179.9656	-DE/DX =	0.0
!					
!	D16	D(12,2,3,7)	-0.0277	-DE/DX =	0.0
!					
!	D17	D(1,2,12,13)	0.0462	-DE/DX =	0.0
!					
!	D18	D(1,2,12,55)	-179.9758	-DE/DX =	0.0
!					
!	D19	D(3,2,12,13)	-179.9311	-DE/DX =	0.0
!					
!	D20	D(3,2,12,55)	0.0469	-DE/DX =	0.0
!					
!	D21	D(2,3,4,5)	0.0017	-DE/DX =	0.0
!					
!	D22	D(2,3,4,8)	-179.995	-DE/DX =	0.0
!					
!	D23	D(7,3,4,5)	179.9948	-DE/DX =	0.0
!					
!	D24	D(7,3,4,8)	-0.0019	-DE/DX =	0.0
!					
!	D25	D(3,4,5,6)	0.0058	-DE/DX =	0.0
!					
!	D26	D(3,4,5,9)	-179.9939	-DE/DX =	0.0
!					
!	D27	D(8,4,5,6)	-179.9974	-DE/DX =	0.0
!					
!	D28	D(8,4,5,9)	0.0029	-DE/DX =	0.0
!					

!	D29	D(4,5,6,1)	-0.006	-DE/DX =	0.0
!					
!	D30	D(4,5,6,10)	-179.9966	-DE/DX =	0.0
!					
!	D31	D(9,5,6,1)	179.9937	-DE/DX =	0.0
!					
!	D32	D(9,5,6,10)	0.003	-DE/DX =	0.0
!					
!	D33	D(1,11,13,12)	0.1147	-DE/DX =	0.0
!					
!	D34	D(1,11,13,14)	-179.7956	-DE/DX =	0.0
!					
!	D35	D(50,11,13,12)	-179.847	-DE/DX =	0.0
!					
!	D36	D(50,11,13,14)	0.2427	-DE/DX =	0.0
!					
!	D37	D(1,11,50,51)	0.0447	-DE/DX =	0.0
!					
!	D38	D(1,11,50,52)	-179.9301	-DE/DX =	0.0
!					
!	D39	D(13,11,50,51)	180.0002	-DE/DX =	0.0
!					
!	D40	D(13,11,50,52)	0.0254	-DE/DX =	0.0
!					
!	D41	D(2,12,13,11)	-0.0998	-DE/DX =	0.0
!					
!	D42	D(2,12,13,14)	179.8116	-DE/DX =	0.0
!					
!	D43	D(55,12,13,11)	179.9228	-DE/DX =	0.0
!					
!	D44	D(55,12,13,14)	-0.1659	-DE/DX =	0.0
!					
!	D45	D(11,13,14,15)	179.9989	-DE/DX =	0.0
!					
!	D46	D(11,13,14,71)	0.0012	-DE/DX =	0.0
!					
!	D47	D(12,13,14,15)	0.104	-DE/DX =	0.0
!					
!	D48	D(12,13,14,71)	-179.8937	-DE/DX =	0.0
!					
!	D49	D(13,14,15,18)	-0.0969	-DE/DX =	0.0
!					
!	D50	D(13,14,15,19)	179.977	-DE/DX =	0.0
!					
!	D51	D(71,14,15,18)	179.9009	-DE/DX =	0.0
!					
!	D52	D(71,14,15,19)	-0.0252	-DE/DX =	0.0
!					
!	D53	D(14,15,18,16)	-179.7846	-DE/DX =	0.0
!					
!	D54	D(19,15,18,16)	0.146	-DE/DX =	0.0
!					
!	D55	D(14,15,19,17)	179.9991	-DE/DX =	0.0
!					
!	D56	D(14,15,19,72)	0.1561	-DE/DX =	0.0
!					
!	D57	D(18,15,19,17)	0.061	-DE/DX =	0.0
!					
!	D58	D(18,15,19,72)	-179.7819	-DE/DX =	0.0
!					

!	D59	D(18,16,17,19)	0.4177	-DE/DX =	0.0
!					
!	D60	D(18,16,17,22)	-179.2264	-DE/DX =	0.0
!					
!	D61	D(20,16,17,19)	-179.6315	-DE/DX =	0.0
!					
!	D62	D(20,16,17,22)	0.7243	-DE/DX =	0.0
!					
!	D63	D(17,16,18,15)	-0.3126	-DE/DX =	0.0
!					
!	D64	D(20,16,18,15)	179.763	-DE/DX =	0.0
!					
!	D65	D(17,16,20,21)	-0.0124	-DE/DX =	0.0
!					
!	D66	D(17,16,20,23)	-179.5711	-DE/DX =	0.0
!					
!	D67	D(18,16,20,21)	179.9146	-DE/DX =	0.0
!					
!	D68	D(18,16,20,23)	0.3558	-DE/DX =	0.0
!					
!	D69	D(16,17,19,15)	-0.3035	-DE/DX =	0.0
!					
!	D70	D(16,17,19,72)	179.5316	-DE/DX =	0.0
!					
!	D71	D(22,17,19,15)	179.2106	-DE/DX =	0.0
!					
!	D72	D(22,17,19,72)	-0.9543	-DE/DX =	0.0
!					
!	D73	D(16,17,22,21)	-1.1543	-DE/DX =	0.0
!					
!	D74	D(16,17,22,61)	-175.1642	-DE/DX =	0.0
!					
!	D75	D(19,17,22,21)	179.3188	-DE/DX =	0.0
!					
!	D76	D(19,17,22,61)	5.3089	-DE/DX =	0.0
!					
!	D77	D(16,20,21,22)	-0.7104	-DE/DX =	0.0
!					
!	D78	D(16,20,21,26)	179.7585	-DE/DX =	0.0
!					
!	D79	D(23,20,21,22)	178.9856	-DE/DX =	0.0
!					
!	D80	D(23,20,21,26)	-0.5455	-DE/DX =	0.0
!					
!	D81	D(16,20,23,25)	-179.9739	-DE/DX =	0.0
!					
!	D82	D(21,20,23,25)	0.4831	-DE/DX =	0.0
!					
!	D83	D(20,21,22,17)	1.1473	-DE/DX =	0.0
!					
!	D84	D(20,21,22,61)	175.1393	-DE/DX =	0.0
!					
!	D85	D(26,21,22,17)	-179.4859	-DE/DX =	0.0
!					
!	D86	D(26,21,22,61)	-5.494	-DE/DX =	0.0
!					
!	D87	D(20,21,26,24)	-179.6034	-DE/DX =	0.0
!					
!	D88	D(20,21,26,25)	0.301	-DE/DX =	0.0
!					

