

**The influence of the oxygen donor capacity of polystearylmethacrylate over polyethylene bulk density  
when using modified methylaluminoxane as co-catalyst.**

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**Supplementary data**

**PSMA1u Spartan 14' Output**

SPARTAN '14 MECHANICS PROGRAM: (Win/64b) Release 1.1.4

Frequency Calculation

Adjusted 19 (out of 372) low frequency modes

Reason for exit: Successful completion

Mechanics CPU Time : .77

Mechanics Wall Time: .49

SPARTAN '14 Semi-Empirical Program: (Win/64b) Release 1.1.4

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Run type: Geometry optimization

(Analytical Gradient)

(Analytical Gradient in FREQ)

(Numerical Frequency)

Model: RHF/PM6

Number of shells: 176

124 S shells

49 P shells

3 5D shells

Number of basis functions: 286

Number of electrons: 286

Use of molecular symmetry disabled

Molecular charge: 0

Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1

This system has 366 degrees of freedom

Initial Hessian option  
Hessian from MMFF94 calculation used.

Max. Max. Neg.

Cycle Energy Grad. Dist. Eigen

1	-1142.8298	0.06274	0.03544
2	-1145.7779	0.01224	0.05608
3	-1146.0780	0.02135	0.01262
4	-1146.6434	0.00239	0.00620
5	-1146.7697	0.00356	0.01638
6	-1146.8720	0.00555	0.02137
7	-1146.9921	0.00325	0.00956
8	-1147.0818	0.00157	0.01252
9	-1147.1722	0.00128	0.01631
10	-1147.2403	0.00357	0.01704
11	-1147.3141	0.00137	0.02127
12	-1147.3794	0.00206	0.02034
13	-1147.4443	0.00113	0.01909
14	-1147.5039	0.00197	0.02370
15	-1147.5571	0.00125	0.02163
16	-1147.6094	0.00108	0.01621
17	-1147.6619	0.00077	0.02007
18	-1147.7079	0.00129	0.01661
19	-1147.7485	0.00111	0.01673
20	-1147.7870	0.00175	0.01736
21	-1147.8150	0.00356	0.01969
22	-1147.8593	0.00099	0.01534
23	-1147.8914	0.00191	0.01996
24	-1147.9240	0.00128	0.01768
25	-1147.9537	0.00109	0.01167
26	-1147.9813	0.00147	0.00830
27	-1148.0049	0.00157	0.00944
28	-1148.0329	0.00167	0.00970
29	-1148.0596	0.00139	0.01274
30	-1148.0865	0.00060	0.01322
31	-1148.0911	0.00352	0.01088
32	-1148.1290	0.00080	0.00748
33	-1148.1459	0.00102	0.00573
34	-1148.1685	0.00067	0.00635
35	-1148.1871	0.00036	0.00674
36	-1148.2075	0.00050	0.00729
37	-1148.2270	0.00076	0.00832
38	-1148.2469	0.00062	0.00833
39	-1148.2617	0.00065	0.00543
40	-1148.2825	0.00041	0.00592
41	-1148.2980	0.00027	0.00565
42	-1148.3145	0.00020	0.00601
43	-1148.3312	0.00032	0.00668
44	-1148.3475	0.00035	0.00902
45	-1148.3617	0.00050	0.00660
46	-1148.3786	0.00036	0.00471
47	-1148.3918	0.00031	0.00464