!	D89	D(22,21,26,24)	1.0424	-DE/DX =	0.0
!					
!	D90	D(22,21,26,25)	-179.0533	-DE/DX =	0.0
!					
!	D91	D(17,22,61,62)	88.9689	-DE/DX =	0.0
!					
!	D92	D(17,22,61,63)	-149.8787	-DE/DX =	0.0
!					
!	D93	D(17,22,61,64)	-31.6971	-DE/DX =	0.0
!					
!	D94	D(21,22,61,62)	-83.8748	-DE/DX =	0.0
!					
!	D95	D(21,22,61,63)	37.2776	-DE/DX =	0.0
!					
!	D96	D(21,22,61,64)	155.4592	-DE/DX =	0.0
!					
!	D97	D(20,23,25,26)	-0.3172	-DE/DX =	0.0
!					
!	D98	D(20,23,25,27)	179.7833	-DE/DX =	0.0
!					
!	D99	D(28,24,26,21)	-179.7692	-DE/DX =	0.0
!					
!	D100	D(28,24,26,25)	0.3279	-DE/DX =	0.0
!					
!	D101	D(26,24,28,27)	-0.4946	-DE/DX =	0.0
!					
!	D102	D(26,24,28,29)	179.9666	-DE/DX =	0.0
!					
!	D103	D(23,25,26,21)	0.0716	-DE/DX =	0.0
!					
!	D104	D(23,25,26,24)	-180.0023	-DE/DX =	0.0
!					
!	D105	D(27,25,26,21)	-180.0049	-DE/DX =	0.0
!					
!	D106	D(27,25,26,24)	-0.0788	-DE/DX =	0.0
!					
!	D107	D(23,25,27,28)	179.5984	-DE/DX =	0.0
!					
!	D108	D(23,25,27,34)	-1.0358	-DE/DX =	0.0
!					
!	D109	D(26,25,27,28)	-0.3026	-DE/DX =	0.0
!					
!	D110	D(26,25,27,34)	179.0632	-DE/DX =	0.0
!					
!	D111	D(25,27,28,24)	0.5553	-DE/DX =	0.0
!					
!	D112	D(25,27,28,29)	-179.7515	-DE/DX =	0.0
!					
!	D113	D(34,27,28,24)	-178.9842	-DE/DX =	0.0
!					
!	D114	D(34,27,28,29)	0.709	-DE/DX =	0.0
!					
!	D115	D(25,27,34,30)	179.4794	-DE/DX =	0.0
!					
!	D116	D(25,27,34,57)	5.5067	-DE/DX =	0.0
!					
!	D117	D(28,27,34,30)	-1.1425	-DE/DX =	0.0
!					
!	D118	D(28,27,34,57)	-175.1153	-DE/DX =	0.0
!					

!	D119	D(24,28,29,30)	179.5647	-DE/DX =	0.0
!					
!	D120	D(24,28,29,33)	-0.3504	-DE/DX =	0.0
!					
!	D121	D(27,28,29,30)	0.0099	-DE/DX =	0.0
!					
!	D122	D(27,28,29,33)	-179.9051	-DE/DX =	0.0
!					
!	D123	D(28,29,30,31)	179.636	-DE/DX =	0.0
!					
!	D124	D(28,29,30,34)	-0.7188	-DE/DX =	0.0
!					
!	D125	D(33,29,30,31)	-0.4213	-DE/DX =	0.0
!					
!	D126	D(33,29,30,34)	179.2238	-DE/DX =	0.0
!					
!	D127	D(28,29,33,32)	-179.7741	-DE/DX =	0.0
!					
!	D128	D(30,29,33,32)	0.314	-DE/DX =	0.0
!					
!	D129	D(29,30,31,32)	0.3079	-DE/DX =	0.0
!					
!	D130	D(29,30,31,65)	-179.5279	-DE/DX =	0.0
!					
!	D131	D(34,30,31,32)	-179.2076	-DE/DX =	0.0
!					
!	D132	D(34,30,31,65)	0.9566	-DE/DX =	0.0
!					
!	D133	D(29,30,34,27)	1.1479	-DE/DX =	0.0
!					
!	D134	D(29,30,34,57)	175.1411	-DE/DX =	0.0
!					
!	D135	D(31,30,34,27)	-179.3238	-DE/DX =	0.0
!					
!	D136	D(31,30,34,57)	-5.3306	-DE/DX =	0.0
!					
!	D137	D(30,31,32,33)	-0.0643	-DE/DX =	0.0
!					
!	D138	D(30,31,32,35)	-179.9942	-DE/DX =	0.0
!					
!	D139	D(65,31,32,33)	179.7793	-DE/DX =	0.0
!					
!	D140	D(65,31,32,35)	-0.1506	-DE/DX =	0.0
!					
!	D141	D(31,32,33,29)	-0.1449	-DE/DX =	0.0
!					
!	D142	D(35,32,33,29)	179.7766	-DE/DX =	0.0
!					
!	D143	D(31,32,35,36)	-179.984	-DE/DX =	0.0
!					
!	D144	D(31,32,35,70)	0.0179	-DE/DX =	0.0
!					
!	D145	D(33,32,35,36)	0.0997	-DE/DX =	0.0
!					
!	D146	D(33,32,35,70)	-179.8984	-DE/DX =	0.0
!					
!	D147	D(27,34,57,58)	-37.044	-DE/DX =	0.0
!					
!	D148	D(27,34,57,59)	84.1038	-DE/DX =	0.0
!					

!	D149	D(27,34,57,60)	-155.2225	-DE/DX =	0.0
!					
!	D150	D(30,34,57,58)	150.1337	-DE/DX =	0.0
!					
!	D151	D(30,34,57,59)	-88.7185	-DE/DX =	0.0
!					
!	D152	D(30,34,57,60)	31.9552	-DE/DX =	0.0
!					
!	D153	D(32,35,36,37)	-0.0944	-DE/DX =	0.0
!					
!	D154	D(32,35,36,38)	-179.9947	-DE/DX =	0.0
!					
!	D155	D(70,35,36,37)	179.9037	-DE/DX =	0.0
!					
!	D156	D(70,35,36,38)	0.0033	-DE/DX =	0.0
!					
!	D157	D(35,36,37,39)	-179.8267	-DE/DX =	0.0
!					
!	D158	D(35,36,37,56)	0.1576	-DE/DX =	0.0
!					
!	D159	D(38,36,37,39)	0.0893	-DE/DX =	0.0
!					
!	D160	D(38,36,37,56)	-179.9265	-DE/DX =	0.0
!					
!	D161	D(35,36,38,40)	179.8091	-DE/DX =	0.0
!					
!	D162	D(35,36,38,45)	-0.235	-DE/DX =	0.0
!					
!	D163	D(37,36,38,40)	-0.1059	-DE/DX =	0.0
!					
!	D164	D(37,36,38,45)	179.85	-DE/DX =	0.0
!					
!	D165	D(36,37,39,40)	-0.0379	-DE/DX =	0.0
!					
!	D166	D(36,37,39,41)	179.9374	-DE/DX =	0.0
!					
!	D167	D(56,37,39,40)	179.9775	-DE/DX =	0.0
!					
!	D168	D(56,37,39,41)	-0.0472	-DE/DX =	0.0
!					
!	D169	D(36,38,40,39)	0.0837	-DE/DX =	0.0
!					
!	D170	D(36,38,40,42)	-179.9097	-DE/DX =	0.0
!					
!	D171	D(45,38,40,39)	-179.8742	-DE/DX =	0.0
!					
!	D172	D(45,38,40,42)	0.1324	-DE/DX =	0.0
!					
!	D173	D(36,38,45,46)	-0.0238	-DE/DX =	0.0
!					
!	D174	D(36,38,45,47)	-179.9947	-DE/DX =	0.0
!					
!	D175	D(40,38,45,46)	179.9251	-DE/DX =	0.0
!					
!	D176	D(40,38,45,47)	-0.0459	-DE/DX =	0.0
!					
!	D177	D(37,39,40,38)	-0.028	-DE/DX =	0.0
!					
!	D178	D(37,39,40,42)	179.9664	-DE/DX =	0.0
!					

!	D179	D(41,39,40,38)	179.9952	-DE/DX =	0.0
!					
!	D180	D(41,39,40,42)	-0.0103	-DE/DX =	0.0
!					
!	D181	D(37,39,41,43)	-179.9625	-DE/DX =	0.0
!					
!	D182	D(37,39,41,69)	0.0295	-DE/DX =	0.0
!					
!	D183	D(40,39,41,43)	0.0098	-DE/DX =	0.0
!					
!	D184	D(40,39,41,69)	-179.9982	-DE/DX =	0.0
!					
!	D185	D(38,40,42,44)	179.9952	-DE/DX =	0.0
!					
!	D186	D(38,40,42,66)	0.0037	-DE/DX =	0.0
!					
!	D187	D(39,40,42,44)	0.0023	-DE/DX =	0.0
!					
!	D188	D(39,40,42,66)	-179.9892	-DE/DX =	0.0
!					
!	D189	D(39,41,43,44)	-0.0014	-DE/DX =	0.0
!					
!	D190	D(39,41,43,68)	179.9957	-DE/DX =	0.0
!					
!	D191	D(69,41,43,44)	-179.9932	-DE/DX =	0.0
!					
!	D192	D(69,41,43,68)	0.0039	-DE/DX =	0.0
!					
!	D193	D(40,42,44,43)	0.0058	-DE/DX =	0.0
!					
!	D194	D(40,42,44,67)	-179.9941	-DE/DX =	0.0
!					
!	D195	D(66,42,44,43)	179.9975	-DE/DX =	0.0
!					
!	D196	D(66,42,44,67)	-0.0024	-DE/DX =	0.0
!					
!	D197	D(41,43,44,42)	-0.0064	-DE/DX =	0.0
!					
!	D198	D(41,43,44,67)	179.9936	-DE/DX =	0.0
!					
!	D199	D(68,43,44,42)	179.9966	-DE/DX =	0.0
!					
!	D200	D(68,43,44,67)	-0.0035	-DE/DX =	0.0
!					

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Stoichiometry C42H18N6O2S4
 Framework group C1[X(C42H18N6O2S4)]
 Deg. of freedom 210
 Full point group C1 NOp 1
 Largest Abelian subgroup C1 NOp 1
 Largest concise Abelian subgroup C1 NOp 1
 Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-10.803371	-0.637271	0.004930