48	-1148.4054	0.00029	0.00553
49	-1148.4188	0.00023	0.00527
50	-1148.4319	0.00017	0.00513
51	-1148.4452	0.00016	0.00524
52	-1148.4591	0.00015	0.00541
53	-1148.4724	0.00042	0.00489
54	-1148.4845	0.00079	0.00445
55	-1148.4967	0.00046	0.00628
56	-1148.5075	0.00083	0.00456
57	-1148.5207	0.00021	0.00348
58	-1148.5323	0.00065	0.00372
59	-1148.5445	0.00048	0.00581
60	-1148.5572	0.00023	0.00364
61	-1148.5685	0.00039	0.00360
62	-1148.5788	0.00037	0.00371
63	-1148.5880	0.00047	0.00401
64	-1148.6001	0.00026	0.00290
65	-1148.6101	0.00031	0.00400
66	-1148.6214	0.00023	0.00452
67	-1148.6324	0.00024	0.00376
68	-1148.6431	0.00016	0.00466
69	-1148.6542	0.00051	0.00510
70	-1148.6649	0.00024	0.00583
71	-1148.6731	0.00067	0.00336
72	-1148.6841	0.00048	0.00270
73	-1148.6930	0.00043	0.00214
74	-1148.7028	0.00034	0.00428
75	-1148.7132	0.00023	0.00296
76	-1148.7240	0.00033	0.00435
77	-1148.7342	0.00100	0.00478
78	-1148.7451	0.00050	0.00529
79	-1148.7473	0.00152	0.00441
80	-1148.7644	0.00037	0.00267
81	-1148.7734	0.00061	0.00411
82	-1148.7833	0.00021	0.00362
83	-1148.7917	0.00051	0.00320
84	-1148.8029	0.00063	0.00458
85	-1148.8126	0.00026	0.00298
86	-1148.8224	0.00017	0.00481
87	-1148.8325	0.00036	0.00381
88	-1148.8426	0.00039	0.00407
89	-1148.8519	0.00021	0.00504
90	-1148.8609	0.00029	0.00277
91	-1148.8705	0.00022	0.00428
92	-1148.8795	0.00023	0.00430
93	-1148.8887	0.00020	0.00357
94	-1148.8955	0.00037	0.00382
95	-1148.9062	0.00028	0.00460
96	-1148.9148	0.00023	0.00339
97	-1148.9243	0.00018	0.00428
98	-1148.9333	0.00030	0.00427
99	-1148.9430	0.00021	0.00524

100	-1148.9510	0.00030	0.00417
101	-1148.9613	0.00026	0.00283
102	-1148.9696	0.00026	0.00508
103	-1148.9790	0.00018	0.00429
104	-1148.9873	0.00025	0.00438
105	-1148.9976	0.00015	0.00376
106	-1149.0066	0.00025	0.00386
107	-1149.0161	0.00032	0.00468
108	-1149.0238	0.00032	0.00444
109	-1149.0348	0.00028	0.00418
110	-1149.0431	0.00020	0.00372
111	-1149.0519	0.00031	0.00263
112	-1149.0595	0.00044	0.00437
113	-1149.0683	0.00020	0.00419
114	-1149.0757	0.00032	0.00345
115	-1149.0840	0.00027	0.00284
116	-1149.0914	0.00018	0.00374
117	-1149.0992	0.00033	0.00409
118	-1149.1071	0.00017	0.00364
119	-1149.1149	0.00016	0.00442
120	-1149.1215	0.00042	0.00412
121	-1149.1296	0.00023	0.00277
122	-1149.1366	0.00027	0.00325
123	-1149.1435	0.00018	0.00357
124	-1149.1497	0.00021	0.00325
125	-1149.1568	0.00020	0.00249
126	-1149.1630	0.00018	0.00273
127	-1149.1692	0.00026	0.00304
128	-1149.1753	0.00012	0.00214
129	-1149.1810	0.00025	0.00300
130	-1149.1874	0.00012	0.00244
131	-1149.1932	0.00012	0.00227
132	-1149.1994	0.00013	0.00204
133	-1149.2057	0.00024	0.00287
134	-1149.2125	0.00013	0.00271
135	-1149.2191	0.00022	0.00295
136	-1149.2260	0.00030	0.00278
137	-1149.2329	0.00050	0.00290
138	-1149.2399	0.00016	0.00257
139	-1149.2468	0.00016	0.00274
140	-1149.2537	0.00013	0.00270
141	-1149.2602	0.00024	0.00276
142	-1149.2668	0.00032	0.00353
143	-1149.2728	0.00033	0.00285
144	-1149.2797	0.00022	0.00264
145	-1149.2859	0.00023	0.00221
146	-1149.2923	0.00013	0.00234
147	-1149.2986	0.00011	0.00275
148	-1149.3049	0.00019	0.00242
149	-1149.3111	0.00025	0.00297
150	-1149.3174	0.00019	0.00276
151	-1149.3237	0.00011	0.00263