2	6	0	-9.994209	-1.788073	0.002849
3	6	0	-10.516716	-3.073085	0.007442
4	6	0	-11.905666	-3.215437	0.014603
5	6	0	-12.726792	-2.081126	0.016920
6	6	0	-12.194771	-0.787500	0.012109
7	1	0	-9.846115	-3.926266	0.005518
8	1	0	-12.353097	-4.204554	0.018445
9	1	0	-13.805578	-2.203111	0.022601
10	1	0	-12.864256	0.060834	0.014179
11	6	0	-9.927078	0.564330	-0.001338
12	6	0	-8.569965	-1.390842	-0.004177
13	6	0	-8.540409	0.088720	-0.005222
14	6	0	-7.404450	0.870095	-0.007426
15	6	0	-6.014476	0.595587	-0.011131
16	6	0	-3.644320	-0.183962	-0.010662
17	6	0	-3.778362	1.228676	-0.016614
18	16	0	-5.182083	-0.989241	-0.012157
19	6	0	-5.099620	1.664929	-0.013038
20	6	0	-2.267214	-0.451795	-0.006598
21	6	0	-1.603923	0.797461	-0.010455
22	7	0	-2.523845	1.820863	-0.032759
23	16	0	-1.150964	-1.806928	-0.007105
24	16	0	1.150915	1.806537	0.008055
25	6	0	0.198420	-0.673774	0.002343
26	6	0	-0.198424	0.673343	-0.001459
27	6	0	1.603937	-0.797878	0.011227
28	6	0	2.267166	0.451409	0.007247
29	6	0	3.644283	0.183683	0.011045
30	6	0	3.778409	-1.228925	0.017023
31	6	0	5.099690	-1.665132	0.013298
32	6	0	6.014493	-0.595734	0.011347
33	16	0	5.181990	0.989050	0.012426
34	7	0	2.523952	-1.821220	0.033317
35	6	0	7.404528	-0.870172	0.007388
36	6	0	8.540398	-0.088684	0.004956
37	6	0	8.569748	1.390882	0.004077
38	6	0	9.927133	-0.564098	0.000737
39	6	0	9.993929	1.788309	-0.002930
40	6	0	10.803248	0.637624	-0.005349
41	6	0	10.516258	3.073402	-0.007267
42	6	0	12.194630	0.788043	-0.012643
43	6	0	11.905183	3.215943	-0.014528
44	6	0	12.726468	2.081741	-0.017202
45	6	0	10.384797	-1.870801	0.002801
46	6	0	9.534100	-3.018676	0.010206
47	6	0	11.769344	-2.222147	-0.001672
48	7	0	8.863977	-3.972415	0.016260
49	7	0	12.886900	-2.551315	-0.005220
50	6	0	-10.384568	1.871088	-0.003704
51	6	0	-11.769079	2.222615	0.000569
52	6	0	-9.533722	3.018856	-0.011178
53	7	0	-12.886594	2.551923	0.003937
54	7	0	-8.863471	3.972505	-0.017293
55	8	0	-7.613055	-2.157586	-0.007884
56	8	0	7.612727	2.157478	0.008003
57	6	0	2.241322	-3.243103	-0.055319
58	1	0	1.319634	-3.467804	0.486037
59	1	0	2.137482	-3.570602	-1.095396
60	1	0	3.054737	-3.799289	0.414699
61	6	0	-2.240714	3.242673	0.055455

Rotational constants (GHZ): 0.1750153 0.0104040 0.0098215

Population analysis using the SCF density.

Orbital symmetries:

[illegible][illegible]

The electronic state is 1-A.

10.21761

Alpha occ. eigenvalues --	-10.21738	-10.21738	-10.21460	-10.21460	-
8.00337					
Alpha occ. eigenvalues --	-8.00337	-7.98820	-7.98820	-5.96817	-
5.96816					
Alpha occ. eigenvalues --	-5.96464	-5.96463	-5.95904	-5.95904	-
5.95285					
Alpha occ. eigenvalues --	-5.95285	-5.94902	-5.94902	-5.94438	-
5.94438					
Alpha occ. eigenvalues --	-1.04937	-1.04936	-1.03135	-1.02917	-
0.93004					
Alpha occ. eigenvalues --	-0.93004	-0.92670	-0.91224	-0.91223	-
0.90604					
Alpha occ. eigenvalues --	-0.90596	-0.90126	-0.90056	-0.87318	-
0.85872					
Alpha occ. eigenvalues --	-0.85768	-0.83100	-0.81819	-0.81119	-
0.80790					
Alpha occ. eigenvalues --	-0.79805	-0.78851	-0.77494	-0.77429	-
0.77319					
Alpha occ. eigenvalues --	-0.77104	-0.75783	-0.75429	-0.72898	-
0.71986					
Alpha occ. eigenvalues --	-0.70452	-0.70257	-0.68446	-0.68149	-
0.67670					
Alpha occ. eigenvalues --	-0.65068	-0.62996	-0.61711	-0.61114	-
0.60527					
Alpha occ. eigenvalues --	-0.60441	-0.59893	-0.59733	-0.58705	-
0.58233					
Alpha occ. eigenvalues --	-0.57770	-0.57024	-0.56049	-0.54556	-
0.54038					
Alpha occ. eigenvalues --	-0.53338	-0.53024	-0.52806	-0.51453	-
0.51024					
Alpha occ. eigenvalues --	-0.50641	-0.50325	-0.50182	-0.49507	-
0.48835					
Alpha occ. eigenvalues --	-0.47679	-0.47434	-0.47082	-0.46758	-
0.45604					
Alpha occ. eigenvalues --	-0.45526	-0.45281	-0.45091	-0.45035	-
0.44915					
Alpha occ. eigenvalues --	-0.44806	-0.44697	-0.44221	-0.44128	-
0.43630					
Alpha occ. eigenvalues --	-0.43538	-0.43485	-0.42588	-0.42509	-
0.41750					
Alpha occ. eigenvalues --	-0.41546	-0.41329	-0.41060	-0.40996	-
0.40937					
Alpha occ. eigenvalues --	-0.40495	-0.38791	-0.38687	-0.38460	-
0.38397					
Alpha occ. eigenvalues --	-0.38049	-0.37924	-0.37910	-0.37661	-
0.37507					
Alpha occ. eigenvalues --	-0.37442	-0.37258	-0.36967	-0.36964	-
0.35962					
Alpha occ. eigenvalues --	-0.35775	-0.35741	-0.35218	-0.34962	-
0.34961					
Alpha occ. eigenvalues --	-0.34231	-0.34223	-0.33951	-0.33946	-
0.33300					
Alpha occ. eigenvalues --	-0.33299	-0.31676	-0.30342	-0.29581	-
0.27859					
Alpha occ. eigenvalues --	-0.27714	-0.27504	-0.27225	-0.26465	-
0.26459					
Alpha occ. eigenvalues --	-0.25875	-0.25349	-0.24315	-0.23187	-
0.22910					
Alpha occ. eigenvalues --	-0.20030				

Alpha virt. eigenvalues -- 0.05404	-0.12502	-0.11025	-0.09588	-0.09099	-
Alpha virt. eigenvalues -- 0.01021	-0.03463	-0.02699	-0.02031	-0.01056	-
Alpha virt. eigenvalues -- 0.01722	-0.00541	0.00273	0.00736	0.01051	
Alpha virt. eigenvalues -- 0.03951	0.01946	0.02141	0.02200	0.03852	
Alpha virt. eigenvalues -- 0.06283	0.04027	0.05121	0.05171	0.05970	
Alpha virt. eigenvalues -- 0.08703	0.06311	0.06927	0.07180	0.07419	
Alpha virt. eigenvalues -- 0.10103	0.08979	0.09146	0.09177	0.10099	
Alpha virt. eigenvalues -- 0.12782	0.11130	0.11417	0.11949	0.12087	
Alpha virt. eigenvalues -- 0.13785	0.13106	0.13539	0.13554	0.13764	
Alpha virt. eigenvalues -- 0.15752	0.14128	0.14486	0.15560	0.15561	
Alpha virt. eigenvalues -- 0.17455	0.15962	0.16188	0.16203	0.16501	
Alpha virt. eigenvalues -- 0.18048	0.17567	0.17856	0.17856	0.17990	
Alpha virt. eigenvalues -- 0.20085	0.18984	0.19159	0.19182	0.19770	
Alpha virt. eigenvalues -- 0.24462	0.22885	0.23297	0.23298	0.23767	
Alpha virt. eigenvalues -- 0.26376	0.24768	0.25202	0.25728	0.25736	
Alpha virt. eigenvalues -- 0.28259	0.26413	0.26840	0.27560	0.28119	
Alpha virt. eigenvalues -- 0.31651	0.29782	0.30813	0.30967	0.31458	
Alpha virt. eigenvalues -- 0.33842	0.31988	0.32023	0.32534	0.33460	
Alpha virt. eigenvalues -- 0.35709	0.34827	0.34897	0.35520	0.35565	
Alpha virt. eigenvalues -- 0.38333	0.35734	0.36111	0.36765	0.38257	
Alpha virt. eigenvalues -- 0.40962	0.39613	0.40246	0.40717	0.40821	
Alpha virt. eigenvalues -- 0.43876	0.42154	0.42775	0.42985	0.43379	
Alpha virt. eigenvalues -- 0.46325	0.44212	0.44806	0.44941	0.46322	
Alpha virt. eigenvalues -- 0.47806	0.46527	0.46539	0.46764	0.46848	
Alpha virt. eigenvalues -- 0.49865	0.47882	0.48021	0.48651	0.48664	
Alpha virt. eigenvalues -- 0.51385	0.50025	0.50035	0.50059	0.51261	
Alpha virt. eigenvalues -- 0.52477	0.51676	0.51843	0.52205	0.52329	
Alpha virt. eigenvalues -- 0.53656	0.52973	0.53254	0.53370	0.53518	
Alpha virt. eigenvalues -- 0.55085	0.54171	0.54304	0.54484	0.55004	
Alpha virt. eigenvalues -- 0.56097	0.55646	0.55742	0.55751	0.56075	

Alpha virt. eigenvalues --	0.57059	0.57277	0.57327	0.57479
0.57811				
Alpha virt. eigenvalues --	0.57908	0.57969	0.58318	0.58580
0.58806				
Alpha virt. eigenvalues --	0.58806	0.58882	0.59668	0.59687
0.59716				
Alpha virt. eigenvalues --	0.59914	0.60425	0.60483	0.61494
0.61608				
Alpha virt. eigenvalues --	0.61922	0.61926	0.62503	0.62886
0.63246				
Alpha virt. eigenvalues --	0.63495	0.63623	0.63781	0.64549
0.64764				
Alpha virt. eigenvalues --	0.65151	0.65160	0.65716	0.65793
0.66514				
Alpha virt. eigenvalues --	0.67267	0.67828	0.67991	0.68154
0.68161				
Alpha virt. eigenvalues --	0.69003	0.69402	0.69424	0.69726
0.69990				
Alpha virt. eigenvalues --	0.70157	0.70901	0.71361	0.71376
0.71496				
Alpha virt. eigenvalues --	0.71748	0.72994	0.74056	0.74194
0.74244				
Alpha virt. eigenvalues --	0.74328	0.75119	0.75494	0.76527
0.77002				
Alpha virt. eigenvalues --	0.77038	0.77067	0.77076	0.77468
0.77511				
Alpha virt. eigenvalues --	0.77770	0.78650	0.78751	0.79110
0.79165				
Alpha virt. eigenvalues --	0.79540	0.79686	0.79695	0.79795
0.80235				
Alpha virt. eigenvalues --	0.81108	0.81222	0.82325	0.82616
0.82687				
Alpha virt. eigenvalues --	0.82757	0.83382	0.83761	0.83983
0.84001				
Alpha virt. eigenvalues --	0.84236	0.85014	0.85310	0.85543
0.85957				
Alpha virt. eigenvalues --	0.85984	0.86430	0.86493	0.86609
0.86825				
Alpha virt. eigenvalues --	0.86890	0.87508	0.87601	0.87946
0.88407				
Alpha virt. eigenvalues --	0.88810	0.88906	0.90201	0.91293
0.92136				
Alpha virt. eigenvalues --	0.92438	0.93096	0.93521	0.93746
0.94438				
Alpha virt. eigenvalues --	0.94630	0.94909	0.95591	0.95771
0.96315				
Alpha virt. eigenvalues --	0.96449	0.96952	0.97193	0.97723
0.97937				
Alpha virt. eigenvalues --	0.98137	0.98410	0.98697	0.99069
0.99441				
Alpha virt. eigenvalues --	0.99647	1.00600	1.01275	1.01743
1.01985				
Alpha virt. eigenvalues --	1.02803	1.02854	1.03213	1.03264
1.03315				
Alpha virt. eigenvalues --	1.03334	1.04013	1.05021	1.05553
1.05889				
Alpha virt. eigenvalues --	1.06209	1.06872	1.07164	1.08779
1.10155				
Alpha virt. eigenvalues --	1.10437	1.10607	1.11993	1.12349
1.13020				