152	-1149.3299	0.00010	0.00291
153	-1149.3361	0.00011	0.00219
154	-1149.3423	0.00012	0.00250
155	-1149.3483	0.00014	0.00264
156	-1149.3543	0.00010	0.00274
157	-1149.3602	0.00012	0.00254
158	-1149.3660	0.00011	0.00292
159	-1149.3714	0.00014	0.00242
160	-1149.3773	0.00012	0.00250
161	-1149.3828	0.00011	0.00253
162	-1149.3883	0.00012	0.00280
163	-1149.3938	0.00012	0.00264
164	-1149.3994	0.00016	0.00262
165	-1149.4048	0.00013	0.00269
166	-1149.4103	0.00008	0.00300
167	-1149.4156	0.00014	0.00243
168	-1149.4210	0.00014	0.00253
169	-1149.4262	0.00010	0.00250
170	-1149.4316	0.00012	0.00262
171	-1149.4369	0.00008	0.00256
172	-1149.4421	0.00009	0.00226
173	-1149.4473	0.00007	0.00199
174	-1149.4522	0.00015	0.00248
175	-1149.4574	0.00009	0.00227
176	-1149.4623	0.00006	0.00220
177	-1149.4675	0.00006	0.00210
178	-1149.4725	0.00007	0.00209
179	-1149.4776	0.00005	0.00220
180	-1149.4826	0.00006	0.00219
181	-1149.4876	0.00006	0.00220
182	-1149.4925	0.00010	0.00221
183	-1149.4974	0.00010	0.00215
184	-1149.5022	0.00008	0.00220
185	-1149.5071	0.00007	0.00209
186	-1149.5119	0.00009	0.00207
187	-1149.5167	0.00008	0.00216
188	-1149.5216	0.00011	0.00210
189	-1149.5263	0.00008	0.00213
190	-1149.5310	0.00010	0.00194
191	-1149.5356	0.00010	0.00223
192	-1149.5403	0.00010	0.00215
193	-1149.5448	0.00008	0.00267
194	-1149.5495	0.00013	0.00229
195	-1149.5544	0.00008	0.00263
196	-1149.5590	0.00009	0.00257
197	-1149.5638	0.00009	0.00306
198	-1149.5685	0.00010	0.00231
199	-1149.5731	0.00009	0.00237
200	-1149.5776	0.00007	0.00250
201	-1149.5821	0.00009	0.00261
202	-1149.5866	0.00009	0.00251
203	-1149.5910	0.00008	0.00267

204	-1149.5954	0.00010	0.00229
205	-1149.5997	0.00007	0.00245
206	-1149.6039	0.00008	0.00256
207	-1149.6082	0.00008	0.00256
208	-1149.6124	0.00014	0.00257
209	-1149.6168	0.00011	0.00241
210	-1149.6211	0.00008	0.00272
211	-1149.6254	0.00009	0.00285
212	-1149.6297	0.00010	0.00268
213	-1149.6338	0.00010	0.00293
214	-1149.6379	0.00010	0.00267
215	-1149.6420	0.00012	0.00287
216	-1149.6459	0.00006	0.00265
217	-1149.6498	0.00006	0.00268
218	-1149.6536	0.00007	0.00253
219	-1149.6573	0.00007	0.00232
220	-1149.6609	0.00009	0.00236
221	-1149.6648	0.00006	0.00225
222	-1149.6685	0.00008	0.00230
223	-1149.6722	0.00005	0.00223
224	-1149.6758	0.00005	0.00224
225	-1149.6794	0.00005	0.00231
226	-1149.6830	0.00009	0.00241
227	-1149.6865	0.00007	0.00222
228	-1149.6899	0.00007	0.00247
229	-1149.6932	0.00008	0.00222
230	-1149.6965	0.00009	0.00249
231	-1149.6998	0.00006	0.00215
232	-1149.7030	0.00007	0.00216
233	-1149.7062	0.00006	0.00206
234	-1149.7095	0.00006	0.00201
235	-1149.7126	0.00011	0.00204
236	-1149.7158	0.00010	0.00176
237	-1149.7187	0.00005	0.00168
238	-1149.7218	0.00006	0.00146
239	-1149.7248	0.00006	0.00153
240	-1149.7278	0.00006	0.00155
241	-1149.7307	0.00007	0.00157
242	-1149.7335	0.00005	0.00135
243	-1149.7364	0.00006	0.00156
244	-1149.7392	0.00006	0.00142
245	-1149.7420	0.00009	0.00160
246	-1149.7447	0.00007	0.00122
247	-1149.7475	0.00008	0.00157
248	-1149.7503	0.00009	0.00128
249	-1149.7530	0.00008	0.00127
250	-1149.7556	0.00005	0.00128
251	-1149.7582	0.00006	0.00116
252	-1149.7608	0.00013	0.00127
253	-1149.7633	0.00006	0.00106
254	-1149.7658	0.00007	0.00122
255	-1149.7683	0.00005	0.00109