Alpha virt. eigenvalues -- 1.19493	1.13186	1.14225	1.14325	1.18876
Alpha virt. eigenvalues -- 1.21397	1.19632	1.20536	1.20894	1.21370
Alpha virt. eigenvalues -- 1.23119	1.21416	1.21775	1.21871	1.22660
Alpha virt. eigenvalues -- 1.25186	1.23152	1.24710	1.24779	1.25021
Alpha virt. eigenvalues -- 1.27697	1.25265	1.25476	1.25930	1.27078
Alpha virt. eigenvalues -- 1.30313	1.28126	1.28622	1.28718	1.28969
Alpha virt. eigenvalues -- 1.31918	1.30640	1.30746	1.30985	1.30991
Alpha virt. eigenvalues -- 1.33430	1.32166	1.32803	1.33291	1.33380
Alpha virt. eigenvalues -- 1.35079	1.33431	1.33709	1.33894	1.34192
Alpha virt. eigenvalues -- 1.38213	1.36596	1.36658	1.36984	1.37244
Alpha virt. eigenvalues -- 1.40109	1.38645	1.38646	1.39585	1.40050
Alpha virt. eigenvalues -- 1.43500	1.40943	1.41262	1.42217	1.42230
Alpha virt. eigenvalues -- 1.46118	1.43639	1.43850	1.45259	1.45510
Alpha virt. eigenvalues -- 1.50458	1.47383	1.48279	1.48903	1.50384
Alpha virt. eigenvalues -- 1.52054	1.50942	1.50944	1.51780	1.51784
Alpha virt. eigenvalues -- 1.55529	1.52258	1.54027	1.54315	1.54935
Alpha virt. eigenvalues -- 1.57628	1.55836	1.56630	1.56665	1.57423
Alpha virt. eigenvalues -- 1.63406	1.59008	1.60951	1.62041	1.62529
Alpha virt. eigenvalues -- 1.65539	1.63935	1.64711	1.65149	1.65155
Alpha virt. eigenvalues -- 1.70297	1.67358	1.67564	1.69464	1.69917
Alpha virt. eigenvalues -- 1.72057	1.70429	1.70613	1.71500	1.71980
Alpha virt. eigenvalues -- 1.74395	1.73441	1.73672	1.74179	1.74182
Alpha virt. eigenvalues -- 1.76531	1.74552	1.75398	1.75408	1.76122
Alpha virt. eigenvalues -- 1.78276	1.76763	1.77290	1.77509	1.77573
Alpha virt. eigenvalues -- 1.80805	1.78293	1.79424	1.79562	1.80061
Alpha virt. eigenvalues -- 1.83475	1.81612	1.82523	1.82905	1.83307
Alpha virt. eigenvalues -- 1.85321	1.83915	1.84517	1.84894	1.85022
Alpha virt. eigenvalues -- 1.88132	1.86140	1.86203	1.87279	1.88067
Alpha virt. eigenvalues -- 1.90201	1.88553	1.88715	1.89637	1.89956
Alpha virt. eigenvalues -- 1.93183	1.90515	1.91438	1.91498	1.91667

Alpha virt. eigenvalues -- 1.95216	1.93448	1.93759	1.93774	1.94370
Alpha virt. eigenvalues -- 1.97533	1.95231	1.96716	1.96717	1.96882
Alpha virt. eigenvalues -- 1.99216	1.98317	1.98319	1.98912	1.98919
Alpha virt. eigenvalues -- 2.00219	1.99643	2.00006	2.00010	2.00135
Alpha virt. eigenvalues -- 2.02955	2.00957	2.01475	2.01596	2.01701
Alpha virt. eigenvalues -- 2.06299	2.03568	2.04290	2.05018	2.05561
Alpha virt. eigenvalues -- 2.07772	2.06849	2.06851	2.06892	2.07012
Alpha virt. eigenvalues -- 2.10294	2.07870	2.08887	2.09202	2.09818
Alpha virt. eigenvalues -- 2.13716	2.10430	2.11683	2.12754	2.13682
Alpha virt. eigenvalues -- 2.15403	2.14470	2.14700	2.14800	2.15117
Alpha virt. eigenvalues -- 2.19380	2.16035	2.16081	2.17595	2.18507
Alpha virt. eigenvalues -- 2.22150	2.20197	2.20983	2.21015	2.22112
Alpha virt. eigenvalues -- 2.25172	2.22270	2.22485	2.22829	2.23341
Alpha virt. eigenvalues -- 2.28997	2.25730	2.26090	2.26100	2.26118
Alpha virt. eigenvalues -- 2.33504	2.31179	2.31201	2.31492	2.32496
Alpha virt. eigenvalues -- 2.35041	2.33867	2.34191	2.34700	2.34817
Alpha virt. eigenvalues -- 2.38897	2.35506	2.36122	2.36935	2.37057
Alpha virt. eigenvalues -- 2.41212	2.39004	2.39050	2.39357	2.41126
Alpha virt. eigenvalues -- 2.45127	2.42057	2.42583	2.42691	2.42742
Alpha virt. eigenvalues -- 2.48991	2.45419	2.45430	2.46152	2.47187
Alpha virt. eigenvalues -- 2.50359	2.49047	2.50117	2.50163	2.50355
Alpha virt. eigenvalues -- 2.54337	2.50470	2.50519	2.52453	2.52672
Alpha virt. eigenvalues -- 2.55990	2.54594	2.54801	2.55302	2.55974
Alpha virt. eigenvalues -- 2.61396	2.57271	2.58052	2.59779	2.60426
Alpha virt. eigenvalues -- 2.62639	2.61400	2.61928	2.61936	2.62394
Alpha virt. eigenvalues -- 2.66017	2.63254	2.63365	2.64815	2.65415
Alpha virt. eigenvalues -- 2.71127	2.66162	2.67505	2.68907	2.68928
Alpha virt. eigenvalues -- 2.73164	2.71255	2.72156	2.72896	2.73093
Alpha virt. eigenvalues -- 2.76842	2.73965	2.74003	2.74305	2.76507
Alpha virt. eigenvalues -- 2.79290	2.77353	2.77353	2.78471	2.79053

Alpha virt. eigenvalues --	2.79901	2.80019	2.80601	2.81885
2.81886				
Alpha virt. eigenvalues --	2.82032	2.83253	2.85596	2.85780
2.86382				
Alpha virt. eigenvalues --	2.86472	2.87328	2.88095	2.89267
2.89987				
Alpha virt. eigenvalues --	2.90063	2.90707	2.91661	2.92700
2.93679				
Alpha virt. eigenvalues --	2.93841	2.94762	2.98331	3.01782
3.01794				
Alpha virt. eigenvalues --	3.02920	3.05287	3.05415	3.06672
3.09808				
Alpha virt. eigenvalues --	3.09985	3.10004	3.13255	3.13595
3.17590				
Alpha virt. eigenvalues --	3.17908	3.20310	3.20549	3.21553
3.22100				
Alpha virt. eigenvalues --	3.22254	3.23269	3.23370	3.25427
3.27292				
Alpha virt. eigenvalues --	3.27651	3.29025	3.29474	3.34645
3.34681				
Alpha virt. eigenvalues --	3.34917	3.34920	3.39574	3.39666
3.40340				
Alpha virt. eigenvalues --	3.40423	3.47487	3.47488	3.48902
3.48914				
Alpha virt. eigenvalues --	3.49909	3.49985	3.56258	3.56324
3.83972				
Alpha virt. eigenvalues --	3.83973	3.89844	3.91393	3.95840
3.96434				
Alpha virt. eigenvalues --	3.97923	3.97970	4.00868	4.00916
4.04372				
Alpha virt. eigenvalues --	4.06752	4.07406	4.07709	4.09443
4.09706				
Alpha virt. eigenvalues --	4.11009	4.11197	4.12558	4.12779
4.14945				
Alpha virt. eigenvalues --	4.16014	4.16550	4.16727	4.17060
4.19599				
Alpha virt. eigenvalues --	4.20128	4.23500	4.24516	4.24644
4.25686				
Alpha virt. eigenvalues --	4.31287	4.32245	4.34053	4.38772
4.40080				
Alpha virt. eigenvalues --	4.44358	4.44944	4.45756	4.47800
4.51996				
Alpha virt. eigenvalues --	4.52727	4.52786	4.55820	4.56203
4.57005				
Alpha virt. eigenvalues --	4.60330	4.62190	4.68677	4.69446
4.69956				
Alpha virt. eigenvalues --	4.72449	4.87294	4.87299	4.88703
4.88704				

Condensed to atoms (all electrons):

Mulliken charges:

1		
1	C	0.043140
2	C	0.041600
3	C	-0.107765
4	C	-0.083833
5	C	-0.089511
6	C	-0.122809
7	H	0.119527
8	H	0.104458
9	H	0.107606

10	H	0.136369
11	C	0.104209
12	C	0.353565
13	C	0.010776
14	C	-0.121209
15	C	-0.165030
16	C	-0.194869
17	C	0.315248
18	S	0.347681
19	C	-0.078087
20	C	-0.187842
21	C	0.318793
22	N	-0.625968
23	S	0.271936
24	S	0.271915
25	C	-0.145973
26	C	-0.145977
27	C	0.318852
28	C	-0.187860
29	C	-0.194832
30	C	0.315204
31	C	-0.078110
32	C	-0.165050
33	S	0.347694
34	N	-0.625957
35	C	-0.121209
36	C	0.010776
37	C	0.353570
38	C	0.104211
39	C	0.041598
40	C	0.043137
41	C	-0.107759
42	C	-0.122805
43	C	-0.083834
44	C	-0.089510
45	C	0.055159
46	C	0.304289
47	C	0.300352
48	N	-0.513460
49	N	-0.505915
50	C	0.055148
51	C	0.300357
52	C	0.304292
53	N	-0.505919
54	N	-0.513468
55	O	-0.493865
56	O	-0.493866
57	C	-0.199937
58	H	0.146715
59	H	0.149169
60	H	0.143868
61	C	-0.199954
62	H	0.149177
63	H	0.146764
64	H	0.143847
65	H	0.131045
66	H	0.136370
67	H	0.107608
68	H	0.104459
69	H	0.119528

70 H 0.130564
71 H 0.130557
72 H 0.131049

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

1
1 C 0.043140
2 C 0.041600
3 C 0.011762
4 C 0.020624
5 C 0.018096
6 C 0.013561
11 C 0.104209
12 C 0.353565
13 C 0.010776
14 C 0.009348
15 C -0.165030
16 C -0.194869
17 C 0.315248
18 S 0.347681
19 C 0.052962
20 C -0.187842
21 C 0.318793
22 N -0.625968
23 S 0.271936
24 S 0.271915
25 C -0.145973
26 C -0.145977
27 C 0.318852
28 C -0.187860
29 C -0.194832
30 C 0.315204
31 C 0.052935
32 C -0.165050
33 S 0.347694
34 N -0.625957
35 C 0.009355
36 C 0.010776
37 C 0.353570
38 C 0.104211
39 C 0.041598
40 C 0.043137
41 C 0.011769
42 C 0.013566
43 C 0.020625
44 C 0.018098
45 C 0.055159
46 C 0.304289
47 C 0.300352
48 N -0.513460
49 N -0.505915
50 C 0.055148
51 C 0.300357
52 C 0.304292
53 N -0.505919
54 N -0.513468
55 O -0.493865
56 O -0.493866
57 C 0.239815
61 C 0.239833