256	-1149.7708	0.00006	0.00118
257	-1149.7734	0.00005	0.00104
258	-1149.7757	0.00006	0.00100
259	-1149.7781	0.00006	0.00097
260	-1149.7804	0.00007	0.00111
261	-1149.7827	0.00008	0.00089
262	-1149.7849	0.00007	0.00091
263	-1149.7871	0.00006	0.00098
264	-1149.7892	0.00007	0.00099
265	-1149.7914	0.00006	0.00113
266	-1149.7936	0.00005	0.00113
267	-1149.7957	0.00006	0.00109
268	-1149.7978	0.00005	0.00116
269	-1149.7999	0.00006	0.00104
270	-1149.8020	0.00004	0.00096
271	-1149.8038	0.00007	0.00090
272	-1149.8057	0.00010	0.00086

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Heat of Formation: -1149.806 kJ/mol

Estimating Force Constant matrix by central-differences

Calculating Hessian

Memory Used: 59.541 Mb

Reason for exit: Successful completion

Semi-Empirical Program CPU Time : 5:24.78

Semi-Empirical Program Wall Time: 5:24.91

SPARTAN '14 Properties Program: (Win/64b) Release 1.1.4

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Modifying values for 96 low frequency terms

Term	ZPE	Enthalpy	Entropy	Cv	% in
	kJ/mol	kJ/mol	J/mol.K	J/mol.K	Ground

Total Vibrations	2680.8778	118.3386	711.9222	626.9069	
Ideal Gas	2.4789				
Translation	3.7184	191.1792	12.4716		
Rotation	3.7184	181.8098	12.4716		
Totals	2809.1321	1084.9113	651.8502		

Vibrational(v) Corrections:

Temp. Correction Hv 2809.1321

Entropy Correction (Hv-TSv) 2485.6658

Reason for exit: Successful completion  
Properties CPU Time : 5.42  
Properties Wall Time: 5.13

### PSMA1u + TMA Spartan 14' Output

SPARTAN '14 MECHANICS PROGRAM: (Win/64b) Release 1.1.4

Frequency Calculation

Warning: global charge (+1.00) does not match input file (+0)!  
Adjusted 18 (out of 411) low frequency modes

Reason for exit: Successful completion  
Mechanics CPU Time : 1.09  
Mechanics Wall Time: 1.02

SPARTAN '14 Semi-Empirical Program: (Win/64b) Release 1.1.4

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Run type: Geometry optimization  
(Analytical Gradient)  
(Analytical Gradient in FREQ)  
(Numerical Frequency)  
Model: RHF/PM6  
Number of shells: 194  
137 S shells  
53 P shells  
4 5D shells  
Number of basis functions: 316  
Number of electrons: 310  
Use of molecular symmetry disabled  
Molecular charge: 0  
Spin multiplicity: 1

Point Group = C1 Order = 1 Nsymop = 1  
This system has 405 degrees of freedom

Initial Hessian option  
Hessian from MMFF94 calculation used.  
Max. Max. Neg.

Cycle Energy Grad. Dist. Eigen  
1 -961.0283 0.26266 0.02106  
2 -1066.7589 0.16360 0.03385  
3 -1123.1696 0.08251 0.01425  
4 -1152.1045 0.04869 0.02030  
5 -1168.4587 0.02442 0.01832  
6 -1180.1223 0.01381 0.01734



7 -1189.7884 0.00861 0.01478  
Lambda correction applied  
8 -1197.5643 0.01725 0.01261  
9 -1203.8873 0.01415 0.01418  
10 -1210.3685 0.01553 0.01402  
11 -1216.1735 0.01443 0.01385  
12 -1221.3606 0.01212 0.01310  
Lambda correction applied  
13 -1225.8882 0.00907 0.01424  
14 -1229.5617 0.00774 0.01233  
15 -1233.3893 0.00534 0.01278  
16 -1236.8242 0.00408 0.01289  
17 -1239.9505 0.00303 0.01378  
18 -1242.7683 0.00282 0.01553  
19 -1245.3499 0.00221 0.01601  
20 -1247.6724 0.00248 0.01753  
21 -1249.7961 0.00227 0.01709  
22 -1251.6992 0.00225 0.01936  
23 -1253.4208 0.00306 0.01656  
24 -1254.9778 0.00226 0.01973  
25 -1256.3826 0.00262 0.01771  
26 -1257.6599 0.00319 0.01647  
27 -1258.8348 0.00243 0.01920  
28 -1259.9075 0.00350 0.01529  
29 -1260.9281 0.00327 0.01811  
30 -1261.8819 0.00355 0.01709  
31 -1262.8023 0.00385 0.01576  
32 -1263.6885 0.00377 0.01655  
33 -1264.5478 0.00400 0.01491  
34 -1265.3898 0.00375 0.01371  
35 -1266.2088 0.00328 0.01268  
36 -1267.0074 0.00310 0.01382  
37 -1267.7921 0.00196 0.01451  
38 -1268.5513 0.00328 0.01553  
39 -1269.3054 0.00200 0.01673  
40 -1270.0294 0.00337 0.01828  
41 -1270.7555 0.00305 0.01752  
42 -1271.4712 0.00265 0.02170  
43 -1272.1925 0.00196 0.01926  
44 -1272.9149 0.00256 0.02191  
45 -1273.6381 0.00291 0.02135  
46 -1274.3694 0.00299 0.02281  
47 -1275.1015 0.00262 0.02201  
Lambda correction applied  
48 -1275.8392 0.00207 0.02226  
Lambda correction applied  
49 -1276.5331 0.00357 0.02188  
50 -1277.2336 0.00386 0.02172  
51 -1277.9539 0.00411 0.02348  
52 -1278.6656 0.00311 0.02235  
53 -1279.3576 0.00458 0.02220  
54 -1280.0187 0.00449 0.02435

55	-1280.6474	0.00239	0.02187
56	-1281.2295	0.00324	0.02447
57	-1281.7721	0.00172	0.02241
58	-1282.2752	0.00330	0.02671
59	-1282.7442	0.00231	0.02338
60	-1283.1842	0.00286	0.02776
61	-1283.6055	0.00264	0.02753
62	-1284.0063	0.00340	0.02786
63	-1284.4006	0.00242	0.02944
64	-1284.7804	0.00300	0.03149
65	-1285.1536	0.00324	0.03188
66	-1285.5129	0.00244	0.03255
67	-1285.8562	0.00379	0.03515
68	-1286.1864	0.00283	0.03272
69	-1286.4965	0.00372	0.03791
70	-1286.7955	0.00284	0.03513
71	-1287.0833	0.00355	0.03672
72	-1287.3589	0.00135	0.03665
73	-1287.6220	0.00398	0.03441
74	-1287.8843	0.00160	0.03413
75	-1288.1217	0.00228	0.03094
76	-1288.3592	0.00287	0.03017
77	-1288.5779	0.00167	0.02718
78	-1288.7872	0.00124	0.03182
79	-1288.9786	0.00142	0.02806
80	-1289.1570	0.00152	0.02875
81	-1289.3294	0.00186	0.02531
82	-1289.4973	0.00148	0.02320
83	-1289.6695	0.00236	0.02168
84	-1289.8276	0.00158	0.01801
85	-1289.9843	0.00339	0.02415
86	-1290.1060	0.00247	0.01577
87	-1290.2314	0.00197	0.01658
88	-1290.3282	0.00346	0.00592
89	-1290.4199	0.00276	0.00573
90	-1290.5301	0.00288	0.00706
91	-1290.5975	0.00381	0.00532
92	-1290.6807	0.00188	0.00864
93	-1290.7451	0.00324	0.00687
94	-1290.8134	0.00303	0.01218
95	-1290.8876	0.00116	0.01005
96	-1290.9492	0.00150	0.00814
97	-1291.0105	0.00195	0.00817
98	-1291.0648	0.00216	0.00690
99	-1291.1150	0.00242	0.00963
100	-1291.1710	0.00139	0.01209
101	-1291.2144	0.00119	0.00719
102	-1291.2591	0.00165	0.01051
103	-1291.2902	0.00176	0.00661
104	-1291.3183	0.00141	0.00487
105	-1291.3534	0.00140	0.00543
106	-1291.3830	0.00155	0.00934