Electronic spatial extent (au): <R**2>= 95533.5276
Charge= 0.0000 electrons
Dipole moment (field-independent basis, Debye):
X= 0.0009 Y= 0.0003 Z= 0.0014
Tot= 0.0017
Quadrupole moment (field-independent basis, Debye-Ang):
XX= -436.6799 YY= -334.4286 ZZ= -334.8476
XY= 102.1689 XZ= -0.7884 YZ= 0.2321
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
XX= -68.0279 YY= 34.2235 ZZ= 33.8044
XY= 102.1689 XZ= -0.7884 YZ= 0.2321
Octapole moment (field-independent basis, Debye-Ang**2):
XXX= -0.1373 YYY= -0.0080 ZZZ= -0.0021
XYY= 0.0726
XXY= 0.0212 XXZ= 0.1988 XZZ= 0.0091
YZZ= -0.0014
YYZ= 0.0362 XYZ= -0.0653
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX= -142660.9943 YYYY= -7969.6522 ZZZZ= -
361.7697 XXXY= 19799.1776
XXXZ= -53.2546 YYYYX= 2374.2670 YYYZ= -
0.6447 ZZZX= -1.5301
ZZZY= 5.8423 XXYY= -24571.5308 XXZZ= -
21669.6649 YYZZ= -1382.8290
XXYZ= -13.2539 YYXZ= -7.4627 ZZXY= -
50.5648

N=N= 6.569682348250D+03 E-N=-2.177052125846D+04 KE= 3.658061155942D+03
1\1\GINC-HPC\FOpt\RB3LYP\6-31G(d,p)\C42H18N6O2S4\CHEM\04-Jan-2019\0\#\#
opt b3lyp/6-31g(d,p) geom=connectivity empiricdispersion=gd3\Title
Card Required\0,1\C,-7.128422668,4.9878800893,1.0188051309\C,-6.1046
214632,5.4192061671,1.8818697072\C,-5.9113873995,6.7532277881,2.209493
3525\C,-6.7765636299,7.6966569336,1.6519017538\C,-7.8012951028,7.28561
01933,0.7905768917\C,-7.9919167364,5.9390357667,0.4635621671\H,-5.1052
846283,7.0307373387,2.8809210623\H,-6.6579080007,8.7505493752,1.883836
3947\H,-8.4683977527,8.027455898,0.3624045263\H,-8.7951469941,5.664729
0511,-0.2053643626\C,-7.0508993202,3.5086976976,0.8854581743\C,-5.3228
63325,4.2521053419,2.3434343206\C,-5.9255336625,3.0582106922,1.7098872
513\C,-5.4951622638,1.7584308084,1.8720836131\C,-4.4519912231,1.146129
7345,2.6098360621\C,-2.5381412645,0.3503595229,3.9988141838\C,-3.22516
15987,-0.6931573976,3.3260415726\S,-3.2295930124,1.90871035,3.67227261
85\C,-4.2904069348,-0.2504822143,2.5480036502\C,-1.5016243008,-0.25873
17957,4.7218717479\C,-1.585176509,-1.6483300557,4.4715814823\N,-2.6444
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9\S,-0.1545616702,-4.0937212895,5.2338879962\C,0.2469796778,-1.5538394
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89,-2.2936367109,6.5714146265\C,1.1613747792,-3.6832355306,6.321179277
\C,2.1976902181,-4.292447115,7.0444033922\C,2.8847707677,-3.2490019265
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,9.1714262683\C,5.5845700293,-7.0006337574,9.3337117353\C,4.9818622886
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\C,5.7635075794,-9.3616083419,9.1613783684\C,6.7871578995,-8.930505043
,10.0247258791\C,5.5702768532,-10.6955607985,8.8334398859\C,7.65048944
08,-9.8818132176,10.5799675359\C,6.4352958943,-11.6391357554,9.3910169
735\C,7.4598693902,-11.2283089252,10.2526431237\C,7.56635582,-6.685732
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173258,-7.2337954201,11.7005096968\N,7.4402091017,-4.1054211483,11.167
4359347\N,9.5216719754,-7.6399365729,12.3415769862\C,-7.9076542402,2.7
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.0678152621,9.0957418356\H,8.4535982721,-9.6076753565,11.2491053344\H,
8.1268444111,-11.9702773871,10.6808014689\H,6.3166517777,-12.692976290
4,9.1588393718\H,4.7642848247,-10.9728959862,8.1618066029\H,5.71592270
89,-4.9508040811,9.7151362977\H,-6.0565900992,1.0083796409,1.328407770
7\H,-4.9422204012,-0.8744377281,1.947646157\\Version=ES64L-G09RevD.01\
State=1-A\HF=-3683.0201218\RMSD=6.221e-09\RMSF=4.971e-06\Dipole=0.0005
372,-0.0002479,-0.0003073\Quadrupole=-52.0017778,70.4942772,-18.492499
4,9.1013648,-58.5485973,13.0491858\PG=C01 [X(C42H18N6O2S4)]\@

TIME GOES, YOU SAY? AH NO!

ALAS, TIME STAYS, WE GO.

-- A. DOBSON (1840-1921)

Job cpu time: 0 days 16 hours 46 minutes 0.3 seconds.

File lengths (MBytes): RWF= 513 Int= 0 D2E= 0 Chk= 57 Scr=
1

Normal termination of Gaussian 09 at Fri Jan 4 09:56:25 2019.