107	-1291.4178	0.00222	0.01294
108	-1291.4536	0.00183	0.00944
109	-1291.4473	0.00287	0.00934
110	-1291.5332	0.00192	0.00874
111	-1291.5730	0.00170	0.00786
112	-1291.6268	0.00130	0.00869
113	-1291.7015	0.00169	0.01061
114	-1291.7682	0.00131	0.01050
115	-1291.8316	0.00112	0.00868
116	-1291.8838	0.00129	0.01292
117	-1291.9366	0.00148	0.00540
118	-1291.9795	0.00144	0.01423
119	-1292.0304	0.00158	0.01727
120	-1292.0389	0.00227	0.00756
121	-1292.1020	0.00141	0.00419
122	-1292.1275	0.00178	0.00804
123	-1292.1726	0.00124	0.01499
124	-1292.2063	0.00136	0.01210
125	-1292.2645	0.00109	0.01114
126	-1292.3028	0.00125	0.01298
127	-1292.3461	0.00096	0.01302
128	-1292.3777	0.00116	0.01226
129	-1292.4249	0.00094	0.00982
130	-1292.4611	0.00119	0.01108
131	-1292.4997	0.00092	0.02043
132	-1292.5348	0.00101	0.01172
133	-1292.5776	0.00096	0.01111
134	-1292.6164	0.00056	0.01570
135	-1292.6555	0.00065	0.01795
136	-1292.6935	0.00072	0.01325
137	-1292.7344	0.00110	0.01170
138	-1292.7615	0.00079	0.01148
139	-1292.7957	0.00105	0.00797
140	-1292.8237	0.00147	0.00741
141	-1292.8534	0.00071	0.00992
142	-1292.8840	0.00092	0.00817
143	-1292.9129	0.00094	0.00992
144	-1292.9414	0.00083	0.00943
145	-1292.9674	0.00116	0.01083
146	-1292.9954	0.00107	0.00936
147	-1293.0199	0.00074	0.01142
148	-1293.0452	0.00065	0.00687
149	-1293.0661	0.00084	0.01096
150	-1293.0879	0.00140	0.00804
151	-1293.1029	0.00072	0.00874
152	-1293.1228	0.00081	0.00438
153	-1293.1348	0.00120	0.00720
154	-1293.1573	0.00059	0.00608
155	-1293.1730	0.00106	0.00503
156	-1293.1924	0.00076	0.00548
157	-1293.2074	0.00152	0.00523
158	-1293.2285	0.00091	0.00667

159	-1293.2470	0.00082	0.00822
160	-1293.2662	0.00063	0.00579
161	-1293.2853	0.00054	0.00601
162	-1293.3019	0.00169	0.00641
163	-1293.3137	0.00223	0.00782
164	-1293.3317	0.00066	0.00343
165	-1293.3366	0.00095	0.00445
166	-1293.3568	0.00119	0.00348
167	-1293.3658	0.00082	0.00409
168	-1293.3828	0.00048	0.00248
169	-1293.3902	0.00064	0.00428
170	-1293.4063	0.00089	0.00339
171	-1293.4123	0.00073	0.00330
172	-1293.4295	0.00038	0.00424
173	-1293.4384	0.00122	0.00302
174	-1293.4523	0.00058	0.00437
175	-1293.4611	0.00064	0.00332
176	-1293.4743	0.00114	0.00209
177	-1293.4809	0.00070	0.00390
178	-1293.4940	0.00086	0.00225
179	-1293.5024	0.00057	0.00238
180	-1293.5140	0.00047	0.00210
181	-1293.5233	0.00051	0.00232
182	-1293.5344	0.00063	0.00312
183	-1293.5367	0.00105	0.00335
184	-1293.5548	0.00043	0.00210
185	-1293.5645	0.00059	0.00150
186	-1293.5749	0.00031	0.00234
187	-1293.5854	0.00047	0.00251
188	-1293.5940	0.00052	0.00358
189	-1293.6062	0.00029	0.00122
190	-1293.6111	0.00052	0.00310
191	-1293.6228	0.00047	0.00121
192	-1293.6274	0.00061	0.00249
193	-1293.6400	0.00055	0.00229
194	-1293.6484	0.00052	0.00234
195	-1293.6590	0.00049	0.00304
196	-1293.6687	0.00067	0.00371
197	-1293.6807	0.00072	0.00242
198	-1293.6910	0.00057	0.00410
199	-1293.7023	0.00070	0.00288
200	-1293.7101	0.00066	0.00499
201	-1293.7247	0.00054	0.00186
202	-1293.7331	0.00046	0.00246
203	-1293.7432	0.00042	0.00195
204	-1293.7500	0.00033	0.00206
205	-1293.7591	0.00043	0.00203
206	-1293.7657	0.00047	0.00203
207	-1293.7739	0.00058	0.00099
208	-1293.7767	0.00068	0.00260
209	-1293.7880	0.00060	0.00165
210	-1293.7931	0.00047	0.00215

211	-1293.8022	0.00031	0.00135
212	-1293.8075	0.00056	0.00161
213	-1293.8158	0.00064	0.00175
214	-1293.8214	0.00042	0.00210
215	-1293.8286	0.00049	0.00061
216	-1293.8299	0.00071	0.00162
217	-1293.8389	0.00069	0.00073
218	-1293.8428	0.00047	0.00116
219	-1293.8486	0.00040	0.00073
220	-1293.8537	0.00036	0.00079
221	-1293.8594	0.00027	0.00172
222	-1293.8650	0.00044	0.00122
223	-1293.8702	0.00076	0.00070
224	-1293.8749	0.00038	0.00086
225	-1293.8805	0.00024	0.00090
226	-1293.8848	0.00058	0.00145
227	-1293.8907	0.00040	0.00062
228	-1293.8934	0.00035	0.00078
229	-1293.8983	0.00042	0.00038
230	-1293.9014	0.00035	0.00054
231	-1293.9058	0.00039	0.00065
232	-1293.9092	0.00081	0.00081
233	-1293.9142	0.00031	0.00049
234	-1293.9189	0.00038	0.00068
235	-1293.9244	0.00033	0.00125
236	-1293.9306	0.00044	0.00127
237	-1293.9353	0.00057	0.00035
238	-1293.9380	0.00039	0.00050
239	-1293.9421	0.00026	0.00052
240	-1293.9437	0.00037	0.00047
241	-1293.9471	0.00022	0.00024
242	-1293.9490	0.00024	0.00031

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Heat of Formation: -1293.949 kJ/mol

Estimating Force Constant matrix by central-differences

Calculating Hessian

Memory Used: 73.536 Mb

Reason for exit: Successful completion

Semi-Empirical Program CPU Time : 9:23.14

Semi-Empirical Program Wall Time: 9:25.85

SPARTAN '14 Properties Program: (Win/64b) Release 1.1.4

Standard Thermodynamic quantities at 298.15 K and 1.00 atm

Modifying values for 107 low frequency terms

Term ZPE Enthalpy Entropy Cv % in  
kJ/mol kJ/mol J/mol.K J/mol.K Ground

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Total Vibrations 2954.5466 134.4633 811.8892 702.8598

Ideal Gas 2.4789

Translation 3.7184 192.3352 12.4716

Rotation 3.7184 182.9574 12.4716

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Totals 3098.9256 1187.1818 727.8031

Vibrational(v) Corrections:

Temp. Correction Hv 3098.9256

Entropy Correction (Hv-TSv) 2744.9674

Reason for exit: Successful completion

Properties CPU Time : 8.42

Properties Wall Time: 8.11